UNIVERSITY OF ADELAIDE

DOCTORAL THESIS

Quantification of uncertainty of geometallurgical variables for mine planning optimisation

---

Author:
Exequiel SEPÚLVEDA ESCOBEDO

Supervisors:
Professor Peter DOWD
Associate Professor Chaoshui XU

A thesis submitted in fulfillment of the requirements for the degree of Doctor of Philosophy

in the

School of Civil, Environmental and Mining Engineering

April 22, 2018

Declaration of Authorship

I, Exequiel SEPÚLVEDA ESCOBEDO, certify that this work contains no material which has been accepted for the award of any other degree or diploma in my name, in any university or other tertiary institution and, to the best of my knowledge and belief, contains no material previously published or written by another person, except where due reference has been made in the text. In addition, I certify that no part of this work will, in the future, be used in a submission in my name, for any other degree or diploma in any university or other tertiary institution without the prior approval of the University of Adelaide and where applicable, any partner institution responsible for the joint-award of this degree.

I give consent to this copy of my thesis when deposited in the University Library, being made available for loan and photocopying, subject to the provisions of the Copyright Act 1968.

I acknowledge that copyright of published works contained within this thesis resides with the copyright holder(s) of those works.

I also give permission for the digital version of my thesis to be made available on the web, via the University's digital research repository, the Library Search and also through web search engines, unless permission has been granted by the University to restrict access for a period of time.

I acknowledge the support I have received for my research through the provision of an Becas Chile Scholarship by Conicyt.

Signed: _____

Date: 19/02/2018

"We have all learned to kill our dreams."

Twenty One Pilots

"Yo también creía que era imposible hasta que lo intenté."

Fausto Murillo

UNIVERSITY OF ADELAIDE

Abstract

Faculty of Engineering
School of Civil, Environmental and Mining Engineering

Doctor of Philosophy

Quantification of uncertainty of geometallurgical variables for mine planning optimisation

by Exequiel SEPÚLVEDA ESCOBEDO

Interest in geometallurgy has increased significantly over the past 15 years or so because of the benefits it brings to mine planning and operation. Its use and integration into design, planning and operation is becoming increasingly critical especially in the context of declining ore grades and increasing mining and processing costs.

This thesis, comprising four papers, offers methodologies and methods to quantify geometallurgical uncertainty and enrich the block model with geometallurgical variables, which contribute to improved optimisation of mining operations. This enhanced block model is termed a geometallurgical block model.

Bootstrapped non-linear regression models by projection pursuit were built to predict grindability indices and recovery, and quantify model uncertainty. These models are useful for populating the geometallurgical block model with response attributes. New multi-objective optimisation formulations for block caving mining were formulated and solved by a meta-heuristics solver focussing on maximising the project revenue and, at the same time, minimising several risk measures. A novel clustering method, which is able to use both continuous and categorical attributes and incorporate expert knowledge, was also developed for geometallurgical domaining which characterises the deposit according to its metallurgical response. The concept of geometallurgical dilution was formulated and used for optimising production scheduling in an open-pit case study.

Acknowledgements

I thank my supervisors Professor Peter Dowd and A/Professor Chaoshui Xu for their supervision, guidance and support during my time as a PhD student.

Many thanks to my family; nothing could be possible without their support and love.

Many old and new friends were very important in this achievement; I acknowledge all of them. I am also very grateful for the support I have received from school staff, professors, PhD students and colleagues.

I am indebted to my dear friend Edgardo Toro who first encouraged me to undertake a PhD almost six years ago; it was the beginning of everything. Special thanks go to all people that helped me during this time in little and big things.

I thank the University of Talca for trusting in me and supporting me with a partial scholarship. A position as assistant professor in the School of Mining Engineering is waiting for me.

Finally, my gratitude to the people of Chile, who support the Becas Chile program, my main sponsorship for my PhD. It is time to pay back.

Contents

List of Figures

List of Tables

Dedicated to my loved Paola, Catalina and Trinidad

Chapter 1

Introduction

The concept of geometallurgy has long been used in mining and many definitions have been proposed. Johnson et al. (2007) used the term geometallurgy to mean the impact of ore quality on mine planning, plant performance and product quality. Geometallurgy requires a complete understanding of geology, mineralogy and metallurgy. Dunham and Vann (2007) defined geometallurgy as a cross-disciplinary approach which aims to improve resource economics by integrating geology, mining planning, operational design, mineral processing and metallurgy. Coward et al. (2009) similarly stated that the value of geometallurgy is in the improvement of mining and ore treatment in both the design phase and operation by improving the understanding of rock properties. All these definitions agree that a proper integration of the available geological and metallurgical information should yield substantial improvement in mine planning and operation.

The term geometallurgy was used for first time by McQuiston and Bechaud (1968) in a textbook in which they emphasised the importance of understanding geology before beginning any mining development. A full understanding of geology can reveal useful, and often critical, relationships between geology and process responses that have not only a critical impact on operations and revenue, but also on risk assessment. Since then, geometallurgy has gained significant interest and application, especially over the last decade. A number of initiatives have been developed and deployed within the mining industry, several dedicated geometallurgical conferences have been held, many academic programmes are now offered, and there has been an increased research focus on geometallurgy.

The increasing attention given to geometallurgy is due to its potential to deliver significant operational advantages and increased profitability. In general, the effective, integrated application of geometallurgy in mining operations is still at a low level and more research is required into the integration of geology and metallurgical performance.

The production of metals and other valuable elements involves the quantitative and qualitative characterisation of geological, metallurgical, operational, and economic variables, each of which is a complex aspect of the mine planning process. Optimal mine planning and design require detailed understanding of the ore, procedures to extract and process the ore, and appropriate measures of economic performance. Planning and design can only be done on the basis of models informed by data, which are often sparse or unknown and subject to uncertainty.

There is strong historical evidence showing that there is a serious problem in reconciling mine production output with predicted output, reflecting the importance of quantifying uncertainty. In the 1980s a survey of 35 Australian gold mines showed that 68% of them could not deliver planned head grade (Burmeister, 1988). Similar results were obtained in a survey of North American projects, where only 10% of the projects achieved the expected results (Harquail, 1991). The study by Ward and McCarthy (1999) revealed that only 50% of nine Australian underground projects achieved designed throughput by the third year and 25% of them never achieved it. A survey by Vallee (2000) showed that for 60% of all mining projects in Canada actual production was less than predicted. Tatman (2001) compared the predicted and final production rates from 60 deposits in the United States and found that 35% did not reach their expected production rates.

These examples show how frequently mining project forecasts differ from the reality of mining. The assessment of uncertainty is critical to reducing the risk associated with achieving expected outcomes.

1.1 Importance of geometallurgy

Understanding how geology impacts on metallurgical performance is critical for mine planning. From the processing perspective, there are many processes, such as blasting and stockpiling, that affect the final product, but both comminution and concentration are critical. For example, grinding is generally the most expensive process representing approximately between 30% and 50% of overall operational expenditure of a mining project (Moema et al., 2009). Additionally, the mineralogical characterisation of a deposit usually provides a better understanding of metallurgical responses (Yildirim et al., 2014). Including the prediction of grinding performance and mineralogy as inputs to production planning optimisation is a key step in improving project profitability and minimising operational risk.

1.1.1 Comminution

Comminution is the process of reducing the size of rocks in order to liberate particles of interest (minerals). Comminution includes primary crushing and milling and constitutes one of the most energy-intensive processes in all the processing chain (Ballantyne et al., 2012; Curry et al., 2014). The rock characteristics play an important role in the response to comminution. Softer rocks will require less energy to yield the required particle size, whereas harder rocks will consume more energy. There are several indices that reflect the responses to different processes in comminution. The Bond crushing work index (CWi) is a measure of the energy consumption required in the primary crushing process. The Bond ball mill work index (BWi) relates to the energy used in a ball mill, whereas the Bond rod mill work index (RWi) is for a rod mill. The Bond abrasion index (Ai) measures the rate at which steel is abraded in contact with ore, which is important for equipment maintenance purposes. The drop weight test is used to derive two comminution metrics: the drop weight index (DWi), which is a measure of the strength of the rock to breakage, and the A×b breakage parameters. Both are used to predict the performance of autogenous and semi-autogenous mills. Another measure of hardness for autogenous and semi-autogenous mills (SAG) is the SAG Power Index (SPI), which is a measure of the energy required to reduce rock to a standard particle size.

Among comminution indices, BWi, SPI and A×b are the most widely used in practice and are very useful for predicting energy consumption.

The energy consumption in ball mills can be modelled by the following equation (Bond, 1961):

$$E = BW_i(10/\sqrt{P_{80}} - 10/\sqrt{F_{80}}) \tag{1.1}$$

where P_{80} and F_{80} are the passing size of product and feed respectively. The energy consumption in SAG mills is given in the following relationship (Starkey and Dobby, 1996):

$$E = C_1 \left(\frac{SPI}{\sqrt{P_{80}}} \right)^{C_2} \tag{1.2}$$

where C_1 and C_2 are calibration parameters. The relationship between the A×b index and the specific comminution energy (kW h/t) is given by:

$$t_{10} = A(1 - e^{-bE}) \tag{1.3}$$

where t_{10} is the percent passing one tenth of the initial mean particle size.

1.1.2 Concentration

After the rock is ground, the next step is to concentrate the valuable elements by separating gangue and ore. There are many processes for concentrating minerals, for example, magnetic separation, gravity separation, but the most commonly used is forth flotation.

The froth flotation process recovers target minerals from an ore feed taking advantage of the hydrophobic and hydrophilic properties of minerals and gangue with the assistance of chemical reagents. The ore is ground to a fine powder and mixed in a cell with water, frothing reagents and collecting reagents to create a feed. When air is forced through the mixture, mineral particles cling to air bubbles that are skimmed from the surface to create a concentrate while waste material sinks to the bottom of the cell to become the tailings. Based on conservation of the ore and contained metal quantity:

$$Q_h = Q_c + Q_t \tag{1.4}$$

$$Recovery = \frac{Q_c}{Q_h} \tag{1.5}$$

where Q_h, Q_c and Q_t are the metal quantity corresponding to the head grade, concentrate grade and tailing grade respectively.

It is possible to measure grinding properties and recoveries under various conditions using laboratory experiments. Including grinding characteristics and recoveries in block models will have a significant impact on the economic valuation and process performance assessment. For example, Gregory et al. (2013) illustrated the importance of recovery in a porphyry copper and gold deposit. Their case study showed that increasing the total gold recovery by 1% increased production by 1.07 million oz. valued at $1.5 billion. A small increase in recovery can significantly increase the economic return.

In the flotation process, the particle size distribution has a critical influence on recovery. Suazo et al. (2010) proposed a model for flotation recovery performance for a copper mine. They successfully incorporated a new parameter, the floatability of the ore for each geometallurgical unit. The importance of this parameter is that it does not depend on mine operating conditions and it can be estimated from laboratory tests in the early stages or from direct measurements in flotation plants. As a result of their fifteen-month case study for six geometallurgical units, they obtained a relative error of 1.8% for recovery estimation. Geological units were defined according to similar geological compositions (lithology and alteration), as well as the volumetric fraction in the material.

1.1.3 Primary-Response framework

The primary-response framework documented in Coward and Dowd (2015) and Coward et al. (2009, 2013) allows primary rock properties (intrinsic rock attributes directly measured from rock samples) to be used to predict processing response properties, such as recovery factors and comminution performance, and incorporate them into the resource model. Using only additive primary variables to predict non-additive response variables minimises the biases related to non-additivity (Carrasco et al., 2008; Newton and Graham, 2001).

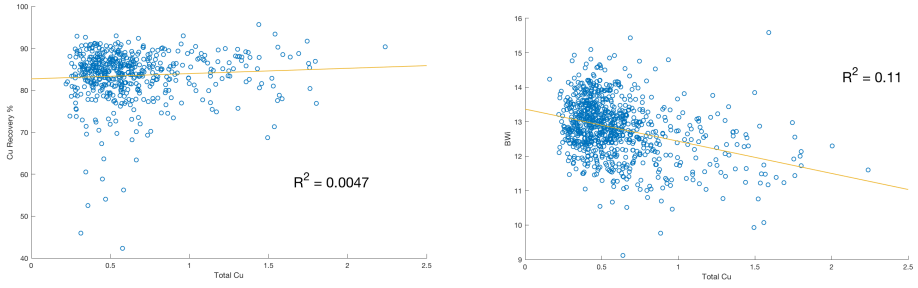
The prediction models for metallurgical responses can be generated by process simulation or regression. Process simulation is, in general, more accurate because it is based on physical and chemical behaviour, which are often very well understood. For example, both JKSimFloat (Runge et al., 1998) and SUPASIM (Hay and Rule, 2003) are flotation circuit simulators used to simulate the flotation process and predict metallurgical recovery. Usually, they need to be calibrated using standardised tests at laboratory scale.

Those laboratory tests can also be used to fit regression models to predict metallurgical responses. The predictions are consequently at the laboratory scale and may need to be scaled up to the block model scale.

Formally, using the primary-response framework, any response variable y can be represented by a function of a multivariate X and an error term:

$$y = f(X) + \epsilon, \tag{1.6}$$

where X is a set of primary variables, the function f can be either a simulation process or a regression function, and $\epsilon \sim \mathcal{N}(0, \sigma)$ is the error.



(A) (B)

FIGURE 1.1: Scatter plot of total Cu vs. (A) Cu Recovery and (B) BWi.

In mining applications, in general, the relationship between X and y is not linear (Barnett and Deutsch, 2012). For example, fig. 1.1 illustrates the relationship between (a) total Cu and Cu Recovery for 930 samples from laboratory testwork, and (b) total Cu and BWi for 840 samples; both scatter plots show a very low coefficient of correlation for a predictive linear model. Despite this observation, multilinear regression is the most commonly used model for predicting geometallurgical variables; examples can be found in Montoya et al. (2011); Boisvert et al. (2013) and Hunt et al. (2013). Very few applications of non-linear regression models can be found in the literature. Keeney and Walters (2011) used explicit non-linear models in three geometallurgical domains using additive variables. Sepúlveda et al. (2017) used a non-parametric regression model and projection pursuit to predict four grinding indices and two recovery rates.

1.1.4 Geometallurgical characterisation

Some primary properties, such as metal content (grades) and qualitative geological features (lithology, alteration and mineralisation style) are abundantly available in most mining projects. Grades are fundamental properties, as they measure the metal content of ore, and they have valuable attributes: they are quantitative, continuous and additive. Geological features are qualitative and subject to the interpretation of geologists (which may be re-interpreted and vary over time). Less abundant variables (compared to grades and geological variables) are mineralogical compositions or mineralogy in short. More expensive acquisition methods are required to obtain mineralogical information, for example, X-ray diffraction (XRS), Semi-quantitative X-ray diffraction (QXRD) and Scanning electron microscopy (QEMSCAN). Mineralogy is a better indicator of grindability and recovery, mainly because mineralogy is closely related to the particle liberation profile (Johnson et al., 2007; Walters, 2008; Lutz et al., 2010; Lamberg, 2011; Bradshaw et al., 2012; Hoal et al., 2013; Tungpalan et al., 2015).

Models based on grades and mineralogy have very good prediction performance (Lamberg, 2011; Hunt et al., 2013; Lund et al., 2015). However, when mineralogy is unavailable, models based only on grades and geological characterisation can perform well (Hunt et al., 2014; Sepúlveda et al., 2017).

A good geometallurgical characterisation provides more variables, which is good in general, but may make it more difficult to build prediction models. Some critical aspects to consider are: (i) compositional data, (ii) redundant

attributes, (iii) mixed continuous and categorical attributes, and (iv) the curse of dimensionality. Feature selection, dimensionality reduction and clustering are data mining techniques that may help to overcome these aspects.

The ultimate goal of geometallurgical characterisation is to enrich the resource model with geometallurgical properties, which is transformed into a geometallurgical block model to be used in mine planning optimisation.

1.2 Quantifying uncertainty

Many sources of uncertainty affect the expected project profitability. These sources can be grouped in two categories: technical and financial (Dowd, 1994; Dimitrakopoulos, 1998). Technical sources are usually classified into geological, mining and metallurgical, such as grades, tonnages, density, lithology, recovery, pit slope, and excavation capacities. Financial sources are related to market conditions. Price is undoubtedly the most significant source of financial uncertainty, affecting not only the long-term economic viability of a mine, but also short-term decision-making. In addition to prices, foreign exchange rates affect non-dollar producers and fuel costs. Moreover, increasingly, environmental variables significantly impact on mine approvals, mine operation and financial matters, for instance, waste disposal, ecology, carbon dioxide emissions and water requirements.

For the purpose of this thesis, the main sources are classified in three groups of uncertainties: financial, geological and metallurgical.

1.2.1 Financial uncertainty

Prices, foreign exchange rates, and operating costs are the most common examples of uncertain financial variables. All these variables are included in the majority of mine planning optimisation problems and have a high impact on project valuation.

Metal price is the most important financial variable because it not only impacts revenue, it also impacts the mine design through ore-waste discrimination (economic cut-off grade). The economic cut-off grade approach is commonly used in the optimisation problem of open-pit mines. In addition, prices can change the mine operation status. In very low-price scenarios the suspension or closure of the mine may be the only alternative. In contrast, in high-price scenarios it can lead to the extension of the life of the mine (by mining

lower grades), increased production and/or the early processing of low-grade stockpiles.

It is common practice to treat metal price as a fixed-value parameter in all evaluation periods or fixed at different values at different periods, which is a rudimentary approach to address the uncertainty concern.

A more sophisticated approach is to treat price as a random variable with a known distribution. Amankwah et al. (2013) assumed that metal prices follow a lognormal distribution. Dowd (1976) used dynamic and stochastic programming to optimise the sequence of cut-off grade grades over the life of a mine and used transition state probability matrices to include price uncertainty. Better price models follow a Wiener process (Dimitrakopoulos and Sabour, 2007; Evatt et al., 2012). Grobler et al. (2011) used the empirical historic distribution of prices. This is a questionable practice because Monte Carlo simulations will reproduce the historical distribution, potentially an unrealistic assumption for future variation.

For producers with domestic currency different to the currencies used in the global markets, such as Australia, South Africa, Canada and Chile, the quantfication of exchange rate uncertainty is critial (Dimitrakopoulos and Sabour, 2007). As exchange rates can be highly volatile, importing and exporting can be favourably or adversely affected by appreciation in the real value of the domestic currency (Bailey and Chung, 1995).

According to Dimitrakopoulos and Sabour (2007), there are two models applied to market and economic variables, prices and exchange rates in particular, the simple geometric Brownian motion (GBM) and mean-reverting process (MRP) model.

The GBM model is represented as

$$\frac{dS}{S} = \mu dt + \sigma dz, \tag{1.7}$$

where S is the financial variable, μ is the expected trend, σ is its standard deviation, dz represents an increment in a standard Weiner process and dt is the time increment. Alternatively, a MRP model is represented as

$$\frac{dS}{S} = \kappa(\mu - ln(S))dt + \sigma dz, \tag{1.8}$$

where κ is the reversion speed at which the log of the variable S reverts back to a long-term equilibrium of log price μ.

Despite its relevance in any mining project evaluation, financial uncertainty is not the focus of this thesis.

1.2.2 Geological uncertainty

The estimation of resources is traditionally done by using drill hole samples to estimate the grades of blocks in a block model of the deposit. The most common method used is the geostatistical estimation technique of kriging, which is a smooth regression of samples that includes spatial and grade correlations (Matheron, 1963). Kriging is the most widely used geostatistical technique in the mining industry. The main problem with the standard linear form of kriging is the smoothing effect (extreme values are not properly represented). Linear kriging gives the minimum variance, unbiased linear estimator, and not the estimated distribution of all possible values except for the special, but unrepresentative, case of normally distributed sample values. Non-linear forms of kriging can provide estimates of grade distributions for blocks. The parametric forms of non-linear kriging assume specific distributions and results may not be robust to departures from this assumption; the non-parametric forms (Journel, 1983) are robust and have been much more widely used. Geostatistical simulation (Journel, 1974) is much more widely used for quantifying spatial uncertainty.

Geostatistical simulation has been the most significant development in quantifying geological uncertainty. Early research (Dowd, 1994; Dimitrakopoulos, 1998) used ore grade simulations in open pit optimisation and production scheduling. Subsequent research continued to focus on integrating these simulations with mining processes using process simulation, stochastic optimisation, traditional integer and mixed programming, heuristic and metaheuristic optimisation (e.g. Dowd and Dare-Bryan, 2004). Most of these studies focussed on open-pit mines with very few applications to underground mines. However, uncertainty of metallurgical variables has only recently begun to be included (Coward et al., 2013; Coward and Dowd, 2015).

In the 1980s, researchers developed various stochastic methods to generate simulations of grades and rock types, the most common being sequential Gaussian, turning bands, multiple indicator and plurigaussian simulation methods (Chilès and Delfiner, 1999).

The use of these simulations for risk analysis started in the 1990s. Dowd (1994) used geostatistical simulations for risk analysis of reserves. Sequential Gaussian simulation was used to generate many equally probable grade scenarios. Each scenario was used to generate the corresponding optimal open-pit design. A proposed framework combined these optimal designs and other distributions of costs and financial variables. The output was a risk analysis using the generated distributions of probable NPV. Dimitrakopoulos (1998)

proposed a framework to deal with geological uncertainty in open-pit design and scheduling. Dimitrakopoulos et al. (2002) extended their earlier work to a probability analysis of NPV. In their work, an important result (in an open-pit gold deposit) was that the NPV of an estimated model had a very low probability of occurring. They raised the concern of high computation cost of using simulations of grades, but this is now less relevant because of the availability of more efficient implementations and more powerful computers. Since this early research, geostatistical simulations have become the standard for quantifying geological uncertainty (e.g. Boisvert et al., 2013; Deutsch et al., 2016; Goodfellow and Dimitrakopoulos, 2017).

Geometallurgical characterisation implies an increasing number of attributes to be simulated (section 1.1.4). Traditional geostatistical simulations for multivariate cases are challenging to use because, as the number of simulation variables increases, the number of direct and cross-variogram models increases in a quadratic manner. Fitting a linear model of coregionalisation for n variables requires $n(n-1)/2$ variogram models. When n is a small number (no more than six), co-simulation methods can be applied with little or moderate effort providing linear models of co-regionalisation can be assumed (Xu and Dowd, 2009; Tehrani et al., 2013; Maleki and Emery, 2015; Adeli et al., 2017). When the number of variables is greater than six, traditional co-simulation methods become difficult to use in practice. The projection pursuit multivariate transformation (PPMT) (Barnett et al., 2014) is able to map multivariate data with very complex relationships into a set of uncorrelated variables following multi-Gaussian distributions. A secondary outcome of PPMT is that transformed variables often show little or no spatial cross-correlation. In this case, the multi-Gaussian transformed variables can be independently simulated by any univariate geostatistical method. In cases where some spatial cross-correlation remains, methods such as Maximum Autocorrelation Factors (MAF) (Desbarats and Dimitrakopoulos, 2000), Uniformly Weighted Exhaustive Diagonalization with Gauss iterations (U-WEDG) (Mueller and Ferreira, 2012), or Minimum Spatial Cross Correlation (MSC) (Sohrabian and Tercan, 2014), among others, can be applied to handle the remaining spatial cross-correlation.

Irrespective of the simulation method, having a block model with many realisations of primary variables provides a means of quantifying the uncertainty of geometallurgical response variables.

1.2.3 Geometallurgical uncertainty

The quantification of the uncertainty of geometallurgical variables could be done by geostatistical simulations similar to the simulation of primary variables. Unfortunately, there are three main problems that often complicate this option. First, there is usually a relatively small number of geometallurgical samples compared to geological and grade variables, largely because geometallurgical sampling is very expensive. This issue imposes a challenge for robust modelling. Second, the non-additivity property of the majority of geometallurgical variables. In mathematical terms, the actual average (or other linear combination) of two non-additive variables is not simply their arithmetic average (Carrasco et al., 2008; Boisvert et al., 2013). Recovery is one example of these variables. This issue is commonly ignored when traditional estimation methods (e.g. kriging) are used and, unfortunately, standard geostatistical estimations or simulations will be biased for non-additive variables. Therefore, a different strategy must be used such as that implemented by Carrasco et al. (2008) in which additive auxiliary variables are used instead. Third, they do not necessarily scale up in a linear manner. Many geometallurgical variables are estimated by laboratory tests on different scales (or supports). Assuming that these variables will linearly scale up from the small laboratory scale to large plant scales may be incorrect. For instance, grindability indices measured in laboratory tests on the scale of core samples, using kilograms of samples with a specific and standardised instrumentation could differ significantly from those measured in plant conditions.

To overcome the first two problems, the quantification of the uncertainty can be done by quantifying the uncertainty of primary variables and the model uncertainty associated with the function f (Eq. 1.6) in the Primary-Response framework. One way of doing the latter is to apply the statistical method of bootstrapping (Efron and Gong, 1983). This method seeks to determine the effect on the model parameters when sample values vary. The application of bootstrapping for quantifying uncertainty of response variables is part of this thesis and is detailed in Chapter 2.

The upscaling problem alone could constitute a PhD thesis and therefore in the work presented in this thesis it is assumed that response variables will scale up from the sample scale to the block scale and to the plant scale.

1.2.4 Risk assessment

Several methodologies have been developed to assess risk; the most common and classic methods are based on scenarios (Schoemaker, 1995). However, scenario-based methods require the definition of a risk measure in order to include them in optimisation problems. According to the literature, there are two relevant risk measures: Value at Risk (VaR) and Conditional Value at Risk (CVaR) (Rockafellar and Uryasev, 2000). The VaR is defined as a threshold at some risk level α, at which the probability of a loss function does not exceed the threshold. The VaR for a loss function Ψ and threshold ζ is:

$$\underset{\alpha}{\text{VaR}} = \inf \zeta \in \mathbb{R} : \Psi(X, \zeta) \geq \alpha. \tag{1.9}$$

CVaR is an improved risk measure defined as the expectation of the loss function L, subject to it being at least the VaR:

$$\text{CVaR}(\alpha) = \mathbb{E}(L|L > \text{VaR}(\alpha)). \tag{1.10}$$

The loss function can be defined as the negative of profit, deviation from production targets or similar objectives.

FIGURE 1.2: Standard deviation, VaR and CVaR in a generic loss distribution.

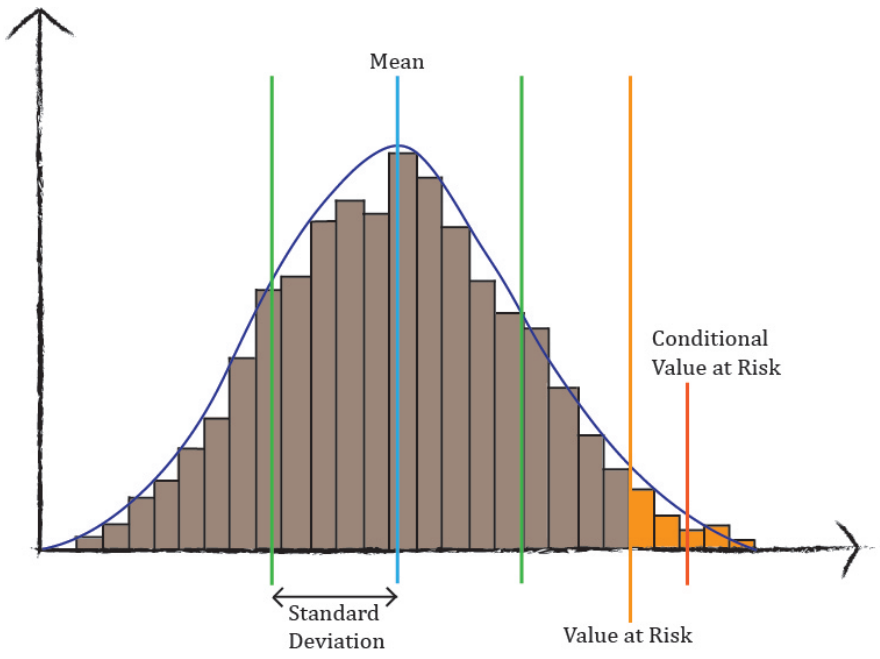


Figure 1.2 depicts three risk measures: the standard deviation, VaR and CVaR for a generic loss distribution. The standard deviation is a basic measure of dispersion, whereas VaR focusses on the tail of the distribution. CVaR is the conditional expected value given the loss is greater than VaR.

Lagos et al. (2011) compared VaR with CVaR approaches under grade uncertainty for an orebody comprising small size veins. They concluded that VaR is risky and only appropriate for less risk-averse scenarios, and CVaR is less risky but expected profits are lower. Similar research by Amankwah et al. (2013), introduced a CVaR measure with both geological and price uncertainties. They formulated a linear programming problem in which the expected profit was maximised and the CVaR was minimised, using synthetic cases in two dimensions. As expected, there are higher expected profits for lower confidence levels.

Chapter 3 details the use of risk measures based on VaR and CVaR to optimise production scheduling in a block caving mine.

1.3 Geometallurgical domaining

The concept of geometallurgical domaining assumes that similar geometallurgical characteristics will have similar responses in mineral processing, which is observed in practice. Geometallurgical domaining is as critical from a processing perspective as geological domaining is for resource estimation; although these two forms of domaining are different they are complementary.

Automated domaining is equivalent to the machine learning method of clustering. Geological clustering, or rock type domaining, is important in understanding the nature of the deposit, however, it does not necessarily explain the responses of the ore to the various processing stages (Keeney and Walters, 2011). Geometallurgical clustering focusses on the geometallurgical characteristics of the orebody to provide a basis for integrated optimisation from mining to processing (Hoal et al., 2013).

The main objective of clustering is to partition the dataset into P different partitions or clusters. These clusters should have two desirable properties: (i) samples within a cluster are very similar, and (ii) samples of different clusters are well separated. These two concepts of similarity and separation are critical to achieve a good partition. The most used method to account for similarity is the variance, whereas for separation it is the distance among cluster centres. A complete review of different cluster indices is given in Halkidi et al. (2001).

Several authors have used different techniques for geometallurgical clustering, for example, Principal Component Analysis (Keeney and Walters, 2011), K-Means (Del Castillo and Dimitrakopoulos, 2016; Goodfellow and Dimitrakopoulos, 2017) , and hierarchical clustering (Nguyen and Keeney, 2014). In Chapter 4 a variation of fuzzy clustering is used for geometallurgical clustering considering also spatial connectivity.

1.4 Geometallurgy applied to mine planning problems

The main benefit of geometallurgy is a substantial improvement in mine planning optimisation. To achieve this benefit, the traditional way of evaluating a mining project and, therefore, the optimisation formulation, needs to be adapted to include geometallurgical variables under uncertainty.

The evaluation of a mining project involves technical, operational and economic factors. Typically, the net present value (NPV) is used to measure the project return in economic terms. In mine projects, it is also the most commonly used method to evaluate project profitability. Specifically, in mine planning, the most accepted formulation for the calculation of the optimal NPV is maximising the total block economic value as follows:

$$max \sum_{i \in B} \frac{v_i}{(1+r)^i} \tag{1.11}$$

where:

$$v_i = t_i g_i RP - t_i C_M - \begin{cases} 0 & \text{if waste} \\ t_i C_P & \text{else} \end{cases}, \forall i \in B, \tag{1.12}$$

and B is the block model, t_i the tonnage of the block i, g_i is the grade of the block i, R is the recovery rate, P the metal price, C_M the cost of mining, C_P the cost of processing and r is the discount rate.

This fundamental formulation has been widely used for several decades, although risk analysis has been incorporated in more recent research with the use of random variables (with their respective distributions). Many scenarios are built using values of these variables generated from their distributions to generate a probability distribution for the NPV. Dowd (1994) identified two main weaknesses in this methodology: the assumption of independence of the variables, and the ignorance of the fact that geological variables are spatially

correlated. The latter requires the use of geostatistical modelling for geological variables.

1.4.1 Open-pit mining

Optimisation problems in open-pit mines make up the majority of past research because open-pit mines are broadly similar compared with underground operations and thus the problem slightly easier. In addition, open-pit design and operation is simpler than underground mining. Open-pit mine optimisation involves three main problems: ultimate pit, pushback design and production scheduling.

The ultimate pit problem consists of determining all blocks that will be mined in order to maximise the NPV subject to slope constraints and fixed cut-off grades. The classic formulation as an integer linear programming is as follows (Newman et al., 2010):

$$max \sum_{i \in B} v_i y_i \tag{1.13}$$

subject to:

$$y_i \leq y_j, \ \forall (i,j) \in PB. \tag{1.14}$$

The objective function to be maximised is given in Eq. 1.13, where v_i is the profit generated by mining and processing the i-th block, y_i is a binary variable with a value of 1 if the i-th block is mined and processed or 0 if not, and B is the set of all blocks. The constraint on slope angles is achieved by Eq. 1.14 where $(i,j) \in PB$ is the precedence set.

This deterministic problem was solved by Lerchs and Grossman (1965) using a graph theory formulation, and by Picard (1976), using a more efficient max-flow algorithm. Whittle (1998) proposed a price parametrisation method based on the Lerchs and Grossman algorithm to select the pushbacks.

The long-term schedule optimisation problem consists of determining all blocks that will be mined in successive periods in order to maximise the NPV subject to slope, technical and operational constraints, given a fixed cut-off discriminator. According to Newman et al. (2010), a typical integer linear programming formulation of long-term schedule optimisation is:

$$max \sum_{i \in B} \sum_{j \in P} v_{ij} y_{ij} \tag{1.15}$$

subject to:

$$\sum_{j \in P} y_{ij} \leq 1, \forall i \in B \tag{1.16}$$

$$C_{min} \leq \sum_{i \in B} c_{ij} y_{ij} \leq C_{max}, \ \forall j \in P \tag{1.17}$$

$$y_{ij} \leq \sum_{j \in P} y_{kj}, \ \forall i, k \in B_i, j \tag{1.18}$$

where Eq. 1.15 is the objective function to be maximised, v_{ij} is the profit of the block, y_{ij} is a binary variable with a value of 1 if the block will be mined and processed or 0 if not, B is the set of all blocks, and P is the set of all periods. c_{ij} is the amount of resource (tonnage) of the block i in the period j. The constraint 1.16 ensures that a block can only be mined once. Eq. 1.17 ensures that the minimum and maximum operational resources capacities are met for each period. Finally, Eq. 1.18 ensures a feasible block extraction sequence is followed in order to mine a block.

The short-term scheduling problem is based on the long-term scheduling but focuses on short periods such as a day, weeks and months of a year period. According to the block mining sequence, operational aspects are considered such as equipment requirements, equipment operative scheduling and plant scheduling.

There is a significant amount of research on production scheduling optimisation in open-pit mining under uncertainty (Marcotte and Caron, 2013; Lamghari et al., 2014; Silva et al., 2015; Goodfellow and Dimitrakopoulos, 2016, 2017; Del Castillo and Dimitrakopoulos, 2016; Montiel and Dimitrakopoulos, 2017; Navarra et al., 2018), but there no formulations that incorporate geometallurgical uncertainty.

1.4.2 Underground mining

Because underground mines are more complex and diverse (Dimitrakopoulos and Grieco, 2009; Epstein et al., 2012), limited research has been undertaken to quantify uncertainty in mining processes. The diversity of underground methods does not allow the generalisation of optimisation methods as used for open-pit mines. Underground designs can be classified into three main groups: artificially supported, unsupported and caving. Examples of artificially supported methods are room and pillar, cut and fill, squared set and long wall. Unsupported methods are, for example, sublevel stoping, shrinkage stoping. Sublevel caving and block caving are examples of caving methods.

In caving methods, the material breaks and flows by gravity. Block caving is the most suitable option for massive mining and is considered the cheapest mining method for large orebodies.

The major complexity in the optimisation of underground mines is the significant number of geomechanical, sequencing and economic constraints that are difficult for mixed integer programming optimisation (MIP) methods to handle (Newman and Kuchta, 2007; Topal, 2008; Epstein et al., 2012). For this reason, a major research focus has been on reducing the number of constraints and creating new algorithms to accommodate this reduction.

Newman and Kuchta (2007) formulated a new MIP optimisation problem based on aggregation for a large underground gold mine using sublevel caving. Their goal was to minimise the difference between production of, and demand for, ore by considering vertical sequencing, horizontal sequencing, and machinery placement constraints. Topal (2008) developed two new optimisation algorithms for the same mine in order to reduce the complexity of the MIP formulation and allow optimal long-term scheduling. Martinez and Newman (2011) proposed a new MIP formulation, focusing on variable elimination and a decomposition based-heuristic in order to cope with realistic problems in reasonable processing times. Bley and Terblanche (2012) focus on selectivity and propose a new MIP formulation of the generic underground mining method. Bai et al. (2013) propose a new algorithm for optimising stopes in sublevel stoping mining using maximum flow algorithms. However, all this research uses only deterministic models and does not consider uncertainties.

Despite all these efforts, the inclusion of grade uncertainty for underground operations remains limited. Dimitrakopoulos and Grieco (2009) developed a new MIP formulation to quantify the uncertainty of grades in a poly-metallic underground mine. They optimised the stope outline using an estimated block model as a base case and used a series of simulated realisations of the block model to quantify uncertainty. The risk profile built from simulations shows a high variability of profit (varying from 1.8 million dollars to as much as 5.9 million). Their proposed solution re-blocked the block model into a set of mineable units called rings. Each ring has a distribution of grades enabling a risk profile after optimisation. The optimisation problem can include a risk level as the probability of each ring to be above some threshold. Nevertheless, the stope design does not constitute part of the optimisation problem and the grade uncertainty is quantified as the probability above the cut-off grade.

There is an additional complexity in caving methods, which is the focus in this research. In these underground operations, rocks move by gravity flow

and the original locations of blocks in the block model change. The simulation of gravity flow enables the understanding of how the rock flows when it is extracted. Simple models do not take this issue into account and use a simple vertical gravity flow. In reality, the rock flow is much more complex than this.

Gravity flow simulation methods can be classified into two categories: empirical and mathematical methods (Castro et al., 2009). Empirical methods are based on volumetric mixing. Probably the most popular empirical method is the commercial software PC-BC (Diering et al., 2010). Mathematical methods may be classified according to the fundamentals and principles on which they have been developed. The two main mathematical methods are dynamic and kinematic based. Dynamic methods model gravity flows through the mechanics of particle interactions. Kinematic models use mass balance principles to balance extraction and moving zones. REBOP software (Pierce, 2010) uses this kinematic principle to track the growth of Isolated Movement Zones (IMZs) at each draw-point. Another kinematic model is based on cellular automata (Sharrock et al., 2004). The fragmented rock particles fill the vacant space (starting in the extraction zone) stochastically following a pattern according to the probability function of their neighbourhood, until an equilibrium state is reached. The software FLOWSIM is an implementation of the cellular automata approach (Castro et al., 2009) and gave very good results in three case studies.

Limited research has been done to incorporate uncertainty into production scheduling optimisation in block caving mining. Rubio and Dunbar (2005) integrated the uncertainty of the deviation from production targets into production scheduling optimisation for block caving. Khodayari and Pourrahimian (2018) propose an optimisation formulation that takes into account the uncertainty of material flow. The material flow uncertainty is quantified with several scenarios of grade mixing.

The use of many simulations of the ore body in underground mine planning optimisation is still a challenge. The same effort to develop models and methodologies applicable to open-pit mines should be applied to underground mines.

1.4.3 Optimisation in mine planning

Because mine planning optimisation requires a stochastic block model in order to incorporate uncertainty, the optimisation process must also follow a stochastic approach.

Stochastic optimisation

There are two main approaches to stochastic optimisation. The first is stochastic programming, which is based on linear, or mixed integer, programming (Dimitrakopoulos, 2011), and the second is metaheuristic optimisation (Kumral and Dowd, 2005; Lamghari and Dimitrakopoulos, 2012).

