# PGE 338 Data Analytics and Geostatistics

## Lecture 12: Spatial Estimation

### Lecture outline . . .

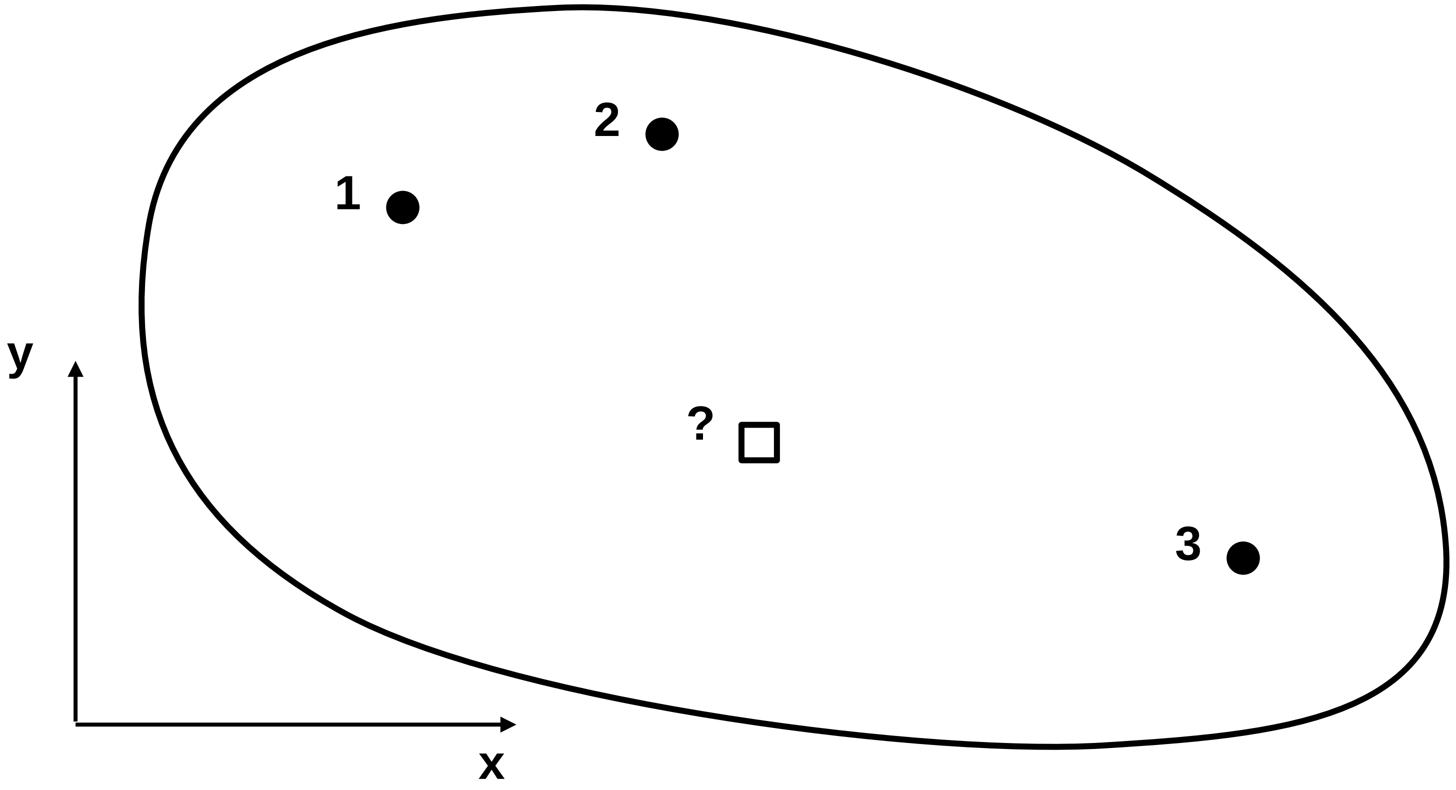
- Spatial Trend Modeling
- Kriging

Michael Pyrcz, The University of Texas at Austin

# Motivation

We need to make predictions away from sampled locations.

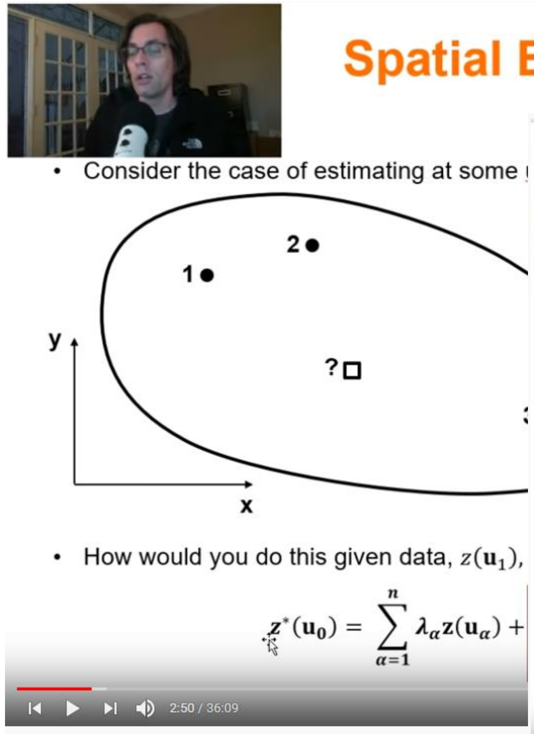
- To determine where to drill next, and to determine how to best develop a reservoir.



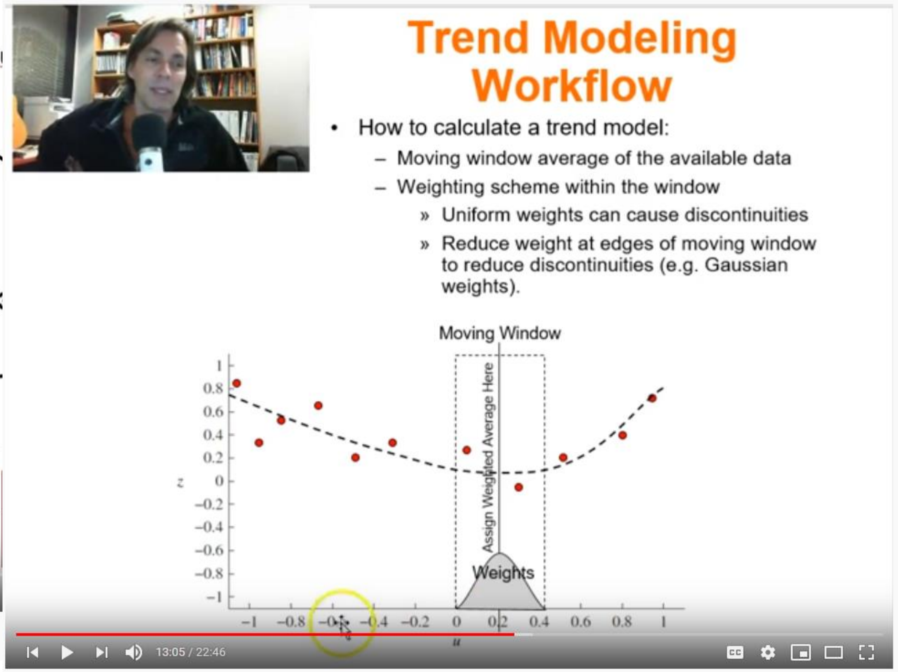

Schematic representation of a spatial prediction problem.

# Resources

Reminder on recorded lectures.



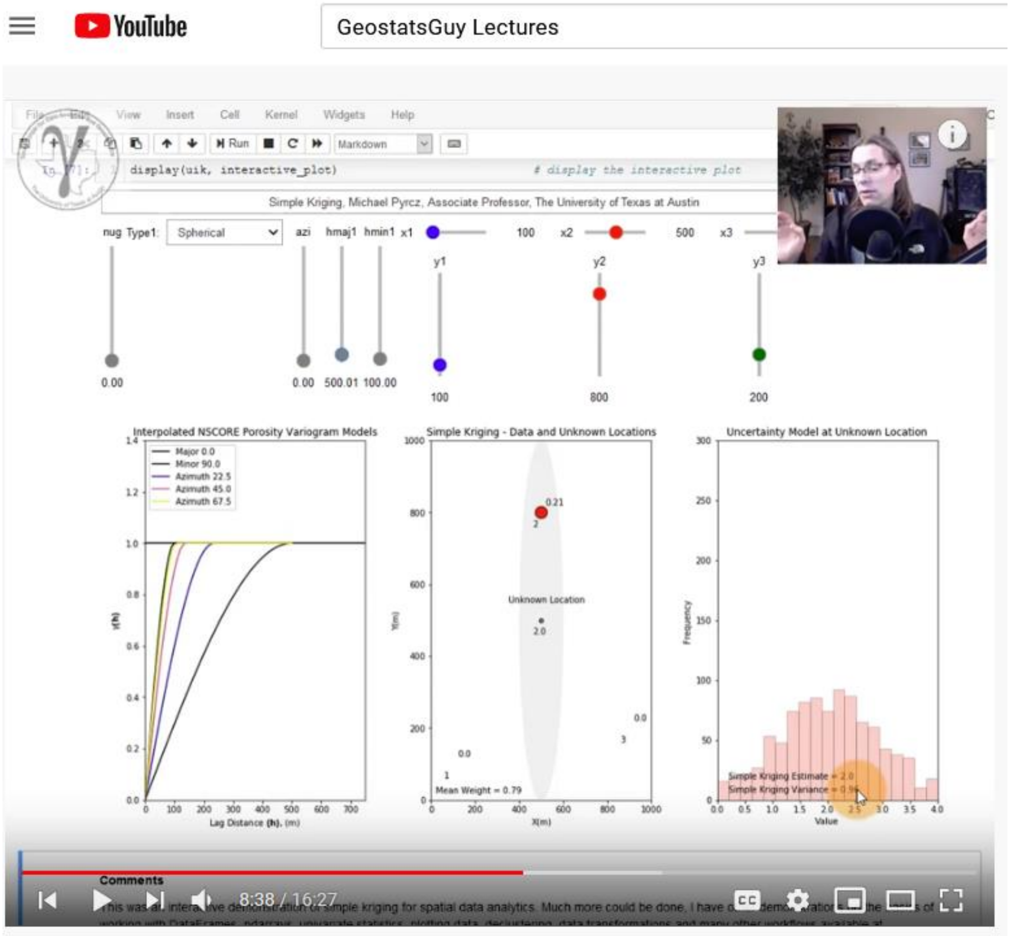

12b Geostatistics Course: Kriging




12a Geostatistics Course: Trend Modeling

# Resources

- Added a recorded walk-though of the Interactive Kriging Demo in Python.



# PGE 338 Data Analytics and Geostatistics

## Lecture 12: Spatial Estimation

**Lecture outline . . .**

- Spatial Trend Modeling



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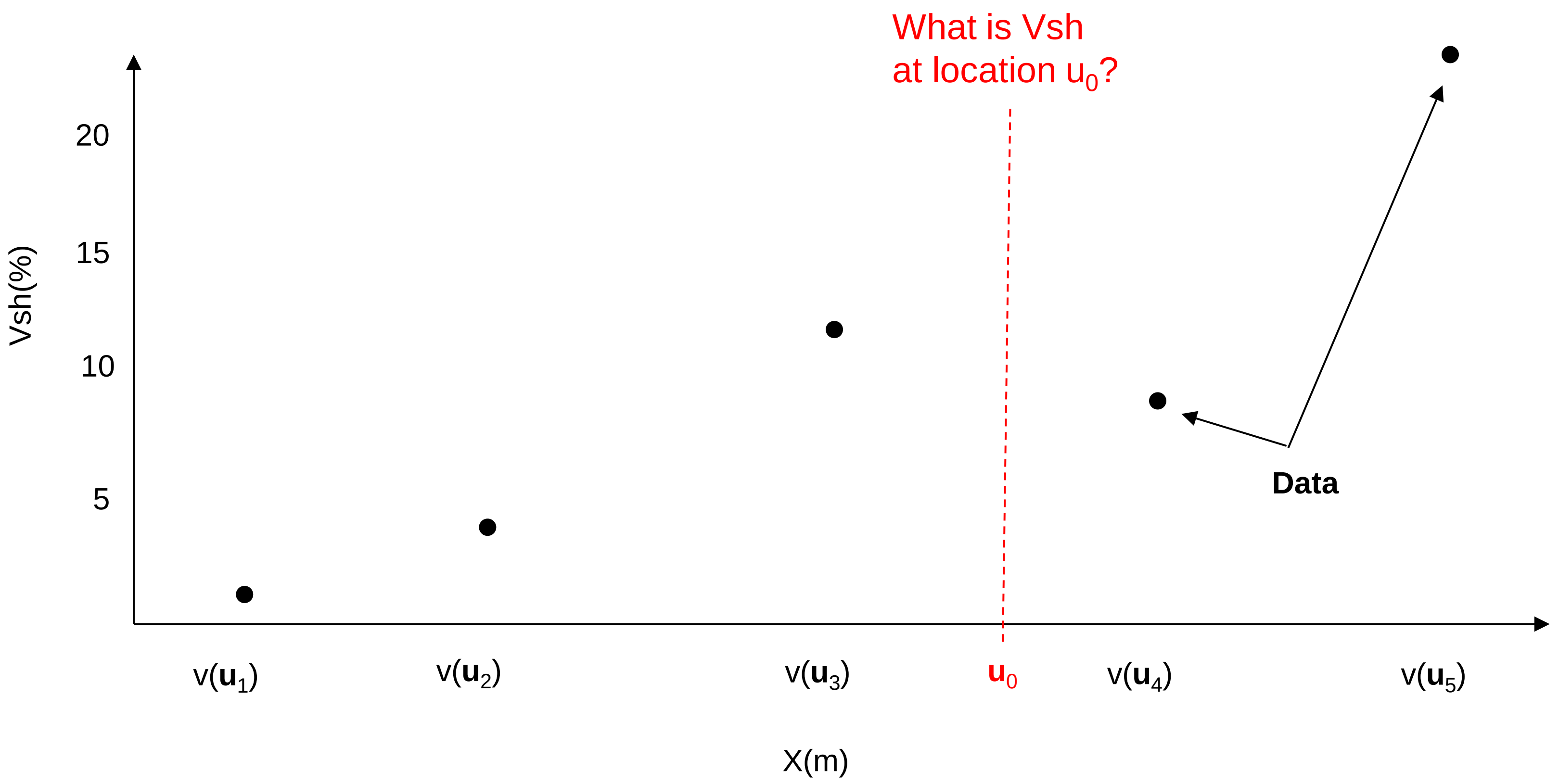
# Trend and Residual Method

Geostatistical spatial estimation methods will make an assumption concerning stationarity

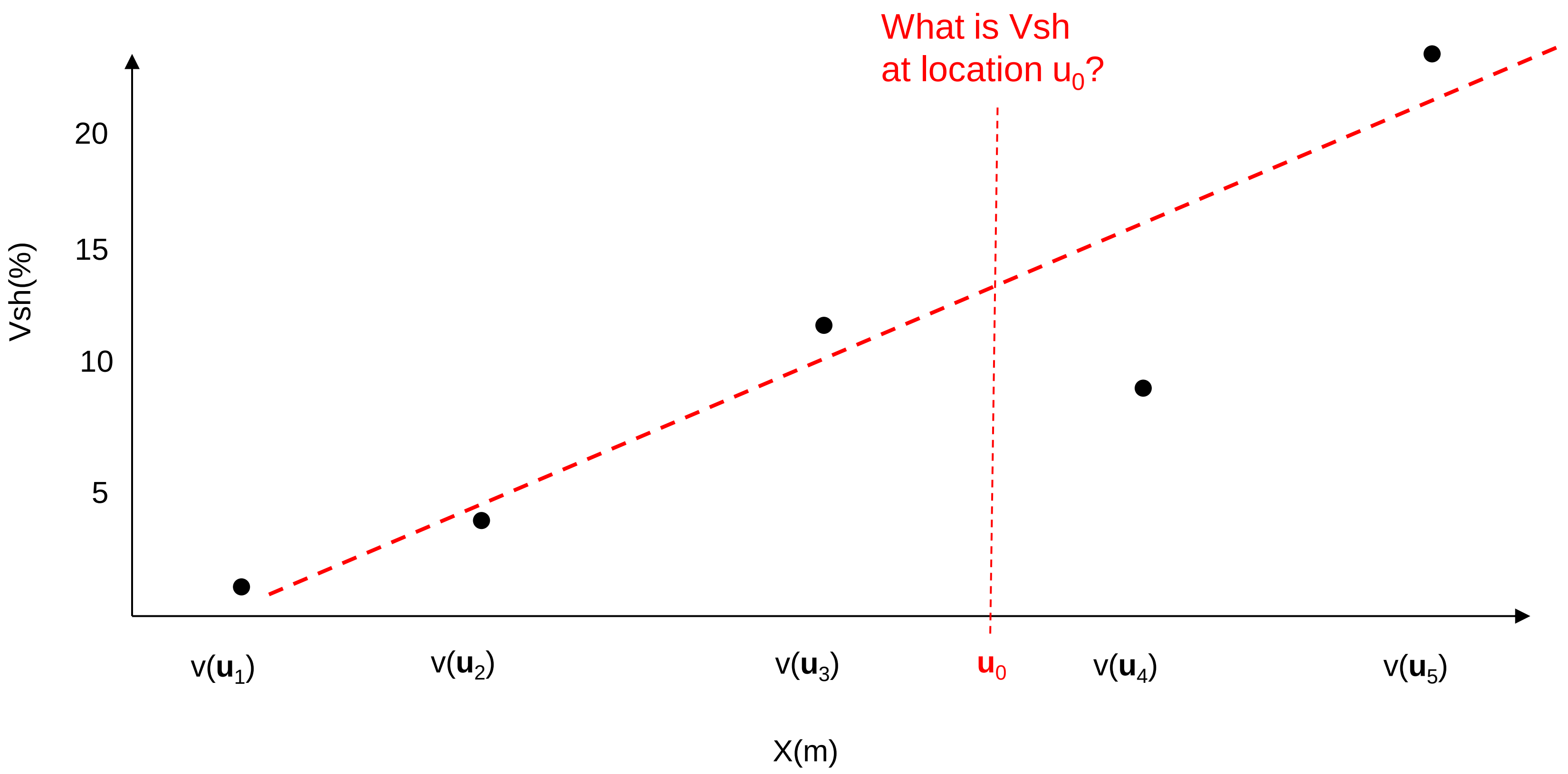
- In the presence of significant nonstationarity we would not rely 100% for spatial estimation on data + spatial continuity model



