Spatial estimation: Concentration of a contaminant in groundwater

Project [MAT-288: Modeling Laboratory I]

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Groundwater Contamination

- Groundwater is the water present beneath Earth's surface in soil pore spaces and in the fractures of rock formations
- Actually, mainly in USA, exists filtration of contaminants in the soil. these contaminants can arriving at populated areas because of groundwater.

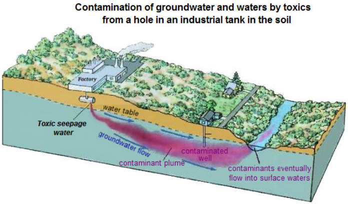

Figure: Example of Grounwater contamination.

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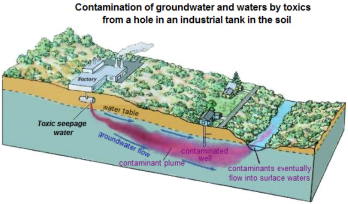

Figure: Example of Grounwater contamination.

The Problem

- C_w is the logarithm of a concentration $\hat{C_w}[ML^{-3}]$ of a contaminant.
  This project's main objective is that from N spatial samples of C_w we can estimate the value of C_w for an domain (3D or 2D).
- For this we have 625000 values of C_w in a 3D domain, these data was obtain of a validated simulation.

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How looks the data: Domain

- We have 625000 values of C_w associated with a 3D domain $[0, 1000] \times [0, 500] \times [0, 10]$ as the figure

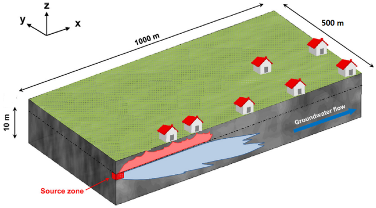

Figure: Sketch domain.

- The C_w data are located in the nodes of the grid with $\Delta x = 4$, $\Delta y = 2$ and $\Delta z = 1$.
So, we can **separate the 3D-domain in 10 2D-layers** with dimensions $[0, 1000] \times [0, 500]$

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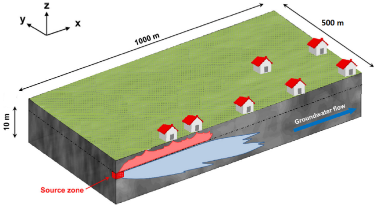

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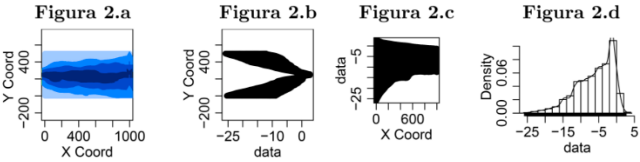
How looks the data: Statistics Analysis of C_w

- **In the nature we don't know this!**, but in our case (because C_w comes of a simulation) this is useful for the a comparison with the results of our prediction.
- For each layer (here's the first one) C_w we analyse the data.



- In 'Figura 2.a' we can see the quartiles increasing with the intensity of blue.
  In 'Figura 2.b' and 'Figura 2.c' we can see (in order) 'Y vs C_w' and 'C_w vs X'.
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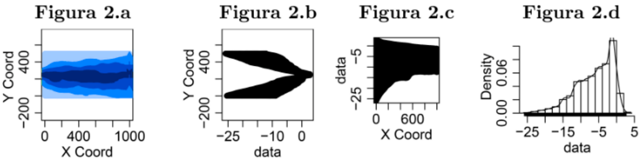

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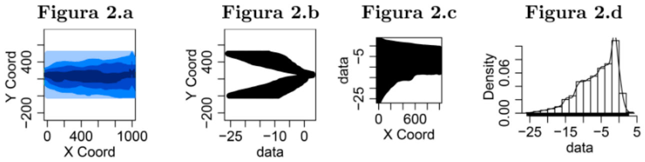

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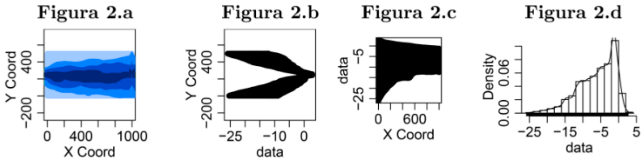

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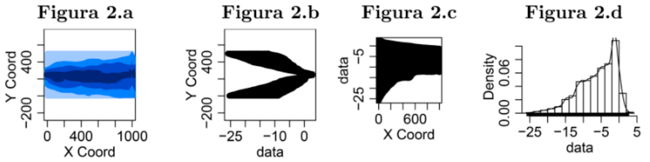

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How looks the data: Statistics Analysis of C_w

- In the next figure we can see a contour plot of the values of C_w in the first layer.