The general idea behind stochastic programming is to extend a deterministic optimisation formulation by using random variables in the objective function and constraints. For example, the objective function that maximises the profit of the ultimate pit for the block model B is:

$$max \sum_{i \in B} v_i y_i \tag{1.19}$$

where v_i is the profit of block i and y_i is a binary variable indicating whether or not block i will be mined and processed. This deterministic formulation can be converted to a stochastic programming formulation as follows:

$$max \sum_{i \in B} \mathbb{E}[v_i] y_i \tag{1.20}$$

where $\mathbb{E}[v_i y_i]$ is the expectation of the profit of block i. Here, the profit depends mainly on grade and the cut-off definition. In a stochastic scenario, grade is a random variable and, therefore, the expectation must be used. If the block model has m equally probable realisations, the expectation is the average profit among all realisations:

$$\mathbb{E}[v_i] = \frac{1}{m} \sum_{k=1}^{m} v_{ik} \tag{1.21}$$

This example illustrates how a deterministic formulation can lead to stochastic programming. Obviously, optimisation formulations for mine planning are more complex, having several constraints on the problem to be solved.

Stochastic programming is an exact approach to optimisation problems but requires considerable computational effort especially in large-scale problems.

Metaheuristic optimisation is a method based on randomly searching a solution space. Contrary to stochastic programming, metaheuristic approaches can deal with large-scale problems at reasonable computing cost, but exact solutions cannot be guaranteed although the solutions are close to the exact ones. Simulated Annealing (SA), Tabu Search (TS), Genetic Algorithms (GA) and Artificial Ant Colony (ACO) are examples of metaheuristic approaches that have been successfully used for mine planning optimisation with grade uncertainty (Denby et al., 1998; Kumral, 2004; Kumral and Dowd, 2005; Lamghari

and Dimitrakopoulos, 2012; Shishvan and Sattarvand, 2015).

Metaheuristic approaches have two crucial properties. The first is the manner in which new solutions are generated from the current solution. This is a key aspect, because new solutions have to explore the solution space as much as possible. The second is to avoid local minima. Table 1.1 summarises these two key aspects for Simulated Annealing, Tabu Search, Genetic Algorithms and Artificial Ant Colony.

TABLE 1.1: Metaheuristic algorithms for optimisation.

Method	Solution space exploration	Escaping from local minima
Simulated Annealing	One new solution at each iteration	Accepting worse solutions randomly
Tabu Search	Several new solutions at each iteration	A short taboo list and defining an aspirational criterion
Genetic Algorithms	Based on a population with many individuals	Selection, crossover and mutation procedures
Artificial Ant Colony	Based on a population with many individuals	An individual stores its best solution so far, combined with the global best solution, and uses a velocity component to move toward a new position in the solution space

Multi-objective optimisation

Complex optimisation problems may require two or more objective functions. Mine planning optimisation problems can include objectives in addition to the typical maximisation of NPV. For instance, the minimisation of deviations from target production, minimisation of energy consumption in the comminution process, secondary metal production, and control of deleterious material presence are also important objectives in mine planning from the geometallurgical perspective.

A multi-objective optimisation formulation is defined as:

$$min[f_1(x), f_2(x), \ldots, f_n(x)] \tag{1.22}$$

where the n objective functions are simultaneously optimised. Multi-objective optimisation methods are capable of building the Pareto-frontier with all Pareto non-dominated solutions found by multi-objective optimisers, giving a complete picture of optimality according to different objectives (Yano and McFadden, 2014). As it is impossible, a priori, to decide which criterion is more relevant, the decision-maker can choose from the Pareto-frontier the optimal solution according to some criterion based on strategic decisions. Figure 1.3 shows the solutions of a two-objective optimisation problem. Minimising only the first objective will increase the second objective and vice versa. Any point at the feasible region is a feasible solution but is dominated by some solution at the Pareto frontier, which means that Pareto frontier solutions are non-dominated solutions and, therefore, they are optimal.

The traditional optimisers, such as mixed integer programming and integer programming are not designed to solve multi-objective problems. For this reason, multi-objective problems are commonly converted into a single-objective problem using a weighted sum objective:

$$min[w_1 f_1(x) + w_2 f_2(x) + \cdots + w_n f_n(x)]. \tag{1.23}$$

The main disadvantages of this approach are that the weights must be defined at the beginning and therefore the results are conditioned to these specified weights, and some non-dominated solutions are missed. In Fig. 1.3, when the feasible solution region is not convex, the solution at B cannot be reached, and the solution at A is the weighted unique optimal solution (the solution at A depends on weights). When the feasible solution region is non-convex, all solutions between A and C are unreachable.

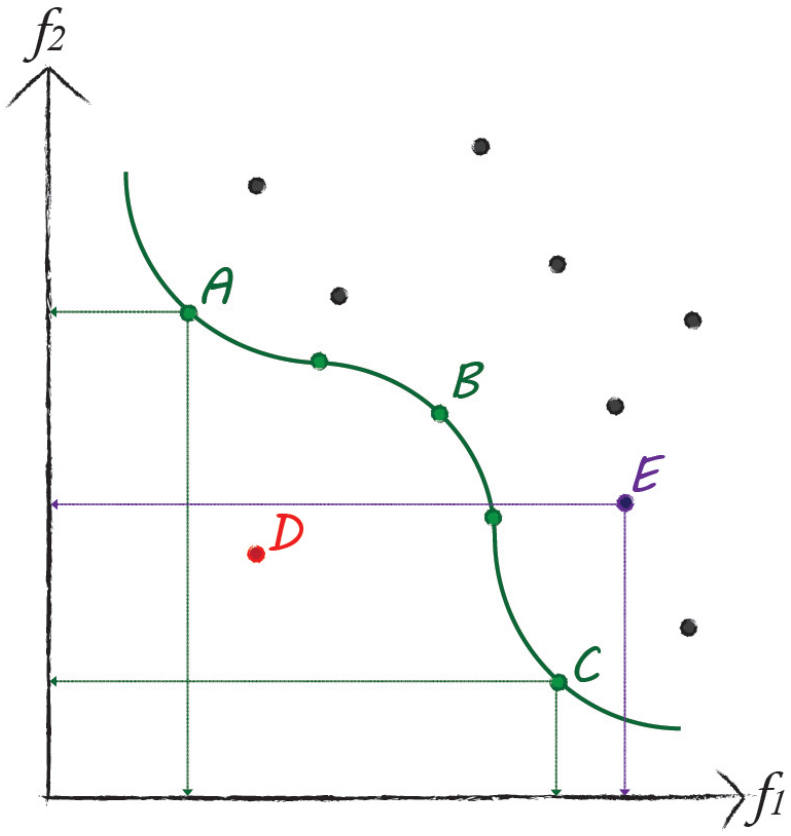


FIGURE 1.3: Pareto front with non-convex feasible regions for two-objective problems.

In conclusion, metaheuristic approaches have the advantage of finding the Pareto frontier in both convex and non-convex regions. They are also efficient in terms of computational costs.

1.5 Addressed gaps in knowledge

The three principal gaps in knowledge addressed in this thesis are:

1. Geometallurgical response properties rarely have linear relationships with primary properties and they are usually non-additive.

2. Mine planning optimisation problems need to be adapted in order to consider geometallurgical variables with uncertainty.

3. Lack of clustering techniques for geometallurgical domaining that consider multivariate, mixed attributes and spatial continuity.

1.6 Research objectives

The main objective of this thesis is to develop methodologies and methods for quantifying the uncertainty of geometallurgical variables and their inclusion in mine planning optimisation problems in a practical way to contribute to the accomplishment of the main goal of geometallurgy which is improving mine planning, plant performance and product quality. To do so, the following research objectives were pursued:

1. Propose a methodology to quantify the uncertainty of geometallurgical variables for practical applications in mine planning optimisation problems.

2. Formulate risk measures to account for geometallurgical uncertainty and their application in mine planning optimisation problems.

3. Improve formulations of production scheduling optimisation problems for open pit and underground mining to include geometallurgical variables and risk measures.

4. Application of metaheuristics to optimise production scheduling problems for open pit and underground mining.

1.7 Thesis overview

Paper 1 (Chapter 2) addresses the problems of non-additivity and non-linear relationships in geometallurgical variables and the quantification of uncertainty of response variables. Applying the primary-response rock property framework and using quantitative and qualitative primary properties, metallurgical response prediction models were built using projection pursuit regression (PPR). Projection pursuit is a statistical modelling technique in which data from a significant number of variables are projected onto a set of directions that optimise the fit of the model with the purpose of revealing underlying relationships. PPR is applied to modelling six geometallurgical variables. The results show a significant improvement compared with traditional multivariate linear regression models. The models were also bootstrapped to generate distributions of feasible scenarios for the response variables, which are critical for assessing the associated uncertainty.

Paper 2 (Chapter 3) optimises the production scheduling of a block caving operation using geometallurgical variables with uncertainty. The optimisation focuses on maximising economic return and minimising the risk arising from the uncertainty associated with several geometallurgical variables. The geometallurgical uncertainty was quantified by geostatistical simulations of primary properties and bootstrapped project pursuit regression models for response variables. Several two-objective optimisation problems were formulated to assess the impact of geometallurgical uncertainty. The first objective is the maximisation of the Net Smelter Return. This objective was combined with four different objectives to measure risk: volatility, value at risk, conditional value at risk and deviation from the planned production target. A genetic algorithm was used to optimise the problems and generate the Pareto fronts to support the decision-making process.

Paper 3 (Chapter 4) proposes a new method for clustering geometallurgical attributes to build geometallurgical domains considering the spatial variability of variables and the uncertainty of cluster membership. Geometallurgical domains can be used to ensure consistent feed to a processing plant by minimising transitions between different feeds coming from different domains. Fuzzy clustering was used to account for the clustering uncertainty and the spatial continuity was achieved by energy minimisation via graph cuts. In addition, two problems with existing clustering methods applied to geometallurgy were addressed: (i) incapability of using subsets of attributes at the cluster level, and (ii) incapability of considering spatial relationships to avoid dispersed and/or overlapped clusters. In addition, a set of new distance metrics were proposed to target geometallurgical responses in the resulting cluster. The resulting clusters can be used directly in mine planning to optimise the ore feed to be delivered to the processing plant.

In paper 4 (Chapter 5), geometallurgical domaining was used to define the concept of geometallurgical dilution. The well-known constrained pit limit optimisation problem (CPIT) is reformulated as a bi-objective formulation that adds to the NPV maximisation objective, the minimisation of geometallurgical dilution. A case study is presented in which clay content has a strong impact on the flotation recovery. Geometallurgical dilution, therefore, is defined as the ratio of the dominant clay domain to the other domains in any time period. The results show that geometallurgical domaining can improve the economic valuation while controlling the negative effect of clay content.

Chapter 6 summarises the key findings and outlines the potential for further research.

References

Adeli, A., Emery, X. and Dowd, PA. (2017), 'Geological modelling and validation of geological interpretations via simulation and classification of quantitative covariates', *Minerals* **8**(1), 7.

Amankwah, H., Larsson, T. and Textorius, B. (2013), Open-pit mining with uncertainty: A conditional value-at-risk approach, *in* 'Optimization Theory, Decision Making, and Operations Research Applications', Springer, pp. 117–139.

Bai, X., Marcotte, D. and Simon, R. (2013), 'Underground stope optimization with network flow method', *Computers & geosciences* **52**, 361–371.

Bailey, W. and Chung, Y. P. (1995), 'Exchange Rate Fluctuations, Political Risk, and Stock Returns: Some Evidence from an Emerging Market', *The Journal of Financial and Quantitative Analysis* **30**(4), 541.

Ballantyne, G., Powell, M. and Tiang, M. (2012), Proportion of energy attributable to comminution, *in* 'Proceedings of the 11th Australasian Institute of Mining and Metallurgy Mill Operator's Conference', pp. 25–30.

Barnett, R. M. and Deutsch, C. V. (2012), Practical implementation of non-linear transforms for modeling geometallurgical variables, *in* 'Geostatistics Oslo 2012', Springer, pp. 409–422.

Barnett, R. M., Manchuk, J. G. and Deutsch, C. V. (2014), 'Projection pursuit multivariate transform', *Mathematical Geosciences* **46**(3), 337–359.

Bley, A. and Terblanche, S. (2012), 'An improved formulation of the underground mine scheduling optimization problem when considering selective mining', *Optimization Online* .

Boisvert, J. B., Rossi, M. E., Ehrig, K. and Deutsch, C. V. (2013), 'Geometallurgical modeling at olympic dam mine, south australia', *Mathematical Geosciences* **45**(8), 901–925.

Bond, F. (1961), Crushing and grinding calculations, Technical report, Allis-Chalmers Manufacturing Company.

Bradshaw, D. J., Triffett, B. and Kashuba, D. (2012), The role of process mineralogy in identifying the cause of the low recovery of chalcopyrite at kucc, *in* 'Proceedings of the 10th International Congress for Applied Mineralogy (ICAM)', Springer, pp. 73–80.

Burmeister, B. (1988), 'From resource to reality: a critical review of the achievements of new australian gold mining projects during the period january 1983 to september 1987', *Macquarie University* .

Carrasco, P., Chilès, J.-P. and Séguret, S. A. (2008), Additivity, metallurgical recovery, and grade, *in* '8th international Geostatistics Congress', pp. on–CD.

Castro, R., Gonzalez, F. and Arancibia, E. (2009), 'Development of a gravity flow numerical model for the evaluation of drawpoint spacing for block/panel caving', *Journal of the Southern African Institute of Mining and Metallurgy* **109**(7), 393–400.

Chilès, J.-P. and Delfiner, P. (1999), 'Conditional simulations', *Geostatistics: Modeling Spatial Uncertainty, Second Edition* pp. 478–628.

Coward, S. and Dowd, PA. (2015), Geometallurgical models for the quantification of uncertainty in mining project value chains, *in* 'International symposium on the application of computers and operations research in the mineral industry (APCOM)', Vol. 37, pp. 360–369.

Coward, S., Dowd, PA. and Vann, J. (2013), 'Value chain modelling to evaluate geometallurgical recovery factors'.

Coward, S., Vann, J., Dunham, S. and Stewart, M. (2009), The primary-response framework for geometallurgical variables, *in* 'Seventh international mining geology conference', pp. 109–113.

Curry, J. A., Ismay, M. J. and Jameson, G. J. (2014), 'Mine operating costs and the potential impacts of energy and grinding', *Minerals Engineering* **56**, 70–80.

Del Castillo, M. F. and Dimitrakopoulos, R. (2016), 'A multivariate destination policy for geometallurgical variables in mineral value chains using coalition-formation clustering', *Resources Policy* **50**, 322–332.

Denby, B., Schofield, D. and Surme, T. (1998), Genetic algorithms for flexible scheduling of open pit operations, *in* 'Computer applications in the minerals industries. International symposium', pp. 605–616.

Desbarats, A. and Dimitrakopoulos, R. (2000), 'Geostatistical simulation of regionalized pore-size distributions using min/max autocorrelation factors', *Mathematical Geology* **32**(8), 919–942.

Deutsch, J. L., Palmer, K., Deutsch, C. V., Szymanski, J. and Etsell, T. H. (2016), 'Spatial modeling of geometallurgical properties: techniques and a case study', *Natural Resources Research* **25**(2), 161–181.

Diering, T., Richter, O. and Villa, D. (2010), Block cave production scheduling using pcbc, *in* 'Proceedings SME conference. Phoenix, USA'.

Dimitrakopoulos, R. (1998), 'Conditional simulation algorithms for modelling orebody uncertainty in open pit optimisation', *International Journal of Surface Mining, Reclamation and Environment* **12**(4), 173–179.

Dimitrakopoulos, R. (2011), 'Strategic mine planning under uncertainty', *Journal of Mining Science* **47**(2), 138–150.

Dimitrakopoulos, R., Farrelly, C. and Godoy, M. (2002), 'Moving forward from traditional optimization: grade uncertainty and risk effects in open-pit design', *Mining Technology* **111**(1), 82–88.

Dimitrakopoulos, R. G. and Sabour, S. A. A. (2007), 'Evaluating mine plans under uncertainty: Can the real options make a difference?', *Resources Policy* **32**(3), 116–125.

Dimitrakopoulos, R. and Grieco, N. (2009), 'Stope design and geological uncertainty: Quantification of risk in conventional designs and a probabilistic alternative', *Journal of Mining Science* **45**(2), 152–163.

Dowd, PA. (1976), 'Application of dynamic and stochastic programming to optimize cutoff grades and production rates', *Mining Technology: IMM Transactions Section A* **85**, 22–31.

Dowd, PA. (1994), 'Risk assessment in reserve estimation and open-pit planning', *Transactions of the Institution of Mining and Metallurgy (Section A: Mining Industry)* **103**.

Dowd, PA. and Dare-Bryan, P. (2004), Planning, designing and optimising using geostatistical simulation, The Australasian Institute of Mining and Metallurgy.

Dunham, S. and Vann, J. (2007), Geometallurgy, geostatistics and project value - does your block model tell you what you need to know?, *in* 'Project evaluation conference, Melbourne, Victoria', pp. 19–20.

Efron, B. and Gong, G. (1983), 'A leisurely look at the bootstrap, the jackknife, and cross-validation', *The American Statistician* **37**(1), 36–48.

Epstein, R., Goic, M., Weintraub, A., Catalán, J., Santibáñez, P., Urrutia, R., Cancino, R., Gaete, S., Aguayo, A. and Caro, F. (2012), 'Optimizing long-term production plans in underground and open-pit copper mines', *Operations Research* **60**(1), 4–17.

Evatt, G. W., Soltan, M. O. and Johnson, P. V. (2012), 'Mineral reserves under price uncertainty', *Resources Policy* **37**(3), 340–345.

Goodfellow, R. C. and Dimitrakopoulos, R. (2016), 'Global optimization of open pit mining complexes with uncertainty', *Applied Soft Computing* **40**, 292–304.

Goodfellow, R. and Dimitrakopoulos, R. (2017), 'Simultaneous stochastic optimization of mining complexes and mineral value chains', *Mathematical Geosciences* **49**(3), 341–360.

Gregory, M. J., Lang, J. R., Gilbert, S. and Hoal, K. O. (2013), 'Geometallurgy of the pebble porphyry copper-gold-molybdenum deposit, alaska: Implications for gold distribution and paragenesis', *Economic Geology* **108**(3), 463–482.

Grobler, F., Elkington, T. and Rendu, J. (2011), Robust decision making-application to mine planning under price uncertainty, *in* '35th APCOM Symposium-Application of Computers and Operations Research in the Minerals Industry, Proceedings', pp. 371–380.

Halkidi, M., Batistakis, Y. and Vazirgiannis, M. (2001), 'On clustering validation techniques', *Journal of intelligent information systems* **17**(2), 107–145.

Harquail, D. (1991), Investing in junior mining companies, *in* 'Proceedings of the 6th Mineral Economics Symposium of CIM'.

Hay, M. and Rule, C. (2003), 'Supasim: a flotation plant design and analysis methodology', *Minerals engineering* **16**(11), 1103–1109.

Hoal, K. O., Woodhead, J. and Smith, K. S. (2013), The importance of mineralogical input into geometallurgy programs, *in* 'The Second AusIMM International Geometallurgy Conference', pp. 17–26.

Hunt, J., Berry, R., Bradshaw, D., Triffett, B. and Walters, S. (2014), 'Development of recovery domains: Examples from the prominent hill iocg deposit, australia', *Minerals Engineering* **64**, 7–14.

Hunt, J., Kojovic, T. and Berry, R. (2013), Estimating comminution indices from ore mineralogy, chemistry and drill core logging, *in* 'GeoMet 2013: The Second AusIMM International Geometallurgy Conference', The Australasian Institute of Mining and Metallurgy (AusIMM), pp. 173–176.

Johnson, R., Scott, G. and Lukey, H. (2007), 'Implications of mineralogy, grain size and texture on liberation and pellet quality of great lakes iron ore', *Iron Ore* **2007**, 109–111.

Journel, A. G. (1974), 'Geostatistics for conditional simulation of ore bodies', *Economic Geology* **69**(5), 673–687.

Journel, A. G. (1983), 'Nonparametric estimation of spatial distributions', *Mathematical Geology* **15**(3), 445–468.

Keeney, L. and Walters, S. (2011), A methodology for geometallurgical mapping and orebody modelling, *in* 'GeoMet 2011-1st AusIMM International Geometallurgy Conference 2011', Australasian Institute of Mining and Metallurgy, pp. 217–225.

Khodayari, F. and Pourrahimian, Y. (2018), 'Production scheduling in block caving with consideration of material flow', *Aspects in Mining & Mineral Science* .

Kumral, M. (2004), 'Genetic algorithms for optimization of a mine system under uncertainty', *Production Planning & Control* **15**(1), 34–41.

Kumral, M. and Dowd, PA. (2005), 'A simulated annealing approach to mine production scheduling', *Journal of the Operational Research Society* **56**(8), 922–930.

Lagos, G., Espinoza, D., Moreno, E. and Amaya, J. (2011), 'Robust planning for an open-pit mining problem under ore-grade uncertainty', *Electronic Notes in Discrete Mathematics* **37**, 15–20.

Lamberg, P. (2011), Particles-the bridge between geology and metallurgy, *in* 'Konferens i mineralteknik', Luleå tekniska universitet.

Lamghari, A. and Dimitrakopoulos, R. (2012), 'A diversified tabu search approach for the open-pit mine production scheduling problem with metal uncertainty', *European Journal of Operational Research* **222**(3), 642–652.

Lamghari, A., Dimitrakopoulos, R. and Ferland, J. A. (2014), 'A variable neighbourhood descent algorithm for the open-pit mine production scheduling problem with metal uncertainty', *Journal of the Operational Research Society* **65**(9), 1305–1314.

Lerchs, H. and Grossman, L. (1965), Optimum design of open-pit mines, *in* 'Operations Research', Vol. 58, CIM Transactions, pp. 17–24.

Lund, C., Lamberg, P. and Lindberg, T. (2015), 'Development of a geometallurgical framework to quantify mineral textures for process prediction', *Minerals Engineering* **82**, 61–77.

Lutz, S. J., Hickman, S., Davatzes, N., Zemach, E., Drakos, P. and Robertson-Tait, A. (2010), Rock mechanical testing and petrologic analysis in support of well stimulation activities at the desert peak geothermal field, nevada, *in* 'Proceedings 35th Workshop on Geothermal Reservoir Engineering'.

Maleki, M. and Emery, X. (2015), 'Joint simulation of grade and rock type in a stratabound copper deposit', *Mathematical Geosciences* **47**(4), 471–495.

Marcotte, D. and Caron, J. (2013), 'Ultimate open pit stochastic optimization', *Computers & geosciences* **51**, 238–246.

Martinez, M. A. and Newman, A. M. (2011), 'A solution approach for optimizing long-and short-term production scheduling at lkab's kiruna mine', *European Journal of Operational Research* **211**(1), 184–197.

Matheron, G. (1963), 'Principles of geostatistics', *Economic geology* **58**(8), 1246–1266.

McQuiston, F. and Bechaud, L. (1968), 'Metallurgical sampling and testing', *Surface mining. New York: The American Institute of Mining, Metallurgical and Petroleum Engineers* pp. 103–121.

Moema, J., Papo, M., Slabbert, G. and Zimba, J. (2009), Grinding media quality assurance for the comminution of gold ores, *in* 'World Gold Conference', The Southern African Institute of Mining and Metallurgy, pp. 27–34.

Montiel, L. and Dimitrakopoulos, R. (2017), 'A heuristic approach for the stochastic optimization of mine production schedules', *Journal of Heuristics* **23**(5), 397–415.

Montoya, P., Keeney, L., Jahoda, R., Hunt, J., Berry, R., Drews, U., Chamberlain, V. and Leichliter, S. (2011), Geometallurgical modelling techniques applicable to prefeasibility projects–la colosa case study, *in* 'The First AUSIMM International Geometallurgy Conference', pp. 103–114.

Mueller, U. A. and Ferreira, J. (2012), 'The u-wedge transformation method for multivariate geostatistical simulation', *Mathematical Geosciences* **44**(4), 427–448.

Navarra, A., Montiel, L. and Dimitrakopoulos, R. (2018), 'Stochastic strategic planning of open-pit mines with ore selectivity recourse', *International Journal of Mining, Reclamation and Environment* **32**(1), 1–17.

Newman, A. M. and Kuchta, M. (2007), 'Using aggregation to optimize long-term production planning at an underground mine', *European Journal of Operational Research* **176**(2), 1205–1218.

Newman, A. M., Rubio, E., Caro, R., Weintraub, A. and Eurek, K. (2010), 'A review of operations research in mine planning', *Interfaces* **40**(3), 222–245.

Newton, M. J. and Graham, J. M. (2001), Estimating comminution indices from ore mineralogy, chemistry and drill core logging, *in* 'GeoMet 2011: The First AusIMM International Geometallurgy Conference', The Australasian Institute of Mining and Metallurgy (AusIMM), pp. 247–261.

Nguyen, K. and Keeney, L. (2014), Spatial domaining of highly variable continuous geometallurgical data, *in* 'XXVII International Mineral Processing Congress-IMPC 2014', Gecamin Digital Publications, pp. 116–127.

Picard, J.-C. (1976), 'Maximal closure of a graph and applications to combinatorial problems', *Management science* **22**(11), 1268–1272.

Pierce, M. E. (2010), *A model for gravity flow of fragmented rock in block caving mines*, University of Queensland.

Rockafellar, R. T. and Uryasev, S. (2000), 'Optimization of conditional value-at-risk', *Journal of risk* **2**, 21–42.

Rubio, E. and Dunbar, S. (2005), Integrating uncertainty in block cave production scheduling, APCOM.

Runge, K., Alexander, D., Franzidis, J., Morrison, R. and Manlapig, E. (1998), Jksimfloat-a tool for flotation modelling, *in* 'Proceedings of the AusIMM Annual Conference', pp. 361–370.

Schoemaker, P. J. (1995), 'Scenario planning: a tool for strategic thinking', *Sloan management review* **36**(2), 25.

Sepúlveda, E., Dowd, PA., Xu, C. and Addo, E. (2017), 'Multivariate modelling of geometallurgical variables by projection pursuit', *Mathematical Geosciences* **49**(1), 121–143.

Sharrock, G., Beck, D., Booth, G. and Sandy, M. (2004), 'Simulating gravity flow in sub-level caving with cellular automata', *Proceedings of MassMin* **189**.

Shishvan, M. S. and Sattarvand, J. (2015), 'Long term production planning of open pit mines by ant colony optimization', *European Journal of Operational Research* **240**(3), 825–836.

Silva, M. d. F., Dimitrakopoulos, R. and Lamghari, A. (2015), 'Solving a large sip model for production scheduling at a gold mine with multiple processing streams and uncertain geology', *Mining Technology* **124**(1), 24–33.

Sohrabian, B. and Tercan, A. E. (2014), 'Multivariate geostatistical simulation by minimising spatial cross-correlation', *Comptes Rendus Geoscience* **346**(3), 64–74.

Starkey, J. and Dobby, G. (1996), 'Application of the minnovex sag power index at five canadian sag plants', *Proceeding Autogenous and Semi-Autogenous Grinding* pp. 345–360.

Suazo, C., Kracht, W. and Alruiz, O. (2010), 'Geometallurgical modelling of the collahuasi flotation circuit', *Minerals Engineering* **23**(2), 137–142.

Tatman, C. (2001), 'Production-rate selection for steeply dipping tabular deposits', *Mining Engineering* **53**(10), 62–64.

Tehrani, M. M., Asghari, O. and Emery, X. (2013), 'Simulation of mineral grades and classification of mineral resources by using hard and soft conditioning data: application to sungun porphyry copper deposit', *Arabian Journal of Geosciences* **6**(10), 3773–3781.

Topal, E. (2008), 'Early start and late start algorithms to improve the solution time for long-term underground mine production scheduling', *Journal of the Southern African Institute of Mining and Metallurgy* **108**(2), 99–107.

Tungpalan, K., Wightman, E. and Manlapig, E. (2015), 'Relating mineralogical and textural characteristics to flotation behaviour', *Minerals Engineering* **82**, 136–140.

Vallee, M. (2000), 'Mineral resource+ engineering, economic and legal feasibility= ore reserve', *CIM bulletin* **93**(1038), 53–61.

Walters, S. (2008), An overview of new integrated geometallurgical research, *in* 'Australasian Institute of Mining and Metallurgy Publication Series', AusIMM, pp. 79–82.

Ward, D. and McCarthy, P. (1999), 'Startup performance of new base metal projects: Adding value to the carpentaria mineral province, mt isa, qld.', *Australian Journal of Mining* .

Whittle, J. (1998), Reference Manual, Technical report, Whittle Programming Pty Ltd.

Xu, C. and Dowd, PA. (2009), 'Conditional simulation of grades controlled by geological indicators'.

Yano, C. A. and McFadden, C. (2014), Mine planning above and below ground: Generating a set of pareto-optimal schedules considering risk and return, *in* 'Essays in Production, Project Planning and Scheduling', Springer, pp. 343–356.

Yildirim, B. G., Bradshaw, D., Powell, M., Evans, C. and Clark, A. (2014), 'Development of an effective and practical Process Alteration Index (PAI) for predicting metallurgical responses of Cu porphyries', *Minerals Engineering* **69**, 91–96.

Chapter 2

Multivariate modelling of geometallurgical variables by projection pursuit

Statement of Authorship

Title of Paper	Multivariate Modelling of Geometallurgical Variables by Projection Pursuit.
Publication Status	☑ Published ☐ Accepted for Publication ☐ Submitted for Publication ☐ Unpublished and Unsubmitted w ork w ritten in manuscript style
Publication Details	Sepulveda E, Dowd PA, Xu C, Addo E. Multivariate Modelling of Geometallurgical Variables by Projection Pursuit. Mathematical Geosciences. 2017 Jan 1;49(1):121-43. DOI: 10.1007/s11004-016-9660-z

Principal Author

Name of Principal Author (Candidate)	Exequiel Manuel Sepulveda Escobedo		
Contribution to the Paper	Develop methodology and methods, conducted programming and execution of methods, wrote manuscript and acted as corresponding author.		
Overall percentage (%)	80%		
Certification:	This paper reports on original research I conducted during the period of my Higher Degree by Research candidature and is not subject to any obligations or contractual agreements with a third party that would constrain its inclusion in this thesis. I am the primary author of this paper.		
Signature		Date	20/02/2018

Co-Author Contributions

By signing the Statement of Authorship, each author certifies that:

i. the candidate's stated contribution to the publication is accurate (as detailed above);

ii. permission is granted for the candidate in include the publication in the thesis; and

iii. the sum of all co-author contributions is equal to 100% less the candidate's stated contribution.

Name of Co-Author	Peter Dowd		
Contribution to the Paper	Supervised development of work and reviewed manuscript.		
Signature		Date	20th February 2018

Name of Co-Author	Chaoshui Xu		
Contribution to the Paper	Supervised development of work and reviewed manuscript.		
Signature		Date	20-02-2018

Name of Co-Author	Emmanuel Addo		
Contribution to the Paper	Wrote and reviewed geological concepts in the manuscript.		
Signature		Date	20-02-2018

Abstract

The integration of geological and geometallurgical data can significantly improve decision-making and optimize mining production due to a better understanding of the resources and their metallurgical performances. The primary-response rock property framework is an approach to the modelling of geometallurgy in which quantitative and qualitative primary properties are used as proxies of metallurgical responses. Within this framework, primary variables are used to fit regression models to predict metallurgical responses. Whilst primary rock property data are relatively abundant, metallurgical response property data are not, which makes it difficult to establish predictive response relationships. Relationships between primary input variables and geometallurgical responses are, in general, complex and the response variables are often non-additive which further complicates the prediction process.

Consequently, in many cases, traditional multivariate linear regression models (MLR) of primary-response relationships perform poorly and a better alternative is required for prediction. Projection pursuit is a powerful exploratory statistical modelling technique in which data from a number of variables are projected onto a set of directions that optimize the fit of the model. The purpose of the projection is to reveal underlying relationships. Projection pursuit regression (PPR) fits standard regression models to the projected data vectors. In this paper, PPR is applied to the modelling of geometallurgical response variables. A case study with six geometallurgical variables is used to demonstrate the modelling approach. The results from the proposed PPR models show a significant improvement over those from MLR models. In addition, the models were bootstrapped to generate distributions of feasible scenarios for the response variables. Our results show that PPR is a robust technique for modelling geometallurgical response variables and for assessing the uncertainty associated with these variables.

Keywords Geometallurgical modelling; Projection pursuit regression; Risk management.

2.1 Introduction

Geometallurgy has the potential to yield substantial improvement in mine planning and operation by properly integrating the available geological and metallurgical information (Dunham and Vann, 2007; Walters, 2008; Coward

et al., 2009, 2013; Coward and Dowd, 2015). The incorporation of metallurgical response variables into the resource model allows not only a more realistic optimization of economic objectives, but also the assessment of processing performances, leading to a more robust project evaluation under uncertainty (Dowd et al., 2016). It also provides the basis for optimizing the net present value of the final product rather than the net present value of a simplistic function of in situ grades and tons. Comminution performance and mineral processing recovery factors are key parameters that directly affect production and the value of the final product and their prediction in the early stages of a mining operation is important for mine planning and project risk assessment.

The most widely used tests for determining comminution performances are the Bond mill work index (BWi), Bond rod mill work index (RWi), resistance to abrasion and breakage index (A$\times$b) and the drop-weight index (DWi). The most common processing recovery tests are based either on flotation or leaching operations. An increasingly better understanding of the physical and chemical principles on which these performance indices are based has contributed to the growing acceptance and use of the concept of geometallurgy. Basic geology and mineral processing knowledge are now enriched with mineralogy (the proportion and/or size distribution of minerals in a rock sample), lithology, textural characteristics and particle liberation profiles that can quantify more precisely the comminution and recovery performances (Keeney and Walters, 2011; Hunt et al., 2013, 2014). However, there remain significant impediments to the incorporation into resource models of these variables and the mineral processing responses in a manner that can be used effectively in practice. In most projects, due to the lack of appropriate geometallurgical data collection and analysis, or their complete absence, there are usually insufficient test-work results for reliable metallurgical response modelling. The significant difference between the large numbers of samples recorded in geological databases (logging, assaying and geotechnical data) and the relatively few metallurgical test-work samples impedes the successful integration of metallurgical responses into the resource model using geostatistical methods (Hunt et al., 2013). Additional issues arise from the non-additivity of many metallurgical response variables (Dunham and Vann, 2007), which may require indirect methods of up-scaling from the laboratory (sample) scale to production scales. The primary-response framework documented in Coward and Dowd (2015) and Coward et al. (2009, 2013) allows primary rock properties (intrinsic rock attributes directly measured from rock samples) to be used to predict processing response properties, such as recovery factors and comminution performance,

and incorporate them into the resource model. Using only additive primary variables to predict non-additive response variables minimizes the biases related to non-additivity (Carrasco et al., 2008).

Under the primary-response framework, two key aspects are considered. The first aspect is the selection of a relationship that has good prediction performance. The statistical model most commonly used to derive relationships for predicting a dependent variable from a set of input variables is regression (Friedman, 1994). Regression is based on the assumption of a functional relationship between a dependent variable and one or more explanatory variables. There are several regression models and methods but the most commonly used is multivariate linear regression (MLR). However, as MLR requires strong linear relationships between dependent and explanatory variables, its predictive performance is extremely poor when the relationships are non-linear.

As strong non-linear relationships are often observed between primary and response geometallurgical variables, MLR is unlikely to be the best option for predicting response variables and other types of regression models should be considered. There are several non-linear regression techniques that are more able to model complex relationships, including machine learning methods, polynomial regression and projection pursuit methods (Friedman, 1994).

The second key aspect is to identify the most important variables in terms of predictive performance given a set of available primary variables. This issue is related to the difficulty in geometallurgy of handling high-dimensional data. Higher dimensions require much more data and are much more difficult to model as when the dimensionality is high, data become sparser and, therefore, finding the best relationship becomes more difficult. In this case, reducing dimensionality could lead to better and simpler models.

Geometallurgical characterization using regression and dimensionality reduction is a common general approach. Keeney and Walters (2011) used principal component analysis (PCA) to define nine geometallurgical domains based on 500 samples using mineralogy and assay data to build prediction models for two comminution indices: BWi and A$\times$b. PCA was used to map multidimensional information onto a two-dimensional scatter plot for the first and second principal components. This mapping was used to identify mineralogical trends and associations for geometallurgical domain definition. Regression models with high coefficients of determination (R^2) were fitted for each defined geometallurgical domain.

Boisvert et al. (2013) merged variables to reduce dimensionality. They used grades, mineralogy and association data, defined as the contact area between

two adjacent minerals within a single grain of crushed material, to predict six plant performance variables. In their model, from a total of 204 input variables, four different subsets were created in several amalgamation steps. Finally, three different kinds of models, each containing different subsets of merged variables, were fitted by multilinear regressions. Reasonable to good correlations between true and estimated values were achieved, ranging from 0.533 to 0.9. These MLR models were used to include plant performance indices in a resource model. Similarly, Hunt et al. (2013) used grades, mineralogy, lithology, and alteration data to predict three comminution indices: SAG power index, BWi and A×b. They applied a feature selection method to select the best predictive variables and used multivariate linear regression models. They reported average relative errors in the range of 6-12%.

Recent research by Hunt et al. (2014) used both qualitative and quantitative primary rock properties (grades, lithology, sulfide class and gangue class). They defined archetypes or geometallurgical domains and established several linear regression models for each different archetype for copper recovery. Using 162 samples, they obtained good model performances with RS between 0.69 and 0.85.

There is no clear or unique set of rules for choosing a particular modelling technique, as the choice is case dependent. In geometallurgical characterizations, there is often no clear linear relationship and a non-linear method may work better than MLR. In the case study presented here, MLR does not perform well.

Although PPR has been successfully applied in many disciplines, it has not been used in geometallurgy modelling but in related disciplines, such as environmental engineering and geoscience (Qianjian and Jianguo, 2011; Ghasemi and Zolfonoun, 2013). PPR is a good alternative for geometallurgical modelling, particularly for this case study, and a robust modelling method that can be easily used for uncertainty and risk assessments applying techniques, such as bootstrapping.

2.2 Method

2.2.1 Projection pursuit

Projection pursuit (PP) is a statistical method developed by Friedman and Tukey (1974) initially for exploratory data analysis. The visualization of a multidimensional dataset is very difficult due to the limitations of finding useful features in a lower dimensional space (two or three dimensions) for easier human interpretation. PP is a linear transformation method that focuses on projections rather than an orthogonal global transformation such as PCA and factor analysis, the two most popular linear transformation methods.

The core component of PP is to find some directions onto which the multidimensional data can be projected to reveal useful characteristics.

Formally, let X be n observations of a k-dimensional random vector $X = (x_1, x_2, ..., x_k), x_i \in \mathbb{R}^n$, where x_i is a random variable representing a feature. A direction α is a normalized vector in $\mathbb{R}^k$ and the projection p of X onto α is $p = \alpha^T X$.

The key aspects of PP are in the definition of a measure of "interestingness" and in the search of a direction onto which the projection of X maximizes "interestingness". This "interestingness" can be represented by a projection index function

$$I(p) = f(p) : \mathbb{R}^n \to \mathbb{R}. \tag{2.1}$$

Since any interesting property is subjective and depends on the problem to be solved, a specific projection index is defined for each specific application and hence different indices are obtained for different projections. For example, projection indices have been defined for exploratory data analysis (Friedman and Tukey, 1974), density estimation (Friedman et al., 1984), regression (Friedman and Stuetzle, 1981), classification (Lee et al., 2005) and de-correlating variables (Barnett et al., 2014). Finally, the PP objective can be seen as an optimization problem in which it is required to find one or more directions that maximize a specific projection index

$$\alpha = \arg\max_{\alpha} \left(I(\alpha^T X)\right), \ \|\alpha\| = 1. \tag{2.2}$$

2.2.2 Projection pursuit regression

Regression is a statistical technique for predicting a dependent variable y using a function of explanatory variables X with an error component ϵ, i.e.,

$$y = f(X) + \epsilon. \tag{2.3}$$

The function f can be linear or non-linear, and the error ϵ is independent and normally distributed with a mean of zero. Due to its simplicity the most commonly used regression technique is multivariate linear regression (Weisberg, 2005)

$$y = b_0 - \sum_{i=1}^{n} b_i x_i + \epsilon, \tag{2.4}$$

where factors bi are found by minimizing the squared error between measured and predicted values of the dependent variable

$$[y - b_0 - \sum_{i=1}^{n} b_i x_i]^2. \tag{2.5}$$

However, when there are strong non-linear relationships between the dependent and explanatory variables, the predictive power of MLR significantly decreases. PPR can handle this problem by adding several linear combinations of smoothed projections.