# Trend and Residual Method

Geostatistical spatial estimation methods will make an assumption concerning stationarity

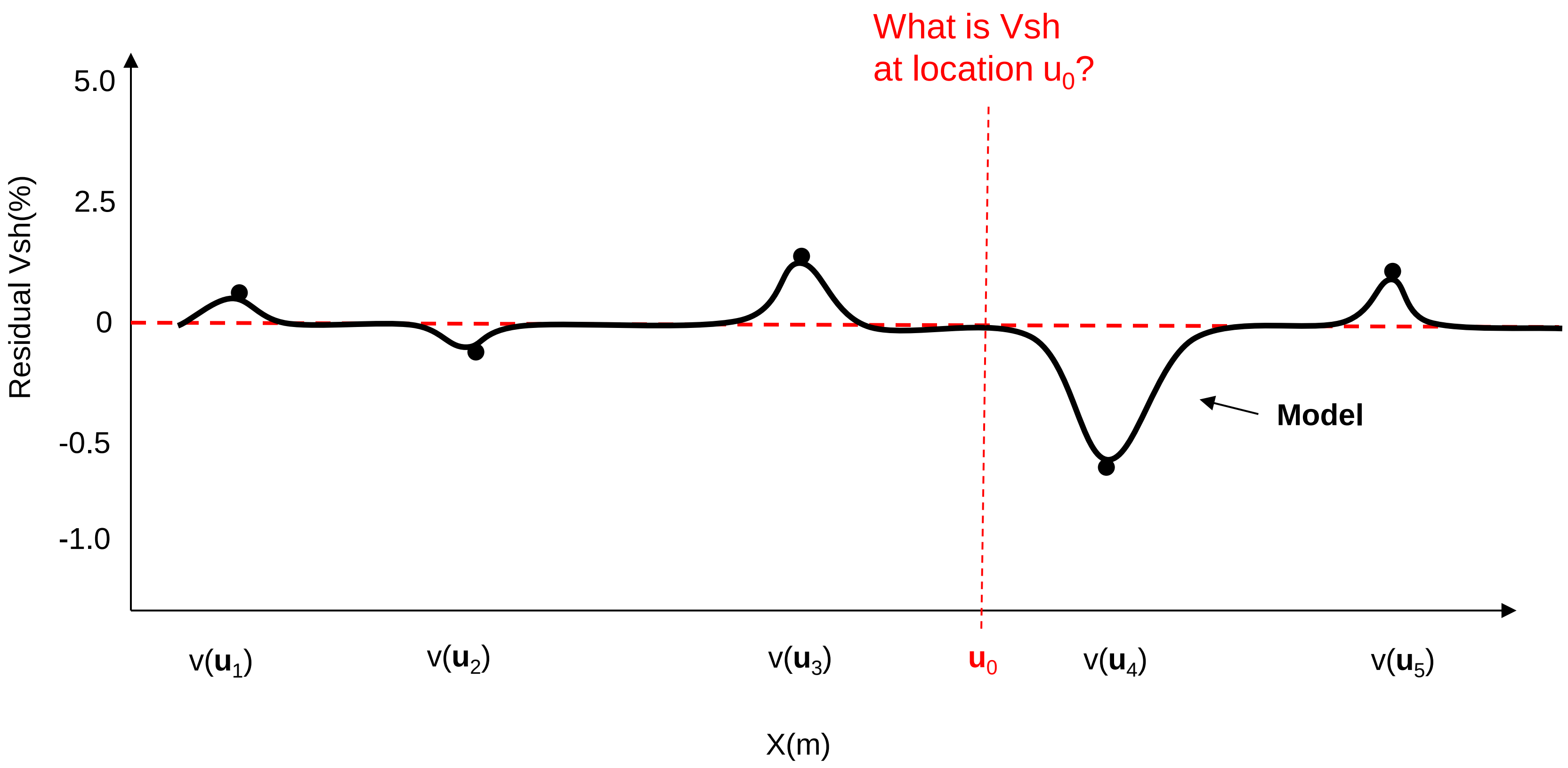
- If we observe a trend, we should model the trend.



# Trend and Residual Method

Geostatistical spatial estimation methods will make an assumption concerning stationarity

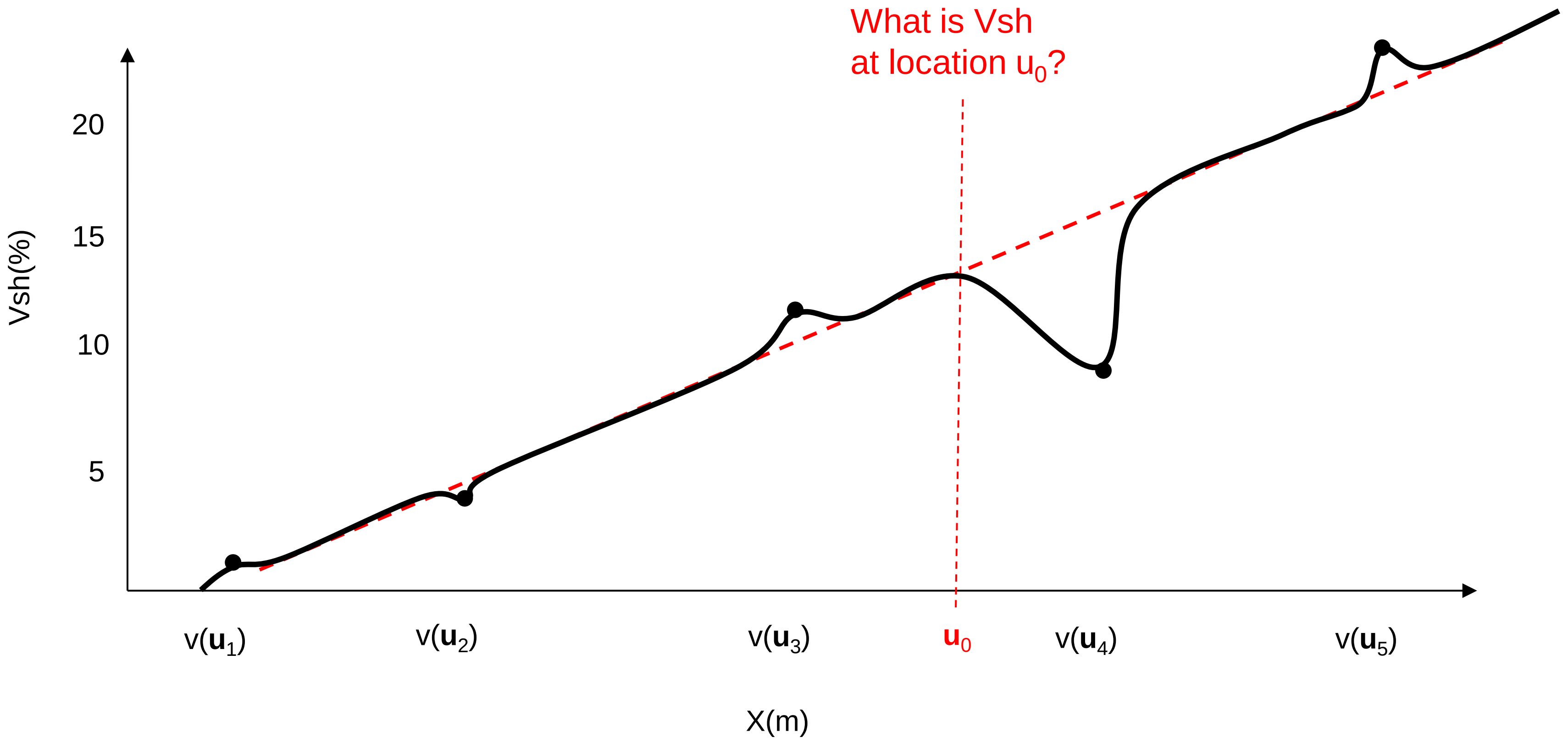
- Then model the residuals stochastically.



# Trend and Residual Method

Geostatistical spatial estimation methods will make an assumption concerning stationarity

- Add the trend back to the modelled residuals



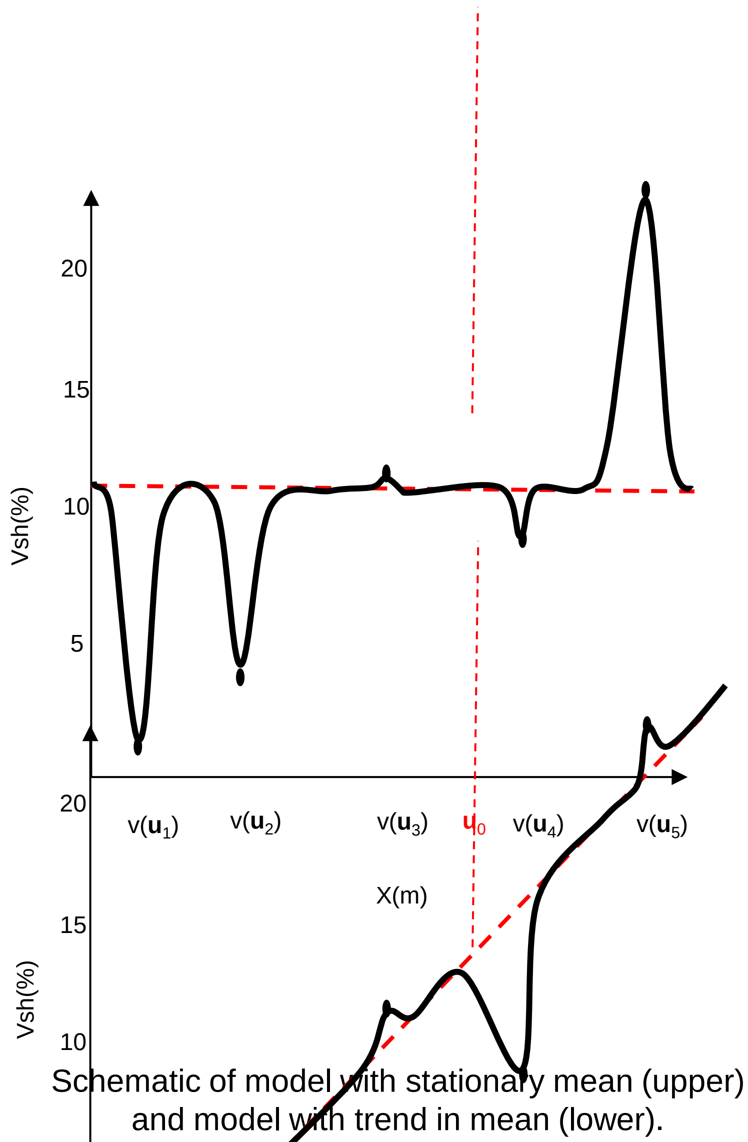
# Trend and Residual Method

How bad could it be if we did not model a trend?

- Geostatistical estimation would assume stationarity and away from data we would estimate with the global mean (i.e., simple kriging)!

**Model with stationary mean + data.**

**Model with mean trend model and residual + data.**




Schematic of model with stationary mean (upper) and model with trend in mean (lower).

# Trend Modeling Method

Trend Modeling

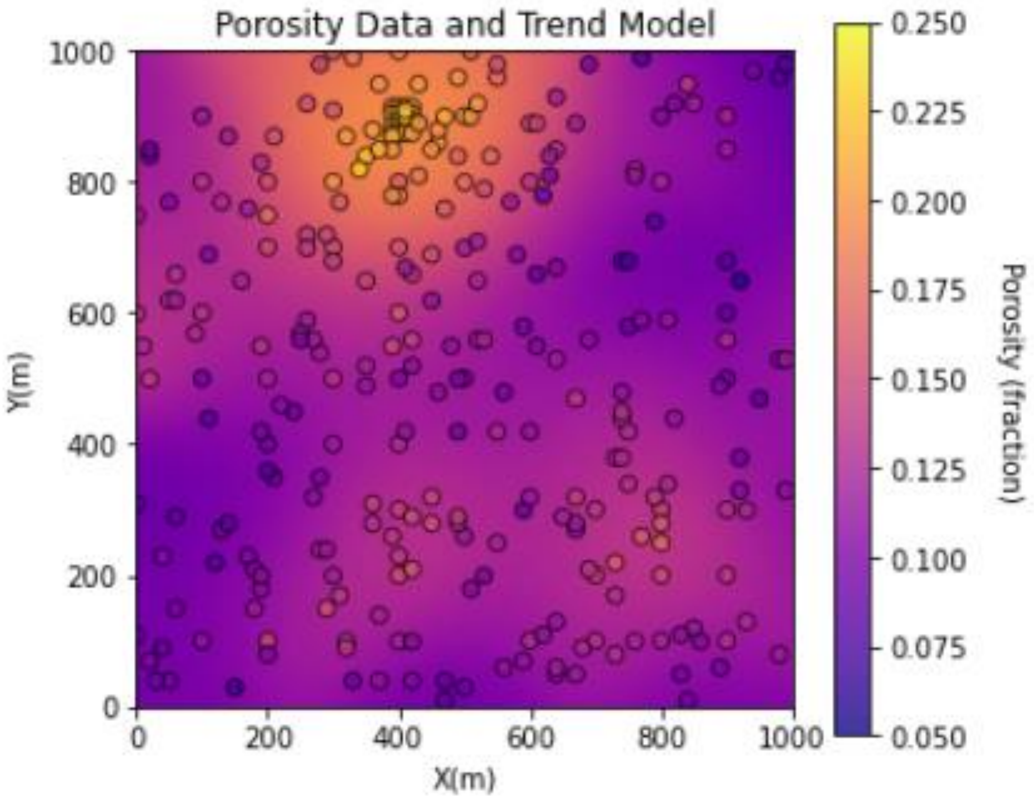
- We must identify and model trends
- Trends in model statistics (e.g., mean) are also known as 'nonstationarities'

We discuss data-driven trend modeling here, but any trend model should include data integration over the entire subsurface asset team

- Geology
- Geophysics
- Petrophysics
- Reservoir Engineering

We are going to build a model by summing 2 components:

1. trend model for the mean
2. residual model



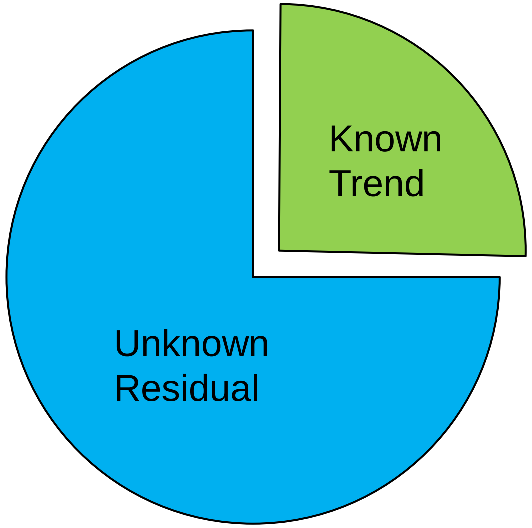

Example porosity data and trend model to model nonstationarity in the mean.

# Trend Modeling Method

Any variance in the [assumed] known trend is removed from the unknown residual:

$$\sigma_X^2 = \sigma_{X_t}^2 + \sigma_{X_r}^2 + 2C_{X_t,X_r}$$

if the $X_t \perp\!\!\!\perp X_r, C_{X_t,X_r} = 0$ $\quad\quad$ $\sigma_{X_r}^2 = \sigma_X^2 - \sigma_{X_t}^2$




Partitioning variance
between trend and residual.

- If $\boldsymbol{\sigma_X^2}$ is the total variance (variability), and $\boldsymbol{\sigma_{X_t}^2}$ is the variability that is deterministically modelled, treated as known, and $\boldsymbol{\sigma_{X_r}^2}$ is the component of the variability that is treated as unknown.
- Result: the more variability explained by the trend the less variability that remains as uncertain.

# Additivity of Variance for Decomposing Trend and Residual

Can we partition variance of random variable $Z$ between trend ($X$) and residual ($Y$)?