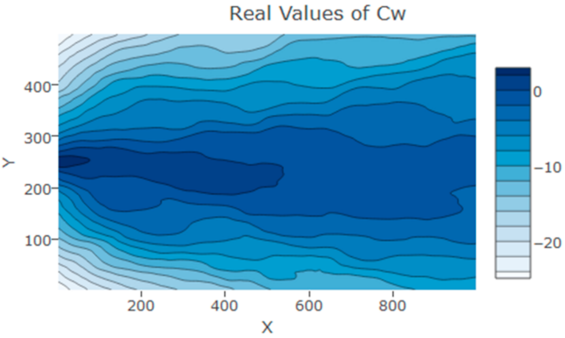

Figure: Contour Plot of Cw (upper layer)

Contents

The Model: Ordinary Kriging
Idea

- Let be $D = \{s \in [0, 1000] \times [0, 500] \subset \mathbb{R}^2\}$ the domain for a layer, defines $Z(s)$, $s \in D$ as a random variable, $Z(s)$ represents the value of C_w at the point s
- Suppose $Z(s) = \mu(s) + e(s)$ with μ constant but unknown and $e(s) \sim (0, \Sigma)$. We want to obtains $\hat{Z}(s_0)$ an estimator of C_w in s_0 since we know N values of C_w in the locations $\{s_1, s_2, ..., s_N\}$ with values $\{Z(s_1), Z(s_2), ..., Z(s_N)\}$.

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The Model: Ordinary Kriging

Definition 1

We define the **variogram** $\gamma(h)$ as:

$$\gamma(h) = \frac{1}{2}\mathbb{V}[Z(s+h) - Z(s)]$$

It's important to say that exists a few **preset families** of variograms that we can associate to a random variable.

Definition 2

We define the **empirical variogram** $\hat{\gamma}(h)$ as:

$$\hat{\gamma}(h) = \frac{1}{2N(h)} \sum_{s_i, s_j \in N(h)} (Z(s_i) - Z(s_j))^2$$

$$N(h) := \{(s_i, s_j) : \|s_i - s_j\| = h, \quad s_i, s_j \in D\}$$

The Model: Ordinary Kriging

Now when we have $\hat{\gamma}(h)$ for all the distances h of the domain D we can adjust (minimizing MeanSquaredError) some preset function $\gamma(h)$, and now we have the theoretical variogram.

The Model: Ordinary Kriging

So, in Ordinary Kriging we obtains the best estimator with the form

$$\hat{Z}(s_0) = \lambda_0 + \sum_{i=1}^{N} \lambda_i Z(s_i)$$

where we demand $\hat{Z}(s_0)$ be an Minimum-variance unbiased estimator.(ie: $\mathbb{E}[\hat{Z}(s_0) - Z(s_0)] = 0$ and minimize $\sigma_E^2 = \mathbb{V}[\hat{Z}(s_0) - Z(s_0)]$)
So it reduces to solving the system

$$\begin{bmatrix} \gamma(s_1 - s_1) & \cdots & \gamma(s_1 - s_N) & 1 \\ \vdots & \ddots & \vdots & 1 \\ 1 & \cdots & 1 & 0 \end{bmatrix} \begin{bmatrix} \lambda_1^{ok} \\ \vdots \\ \lambda_N^{ok} \\ \mu_{ok} \end{bmatrix} = \begin{bmatrix} \gamma(s_1 - s_0) \\ \vdots \\ \gamma(s_N - s_0) \\ 1 \end{bmatrix}$$