PPR has two main features: (i) instead of using the raw input, it uses a projection; and (ii) the projection is smoothed to capture the main trend in the relationship. The smoothing procedure is important, since its application gives a good generalization and attenuates extreme values. Figure 2.1 illustrates the projection and its smoother for the response variable BWi using the first direction. In addition, PPR uses an iterative algorithm to find more appropriate projection directions. The PPR can be expressed as

$$y = \sum_{k=1}^{m} s_k(\alpha_k^T X), \tag{2.6}$$

where s is the smoother and Îś is the direction at step k. There are several types of smoothers. The most common is the spline smoother (Silverman, 1984), but the super-smoother (Friedman, 1984) is used in this work. The super-smoother uses short, middle and large spans at 5%, 20% and 50% of the number of samples respectively, to determine an optimal span by cross-validation. The use of a smoother enhances the capability of PPR to deal with non-linear relationship

problems.

The critical component of PPR is to define an appropriate projection index. For regression models, the explained variance is an effective indicator of model accuracy. As the explained variance is 1.0 for a perfect model, the projection index can be defined as

$$I(\alpha) = 1 - \frac{[\sum_{i=1}^{n} r_i - s_\alpha(\alpha X)]^2}{\sum_{i=1}^{n} r_i^2}, \tag{2.7}$$

where r_i are the current residuals.

The best direction is the one that maximizes $I(\alpha)$. When the projection index for a direction is close to zero, the contribution of that direction is not significant and no more directions are needed. This projection index is differentiable if the smoother is differentiable. Although the super-smoother is not differentiable and, therefore the global optimum is not guaranteed, finding successively local-optimum directions using a gradient-based optimization algorithm leads to satisfactory results.

The final PPR algorithm is as follows:

1. Let y be the dependent variable, initially standardized (centered with unit variance).

2. Let $r_1 = y$ be the initial residuals.

3. Let α and $s\alpha$ be the best direction and smoother respectively, where the smoothed projection onto α maximizes the projection index (Eq. 2.7).

4. If the explained variance is not sufficiently small (a user-defined value, but a variation less than 1% is a good value in practice), store the direction and the smoother, update the residual: $r_{i+1} = r_i - s_\alpha(\alpha X)$ and go to step 2 to find a new direction.

PPR is very efficient in terms of computational cost. For a dataset of n samples, k dimensions and m projections, the required computation is of the order of $m * k * n * log(n)$.

2.3 Methodology

Projection pursuit is used in this work to build prediction models for response properties under the primary-response framework discussed above. Both geological and metallurgical variables are used initially in this case to construct the

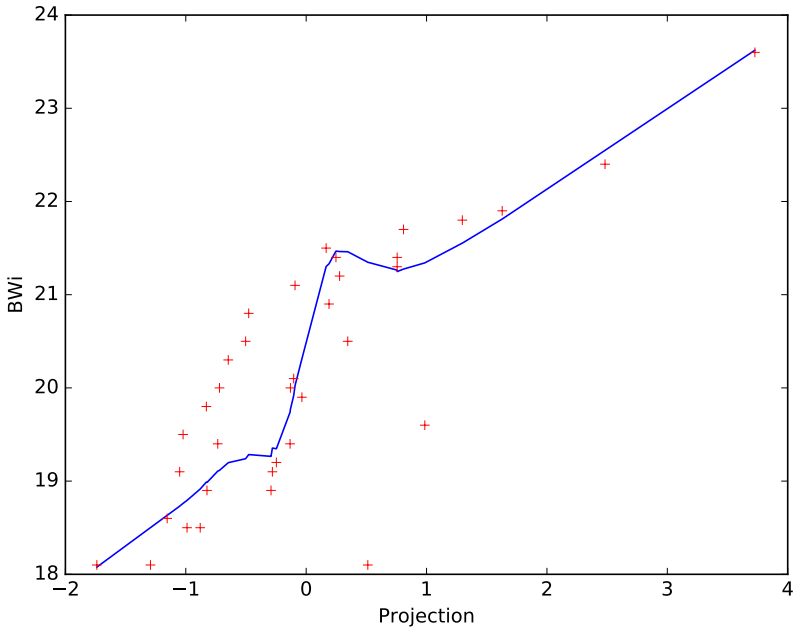


FIGURE 2.1: Projection and its smoother of the first direction found by PPR for BWi.

PPR models, which must be based on a good training data set. Training regression models with a reduced number of data may be challenging as models may be very sensitive to the presence/absence of a datum. There is a temptation to use all data available without any validation. This approach may produce a very good fit for the data available but the final outcome may be misleading. A good model should predict unknown data as well as training data. A common approach involves randomly partitioning the input data into two datasets: one for training and one for validation. This procedure, however, is very biased on small datasets, because obtaining similar distributions on both sets is hard to achieve in practice. For example, if there are outlier data, the probability of having outliers in the validation set is higher if the dataset is small. The k-fold cross-validation technique was developed to overcome this drawback by varying the training and validation datasets. A more robust validation technique is bootstrapping. This technique involves sampling randomly from the original dataset with replacement to form a subset of samples, which is then used to train the regression model. The trained regression model is then tested on the complete original dataset. An additional advantage of this approach is that, by repeating the process a certain number of times, a complete distribution of models can be generated to assess the uncertainty involved. This could be very useful in the case of modelling metallurgical responses. A good discussion of

these cross-validation methods can be found in (Efron and Gong, 1983) and (Arlot et al., 2010).

Five goodness-of-fit measurements are used to evaluate the performance of regression models: correlation coefficient (R), coefficient of determination (R^2), root mean squared error (RMSE), mean absolute error (MAE), and the mean error (ME)

$$R(y, \hat{y}) = \frac{cov(y, \hat{y})}{\sigma_y \sigma_{\hat{y}}}, \tag{2.8}$$

$$R^2(y, \hat{y}) = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}, \tag{2.9}$$

$$RMSE(y, \hat{y}) = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}, \tag{2.10}$$

$$MAE(y, \hat{y}) = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i|, \tag{2.11}$$

$$ME(y, \hat{y}) = \frac{1}{n}\sum_{i=1}^{n}[(y_i - \hat{y}_i) - \overline{(y_i - \hat{y}_i)}], \tag{2.12}$$

where $cov(y, \hat{y})$ is the covariance between y and its prediction $\hat{y}$; $\bar{y}$ is the mean value of y and σ is the standard deviation.

A value of R, between true and predicted values, close to -1 or 1 is an indication of good prediction performance. A good model should also explain as much as possible the variance of the true value; $R^2 = 1.0$ means that the model fully explains the total variance and $R^2 = 0.0$ means that the model does not explain any of the variance. RMSE and MAE are different measurements of prediction error. ME gives an indication of the level of bias; a value close to 0 indicates that the prediction is globally unbiased.

The following four steps are used to derive the best PPR model:

1. Feature selection.
2. Optimal number of directions.
3. Bootstrapping.
4. Model selection.

The main purpose of feature selection is to choose the subset of input variables that has the best predictive capability. This procedure in general leads to dimensionality reduction as usually the subset is substantially smaller than the

TABLE 2.1: Basic statistics of six geometallurgical response variables.

Variable	#Samples	Minimum	Mean	Maximum	Variance
Resistance to abrasion breakage (A×b)	64	24.4	31.45	51.20	19.28
Drop-weight index (DWi)	58	5.5	8.90	10.77	1.10
ond ball mill work index (BWi)	36	18.1	20.14	23.60	1.81
Bond rod mill work index (RWi)	33	22.9	28.45	34.00	10.36
Gold rougher recovery (Au Rec)	247	42.9	80.36	94.70	77.40
Copper rougher recovery (Cu Rec)	247	55.9	88.93	98.50	69.19

complete set of input variables. A combination of a forward selection and the meta-heuristic optimization method are used in this work. Forward selection (Chatterjee and Hadi, 2015) adds variables one by one by selecting the variable that best improves the model when it is included. Forward selection does not necessarily select the best subset of input variables because it is a greedy procedure. For this reason, the forward selection result is the initial solution that is further refined using the Tabu search meta-heuristic optimizer (Glover, 1990).

After the best features are selected, the number of directions used by PPR can be optimized. Since the most critical parameters are now fixed, all models are exhaustively bootstrapped using the five goodness-of-fit measurements to conduct the final model selection. A good model should not only have good performance indices, but should also be unbiased. The structure of the residuals is, therefore, very important in the final choice of model.

A stochastic geometallurgical block model may be derived from simulations of all primary input variables, which could be generated by geostatistical simulation techniques. Since all PPR models are based on testwork values at the laboratory scale they must be scaled up to the block volumes before being included into the block model. The up-scaling problem is not addressed in the work presented here.

Finally, a complete geological and geometallurgical block model such as this will contribute to improved mine planning and mine-to-mill optimization.

2.4 Case study

PPR is applied to the geometallurgical characterization of a poly-metallic deposit in which gold-copper mineralization occurs in a porphyry intrusion and adjacent wall rock. The rocks in the study area are feldspathic siltstones with lesser sandstones, underlain by volcanic rocks. Several geological and metallurgical samples were taken from the study area and were used as proxies to

predict key metallurgical and processing responses. There are six geometallurgical response variables to be modelled: the recovery rates of two metals in a rougher flotation circuit and four comminution indices. Table 2.1 shows the basic statistics for the six response variables. The main difficulties in this case study are the small number of samples for the four comminution indices and the high variance of recovery variables.

As all test-work results are recorded against the drill holes from which the core samples were taken it is easy to link the geometallurgical response variables to the geological and assay databases. In this case study, grades, lithology, alteration and mineralization style are available as input variables. Grades are quantitative (continuous) variables while lithology, alteration and mineralization styles are qualitative (categorical) variables. Qualitative data are specified as proportions of each category, for example, a volcaniclastic lithology value of 0.8 means that 80% of the sample comprises that particular lithology.

Within the primary-response framework, models are sought to estimate the six response variables using the available primary variables. This process is not difficult if the relationships are simple. However, in this case study, there are two problems. The first one is the high dimensionality of the input space (57 variables) especially when combined with less number of samples than dimensions, such as BWi, RWi and DWi. The second is the complexity of the relationships between primary and response variables. The first problem is addressed by the application of a feature selection method and the second problem by PPR. Details are given below.

There are two objectives in the multivariate modelling. The first is to determine whether the inclusion of the qualitative information (alteration, mineralization and lithology) improves the performance of models compared with using only quantitative information (grades). Two models are defined: the "Base Model" which includes only grade variables and the "Optimized Model" which includes the best selection from the feature selection process of both quantitative and qualitative variables. The second objective is to compare the performances of the derived PPR models with those of the traditional MLR models.

To select the best features for fitting a regression model, the correlation coefficients between dependent and all explanatory variables are examined, as shown in Table 2.2. In general, there are no strong correlations between primary and response variables.

For A$\times$b and DWi, there is no strong correlation as all absolute coefficients are less than 0.3. BWi has an absolute correlation coefficient greater than 0.5 with Fe and Ql mineralization and 0.4 with Se alteration and ST lithology.

TABLE 2.2: Correlations between primary and response variables. The symbol "-" denotes missing value. Correlations with absolute value greater than 0.4 are highlighted.

Variable		A×b	BWi	DWi	RWi	Au Rec	Cu Rec
Grades	Au	0.068	-0.254	-0.163	-0.085	0.245	0.003
	Cu	0.056	-0.105	-0.092	-0.120	0.216	0.344
	S	-0.062	0.160	0.023	-0.019	0.286	0.192
	Fe	-0.100	0.559	0.177	**0.395**	-0.270	-0.195
	Mo	0.173	-0.178	-0.219	-0.195	-0.376	**-0.499**
Alteration	Ab	-0.209	0.352	0.183	0.163	-0.120	-0.347
	B	0.002	-	0.009	-	-0.082	0.064
	Bt	-0.095	0.223	0.092	0.388	0.021	0.097
	Ca	-0.095	-0.209	0.120	-0.181	-0.071	-0.114
	Cb	0.156	-0.170	-0.115	0.134	-0.005	-0.084
	Ch	0.030	0.183	0.006	0.141	0.030	-0.074
	Cy	0.101	0.194	-0.138	0.124	-	-
	Ep	0.128	-	-0.161	-	-	-
	H	-0.071	-0.069	0.064	-0.109	0.019	-0.153
	He	-	-	-	-	0.130	0.246
	I	-0.053	-0.315	0.075	-0.346	0.013	-0.013
	Ka	0.117	-	-0.165	-	0.068	0.246
	Kf	-0.006	0.115	-0.015	0.162	-0.010	-0.015
	Mt	0.076	0.047	-0.061	-0.253	0.076	0.213
	Py	0.099	0.022	-0.136	0.007	-0.095	-0.109
	Q	-0.075	0.111	-0.136	**0.445**	0.042	0.136
	R	0.174	-0.099	-0.163	0.072	0.091	-0.098
	S	0.073	-0.060	-0.060	-0.122	0.025	0.179
	Se	0.058	**-0.410**	-0.028	-0.385	-0.265	**-0.421**
	To	-0.132	-0.301	0.154	-0.363	-0.071	-0.103
	U	-0.013	-	0.052	-	-0.238	-0.242
Mineralization	Bo-Cp-Mo	0.016	0.011	-0.038	**-0.435**	0.037	0.033
	BV	-	-	-	-	-0.007	0.149
	CP	0.064	-0.038	-0.076	-0.126	-0.030	-0.026
	Cp-Bo	0.016	0.097	-0.038	-0.215	-	-
	CV	0.006	-0.167	-0.059	-0.234	-0.015	-0.080
	EV	-	-	-	-	0.113	-0.032
	GQZ	-0.181	0.199	0.239	0.180	-0.041	-0.141
	MV	-0.136	0.085	-0.055	0.168	-0.144	-0.149
	PY	0.056	-0.009	-0.088	-0.112	0.030	-0.019
	Py-Cp	0.161	0.073	-0.191	-0.082	0.024	-0.032
	QCK	-0.263	0.180	0.271	**0.572**	0.022	0.096
	QCP	0.212	-0.215	-0.183	-0.210	-0.063	-0.045
	Ql	-0.119	**0.659**	0.185	**0.482**	0.114	0.017
	QPY	0.163	-0.057	-0.146	0.078	-0.036	0.014
	QZB	0.120	-0.045	-0.155	-0.040	0.019	-0.066
	QZC	-0.029	0.044	0.032	0.070	0.133	-0.007
Rock type	A	-0.019	-0.078	-0.033	0.175	-0.206	**-0.419**
	BX	0.095	-0.160	-0.191	-0.149	-0.022	-0.122
	CC	0.179	0.020	-0.214	-0.299	-0.009	-0.130
	CP	-0.137	0.204	0.162	0.203	-0.069	0.058
	FT	0.104	0.169	-0.150	0.247	0.013	0.016
	G	-0.008	-0.057	-0.045	0.024	-0.021	-0.049
	M	-0.064	-0.148	0.031	0.089	0.019	0.130
	PF	0.157	0.086	-0.126	-0.021	-0.128	-0.163
	PP	0.181	-0.140	-0.141	-0.105	-0.025	0.013
	ST	-0.131	**0.440**	0.182	0.154	-0.062	-0.200
	V	-0.293	0.141	0.323	0.235	0.122	0.230
	VB	-0.081	-0.092	-0.088	-0.060	0.090	-0.073
	VC	-0.017	0.129	0.039	-0.311	-0.028	0.086
	VP	-0.007	-0.062	-0.032	0.173	0.142	0.041
	VX	0.023	-0.134	0.001	-0.202	0.008	-0.005

TABLE 2.3: Final feature selection for PPR and MLR models.

Response variable	Inputs variables				
	Total number of variables	Grades	Lithology codes	Alteration codes	Mineralization codes
PPR models					
A×b	5	Mo	V, VX	Ch, Cy	
BWi	3	Fe	G		Ql
DWi	6	Au, Fe	V	Ab, Q	QCK
RWi	7	Fe, Mo		I, Mt, Q, Bt	Ql
Au Recovery	20	Au, Mo	PF, G, CP, VX, VC, FT, BX	Ab, B, He, Q, R, S, U	EV, QCK, QZC, Ql
Cu Recovery	20	Cu, Mo, S	A, BX, CC, CP, PP, ST, VB	Ab, B, He, I, Ka, R, S	BV, Py-Cp, Ql
MLR models					
A×b	10	Au, Cu	G, V, VC	Ab, I, Q, R	QCK
BWi	9	Au, Cu	G, VC, FT	Se	Ql, GQZ, CP
DWi	8	Au, Cu	V, VC	Ab, I, R	QCK
RWi	7	Fe	VC	R, Q, Se	GQZ, QCK
Au Recovery	22	Au, Cu, Fe, Mo	PF, G, CP, CC, VC, FT	He, B, Kf, I, U, Se	QCK, QZC, QZB, PY, Ql, EV
Cu Recovery	25	Cu, Mo, S	PF, G, CC, VB, M, VC, BX, ST, PP, V, A	QZB, GQZ, Ql, BV	He, Ka, Kf, I, H, Q, R, U, Se, Ab

RWi is moderately correlated with Q alteration (positive) and three mineralization styles: Bo-Cp-Mo (negative), QCK and Ql (both positive). Gold recovery shows negligible correlation with primary variables. Copper recovery correlates positively, but only moderately, with copper grade; and negatively with molybdenum, Se alteration and A lithology.

2.4.1 Feature selection

Weak correlations make it difficult to find the most appropriate input variables. Feature selection techniques seek to reduce the number of input variables by identifying and discarding variables that do not contribute significantly to the performance of a regression model. In our study, the optimal subset of input variables was found for each response variable by using the forward selection and meta-heuristic optimization procedures explained in Sect. 2.3. Table 2.3 shows the input variables found by the optimization procedure for each response variable.

2.4.2 Optimal number of directions

The number of projections is one of the most important parameters of PPR. Although, in general, the predictability increases as the number of projections increases, too many projections can result in over-fitting. Figure 2.2 shows the improvement in R^2 between predicted and true values of all response variables as the number of projections increases from 1 to 20.

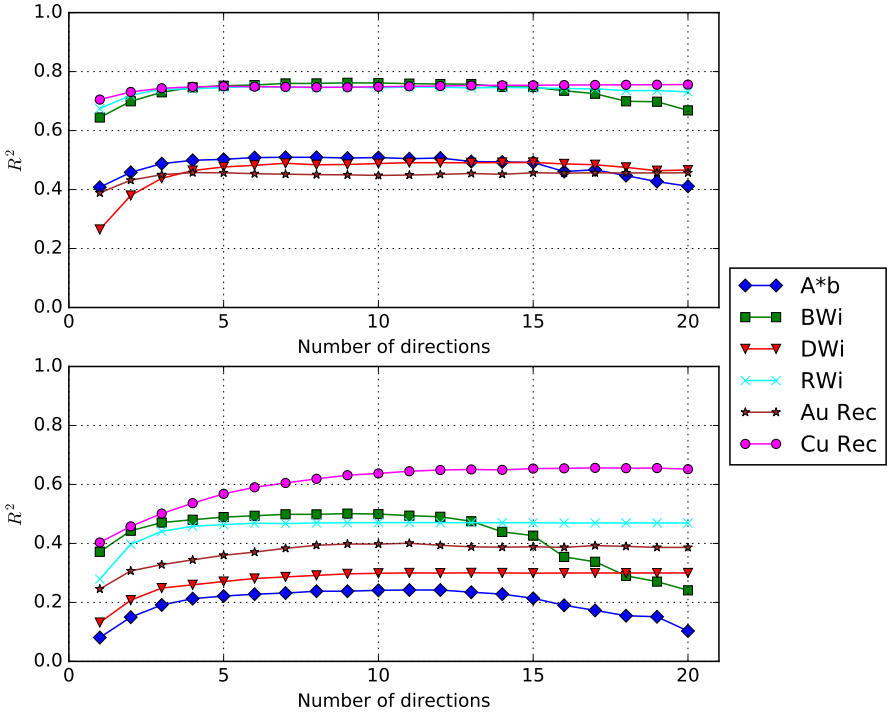
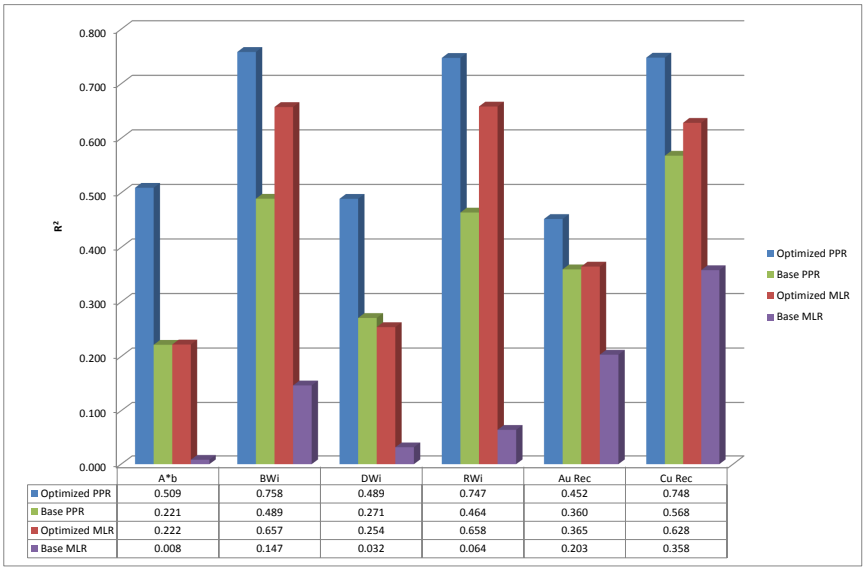


FIGURE 2.2: R^2 coefficient using from one to twenty directions. Optimized models and base models correspond to upper and lower charts respectively.

TABLE 2.4: Summary of R^2 coefficient for PPR models.

	Optimized		Base		Improvement
	R^2	Directions	R^2	Directions	
A×b	0.509	8	0.242	11	110%
BWi	0.762	9	0.501	9	52%
DWi	0.492	15	0.300	13	64%
RWi	0.749	6	0.471	11	59%
Au Rec	0.457	4	0.401	11	14%
Cu Rec	0.756	20	0.656	17	15%



	A*b	BWi	DWi	RWi	Au Rec	Cu Rec
Optimized PPR	0.509	0.758	0.489	0.747	0.452	0.748
Base PPR	0.221	0.489	0.271	0.464	0.360	0.568
Optimized MLR	0.222	0.657	0.254	0.658	0.365	0.628
Base MLR	0.008	0.147	0.032	0.064	0.203	0.358

FIGURE 2.3: Comparison of performance (R^2) of optimized and base models for PPR and MLR.

All optimized models reach a plateau using seven or more projection directions. For base models, between 5 and 12 directions are required for R^2 to stabilize. The comparison of the performances at the maximum R^2 (Table 2.4) shows that optimized models consistently out-perform the base models with a significant improvement of 110% in the A$\times$b index model. Both recovery rates show modest improvements. For copper recovery, the base model explains nearly 65% and the optimized model explains a little more than 75% of the variance. This is still considered a significant improvement in terms of reducing the variability of predictions.

2.4.3 PPR compared with MLR

MLR models were also generated and bootstrapped to compare the prediction performances of the traditional approach with those of the proposed PPR models. To obtain the optimized MLR models, the same procedure of feature selection and optimization was followed. Note that the optimized subsets of variables for PPR and MLR are different (Table 2.3). For base models, the same five grade variables were used.

It can be observed from Figure 2.3 that optimized PPR models consistently out-perform the MLR models. In the case of A$\times$b, DWi and Au recovery, even

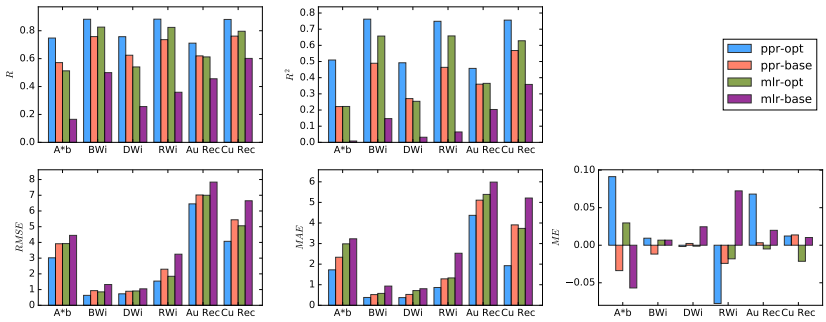


FIGURE 2.4: Average values of R, R^2, RMSE, MAE and ME of optimized and base PPR models.

base PPR models have performances similar to those of the optimized MLR models. While the base MLR models for three grindability indices perform extremely poorly (with R^2 close to zero), base PPR models can still be used if simple models are required. It is clear from this comparison study that models perform significantly better when qualitative information is included.

Finally, Figure 2.4 summarizes the five goodness-of-fit indices for both optimized models and base models from the bootstrapping procedure for both PPR and MLR models. All values show clearly the advantage of using PPR over MLR. Not only is R^2 substantially improved, both error measurements, RMSE and MAE, are significantly reduced.

2.4.4 Bootstrapping

To assess the accuracy and final predictive performance, both the optimized and base PPR models were bootstrapped. A total of 500 samples with replacement were generated from the original dataset in order to assess the variability and uncertainty associated with each model. This number of samples was selected as it is the number at which all indices become stable, and also avoids having different numbers of samples for the variables. This is specifically useful in cases where some variables have fewer data, which may require a smaller number of samples. Figure 2.5 shows boxplots of all goodness-of-fit indices for optimized and base PPR models. Comparing the performance of both models based on the bootstrapping results, it is evident that for the four grindability indices, the inclusion of categorical variables has significantly improved the model predictability. Although for recovery variables the improvement is only marginal, categorical variables increase the predictive performance of the models. This observation is consistent with the geology as grindability indices

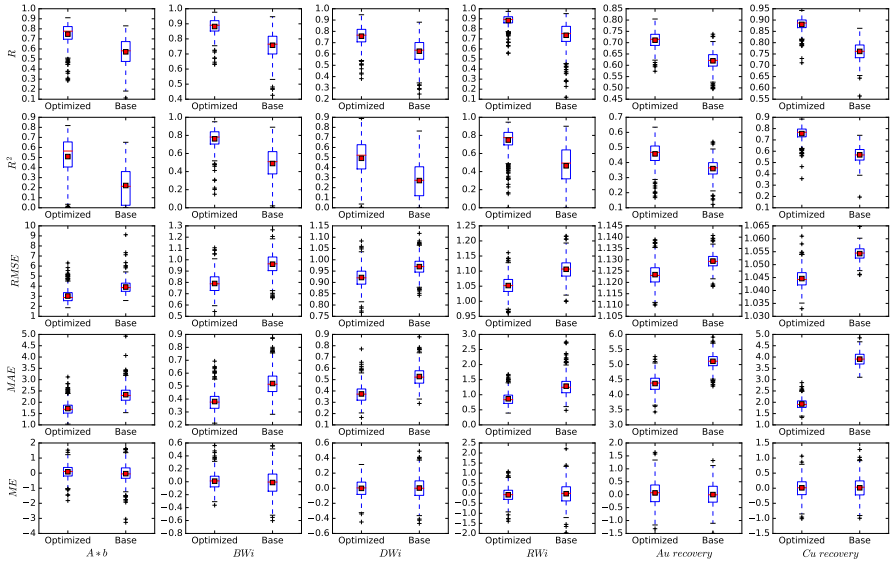


FIGURE 2.5: Boxplot of optimized and base PPR bootstrapped models. Rows are R, R^2, RMSE, MAE and ME; columns are the six response variables.

depend largely on geological rock properties rather than on chemical element concentrations.

Copper recovery (Cu Rec) has the lowest variability for R^2, which indicates that the PPR models are very stable. Low variability is observed for BWi, RWi and gold recovery (Au Rec), but A$\times$b and DWi have higher variability of R^2. As expected, most of the optimized models vary less than the base models. Only for gold recovery, do the optimized models have higher variability, which suggests that some goodness-of-fit measures are very dependent on the selected features. Overall, the optimized models have consistently lower error measures and their biases, given by the mean errors (fifth row Figure 2.5), indicate that mean prediction errors are concentrated close to zero; nevertheless, some models with high mean error (bias) should be rejected.

2.4.5 Model selection

To incorporate the uncertainty of a model for risk assessment, a subset of valid bootstrapped models should be used to guarantee a good reproduction of all possible predictions. To ensure unbiasedness, only models with mean prediction errors between -0.05 and 0.05 are considered valid models. The mean and standard deviation of measured (true) and predicted values are very similar

TABLE 2.5: Summary of statistics of true and predicted values of selected optimized PPR models.

Variables	Models	True Value		Prediction	
		μ	σ	μ	σ
A×b	42	31.447	4.356	31.446	4.186
BWi	164	20.142	1.328	20.117	1.325
DWi	169	8.895	1.039	8.853	1.118
RWi	56	28.448	3.164	28.439	3.609
Au Recovery	42	80.355	8.780	80.356	7.805
Cu Recovery	63	88.933	8.301	88.814	7.702

TABLE 2.6: Directions of the best selected PPR model for BWi.

Direction	[Ql] Quartz Limonite Vein Style Mineralization	[Fe] Iron Grade	[G] Volcaniclastic - Conglomerate Lithology
1	0.994	0.076	-0.079
2	0.837	-0.439	0.326
3	-0.104	-0.447	0.888
4	0.170	-0.050	0.984
5	0.880	-0.225	0.418
6	-0.960	0.273	-0.062
7	1.000	-0.020	0.019

(Table 2.5). All QQ-plots show that optimized and base PPR models produce values very close to the true distributions (Figure 2.6). In contrast, the MLR models do not reproduce the true value distributions especially in the tails.

It is useful to inspect the projection directions of the PPR models and, to do so, the best model for BWi is used as an example. The best model is chosen as the one with the best balance of all five goodness-of-fit indices.

There is no obvious interpretation of PPR beyond the first direction because each additional direction operates over the residuals; nevertheless, some findings are highlighted.

Table 2.6 shows that in the first direction the most relevant variable for BWi is Ql mineralization. Because all proportions of qualitative variables are within the range of (0.0 - 1.0) and the values of iron content are within the range of (0.0 - 6.0), the second most important variable is iron. The R^2 plot for BWi (Figure 2.2), indicates clearly that the performance of the model is sufficient using only the first direction whereas contributions from additional directions are insignificant compared with the first.

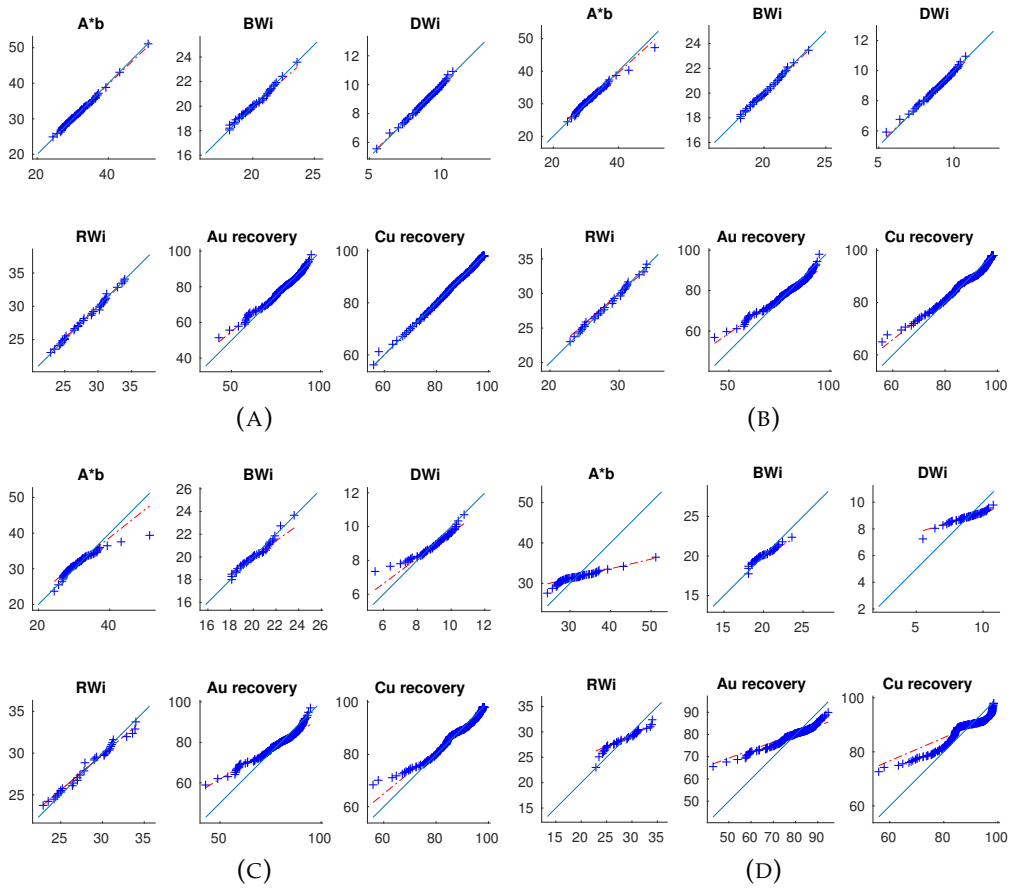


FIGURE 2.6: QQ-plots of true value and predictions: optimized (A) and base (B) PPR models, and optimized (C) and base (D) MLR models.

2.5 Discussion

The success of geometallurgical modelling depends largely on the available data. Access to quantitative data such as mineralogy, liberation profiles and particle size distribution surely will improve geometallurgical modelling, but quite often these data are not collected or are collected in insufficient numbers. This case study focusses on modelling geometallurgical response variables using data that are abundant in most mining operations (assays and geological logging). When the number of testwork samples is limited, the selection of an appropriate regression model is critical to the derivation of an accurate prediction model.

Two different models were defined to quantify the impact of including qualitative information. The base models are defined to assess the performance of a model using only grade variables which are usually considered the most relevant. When all variables are included to derive the optimized models, the modelling becomes a high dimensionality problem. Feature selection techniques are then used to identify the most significant input variables, defined as the set of variables that best balances the amount of data with a coherent representation of geology and metallurgy.

For BWi, the most relevant variables selected were quartz limonite mineralization (Ql code), iron grade and volcaniclastic conglomerate lithology (G code). The quartz-limonite mineralization silicifies the surrounding rocks. The degree of silicification has an effect on the hardness of surrounding rocks. Lutz et al. (2010) showed in their mechanical rock testing of siliceous rocks that these rocks are stronger and harder compared to the non-siliceous rocks. Also, high iron content makes the rocks denser and the hardness of the rock will increase as the amount of contained iron increases. Finally, the volcaniclastic conglomerate lithology is normally made up of volcanic breccias and clastic material with a high percentage of quartz and feldspar-bearing minerals. These quartz and feldspar-bearing breccias and clastic materials have hardness of 6.0 to 7.0 on the Mohs scale and will affect the overall hardness of the volcaniclastic conglomerates lithology. All variables selected by the model have an impact on rock hardness, which is directly related to the BWi. These relationships support the inclusion of quartz limonite mineralization, iron grades and volcaniclastic conglomerates as the most relevant variables for predicting BWi. For other response variables, similar conclusions can also be drawn from the perspectives of geology and metallurgy to support the features selected to fit the PPR models. These selected features are also optimal in the sense of predictive

performance.

All PPR models only use additive variables which overcomes the non-additivity problem when geostatistical methods are applied. When qualitative information is included, all optimized models perform significantly better with better goodness-of-fit measures compared with base models. For grindability response models, this improvement is much more noticeable because rock characteristics are more relevant than grades to these response variables.

Base PPR models are capable of performing at similar levels to optimized MLR models. This is a clear demonstration of the power of the PPR technique. Projections can reveal structures and relationships where simple linear combinations cannot. Moreover, optimized PPR models consistently out-perform their corresponding base MLR models.

Reducing the number of inputs is important as it will greatly simplify the process of populating the response variables into the resource model using geostatistical estimation or simulation. Traditionally in geostatistics, spatially correlated variables require modelling of auto- and cross-variograms in estimation or simulation, and the complexity of this procedure increases as the number of input variables increases (Goulard and Voltz, 1992). An additional complexity may be present when some variables are categorical and spatially correlated with the continuous variables. Joint geostatistical modelling of a large number of continuous and categorical variables is still very challenging, although there are approaches to do so with one categorical variable (Xu and Dowd, 2009; Emery and Silva, 2009; Maleki and Emery, 2015).

The bootstrapping procedure is highly recommended for uncertainty and risk assessment. The uncertainty of models due to small numbers of samples can be assessed. Among all bootstrapped models, unbiased models are recommend, i.e., with the lowest possible prediction error, for a more realistic incorporation of uncertainty. For the best model, the recommendation is to select the one with the best balance of goodness-of-fit indices.

Response properties can be incorporated into the resource model assuming that the PPR models, built at the scale (support) of laboratory samples, can be up-scaled to block model volumes. If the focus is on minimum variance unbiased estimates, using kriged inputs, the best selected models should be used to predict the response variables. If the focus is on uncertainty quantification and risk assessment, geostatistical simulations should be used to generate many realizations of the block model. For each realization, all selected PPR models should be applied to quantify the metallurgical response variables. Some authors suggest that few realizations, from 10 to 25, are sufficient for

optimization problems (Ramazan and Dimitrakopoulos, 2013; Marcotte and Caron, 2013; Kumral, 2013) and others use more than 25 realizations (Armstrong and Galli, 2012; Lagos et al., 2011; Amankwah et al., 2013). For example, if there are 100 realizations of the block model and 20 different bootstrapped recovery models, the total number of realizations incorporating geometallurgical variables would be 2,000. A large number of realizations such as this can effectively quantify the uncertainty in mine planning and design, although the optimization procedures in this context remain extremely challenging. Fortunately, the combination of increasing computing power and more efficient optimizers should enable large numbers of realizations to be dealt with, a topic that the authors are working on.

2.6 Conclusions

The presented results have demonstrated that PPR models are superior to MLR models mainly due to their ability to find the best directions onto which data can be projected to reveal underlying relationships and correlations. The improvement in prediction performances of PPR over MLR models is consistent and in some cases very significant. Feature selection proved to be efficient in the case study. For comminution response variables, the inclusion of qualitative information significantly enhanced the performance of the models, suggesting that rock properties are more important than grade variables for these response variables. For recovery response variables, the inclusion of qualitative information also improves (but more modestly) the prediction capability of the PPR models. A selected subset of unbiased bootstrapped models can provide a means of quantifying uncertainty for risk assessment purposes. Further research could be done on formulating interestingness indices other than explained variance; in particular, an index that measures the linearity of relationships between predictors and dependent variable may provide an effective means of dealing with non-additivity of many geometallurgical variables. This could be an initial step towards transforming a non-linear problem into a linear one, and thereby solve the upscaling problem.

Acknowledgements

This work was supported with supercomputing resources provided by the Phoenix HPC service at the University of Adelaide. The first author acknowledges the support of CONICYT in the form of a Becas Chile scholarship.

References

Amankwah, H., Larsson, T. and Textorius, B. (2013), Open-pit mining with uncertainty: A conditional value-at-risk approach, *in* 'Optimization Theory, Decision Making, and Operations Research Applications', Springer, pp. 117–139.

Arlot, S., Celisse, A. et al. (2010), 'A survey of cross-validation procedures for model selection', *Statistics surveys* **4**, 40–79.

Armstrong, M. and Galli, A. (2012), 'New approach to flexible open pit optimisation and scheduling', *Mining Technology* **121**(3), 132–138.