- Start with the variance of $Z$:

$$\sigma_Z^2 = E(Z^2) - [E(Z)]^{\,2}$$

- Substitute: $Z = \mathrm{X} + \mathrm{Y}$

Recall Covariance is
$C_{XY} = E(XY) - E(X)E(Y)$

$$\sigma_{X+Y}^2 = E\big((X+Y)^2\big) - [E(X+Y)]^{\,2}$$

$$\sigma_{X+Y}^2 = E(X^2 + 2XY + Y^2) - [E(X) + E(Y)]^{\,2}$$

$$\sigma_{X+Y}^2 = E(X^2) + 2E(XY) + E(Y^2) - \left(E(X)^2 + 2E(X)E(Y) + E(Y)^2\right)$$

$$\sigma_{X+Y}^2 = \underbrace{\boxed{E(X^2) - E(X)^2}}_{\boldsymbol{\sigma_X^2}} + \underbrace{\boxed{E(Y^2) - E(Y)^2}}_{\boldsymbol{\sigma_Y^2}} + 2\underbrace{\boxed{\big(E(XY) - E(X)E(Y)\big)}}_{\boldsymbol{C_{XY}(0)}}$$

$$\sigma_{X+Y}^2 = \sigma_X^2 + \sigma_Y^2 + 2C_{XY}(0)$$ ← Additivity of variance

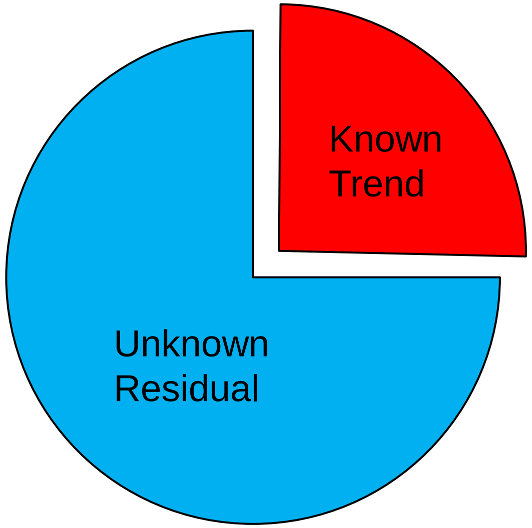
If the $X \perp\!\!\!\perp Y, C_{XY}(0)$ = 0, then $\sigma_{X+Y}^2 = \sigma_X^2 + \sigma_Y^2$

# Definition
# Deterministic Model

Model that assumes perfect knowledge, without uncertainty

- Based on knowledge of the phenomenon or trend fitting to data

- Most subsurface models have a deterministic component (trend) to capture expert knowledge and to provide a stationary residual for geostatistical modeling.



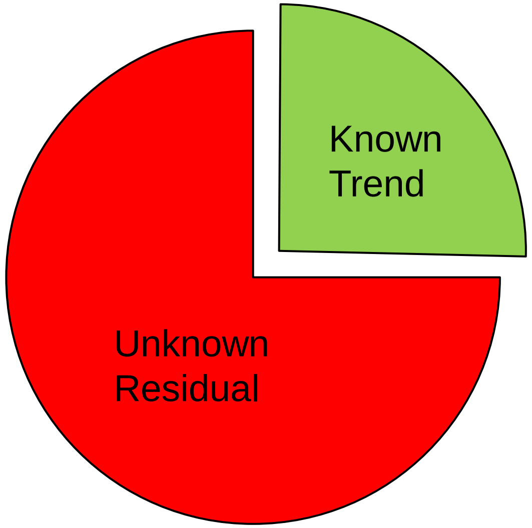

Partitioning variance between trend and residual.

# Definition Stochastic Model

The unknown residual is modeled as a **stochastic, statistical model**

- Model that integrates uncertainty through the concept of random variables and functions
- Based primarily on data-driven statistics and various forms of integration of domain and local knowledge
- Most subsurface models have a stochastic component (residual) to quantify the uncertain component of the model (as opposed to the certain component from the trend model)

Note, more about stochastic, statistical models later this lecture and over the next few lectures.




Partitioning variance between trend and residual.

# Trend Modeling Method

Trend Modeling Workflow

- Start with spatial data, $Z(\mathbf{u}_\alpha)$, $\alpha = 1, \dots, n$ data

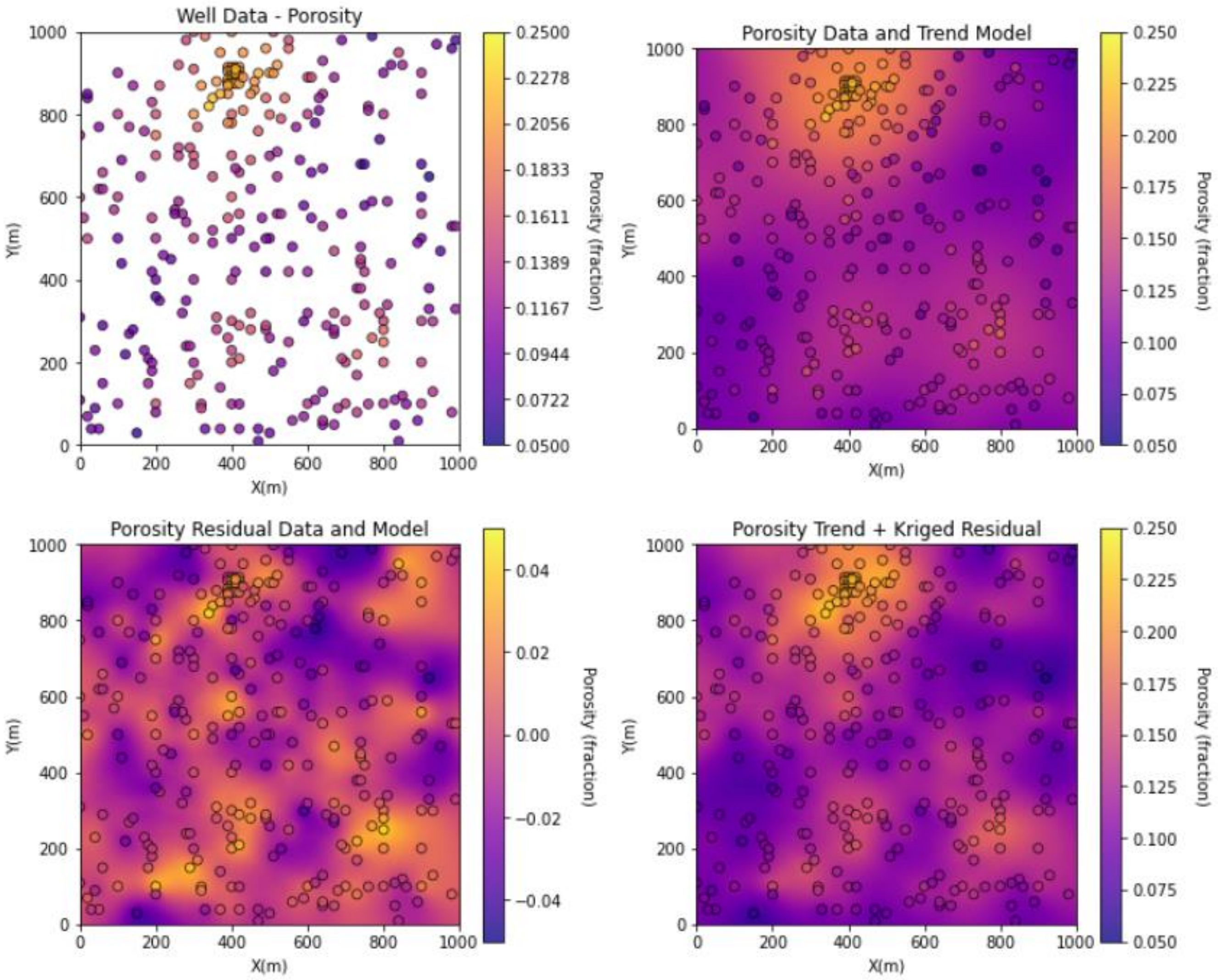
- Fit a deterministic trend model to the data to model nonstationarity in the mean, at data $Z_t(\mathbf{u}_\alpha)$ and away from data, $Z_t(\mathbf{u}_\beta)$, $\beta = 1, \dots, n_c$ model cells

- Calculate the residual at data locations, $Z_r(\mathbf{u}_\alpha) = Z(\mathbf{u}_\alpha) - Z_t(\mathbf{u}_\alpha)$

- Calculate a statistical residual away from the data, $Z_r(\mathbf{u}_\beta)$

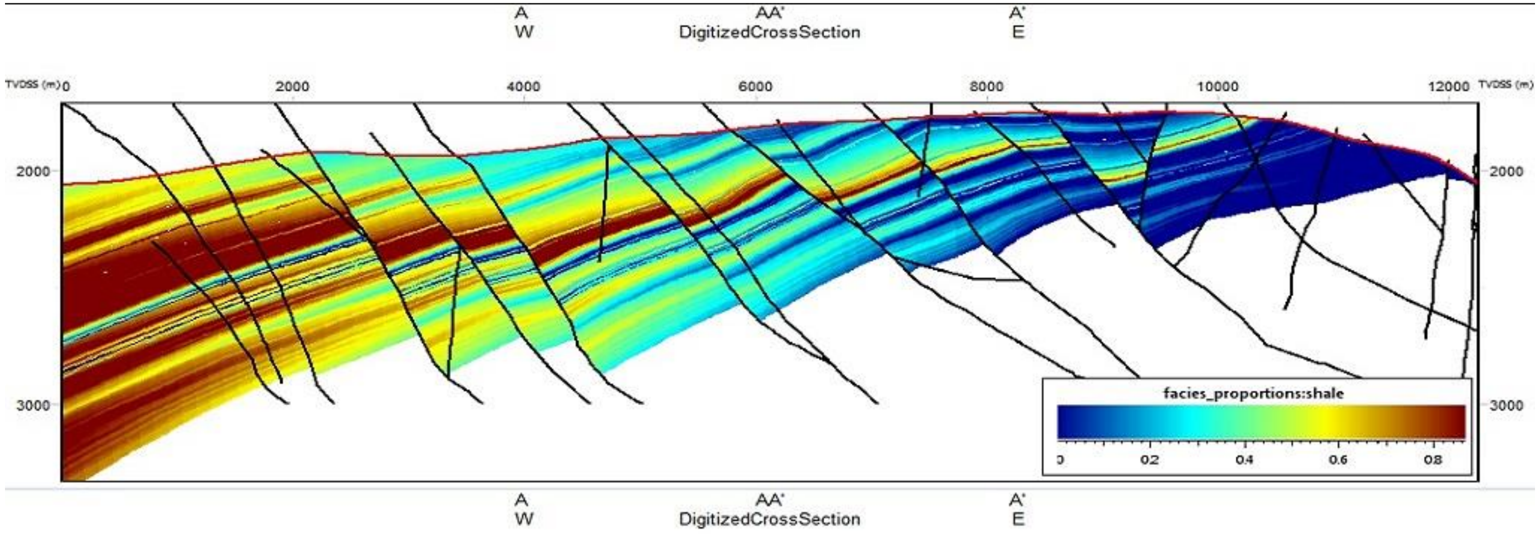
- Add the trend and residual models to calculate the trend + residual model

$$Z(\mathbf{u}_\beta) = Z_t(\mathbf{u}_\beta) + Z_r(\mathbf{u}_\beta)$$



Complete additive trend and residual modeling workflow, from GeostatsPy_trends.ipynb.

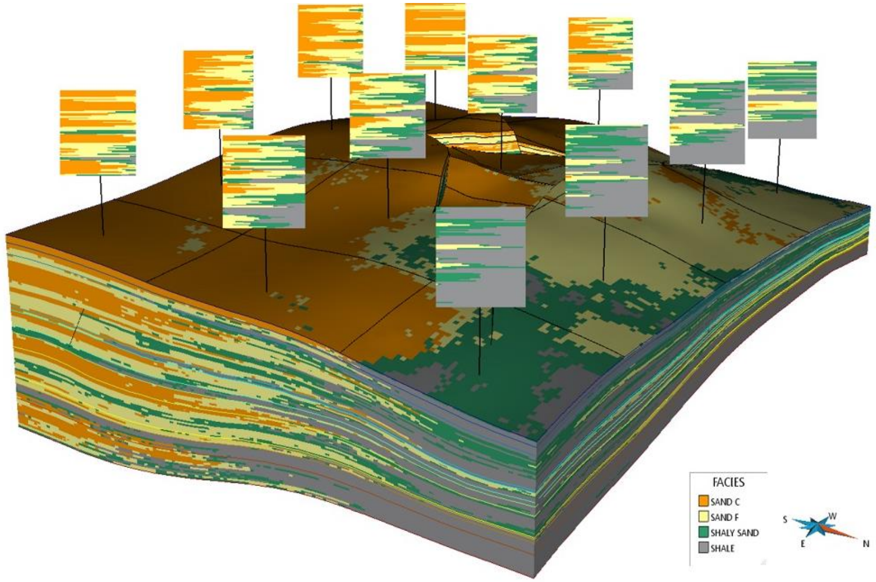
# Trend Modeling Methods




Example facies trend model Gocad SKUA. http://www.pdgm.com/getdoc/b24891f9-7470-4728-8cb7-0ddd7df196df/skua-facies-modeling/

Trend models:

- Tend to be smooth, based on data and interpretation
- May be complicated (see above)
- Parameterized by vertical proportion curves (see right) and areal trend maps

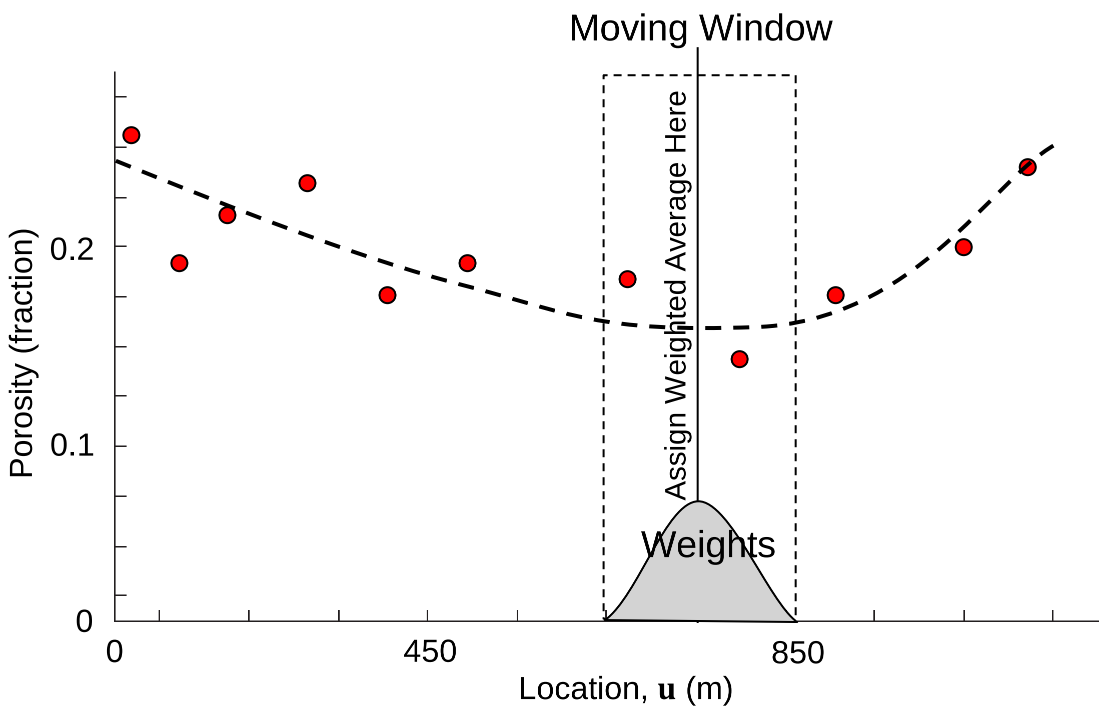



Example facies trend model Gocad. http://www.pdgm.com/getdoc/bd9ab6b6-7dbb-4023-8f79-de34238d5136/skua-reservoir-data-analysis/

# Trend
# Modeling Methods

How to calculate a trend model? E.g.:

- Moving window average of the available data
- Weighting scheme within the window
  - Uniform weights can cause discontinuities
  - Reduce weight at edges of the moving window to reduce discontinuities (e.g., Gaussian distributed weights).




Schematic of 1D data (●) , moving window weights and trend model ( ).

