On the effect of parametric uncertainty in Gaussian Processes applied to geostatistical estimation: an in-silico case study

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INTRODUCTION

- In mining exploration and production, **models of the subsurface** are constructed **using Gaussian Processes (GPs)** to interpolate between samples of the ground (drill core).
- **Drilling** the ground for samples is **expensive and time-consuming**. In value-dense commodities, sampling is a production bottleneck. **Optimal sampling** is thus desirable.
- Commonly in industry, **samples target** the location with the **highest Kriging variance**.
- However, this variance implicitly **depends on estimates of the kernel parameters**.
- A methodology is proposed that fits multiple GPs with sets of parameter estimates from **Monte Carlo Simulations** to account for parametric and model prediction uncertainty.
- The **goal** is to produce maps to make **quantitative uncertainty assessments** possible. These shall be used as one of the optimality criteria **for optimal experimental designs.**

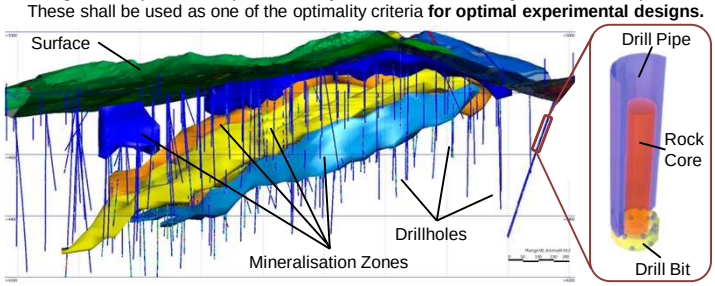
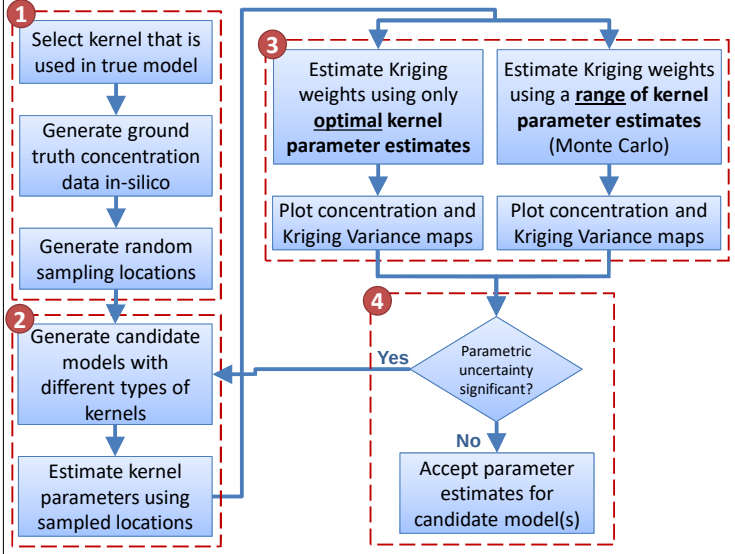


Figure 1: 3D model of a mineral deposit [1] with different concentrations in the blue, yellow and orange clouds. Drilled samples are in dark blue and a schematic of a drill is shown.

METHODOLOGY

Approach for Quantifying Parametric Uncertainty

1. **Generating Ground Truth & Sampling**: A known kernel, which describes the spatial correlation structure of concentration likelihood at different points, is used to generate ground truth concentration data. Some points are sampled; the rest are to be modelled.
2. **Estimation of Kernel Parameters:** Models based on different kernels are suggested and the kernel parameters are estimated based on magnitude and position of samples.
3. **Estimation of Kriging Weights:** Kriging weights determine the relative importance of samples for the GP. They are estimated for all proposed kernels; once with the optimal kernel parameters and once with the range of likely kernel parameters (MC simulation).
4. **Parameter identifiability:** Compare predicted concentrations and variances from the single-pass and the Monte Carlo GP. If the difference is significant, reducing parametric uncertainty must be prioritised in experiment designs or the model rejected altogether.



Formulation of Models

- The **kernel of the GP** consists of a **correlation function** $R(h)$, relating the semivariance $\gamma(h)$ of concentration at distance h and the distribution variance σ_Z^2 of concentrations.

$$\gamma(h) = \sigma_Z^2 - R(h) \quad (1)$$

- **Simple (biased) Kriging** is a form of GP which gives the **best linear estimate** of the **mean expected concentration** at an unsampled location Z using the estimator $\hat{Z}$, and the **variance of estimates** (σ_{BK}^2) based on the expected square error to the mean.

$$\sigma_{BK}^2 = E\left[\left(Z - \hat{Z}\right)^2\right] \quad (2)$$

- The estimators are based on the samples Z_i and their relative importance weights w_i.

$$\hat{Z} = \sum_{i=1}^{N} w_i Z_i \quad (3)$$

- The **optimal weights** w_i can be found from samples i and j by substituting (3) into (2):

$$\sigma_{BK}^2 = \sigma_Z^2 - 2\sum_{i=1}^{N} w_i R(Z, Z_i) + \sum_{i=1}^{N}\sum_{j=1}^{N} w_i w_j R(Z_i, Z_j) \quad (4)$$

- And then **minimising the Kriging variance**: $\partial\, \sigma_{BK}^2 / \partial\, w_i = 0$:

$$\sum_{i=1}^{N} R(Z_i, Z_j)\, w_i = R(Z, Z_j) \quad (5)$$

- For all unsampled locations this results in a weights matrix **W** and correlation matrices between sampled points **A**, and sampled and unsampled locations **P**. This can be solved as it is a linear system of equations with no degrees of freedom.[2]