Barnett, R. M., Manchuk, J. G. and Deutsch, C. V. (2014), 'Projection pursuit multivariate transform', *Mathematical Geosciences* **46**(3), 337–359.

Boisvert, J. B., Rossi, M. E., Ehrig, K. and Deutsch, C. V. (2013), 'Geometallurgical modeling at olympic dam mine, south australia', *Mathematical Geosciences* **45**(8), 901–925.

Carrasco, P., Chiles, J.-P. and Séguret, S. A. (2008), Additivity, metallurgical recovery, and grade, *in* '8th international Geostatistics Congress', pp. on–CD.

Chatterjee, S. and Hadi, A. S. (2015), *Regression analysis by example*, John Wiley & Sons.

Coward, S. and Dowd, PA. (2015), Geometallurgical models for the quantification of uncertainty in mining project value chains, *in* '37th APCOM Conference', Vol. 37, pp. 360–369.

Coward, S., Dowd, PA. and Vann, J. (2013), Value chain modelling to evaluate geometallurgical recovery factors, *in* '36th APCOM Conference', Fundacao Luiz Englert, pp. 288–289.

Coward, S., Vann, J., Dunham, S. and Stewart, M. (2009), The primary-response framework for geometallurgical variables, *in* 'Seventh international mining geology conference', pp. 109–113.

Dowd, PA., Xu, C. and Coward, S. (2016), 'Strategic mine planning and design: some challenges and strategies for addressing them', *Mining Technology* **125**(1), 22–34.

Dunham, S. and Vann, J. (2007), Geometallurgy, geostatistics and project value - does your block model tell you what you need to know?, *in* 'Project evaluation conference, Melbourne, Victoria', pp. 19–20.

Efron, B. and Gong, G. (1983), 'A leisurely look at the bootstrap, the jackknife, and cross-validation', *The American Statistician* **37**(1), 36–48.

Emery, X. and Silva, D. A. (2009), 'Conditional co-simulation of continuous and categorical variables for geostatistical applications', *Computers & Geosciences* **35**(6), 1234–1246.

Friedman, J. H. (1984), A variable span smoother, Technical report, Stanford Univ CA lab for computational statistics.

Friedman, J. H. (1994), An overview of predictive learning and function approximation, *in* 'From Statistics to Neural Networks', Springer, pp. 1–61.

Friedman, J. H. and Stuetzle, W. (1981), 'Projection pursuit regression', *Journal of the American statistical Association* **76**(376), 817–823.

Friedman, J. H., Stuetzle, W. and Schroeder, A. (1984), 'Projection pursuit density estimation', *Journal of the American Statistical Association* **79**(387), 599–608.

Friedman, J. H. and Tukey, J. W. (1974), 'A projection pursuit algorithm for exploratory data analysis', *IEEE Transactions on computers* **100**(9), 881–890.

Ghasemi, J. B. and Zolfonoun, E. (2013), 'Simultaneous spectrophotometric determination of trace amount of polycyclic aromatic hydrocarbons in water samples after magnetic solid-phase extraction by using projection pursuit regression', *Environmental Monitoring and assessment* **185**(3), 2297–2305.

Glover, F. (1990), 'Tabu search: A tutorial', *Interfaces* **20**(4), 74–94.

Goulard, M. and Voltz, M. (1992), 'Linear coregionalization model: tools for estimation and choice of cross-variogram matrix', *Mathematical Geology* **24**(3), 269–286.

Hunt, J., Berry, R., Bradshaw, D., Triffett, B. and Walters, S. (2014), 'Development of recovery domains: Examples from the prominent hill iocg deposit, australia', *Minerals Engineering* **64**, 7–14.

Hunt, J., Kojovic, T. and Berry, R. (2013), Estimating comminution indices from ore mineralogy, chemistry and drill core logging, *in* 'GeoMet 2013: The Second AusIMM International Geometallurgy Conference', The Australasian Institute of Mining and Metallurgy (AusIMM), pp. 173–176.

Keeney, L. and Walters, S. (2011), A methodology for geometallurgical mapping and orebody modelling, *in* 'GeoMet 2011-1st AusIMM International Geometallurgy Conference 2011', Australasian Institute of Mining and Metallurgy, pp. 217–225.

Kumral, M. (2013), 'Optimizing ore–waste discrimination and block sequencing through simulated annealing', *Applied Soft Computing* **13**(8), 3737–3744.

Lagos, G., Espinoza, D., Moreno, E. and Amaya, J. (2011), 'Robust planning for an open-pit mining problem under ore-grade uncertainty', *Electronic Notes in Discrete Mathematics* **37**, 15–20.

Lee, E.-K., Cook, D., Klinke, S. and Lumley, T. (2005), 'Projection pursuit for exploratory supervised classification', *Journal of Computational and Graphical Statistics* **14**(4), 831–846.

Lutz, S. J., Hickman, S., Davatzes, N., Zemach, E., Drakos, P. and Robertson-Tait, A. (2010), Rock mechanical testing and petrologic analysis in support of well stimulation activities at the desert peak geothermal field, nevada, *in* 'Proceedings 35th Workshop on Geothermal Reservoir Engineering'.

Maleki, M. and Emery, X. (2015), 'Joint simulation of grade and rock type in a stratabound copper deposit', *Mathematical Geosciences* **47**(4), 471–495.

Marcotte, D. and Caron, J. (2013), 'Ultimate open pit stochastic optimization', *Computers & geosciences* **51**, 238–246.

Qianjian, G. and Jianguo, Y. (2011), 'Application of projection pursuit regression to thermal error modeling of a cnc machine tool', *The International Journal of Advanced Manufacturing Technology* **55**(5), 623–629.

Ramazan, S. and Dimitrakopoulos, R. (2013), 'Production scheduling with uncertain supply: a new solution to the open pit mining problem', *Optimization and Engineering* **14**(2), 361–380.

Silverman, B. W. (1984), 'Spline smoothing: the equivalent variable kernel method', *The Annals of Statistics* pp. 898–916.

Walters, S. (2008), An overview of new integrated geometallurgical research, *in* 'Australasian Institute of Mining and Metallurgy Publication Series', AusIMM, pp. 79–82.

Weisberg, S. (2005), *Applied linear regression*, Vol. 528, John Wiley & Sons.

Xu, C. and Dowd, PA. (2009), Conditional simulation of grades controlled by geological indicators, *in* 'Orebody Modelling and Strategic Mine Planning', AusIMM, pp. 43–49.

Chapter 3

The optimisation of block caving production scheduling with geometallurgical uncertainty - A multi objective approach

Statement of Authorship

Title of Paper	The optimisation of block-caving production scheduling with geometallurgical uncertainty - A multi-objective approach.
Publication Status	☐ Published ☑ Accepted for Publication ☐ Submitted for Publication ☐ Unpublished and Unsubmitted w ork w ritten in manuscript style
Publication Details	Sepulveda E, Dowd PA and Xu C. The optimisation of block-caving production scheduling with geometallurgical uncertainty - A multi-objective approach. Mining Technology. Accepted for Publication on 13/02/2018. DOI: 10.1080/25726668.2018.1442648

Principal Author

Name of Principal Author (Candidate)	Exequiel Manuel Sepulveda Escobedo		
Contribution to the Paper	Develop methodology and methods, conducted programming and execution of methods, wrote manuscript and acted as corresponding author.		
Overall percentage (%)	80%		
Certification:	This paper reports on original research I conducted during the period of my Higher Degree by Research candidature and is not subject to any obligations or contractual agreements with a third party that would constrain its inclusion in this thesis. I am the primary author of this paper.		
Signature		Date	20/02/2018

Co-Author Contributions

By signing the Statement of Authorship, each author certifies that:

i. the candidate's stated contribution to the publication is accurate (as detailed above);

ii. permission is granted for the candidate in include the publication in the thesis; and

iii. the sum of all co-author contributions is equal to 100% less the candidate's stated contribution.

Name of Co-Author	Peter Dowd		
Contribution to the Paper	Supervised development of work and reviewed manuscript.		
Signature		Date	20th February 2018

Name of Co-Author	Chaoshui Xu		
Contribution to the Paper	Supervised development of work and reviewed manuscript.		
Signature		Date	20-02-2018

Abstract

The incorporation of the uncertainties of geometallurgical variables in mine planning provides new opportunities for decision-makers to analyse, compare and choose among many scenarios to achieve an optimal balance between economic and operational objectives. This research focuses on maximising economic return and minimising the risk arising from the uncertainty associated with geometallurgical variables. We formulate two-objective optimisation problems based on an underground mining operation. The first objective is the maximisation of the Net Smelter Return, which includes penalties associated with deleterious elements in concentrates. Four different objectives were tested as candidates for the second objective: Volatility, Value at Risk, Conditional Value at Risk and deviation from the planned production target. The first three are measures of economic risk and the fourth is a measure of operational risk. Uncertainties in metal grades, geometallurgical recoveries and grades in concentrate are included in the proposed model. Our results demonstrate that geometallurgical uncertainties can be successfully integrated into production scheduling optimisation in a multi-objective approach and the problem can be solved using genetic algorithms to yield useful conclusions to support the decision-making process.

Keywords Geometallurgy; uncertainty; risk assessment; production scheduling optimisation; multi-objective optimisation; block caving.

3.1 Introduction

The complete value chain of a mining project is subject to uncertainties that complicate the decision-making process. Internal uncertainties are present in resource models and in processes such as blasting, grinding and mineral processing, whereas external uncertainties are present in, but not limited to, prices, commodities costs and other externalities (Vann et al., 2012). These uncertainties are probably the most significant causes of projects not meeting initial expectations and it is, therefore, crucial to quantify them to assess completely the risk of not achieving expected outcomes. McCarthy (2003) reports that, among the causes of project failure, the three most important are mine design and scheduling, geology, and metallurgy. The sources of risk in a mining operation that can affect its feasibility can be classified into three groups: technical, financial and environmental (Dimitrakopoulos, 1998; Dowd, 1994, 1997).

Commodity prices, foreign exchange rates and production costs are the most common examples of uncertain financial variables, while geological, geotechnical, and metallurgical variables are examples of technical risk sources. Environmental risk is largely technical in nature and has consequences that are technical, financial, organisational, and the social licence to operate.

Financial uncertainty is regarded as a critical component and has been a significant focus of research in uncertainty assessments of mining operations. Grobler et al. (2011) presented a strategic mine planning optimisation problem considering multiple processing and mining capacities as well as the price uncertainty. This study showed a trade-off between return and risk, which is defined as the probability of making a loss. Groeneveld and Topal (2011) modelled the uncertainties in metal prices, capital costs, operating costs and plant performance using Monte Carlo simulations with some well-known distributions. They developed a new algorithm based on dynamic programming and the branch and bound method with price uncertainty. Amankwah et al. (2013) modelled the uncertainty in metal prices using the lognormal distribution while others used the Wiener process (Dimitrakopoulos and Sabour, 2007; Evatt et al., 2012). Whilst financial uncertainty assessment is obviously important for mining operations, the focus of the work reported here is geological and metallurgical uncertainty.

Geometallurgy is emerging as a specific sub-discipline in the assessment, evaluation and design of mining projects. It combines expert knowledge and data from geology and metallurgy, and it claims to have made a substantial improvement in the design, operation and evaluation of mining operations (Dunham and Vann, 2007; Coward and Dowd, 2015). Among all technical risks, geometallurgy plays a critical role. Geological uncertainty has been a focus of research for many years and geostatistical simulation (Journel, 1974; Dowd, 1994) is widely used to quantify geological risk and its impact on planning, design and production. Geostatistical simulations overcome the problems of bias and unrealistic production expectations associated with conventional approaches that are in general, based on a fixed (deterministic) resource model, often generated by kriging or other spatial weighting methods (Dowd and Dare-Bryan, 2004; Dimitrakopoulos, 2011). Early work in minerals project risk assessment focused on generating stochastic block models and independently optimising realisations of the block model to generate a complete distribution of possible values of an objective, usually the NPV (Dowd, 1994, 1997) as a means of quantifying risk. The next development in stochastic

risk assessment was the application of stochastic optimisation. Dimitrakopoulos (2011) optimised the scheduling of an open-pit mine including geological uncertainty and offered two stochastic methods. In another development, a two-stage simultaneous stochastic optimisation method was used to solve simultaneously the problems of ore-waste discrimination and block sequencing (Kumral, 2013). Similarly, grade uncertainty was included in the production scheduling problem using meta-heuristic stochastic optimisation (Lamghari and Dimitrakopoulos, 2012). Benndorf and Dimitrakopoulos (2013) combined three objectives - the maximisation of NPV, minimisation of deviations from production targets, and smoother mining sequences - into a single optimisation problem using 20 simulated orebodies generated by geostatistical co-simulations. Montiel et al. (2016) presented a method that optimises mining complexes (open-pit and underground operations) and multiple processing destinations. They accounted for geological uncertainty by orebody simulations and the optimisation was performed using the Simulated Annealing metaheuristic. Their results showed a higher NPV and a reduced risk. Here, risk is quantified by deviations from capacities in mines, transport systems, processing destinations and operational properties.

Geometallurgy enriches the block model with additional information that should improve the overall optimisation of a mining operation. Important metallurgical performance indices, such as recovery and grindability, can be predicted largely by indirect methods such as regressions or simulations of the milling and recovery processes.

The element-to-mineral approach (Lamberg, 2011; Lund et al., 2015; Parian et al., 2015) is based on regressing mineralogy data on metallurgical performance measures. Grades may be good predictors of mineralogy but, in general, they do not directly explain metallurgical performance. Techniques such as QEMSCAM, X-ray diffraction and scanning electron microscopy are normally used to characterise mineralogy, which is then used to improve the prediction of mineral grades and metallurgical response properties. Boisvert et al. (2013) modelled head grades, mineralogy (mineral size and distribution) and mineral associations using multivariate linear regressions and these regression models were used to predict several plant performance variables. Hunt et al. (2014) used both qualitative and quantitative primary rock properties such as multi-element geochemistry and sulphide speciation classes, and derived linear regression models for copper recovery. Similar qualitative and quantitative primary rock properties were also used recently to build models that can overcome non-linearity by project pursuit regression (Sepúlveda et al., 2017).

An alternative to regression models is via direct simulations of metallurgical processes. For example, Tungpalan et al. (2015) used mineralogical characterisation to simulate the processes of comminution, classification and flotation to predict metallurgical performance. This simulation approach is promising but it remains a challenge to include it directly in planning optimisation problems because process simulations are generally computationally expensive and highly time-consuming.

Regression models and simulations can be used to populate block models with geometallurgical values to improve decision-making. Whilst this is the primary purpose of geometallurgical modelling, there has thus far been very little research into incorporating geometallurgical variables and their uncertainties directly into mine optimisation.

Production scheduling is an integral part of mine optimisation. The stochastic scheduling problem for open-pit mines has been covered extensively by many researchers (Gholamnejad and Osanloo, 2007; Ramazan and Dimitrakopoulos, 2013; Lamghari and Dimitrakopoulos, 2012; Silva et al., 2015; Goodfellow and Dimitrakopoulos, 2016). The problem for underground mines is much more complex because there are many variations in mining methods and a generalized approach is impractical. In this research, we target a block caving mining operation because this mining method is increasingly being used in deeper and lower grade orebodies.

The deterministic scheduling problem has been solved using various methods. By way of example, Yashar et al. (2013) used a multi-step, mixed integer linear programming (MILP) formulation. To overcome the size problem, a clustering technique was applied to solve the problem at different scales. The NPV was maximised for 298 draw-points over 15 years. Rahal et al. (2003) used a different MILP formulation to reduce deviations in two objectives: the ideal depletion rate and the deviation from production targets. Compared with open-pit mining, there has been very little research into stochastic scheduling of block caving; this view is supported by the review of mathematical methods for block caving scheduling problem undertaken by Khodayari and Pourrahimian (2015). Rubio and Dunbar (2005) used historical forecasts and production data to define the reliability of a draw-point in a block caving operation as the ability of different production strategies to achieve production targets. The reliability index, defined as an indicator of the deviation of planned tonnage to be drawn from a draw-point, could be used as a measure of risk. Nezhadshahmohammad et al. (2017) presented a MILP formulation to optimise the scheduling of draw columns in a block caving operation subject to

the depletion rates of all adjacent draw-points. They applied the model to a case study of 325 draw-points over 15 production periods.

Including some risk minimisation is a significant step forward in realistic stochastic optimisation. However, the issue of providing a meaningful final decision remains, i.e., the selection of a schedule given all available information and the associated risk. This is not a simple issue and, in general, it is a compromise between economic and operational objectives. In other words, pursuing higher economic returns would attract higher risk, but less risky schedules may be less attractive in terms of potential economic returns. In general, this trade-off can be quantified by using multi-objective optimisations. However, the majority of formulations in published research in this area are based on weighted objectives that transform the problem into a supposedly equivalent single objective problem, which does not guarantee that the original multiple objectives are optimised. The work reported in this paper offers a methodology to formulate a multi-objective optimisation that can be used to assist effective decision-making in block caving mining operations, including the uncertainties in the geometallurgical variables.

In the following sections the methodology is explained in detail, the concepts of quantifying uncertainty, risk measures and optimisation under uncertainty are discussed, and a set of bi-objective formulations is proposed. The proposed methodology is implemented on a case study and the results and further research recommendations are discussed.

3.2 Methodology

3.2.1 Quantification of uncertainty

Uncertainties are present in the entire mining value chain. In resource models, uncertainty of grades and tonnage are usually quantified by geostatistical simulations. Geological uncertainty may be misunderstood or underestimated due to averaging at different scales, producing a double-smoothing effect, which can impact on the prediction of processing performances. In processing, there are additional uncertainties related to deleterious elements and contaminants that affect performance, and they must be incorporated. Other sources of uncertainties can be included by incorporating them at appropriate stages, for example, mining depletion, mining allocation, stockpiling and blending, mineral processing. Metallurgical responses (and their uncertainties) can be predicted by process simulation, which may be accurate but require

calibration using standardised laboratory-scale tests. Linear, or non-linear, regression models based on laboratory tests are also used for predicting metallurgical responses (Vann et al., 2012). The uncertainties in geology and mineral processing can be classified as geometallurgical uncertainties.

The primary-response framework (Coward et al., 2009) allows the quantification of geometallurgical uncertainties. In this framework, primary geological variables, such as grades, mineralogy and rock type, are identified as proxies for some response variables such as recoveries and grindability indices. The prediction models for metallurgical responses can be generated by regressions or process simulations, as discussed above.

In this paper, the focus is solely on quantifying geometallurgical uncertainties, but the methodology can also be used to incorporate other uncertainties in the value chain.

Geometallurgical uncertainty

Geostatistical techniques can be used to quantify the uncertainties of variables that are spatially correlated. The kriging estimator, for instance, gives smoothed, minimum variance, unbiased estimations of the variables, which gives a rudimentary measure of the uncertainty associated with the estimated values of the variables. Geostatistical simulation provides a more comprehensive and realistic quantification of uncertainty that can give a full distribution of possible values at the desired scale. However, many geometallurgical variables, such as recovery rate and comminution energy consumption, have non-linear relationships with primary variables and are non-additive. These issues make it inappropriate to use standard geostatistical methods to simulate the variables directly. A data-driven approach is used in this research to derive a clear relationship between primary and metallurgical response variables. The method used is projection pursuit regression (PPR), which can deal effectively with non-linearity and performs very well in geometallurgical variable modelling (Sepúlveda et al., 2017).

3.2.2 Risk measures

The following basic risk measure is used in this research. Let X be a random variable with a cumulative distribution function:

$$\Psi(X, \zeta) = P(X|X < \zeta). \tag{3.1}$$

If the distribution of X represents a loss function, the focus would be on its upper tail. For instance, for the distribution of deviations from production targets, the interest would be in the deviations that exceed certain thresholds. On the other hand, if the distribution is for the financial return or revenue, the focus would be in the lower tail, i.e., the value of the economic return less than a minimum target value. In this case, the risk measure can be quantified using the probability function (Eq. 3.1) and the threshold.

Volatility

The simplest and most widely used measurement of risk is the variance (or some function of variance, such as the coefficient of variation), which quantifies the variability or volatility of the variable.

Volatility is a non-negative value. Zero volatility means there is no uncertainty. Higher values mean higher dispersion, implying higher risk.

Value at risk

The value at risk (VaR) is a measure of the risk of extreme events occurring (Rockafellar and Uryasev, 1997). For a given confidence interval α, the VaR is the value ζ such that the probability of all values is greater than ζ is at least α, i.e.,

$$\underset{\alpha}{\text{VaR}} = \inf \zeta \in \mathbb{R} : \Psi(X, \zeta) \geq \alpha. \tag{3.2}$$

Taking the economic return as an example, a 95% VaR of \$10M means that there is 95% of probability that the economic return will be at least \$10M. If the random variable represents deviation from production targets, a 90% VaR of 10Mt means that there is a 90% chance that production will deviate from target for less than 10Mt.

Conditional value at risk

The VaR indicates only a threshold of a distribution at a certain confidence level but it does not indicate the magnitude of possible values greater than the threshold. For the former example, a VaR for the deviation from a target of more than 10Mt at 90% probability does not give the expected deviation of all deviations greater than the threshold. From an operational point of view, quantifying the expected deviation from the production target in an extreme

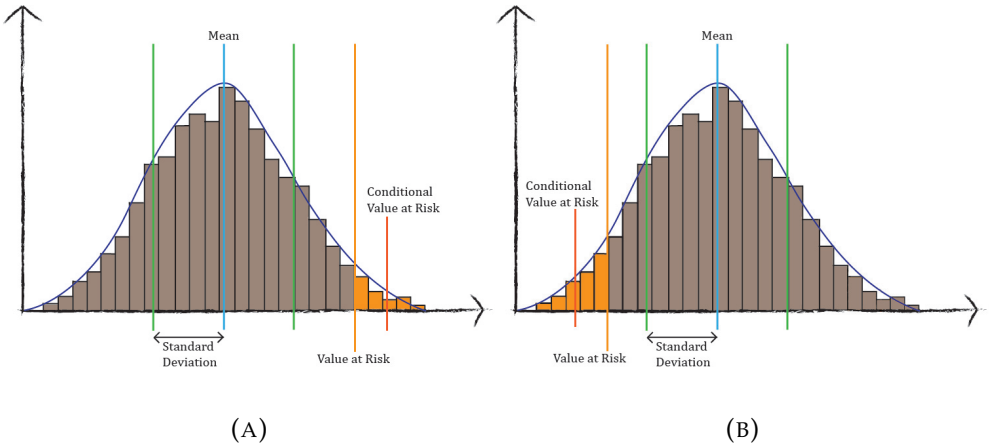


FIGURE 3.1: Volatility, VaR and CVaR in a (A) loss and (B) revenue distribution.

event (VaR) would be helpful and the minimisation of this value may assist in identifying less risky scenarios.

Conditional value at risk (CVaR) is therefore defined as the expectation of a revenue function for an extreme event (VaR) at some level of risk (Rockafellar and Uryasev, 1997). Formally CVaR is defined as:

$$CVaR_\alpha = E(R|R < VaR_\alpha). \tag{3.3}$$

The relationships between VaR and CVaR defined above are shown in Fig. 3.1 using both a generic (A) loss and (B) revenue distribution (Sarykalin et al., 2008).

Once the distribution is known, the risk measures discussed above can then be quantified at a desired confidence level. For the geometallurgical problem, there are two basic distributions to be derived for risk quantification. The first is the distribution of variables at block scale, such as metal content (grades), recoveries and concentration of deleterious elements in each block. The second distribution corresponds to derived variables as a function of the stochastic block model and the operations, such as total NSR, energy costs and concentration of deleterious elements in concentrates for a given schedule. Both these distributions will be used in the following sections to formulate the optimisation problems.

3.2.3 Optimisation under uncertainty

The mine optimisation problem with deterministic variables has been extensively studied. If the problem can be formulated as a linear problem with linear constraints, techniques such as linear programing (LP) and mixed integer linear programming (MILP) can be used to find the exact optimum solution. For non-linear optimisation problems, the common approach is to formulate the optimisation as a linear or quadratic problem and then solve the problem using LP, but unfortunately not all problems can be transformed into a linear formulation. A method for solving LP and MILP is the branch and bound technique, which involves representing the solution space (set of all feasible solutions) by a rooted tree (with branches representing subsets of the space) and reducing this space as quickly as possible after discarding branches that are non-optimal. The branch and bound technique, devised by Land and Doig (1960), is particularly useful for solving combinatorial optimisation problems. Although exact optimisers for solving LP and MILP models are ideal, many problems either cannot be formulated in the manner required by exact algorithms or the size of the problem makes it computationally intractable for them.

The complexity increases significantly for optimisation problems that include stochastic variables. If the stochastic variables can be defined analytically there is a good chance that the problem can be solved mathematically under the condition of convexity. Unfortunately, this condition is frequently not met. If an analytical solution is not possible, the problem can be solved numerically using Monte Carlo sampling. In this approach, the decision variables are repeatedly sampled a certain number of times to form the sample space within which the problem becomes deterministic. This method is simple but may be difficult to implement in practice when there are many stochastic variables involved and Monte Carlo sampling may become computationally expensive. In addition, objectives and constraints might include some features of these variables, such as their expectation, variance and probabilities. Another solution method is stochastic programming with two-stage programming as the most popular option. To solve the problem, a decision needs to be taken (first stage), and once that decision is taken the problem becomes deterministic (second stage). This strategy can be extended to multi-stage formulations. For large-size problems, this method is often more computationally expensive to solve that LP and MILP problems.

To overcome these practical problems, heuristic approaches can be applied

to obtain good solutions in a reasonable amount of time. Among these approaches, meta-heuristic methods have shown excellent capabilities for solving complex stochastic optimisation problems. One significant advantage of the meta-heuristic approaches is that they are algorithmic-oriented, i.e., objectives and constraints are defined as functions of stochastic variables. Thus, provided an efficient computing algorithm is used to evaluate these functions, the meta-heuristic method can solve the problem irrespective of the complexity of the functions and problem size, giving good scaling properties. This feature makes meta-heuristic methods a very attractive option for solving complex optimisation problems. For example, although in principle VaR and CVaR can be formulated as a MILP, the optimisation can be very complex (Rockafellar and Uryasev, 1997; Schultz and Tiedemann, 2006). If the meta-heuristic method is used, the computation of objectives and constraints becomes much easier. For example, VaR and CVaR are computed by building the cumulative sample distribution and selecting the desired quantile.

Necessity for multi-objective optimisation

In a decision-making process, there are very often two or more competing objectives. If uncertainties are included, any objective may be restricted by a risk threshold defined by the decision-maker. When the only criterion is the maximisation of the economic return, other criteria may be affected; for example, it may be that the schedule with the highest revenue incurs the highest deviation from some production target or that it has the highest variance among all scenarios. It is important to understand this trade-off, which in multi-objective optimisation, is expressed as the Pareto front (PF) (Marler and Arora, 2004). For two objectives, the PF is a curve but it can easily be generalised. The PF has an important characteristic: for any pair of solutions S_1 and S_2 on the PF, S_1 does not dominate S_2 and vice versa, but both dominate any feasible solution S_3 not on the PF. The concept of dominance allows the finding of solutions that are optimal but different. Formally, a solution S_1 dominates a solution S_2: (i) if at least one objective is improved, (ii) any objective does not worsen. In the example shown in Fig. 3.2, C improves both objectives compared to E, therefore C dominates E, but A does not dominate C because A improves f_1 but worsens f_2. Finding this PF is not trivial.

A general multi-objective optimisation problem can be formulated as follows:

$$\arg\min f_1(x, Y), f_2(x, Y), \ldots, f_n(x, Y) \tag{3.4}$$

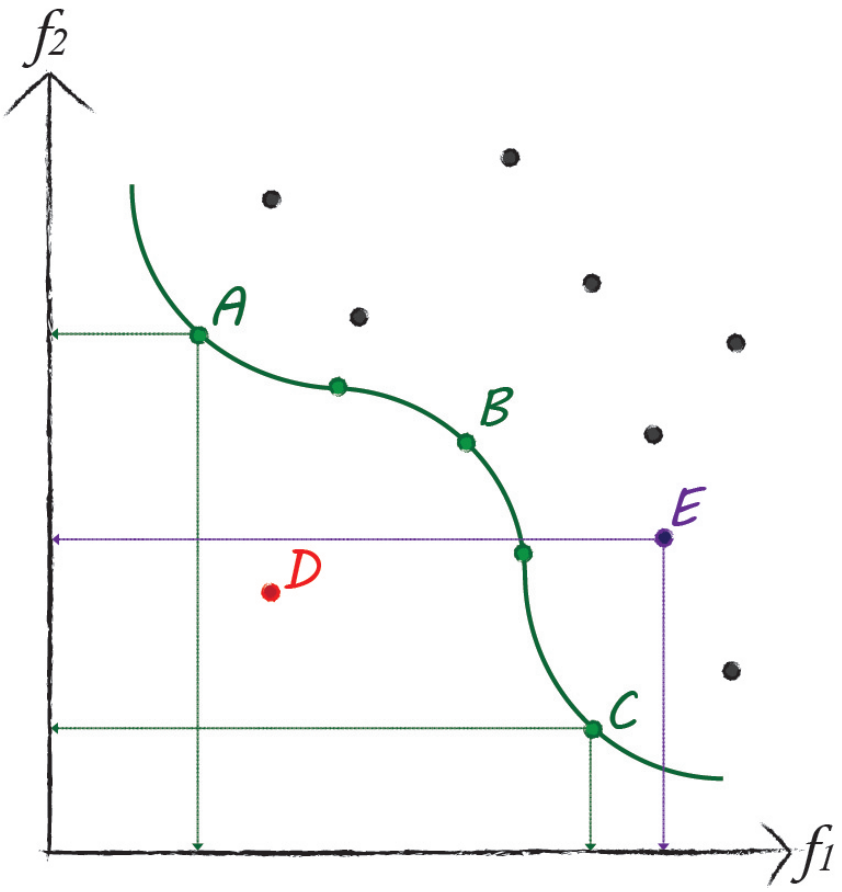


FIGURE 3.2: Pareto Front diagram. A, B and C are non-dominated solutions. D is unfeasible and E is feasible but dominated.

$$g(x, Y) \leq 0 \tag{3.5}$$

$$h(x, Y) = 0 \tag{3.6}$$

$$LB \leq x \leq UB \tag{3.7}$$

where $f_i(x, Y)$ is the set of objective functions being optimised, $g(x, Y)$ represents the inequality constraints, $h(x, Y)$ the equality constraints, and LB/UB are the lower and upper bounds of the decision variable x. The variable Y denotes the variable under uncertainty.

For convex PF, the problem can be reduced to a weighted single objective problem:

$$\arg\min \sum_{i-1}^{n} w_i f_i(x). \tag{3.8}$$

The PF can be approximated by using appropriate values of w, which are unknown in practice and hard to calibrate. When the PF is not convex, this approach fails to find hidden optimal solutions, solution B in Fig. 3.2 for example, which may be relevant to decision-making processes, and they should not be ignored.

Meta-heuristic approaches have several important characteristics: first, they are algorithmic-oriented, which facilitates the computation of complex objectives and constraints; second, they offer a good approximate solution to the PF for convex and non-convex problems, and third, they can solve large problems that cannot be solved by traditional solvers. However, these approaches cannot guarantee that the PF solution is optimal, but they do provide good quality solutions in a reasonable amount of time.

Genetic algorithms

There are several meta-heuristic methods that have been successfully used for multi-objective optimisation problems. These include: local search, tabu search, simulated annealing, evolutionary algorithms and swarm intelligence (Bianchi et al., 2009). Among evolutionary algorithms, genetic algorithms (GA) have been extensively and successfully used in many areas of engineering. It is not the intention in this paper to give an exhaustive account of GA, but a general overview is given below.

GA imitates the evolutionary process in nature by applying selection, mutation and mating to a population over many generations. A population in this

case is formed by a set of individuals that represent the solutions. An individual has a genome, which is improved (as measured by objective functions) by genetic operations in the evolutionary process. For a specific problem, coding a solution into a genome is one of the most important steps in a GA approach. Whitley (1994) gives a detailed review of GA.

GA has been a very active research topic and it has many specific implementations. In the case of multi-objective optimisation, the fast non-dominated sorting genetic algorithm, NSGA-II, performs well in approximating the PF (Deb et al., 2002) and has been used in the research presented here.

3.2.4 Mathematical formulation

The formulation for optimising block caving scheduling presented here is based on a simplified formulation of the work by Nezhadshahmohammad et al. (2017). In that formulation, which uses a deterministic model instead of simulated scenarios, the objective function is the maximisation of the NPV. The constraints are mining capacity, production grade, maximum number of active draw-points, precedence of draw-points, continuous extraction, number of new draw-points, reserves and, draw rate. Three decision variables were used: a) a continuous variable defined as the portion of a draw column to be extracted in a period, b) a binary variable that indicates whether a draw-point is active in a period, and c) a binary variable that controls the starting period for extraction from a draw-point. They used simulations to characterise the material drawn from a draw column comprised of several consecutive slices. Each slice contains an economic value, tonnage, grade and dilution.

In our simplified formulation, the most significant differences are that we use only one decision variable, include geometallurgical variables under uncertainty, and use block-scale revenue. A simple gravity flow procedure determines the blocks that will be drawn from a draw-point as a deterministic sequence. Also, for simplicity, the only constraints used here are mining capacity and reserves, as we assume all draw-points are active from the first period. However, any additional constraints can be included in the GA algorithm.

The use of block-scale revenue, which is a distribution of possible values depending on the scenarios, allows geometallurgical variables to be incorporated at the appropriate scale as we show in the formulation section.

Definitions and parameters

The following definitions are used in the formulation of objectives and constraints:

B	the number of blocks in the block model.
S	the number of scenarios.
T	the number of periods.
D	the number of drawpoints.
b	index for blocks, $b \in [1, 2, \ldots, B]$.
s	index for scenarios, $s \in [1, 2, \ldots, S]$.
t	index for periods, $t \in [1, 2, \ldots, T]$.
d	index for draw-points, $d \in [1, 2, \ldots, D]$.
F^d	the queue of all blocks to be drawn from the d-th draw-point. F^d_j denotes the j-th index of F^d.
$nsr_{b,s}$	pre-calculated net smelter return (NSR) value for each block per scenario. This is a matrix of rank (B, S).
$tons_b$	tonnage for each block. This is a vector of size B and calculated as the product of density and volume.
dr	discount rate.
C	production target.
LT	lower bound for tonnage.
UT	upper bound for tonnage.
$MAXB_d$	maximum number of blocks to be extracted from any draw-point d in any period.
α	confidence level for VaR and CVaR.

Decision variables

Production scheduling is defined as the tonnage drawn from each draw-point in each time period. This is equivalent to determining the number of blocks that can be extracted from each draw-point in each time period. Once the sequence F is determined for each draw-point, it is straightforward to calculate the subset of blocks to be drawn from a draw-point in any period. For example, if the numbers of extracted blocks are 40 and 50 for the first and second periods respectively, the extracted blocks in the first period are the first 40 elements of F and for the second period, are the following 50 elements of F starting at position 41. In general terms, the blocks extracted in any period depend on the accumulated extraction of all previous periods. For such a simplified approach for ore-drawing, the only decision variable related to ore extraction is:

x_{dt}: number of blocks to be extracted from the draw-point d in period t.

We can, therefore, define the following function $EB(x, d, t)$ to determine the subset of blocks to be extracted from draw-point d in any period t that depends on x and F:

$$EB(x, d, t) = \{F_j^d\}, \forall j \in \{k, \ldots, k + x_{dt}\}, k = \sum_{i=1}^{t-1} x_{d,i}. \tag{3.9}$$

The EB function is the base function for the calculation of several different objectives.

Objective formulations

The traditional net present value (NPV) approach does not usually take into account the effect of geometallurgical variables and is generally calculated as $NPV = grade * tonnage * recovery$. The use of the net smelter return (NSR), as an alternative to the traditional NPV, is a more useful way of incorporating geometallurgical variables. NSR is defined as the value of minerals after the deduction of all off-mine processing and selling costs (Goldie and Tredger, 1991). The NSR calculation involves not only grades, but also recoveries, grade in concentrate, smelting and treatment charges, marketing, freight costs, metal prices and any deductions such as penalties for high concentrations of deleterious elements and other losses. The NSR valuation is clearly closely related to the purpose of including geometallurgy in mine optimisation, i.e., to improve decision-making through the integration of geology and metallurgical knowledge. The NSR calculation involves both primary variables and geometallurgical response variables.

NSR calculation The Net Smelter Return includes the value of any element of interest, such as copper and gold, in concentrate after any deductions.

The NSR value for each block model is a function of ore grades, geometallurgical variables, costs and prices as listed in the following table:

Symbol	Description	Example
G_{cu}	Copper grade (geometallurgical).	2.3%
R_{cu}	Recovery rate of copper to concentrate (geometallurgical).	80%
C_{cu}	Copper grade in concentrate (geometallurgical).	31.2%
P_{cu}	Copper price.	3.10 \$/lb
G_{au}	Gold grade (geometallurgical).	0.3g/t
R_{au}	Recovery rate of gold in concentrate (geometallurgical).	72%
C_{au}	Gold grade in concentrate (geometallurgical).	5.7g/t
P_{au}	Gold price.	1,316.43 \$/oz
D_{cu}	Copper deduction.	1.0 untis
Y_{cu}	Payable copper percentage.	100%
RF_{cu}	Copper refining charge.	\$0.08
D_{au}	Gold deduction.	0.7 oz/t
Y_{au}	Gold deduction percentage.	88%
RF_{au}	Gold refining charge.	\$6.0
K_f	Penalty charge of fluorine.	\$1.5 each 100ppm
TK_f	Threshold to apply penalty (in concentrate).	300ppm
S:	Smelter charge.	\$80
F	Freight cost.	\$1.94

Gross value in concentrate is:

$$CG_{cu} = (\boldsymbol{C_{cu}}/100.0) * P_{cu} * 2204.6$$
$$CG_{au} = \boldsymbol{C_{au}} * P_{au} * 0.03215$$

Payable metal in concentrate:

$$
\begin{aligned}
PY_{cu} &= (\boldsymbol{C_{cu}} - D_{cu}) * Y_{cu} \\
PYM_{cu} &= PY_{cu} * P_{cu} * 2204.6/100.0 \\
PY_{au} &= (\boldsymbol{C_{au}} - D_{au}) * Y_{au} \\
PYM_{au} &= PY_{au} * P_{au} * 0.03215 \\
TP &= PYM_{cu} + PYM_{au}
\end{aligned}
$$

Penalties due to fluorine in concentrate:

$$N_f = 0 \textbf{ if}(\boldsymbol{C_f} > TK_f) \textbf{ else } \boldsymbol{C_f} * K_f$$

Payable gross value:

$$TGP = TP - (S + F + N_f)$$

NSR per metal:

$$
\begin{aligned}
PP_{cu} &= PY_{cu}/TP \\
GP_{cu} &= PP_{cu} * TGP \\
RV_{cu} &= \boldsymbol{R_{cu}} * 2204.6 * (PY_{cu}/100.0) \\
PP_{au} &= PYM_{au}/TP \\
GP_{au} &= PP_{au} * TGP \\
RV_{au} &= \boldsymbol{R_{au}} * 0.03215 * PY_{cu} \\
CNSR_{cu} &= GP_{cu} - RF_{cu} - N_f \\
CNSR_{au} &= GP_{au} - RF_{au} \\
NSR_{cu} &= CNSR_{cu}/\boldsymbol{C_{cu}} * (R_{cu}/100.0) * \boldsymbol{G_{cu}} \\
NSR_{au} &= CNSR_{au}/\boldsymbol{C_{au}} * (R_{au}/100.0) * \boldsymbol{G_{au}} \\
nsr &= NSR_{cu} + NSR_{cu}
\end{aligned}
$$

A complete guide to NSR calculation can be found in Goldie and Tredger (1991).