# Trend 2D + 1D Workflow

Calculate a 2D Areal trend and 1D Vertical trends:

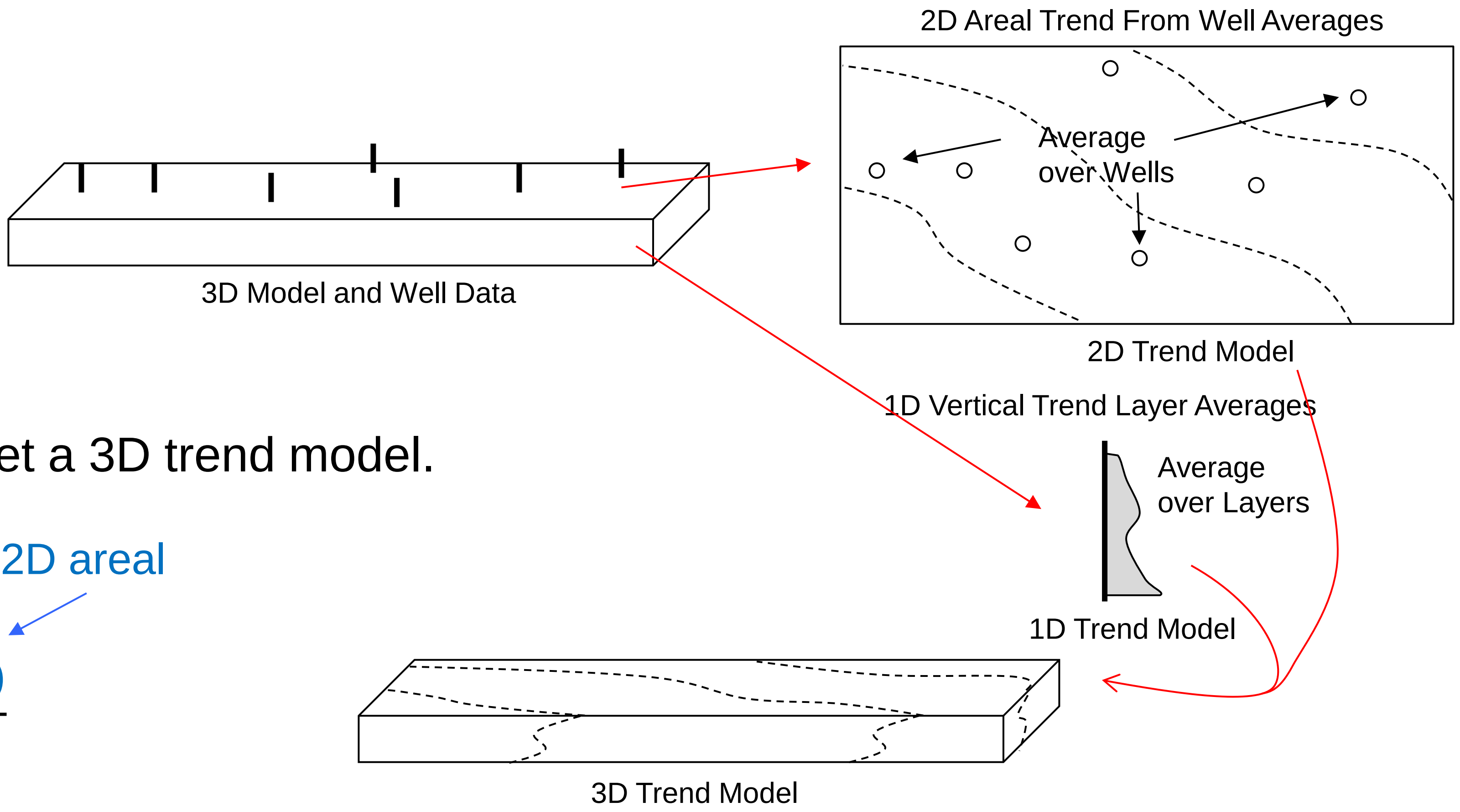
- Combine 1D and 2D trends to get a 3D trend model.

1D vertical

2D areal

$$\bar{X}(\mathbf{x},\mathbf{y},\mathbf{z}) = \bar{X}(\mathbf{z}) \cdot \frac{\bar{X}(\mathbf{x},\mathbf{y})}{\bar{X}}$$

global average




Schematic of the 1D vertical trend + 2D areal trend to calculate a 3D trend model workflow.

# Trend 2D + 1D Workflow

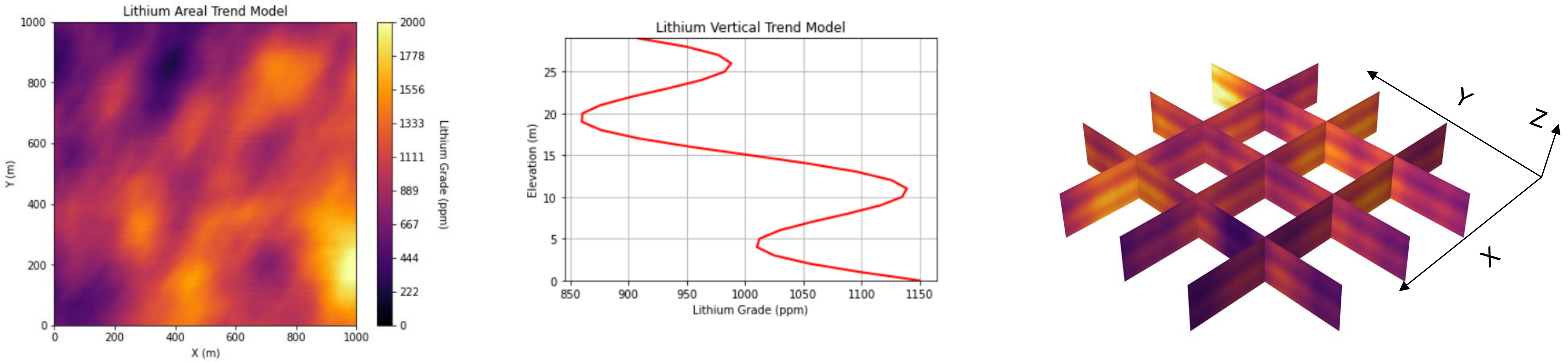
How to calculate a trend model with sparse data

- Break the problem up into a 1D and 2D trend inference problem and then combine to calculate a reasonable 3D trend
- Calculate the 2D areal trend by interpolating over vertically averaged wells.
- Calculate the 1D vertical trend by averaging layers
- Combine the 1D vertical and the 2D areal trends:

3D Trend
1D Vertical Trend
2D Areal Trend

$$\overline{X}(x,y,z) = \overline{X}(z) \cdot \frac{\overline{X}(x,y)}{\overline{X}}$$

Global Mean




Lithium 3D trend (right) from 2D areal trend (left), 1D vertical trend (center).

# Trend Definition

Common Uses of the Term **Trend**

1. Observation of nonstationarity in any statistic, metric of interest

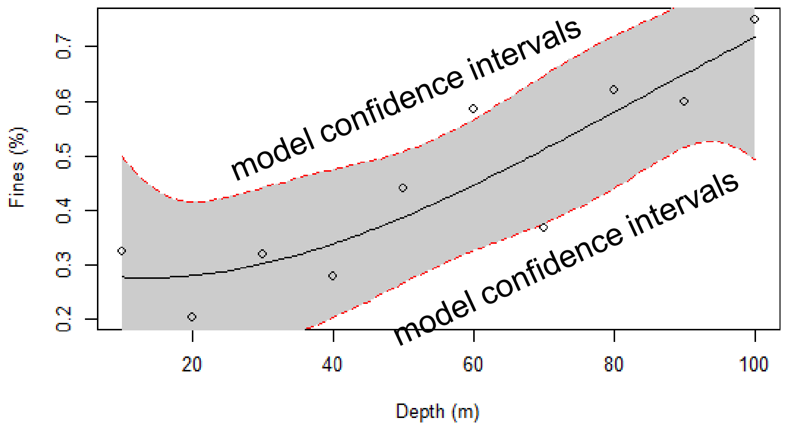
2. A model of the nonstationarity in any statistic, metric of interest

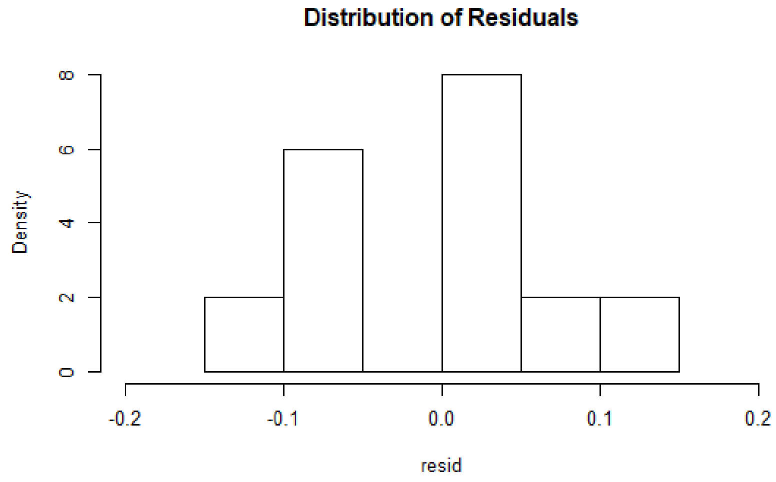
Typically modeled with support of data and expert knowledge in a deterministic manner (without uncertainty).

# Overfitting

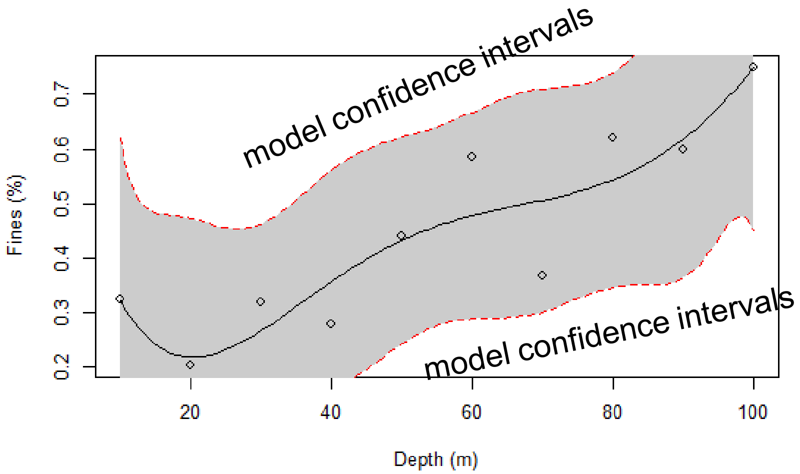
Example of trend fits:

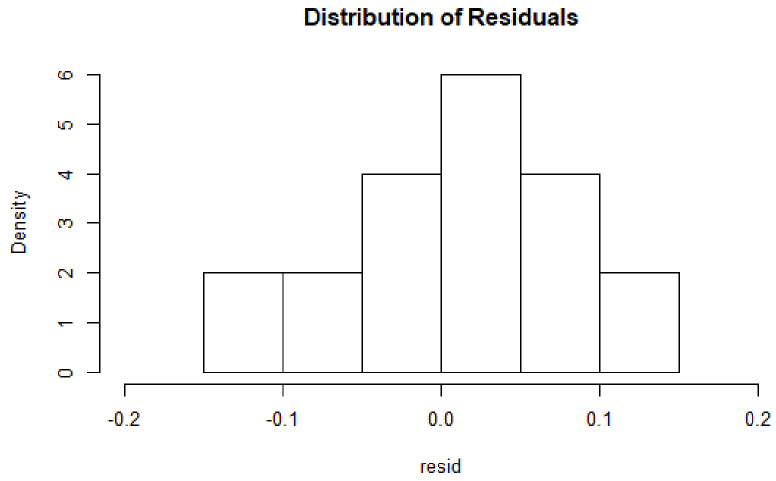
- 3rd Ordered Polynomial




- 5th Order Polynomial




Overfit demonstration in R, code is here: https://github.com/GeostatsGuy/geostatsr/blob/master/overfit.R

# Overfitting

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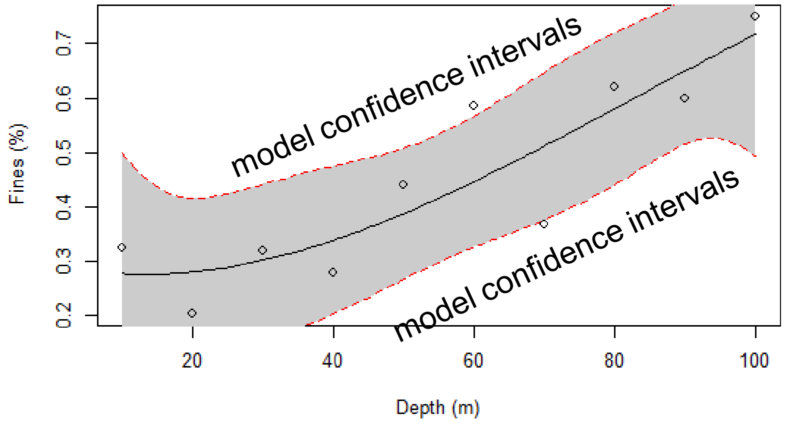
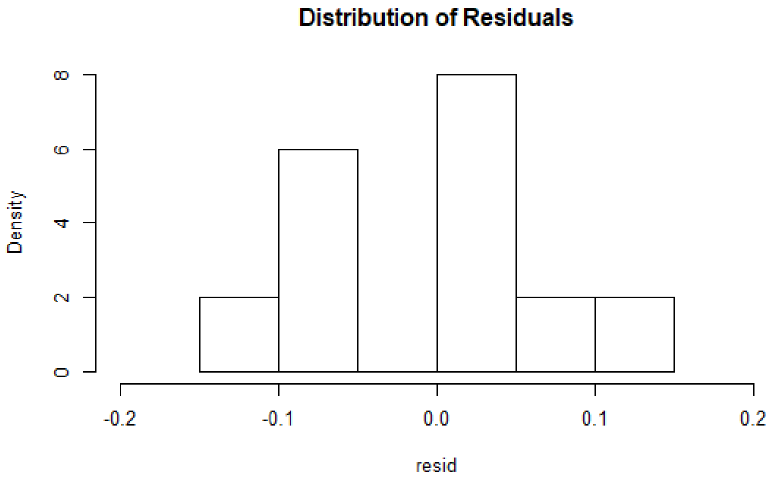
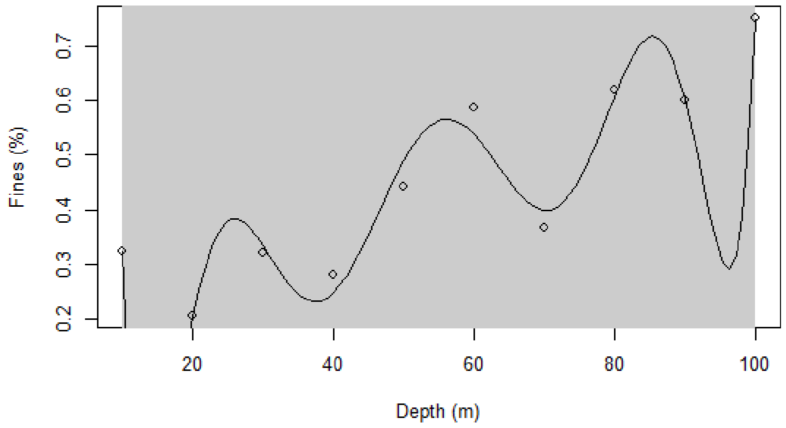
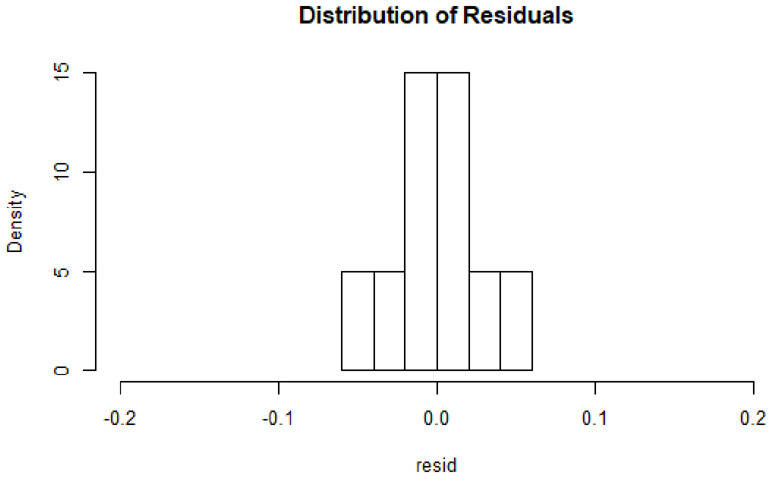



- 8th Order Polynomial



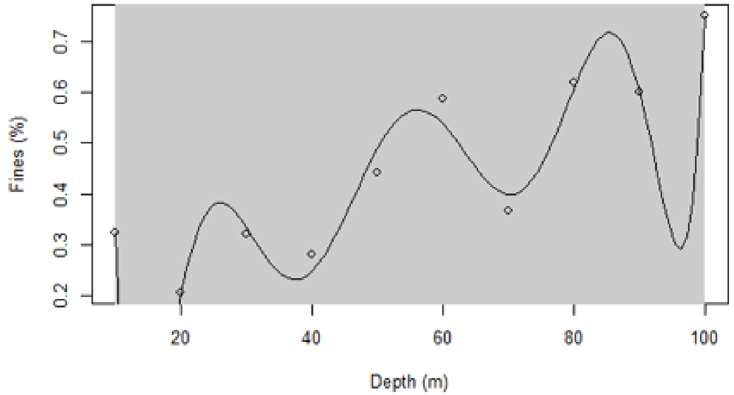

Overfit demonstration in R, code is here: https://github.com/GeostatsGuy/geostatsr/blob/master/overfit.R

# Definition of Overfitting

Overfitting

- Overly complicated model to explain “idiosyncrasies” of the data, capturing data noise in the model
- More parameters than can be justified with the data

- Results in likely very high error away from the data
- But, results in low residual variance that cannot be defended with available data!
- High $R^2$ - proportion of variance explained
- Very accurate at the data! - *Claim you know more than you do away from data!*

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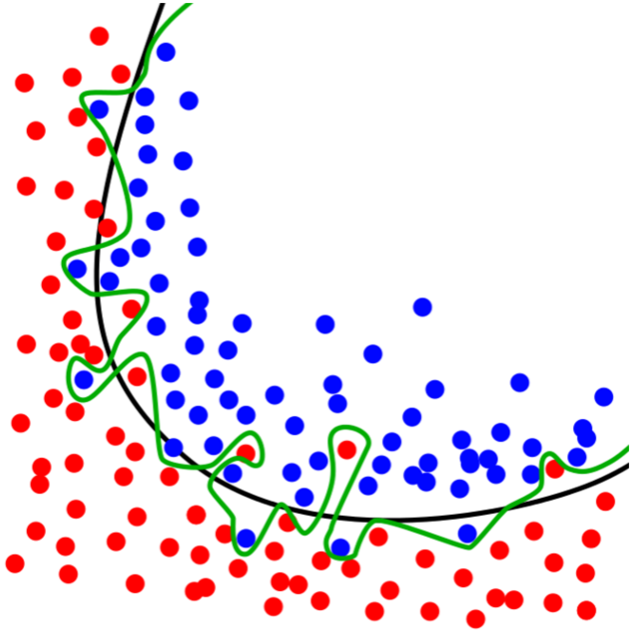


Overfit classification model example from: https://en.wikipedia.org/wiki/Overfitting#/media/File:Overfitting.svg

# Spatial Trend Modeling in Python

**Univariate Spatial Trend Modeling for Subsurface Data Analytics in Python**

**Michael Pyrcz, Associate Professor, University of Texas at Austin**

*Twitter* | *GitHub* | *Website* | *GoogleScholar* | *Book* | *YouTube* | *LinkedIn*

Here's a simple workflow with basic univariate spatial trend modeling for subsurface modeling workflows. This should help you get started with building subsurface models that include deterministic and stochastic components.