CASE STUDY

1. Generation of Candidate Models & Ground Truth

Spherical Kernel [2]**:**

True Model if $h < r$ $\quad \gamma(h) = (s)\left(\frac{3h}{2r} - \frac{1}{2}\left(\frac{h}{r}\right)^3\right) + \mathrm{n}$; if $h \geq r$ $\quad \gamma(h) = s + n$ (6)

Gaussian Kernel [2]**:**

if $h < r$ $\quad \gamma(h) = (s)\left(1 - e^{-a\frac{h^2}{r^2}}\right) + \mathrm{n}$; if $h \geq r$ $\quad \gamma(h) = s + n$ (7)

Where s is the sill, n the nugget effect, r the characteristic range of correlations and a is constant.

2. Estimation of Kernel Parameters from Sampled Locations

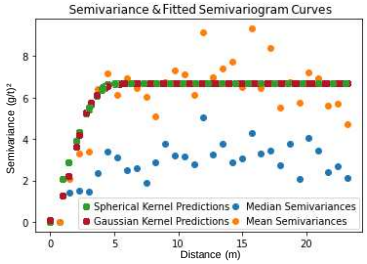


Figure 2 – Semivariance (squared concentration difference) between sampled point pairs vs. distance between them

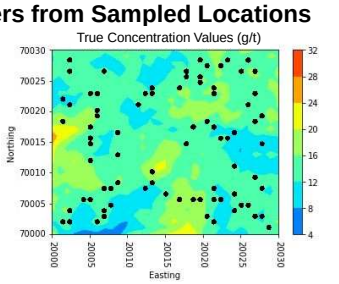


Figure 3 – True distribution of metal grade with 80 random sampling locations used in analysis

Kernel Parameters

Parameter	True Values	Spherical Kernel Estimates	Gaussian Kernel Estimates
r	17	8.68	8.68
n	3	2.31	2.31
s	20	4.23	4.23
a	-	-	251.62

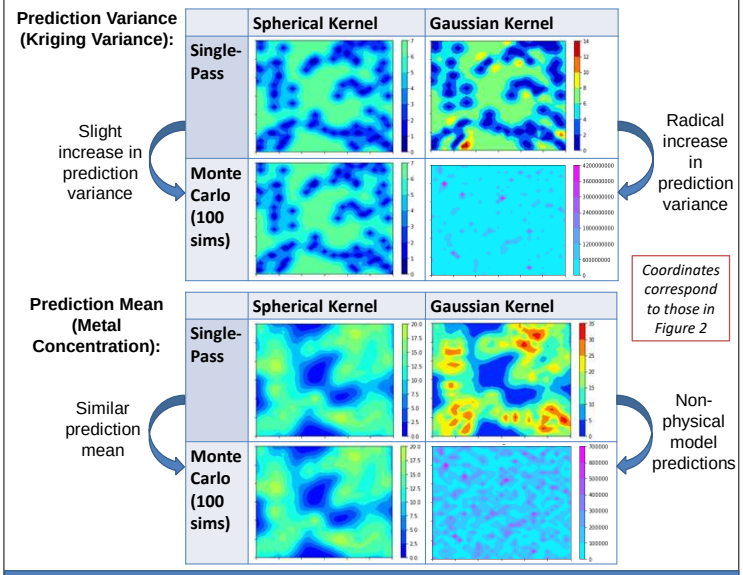
Spherical Kernel: Variance-Covariance Matrix for Parameters

	1	2	3
1	4.14		
2	-0.39	0.20	
3	0.54	-0.18	0.18

Gaussian Kernel: Variance-Covariance Matrix for Parameters

	1	2	3	4
1	3.95×10^{15}			
2	3.98×10^{6}	0.78		
3	-4.18×10^{6}	-0.77	0.77	
4	5.50×10^{16}	5.54×10^{7}	-5.83×10^{7}	7.66×10^{17}

3. Estimation of Kriging Weights & Fitting Gaussian Processes



CONCLUSIONS & FUTURE WORK

- Kernels with **structurally unidentifiable parameters**, e.g. the **Gaussian kernel** in Sahimi[2], should be avoided. Alternative formulations that fix the numerical parameter a = 1/3, e.g. in Rossi and Deutsch[3], should be used instead.
- In industry practice, kernel parameter uncertainty, local anisotropies and qualitative factors are often accounted for by fitting the kernel by hand[3]. Instead, regression should be used and the **variance-covariance matrix** should be computed so that the **effect of parametric uncertainty** can be **quantified** and propagated to the GP.
- Future **Model-based optimal experiment designs** will include a criterion to capture the effect of parametric uncertainty on the GP. This will be based on the **Fisher Information Matrix** and constitute second design objective in model discrimination work.

REFERENCES

[1]Dominy, S., O'Connor, L., Parbhakar-Fox, A., Glass, H., Purevgerel, S. (2018) Geometallurgy – a route to more resilient mine operations, *Minerals,* 8(12).
[2]Sahimi, M. (2011) Flow and Transport in Porous Media and Fractured Rock, 2nd Ed., Wiley.
[3] Rossi, M. and Deutsch, C. (2014) Mineral Resource Estimation, 1st Ed, Springer.

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