NSR function Five of the six objectives used in our formulations depend on the distribution of NSR calculated for a feasible solution over all scenarios. The calculation of NSR for a scenario s is the basis for generating the NSR distribution. NSR is given by:

$$NSR_s(x) = \sum_{d=1}^{D} \sum_{t=1}^{T} \frac{1}{(1-dr)^{t-1}} \sum_{b \in EB(x_{dt})} nsr_{bs}. \tag{3.10}$$

The distribution of NSR is denoted as $PDF(NSR)$ and it is represented by the discrete set given by:

$$PDF(NSR) = \{NSR_s(x), \forall s \in S\}. \tag{3.11}$$

Expectation and variance of NSR The expected NSR value is calculated as the expected value of $PDF(NSR)$:

$$f_1(x) = [PDF(NSR)] = 1/S \sum_{s=1}^{S} NSR_s(x). \tag{3.12}$$

The standard deviation of NSR is also straightforward to calculate:

$$f_2(x) = \sqrt{1/S \sum_{s=1}^{S} [NSR_s(x)]^2 - [1/S \sum_{s=1}^{S} NSR_s(x)]^2}. \tag{3.13}$$

Value at risk and conditional value at risk of NSR The calculation of VaR and CVaR is done over the NSR distribution. Conceptually both are simple to formulate and calculate, but difficult to optimise as MILP formulations. However, as the formulation here are not necessarily MILP, only their evaluations are needed.

The objective function for maximising VaR is given by:

$$f_3(x) = VaR_\alpha(NSR(x)), \tag{3.14}$$

for this case, $\Psi(x, \zeta)$ (from Eq. 3.2) is calculated algorithmically, this is, sorting all NSR values and finding the NSR value at the location $\lfloor (1-\alpha)S \rfloor$. For example, for $S = 100$ and $\alpha = 90\%$, the VaR_α is located at the 10-th sorted NSR value.

Consequently, the objective function to maximise the CVaR is given by:

$$f_4(x) = CVaR_\alpha(NSR(x)). \tag{3.15}$$

Similar to VaR, CVaR is calculated sorting all NSR and calculating the average of all NSR located to the left where the VaR value is located.

Deviations from production targets Under the assumption of fixed density of any block, the deviation from production targets calculation is given by:

$$f_5(x) = |C - \sum_{d=1}^{D} \sum_{t=1}^{T} \sum_{b \in EB(x_{dt})} tons_b|. \tag{3.16}$$

NSR of VaR at block scale An alternative for risk minimisation is to use the VaR at block scale, i.e. the VaR of all nsr_{bs}, for any block b. This is a measure of the worst possible case for each block, which is a very pessimistic, and highly unlikely, case. This value, denoted by VaR(nsr_b), transforms the discrete random variable nsr into to a deterministic value and the objective function is, therefore, also deterministic, as opposed to Eq. 3.12, in which the expectation is used.

The calculation of NSR using VaR(nsr_b) is given by:

$$f_6(x) = NSR^{\text{VaR}}(x) = \sum_{d=1}^{D} \sum_{t=1}^{T} 1/(1-dr)^{t-1} \sum_{b \in EB(x_{dt})} \text{VaR}(nsr_b). \tag{3.17}$$

Note that VaR(nsr_b) can be pre-calculated for all blocks.

Bi-objective optimisation problems Maximising NSR is one of the most important objectives for medium- and long-term mine planning. Operational objectives, such as meeting production targets, are also important especially when there are contractual obligations. In this case, the minimisation of deviations from production targets (DPT) will contribute to reducing operational risk. For both objectives, the risk associated with geometallurgical uncertainty can also can be minimised using the proposed risk measures.

The traditional approach of optimising each scenario independently is useful as a general way to assess risk. When each scenario is independently optimised, the resulting distribution of all maxima can be used to quantify the risk involved (Fig. 3.3). The objectives of economic valuation and deviation from production targets are combined to define the following five bi-objective problems (also denominated cases):

A Maximisation of the expected NSR and minimisation of the standard deviation of NSR (Eq. 3.12 and 3.13).

B Maximisation of the expected NSR and maximisation of VaR(NSR) (Eq. 3.12 and 3.14).

C Maximisation of the expected NSR and maximisation of CVaR(NSR) (Eq. 3.12 and 3.15).

D Maximisation of the expected NSR and minimisation of DPT (Eq. 3.12 and 3.16).

E Maximisation of the NSR of the VaR at block scale and minimisation of DPT (Eq. 3.17 and 3.16).

The first four problems involve the maximisation of the expected NSR. There is a subtle difference between the fifth problem and the other problems. Instead of calculating the NSR for all scenarios, the VaR of the NSR are calculated at block scale, which represents the extreme event for each block over all scenarios.

Constraints

Mining capacities

$$LT \leq g_1(x) = \sum_{d=1}^{D} \sum_{t=1}^{T} \sum_{b \in EB(x_{dt})} tons_b \leq UT. \tag{3.18}$$

Lower and upper bounds on decision variables As x_{dt} represents the number of blocks drawn from draw-point d in the period t, $X \geq 0$ and the upper bound is the parameter $MAXB_d$:

$$0 \leq x_{dt} \leq MAXB_d, \forall d, \forall t. \tag{3.19}$$

3.3 Case Study

3.3.1 Description

This case study uses real data from an operating mine but with a set of fictitious parameters. The mine is a massive panel caving operation and the main metals are gold and copper, which are mainly sold in copper concentrates. A block caving plan has been defined for a volume of approximately 380×120×150 m; it contains 231 draw-points with an average draw of 464.4 kt per draw-point per year.

The block model for this caving volume comprises 560,000 blocks of size 5×5×5 m. In addition to gold and copper, the block model has five additional elements: iron, sulphur, molybdenum, copper cyanide and fluorine. Fluorine is a deleterious element and a high level in the concentrate will attract a penalty as it will have a negative impact on the smelting process. As the impact of deleterious elements could be high, the use of the NSR valuation model incorporating geometallurgy is more realistic than the simple NPV valuation.

The NSR calculation requires the grades of copper and gold, grade of fluorine as a deleterious element, ore recovery of copper and gold, and grade in concentrate for copper, gold and fluorine.

From more than 200 metallurgical tests at laboratory scale, regression models for ore recovery a) of copper and b) gold, grade in concentrate for c) copper, d) gold and e) fluorine were built using projection pursuit regression (PPR), as detailed in Sepúlveda et al. (2017). The input variables for these five PPR models are seven ore grades: copper, gold, iron, sulphur, molybdenum, copper cyanide and fluorine. To quantify the model uncertainty, 25 bootstrapped PPR models were evaluated. The regression models were applied under the assumption that the response variables are linearly scalable.

To quantify geological uncertainty, geostatistical simulations of these seven inputs (grade variables) were used to build 25 realisations of the block model. The framework of projection pursuit multivariate transform (Barnett et al., 2014, 2016) was used in together with sequential Gaussian geostatistical simulation.

In summary, the inclusion of geometallurgical uncertainty involves 625 combined realisations from the 25 geostatistical realisations of input variables and the 25 PPR bootstrapped models applied to predict recoveries and grades in concentrate. These 625 realisations are the scenarios used in all formulations (parameter $S = 625$).

The geometallurgical block model used contains:

- Primary variables:
  - Copper grade
  - Gold grade
  - Fluorine grade
  - Specific gravity (to calculate tonnage)
- Secondary variables:
  - Iron grade

  - Sulphur grade
  - Molybdenum grade
  - Copper cyanide grade

- Response variables:
  - Copper recovery
  - Gold recovery
  - Copper grade in Concentrate
  - Gold grade in Concentrate
  - Fluorine grade in Concentrate

- Economic variables:
  - Net smelter return

A hypothetical life of mine of 12 periods of one year each are used for this study. All economic values are expressed in a fictitious monetary unit, but using the dollar symbol $, to maintain the confidentiality of the real data used in this paper.

3.3.2 Assumptions

As the main objective of this paper is to demonstrate a method for including geometallurgical uncertainty in mine optimisation, four main assumptions and simplifications were used:

- The caving process was simulated as a simple vertical particle flow with no horizontal interactions.
- All draw-points are developed and active from the beginning.
- No operational constraints are imposed on neighbouring draw-points.
- Recovery and concentrate models derived from laboratory tests on samples can be scaled up to blocks.

More complex models without using these assumptions can also be built. For example, instead of using a simple vertical flow for ore extraction, a more realistic ore draw model can be used but with an increase in computational cost. We are addressing the general upscaling problem (for the case of non-linearity) in on-going research. The addition of more constraints is also simple

TABLE 3.1: Parameters used in block caving optimisation.

Parameter	Value
D	231
T	12
S	625
dr	10%
C	7500kt.
LT	7000kt.
UT	8000kt.
MAXB	200
α	90%

TABLE 3.2: Parameters used in GA.

Parameter	Value
Population size	100
Number of generations	100
Probability of crossover	1.0
Probability of mutation	0.4
Tournament size	20

in the GA approach. Each constraint is simply a function to be evaluated and evolution will ensure that bad (unfeasible) solutions are eliminated.

The values of the parameters used in the case study are presented in Table 3.1.

3.3.3 GA enconding

The GA coding is simple in this case and is based on the definition of the decision variables. For D draw-points and T periods, the genome is a two-dimensional array of integers of size (D, T). In any period, the maximum number of blocks to be extracted is 200 in any draw-point, and thus the maximum tonnage in any period is 69.6 kt.

Three operators must be specified for GA: crossover, mutation and selection. For this case study, we have chosen the uniform binary crossover as the operator. The mutation operator uses the uniform integer mutation and for selection, the operator is tournament selection. We do not tune these operators or their parameters (Table 3.2). The optimisation was performed several times with different random number seeds all with similar results. As the focus of this paper is not the GA optimisation itself, one representative instance is used for illustration.

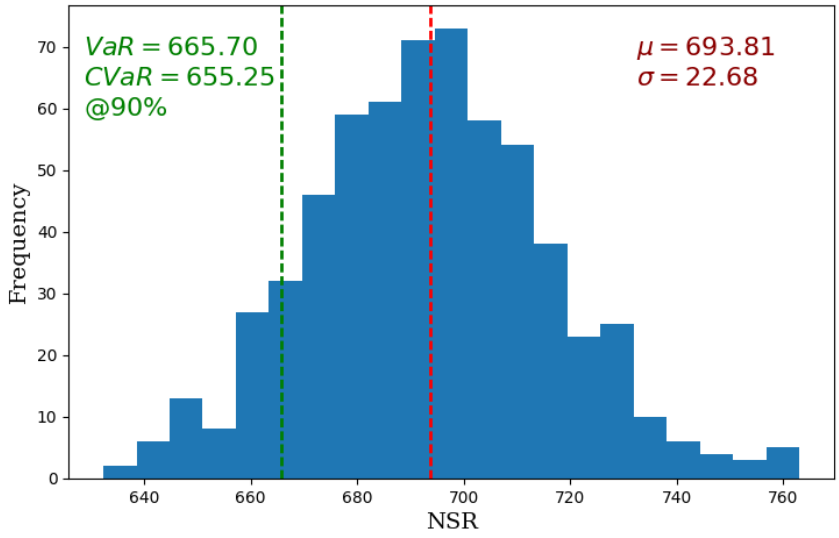


FIGURE 3.3: Distribution of maximum NSR values for each scenario.

3.4 Discussion

3.4.1 Independent maximisation of each scenario

The traditional approach for examining multiple scenarios in an optimisation problem is to optimise them independently to produce the distribution of all optimum values for each scenario (Dowd, 1994; Coward et al., 2013; Dowd et al., 2016).

For the case study, as a result of maximising the NSR for each scenario, there are 625 equally probable optimum schedules. Given all these schedules, and assuming that all data are known with certainty, it is possible to calculate the distribution of NSR (Fig. 3.3) and the deviation from production targets. This provides an upper bound for the stochastic optimisation formulations; for example, with 90% confidence the NSR will be at least $665.70 (VaR) and the expected NSR for all values less than the VaR will be $655.25 (CVaR).

The results from this single objective approach will be compared to those obtained from the bi-objective formulations discussed below.

3.4.2 Optimisation of the expected NSR and volatility

Volatility is the simplest measure of risk and it is added as a secondary objective in this combination. The primary objective is still the maximisation of the

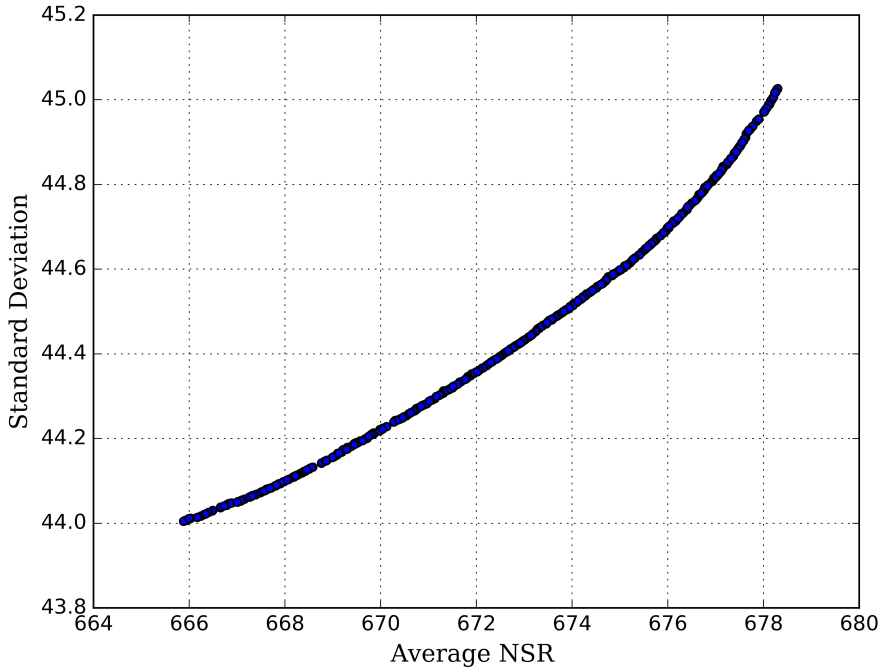


FIGURE 3.4: Pareto front of maximisation of NSR and minimisation of volatility.

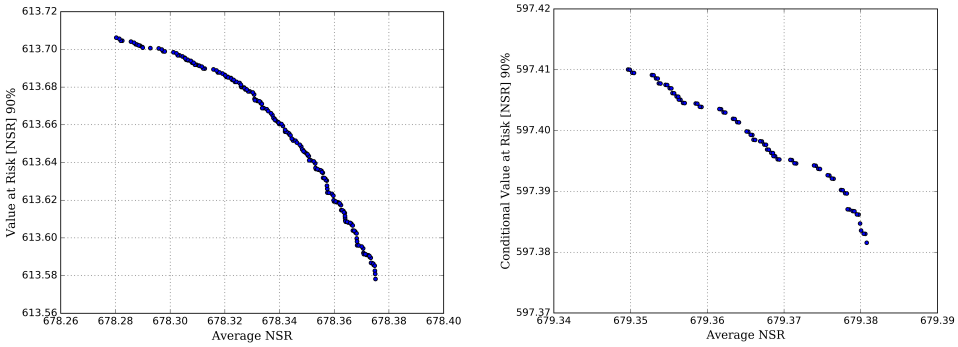
expected NSR. The standard deviation of the distribution of NSR in all scenarios is used here as a volatility measure.

The Pareto front in this case shows the expected economic return that would have to be sacrificed to reduce the volatility or risk (Fig. 3.4). For example, 1.0 unit of risk volatility reduction corresponds to an approximate $14M reduction in expected NSR for this operation.

3.4.3 Optimisation of the expected NSR and the VaR and CVaR of NSR

One of the shortcomings of the volatility risk measure is that it does not describe the shape of the distribution and, in particular, the critical part of the distribution, i.e., the tails. For example, two distributions could have similar volatility but very different extreme values. Value at risk and conditional value at risk take this into account. From a risk perspective, maximising the VaR and CVaR of NSR would force the optimiser to find less risky solutions because higher VaR and CVaR may imply a solution with favourable extreme events.

These two secondary objectives show a very narrow range for the case study (Fig. 3.5). For example, VaR ranges from $613.58 to $613.71. The same



(A) (B)

FIGURE 3.5: Pareto front of maximisation of NSR and maximisation of (A) VaR and (B) CVaR.

occurs with CVaR with values ranging from $597.38 to $597.41. The reason is that the distribution of the global NSR changes very little in the left tail. This is consistent with the scale effect. At block cave scale the VaR (at 90% confidence) is very stable. This observation indicates that the global VaR and CVaR are not good measures of risk for this case study.

3.4.4 Optimisation of NSR and deviation from targets

Another important objective from the operational perspective is to keep the production tonnage as close as possible to the target so as to feed the plant. When this objective is not considered in the maximisation of economic returns, the resulting schedules usually have higher tonnages in early periods and lower tonnages in later periods so as to maximise the return as soon as possible, even if lower and upper bounds are imposed as in this case study. Unfortunately, imposing a small, hard bound for tonnage could lead to infeasible solutions. A better approach is to use a larger bound and minimise the deviations. Understanding the cost of such deviations is important for risk assessment. The Pareto front of this bi-objective problem, shown in Fig. 3.6, reflects exactly this point.

The two tails of the Pareto front show that there is a difference of 120k tonnes from production targets with a value of $12M. Decision-makers can evaluate the cost per tonne of deviation. Some researchers have introduced penalties for each unit of deviation so that the optimiser seeks to reduce such penalties in open-pit problems (Ramazan and Dimitrakopoulos, 2013; Goodfellow and Dimitrakopoulos, 2016). This approach, however, has two main

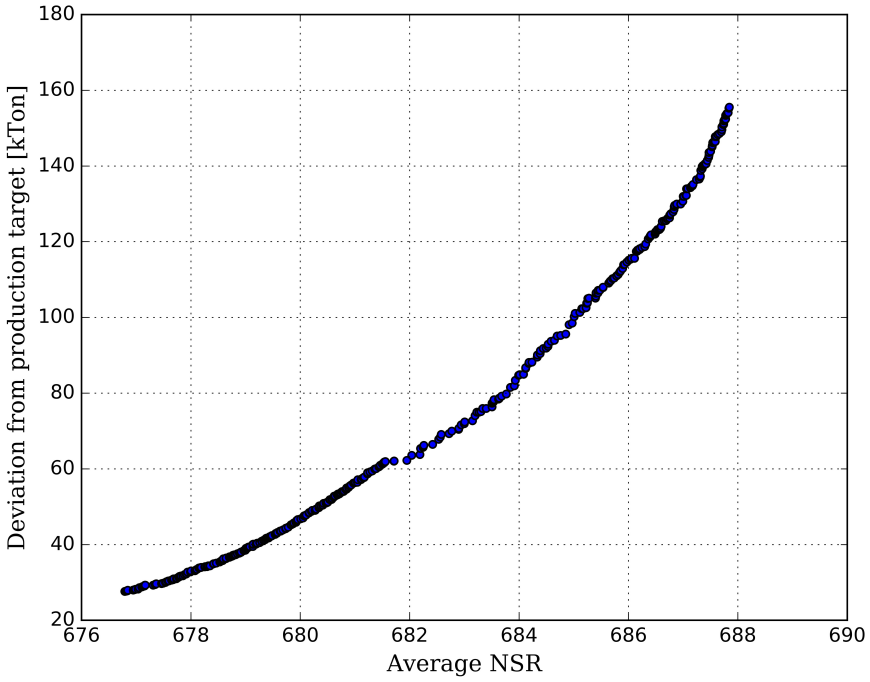


FIGURE 3.6: Pareto front of maximisation of NSR and minimisation of deviation from production targets.

drawbacks: (i) the optimal solution depends largely on the calibration of the magnitude of the penalties, and (ii) it is not easy to discern the cost of the deviation in terms of economic valuation. The bi-objective optimisation presented here overcomes these drawbacks. No parameters are required except for the production targets, which are known, and the generated Pareto front reveals the structure of the cost of deviation.

The inclusion of the minimisation of the deviation from production targets is very useful for minimising one particular component of operational risk. The addition of the minimisation of economic risk would be better for general risk assessment. One way to do so is to formulate a three-objective optimisation problem: (i) the maximisation of average NSR, (ii) the minimisation of deviations from production targets, and (iii) the minimisation of any risk measure such as volatility, VaR and CVaR. In practice, the Pareto front for a three-objective problem is hard to visualise and interpret. A simplified and useful alternative is to merge the objectives of maximising the economic return and minimising economic risk. A combined strategy can be applied as the block model contains the complete distribution of NSR at the block scale, which can be used directly instead of using the expected NSR at block scale to compute

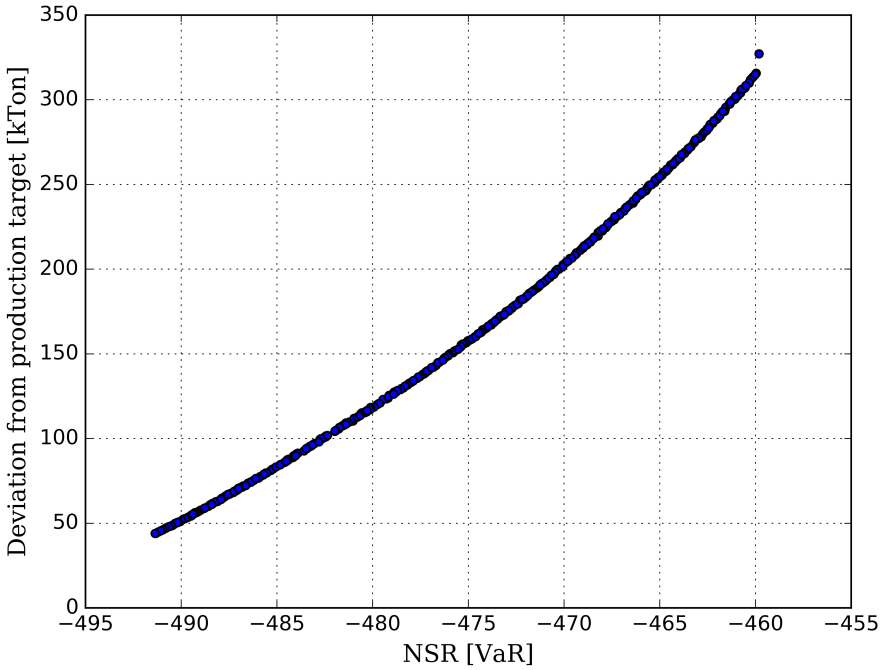


FIGURE 3.7: Pareto Front of maximisation of NSR-VaR and minimisation of deviation from production targets.

the global NSR and minimising the VaR of the generated global NSR distribution. The VaR of the NSR distribution at block scale can be used as a risk measure at that scale. The main goal can then be achieved by maximising the global NSR using the VaR at block scale where the optimiser finds a good solution based on a pessimistic situation (which is the VaR) and therefore the risk is minimised jointly with maximised NSR. This approach allows the definition of a new bi-objective optimisation problem: the maximisation of the NSR-VaR and the minimisation of deviations from production targets.

The Pareto front shown in Fig. 3.7 may be difficult to interpret compared with the previous ones. The NSR in this case is in fact the VaR at block scale, which is negative in this case study, indicating losses, but these losses are minimised assuming the pessimistic event occurs. To see the actual NSR value, all solutions from the Pareto front need to be used to calculate the average NSR.

3.4.5 Detailed view of some solutions from the Pareto front

The bi-objective formulations discussed above try to find optimal solutions that maximise economic returns and minimise some risk measures. The results are summarised in Table 3.3 in which the extreme solutions at the Pareto

TABLE 3.3: Statistics of all bi-objective formulations. Good solutions are highlighted.

Schedule Statistic	NSR vs Volatility (A)		NSR vs VaR (B)		NSR vs CVaR (C)		NSR vs DFT (D)		NSR-VaR vs DFT (E)	
	LT	UT	LT	UT	LT	UT	LT	UT	LT	UT
NSR-Mean	665.88	678.30	678.28	678.38	679.35	679.38	678.81	**687.84**	676.48	**682.80**
NSR-VaR	604.45	615.66	613.71	613.58	614.46	614.46	616.41	**625.03**	616.01	**620.02**
NSR-CVaR	588.81	599.16	596.67	596.77	597.76	597.73	598.56	**606.53**	598.82	**602.99**
Tonnage-1	7654.92	7857.65	7994.75	7986.07	7992.03	7995.16	7540.70	7861.10	7002.49	7232.99
Tonnage-2	7613.60	7752.75	7992.37	7992.38	7981.91	7981.91	7700.84	7833.51	7016.47	7331.48
Tonnage-3	7690.83	7818.97	7984.95	7984.95	7993.92	7993.92	7509.42	7814.38	7029.75	7431.58
Tonnage-4	7758.80	7849.92	7992.35	7999.64	7986.61	7986.61	7500.87	7609.87	7037.28	7493.37
Tonnage-5	7796.18	7913.80	7970.54	7970.54	7992.80	7996.28	7499.98	7613.75	7016.23	7498.93
Tonnage-6	7795.53	7890.76	7999.02	7999.02	7962.95	7972.66	7499.98	7567.24	7318.01	7499.67
Tonnage-7	7694.57	7842.07	7978.11	7978.47	7992.05	7994.13	7501.29	7531.84	7215.85	7500.87
Tonnage-8	7462.95	7533.80	7847.16	7856.89	7896.85	7896.86	7499.96	7502.43	7322.41	7498.15
Tonnage-9	7003.59	7027.19	7115.29	7124.65	7171.54	7171.53	7498.70	7508.29	7224.66	7499.39
Tonnage-10	7001.71	7003.80	7002.71	7020.17	7053.31	7052.61	7501.80	7484.93	7263.81	7494.21
Tonnage-11	7001.02	7008.49	7019.19	7019.11	7002.67	7006.15	7490.31	7328.56	7281.34	7499.09
Tonnage-12	7002.30	7004.31	7011.48	7016.67	7000.80	7006.69	7317.94	7161.87	7346.56	7494.52
DFT	294.41	368.00	467.55	465.61	464.23	465.05	**37.34**	155.59	327.10	**43.96**

front are evaluated (LT and UT stand for lower and upper tails of the PF). Extreme solutions here represent extreme schedules reflecting the trade-off between two objectives. The mean global NSR and the VaR and CVaR are included. The tonnage for each period is also included together with the mean deviation from the production target (DFT).

Note the values when all scenarios are optimised independently: the mean NSR is \$693.81, VaR is \$665.70 and CVaR is \$655.25. These values can be compared with the results presented in Table 3.3 to assess the effect of multiple-objective optimisations.

Overall, if the DFT objective is not included in the optimisation, the deviation is consistently higher (cases A, B and C). This is as expected as in earlier periods the optimiser will try to use a schedule to extract as much as possible (but less than the set upper bound) to maximise the expected NSR. The solutions are very similar when VaR and CVaR are used as risk measures because schedules show similar economic returns in the pessimistic case. VaR and CVaR of NSR are not particularly useful in quantifying risks for this case study. On the other hand, if the DFT objective is included in the optimisation, (i.e., all risk components, economic valuation and operational constraints are considered together in the optimisation), solutions appear to be more realistic. For case D, as the expected NSR is jointly maximised with minimising DFT, the corresponding DFT is lower than for cases A, B and C. Case D and E produce a balanced trade-off among economic valuation, economic risk and operational risk. The minimum DFT for case E is also a very good solution, because it also has a high average NSR, and is better than the average solution from all scenarios.

These bi-objective optimisations offer two benefits compared with the independent optimisation of all scenarios. Firstly, any solution in the Pareto fronts is a good schedule and can be chosen by the decision-maker based on the preferred criteria and potential risks involved. Secondly, not only can the economic return be maximised, which is the de facto objective for most optimisation formulations, the minimisation of risk has also been successfully included in the evaluations as demonstrated in this study.

3.5 Conclusions

This paper presents some techniques for the optimisation under uncertainty of a block caving mining operation using meta-heuristic approaches. Five bi-objective formulations are described which can incorporate risk measures related to geometallurgical uncertainties. The Pareto fronts show the relationship and trade-off between the two objectives, which provides a useful tool for decision-makers in understanding and selecting the optimal solution at the desired risk level. The total NSR values, based on VaR and CVaR, do not show significant uncertainty at the caving scale but some useful results are obtained by using the VaR at the block scale. The maximisation of the NSR-VaR formulation combined with the minimisation of the deviations from production targets yields better results in terms of risk reduction. In addition, it was demonstrated that the genetic algorithm is capable of producing an approximate Pareto front for real-sized problems for which traditional optimisation methods will struggle. Further research could focus on using more advanced simulations of the caving flow of rock and incorporating other constraints such as the control of relative draw rates between adjacent draw-points. These additional variables can readily be included in the proposed algorithm-oriented methodology described in this paper.

Acknowledgements

The authors acknowledge Professor Emmanuel Chanda for his very useful review of this paper and Catalina Sepúlveda for designing and drawing diagrams. This work was supported with supercomputing resources provided by the Phoenix HPC service at the University of Adelaide. The first author acknowledges the support of CONICYT in the form of a Becas Chile scholarship.

References

Amankwah, H., Larsson, T. and Textorius, B. (2013), Open-pit mining with uncertainty: A conditional value-at-risk approach, *in* 'Optimization Theory, Decision Making, and Operations Research Applications', Springer, pp. 117–139.

Barnett, R. M., Manchuk, J. G. and Deutsch, C. V. (2014), 'Projection pursuit multivariate transform', *Mathematical Geosciences* **46**(3), 337–359.

Barnett, R. M., Manchuk, J. G., Deutsch, C. V. et al. (2016), 'The projection-pursuit multivariate transform for improved continuous variable modeling', *SPE Journal* **21**(6).

Benndorf, J. and Dimitrakopoulos, R. (2013), 'Stochastic long-term production scheduling of iron ore deposits: Integrating joint multi-element geological uncertainty', *Journal of Mining Science* **49**(1), 68–81.

Bianchi, L., Dorigo, M., Gambardella, L. M. and Gutjahr, W. J. (2009), 'A survey on metaheuristics for stochastic combinatorial optimization', *Natural Computing* **8**(2), 239–287.

Boisvert, J. B., Rossi, M. E., Ehrig, K. and Deutsch, C. (2013), 'Geometallurgical Modeling at Olympic Dam Mine, South Australia', *Mathematical Geosciences* **45**(8), 901–925.

Coward, S. and Dowd, PA. (2015), Geometallurgical models for the quantification of uncertainty in mining project value chains, *in* '37th APCOM Conference', Soc. Mining, Metallurgy and Exploration (SME) ISBN 978-0-87335-417-2, pp. 360–69.

Coward, S., Dowd, PA. and Vann, J. (2013), Value chain modelling to evaluate geometallurgical recovery factors, *in* '36th APCOM Conference', Fundação Luiz Englert, Brazil; ISBN 978-85-61155-02-5, Porto Alegre, Brazil, pp. 288–289.

Coward, S., Vann, J., Dunham, S. and Stewart, M. (2009), The primary-response framework for geometallurgical variables, *in* 'Seventh international mining geology conference', pp. 109–113.

Deb, K., Pratap, A., Agarwal, S. and Meyarivan, T. (2002), 'A fast and elitist multiobjective genetic algorithm: Nsga-ii', *IEEE transactions on evolutionary computation* **6**(2), 182–197.

Dimitrakopoulos, R. (1998), 'Conditional simulation algorithms for modelling orebody uncertainty in open pit optimisation', *International Journal of Surface Mining, Reclamation and Environment* **12**(4), 173–179.

Dimitrakopoulos, R. (2011), 'Strategic mine planning under uncertainty', *Journal of Mining Science* **47**(2), 138–150.

Dimitrakopoulos, R. G. and Sabour, S. A. A. (2007), 'Evaluating mine plans under uncertainty: Can the real options make a difference?', *Resources Policy* **32**(3), 116–125.

Dowd, PA. (1994), 'Risk assessment in reserve estimation and open-pit planning', *Transactions of the Institution of Mining and Metallurgy (Section A: Mining Industry)* **103**.

Dowd, PA. (1997), 'Risk in minerals projects: analysis, perception and management', *Transactions of the Institutions of Mining and Metallurgy, Section A: Mining Technology* (108), 9–18.

Dowd, PA. and Dare-Bryan, P. (2004), Planning, designing and optimising using geostatistical simulation, *in* 'Proceedings of the International Symposium on Orebody Modelling and Strategic Mine Planning', The Australasian Institute of Mining and Metallurgy, Melbourne, Australia, pp. 363–379.

Dowd, PA., Xu, C. and Coward, S. (2016), 'Strategic mine planning and design: some challenges and strategies for addressing them', *Mining Technology* **125**(1), 22–34.

Dunham, S. and Vann, J. (2007), Geometallurgy, Geostatistics and Project Value - Does Your Block Model Tell You What You Need to Know?, *in* 'Project Evaluation Conference', Melbourne, pp. 189–196.

Evatt, G. W., Soltan, M. O. and Johnson, P. V. (2012), 'Mineral reserves under price uncertainty', *Resources Policy* **37**(3), 340–345.

Gholamnejad, J. and Osanloo, M. (2007), 'Incorporation of ore grade uncertainty into the push back design process', *Journal of the South African Institute of Mining & Metallurgy* **107**(3), 177.

Goldie, R. and Tredger, P. (1991), 'Net smelter return models and their use in the exploration, evaluation and exploitation of polymetallic deposits', *Geoscience Canada* **18**(4).

Goodfellow, R. C. and Dimitrakopoulos, R. (2016), 'Global optimization of open pit mining complexes with uncertainty', *Applied Soft Computing* **40**, 292–304.

Grobler, F., Elkington, T. and Rendu, J. (2011), Robust decision making-application to mine planning under price uncertainty, *in* '35th APCOM Symposium-Application of Computers and Operations Research in the Minerals Industry, Proceedings', pp. 371–380.

Groeneveld, B. and Topal, E. (2011), 'Flexible open-pit mine design under uncertainty', *Journal of Mining Science* **47**(2), 212–226.

Hunt, J., Berry, R., Bradshaw, D., Triffett, B. and Walters, S. (2014), 'Development of recovery domains: Examples from the Prominent Hill IOCG deposit, Australia', *Minerals Engineering* **64**, 7–14.

Journel, A. G. (1974), 'Geostatistics for conditional simulation of ore bodies', *Economic Geology* **69**(5), 673–687.

Khodayari, F. and Pourrahimian, Y. (2015), 'Mathematical programming applications in block-caving scheduling: a review of models and algorithms', *International Journal of Mining and Mineral Engineering* **6**(3), 234–257.

Kumral, M. (2013), 'Optimizing ore–waste discrimination and block sequencing through simulated annealing', *Applied Soft Computing* **13**(8), 3737–3744.

Lamberg, P. (2011), Particles-the bridge between geology and metallurgy, *in* 'Konferens i mineralteknik 2011: 08/02/2011-09/02/2011', Luleå tekniska universitet.

Lamghari, A. and Dimitrakopoulos, R. (2012), 'A diversified tabu search approach for the open-pit mine production scheduling problem with metal uncertainty', *European Journal of Operational Research* **222**(3), 642–652.

Land, A. H. and Doig, A. G. (1960), 'An automatic method of solving discrete programming problems', *Econometrica: Journal of the Econometric Society* pp. 497–520.

Lund, C., Lamberg, P. and Lindberg, T. (2015), 'Development of a geometallurgical framework to quantify mineral textures for process prediction', *Minerals Engineering* **82**, 61–77.

Marler, R. T. and Arora, J. S. (2004), 'Survey of multi-objective optimization methods for engineering', *Structural and multidisciplinary optimization* **26**(6), 369–395.

McCarthy, P. (2003), Managing technical risk for mine feasibility studies, *in* 'Mining Risk Management 2003', pp. 21–27.

Montiel, L., Dimitrakopoulos, R. and Kawahata, K. (2016), 'Globally optimising open-pit and underground mining operations under geological uncertainty', *Mining Technology* **125**(1), 2–14.

Nezhadshahmohammad, F., Aghababaei, H. and Pourrahimian, Y. (2017), 'Conditional draw control system in block-cave production scheduling using mathematical programming', *International Journal of Mining, Reclamation and Environment* pp. 1–24.

Parian, M., Lamberg, P., Möckel, R. and Rosenkranz, J. (2015), 'Analysis of mineral grades for geometallurgy: Combined element-to-mineral conversion and quantitative x-ray diffraction', *Minerals Engineering* **82**, 25–35.

Rahal, D., Smith, M., Van Hout, G. and Von Johannides, A. (2003), The use of mixed integer linear programming for long-term scheduling in block caving mines, *in* 'Proceedings of the 31st International APCOM Symposium, Cape Town, South Africa', pp. 123–131.

Ramazan, S. and Dimitrakopoulos, R. (2013), 'Production scheduling with uncertain supply: a new solution to the open pit mining problem', *Optimization and Engineering* **14**(2), 361–380.

Rockafellar, R. T. and Uryasev, S. (1997), 'Optimization of conditional value-at-risk', *Journal of Risk* **2**, 21–41.

Rubio, E. and Dunbar, W. S. (2005), Integrating Uncertainty in Block Cave Production Scheduling, *in* '32nd International Symposium on the Application of Computers and Operations Research in the Mineral Industry', Arizona.

Sarykalin, S., Serraino, G. and Uryasev, S. (2008), Value-at-risk vs. conditional value-at-risk in risk management and optimization, *in* 'State-of-the-Art Decision-Making Tools in the Information-Intensive Age', Informs, pp. 270–294.

Schultz, R. and Tiedemann, S. (2006), 'Conditional value-at-risk in stochastic programs with mixed-integer recourse', *Mathematical Programming* **105**(2-3), 365–386.

Sepúlveda, E., Dowd, PA., Xu, C. and Addo, E. (2017), 'Multivariate modelling of geometallurgical variables by projection pursuit', *Mathematical Geosciences* **49**(1), 121–143.

Silva, M. d. F., Dimitrakopoulos, R. and Lamghari, A. (2015), 'Solving a large sip model for production scheduling at a gold mine with multiple processing streams and uncertain geology', *Mining Technology* **124**(1), 24–33.

Tungpalan, K., Manlapig, E., Andrusiewicz, M., Keeney, L., Wightman, E. and Edraki, M. (2015), 'An integrated approach of predicting metallurgical performance relating to variability in deposit characteristics', *Minerals Engineering* **71**, 49–54.

Vann, J., Jackson, S., Bye, A., Coward, S., Moayer, S., Nicholas, G. and Wolff, R. (2012), Scenario thinking: a powerful tool for strategic planning and evaluation of mining projects and operations, *in* 'Project Evaluation 2012: Proceedings. Project Evaluation Conference', pp. 5–14.

Whitley, D. (1994), 'A genetic algorithm tutorial', *Statistics and computing* **4**(2), 65–85.

Yashar, P., Hooman, A.-N. et al. (2013), 'A multi-step approach for block-cave production scheduling optimization', *International Journal of Mining Science and Technology* **23**(5), 739–750.

Chapter 4

A new clustering method with spatial correction and its application to geometallurgical domaining

Statement of Authorship

Title of Paper	A new clustering method with spatial correction and its application to geometallurgical domaining.
Publication Status	☐ Published ☐ Accepted for Publication ☑ Submitted for Publication ☐ Unpublished and Unsubmitted w ork w ritten in manuscript style
Publication Details	Sepulveda E, Dowd PA and Xu C. A new clustering method with spatial correction and its application to geometallurgical domaining. Mathematical Geosciences. Submitted on 2017 Nov 23.

Principal Author

Name of Principal Author (Candidate)	Exequiel Manuel Sepulveda Escobedo		
Contribution to the Paper	Develop methodology and methods, conducted programming and execution of methods, wrote manuscript and acted as corresponding author.		
Overall percentage (%)	80%		
Certification:	This paper reports on original research I conducted during the period of my Higher Degree by Research candidature and is not subject to any obligations or contractual agreements with a third party that would constrain its inclusion in this thesis. I am the primary author of this paper.		
Signature		Date	20/02/2018

Co-Author Contributions

By signing the Statement of Authorship, each author certifies that:

i. the candidate's stated contribution to the publication is accurate (as detailed above);

ii. permission is granted for the candidate in include the publication in the thesis; and

iii. the sum of all co-author contributions is equal to 100% less the candidate's stated contribution.