**Trend Modeling**

Trend modeling is the modeling of local features, based on data and interpretation, that are deemed certain (known). The trend is substracted from the data, leaving a residual that is modeled stochastically with uncertainty (treated as unknown).

- geostatistical spatial estimation methods will make an assumption concerning stationarity
  - in the presence of significant nonstationarity we can not rely on spatial estimates based on data + spatial continuity model
- if we observe a trend, we should model the trend.
  - then model the residuals stochastically

Steps:

1. model trend consistent with data and intepretation at all locations within the area of itnerest, integrate all available information and expertise.

$$m(\mathbf{u}_\beta), \forall \beta \in \textbf{AOI}$$

2. substract trend from data at the $n$ data locations to formulate a residual at the data locations.

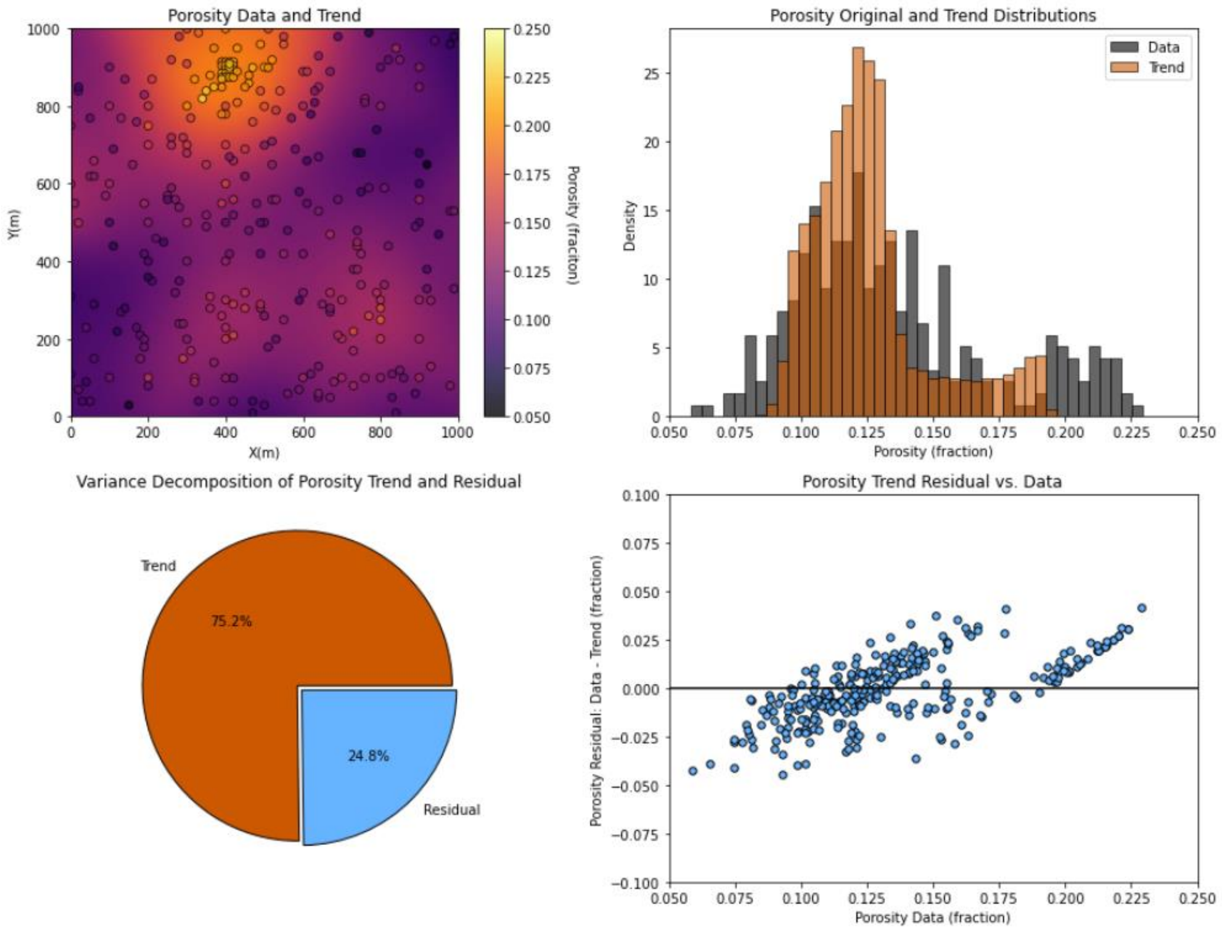
$$y(\mathbf{u}_\alpha) = z(\mathbf{u}_\alpha) - m(\mathbf{u}_\alpha), \forall \alpha = 1, \ldots, n$$

3. characterize the statistical behavoir of the residual $y(\mathbf{u}_\alpha)$ integrating any information sources and interpretations. For example the global cumulative distribution function and a measure of spatial continuity shown here.

$$F_y(y) \quad \gamma_y(\mathbf{h})$$

4. model the residual at all locations with $L$ multiple realizations.

2D trend modeling and checking workflow GeostatsPy_trends.ipynb.




Trend model and trend checking, trend diagnostic plots.

# Interactive Spatial Trend Modeling in Python

### Interactive Trend Modeling for Spatial Estimation Demonstration

#### Michael Pyrcz, Associate Professor, University of Texas at Austin

*Twitter* | *GitHub* | *Website* | *GoogleScholar* | *Book* | *YouTube* | *LinkedIn*

#### The Interactive Workflow

Here's a interactive demonstration of:

* trend fitting
* spatial estimation with a trend model vs. a stationary mean

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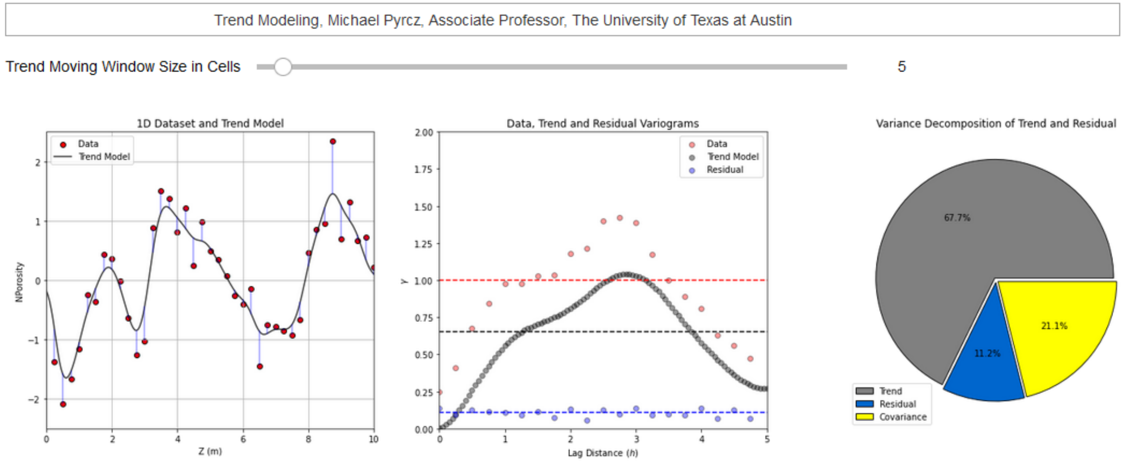
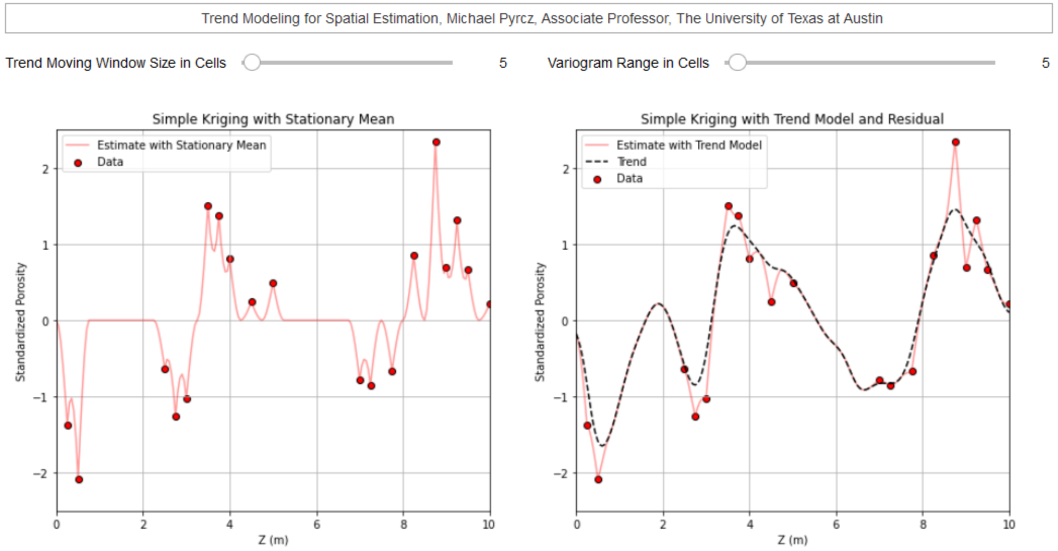
Interactive trend modeling demonstration Interactive_Trend.ipynb.




Trend and residual variance and variograms.




Additive trend and residual model in 1D.

# PGE 338 Data Analytics and Geostatistics

## Lecture 12: Spatial Estimation

**Lecture outline . . .**

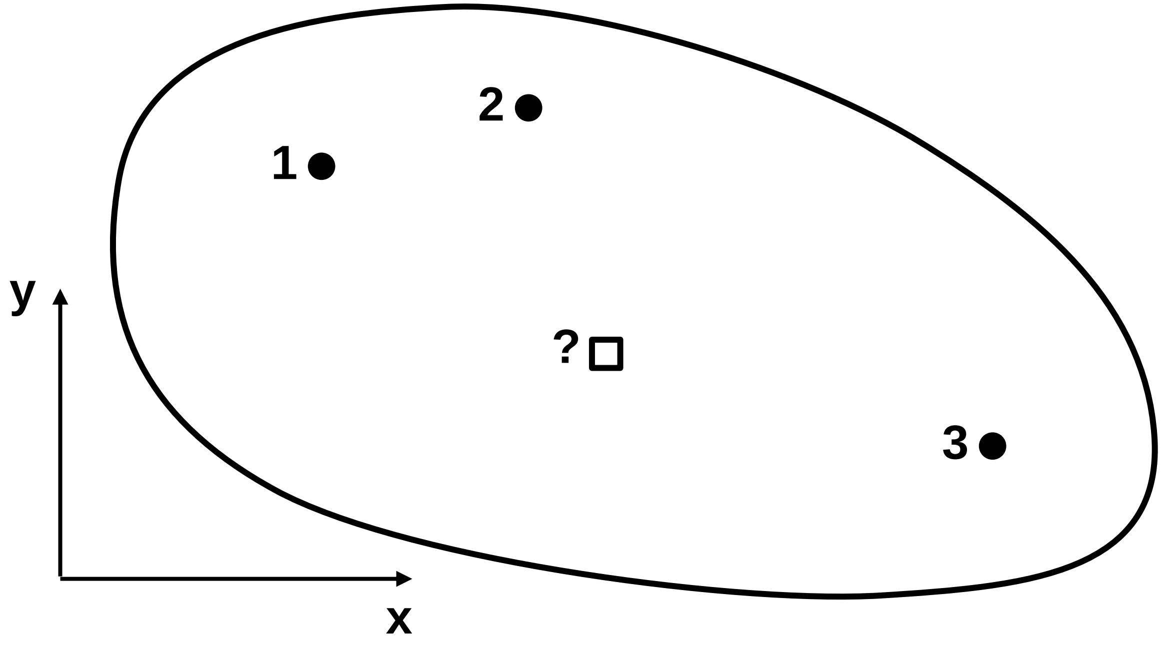
- Kriging



Michael Pyrcz, The University of Texas at Austin

# Spatial Estimation

Consider the case of estimating at an unsampled location:

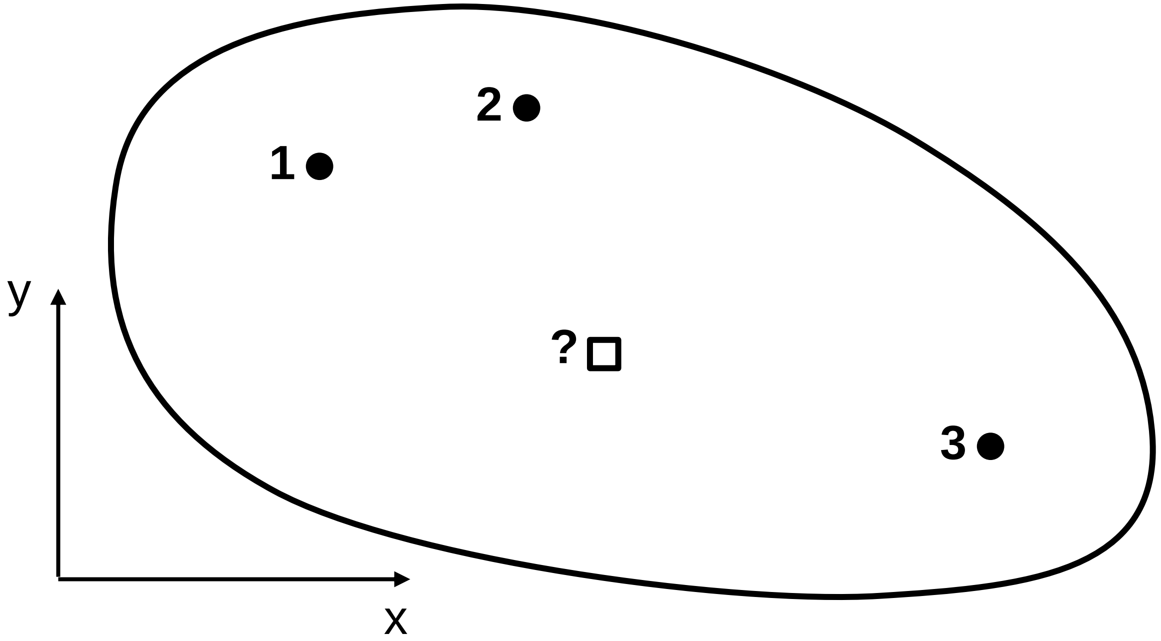



- How would you do this given data, $z(\mathbf{u}_1)$, $z(\mathbf{u}_2)$, and $z(\mathbf{u}_3)$?

Note: z is the variable of interest (e.g., porosity etc.) and $\mathbf{u}_i$ are the $i = [1,2,3]$ data locations.

# Spatial Estimation

Consider the case of estimating at an unsampled location:




$\mathbf{z}(\mathbf{u}_\alpha)$ **are the data values**

$z^*(\mathbf{u}_0)$ **is an estimate**

$\lambda_\alpha$ **are the data weights**

$m_z$ **is the global mean**

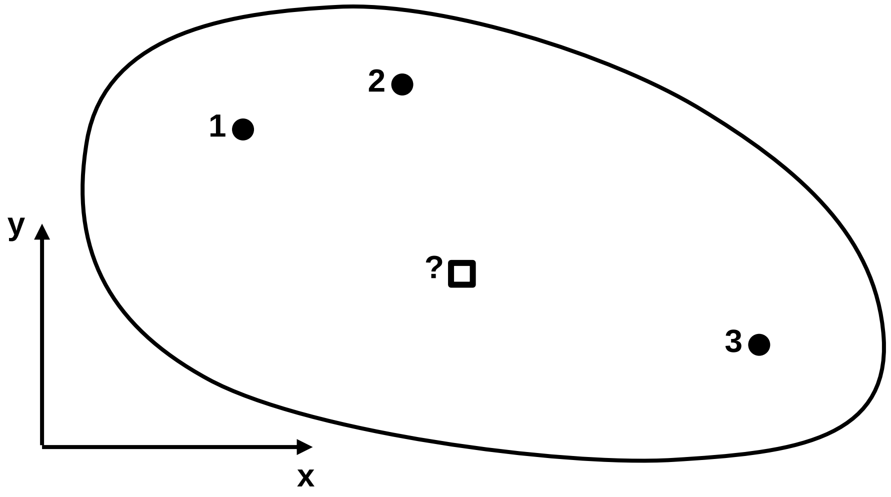
- How would you do this given data, $z(\mathbf{u}_1)$, $z(\mathbf{u}_2)$, and $z(\mathbf{u}_3)$?

$$z^*(\mathrm{u}_0) = \sum_{\alpha=1}^{n} \lambda_\alpha \mathrm{z}(\mathrm{u}_\alpha) + \boxed{\left(1 - \sum_{\alpha=1}^{n} \lambda_\alpha\right) m_z}$$

**Unbiasedness Constraint Weights sum to 1.0.**

# Spatial Estimation

Consider the case of estimating at an unsampled location:




- How do we get the weights? $\boldsymbol{\lambda_{\alpha}, \alpha = 1, \ldots, n}$

It would be good to use weights that account for,

1. closeness,
2. redundancy,
3. Variogram (covariance) model

How can we do that?