Results

The next figure consists in contours plots of the results of Ordinary Kriging to some sizes of samples(the samples are coloured in orange)

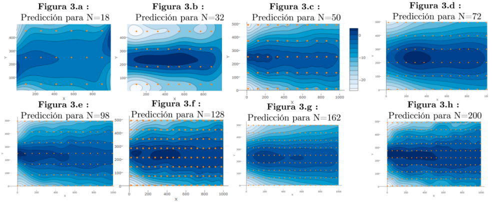

Figure: Prediction of Cw for some sizes of sample N

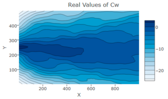

Figure: Real Values of Cw

Results

Particularly for $N = 50$ we analyse the prediction.

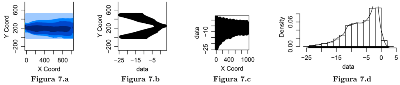

Figure: Statistics analysis of the prediction for N=50

In 'Figura 7.a' we can see the quartiles increasing with the intensity of blue. In 'Figura 7.b' and 'Figura 7.c' we can see (in order) 'Y vs C_w' and 'C_w vs X'.

In 'Figura 7.d' we can see the histogram for C_w

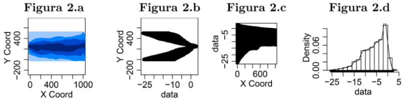

Figure: Statistics analysis Cw (Real Data)

Results

Particularly for $N = 50$ we observe the next figure that represents the variance of prediction in a contour plot. Again, the orange dots represents the sample.

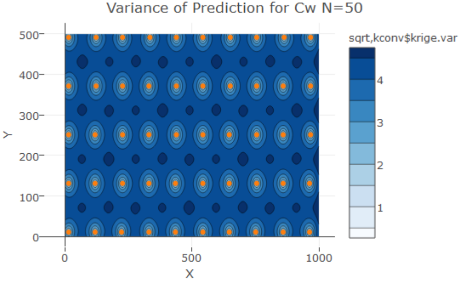

Figure: Variance of prediction for N=50

We note the variance is higher away from samples.

Results

Particularly for $N = 50$ we observe the next figure that represents a 3D plot of the prediction P (red), the real values C_w (blue) and the residue $R = P - C_w$ (green).

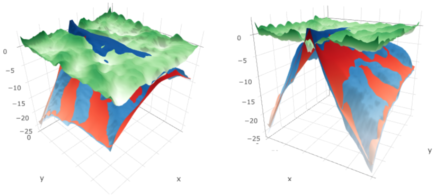

Figure: 3D comparison plot

OBS: If the prediction is perfect, $R = P - C_w$ correspond to the plane $z = 0$. R is positive where prediction is overestimated, and is negative where the prediction is underestimates.

Error

A measure of the goodness of prediction is the MSE. So in the next figure we can see 'MSE vs N'

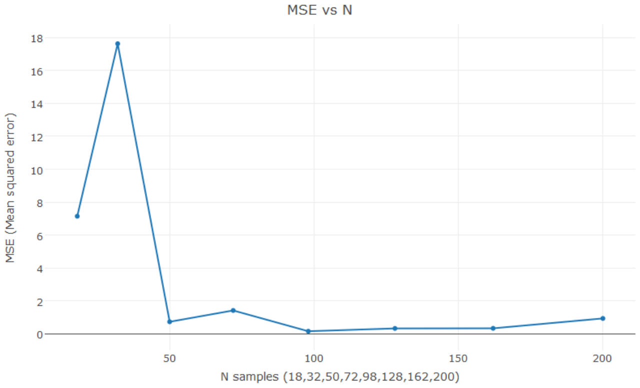

Figure: Mean Squared Error vs N

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Conclusions

- A prediction for C_w was achieved with good goodness of fit. In particular for N=50 obtains MSE=0.74
- 'MSE vs N' provides a comparison between the error of prediction and the number of samples N.
- This method is 'cheaper' and faster than trying to solve an diffusion equation, and do not handle assumptions regarding soil or nature parameters.
- It is possible in the future to develop a time serie to analyze the evolution over time of C_w

Thanks for your attention!