Name of Co-Author	Peter Dowd		
Contribution to the Paper	Supervised development of work and reviewed manuscript.		
Signature		Date	20th February 2018

Name of Co-Author	Chaoshui Xu		
Contribution to the Paper	Supervised development of work and reviewed manuscript.		
Signature		Date	20-02-2018

Abstract

This paper describes a proposed method for clustering attributes on the basis of their spatial variability and the uncertainty of cluster membership. The method is applied to geometallurgical domaining in mining applications. The main objective of geometallurgical clustering is to ensure consistent feed to a processing plant by minimising transitions between different types of feed coming from different domains (clusters). For this purpose, clusters should contain not only similar geometallurgical characteristics but also be located in as few contiguous and compact spatial locations as possible so as to maximise the homogeneity of ore delivered to the plant. Most existing clustering methods applied to geometallurgy have two problems. Firstly, they are unable to differentiate subsets of attributes at the cluster level and therefore cluster membership can only be assigned on the basis of exactly identical attributes, which may not be the case in practice. Secondly, they do not take account of the spatial relationships and therefore they can produce clusters which may be spatially dispersed and/or overlapped. In the work described in this paper a new clustering method is introduced that integrates three distinct steps to ensure quality clustering. In the first step, the fuzzy membership information is used to minimise compactness and maximise separation. In the second step, the best subsets of attributes are defined and applied for domaining purposes. These two steps are iterated to convergence. In the final step a graph-based labelling method, which takes spatial constraints into account, is used to produce the final clusters. Three examples are presented to illustrate the application of the proposed method. These examples demonstrate that the proposed method can reveal useful relationships among geometallurgical attributes within a clear and compact spatial structure. The resulting clusters can be used directly in mine planning to optimise the ore feed to be delivered to the processing plant.

Keywords Geometallurgy; Clustering; Geometallurgical Domaining.

4.1 Introduction

Geometallurgy provides new opportunities for mine planning by integrating primary and response properties to enhance the value of information for decision-making processes (Coward et al., 2009, 2013; Coward and Dowd, 2015). Even

though significant progress has been made in sensing and collecting geometallurgical data, there is still a significant gap in achieving effective use of these data in practical applications. Discriminating among geometallurgical characteristics is a step towards an effective use of geometallurgy for mine planning, as similar geometallurgical characteristics will have similar responses in mineral processing. From this perspective, a proper clustering of *in-situ* resources based on geometallurgical characteristics is essential to optimising operations across the entire value chain from mining to mineral processing.

Traditional geological clustering, commonly known as rock type domaining, is important in understanding the nature of the deposit but it does not necessarily reflect the responses of the ore to the various processing stages. Geometallurgical clustering (or domaining) is similar to geological clustering but focusses on the geometallurgical characteristics of the orebody to provide a basis for integrated optimisation from mining to processing (Hoal et al., 2013).

Clustering is an important problem in machine learning and, for unsupervised problems, it is one of the hardest to formulate and solve. Regression or classification is supervised because the response is known, whereas clustering partitions data on the basis of similar characteristics and, at the same time, maximises the separation of those partitions.

The classic cut-off grade approach to ore selection clearly does not consider the mineral complexity and its responses to processing, such as the energy consumption due to different hardness and grindability, concentration of deleterious elements, different recovery rates due to different geometallurgical attributes. Clustering based on geometallurgical attributes has been an active research topic over the past decade. Having more material classes (clusters) may improve the ability to select the best processing route for each parcel of mined ore so that the overall operation is optimised (Dunham and Vann, 2007; Hunt et al., 2013). However, the risk of misclassification increases as more clusters are defined and this risk must be considered in any geometallurgical clustering.

Geological domains are not necessarily useful in defining processing domains that are required to reflect characteristics such as the Bond Ball Mill Work index (BMWi), which relates to the energy used in a ball mill (Bond, 1961), or the A$\times$b comminution index (Napier-Munn et al., 1996), which is a measure of the ore impact breakage resistance. To remediate this problem, Keeney and Walters (2011) used Principal Component Analysis (PCA) (Wold et al., 1987) to project variables onto a two-dimensional space representing

geometallurgical attributes such as mineralogy and grindability indices. Different classes were then manually defined by drawing polygons around spatially contiguous projected points on the basis of mineralogical association. These classes were used to build predictive models and propagate them into the block model using standard geostatistical indicator approaches. The same method was used in a similar case study to define four geometallurgical domains at drill-hole scale which were then scaled up to block scale by four different methods: sectional interpretation and wireframe modelling, nearest neighbour assignment, indicator kriging, and stochastic trend analysis (Newton and Graham, 2011). The two comminution parameters, A$\times$b and BMWi, were then populated into the block model by applying specific regression models in each geometallurgical domain.

Leichliter and Larson (2013) developed a geometallurgical model to cluster a deposit into two classes for two different recovery circuits: flotation circuit for less oxidized ore and heap leaching for oxidized ore. They used the variables of assays, geological mapping, mineralogy, hardness, gravity and floatability attributes to define the classes.

Hunt et al. (2014) manually clustered copper recovery domains on the basis of Al and Fe content (Low Al - High Fe and High Al - Low Fe). They pre-clustered 24 archetypes using chemical and mineralogical information. For each recovery domain, they built linear regression models using Al, Cu, Fe and grinding index from drill hole data and batch flotation tests. These models were scaled up for the block model using standard geostatistical methods.

A geometallurgical domaining system was built by hierarchical clustering at sample scale using assay values, geotechnical logging and petrophysical attributes to model and estimate grindability response indices (Nguyen and Keeney, 2014). Goodfellow and Dimitrakopoulos (2017) performed clustering using grades and material types to define different ore destination policies, which were used to optimise scheduling.

Garrido et al. (2017) used clay content as a measure to define the concept of geometallurgical dilution in a manner similar to mining dilution. Here, the geometallurgical dilution is formally defined as the ratio between the most common clay cluster and all other clusters. This dilution concept can be used in scheduling optimisation to avoid excessive changes in clay content in the ore to be sent to the processing plant.

The research discussed above demonstrates the use and ability of geometallurgical domaining in improving processing decisions and optimising scheduling to processing plants. However, most of this research uses standard clustering methods and the resulting clusters are then up-scaled to the block model using geostatistical approaches. There is no explicit imposition of spatial contiguity and compactness in the determination of clusters. In addition, the uncertainty of the clustering is not assessed.

For the explicit use of the spatial component, Oliver and Webster (1989) incorporated into the dissimilarity measure a spatial variogram model, using an isotropic exponential structure with parameters of nugget effect, sill and range. Bourgault et al. (1992) generalised the Oliver and Webster (1989) method by using a multivariate (co)variogram to account for both spatial and attributes correlations in clustering. Allard and Guillot (2000) modelled the hard clustering problem as a mosaic of independent stationary normal random functions for the univariate case. Three different optimisation approaches were tested. One approach was based on minimising the ratio between the variance inside a cluster and the variance between clusters. The second optimisation method used negative log-likelihood to estimate the parameters. Finally, in the third approach they used the Expectation-Maximisation (EM) algorithm. The spatial structure is accounted for by the kriged (estimated) mean of the random function and the associated kriging variance. Guillot et al. (2006) assumed that the spatial component is characterised by a second order stationary random field. The inference of the parameters that define the covariance function and the clusters are found by a Markov Chain Monte Carlo algorithm. This method uses quantitative and categorical multivariate data. For hard clustering in the univariate case, Carlo et al. (2017) incorporated the spatial component as a non-stationary Markov random field conditioned to the k-nearest neighbourhood structure. The optimisation was performed by the EM algorithm. The method allows each cluster to have different spatial interaction modulated by a spatial covariate. Fouedjio (2016) incorporated the spatial component in the definition of the dissimilarity measure in the agglomerative hierarchical clustering method. The dissimilarity/similarity between two observations is not a simple Euclidean measure but rather a function of their spatial correlation. It is not clear what effect negative correlations in cross-variograms have on this dissimilarity measure and its performance when the spatial correlation is low, but the method is consistent with geostatistical approaches.

Based on Gaussian mixture models, Ambroise et al. (1996) proposed a method that adds a regularisation component, derived from the spatial structure, to the

clustering optimisation formulation. This method takes into account the membership of all neighbours of any observation for clustering. Romary et al. (2015) incorporated the spatial component into the distance metric using a hierarchical clustering method. The distance function takes into account the spatial connectivity introduced by a moving neighbourhood. Weights for each attribute can be defined by the user and incorporated into the distance function. The coordinates are also included as attributes.

In addition to clustering methods that incorporate a spatial component, cleaning realisations of lithofacies in a regular grid, or image, helps to preserve spatial continuity. Schnetzler (1994) used two image processing pixel-base methods of dilatation and erosion, to produce cleaner images. The resulting grid does not necessarily reproduce the original statistics of the lithofacies. To overcome this issue, a post-process changes the categorical value of the pixels to match the original statistics. The probability of accepting changes is defined as the ratio of the kriging variance to the total variance. This method is only applicable to a regular grid as it was designed to correct 'noisy' grids for visualisation purposes. Deutsch (1998) improved the method of Schnetzler (1994) by using the quantile transformation to correct proportions and produce less-noisy realisations. Locations in the borders between regions are candidates for relocation. The maximum a posteriori selection algorithm replaces each location by the most probable value according to the local neighbourhood structure, based on three aspects: closeness, conditioning data, and target proportions.

In this paper, a new adapted method is proposed to cluster diverse attributes to build geometallurgical domains. The method, Spatial Weighted Fuzzy Clustering (SWFC), is based on traditional fuzzy clustering (Dunn, 1973) with a novel adaptation to support mixed attributes together with the capacity to include expert knowledge and spatial structures. The formulation of the clustering algorithm based on fuzzy clustering, flexible distance metrics and feature selection is given in the methodology section. The mathematics of the proposed SWFC method is then described in the following section. Three case studies are presented to illustrate the application of SWFC, starting with a very simple illustrative example, followed by a two-dimensional case, and finally, a comprehensive three-dimensional synthetic geometallurgical block model.

4.2 Methodology

A dataset is defined as a set of observations or samples. Each sample is a k-dimensional vector, where each dimension represents a feature or an attribute. Each attribute can be a continuous or a categorical variable (ordinal or nominal). The goal of clustering is to partition the dataset into P sets where samples within a partition are similar and partitions are well separated. The concept of similarity within a cluster (defined as compactness, see below) and separation distance between clusters are key aspects of clustering.

4.2.1 Definition of symbols and indices

Symbols:

- $\mathcal{P}$ is a set of partitions or clusters.
- P is the number of partitions or clusters.
- K is the number of dimensions of a multivariate sample.
- N is the total number of samples.
- S_j is the number of samples in the j^{th} cluster.
- v_j is the centroid of the j^{th} cluster.
- m is the fuzzier used in the fuzzy clustering algorithm.
- u is the membership matrix with N rows and P columns.
- w are the weights of attributes.

Indices:

- i indicates the i^{th} sample, $1 <= i <= N$. For example x_i.
- j indicates the j^{th} cluster, $1 <= j <= P$. For example v_j.
- k indicates the k^{th} dimension, $1 <= k <= K$. For example w_k.

4.2.2 Hard clustering

Hard clustering, or crisp clustering in the machine learning literature, seeks a non-overlapped, hard partition of a dataset and therefore the partitions $\mathcal{P}$ are disjoint sets and each sample belongs only to one partition. One option for clustering is to find the centroids of clusters that minimise the overall distance of each sample to the centroid of its cluster, i.e.,

$$(v_i^*, \ldots, v_p^*) = \underset{v_i,\ldots,v_p}{\arg\min} \sum_{j=1}^{P} \sum_{i=1}^{S_j} D(x_i, v_j),\ \sum_{j=1}^{P} S_j = N, \tag{4.1}$$

where D is any distance metric, x_i is the i^{th} sample belonging to the j^{th} cluster.

There are many hard clustering methods and among the most used are K-Means, for continuous variables, K-Mode for categorical variables and several variants for mixed variables.

K-Means is probably the most used clustering method due to its simplicity. K-Means is solved by a two-stage iterative procedure to minimise the variance of the distances within clusters. In the first stage the centroids of clusters are assumed to be fixed and each sample is assigned to the closest centroid. In the second stage, the centroids are updated as the average of all samples within a cluster. The two stages are iterated until overall variance of clusters is minimised. It is common to select initial centroids at random.

A very common variation is to perform an initial dimension reduction to compress the information into two or three dimensions by PCA (Ding and He, 2004). After the dimensionality has been reduced, K-Means is applied to the compressed data.

For geometallurgical applications, it is important to quantify the uncertainty of belonging to a cluster but hard clustering cannot provide this assessment. The fuzzy clustering method assigns the grade of cluster membership to all samples. This grade can be used as a probability measure and, therefore, it can provide a simple way to quantify the uncertainty of clustering.

4.2.3 Fuzzy clustering

Fuzzy clustering, as opposed to hard clustering, is a method that seeks to find the grade of membership of a sample with regard to each cluster (Ruspini, 1969). The objective for optimisation, therefore, changes to

$$u^* = \arg\min_u \sum_{i=1}^{N}\sum_{j=1}^{P}(u_{ij})^m D(x_i, v_j),\ \sum_{j=1}^{P} u_{ij} = 1, \forall i = 1, \ldots, N \tag{4.2}$$

and

$$u_{ij}^{-1} = \sum_{j'=1}^{P}\left[\frac{D(x_i, v_j)}{D(x_i, v_{j'})}\right]^{2/(m-1)} \tag{4.3}$$

where m is the fuzzier, which controls the degree of fuzziness. When m is close to 1, the fuzzy partition becomes a hard partition, i.e. u_{ij} will be 0 or 1 (Pal and Bezdek, 1995; Ren et al., 2016), and when m is large, u_{ij} will tend to be uniformly distributed, but always subject to $\sum_{j=1}^{P} u_{ij} = 1, \forall i$.

There are several methods to find the optimal membership, for example, fuzzy c-means, fuzzy k-modes and fuzzy k-prototypes. These methods are not

designed to use mixed attributes and they do not perform feature selection. To take these features into account, a distance-based approach must be used.

4.2.4 Distance metrics

Clustering essentially relies on similarity among observations and therefore the most critical aspect is the definition of a distance metric between observations. In general, the Euclidian distance (Eq. 4.4) is the default selection when all attributes are continuous, however when there is a mix of continuous and categorical attributes the Euclidian distance is not the best choice.

$$D_{\text{euclidean}}(x,y) = \sqrt{\sum_{k=1}^{K}(x_k - y_k)^2}. \tag{4.4}$$

For two multivariate attributes x and y, the distance function can be formulated as the contribution of each dimension to the total distance (Friedman and Meulman, 2004)

$$D^{(1)}(x,y) = \sum_{k=1}^{K} d_k(x_k, y_k). \tag{4.5}$$

This formulation gives a high degree of flexibility in the definition of specific distance functions for different kinds of attributes.

Continuous attributes

For continuous attributes, such as grades, recovery rates and milling indices, the distance function is defined as

$$d_k(x,y) = |x - y|/s_k, \tag{4.6}$$

where s_k is any measure of dispersion, such as variance, standard deviation, interquartile range (Friedman and Meulman, 2004). The importance of including dispersion is to avoid distortions with different scale values of the attributes. In this paper the standard deviation was used as dispersion measure.

Categorical attributes

For categorical attributes, such as lithology, alteration types and mineralisation styles, the distance function is defined by a distance matrix, which is a symmetric square matrix of size $M \times M$, where M is number of unique values of that attribute. For example, for a categorical attribute taking a set of possible

values $h_1, h_2, \ldots, h_M$, the distance matrix is

$$\begin{bmatrix} 0 & \ldots & \theta_{1j} & \ldots & \theta_{1M} \\ \vdots & 0 & \vdots & \vdots & \vdots \\ \theta_{j1} & \ldots & 0 & \ldots & \theta_{jM} \\ \vdots & \vdots & \vdots & 0 & \vdots \\ \theta_{M1} & \ldots & \theta_{Mj} & \ldots & 0 \end{bmatrix},$$

where each θ_{ij} is a fixed value corresponding to the distance between the value h_i and h_j and $\theta_{ij} = \theta_{ji}, \forall i, j$ as the distance is symmetric.

If the categorical attribute has no preference among values, θ_{ij} can be a constant positive value for all i and $j \in 1, \ldots, M$. For example, when θ_{ij} is 1, the matrix becomes the traditional transformation to indicators, and is equivalent to

$$d_k(x, y) = \begin{cases} 0, & \text{if } x = y \\ 1, & \text{else} \end{cases}. \tag{4.7}$$

The flexibility of the matrix distance function allows for the definition of distance between categorical values, which is very useful for geometallurgical applications since there are, in general, categorical variables related to rock property attributes involved. For example, silication and silicification alterations are more similar compared to silication and argillic alteration. In this case, the distance between silication and silicification alterations should be smaller than that between silication and argillic alterations based on the definition above. The same can be considered in the case of metamorphic rocks, for example, phyllite and schist rocks are more similar compared to slate and gneiss.

The distance for the categorical attribute can be defined as

$$d_k(x, y) = \theta_{h(x)h(y)} / s_k, \tag{4.8}$$

where $h(x)$ denotes the value of the categorical variable x used in the definition of its distance matrix.

Targeted attributes

Another flexibility of the proposed distance function is the option of including a target value in any distance function. There are situations when similarity needs to be defined as closeness to a target value; for example, we could be interested in low, medium and high recoveries. Setting specific low, medium

and high values of recoveries will tend to yield clusters according to those targets. Friedman and Meulman (2004) defined a distance function for one and two targets, t and u, as

$$g_k(x, y, t) = \max(d_k(x, t), d_k(y, t)) \tag{4.9}$$

and

$$g_k(x, y, t, u) = \min\left(g_k(x, y, t), g_k(x, y, u)\right). \tag{4.10}$$

These two metrics are not strictly distance metrics because they violate the identity property, but they work in practice. The problem arises when they are used to compare two values very close to each other. For example, both distances, $g_k(x, y, t)$ and $g_k(x + \epsilon, y, t)$ with $x + \epsilon < y$, are the same, due to the maximisation criterion in Eq. 4.9.

To correct this problem a new criterion for a single target t is defined as

$$g_k(x, y, t) = d_k(x, t) + d_k(y, t) \tag{4.11}$$

and its extension to multiple targets T is given by

$$g_k(x, y, T) = \min(g_k(x, y, t)), \forall t \in T. \tag{4.12}$$

Including the target is applicable to both continuous and categorical distance functions.

4.2.5 Feature selection

In geometallurgy there are, in general, many attributes that can be used for clustering. The contributions of attributes to clustering may vary from very important to little or no importance. It is desirable that the clustering procedure considers the degree of importance of different attributes, which can sometimes be defined by expert knowledge. In this context, feature selection is an important procedure to determine the involvement of attributes and their degree of involvement as part of the clustering process. The most basic method is to consider all permutations of attributes and to select a set which performs the best. This approach obviously is computationally intensive and, as the number of attributes increases, the number of possible permutations increases exponentially. Note that the number of permutations of n attributes without repetitions is $2^n - 1$, which is equal to 1,048,575 permutations for a reasonable case of 20 attributes. On the other hand, forward and backward methods

are greedy methods for feature selection. The forward method starts with one attribute and iteratively adds the attribute that most improves the distance metric. The backward method starts with all variables and removes the least useful attribute one at a time.

Another strategy is based on weights. Each attribute has, as an indicator of its degree of importance, a positive number within the range of $[0, 1]$ as its weight. This weight can then be included in the distance metric as follows

$$D^{(2)}(x, y, w) = \sum_{k=1}^{K} w_k d_k(x_k, y_k), \tag{4.13}$$

where w_k is the weight of the k-feature, subject to $\sum_{k=1}^{K} w_k = 1$.

In the case of clustering, by default all attributes have the same weight in different clusters. In practice, it may be desired in some cases to impose different weights for attributes in different clusters, i.e.,

$$D^{(3)}(x, y, w, c) = \sum_{k=1}^{K} w_{ck} d_k(x_k, y_k), \tag{4.14}$$

where w_{ck} is the weight of the attribute k in the cluster c, subject to

$$\sum_{k=1}^{K} w_{ck} = 1, \forall c. \tag{4.15}$$

This weight-based feature selection mechanism can also be included in the optimisation process to determine the best weights for each attribute in each cluster.

As pointed out by Friedman and Meulman (2004), the best minimisation strategy is to assign all weight to the attribute with the lowest dispersion of observations in each cluster, which provides an incentive to spread the weights to more attributes, the distance is defined as

$$d^{(4)}(x, y, w, c, \lambda) = w_{ck} d_k(x_k, y_k) + \lambda w_{ck} \log(w_{ck}) \tag{4.16}$$

$$D^{(4)}(x, y, w, c, \lambda) = \sum_{k=1}^{K} d^{(4)}(x, y, w, c, \lambda) + \lambda \log(K). \tag{4.17}$$

The parameter λ controls how the weights are spread to other attributes. For larger λ, the weights will tend to be similar for all attributes whereas for smaller λ the weights will tend to be given one or a few attributes.

4.2.6 Spatial correction

Another important characteristic is the spatial structure. Traditional clustering methods do not incorporate any spatial structure. In fact, if coordinates of samples are included as attributes, traditional methods are likely to produce erroneous results as samples in the same cluster are not necessarily spatially connected and these clustering procedures will tend to separate them into different clusters on the basis of their coordinates. Within the geometallurgical context, a cluster (ore parcels with similar geometallurgical characteristics) may be in many sectors not directly spatially connected across the deposit, and therefore a more advanced technique is required for taking the coordinates into account. As one of the goals of geometallurgical clustering is to generate clusters as spatially connected as possible, it is essential to apply a spatial correction to avoid compact zones that include a few observations that belong to a cluster different than that to which the majority belong.

Spatial correction is conceptually similar to image segmentation. In computer vision, image segmentation tries to simplify any image by assigning to each pixel a label (here equivalent to a cluster) from a small set of labels. Image segmentation has been successfully applied for applications such as cancer detection and automated driving (López and Malpica, 2008; Tarabalka and Charpiat, 2013; Tarabalka and Rana, 2014; Wang et al., 2016).

There are many techniques for image segmentation, but the graph cut method (Boykov and Veksler, 2006) is of special interest in this work because it can be integrated easily with fuzzy clustering.

The image segmentation, or labelling, problem can be formulated as an energy minimisation problem in a graph,

$$E(L) = \sum_{p \in I} D_p(L_p) + \sum_{pq \in \mathcal{N}} V_{pq}(L_p, L_q), \tag{4.18}$$

where L_p represents the label of a pixel p of the image I, D_p is the data penalty function, V_{pq} is the interaction potential, or the spatial relationship, and $\mathcal{N}$ is the neighbourhood (spatial connectivity).

Clearly there are some similarities between the image segmentation problem and our proposed clustering method. An image corresponds to the entire deposit whereas a pixel corresponds to an observation and the pixel value corresponds to an attribute of a sample. The fuzzy membership information (Eq. 4.3) of each observation can be interpreted as the data penalty function. This means that each observation has a probability of belonging to a cluster and using $D_p(L_p) = -\log(u_{pL_p})$ assigns a lower data cost when the membership

probability is higher and *vice versa*. The interaction potential V_{pq} corresponds to the spatial relationship among observations.

The neighbourhood can be determined by the k-nearest neighbour in the case of unstructured locations, or the surrounding cells in the case of a regular grid, which defines the connections of data in the form of a graph. Complex interaction potential functions can be formulated in the form of geostatistical (co)variograms or correlograms as defined in Bourgault et al. (1992), but a simpler one is the Potts model, which focuses on discontinuities. The Potts model is defined as

$$V_{pq}(L_p, L_q) = K_{pq} * \begin{cases} 1, & \text{if } L_p = L_q \\ 0, & \text{else} \end{cases}, \tag{4.19}$$

where K_{pq} may be a constant value or the cost of the spatial relationship between p and q, for example, the distance between p and q. The Potts model favors a clearer segmentation among clusters, opposite to smooth transitions, which is desired for domaining.

4.3 Proposed method

Our proposed method, Spatial Weighted Fuzzy Clustering (SWFC), combines two components: (a) an adapted version of fuzzy clustering, termed Weighted Fuzzy Clustering (WFC), and (b) the spatial correction by the graph cut method. Both components are formulated as optimisation problems.

4.3.1 Optimisation formulations

For the proposed fuzzy clustering, the concepts of compactness and separation are combined in a single objective formulation, and they are defined below.

Compactness

$$COMP(m, u, v, w, \lambda) = \sum_{j=1}^{P} \sum_{i=1}^{N} u_{ij}^{m} D^{(4)}(x_i, v_j, w, j, \lambda), \tag{4.20}$$

where λ controls the weight values among attributes. The u matrix is given by

$$u_{ij}^{-1} = \sum_{j'=1}^{P} \sum_{k=1}^{K} \left[\frac{d_k^{(4)}(x_i, v_j, w, j, \lambda)}{d_k^{(4)}(x_i, v_{j'}, w, j', \lambda)} \right]^{2/(m-1)}. \tag{4.21}$$

Separation

$$SEP(m, v, w, \lambda) = \sum_{j=1}^{P} \sum_{j'=1, i \neq j'}^{P} \sum_{k=1}^{K} d_k^{(4)}(v_{ik}, v_{j'k}, \max(w_j, w_{j'}), j, \lambda). \tag{4.22}$$

The maximum criterion in Eq. (4.22) is required because different clusters may not share the same weights, in which case the maximum weight is used for the k^{th} dimension.

Objective

The proposed clustering seeks to minimise compactness of clusters and, at the same time, to maximise separation between clusters. A single objective formulation that incorporates both aims is defined as

$$(v^*, w^*) = \arg\min_{v,w}(COMP(m, u, v, w, \lambda) + \frac{C}{SEP(m, v, w, \lambda)}), \tag{4.23}$$

where C is a constant which scales the importance of separation as a criterion in the optimisation formulation. The lower the value of C, the less important is any increment in separation. Our experiments indicate that a value of $C = 15$ is appropriate to give more relative importance to compactness over separation but we recommend a complete assessment of the impact of different values. Other expressions that combine compactness and separation in a single objective may also be explored.

There are two main obstacles to solving this optimisation problem. The first is the non-convexity of the problem, meaning that the global minimum is hard to find. The second is the difficulty of finding the cluster centroids and defining a proper set of weights that can be used.

The first obstacle can be dealt with by the use of metaheuristics, which is a simple technique to solve optimisation problems with many local optima. The second obstacle is solved by a two-stage procedure in the proposed method. In the first stage, the optimal centroids and membership are found for a given set of fixed weights. In the second stage, the weights are optimised given the clusters and memberships found in the first stage. These two steps are iterated until convergence.

4.3.2 Implementations

We use a genetic algorithm (GA) metaheuristic not only because of its simplicity, flexibility and good performance, but also because GA has been successfully used as an optimisation method for clustering (Maulik and Bandyopadhyay, 2000; Nanda and Panda, 2014; Luchi et al., 2016).

Genetic algorithm

A genetic algorithm is a metaheuristic optimisation method that emulates the process of evolution. There are three main concepts involved in GA: selection, crossover and mutation.

The selection operation imitates the natural selection process in which better individuals have more chances to pass their genes to the next generation. A fitness value is assigned to each individual, which corresponds to the evaluation function to be optimised. Crossover produces new individuals combining the genes of the parents. Mutation produces a new individual by mutating a small part of the gene of an individual. We refer to both operations as generic functions $crossover()$ and $mutation()$ respectively in the description of the algorithms which are problem dependent.

These three operations are executed for many generations to ensure that the best final individual of the population is a good local optimum. A complete tutorial on GA can be found in Whitley (1994).

The hyper-parameters of GA are the number of individuals in the population, the number of generations, the operations of selection, crossover and mutation, and the probabilities of crossover and mutation. Given these hyper-parameters, which depend on the problem to be solved, the GA procedure for minimisation is given by algorithm 1.

The most important design aspect of any GA is the solution codification (genome), which is problem dependent. For a given problem codification, its corresponding crossover and mutation operations must also be defined. In our implementations, the crossover function is the standard uniform crossover. Selection is performed by tournament selection.

GA for optimising centroids

For the first stage discussed above, the problem reduces to finding the cluster centroids that minimise the objective function given in Eq 4.23. Thus, the genome in this case represents the centroids of each cluster.

Algorithm 1: Minimisation by GA

```
Result: best_individual, best_fitness
Data: npop: size of the population, ngen: number of generations
population ← set of random individuals of size npop;
foreach ind ∈ population do
    fitness (ind) ← evaluation(ind);
end
fitness (ind) ← set of random individuals of size npop;
for iteration ← 1 to ngen do
    offspring ← selection(population);
    foreach ind ∈ offspring do
        if rand() < prbcx then ind ← crossover(ind);
        if rand() < prbmut then ind ← mutation(ind);
        fitness (ind) ← evaluation(ind);
        if fitness (ind) < best_fitness then
            best_fitness ← fitness (ind);
            best_individual ← ind;
        end
    end
end
```

The initial centroids are selected from samples at random. The mutation operation perturbs one dimension of one centroid: for continuous variables, the perturbation corresponds to a random value drawn from a normal distribution $\mathcal{N}(\mu = 0, \sigma = 0.1)$, whereas for categorical variables, the perturbation simply selects a different value of their categories at random.

The evaluation function for optimising centroids is given by algorithm 2 and the mutation operator is given by algorithm 3. The function $\dim(A)$ returns the number of the rows and columns of a matrix A.

Algorithm 2: Evaluate clustering criteria for optimising centroids

Result: compactness $+\frac{C}{\text{separation}}$
Data: V: centroids
Parameters: m: the fuzzier, λ: weight strenght, w: weights, C: constant for the contribution of separation

$U \leftarrow$ Equation 4.21;
compactness $\leftarrow$ Equation 4.20;
separation $\leftarrow$ Equation 4.22;

Algorithm 3: Mutation for finding centroids

Result: mutated V
Data: V: centroids
Parameters: C: set of categorical values for the attribute k
$P, K \leftarrow dim(V)$;
$j \leftarrow randint(1, P)$;
$k \leftarrow randint(1, K)$;
if *attribute k is continuous* **then** $V[j,k] \leftarrow V[j,k] + randnorm(0, 0.1)$;
else $V[j,k] \leftarrow$ select at random from $C - V[j,k]$;

GA for optimising weights

In the second stage, the weights are optimised with fixed centroids, and the problem reduces to finding the weights that minimise the objective function given in Eq. 4.23.

As the weights are within the range $[0, 1]$, the mutation adds a small number drawn from the normal distribution, $\mathcal{N}(\mu = 0.0, \sigma = 0.01)$. Two integer numbers are selected at random, one for a cluster and the other for an attribute to modify.

Note the weights must sum to one. In addition, if there is expert knowledge to set a specific weight to an attribute, the perturbation can preserve these values.

The optimisation of weights is given by algorithm 4 and mutation operator by algorithm 5.

Algorithm 4: Evaluate clustering criteria for optimising weights

Result: $\mathsf{compactness} + \frac{C}{\mathsf{separation}}$
Data: W: weights
Parameters: m: the fuzzier, λ: weight strenght, V: centroids, C: constant for the contribution of separation
$U \leftarrow$ Equation 4.21;
$\mathsf{compactness} \leftarrow$ Equation 4.20;
$\mathsf{separation} \leftarrow$ Equation 4.22;

Proposed clustering method (SWFC)

The final proposed method is shown in the algorithm 6 and the spatial correction is given by algorithm 7.

Algorithm 5: Mutation for optimising weights

Result: mutated W
Data: W: weights
$P, K \leftarrow dim(W)$;
$j \leftarrow randint(1, P)$;
$k \leftarrow randint(1, K)$;
$W[j,k] \leftarrow W[j,k] + randnorm(0, 0.01)$;
//Normalisation
$W[j] = W[j] / \sum_{k=1}^{K} W[j,k], \forall j$;

Algorithm 6: Spatial Weighted Fuzzy Clustering

Result: *clusters*: clusters assigned to each sample, U: membership matrix, V: centroids, W: weights,
Data: *locations*: coordinates of observations, *samples*: multivariate attributes of observations, P: number of clusters
Parameters: m: the fuzzier, λ: weight strength, V: centroids, C: constant for the contribution of separation,
//N samples of K attributes
$N, K \leftarrow dim(samples)$;
//start with uniform weights on all attributes
$CurrentW \leftarrow ones(P, K)$;
$CurrentW \leftarrow CurrentW / K$;
repeat
  //stage1
  $V \leftarrow$ OptimiseCentroids$(CurrentW, samples, P, C)$;
  //stage2
  $W \leftarrow$ OptimiseWeights$(CurrentW, V, m, C)$;
  $CurrentW \leftarrow W$;
until $\sum |W - CurrentW| < \epsilon$;
//Spatial correction
$clusters \leftarrow$ SpatialCorrection$(locations, U)$;

Algorithm 7: Spatial Correction by graph cut method

Result: *clusters*: clusters assigned to each sample
Data: U: membership matrix, *locations*: coordinates of observations,
//N samples and P clusters
$N, P \leftarrow dim(U)$;
//Use K-Nearest-Neighbour or regular grid
edges $\leftarrow$ BuildNeighbourhood(*locations*);
//Data penalty is lower for higher probabilities and higher for lower probabilities
$D \leftarrow -\log(U)$;
//Interaction potential by Potts model
for $i \leftarrow 1$ **to** P **do**
  for $j \leftarrow 1$ **to** P **do**
    if $i = j$ **then** $V[i, j] \leftarrow 0$;
    else $V[i, j] \leftarrow 1$;
  end
end
clusters $\leftarrow$ GraphCut(edges,D,V);

The function BuildNeighbourhood$(locations)$ returns the edges of the spatial structure of the *locations*. The spatial structure can be defined using Delaunay tessellation, k-nearest neighbour, or the surrounding blocks in a structured block model.

Efficiency and scalability

The efficiency of SWFC relies mainly on its two components, the optimisation of the centroids and weights and the spatial correction by the graph-cut method.

When the centroids are optimised, GA calculates, for each individual, the membership matrix, separation and compactness. The complexity of the calculation of the membership matrix is $\mathbf{O}(N * P^2)$, separation is $\mathbf{O}(N * P * K)$, and compactness is $\mathbf{O}(K * P^2)$. As usually $N \gg K$ and assuming that $K > P$, an upper bound for the complexity of the evaluation of each individual is $\mathbf{O}(N * P * K)$.

The GA algorithm needs to evaluate $npop$ individuals over $ngen$ generations, therefore, the total complexity of the WFC algorithm is $\mathbf{O}(N * P * K * npop * ngen)$. Our results indicate that WFC converges in less than 20 iterations (main loop in algorithm 6).

The complexity of the graph-cut algorithm used is $\mathbf{O}(N * P^2)$ (Boykov and Veksler, 2006).

The complexity of the fuzzy clustering is comparable to the K-Means algorithm at each iteration, but the difference is in the optimisation procedure, where SWFC is more computational intensive. Nevertheless, it overcomes two aspects: the use of GA helps in escaping from local minima and both fuzzy clustering and feature selection are jointly optimised.

The complexity of SWFC does not have a high impact on the number of samples N, since it scales linearly as a function of N. Also, P is usually small for practical reasons (no greater than 10) and K is, in general, less than 100.

GA is a stochastic optimisation method and the results may be affected by the initial random seed. Our experiments showed that different seeds produce very stable results. All results reported are based on a single, representative run.

Assessing the number of clusters

There is no common choice for the number of clusters and this selection largely depends on the data and the application of the clusters. However, there are several indices that can be used to assess the cluster quality. The silhouette index (SI) (Eq. 4.24) comprises compactness and separation (Rousseeuw, 1987). This index is a real number in the range [-1,1]. An index close to -1 means there is little or no cluster structure and close to 1 indicates perfect compactness within clusters and clear separation between clusters. This index uses only the distance among observations.

$$SI = \frac{1}{N}\sum_{k=1}^{N} SI_k \tag{4.24}$$

and

$$SI_k = \frac{1}{N}\sum_{i=1}^{N}((b_i - a_i))/(\max(b_i - a_i)), \tag{4.25}$$

where N is the total number of points, a_i is the average distance between point i and all other points in its own cluster and b_i is the minimum of the average distances between i and points in other clusters.

Another index for assessing the quality of clusters is the Davies-Bouldin index (DBI), which describes how well the clustering has been done as measured by the distance between observations and cluster centroids. Values of this index close to 0 suggest better cluster structures (Davies and Bouldin, 1979). DBI

is calculated using the following equations:

$$DBI = \frac{1}{P}\sum_{i=1}^{P} D_i \tag{4.26}$$

$$D_i = \max(R_{ij}),\ i = 1,\ldots,P, j = 1,\ldots,P \tag{4.27}$$

$$R_{ij} = \frac{T_i + T_j}{M_{ij}} \tag{4.28}$$

$$M_{ij} = \left(\sum_{k=1}^{K} |v_{ik} - v_{jk}|^p\right)^{1/p} \tag{4.29}$$

$$T_i = \left(\frac{1}{S_i}\sum_{j=1}^{S_i} |x_j - v_i|^p\right)^{1/p} \tag{4.30}$$

with $p = 2$ for the Euclidean norm.

4.4 Application

We present three examples to demonstrate the application of the proposed method. The first example is a simple synthetic case that illustrates the difficulties of traditional methods when clustering using different attributes. The second example is a cross-section of a simulated copper porphyry deposit (Garrido et al., 2017). The third example is a full synthetic geometallurgical block model (Lishchuk, 2016).

The results of K-Means and PCA clustering methods are compared. The spatial correction also is applied to K-Means and PCA, using the membership matrix as the inverse of the squared distance between each sample to the centroids

$$u_{ij} = \frac{1/\left\|x_i - v_j\right\|^2}{\sum_{j'=1}^{P} 1/\left\|x_i - v_{j'}\right\|^2}. \tag{4.31}$$

K-Means and PCA with spatial correction are denoted by SK-Means and SPCA respectively.

Table 4.1 shows the values of the parameters used in the algorithms for the three examples.

TABLE 4.1: Parameters used in the algorithms

Parameter	Value	Observation
npop	100	Population size
ngen	100	Number of generations
prbcx	0.8	Probability of crossover
prbmut	0.4	Probability of mutation
Tournament size	9	9 individuals used in the tournament selection
λ	0.25	Weight strength
m	2.0	Fuzzier
C	15	Constant for the contribution of separation

TABLE 4.2: The design of four clusters based on combination of Cu, Fe, Au and Rec

Attribute	Default	C1 (red)	C2 (blue)	C3 (green)	C4 (yellow)
Cu	$\mathcal{N}(0.68, 0.3)$	$\mathcal{N}(0.8, 0.05)$	$\mathcal{N}(0.9, 0.05)$	$\mathcal{N}(0.4, 0.05)$	
Fe	$\mathcal{N}$(2.56,1.15)		$\mathcal{N}$(1.5,0.1)	$\mathcal{N}$(1.2,0.1)	$\mathcal{N}$(4.0,0.1)
Au	$\mathcal{N}$(21.5,11.08)	$\mathcal{N}$(30.0,1.0)	$\mathcal{N}$(15.0,1.0)		$\mathcal{N}$(40.0,1.0)
Rec	$\mathcal{N}$(81.43,6.04)	$\mathcal{N}$(88.0,1.0)		$\mathcal{N}$(70.0,2.0)	

4.4.1 Illustrative example

In this example, there are four attributes: grades of copper, gold and iron, and recovery of copper, denoted as Cu, Au, Fe and Rec respectively. Although these attributes do not usually follow normal distributions, for the sake of simplicity, they were taken from normal distributions, but their means and standard deviations are different so as to form four clusters, see Table 4.2.

All attributes follow their default normal distributions but for specific clusters, they follow normal distributions with different means and lower variances. Cluster 1 includes only Cu, Fe and Rec; cluster 2: Cu, Fe and Au; cluster 3: Cu, Fe, Rec; and cluster 4 only Fe and Au.