# Derivation of Simple Kriging Equations

Consider a linear estimator:

$$Y^*(\mathbf{u}) = \sum_{i=1}^{n} \lambda_i \cdot Y(\mathbf{u}_i)$$

where $Y(\mathbf{u}_i)$ are the residual data (data values minus the mean) and $Y^*(\mathbf{u}_i)$ is the estimate (add the mean back in when we are finished)

Stationary Mean, Variogram

$$E\{Y\} = 0$$

$$2\gamma(\mathbf{h}) = E\left\{\left[Y(\mathbf{u}) - Y(\mathbf{u}+\mathbf{h})\right]^2\right\}$$

- The **estimation variance** is defined as:

$$E\left\{\left[Y^*(u) - Y(u)\right]^2\right\} = \ldots$$

$$= E\left\{\left[Y^*(u)\right]^2\right\} - 2\,E\left\{Y^*(u)\;Y(u)\right\} + E\left\{\left[Y(u)\right]^2\right\}$$

$$= \sum_{i=1}^{n}\sum_{j=1}^{n} \lambda_i \lambda_j E\left\{Y(u_i)\;Y(u_j)\right\} - 2\sum_{i=1}^{n} \lambda_i E\left\{Y(u)\;Y(u_i)\right\} + C(0)$$

$$= \sum_{i=1}^{n}\sum_{j=1}^{n} \lambda_i \lambda_j C(u_i,u_j) - 2\sum_{i=1}^{n} \lambda_i C(u,u_i) + C(0)$$

**redundancy** **closeness** **variance**

$C(\mathbf{u}_i,\mathbf{u}_j)$ – covariance between data i and j, $C(\mathbf{u}_i,\mathbf{u})$covariance between data and unknown location and $C(0)$ is the variance.

# Derivation of Simple Kriging Equations

- Optimal weights $\lambda_i, i = 1, \ldots, n$ may be determined by taking partial derivatives of the error variance w.r.t. the weights

$$\frac{\partial[\quad\quad]}{\partial \lambda_i} = \sum_{j=1}^{n} \lambda_j C(\mathbf{u}_i, \mathbf{u}_j) - 2 \cdot C(\mathbf{u}, \mathbf{u}_i), i = 1, \ldots, n$$

and setting them to zero

$$\sum_{j=1}^{n} \lambda_j C(\mathbf{u}_i, \mathbf{u}_j) = \cdot\, C(\mathbf{u}, \mathbf{u}_i), i = 1, \ldots, n$$

- This system of *n* equations with *n* unknown weights is the simple kriging (SK) system

# Kriging Definition

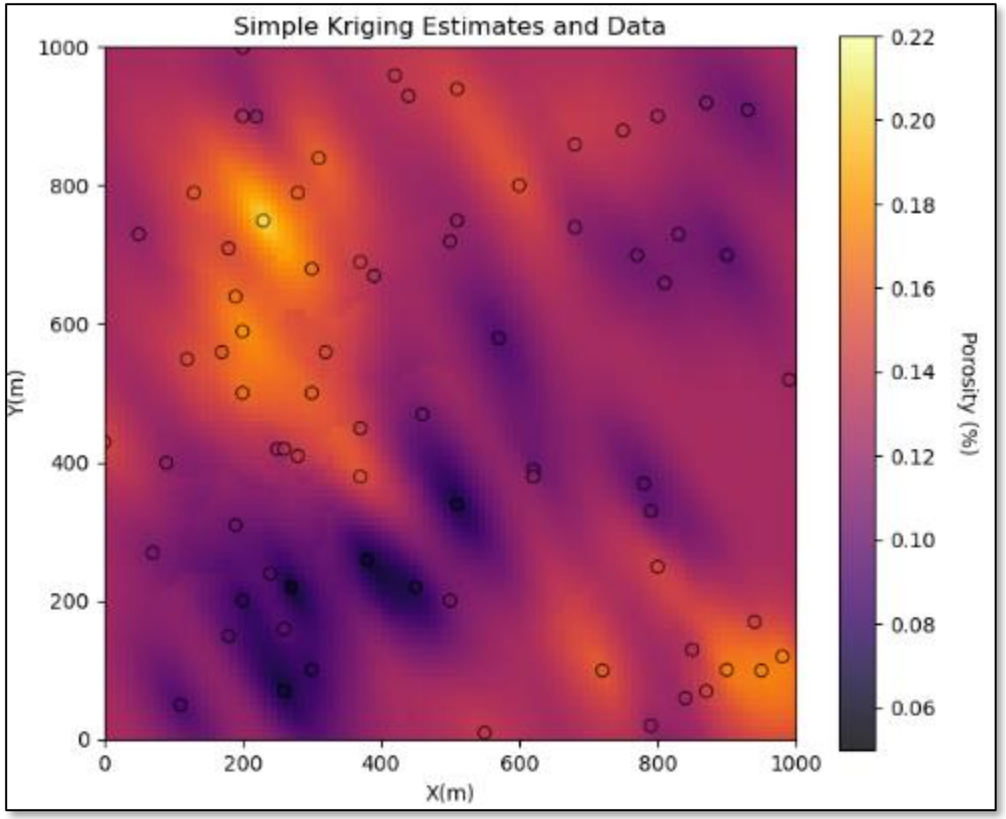
Spatial estimation method that,

- relies on linear weights

that account for,

- spatial continuity (variogram),
- data closeness and,
- redundancy.

Linear kriging estimates are unbiased and the weights minimize the estimation variance.

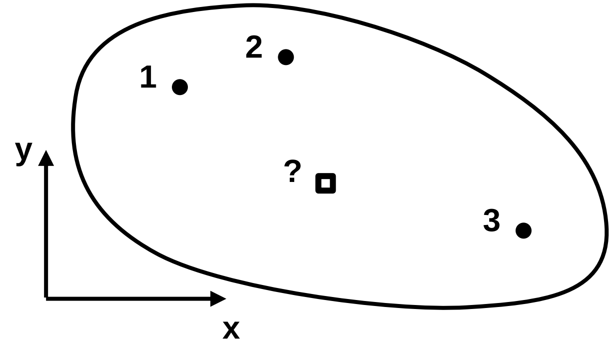



Map of porosity kriging estimates, from the Simple and Ordinary Kriging chapter of my Applied Geostatistics in Python e-book.

# Simple Kriging System of Equations

There are $n$ equations to determine the $n$ weights:

$$\lambda_1 \cdot C(\mathbf{u}_1,\mathbf{u}_1) + \lambda_2 \cdot C(\mathbf{u}_1,\mathbf{u}_2) + \lambda_3 \cdot C(\mathbf{u}_1,\mathbf{u}_3) = C(\mathbf{u},\mathbf{u}_1)$$
$$\lambda_1 \cdot C(\mathbf{u}_2,\mathbf{u}_1) + \lambda_2 \cdot C(\mathbf{u}_2,\mathbf{u}_2) + \lambda_3 \cdot C(\mathbf{u}_2,\mathbf{u}_3) = C(\mathbf{u},\mathbf{u}_2)$$
$$\lambda_1 \cdot C(\mathbf{u}_3,\mathbf{u}_1) + \lambda_2 \cdot C(\mathbf{u}_3,\mathbf{u}_2) + \lambda_3 \cdot C(\mathbf{u}_3,\mathbf{u}_3) = C(\mathbf{u},\mathbf{u}_1)$$




In matrix notation:

$$\underbrace{\begin{bmatrix} C(\mathbf{u}_1,\mathbf{u}_1) & C(\mathbf{u}_1,\mathbf{u}_2) & C(\mathbf{u}_1,\mathbf{u}_3) \\ C(\mathbf{u}_2,\mathbf{u}_1) & C(\mathbf{u}_2,\mathbf{u}_2) & C(\mathbf{u}_2,\mathbf{u}_3) \\ C(\mathbf{u}_3,\mathbf{u}_1) & C(\mathbf{u}_3,\mathbf{u}_2) & C(\mathbf{u}_3,\mathbf{u}_3) \end{bmatrix}}_{\textbf{redundancy}} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{bmatrix} = \underbrace{\begin{bmatrix} C(\mathbf{u},\mathbf{u}_1) \\ C(\mathbf{u},\mathbf{u}_2) \\ C(\mathbf{u},\mathbf{u}_3) \end{bmatrix}}_{\textbf{closeness}}$$

**redundancy**

Covariance between all combinations of data locations, $\mathbf{u}_\alpha$.

**closeness**

Covariance between all data locations, $\mathbf{u}_\alpha$, and the unknown location, $\mathbf{u}$, combinations of data.

## Notation Reminder

Locations of the data:

$$\mathbf{u}_\alpha, \alpha = 1, \dots, n$$

Estimate location:

$$\mathbf{u}$$

Data values at those locations:

$$y(\mathbf{u}_\alpha), \alpha = 1, \dots, n$$

Covariance between points, $\mathbf{u}_1$ and $\mathbf{u}_2$:

$C(\mathbf{u}_1,\mathbf{u}_2) = \sigma^2 - \gamma(\mathbf{u}_1,\mathbf{u}_2)$

# Properties of Simple Kriging

- Solution exists and is unique if matrix $C(\mathbf{u}_i, \mathbf{u}_j)$, kriging system left-hand side is positive definite, guaranteed by using nested, permissible variogram models.
  – additive nugget, spherical, exponential, Gaussian, etc. variogram structures

- Kriging estimator is unbiased, $E\{Y^* - Y\} = 0.0$, due to unbiasedness constraint,

$$z^*(\mathrm{u}_0) = \sum_{\alpha=1}^{n} \lambda_\alpha \mathrm{z}(\mathrm{u}_\alpha) + \left(1 - \sum_{\alpha=1}^{n} \lambda_\alpha\right) m_z$$

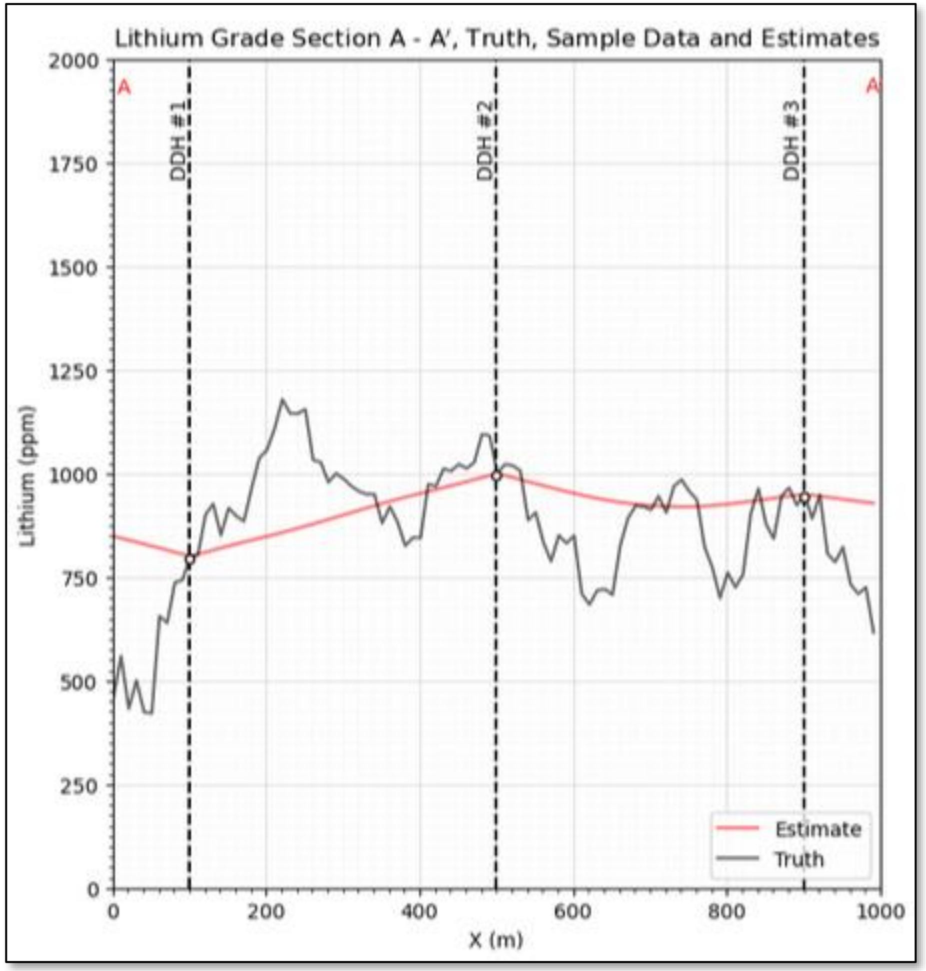
or use of a trend model, and kriged residual with mean of 0.0, $y^*(u_0) = \sum_{\alpha=1}^{n} \lambda_\alpha \, \mathrm{y}(u_\alpha)$ given, $y = z - m$

- Minimum error variance estimator (just try to pick weights, you won't bet it)

- Best Linear Unbiased Estimator (BLUE)

# Properties of Simple Kriging

- Exact interpolator, estimates with the data values at the data locations

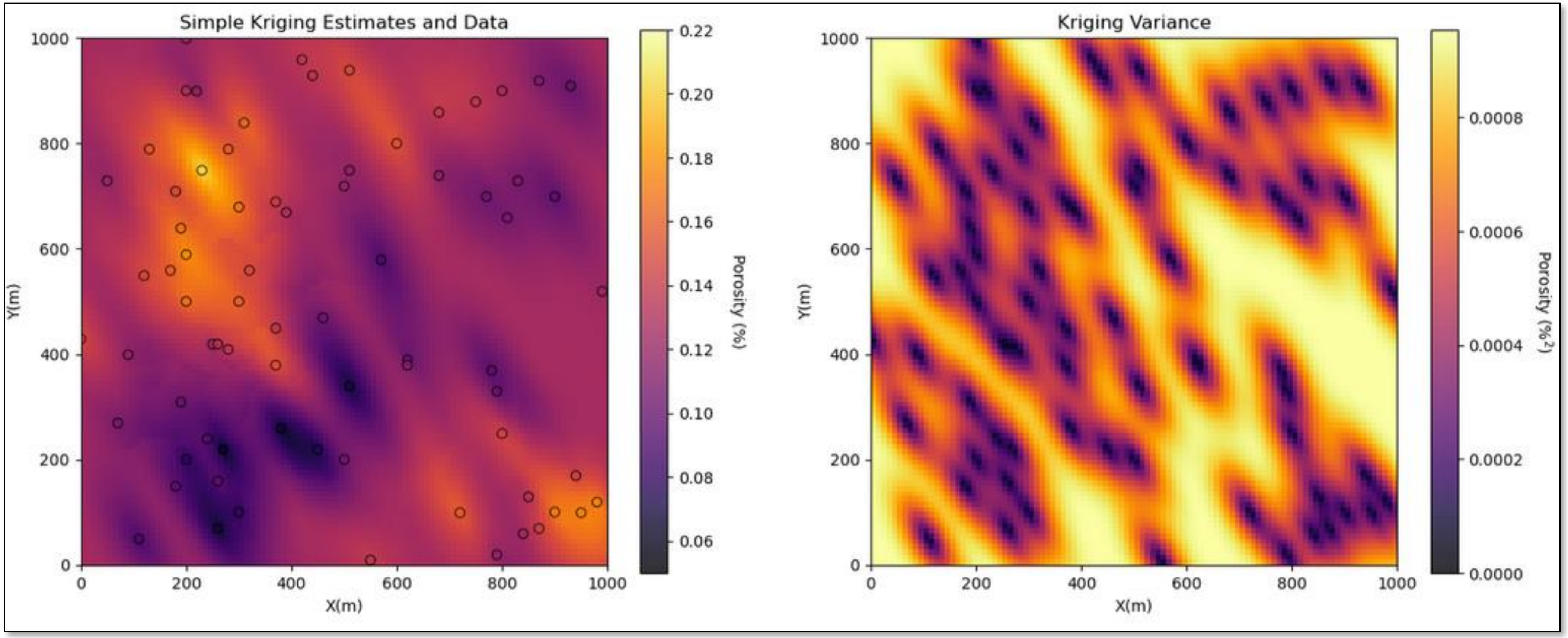



1D section with 3 drill holes, unknown truth (black) and kriging estimates (red), from the “Kriging vs. Simulation, 1D” chapter of my Applied Geostatistics in Python e-book.

# Properties of Simple Kriging

- Provides a measure of the estimation (or kriging) variance (uncertainty) in the kriging estimate:

$$\sigma_k^2(\mathbf{u}) = C(0) - \sum_{\alpha=1}^{n} \lambda_\alpha C(\mathbf{u} - \mathbf{u}_\alpha) \qquad \sigma_k^2 \in [0, \sigma_z^2]$$




Map of porosity kriging estimates, from the Simple and Ordinary Kriging chapter of my Applied Geostatistics in Python e-book.

# Properties of Simple Kriging

- Kriging variance can be calculated before getting the sample information, homoscedastic, i.e., depends on the data locations, not their values!

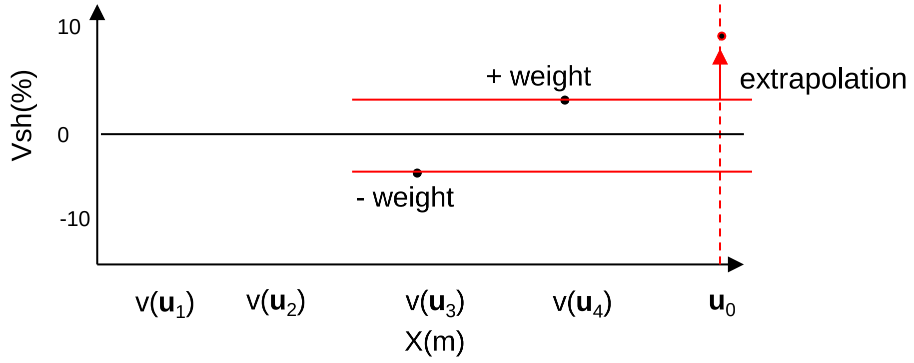
$$\sigma_k^2(\mathbf{u}) = C(0) - \sum_{\alpha=1}^{n} \lambda_\alpha C(\mathbf{u} - \mathbf{u}_\alpha)$$

- Kriging takes into account:
  - closeness of the data to the estimate, $C(\mathbf{u}_i, \mathbf{u})$
  - redundancy between the data, $C(\mathbf{u}_i, \mathbf{u}_j)$
  - structural continuity of the variable being considered, $C(\mathbf{h})$
- The smoothing effect of kriging can be forecast – we will return to this with simulation.

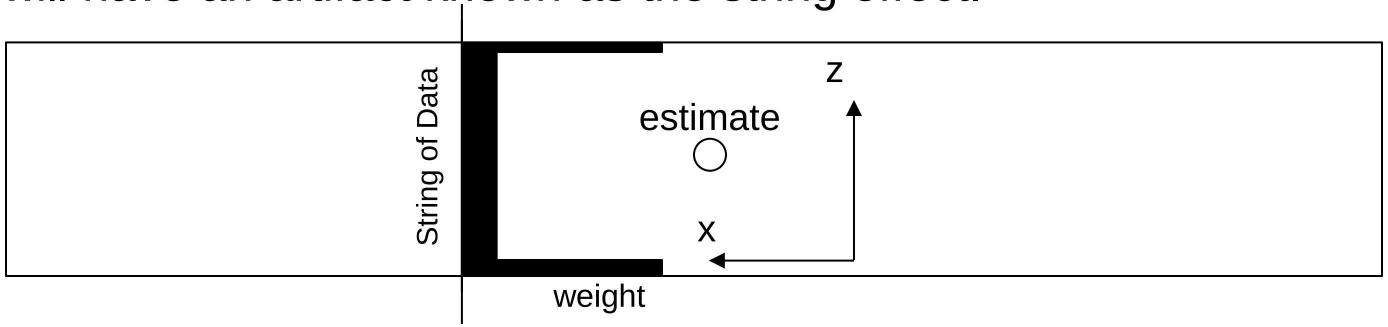
# Properties of Simple Kriging

- Outside range of the data, simple kriging weights all equal 0.0.  The best estimate is the provided mean!

- Screened data will sometimes have negative weights!  This allows kriging to extrapolate.




- Strings of data will have an artifact known as the string effect.



# Simple Kriging Exercise in Excel

To explore the nuts and bolts of simple kriging

- simple kriging to make 1 spatial estimate with Excel

- using a single variogram structure and assumed global mean

**Simple Kriging Demonstration**

*Michael Pyrcz, Geostatistics at Petroleum and Geosystems Engineering, University of Texas at Austin (mpyrcz@austin.utexas.edu)*

**1. Data and Estimate Locations and Values**

| Point | x | y | value | residual |
|---|---|---|---|---|
| 1 | 60 | 80 | 0.1 | -0.040 |
| 2 | 25 | 50 | 0.12 | -0.020 |
| 3 | 80 | 10 | 0.2 | 0.060 |
| unknown | 50 | 50 | | |
| mean | | | 0.140 | |

**2. Distance Matrix**

| | | | |
|---|---|---|---|
| 0.00 | 46.10 | 72.80 | 31.62 |
| 46.10 | 0.00 | 68.01 | 25.00 |
| 72.80 | 68.01 | 0.00 | 50.00 |

**3. Variogram Model**

| | |
|---|---|
| Nugget | 0 |
| Spherica | 1 |
| Range | 300 |

**4. Variogram Matrix**

| | | | |
|---|---|---|---|
| 0.000 | 0.229 | 0.357 | 0.158 |
| 0.229 | 0.000 | 0.334 | 0.125 |
| 0.357 | 0.334 | 0.000 | 0.248 |

**5. Covariance Matrix**

| | | | |
|---|---|---|---|
| 1.000 | 0.771 | 0.643 | 0.842 |
| 0.771 | 1.000 | 0.666 | 0.875 |
| 0.643 | 0.666 | 1.000 | 0.752 |

**6. Inverse Left Side**

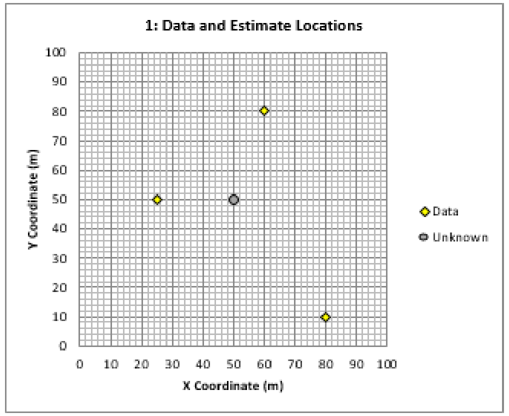
| | | |
|---|---|---|
| 2.667 | -1.644 | -0.621 |
| -1.644 | 2.810 | -0.813 |
| -0.621 | -0.813 | 1.941 |

**7. Weights**

| | |
|---|---|
| | 0.341 |
| | 0.462 |
| | 0.225 |
| *Sum Weights* | 1.029 |
| Mean Weight | -0.029 |

**8. Kriging Results**

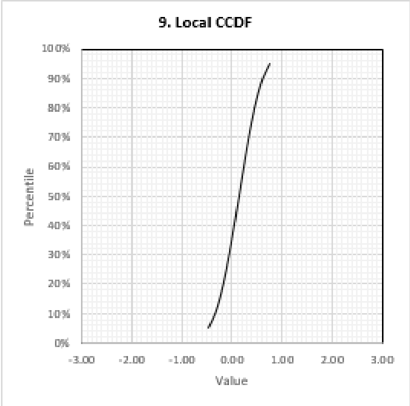
| | |
|---|---|
| *Kriging Estimate* | 0.131 |
| *Kriging Variance* | 0.139 |




Legend

| |
|---|
| Information |
| User Input |
| Calculation |
| Redundancy Measure |
| Closeness Measures |

| p-value | $F^{-1}(p)$ |
|---|---|
| 5% | -0.48 |
| 10% | -0.35 |
| 15% | -0.26 |
| 20% | -0.18 |
| 25% | -0.12 |
| 30% | -0.06 |
| 35% | -0.01 |
| 40% | 0.04 |
| 45% | 0.08 |
| 50% | 0.13 |
| 55% | 0.18 |
| 60% | 0.22 |
| 65% | 0.27 |
| 70% | 0.33 |
| 75% | 0.38 |
| 80% | 0.44 |
| 85% | 0.52 |
| 90% | 0.61 |
| 95% | 0.74 |




**Description**

This sheet provides an illustration of Simple Kriging at a single estimated location.

Step 1: Input the data locations and values, the unknown simulated location. At any point these locations and values may be changed to observed their influence on the simulation.
Step 2: The distance matrix is automatically calculated, that is the distance between the data and the unknown locations.
Step 3: Enter the model of spatial continuity in the form of an isotropic spherical variogram and nugget effect (contributions should sum to one). This model may be changed at any time to observed sensitivities to spatial continuity.
Step 4: Variogram matrix is calculated by applying the distance matrix to the isotropic variogram model.
Step 5: Covaraince matrix is calculated by subtracing the variogram from the variance (1 for standard normal distribution). This is applied to improve numerical stability as a diagonally dominant matrix is more readily invertable.
Step 6: The left hand side of the covariance matrix is inverted.
Step 7: The inverted left handside matrix is multiplied by the right hand side matrix to calculate the simple kriging weights.
Step 8: The kriging estimate and kriging variance are calculated with the weights and covariances.
Step 9: With the Gaussian assumption the complete local conditional cumulative distribution function is available.

Simple kriging in Excel, file is Simple_Kriging_Demo.xlsx

# Simple Kriging Exercise in Excel

Some ideas for experimenting with simple kriging. Do the following and pay attention to the weights, the estimate and the estimation variance.

1. Set points 1 and 2 closer together.

2. Put point 1 behind point 2 to create screening.

3. Put all points outside the range.

4. See the range very large.

# Ordinary Kriging

Add the constraint to the simple kriging system:

$$\sum_{\alpha=1}^{n} \lambda_\alpha = 1.0$$

$$\begin{bmatrix} C(\mathbf{u}_1,\mathbf{u}_1) & C(\mathbf{u}_1,u_2) & C(\mathbf{u}_1,\mathbf{u}_3) & 1 \\ C(\mathbf{u}_2,\mathbf{u}_1) & C(\mathbf{u}_2,u_2) & C(\mathbf{u}_2,\mathbf{u}_3) & 1 \\ C(\mathbf{u}_3,\mathbf{u}_1) & C(\mathbf{u}_3,u_1) & C(\mathbf{u}_3,\mathbf{u}_3) & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \mu \end{bmatrix} = \begin{bmatrix} C(\mathbf{u}_0,\mathbf{u}_1) \\ C(\mathbf{u}_0,\mathbf{u}_2) \\ C(\mathbf{u}_0,\mathbf{u}_3) \\ 1 \end{bmatrix}$$

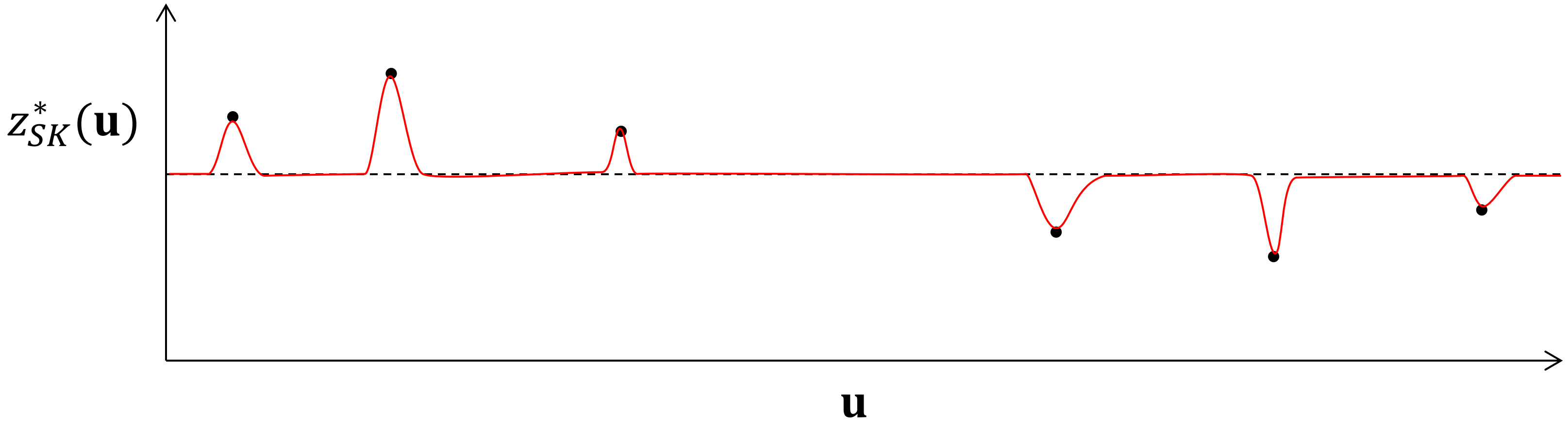
Recall: $C(\mathbf{h}) = C(0) - \gamma(\mathbf{h})$

Now we have:

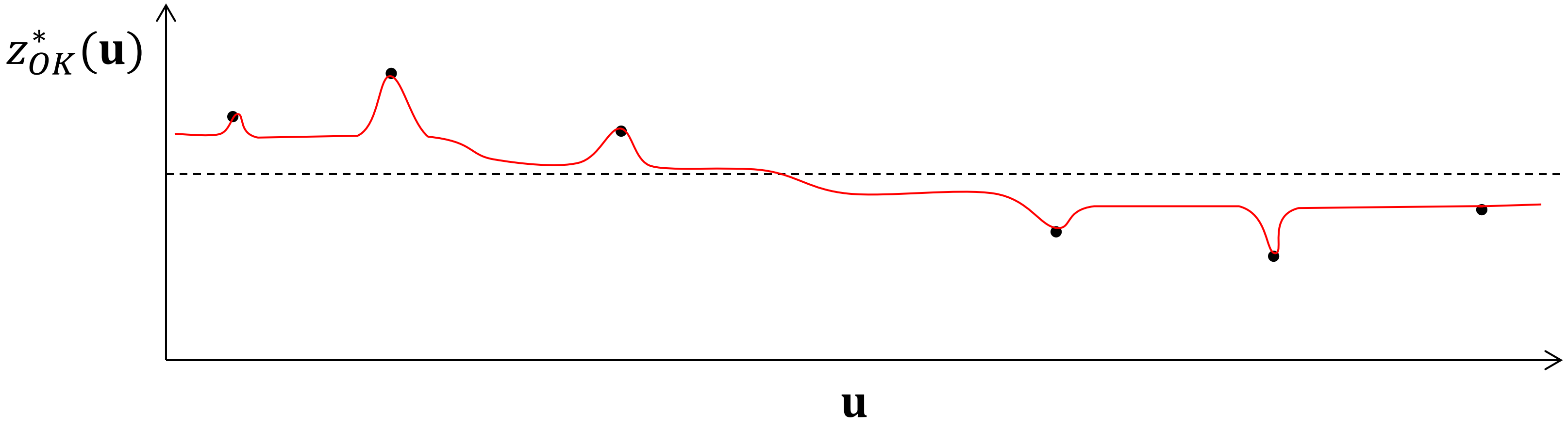
$$z^*(\mathrm{u}_0) = \sum_{\alpha=1}^{n} \lambda_\alpha z(\mathrm{u}_\alpha) + \cancelto{0}{\left(1 - \sum_{\alpha=1}^{n} \lambda_\alpha\right) m_z}$$

With ordinary kriging the mean does not need to be known. Ordinary kriging estimates the mean locally!

# Simple Kriging vs. Ordinary Kriging




Beyond the range of correlation, Simple Kriging estimates the global mean.




Beyond the range of correlation, Ordinary Kriging estimates with an estimated local mean. Relaxes the stationary mean assumption.

# Kriging Summary

- Kriging is a procedure for constructing a minimum error variance linear estimate at a location where the true value is unknown

- The main controls on the kriging weights are:
  - closeness of the data to the location being estimated
  - redundancy between the data
  - the variogram

- Simple Kriging (SK) does not constrain the weights and works with the residual from the mean

- Ordinary Kriging (OK) constrains the sum of the weights to be 1.0, therefore, the mean does not need to be known

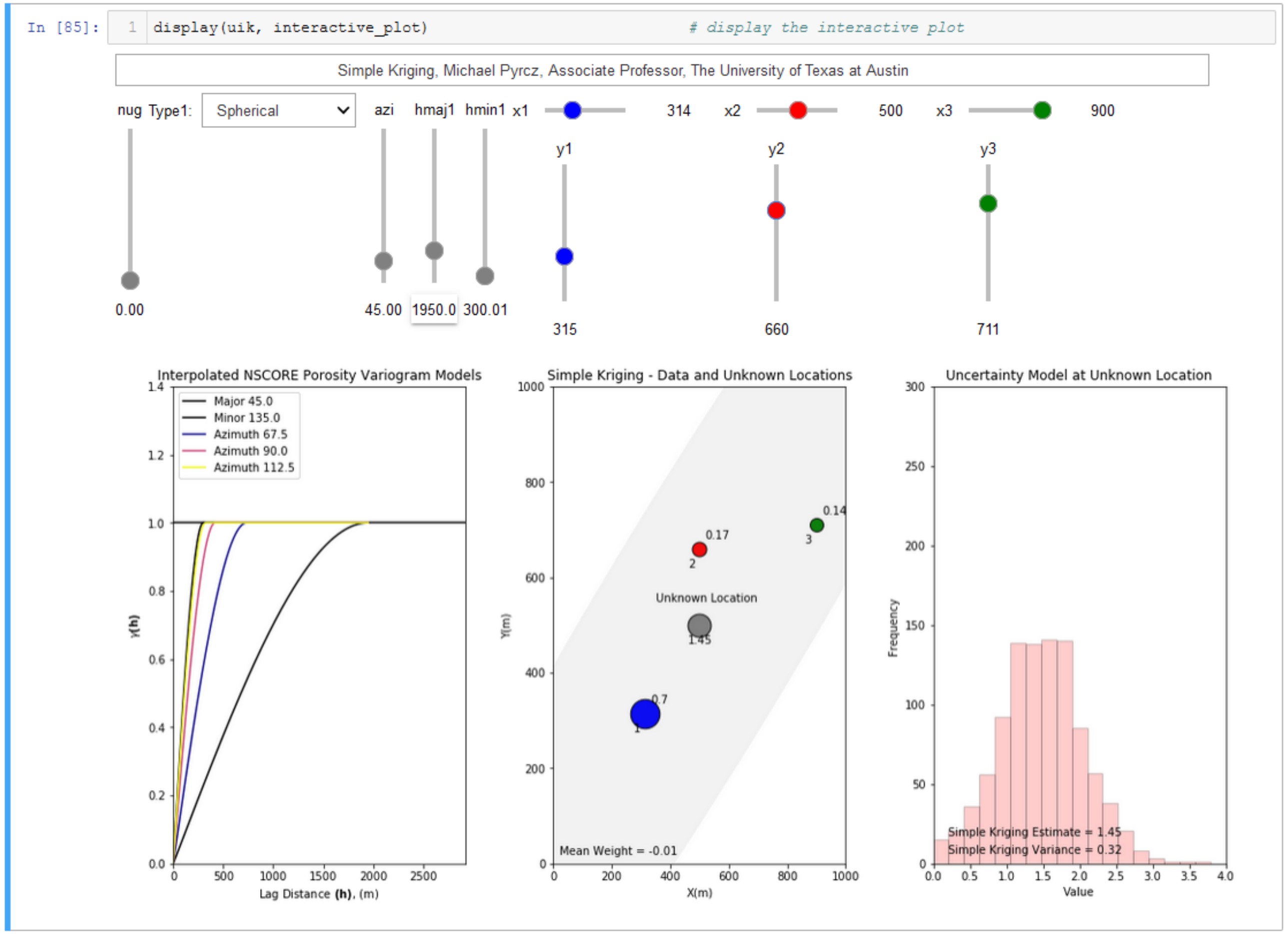
- There are many different types of kriging:
  - e.g., universal kriging fits a parametric trend model over location while calculating the optimum weights.