A spatial component was assigned to each cluster: half of cluster 1 is uniformly located in the region of $[(10.0 - 35.0), (10.0 - 35.0)]$ and the other half in $[(65.0 - 85.0), (65.0 - 85.0)]$; all of cluster 2 is located uniformly in the region of $[(0.0 - 100.0), (30.0 - 70.0)]$; all of cluster 3 is located uniformly in the region of $[(5.0 - 45.0), (65.0 - 100.0)]$; and finally, cluster 4 is located uniformly in $[(55.0 - 100.0), (0.0 - 35.0)]$.

The illustrative example comprises 200 samples of cluster 1, 200 samples of cluster 2, 400 samples of cluster 3, and 100 samples of cluster 4. Of these 900 samples, the locations of 100 samples are randomised uniformly for the entire region of $[(0.0 - 100.0), (0.0 - 100.0)]$. Figure 4.1 shows the final locations of all samples.

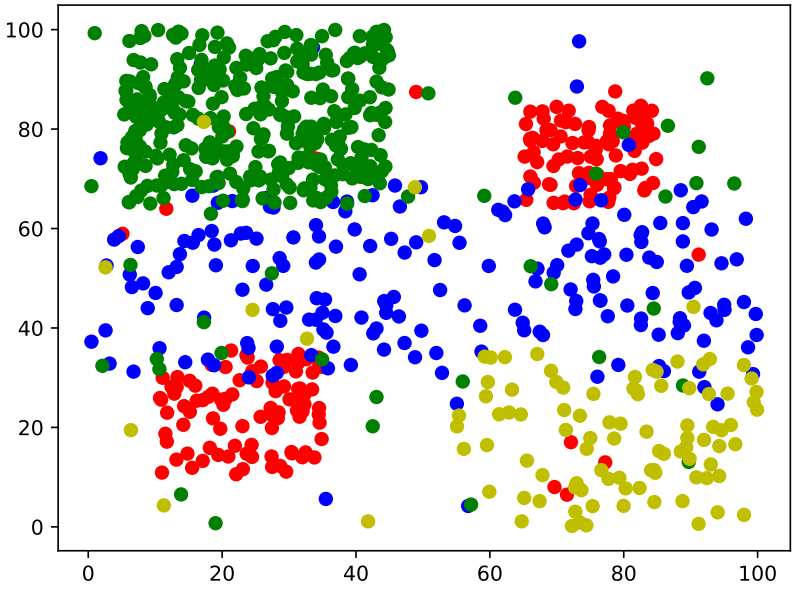


FIGURE 4.1: Scatter plot of true four clusters

TABLE 4.3: Davies-Bouldin and Silhouette indices of K-Means, PCA, and WFC for different number of clusters

Clusters	K-Means		PCA		WFC	
	DBI	SI	DBI	SI	DBI	SI
2	0.852	0.504	1.026	0.496	0.234	0.802
3	0.819	0.537	0.801	0.537	0.306	0.776
4	0.974	0.427	0.818	0.520	0.185	0.866
5	0.907	0.452	0.856	0.442	1.771	0.577
6	0.923	0.439	0.931	0.426	1.231	0.600

In this example, the number of clusters is known and therefore, the example can be used to assess the efficacy of different clustering methods. Both K-Means and PCA perform better with three clusters, although PCA has similar results with four clusters. The proposed method, with or without spatial correction, significantly outperforms K-Means and PCA in finding the correct number of clusters (Table 4.3).

Using four clusters, the performance of different clustering methods can be further assessed. The imposed spatial structure and added noise make it difficult for the K-means clustering method to reproduce four clusters (Fig. 4.3A). The poor performance of the K-means method is clearly shown in the figure in which green and blue clusters are correctly identified but the other two clusters are not. In addition, the importance of different attributes is not identified. For example, the Cu attribute is well clustered (good separation and low variance) across all clusters (see Fig. 4.2A) despite the fact that no Cu

TABLE 4.4: Explained variance of PCA components

Component	Explained variance (%)
1	53.55
2	30.14

dependency is imposed in cluster 4 (Table 4.2).

PCA overcomes some of the problems of K-Means. Two components were used. Table 4.4 depicts the contribution of each component to the total variance. When the data are projected, and therefore compressed to only two dimensions, the cluster structure can be clearly seen by visual inspection (Fig. 4.5). Despite the obvious cluster structure, PCA clustering performs better than K-Means but clusters 1 and 4 are still misclassified to some extent (Fig. 4.4).

There are two hyper-parameters that need to be defined to apply SWFC: the fuzzier m and the parameter λ for weights. Most cases reported in the literature suggest that a value of 2.0 for m is a reasonable choice to account for uncertainty (Pal and Bezdek, 1995; Ren et al., 2016), and $m = 2.0$ is used in all applications of SWFC discussed in this paper. For parameter λ, there is no rule of thumb guidance in the literature. A small value close to 0 means that all weight will be assigned to one attribute, while a large value will tend to assign the same weights to all attributes. For this example, the influences of different λ values between 0.05 and 1.0 on the weights assigned to different attributes are shown in Fig. 4.6. This figure is useful for assessing the impact of λ on the number of attributes that are considered significant for finding the cluster structure so that an appropriate λ value can be selected. For this example, a value of 0.25 was selected for λ because it tends to give importance to two or three attributes for clustering, which matches the number used to create the clusters in the first place.

The spatial correction was also applied to the three clustering algorithms, K-Means, PCA and WFC, to compare the effect of this correction. The spatial correction applied to K-Means results in the loss of cluster 1 (Fig. 4.4B), due to its weak membership values, which are reassigned to cluster 4 (Fig. 4.3B). Although the correction improves PCA compared to K-Means, its performance remains the same as WFC (Fig. 4.3E). The spatial correction applied to PCA gives results that are similar to SWFC (Fig. 4.4 D and F). WFC is impressively exact, even identifying the correct clusters for the randomly located observations. The performance of SWFC slightly decreases but it still significantly outperforms SK-Means (Fig. 4.4 B and F). The spatial correction alters the final

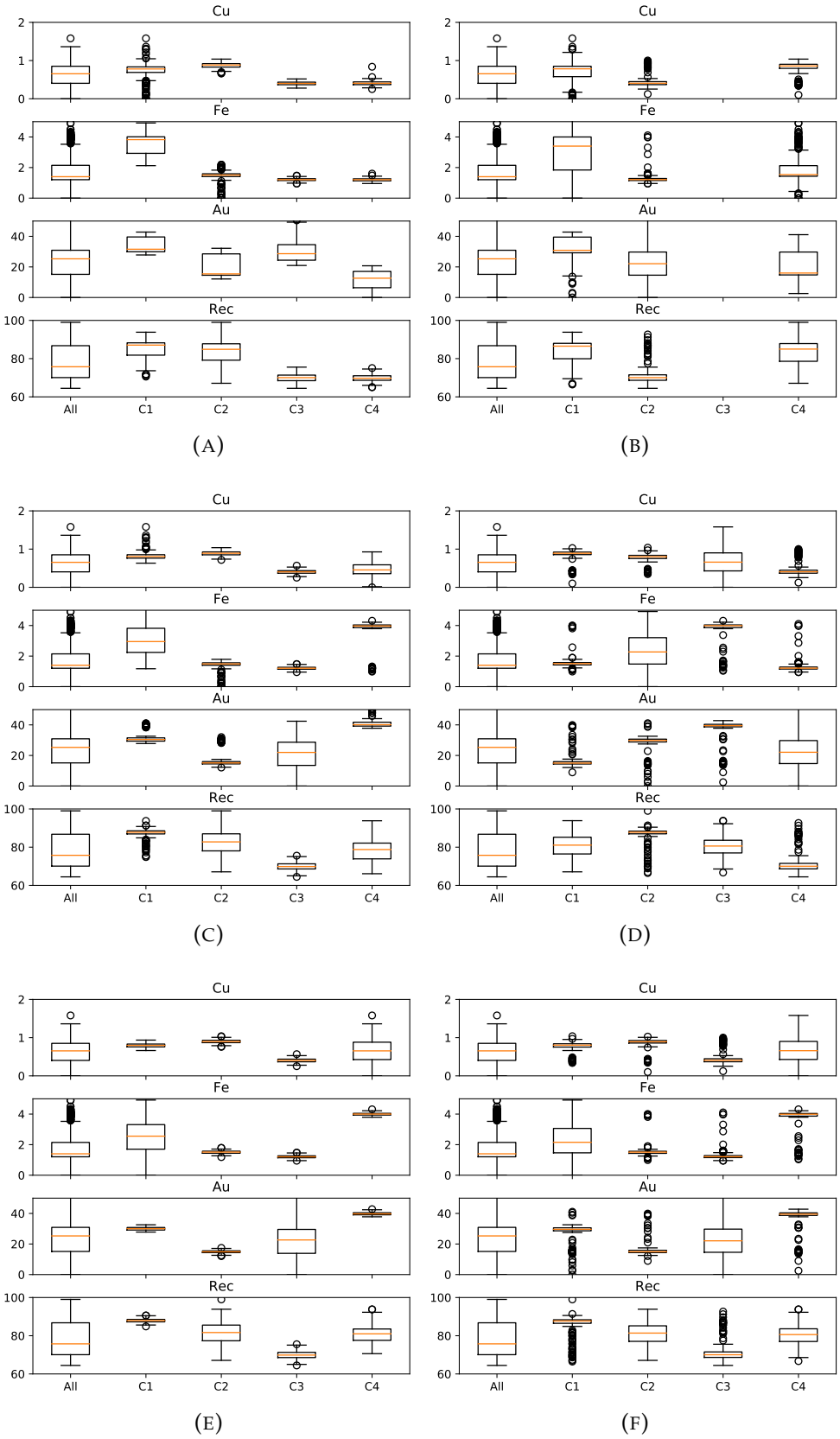


FIGURE 4.2: Boxplots of all attributes in clusters found by (A) K-Means, (B) SK-Means, (C) PCA, (D) SPCA, (E) WFC, and (F) SWFC. Attributes from top to down are Cu, Fe, Au and Re

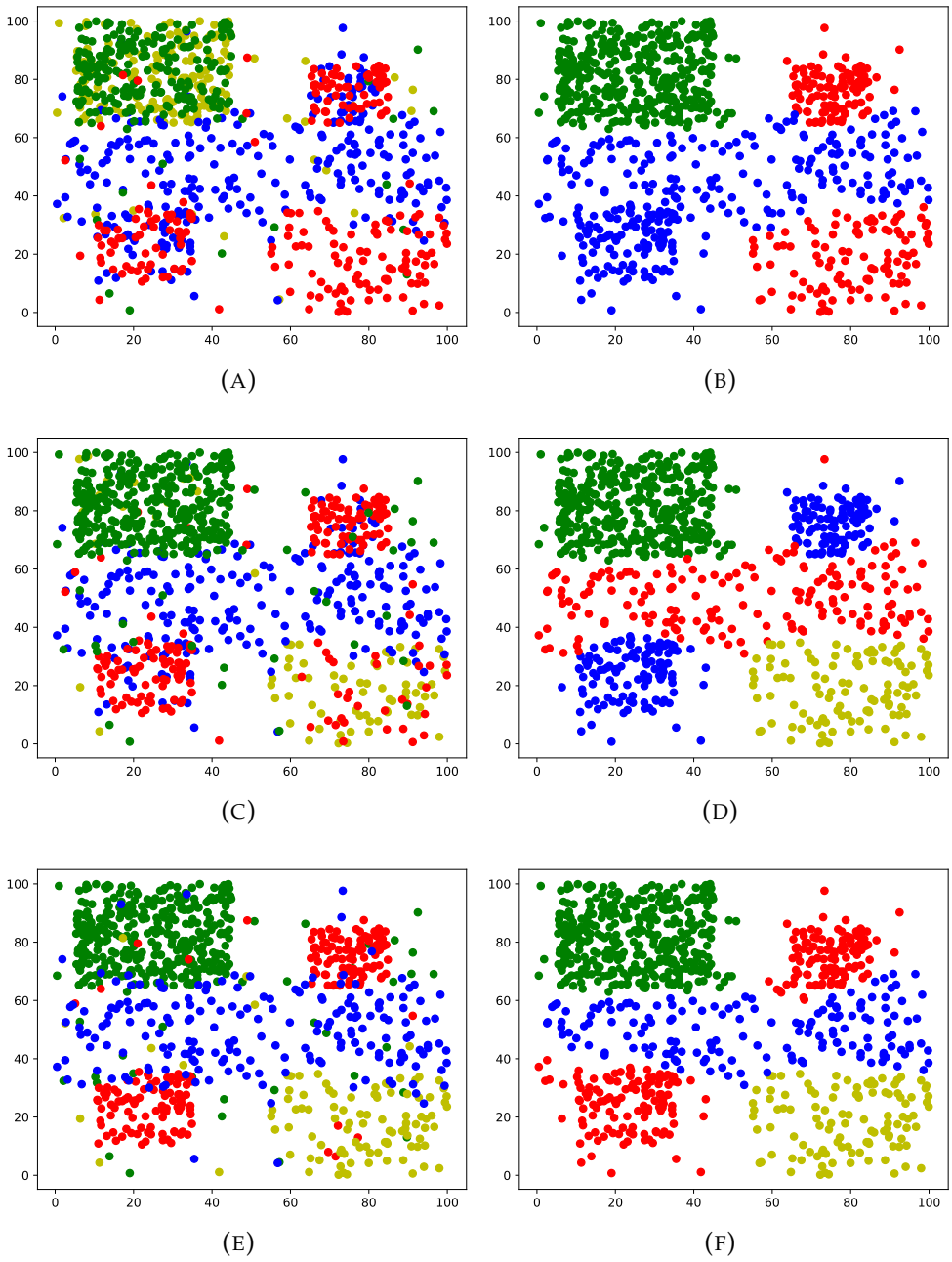
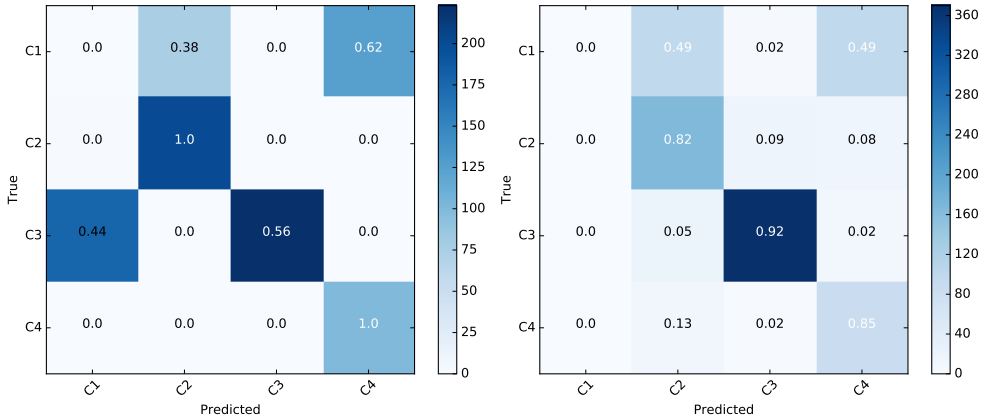
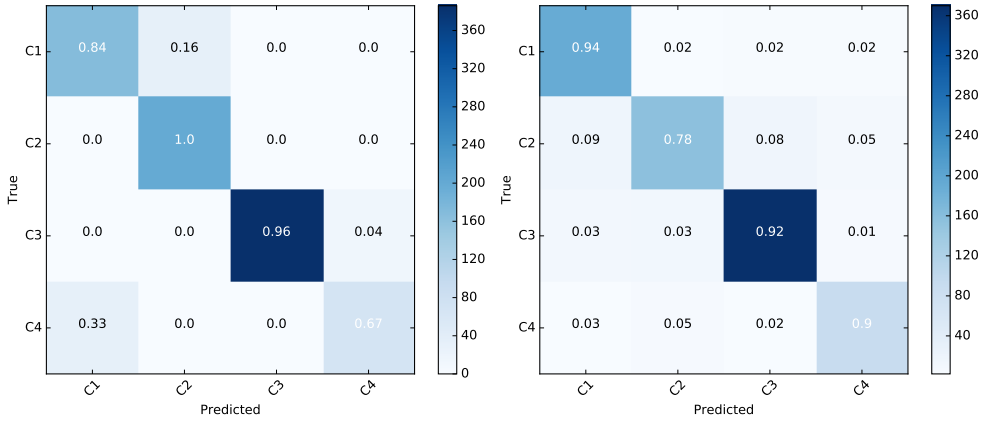


FIGURE 4.3: Scatter plot of clusters found by (A) K-Means, (B) SK-Means, (C) PCA, (D) SPCA, (E) WFC, and (F) SWFC



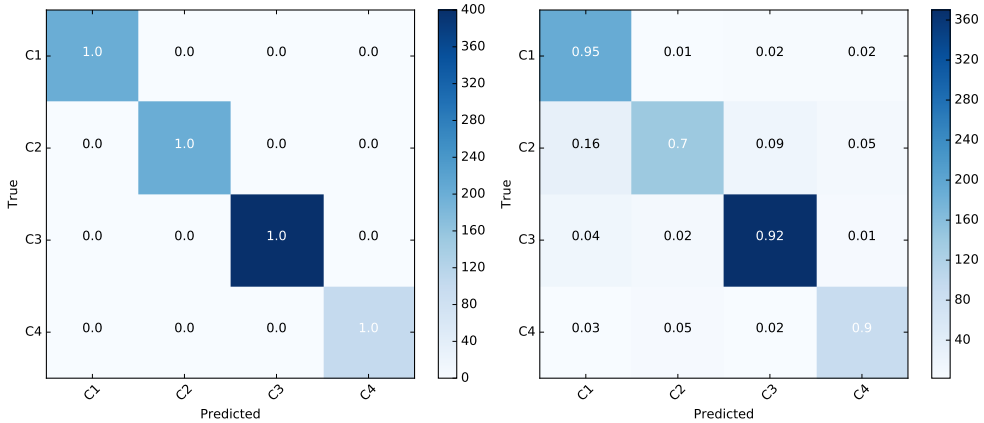
(A)

(B)



(C)

(D)



(E)

(F)

FIGURE 4.4: Confusion matrix of clusters found by (A) K-Means, (B) SK-Means, (C) PCA, (D) SPCA, (E) WFC, and (F) SWFC

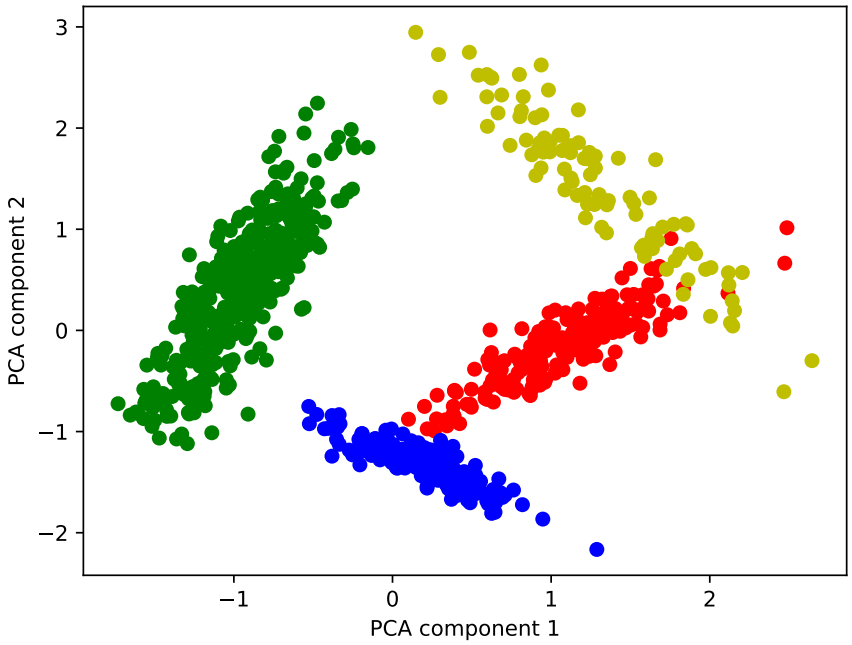


FIGURE 4.5: Projection on first and second principal components of PCA

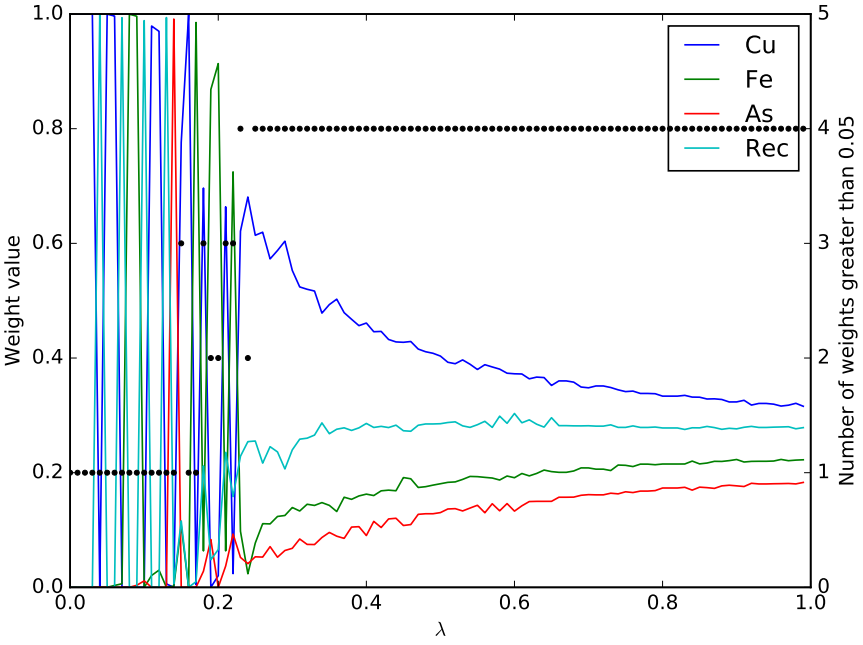


FIGURE 4.6: Weights (left y-axis) of the four attributes for different values of λ (x-axis). The black points indicate the number of weights greater than 0.05 (right y-axis) at each value of λ

TABLE 4.5: Explained variance of PCA components

Component	Explained variance (%)
1	53.15
2	17.13
3	14.50

cluster membership of only a few observations in order to make the clusters more spatially compact (Fig. 4.4F). The boxplots for WFC and SWFC show no substantial difference in their performance statistics (Fig. 4.2 E and F).

This simple illustrative example clearly shows that traditional methods struggle to find the cluster structure correctly when those clusters are defined by different attributes. The proposed method significantly outperforms the traditional methods and can perfectly reveal the cluster structure in this case as well as producing compact clusters in terms of spatial connectivity.

4.4.2 Simulated copper porphyry deposit example

This example is a simulated deposit based on actual data from a copper porphyry deposit (Garrido et al., 2017). The orebody is mainly dominated by disseminated chalcopyrite and with four categories of large, moderate, small and minimum presence of clay. A cross-section, comprising 6,462 blocks is used to illustrate the results of SWFC in two dimensions. The first level clustering results in 4,268 blocks of waste and 2,194 blocks of ore. The ore cluster has two grade elements (copper and arsenic), two response attributes (copper recovery and bond index), and one categorical attribute (presence of clay in low, medium and high degree). SWFC is applied to the ore super-cluster to find four sub-clusters using these 5 attributes. For PCA clustering, three principal components were used. Table 4.5 depicts the explained variance of each component of the total variance.

Cluster 1 is characterised by high content of clay (category 2), low grade values of copper and arsenic (detection limit of 20 for arsenic), and low recovery due to the clay content and low hardness. Cluster 2 is characterised by medium content of clay (category 1), low grade values of copper and arsenic, and slightly higher recovery. Interestingly, SWFC has identified two additional clusters for low content of clay (cluster 3 and 4), which are characterised by high recovery and high bond index but are well separated by arsenic content (low and high), see Table 4.6.

Table 4.7 lists the weights assigned to different attributes in SWFC, which effectively shows the degree of importance of each attribute for each cluster.

TABLE 4.6: Centroids of the four clusters found by SWFC

Cluster	Clay	Copper	Arsenic	Recovery	Bond index
1	2	0.436	20.00	76.48	10.65
2	1	0.454	20.00	83.03	12.70
3	0	0.968	63.34	94.11	16.04
4	0	0.780	20.00	94.98	16.49

TABLE 4.7: Weights of the four clusters found by SWFC

Cluster	Clay	Copper	Arsenic	Recovery	Bond index
1	0.5275	0.0971	0.3152	0.007	0.0533
2	0.4017	0.1102	0.3877	0.0357	0.0647
3	0.5159	0.0241	0.0034	0.2786	0.1780
4	0.4595	0.0118	0.2403	0.2039	0.0846

Clay content is the most important attribute for all clusters, which is consistent with the copper recovery performance and hardness as high clay content is related to low copper recovery and softer rocks. The second most relevant attribute differs for different clusters. Arsenic content is more relevant for clusters 1, 2 and 4, whereas recovery is for cluster 3. One interpretation is that SWFC was capable of separating clusters 3 and 4 in terms of arsenic attribute although both have low clay content.

Fig. 4.7 shows the statistics of the four most relevant attributes for K-Means, PCA and WFC. Clay content is well separated, but K-Means separates clays in a different way. The clusters found by PCA and WFC look very similar, except for the size of cluster 3. For all methods, copper grade is split into two main groups: low and high. High content of arsenic is very relevant for cluster 3 in both PCA and WFC, whereas recovery is well separated among clusters. In general, PCA and WFC perform similarly and both are superior to K-Means.

The spatial connectivity of the clusters is another important aspect for SWFC. The results in terms of spatial connectivity for SK-Means, SPCA, and SWFC are shown in Fig. 4.8. SK-Means does not preserve cluster 2 (Fig. 4.8 A and B) and SPCA does not preserve cluster 4 (Fig. 4.8 C and D) due to the poor connectivity of the clusters. For WFC, there are several blocks in cluster 4 (blue) that are spatially unconnected (Fig. 4.8E); the spatial correction generates much more spatially compact clusters (Fig. 4.8F), which is a desirable property achieved by the proposed method.

This simple two-dimensional case study illustrates the power of SWFC to produce compact and well separated clusters while preserving their spatial connectivity. It does so by selecting the appropriate attributes relevant for the

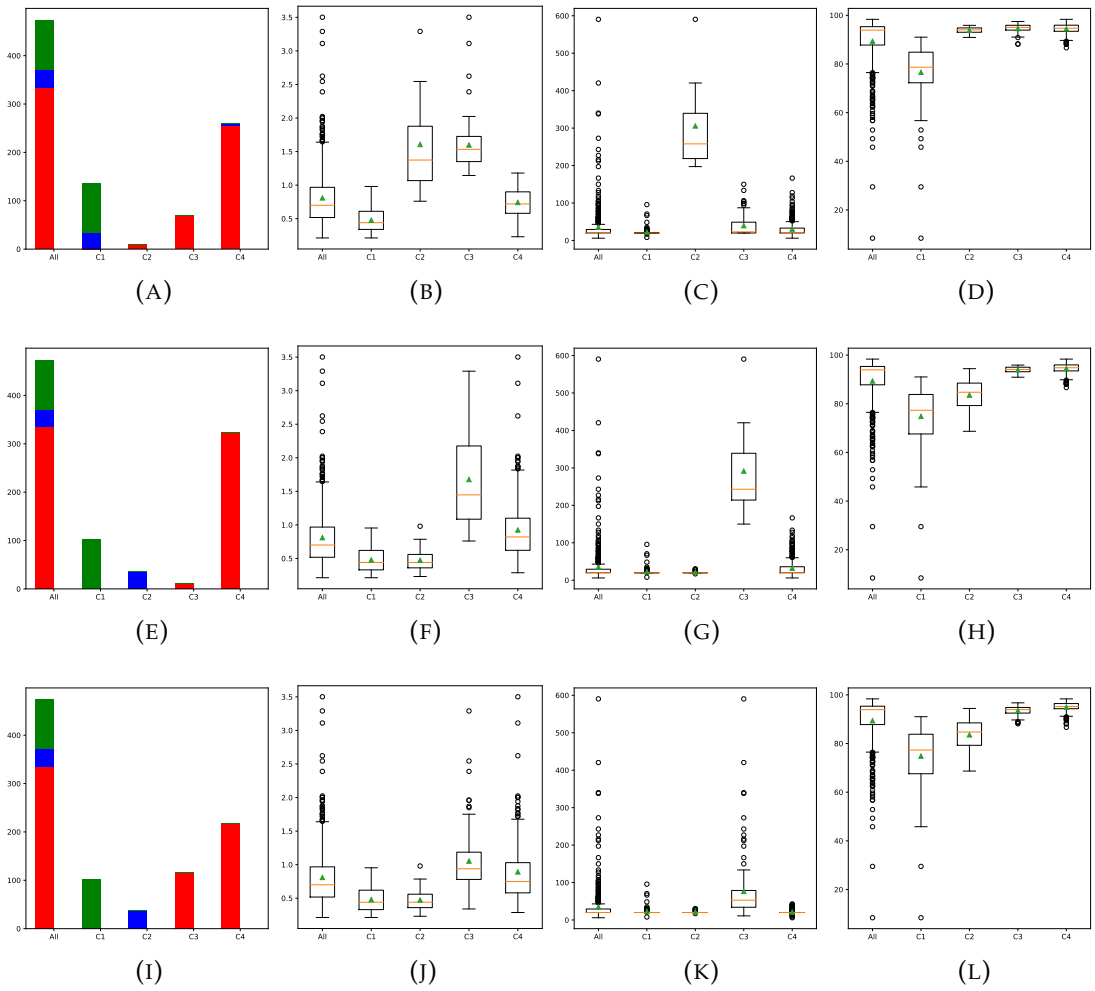
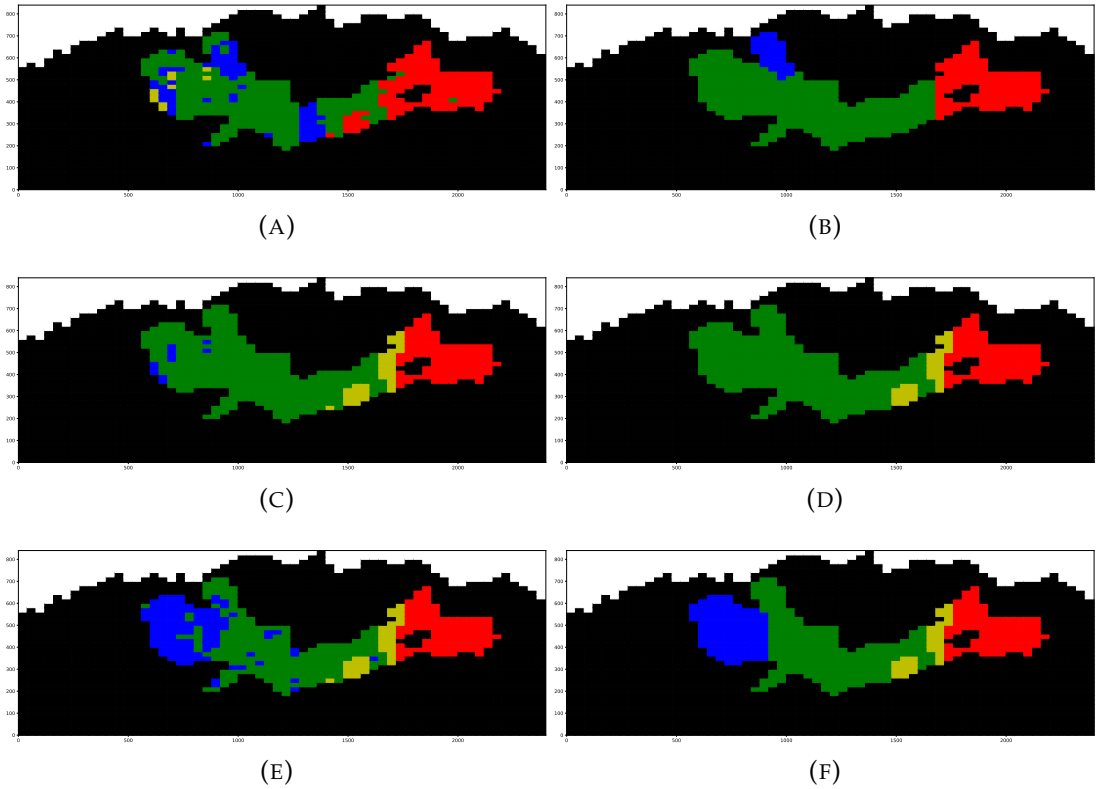


FIGURE 4.7: Statistics of the four most relevant attributes for all observations and for the four clusters by (A-D) K-Means, (E-H) PCA, and (I-L) WFC. Attributes are from left to right: clay content, copper, arsenic, and recovery



(A) (B)

(C) (D)

(E) (F)

FIGURE 4.8: Map of (A) K-Means, (B) SK-Means, (C) PCA, (D) SPCA, (E) WFC, and (F) SWFC. Black represents waste rock. Red, Yellow, Green and Blue represent the four clusters

cluster structure using the optimisation technique discussed above. The resulting clusters can then be much more effectively used for scheduling. Taking into account the characteristics of each cluster, for example, the scheduler may avoid too many jumps between different clusters in order to derive sets of blocks with similar characteristics to be delivered to the plant for a particular time period.

4.4.3 Simulated geometallurgical block model example

This geometallurgical block model was built based on the Malmberget iron deposit in northern Sweden using simulation modules for geology, sampling, production and mining economics. The complete methodology used to build this geometallurgical block can be found in (Lund et al., 2015; Lishchuk, 2016).

This geometallurgical model has $50 \times 50 \times 50$ number of blocks of size $5 \times 5 \times 5$m, where 21,710 of them are ore blocks. The 23 attributes used for clustering are: lithology, 6 mineral grades, 14 chemical element grades, specific gravity, and iron recovery (Table 4.8).

In this example, we are interested in building geometallurgical domains for iron recovery. Lithology should play an important role in clustering, but lithology alone in this case is not sufficient to discriminate iron recovery.Finding the other attributes that can contribute to a better identification of clusters is very important.

We illustrate the flexibility of SWFC by setting the objective as achieving a geometallurgical domaining for Fe recovery. To do so, we use the targeted distance for iron recovery with the values at 15%, 50% and 85% percentiles in its distribution, corresponding to recovery values of 82.41%, 88.98% and 91.22% respectively, and use a weight of 15% for the recovery attribute. These conditions provide a guide for SWFC to find three clusters. The purpose of imposing the target and weight to Fe recovery is to find which secondary attributes would be useful for clustering the structure as we can expect that clusters thus found will tend to have Fe recovery values close to the defined targets.

The number of clusters is set to three according to both DBI and SI values (Table 4.10). For PCA clustering, three principal components were used. Table 4.9 depicts the explained variance of each component of the total variance.

The results for apatite, magnetite, iron, iron recovery, and rock type are used to compare the performance of the clustering methods.

Some interesting observations can be made about the centroids of the three clusters (Table 4.11). The targeted distance applied to iron recovery is very

TABLE 4.8: Attribute descriptions of the geometallurgical block model

Type of Attribute	Attributes	Observation
Rock properties	Lithology, Specific gravity	Lithology codes: 1: Semi-massive ore. Feldspar rich dominated with albite. 2: Massive ore. Amphibole dominated with minor apatite and biotite. 3: Massive ore. Apatite dominated with minor Amphibole.
Mineral groups	Magnetite (Mgt), Hematite (Hem), Albite (Ab), Actinolite (Act), Apatite (Ap), Biotite (Bt)	Fe minerals: magnetite and hematite. Gangue: albite, actinolite, Apatite and biotite. Actinolite has some recoverable content of Fe.
Chemical elements	O, F, Na, Mg, Al, Si, P, Cl, K, Ca, Ti, V, Mn and Fe	
Processing	Iron recovery	Recovery in magnetic separation process

TABLE 4.9: Explained variance of PCA components

Component	Explained variance (%)
1	50.51
2	24.65
3	12.26

TABLE 4.10: DBI and SI of K-Means, PCA, and WFC for different number of clusters

Clusters	K-Means		PCA		WFC	
	DBI	SI	DBI	SI	DBI	SI
2	0.98	0.50	1.05	0.46	0.53	0.69
3	0.95	0.39	1.38	0.33	0.48	0.71
4	0.96	0.44	0.97	0.43	0.63	0.61
5	1.20	0.43	1.27	0.41	1.00	0.53
6	1.21	0.42	1.38	0.41	1.56	0.42
7	1.24	0.41	1.28	0.39	2.57	0.44
8	1.36	0.40	1.27	0.31	2.59	0.36
9	1.34	0.32	1.38	0.30	4.13	0.36
10	1.41	0.32	1.32	0.30	6.40	0.29

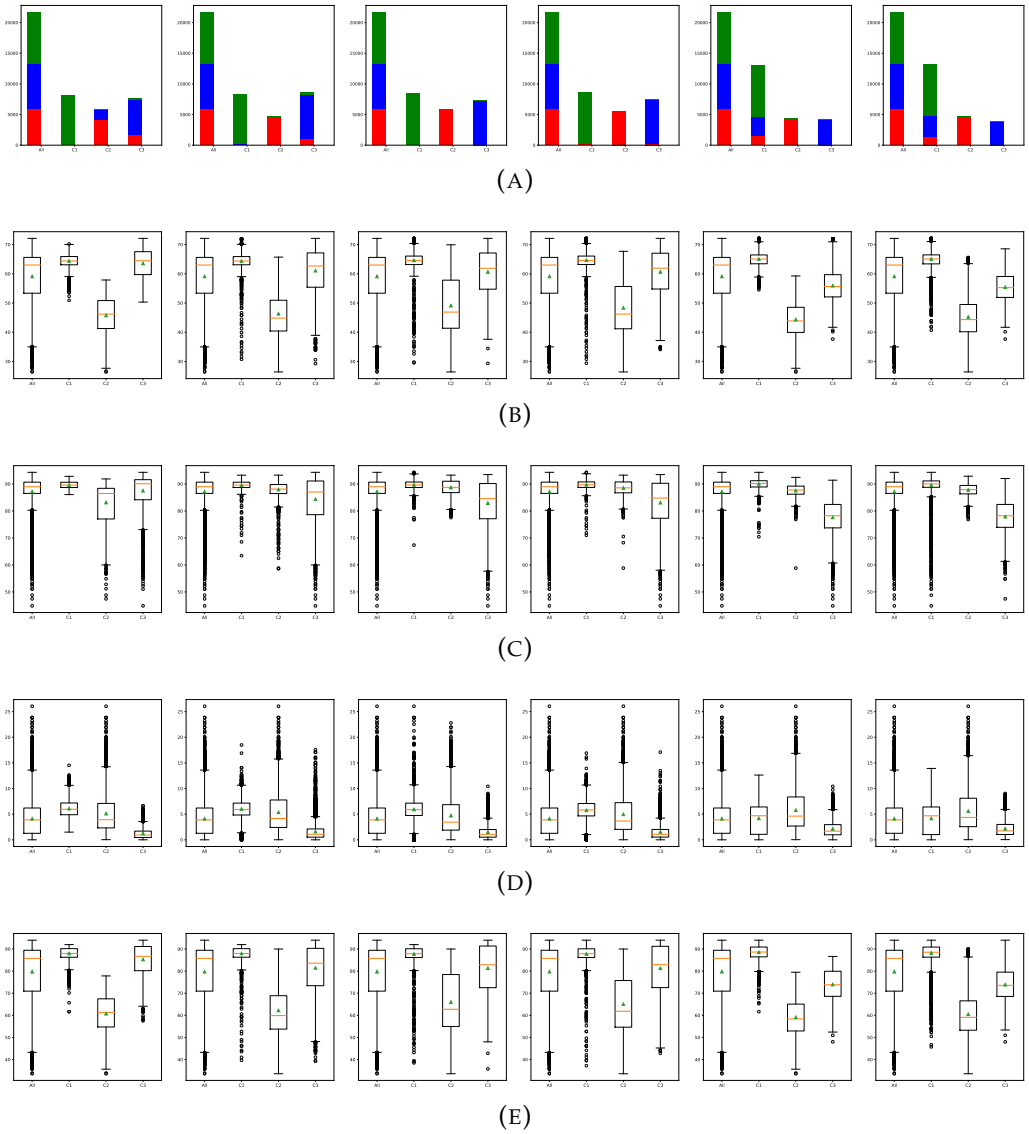
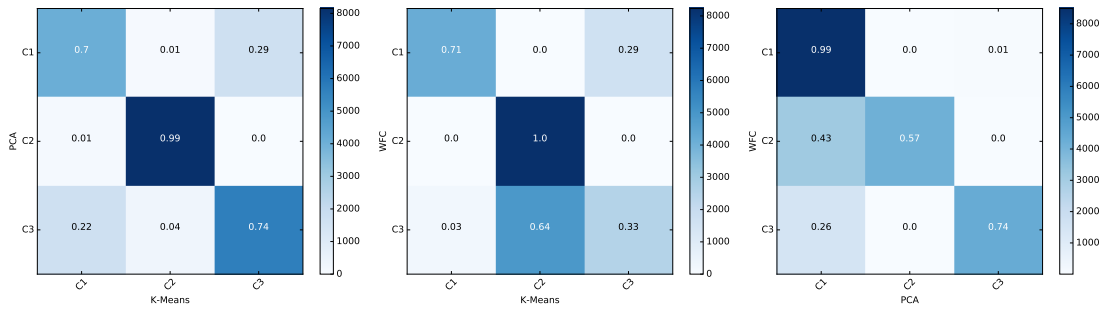


FIGURE 4.9: Distribution of (A) Lithology, (B) Fe, (C) Fe recovery, (D) Apatite, and (E) Magnetite. Clustering methods from left to right are: K-Means, SK-Means, PCA, SPCA, WFC and SWFC

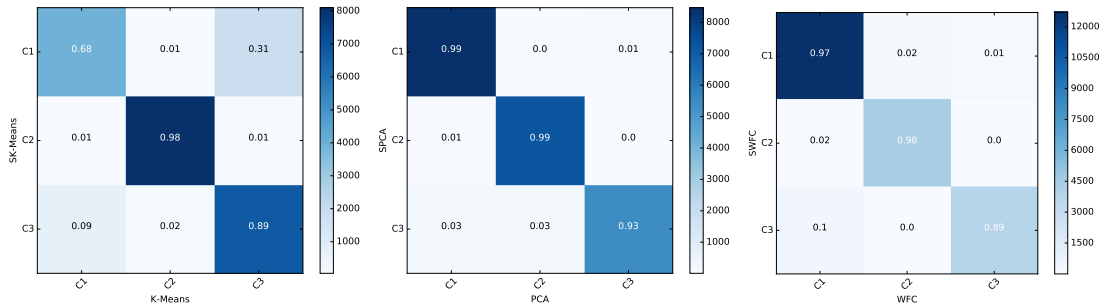
well represented by the SWFC method, but not so by SK-Means and SPCA because they do not use targeted distance functions. Lithology is also well discriminated and the positive correlation between apatite and iron recovery is maintained. Apatite is separated only as low content for cluster 3 in SWFC, whereas SK-Means and SPCA do not separate apatite to the same extent in cluster 3 but are similar for clusters 1 and 2. The centroids of the three clusters for Iron grade show a similar separation for the three methods.