# Kriging Hands-On in Python

## Interactive Kriging Demonstration in Python

Walkthrough:

- Change the variogram parameters.
- Change the data locations.
- Investigate:
    - closeness
    - redundancy
    - mean weight
    - screening effect




Interactive simple kriging dashboard in Python, file is Interactive_Simple_Kriging.ipynb

# Spatial Uncertainty Hands-on

Here's an opportunity for experiential learning with Simple Kriging for spatial uncertainty. The kriging estimation variance is very useful.

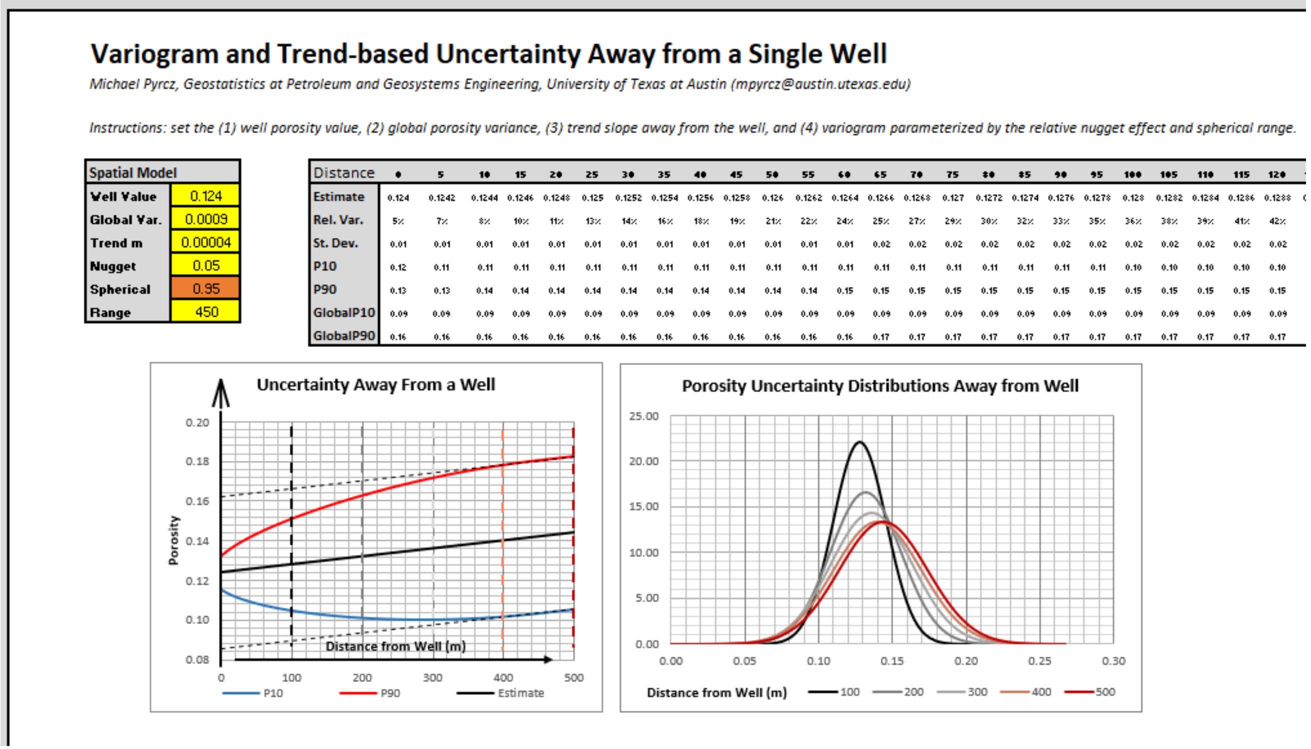
**Things to try:**

Pay attention to the kriging uncertainty P10, mean and P90 away from the well as you:

1. Change the spatial continuity range.

2. Add and adjust the nugget effect.

3. Modify the trend slope.




| Distance | 0 | 5 | 10 | 15 | 20 | 25 | 30 | 35 | 40 | 45 | 50 | 55 | 60 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Estimate | 0.124 | 0.1242 | 0.1244 | 0.1246 | 0.1248 | 0.125 | 0.1252 | 0.1254 | 0.1256 | 0.1258 | 0.126 | 0.1262 | 0.1264 |
| Rel. Var. | 5% | 7% | 8% | 10% | 11% | 13% | 14% | 16% | 18% | 19% | 21% | 22% | 24% |
| St. Dev. | 0.01 | 0.01 | 0.01 | 0.01 | 0.01 | 0.01 | 0.01 | 0.01 | 0.01 | 0.01 | 0.01 | 0.01 | 0.01 |
| P10 | 0.12 | 0.11 | 0.11 | 0.11 | 0.11 | 0.11 | 0.11 | 0.11 | 0.11 | 0.11 | 0.11 | 0.11 | 0.11 |
| P90 | 0.13 | 0.13 | 0.14 | 0.14 | 0.14 | 0.14 | 0.14 | 0.14 | 0.14 | 0.14 | 0.14 | 0.14 | 0.15 |
| GlobalP10 | 0.09 | 0.09 | 0.09 | 0.09 | 0.09 | 0.09 | 0.09 | 0.09 | 0.09 | 0.09 | 0.09 | 0.09 | 0.09 |
| GlobalP90 | 0.16 | 0.16 | 0.16 | 0.16 | 0.16 | 0.16 | 0.16 | 0.16 | 0.16 | 0.16 | 0.16 | 0.16 | 0.16 |

| Distance | 65 | 70 | 75 | 80 | 85 | 90 | 95 | 100 | 105 | 110 | 115 | 120 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Estimate | 0.1266 | 0.1268 | 0.127 | 0.1272 | 0.1274 | 0.1276 | 0.1278 | 0.128 | 0.1282 | 0.1284 | 0.1286 | 0.1288 |
| Rel. Var. | 25% | 27% | 29% | 30% | 32% | 33% | 35% | 36% | 38% | 39% | 41% | 42% |
| St. Dev. | 0.02 | 0.02 | 0.02 | 0.02 | 0.02 | 0.02 | 0.02 | 0.02 | 0.02 | 0.02 | 0.02 | 0.02 |
| P10 | 0.11 | 0.11 | 0.11 | 0.11 | 0.11 | 0.11 | 0.11 | 0.10 | 0.10 | 0.10 | 0.10 | 0.10 |
| P90 | 0.15 | 0.15 | 0.15 | 0.15 | 0.15 | 0.15 | 0.15 | 0.15 | 0.15 | 0.15 | 0.15 | 0.15 |
| GlobalP10 | 0.09 | 0.09 | 0.09 | 0.09 | 0.09 | 0.09 | 0.09 | 0.09 | 0.09 | 0.09 | 0.09 | 0.09 |
| GlobalP90 | 0.17 | 0.17 | 0.17 | 0.17 | 0.17 | 0.17 | 0.17 | 0.17 | 0.17 | 0.17 | 0.17 | 0.17 |

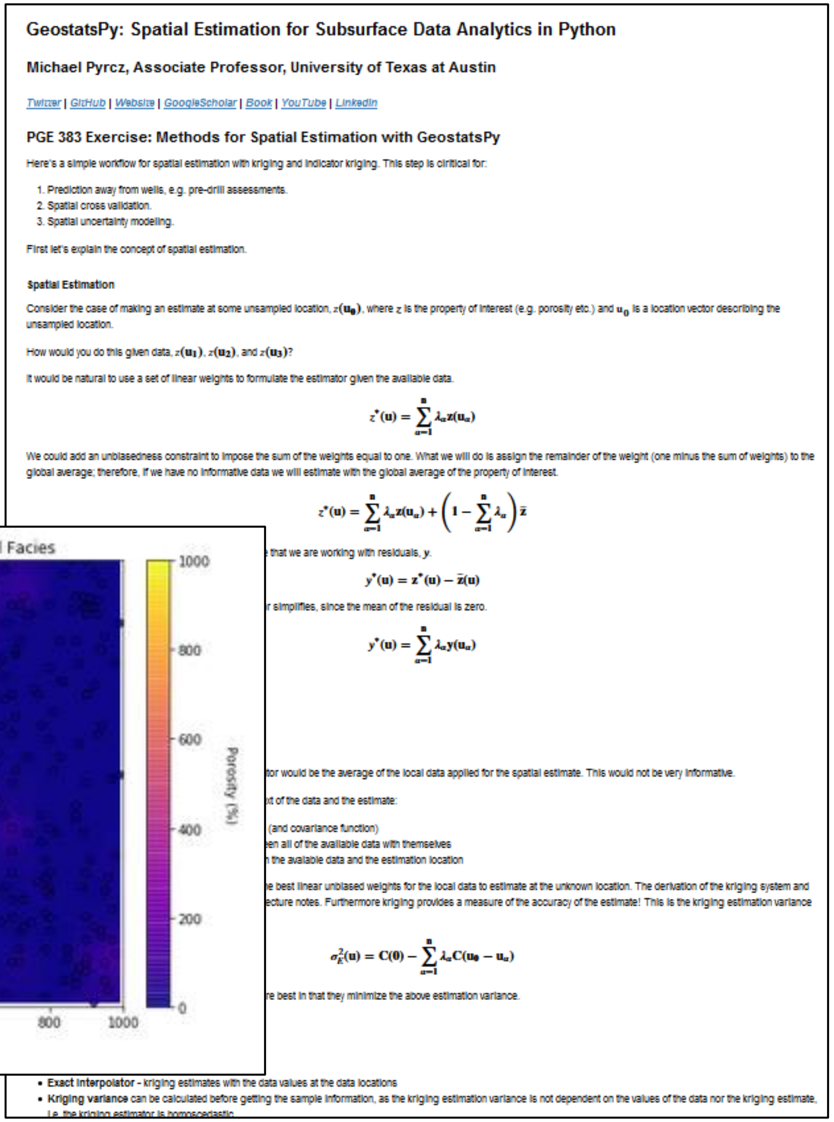
Simple kriging uncertainty away from a well workflow in Excel, file is Uncertainty_Away_from_Well_Demo.

# Complete Kriging Workflow in Python

## Kriging Workflow in Python

- Walkthrough and try to:

- Change the variogram and search parameters.


### GeostatsPy: Spatial Estimation for Subsurface Data Analytics in Python

#### Michael Pyrcz, Associate Professor, University of Texas at Austin

Twitter | GitHub | Website | GoogleScholar | Book | YouTube | LinkedIn

#### PGE 383 Exercise: Methods for Spatial Estimation with GeostatsPy

Here's a simple workflow for spatial estimation with kriging and indicator kriging. This step is cirtical for:

1. Prediction away from wells, e.g. pre-drill assessments.
2. Spatial cross validation.
3. Spatial uncertainty modeling.

First let's explain the concept of spatial estimation.

**Spatial Estimation**

Consider the case of making an estimate at some unsampled location, $z(\mathbf{u}_0)$, where $z$ is the property of interest (e.g. porosity etc.) and $\mathbf{u}_0$ is a location vector describing the unsampled location.

How would you do this given data, $z(\mathbf{u}_1)$, $z(\mathbf{u}_2)$, and $z(\mathbf{u}_3)$?

It would be natural to use a set of linear weights to formulate the estimator given the available data.

$$z^*(\mathbf{u}) = \sum_{\alpha=1}^{n} \lambda_\alpha z(\mathbf{u}_\alpha)$$

We could add an unbiasedness constraint to impose the sum of the weights equal to one. What we will do is assign the remainder of the weight (one minus the sum of weights) to the global average; therefore, if we have no informative data we will estimate with the global average of the property of interest.

$$z^*(\mathbf{u}) = \sum_{\alpha=1}^{n} \lambda_\alpha z(\mathbf{u}_\alpha) + \left(1 - \sum_{\alpha=1}^{n} \lambda_\alpha\right) \bar{z}$$

that we are working with residuals, $y$.

$$y^*(\mathbf{u}) = z^*(\mathbf{u}) - \bar{z}(\mathbf{u})$$

r simplifies, since the mean of the residual is zero.

$$y^*(\mathbf{u}) = \sum_{\alpha=1}^{n} \lambda_\alpha y(\mathbf{u}_\alpha)$$

tor would be the average of the local data applied for the spatial estimate. This would not be very informative.

t of the data and the estimate:

(and covariance function)

en all of the available data with themselves

the available data and the estimation location

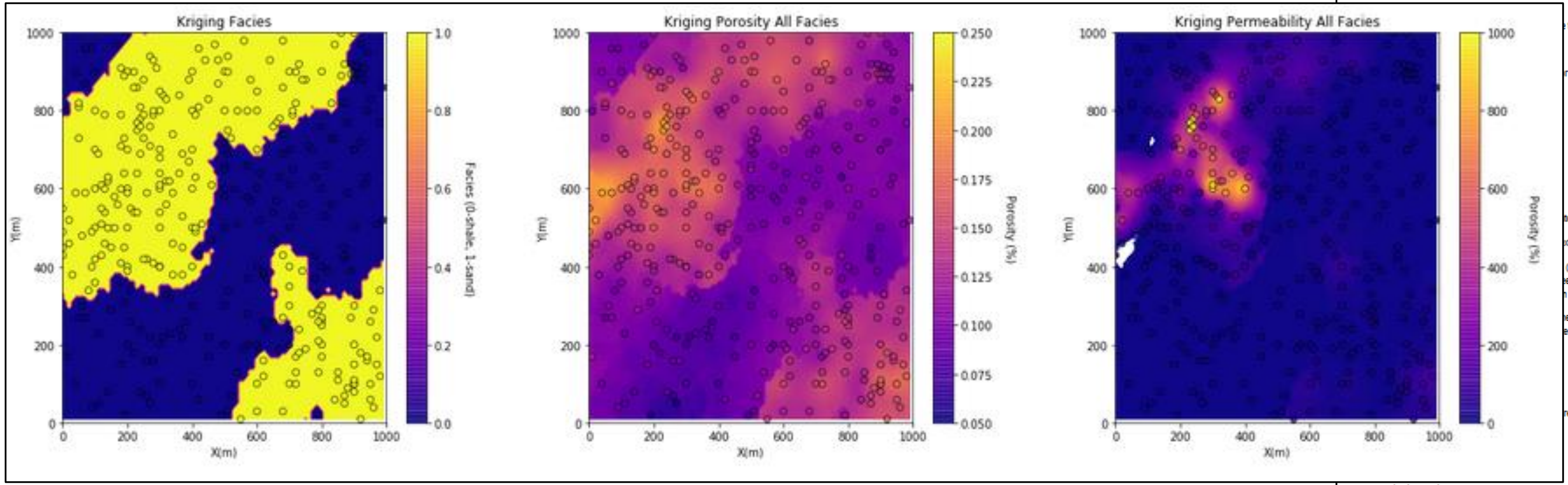
e best linear unbiased weights for the local data to estimate at the unknown location. The derivation of the kriging system and

ecture notes. Furthermore kriging provides a measure of the accuracy of the estimate! This is the kriging estimation variance

$$\sigma^2_E(\mathbf{u}) = C(0) - \sum_{\alpha=1}^{n} \lambda_\alpha C(\mathbf{u}_0 - \mathbf{u}_\alpha)$$

re best in that they minimize the above estimation variance.

- **Exact interpolator** - kriging estimates with the data values at the data locations
- **Kriging variance** can be calculated before getting the sample information, as the kriging estimation variance is not dependent on the values of the data nor the kriging estimate, i.e. the kriging estimator is homoscedastic.




Complete kriging modeling workflow, file is GeostatsPy_kriging.ipynb

# PGE 338 Data Analytics and Geostatistics

## Lecture 12: Spatial Estimation

**Lecture outline . . .**

- Spatial Trend Modeling
- Kriging

Michael Pyrcz, The University of Texas at Austin