Figure 4.9 shows the statistics of the six clustering methods. SPCA separates each lithology into each cluster as does SK-Means. SWFC clusters lithology in a different way, for example, cluster 1 contains the three lithologies, but clusters 2 and 3 contain only lithology 1 and 3 respectively. This difference may be explained by the fact that WFC and SWFC seek the imposed targets for iron recovery.

A summary of the differences of clustering among K-Means, PCA and WFC is given in Fig. 4.10A. K-Means shows some differences compared to PCA and WFC, while PCA and WFC are very similar in performance (Fig. 4.10B).



(A)



(B)

FIGURE 4.10: (A) Pairwise cluster discrepancy between K-Means, PCA and WFC. (B) Pairwise cluster comparison between each clustering method before and after spatial correction

This case study of a complete three-dimensional geometallurgical block

TABLE 4.11: Centroids of the three clusters for lithology, apatite, magnetite, iron and iron recovery found by SK-Means, SPCA and SFWC.

Cluster	Lithology	Apatite	Magnetite	Iron	Iron recovery
SK-Means					
1	3	2.85	87.96	64.37	89.60
2	1	3.81	62.20	46.33	87.94
3	2	2.14	81.48	61.07	84.33
SPCA					
1	3	2.73	87.78	64.66	89.71
2	1	3.49	65.04	48.35	88.51
3	2	2.30	81.29	60.64	83.07
SWFC					
1	3	4.51	88.08	64.87	91.22
2	1	4.88	57.05	42.98	88.98
3	2	1.82	72.87	54.83	82.41

model demonstrates the flexibility of applying SWFC in practice. The objective was for the three clusters to be centred in specific values of iron recovery, which was fully achieved. The spatial correction step in the three clustering methods makes some changes in the final membership (Fig. 4.10B). Although these changes are small, they are worthwhile as they ensure that the derived clusters are as spatially compact as possible.

4.5 Conclusions and future work

Identifying geometallurgical clusters or domains in mining applications is very important not just to characterise geology and geochemistry, but also to assist in choosing optimal processing routes for parcels of ore with different properties. Geometallurgy is increasingly incorporating more information and more variables, which makes it more difficult to find useful cluster structures for mine planning purposes.

In this paper, the difficulty of traditional clustering methods is demonstrated when dealing with multivariate scenarios in which the cluster structures depend on different attributes, as is commonly the case in practice. A new clustering method is proposed which is based on fuzzy clustering but incorporates additional valuable characteristics such as feature selection, spatial correction and the flexibility of including expert knowledge. Expert knowledge in the proposed method can be incorporated through an appropriate distance definition (categorical or targeted distances) and forcing a specific weight

to a particular attribute.

Three case studies were presented to illustrate the application of SWFC. The first case study was explicitly designed to construct clusters that depend on different subsets of attributes. While the traditional methods fail to discover the true clusters, WFC and SWFC can readily find the designed cluster structure and SWFC also constructs well-connected clusters by incorporating spatial information. The second case study was used to illustrate graphically the effectiveness of SWFC using a two-dimensional synthetic geometallurgical model. The clusters found by SWFC are spatially well-connected and the most compact. Finally, SWFC was applied to a complete synthetic geometallurgical block model to demonstrate its capability and flexibility in building clusters, which in this case are geometallurgical domains for iron recovery. By imposing a targeted distance for iron recovery and weight, SWFC can find the relevant secondary attributes that control the cluster structures.

In summary, SWFC has been demonstrated to be capable of defining meaningful geometallurgical domains for different application scales, based either on samples or complete block models.

In future research, the geometallurgical uncertainty may be also taken into account for the clustering method. Uncertainty can be introduced by generating many realisations of the block model. The SWFC method can then include the distances between realisations to account for uncertainty. Also, the interaction potential could be reformulated to incorporate some form of multivariate spatial correlation, such as semivariogram or correlogram, instead of the Potts model. It is also necessary to investigate an optimisation formulation that can include the minimisation of compactness, maximisation of separation, feature selection and spatial correction all within a single integrated step.

Acknowledgements

This work was supported with the supercomputing resources provided by the Phoenix HPC service at the University of Adelaide. The first author acknowledges the support of CONICYT in the form of a Becas Chile scholarship.

References

Allard, D. and Guillot, G. (2000), Clustering geostatistical data, *in* 'Proceedings of the sixth geostatistical conference'.

Ambroise, C., Dang, M. and Govaert, G. (1996), Clustering of Spatial Data by the EM Algorithm, *in* 'Geostatistics for environmental applications', Lisboa, pp. 493–504.

Bourgault, G., Marcotte, D. and Legendre, P. (1992), 'The multivariate (co) variogram as a spatial weighting function in classification methods', *Mathematical Geology* **24**(5), 463–478.

Boykov, Y. and Veksler, O. (2006), 'Graph cuts in vision and graphics: Theories and applications', *Handbook of Mathematical Models in Computer Vision* pp. 79–96.

Carlo, G., Paolo, G. and Roberto, P. (2017), 'Spatial clustering of curves with an application of satellite data', *Spatial statistics* **20**, 110–124.

Coward, S. and Dowd, PA. (2015), Geometallurgical models for the quantification of uncertainty in mining project value chains, *in* '37th APCOM Conference', Alaska, pp. 360–369.

Coward, S., Dowd, PA. and Vann, J. (2013), Value chain modelling to evaluate geometallurgical recovery factors, *in* '36th APCOM Conference', Fundação Luiz Englert, Brazil; ISBN 978-85-61155-02-5, Porto Alegre, Brazil, pp. 288–289.

Coward, S., Vann, J., Dunham, S. and Stewart, M. (2009), The Primary-Response Framework for Geometallurgical Variables, *in* 'Seventh International Mining Geology Conference', pp. 109–113.

Davies, D. L. and Bouldin, D. W. (1979), 'A cluster separation measure.', *IEEE transactions on pattern analysis and machine intelligence* **1**(2), 224–227.

Deutsch, C. V. (1998), 'Cleaning categorical variable (lithofacies) realizations with maximum a-posteriori selection', *Computers & Geosciences* **24**(6), 551–562.

Ding, C. and He, X. (2004), K-means clustering via principal component analysis, *in* 'Twenty first international conference on Machine learning', ACM, Banff, Canada, p. 29.

Dunham, S. and Vann, J. (2007), Geometallurgy, Geostatistics and Project Value - Does Your Block Model Tell You What You Need to Know?, *in* 'Project Evaluation Conference', Melbourne, pp. 189–196.

Dunn, J. C. (1973), 'A fuzzy relative of the isodata process and its use in detecting compact well-separated clusters', *Cybernetics* **3**, 32–57.

Fouedjio, F. (2016), A Clustering Approach for Discovering Intrinsic Clusters in Multivariate Geostatistical Data, *in* 'Machine Learning and Data Mining in Pattern Recognition', Vol. 9729, pp. 491–500.

Friedman, J. H. and Meulman, J. J. (2004), 'Clustering objects on subsets of attributes', *Journal of the Royal Statistical Society. Series B: Statistical Methodology* **66**(4), 815–839.

Garrido, M., Sepúlveda, E. and Navarro, F. (2017), Optimization of planning and scheduling of ore body with open pit extraction considering homogeneity in clays as geometallurgical variables, *in* '5th International Seminar on Mine Planning', Santiago, pp. 1–7.

Goodfellow, R. and Dimitrakopoulos, R. (2017), 'Simultaneous stochastic optimization of mining complexes and mineral value chains', *Mathematical Geosciences* **49**(3), 341–360.

Guillot, G., Kan-King-Yu, D., Michelin, J. and Huet, P. (2006), 'Inference of a hidden spatial tessellation from multivariate data: application to the delineation of homogeneous regions in an agricultural field', *Journal of the Royal Statistical Society: Series C (Applied Statistics)* **55**(3), 407–430.

Hoal, K. O., Woodhead, J. and Smith, K. S. (2013), The Importance of Mineralogical Input into Geometallurgy Programs, *in* 'The second AUSIMM international geometallurgy conference', number October, Brisbane, QLD, pp. 17–25.

Hunt, J., Berry, R., Bradshaw, D., Triffett, B. and Walters, S. (2014), 'Development of recovery domains: Examples from the Prominent Hill IOCG deposit, Australia', *Minerals Engineering* **64**, 7–14.

Hunt, J., Kojovic, T. and Berry, R. (2013), Estimating Comminution Indices from Ore Mineralogy , Chemistry and Drill Core Logging, *in* 'The Second AusIMM International Geometallurgy Conference', number October, Brisbane, QLD, pp. 173–176.

Keeney, L. and Walters, S. G. (2011), A Methodology for Geometallurgical Mapping and Orebody Modelling, *in* 'The First AusIMM International Geometallurgy Conference', number September, Brisbane, QLD, pp. 217–225.

Leichliter, S. and Larson, D. (2013), 'Geometallurgy for two recovery process operations at Cripple Creek & Victor gold mine', *Mining Engineering* (January), 29–33.

Lishchuk, V. (2016), Geometallurgical Programs - Critical Evaluation of Applied Methods and Techniques, Licentiate thesis, Lulea University of Technology.

López, A. A. and Malpica, J. A. (2008), 'High resolution satellite classification with graph cut algorithms', *Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics)* **5359 LNCS**(PART 2), 105–112.

Luchi, D., Rodrigues, A., Varejão, F. M. and Santos, W. (2016), A genetic algorithm approach for clustering large data sets, *in* 'Tools with Artificial Intelligence (ICTAI), 2016 IEEE 28th International Conference on', IEEE, pp. 570–576.

Lund, C., Lamberg, P. and Lindberg, T. (2015), 'Development of a geometallurgical framework to quantify mineral textures for process prediction', *Minerals Engineering* **82**, 61–77.

Maulik, U. and Bandyopadhyay, S. (2000), 'Genetic algorithm-based clustering technique', *Pattern Recognition* **33**, 1455–1465.

Nanda, S. J. and Panda, G. (2014), 'A survey on nature inspired metaheuristic algorithms for partitional clustering', *Swarm and Evolutionary Computation* **16**, 1–18.

Napier-Munn, T. J., Morrell, S., Morrison, R. D. and Kojovic, T. (1996), *Mineral comminution circuits: their operation and optimisation*, Vol. 2, Julius Kruttschnitt Mineral Research Centre, University of Queensland.

Newton, M. and Graham, J. (2011), Spatial modelling and optimisation of geometallurgical indices, *in* 'The First AusIMM International Geometallurgy Conference', Brisbane, pp. 247–261.

Nguyen, K. and Keeney, L. (2014), Spatial domaining of highly variable continuous geometallurgical data, *in* 'XXVII International Mineral Processing Congress - IMPC 2014', Gecamin Digital Publications, pp. 116–127.

Oliver, M. A. and Webster, R. (1989), 'A geostatistical basis for spatial weighting in multivariate classification', *Mathematical Geology* **21**(1), 15–35.

Pal, N. R. and Bezdek, J. C. (1995), 'On cluster validity for the fuzzy c-means model', *IEEE Transactions on Fuzzy systems* **3**(3), 370–379.

Ren, M., Liu, P., Wang, Z. and Yi, J. (2016), 'A Self-Adaptive Fuzzy c-Means Algorithm for Determining the Optimal Number of Clusters', *Computational Intelligence and Neuroscience* **2016**(1).

Romary, T., Ors, F., Rivoirard, J. and Deraisme, J. (2015), 'Unsupervised classification of multivariate geostatistical data: Two algorithms', *Computers & Geosciences* **85**, 96–103.

Rousseeuw, P. J. (1987), 'Silhouettes: A graphical aid to the interpretation and validation of cluster analysis', *Journal of Computational and Applied Mathematics* **20**(C), 53–65.

Ruspini, E. H. (1969), 'A new approach to clustering', *Information and control* **15**(1), 22–32.

Schnetzler, E. (1994), Visualization and cleaning of pixel-based images, PhD thesis, Stanford University.

Tarabalka, Y. and Charpiat, G. (2013), 'A graph-cut-based method for spatio-temporal segmentation of fire from satellite observations', *International Geoscience and Remote Sensing Symposium (IGARSS)* **2**, 3494–3497.

Tarabalka, Y. and Rana, A. (2014), Graph-Cut-Based Model for Spectral-Spatial Classification of Hyperspectral Images, *in* 'International Geoscience and Remote Sensing Symposium', Quebec, Canada.

Wang, Y., Song, H. and Zhang, Y. (2016), 'Spectral-Spatial Classification of Hyperspectral Images Using Joint Bilateral Filter and Graph Cut Based Model', *Remote Sensing* **8**(9), 748.

Whitley, D. (1994), 'A genetic algorithm tutorial', *Statistics and computing* **4**(2), 65–85.

Wold, S., Esbensen, K. and Geladi, P. (1987), 'Principal component analysis', *Chemometrics and intelligent laboratory systems* **2**(1-3), 37–52.

Chapter 5

Optimization of planning and scheduling of ore body with open pit extraction considering homogeneity in clays as geometallurgical variables

Statement of Authorship

Title of Paper	Optimization of planning and scheduling of ore body with open pit extraction considering homogeneity in clays as geometallurgical variables.
Publication Status	☑ Published ☐ Accepted for Publication ☐ Submitted for Publication ☐ Unpublished and Unsubmitted w ork w ritten in manuscript style
Publication Details	Garrido, M., Sepulveda, E. and Navarro, F. (2017), Optimization of planning and scheduling of ore body with open pit extraction considering homogeneity in clays as geometallurgical variables, GEOMIN-MINEPLANNING in 5th International Seminar on Geology for the Mining Industry, Santiago, Chile, pp. 294-300.

Secondary Author

Name of Secondary Author (Candidate)	Exequiel Manuel Sepulveda Escobedo		
Contribution to the Paper	Development of geometallurgical dilution concept, optimisation formulations and helped with edition of manuscript.		
Overall percentage (%)	40%		
Certification:	This paper reports on original research I conducted during the period of my Higher Degree by Research candidature and is not subject to any obligations or contractual agreements with a third party that would constrain its inclusion in this thesis. I am the secondary author of this paper.		
Signature		Date	20/02/2018

Co-Author Contributions

By signing the Statement of Authorship, each author certifies that:

i. the candidate's stated contribution to the publication is accurate (as detailed above);

ii. permission is granted for the candidate in include the publication in the thesis; and

iii. the sum of all co-author contributions is equal to 100% less the candidate's stated contribution.

Name of Co-Author	Mauricio Garrido		
Contribution to the Paper	Principal Author (50%), Development of geometallurgical dilution concept, optimisation formulations and main writer of manuscript.		
Signature		Date	20/02/2018

Name of Co-Author	Felipe Navarro		
Contribution to the Paper	Helped with writing the program for optimisation and revision of manuscript.		
Signature		Date	22/02/2018

Abstract

Mine planning in open pit operations defines the material to be extracted, when it will be extracted and its final destination. Conventional scheduling usually considers block values based on geological parameters such the grade of the metal of interest, its mineralogy, and parameters external to geology. The latter parameters correspond, for example, to economic parameters, opportunity costs, types of plant and plant processes. The scope of this research is to include geometallurgical constraints into the optimization problem known in mine planning as the constrained pit-limit problem.

In recent years, numerous works have proven that clays have a strong on the flotation recovery process for chalcopyrite or bornite minerals. This impact generates operational problems that, if not controlled, can decrease metallurgical recovery. For example, clays are usually soft rocks and hence the grinding time is modified, thus affecting the operational performance and final recovery. In addition, clays increase the costs associated with water input as they require additional consumption to obtain the expected recovery. All these factors can be handled when they are incorporated in medium to long-term plans, but they are challenging in short-term planning and make most projects uneconomical.

In this work, we propose a methodology which adds a homogeneity condition to the optimization problem. The condition is that minerals with similar geometallurgical properties (in this case, the estimated clay content) should be extracted in each period so that the operational mineral processing parameters would remain relatively similar. The algorithm was applied to a case study where zones with different levels of alteration and clay content were modelled. The valuation used standard mining industry economic parameters.

5.1 Introduction

An approach often used in mine planning is to determine the time-sequence of blocks to be extracted from a block model so as to maximize the net present value (NPV) subject to different operational conditions, creating an optimization problem that can include many constraints (Lane, 1988). In the case of an open pit, they include precedence constraints, which are geometric constraints associated with the access to blocks and rock slope stability (Whittle, 2009). Current algorithms for this optimization deliver satisfactory solutions by defining different pushbacks and a final pit, which maximizes the NPV over

the life of the mining project (Fytas et al., 1993; Johnson, 1968). Often, these numerically correct solutions are not operationally feasible and hence require design modifications to define a feasible extraction plan.

Different restrictions can be added to the optimization problem, for example: mine production, plant capacity, multiple destinations (stockpile), schedule or sequences (Kim and Zhao, 1994), secondary variables of interest, among others. However, by adding additional constraints, the optimization problem becomes very complex, requiring large computing times and sometimes exceeding the available memory. This scenario motivated us to search for alternative methodologies capable of handling the computational complexity.

In this research, we consider geometallurgical variables for the optimization problem. Different types of clays cause operational metallurgical problems in flotation processes. The clay minerals, kaolinite (stratified silicate) and illite (phyllosilicate), are grouped into four categories according to their presence in the ore: large (> 30%), moderate (10% -30%), small (2% -10%) and minimum (<2%) (Chipera and Bish, 2001). Models of clay are usually built using categorical variables based on geological mapping and/or X-ray diffraction (analysis of clay speciation XRD). Clay variability in the metallurgical plant generates many operational problems which negatively influence the recovery of the metal of interest, generating mineral and economic losses. Bulatovic states: "Clays are the main reason for low recoveries of copper and gold by flotation" (Bulatovic, 1997).

The focus of this research is to generate a multi-objective optimization formulation to minimize the variation of clay to be processed in the short term. This optimization problem was constructed as the constrained pit limit problem (CPIT) subject to minimising variation in the clay content per period. CPIT consists of maximising the NPV over a time horizon, subject to block precedence and operational constraints. We used metaheuristic tabu search (TS) (Glover and Laguna, 1993) to solve this multi-objective optimisation problem because it can find solutions with a high level of accuracy in reasonable computational time.

The following section describes the methodology used to simulate a deposit that was used to test the proposed optimisation method. In this study, we apply TS to the synthetic deposit to maximize NPV and minimize the variation in clays content. The results are discussed in the conclusions.

5.2 Methodology

The simulated case study corresponds to the surface area of a copper porphyry deposit (Camus, 2003). The hydrothermal system which generated the deposit is much larger than the deposit and has also altered the surrounding rocks (Burnham, 1979). The rock mass is composed primarily of andesite. The deposit dates from the late-eocene and the intrusive complex is of the diorite-type. Kaolinite clays are strongly associated with sericitic alteration, which is presented superficially and covers the largest area of the study. The mineralization is composed mainly of disseminated chalcopyrite (ore of economic value) with poor indicators of secondary supergene processes. The dimensions of the deposit are not known at depth; however, we focused our research on portions of the deposit with low uncertainty (measured-indicated resources). For more information on porphyry deposits and hydrothermal systems, see (Feiss, 1978; Robb et al., 2004). Figure 5.1 shows a typical cross-section of the orebody.

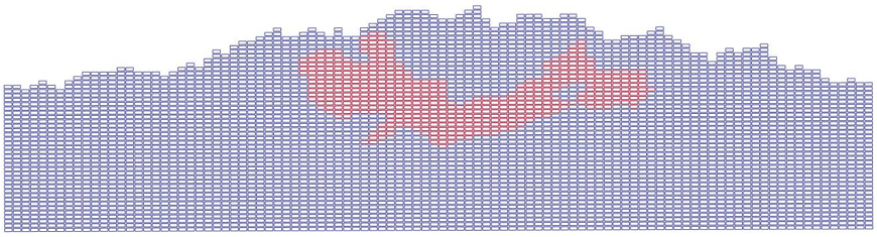


FIGURE 5.1: Typical cross-section of the orebody used for the optimisation. Red and blue blocks are ore and waste blocks respectively.

The clay minerals were modelled on the basis of geological mapping of sericitic alteration from cores from diamond and reverse circulation drilling. Four main categories were proposed as areas of large, moderate, small and minimum presence of clay (increasing towards the edges and surface of the area) (Figure 5.2).

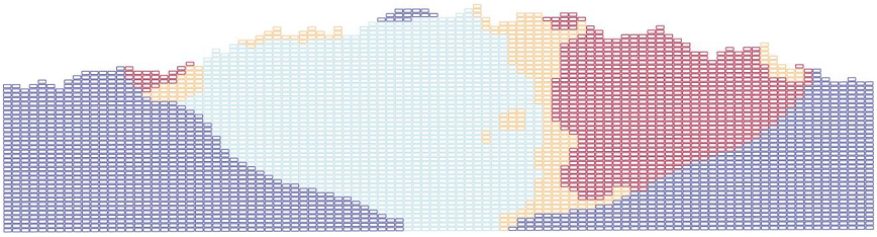


FIGURE 5.2: Clays modelled on a typical cross-section: Blue is minimum clay presence, cyan represents small clay presence, yellow is moderate clay presence, and red is large clay presence.

The multi-objective optimization problem is defined as follows. The main objective is formulated according to CPIT (Espinoza D, 2013) which is the maximization of the NPV subject to precedence constraints (pit form) and temporal constraints (schedule) (Lambert et al., 2014; Lamghari, 2017). The second objective is addressed as the minimization of dilution of the exploitation over the time horizon T (Equation 5.1). Dilution (in mining) is the relationship between waste and ore in the extraction process. In the case of geometallurgical dilution, ore and waste are redefined; in the case of ore, corresponds to the most frequent clay domain in a period, and, in the case of waste, to the rest of the domains. Using this definition, geometallurgical dilution can be described as the proportion of waste in a period (Equation 5.2). Clay attributes represented as $a_i = 0, 1, 2, 3$ where 0 is minimum clay presence and 3 is large clay presence.

The minimization of dilution problem is specified as:

$$\min \sum_{t=1}^{T} D_t, \tag{5.1}$$

where D_t is dilution in the period t:

$$D_t = \frac{E_t}{E_t + M_t}. \tag{5.2}$$

Mineral (M_t) and Waste (E_t) in the period t are defined as follows:

$$M_t = \sum_{i=1}^{N(t)} I_i \tag{5.3}$$

$$E_t = \sum_{i=1}^{N(t)} J_i, \tag{5.4}$$

where I_i and J_i are respectively:

$$I_i = \begin{cases} 0, & \text{if } a_i \neq m_t \\ 1, & \text{if } a_i = m_t \end{cases} \tag{5.5}$$

$$J_i = \begin{cases} 0, & \text{if } a_i \neq e_t \\ 1, & \text{if } a_i = e_t \end{cases}, \tag{5.6}$$

and the parameters determining waste or mineral are defined as:

$$\begin{aligned} m_t &= \text{mode } a_i \\ e_t &= a_i | a_i \neq m_t \end{aligned}. \tag{5.7}$$

Tabu search was developed by Glover at the end of the 1990s (Glover and Laguna, 1993) and is a metaheuristic optimization method that takes advantage of local search and internal memory. Giving the combinatorial aspect of the formulation, we considered it appropriate to use of these algorithms that sacrifice accuracy in the solution to significantly reduce the processing times, allowing us to have good solutions in a reasonable execution time.

5.3 Results and discussion

Figure 5.3 shows the resources to be extracted in the different time periods. It should be noted that the solution seeks to maximize the NPV and decrease the "geometallurgical dilution" per period. In addition, Figure 5.4 shows the variability of dilution by period, specifying the times at which higher dilution can be expected. The information generated by this process can used, from a predictive point of view, to manage operational parameters at the processing plant as a function of the variability of clay content, which was modelled as dilution.

The chart in Figure 5.4 summarizes the general schedule for the different periods of time in terms of tonnage and grade. The optimization did not consider keeping mine or plant tonnages constant over time (this condition could be added in future work).

The results obtained with the TS algorithm were compared with the optimization problem solved without dilution restriction (CPIT). Table 5.1 shows the values of NPV for the dilution case and the base case. The dilution case gives results very similar to the base case in terms of grades and extracted tonnages. Both cases have low differences in tonnage by period, which results in a

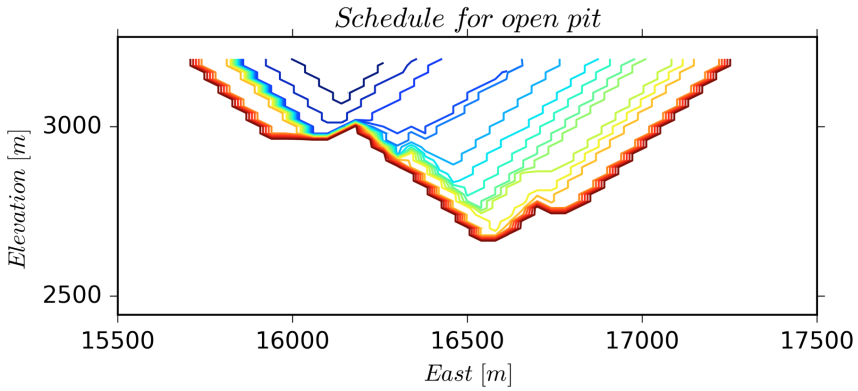


FIGURE 5.3: Schedules for different periods. Each contour plot corresponds to the pit limit in a period.

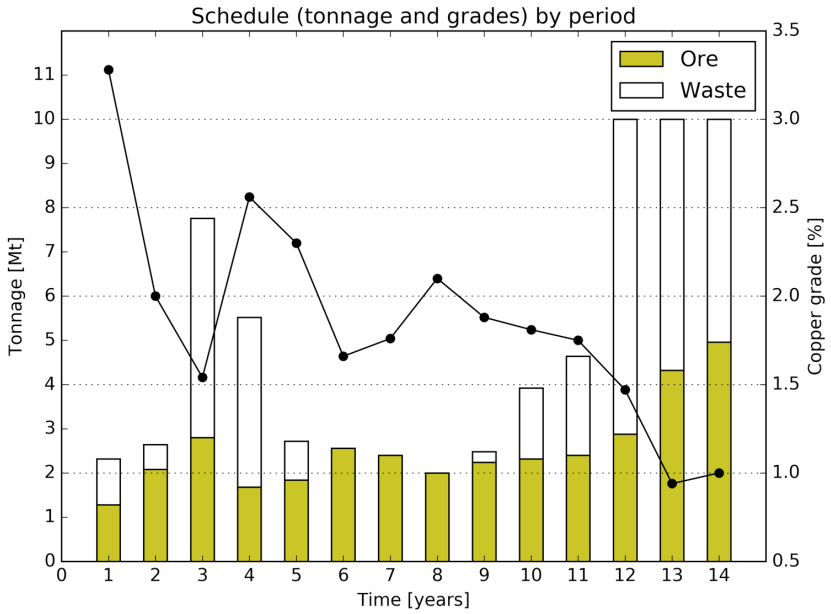


FIGURE 5.4: Tonnage and grades average by period.

TABLE 5.1: Comparison between base case and dilution case. Base case does not consider plant processing costs.

	Base case		Dilution case		Difference	
Period	Dilution	NPV [MUS$]	Dilution	NPV [MUS$]	Dilution	NPV [MUS$]
1	10%	135	2.5%	95	-76.0%	-30%
2	0.0%	249	0.0%	201	-	-19%
3	0.0%	327	0.0%	294	-	-10%
4	0.0%	413	0.0%	396	-	-4%
5	0.0%	500	0.0%	486	-	-3%
6	0.0%	577	0.0%	562	-	-3%
7	0.0%	649	0.0%	631	-	-3%
8	0.0%	716	0.0%	698	-	-2%
9	0.0%	775	0.0%	756	-	-2%
10	4.1%	825	2.4%	808	-42%	-2%
11	14%	868	15%	851	7.0%	-2%
12	32%	896	24%	879	-26%	-2%
13	28%	910	16%	883	-43%	-3%
14	9.6%	928	8.8%	901	-8.3%	-3%

decrease of the NPV in dilution case (6% of difference in average). The dilution decreases notably in most periods, generating a more homogeneous feed to the metallurgical processing plant. The reduction in dilution may avoid economic losses that are not often considered in the standard evaluation since they are difficult to quantify.

5.4 Conclusions

We propose an addition to traditional optimization of the NPV, by considering other variables. Considering additional variables can improve the operation in the short and medium term, but the complexity of the optimization problem is increased. We considered the deleterious effect on metallurgical processing of the clay dilution of ore and included the minimisation of clay variability in the optimisation of production schedules. The problem was solved using the tabu search metaheuristic and compared the results to the CPIT formulation used as base case. In terms of tonnage and grade of metal, the application of this methodology shows promising results. In addition, the methodology delivers production sequences with lower temporal dilution (higher homogeneity), which improves the predictive metallurgical capacity.

The metaheuristic approach used in this work enabled additional constraints to be included in the optimisation which is not possible in traditional formulations because the complexity of the numerical model makes it impossible to find an optimal solution. We strongly recommend the use of this metaheuristic (or any other) to tackle additional constraints that are not usually considered.

Acknowledgements

The authors would like to thank the industrial supporters of ALGES Laboratory, as well as the support from the Advanced Mining Technology Center (AMTC), the Department of Mining Engineering and the financial support from project Fondef "Caracterización y Modelamientos Geo-Minero-Metalúrgicos Predictivos: Camino a la Minería del Futuro" (IT16M10021). The second author acknowledges the support of CONICYT in the form of a Becas Chile scholarship.

References

Bulatovic, S. (1997), 'Flotation behaviour of gold during processing of porphyry copper-gold ores and refractory gold-bearing sulphides', *Minerals Engineering* **10**(9), 895–908.

Burnham, C. W. (1979), 'Magmas and hydrothermal fluids', *Geochemistry of Hydrothermal Ore Deposits*. pp. 71–136.

Camus, F. (2003), 'Geología de los sistemas porfíricos en los andes de chile', *Servicio Nacional de Geología y Minería* .

Chipera, S. J. and Bish, D. L. (2001), 'Baseline studies of the clay minerals society source clays: powder x-ray diffraction analyses', *Clays and Clay Minerals* **49**(5), 398–409.

Espinoza D, Goycoolea M, M. E. N. A. (2013), 'Minelib: a library of open pit mining problems', *Annals of Operations Research* **206**(1), 93–114.

Feiss, P. G. (1978), 'Magmatic sources of copper in porphyry copper deposits', *Economic geology* **73**(3), 397–404.

Fytas, K., Hadjigeorgiou, J. and Collins, J. (1993), 'Production scheduling optimization in open pit mines', *International Journal of Surface Mining and Reclamation* **7**(1), 1–9.

Glover, F. and Laguna, M. (1993), *Tabu search*, John Wiley & Sons, Inc.

Johnson, T. B. (1968), Optimum open pit mine production scheduling, Technical report, University of California Berkeley, Operations Research Center.

Kim, Y. and Zhao, Y. (1994), 'Optimum open pit production sequencing-the current state of the art', *Preprints - Society of Mining Engineers of AIME* .

Lambert, W. B., Brickey, A., Newman, A. M. and Eurek, K. (2014), 'Open-pit block-sequencing formulations: a tutorial', *Interfaces* **44**(2), 127–142.

Lamghari, A. (2017), 'Mine planning and oil field development: a survey and research potentials', *Mathematical Geosciences* **49**(3), 395–437.

Lane, K. F. (1988), *The economic definition of ore: cut-off grades in theory and practice*, Mining Journal Books.

Robb, L. et al. (2004), *Introduction to ore-forming processes.*, Blackwell Publishing.

Whittle, J. (2009), 'Whittle consulting global optimization software. melbourne, australia'.

Chapter 6

Conclusions, limitations, and future work

The main aim of geometallurgy is the improvement of mine planning by integrating data and knowledge of geology and metallurgical responses. In addition to building predictive models of metallurgical responses, it is critical to incorporate them into the block model. In many mining operations, the integrated geometallurgical component of this enriched block model can significantly improve the outcomes of mine planning optimisation. Geometallurgical block models also bring new challenges: the incorporation of many new geometallurgical variables increases the total number of variables in the model; more predictive models have to be fitted; and finding significant relationships between geological and metallurgical response variables is often difficult. From a decision-making perspective, not only the prediction of metallurgical responses is required but also the quantification of their uncertainty in order to assess economic and operational risk. The benefit of geometallurgy relies on the ability to integrate geometallurgical variables, together with their uncertainty, into mine planning.

6.1 Conclusions

This thesis achieves the proposed objectives as exemplified by the following outcomes:

- Paper 1:
  - Paper 1 proposes bootstrapped Projection Pursuit Regression (PPR) models to quantify the geometallurgical uncertainty of comminution and recovery responses.

  - PPR has systematically better predictive performance compared to multilinear regression models despite non-linear relationships found among predictors and the dependent variables.
  - Bootstrapping PPR models provide a means of quantifying the model uncertainty when the number of samples is limited, which is often the case in geometallurgical modelling.

- Paper 2:

  - The models developed in paper 1 are used to enrich the block model with several geometallurgical variables for a block caving mine. This enhanced block model contains many realisations to account for geometallurgical uncertainty.
  - The traditional form of economic valuation using standard NPV needs to be expanded in order to incorporate geometallurgical variables, for example, by using the Net Smelter Return valuation method.
  - Diverse risk measures are tested in multi-objective formulations to find the Pareto front for the decision-making process.
  - The genetic algorithms metaheuristic is used to optimise the stochastic formulations in a real-size problem. One advantage of using metaheuristics is that objective functions and constraints do not need to be linear which provides greater flexibility to incorporate non-linear functions or their evaluation by an algorithm.

- Paper 3:

  - One practical application of machine learning techniques in geometallurgy is building geometallurgical domains. Geometallurgical domaining is very useful in identifying contiguous in-situ rock volumes that have similar mineral processing characteristics. Discriminating processing streams according to the characteristics of each geometallurgical cluster may improve ore processing and metal beneficiation.
  - A new clustering method is presented. The clustering method combines fuzzy clustering and spatial continuity to generate potential geometallurgical domains.
  - This new clustering method allows for incorporating expert knowledge by weighting attributes and defining targets in the distance metric used in fuzzy clustering.

  - Another advantage of this new method is that the weights are found automatically in the optimisation process that minimises the size of the set of attributes. This subset of attributes may be different in each cluster.

- Paper 4:
  - This paper shows how geometallurgical clustering helps in production scheduling optimisation problems to achieve homogeneity in ore sent to the processing plant.
  - The concept of geometallurgical dilution is introduced as a measure of the discontinuity of geometallurgical domains.
  - The scheduling optimisation problem is reformulated as a bi-objective problem with a secondary objective being to minimise the geometallurgical dilution.

6.2 Limitations

The research conducted in this thesis has some limitations:

- Geometallurgical responses are assumed to scale up linearly from the laboratory scale to the block model scale and the plant scale. This is a strong assumption that, in many cases, is invalid.
- The rock flow in block caving mining has been represented only by vertical interactions. Horizontal interactions are not considered, despite the fact that, in reality, rock flow is a much more complicated process.
- Although metaheuristics can deal with large optimisation problems, they do not guarantee near-optimal solutions. In addition, metaheuristics are stochastic methods and, therefore, different runs may lead to different results.
- The clustering of geometallurgical data was done only for synthetic datasets due to the lack of access to large real geometallurgical datasets.
- For assessing risk in project evaluation, only geometallurgical uncertainty was considered. For an integrated risk assessment, other sources of uncertainty should be included, such as financial, operating and environmental.

6.3 Future work

The research conducted in this thesis has identified new research opportunities for future work. From paper 1 (Chapter 2), projection pursuit appears to have significant potential for new applications to address the non-additivity and upscaling issues. Instead of finding projections where the explained variance is maximised, a new index that measures the linearity of relationships between predictors and dependent variables may be useful to transform those variables into a new set of variables that show 'more' linearity in their relationships, similar to the PPMT technique. If this is feasible, the new variables can be used to estimate or simulate at the block-model scale, applying linear geostatistics and transforming the values back to the original scale.

In paper 2 (Chapter 3), the uncertainty of geometallurgical variables is quantified by geostatistical simulations and predictive models. These stochastic block models, which have 625 scenarios, make the bi-objective formulations very difficult to optimise. In the case of the block caving scheduling problem, if the uncertainty of the flow process is also included, the number of scenarios becomes even larger. Metaheuristics can cope with this issue, but further research is needed to assess the quality of the Pareto fronts found by metaheuristics. In addition, more research in computational efficiency and parallelism is required to solve these large real problems in a tractable computational time.

The new method for geometallurgical domaining, proposed in paper 3 (Chapter 4), also requires further research. Although it was applied to three synthetic cases, an application to a real geometallurgical database is recommended to determine whether the generated clusters are coherent with geology and reconciliation data from the plant.

The concept of geometallurgical dilution, introduced in paper 4 (Chapter 5), is promising but more research is needed to develop properly this concept and its practical use as a risk index to be minimised.