Uncertainty in Spatial Models
Geostatistics and Machine Learning

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Sources of Uncertainty

Natural system modelling is subject to:

- observation errors (calibration, positioning, etc)
- unknown free model parameters
- computational discretisation – solution errors
- conceptual uncertainty – model inadequacy

Uncertainty Modelling Questions

- How accurate is the prediction?
- What is the risk of taking a decision on the prediction?
- How variable and uncertain are spatial predictions?
- How the model uncertainty is propagated into further predictions?
- Where to obtain further measurements to improve the prediction quality?

Modelling Approaches

- Geostatistics
- Machine Learning
- Bayesian Maximum Entropy
- Uncertainty Quantification in Inverse Problems

Spatial Modelling Approaches

- Deterministic
  - rely on analytical assumptions about model dependencies
  - uncertainty quantification is limited to parameter selection
- Geostatistics
  - stochastic nature of data $Z(x) = m(x) + S(x)$
  - spatial correlation (covariance) model
  - family of kriging models (regression)
  - stochastic simulations (multiple realisations)
- Machine learning
  - data driven approach
  - model choice is based on the learning principles
  - suffer from poor quality and insufficient amount of data

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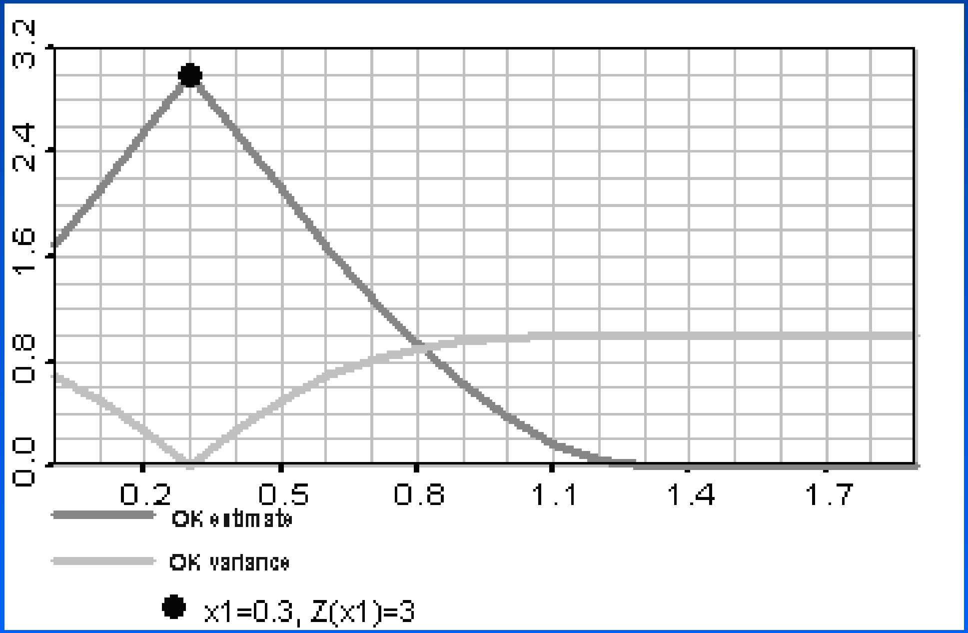
Geostatistical Predictors

Kriging:

- Unbiased linear estimator
- “Best” in terms of minimum variance
- Honours the data



Ordinary kriging estimate:

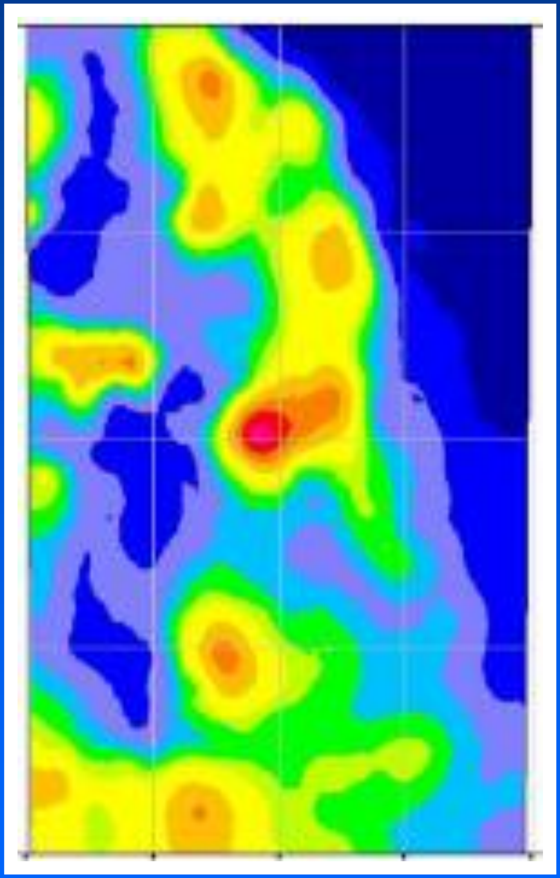
$$Z^*(x_0) = \sum_{j=1}^{n} w_j Z(x_j)$$

Ordinary kriging variance:

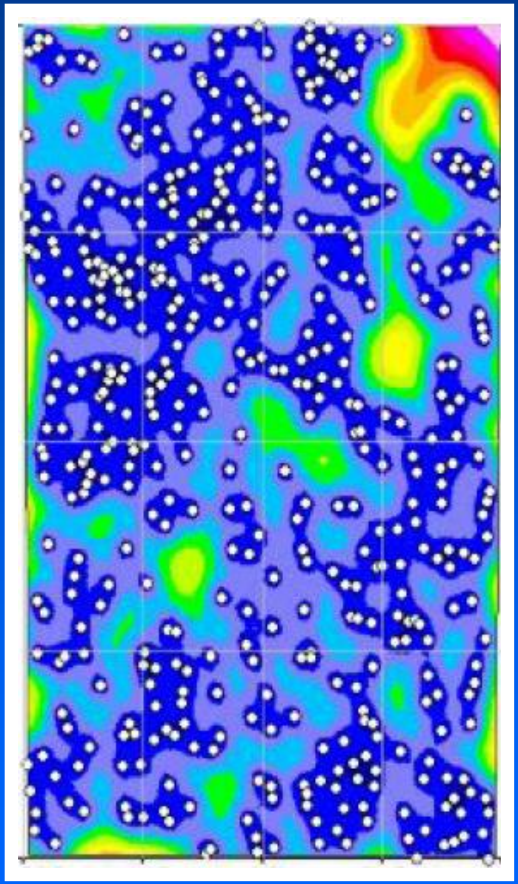
$$\sigma_{OK}^2(x) = \sigma_Z^2 - \sum_{j=1}^{n(x)} w_j(x) C_{j0} + \mu(x)$$

Kriging Predictions

Kriging estimate



Kriging variance



Kriging variance is unconditional:

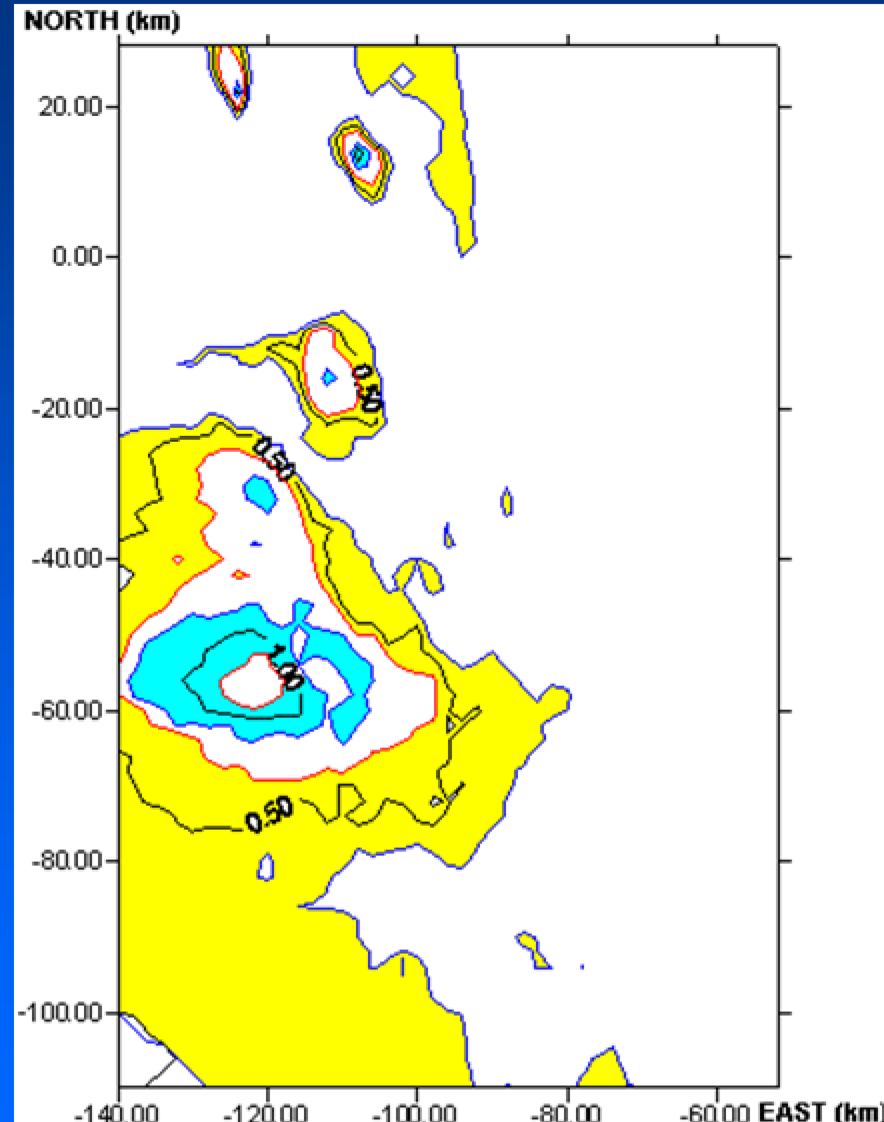
- depends on the data density
- does not reflect function value

Chernobyl radioactive soil contamination

Uncertainty Visualisation: Thick Contours

Kriging variance determines the thickness of the uncertainty interval around the kriging estimate contour

Chernobyl radioactive soil contamination



Uncertanity contours for isoline at 0.5 Ci/sq.km

Uncertanity contours for isoline at 1.0 Ci/sq.km

M. Kanevski, et.al. Mapping of Radioactively Contaminated Territories with Geostatistics and Artificial Neural Networks. Contaminated Forests , Kluwer 1999

Learning from Data

- Conventional model driven approach
  - Develop a model with known functional dependencies
  - Fit the model parameters to the available data
- Data driven approach
  - Model dependencies are not explicitly defined in functional form due to their complexity or lack of knowledge
  - Model dependencies are extracted from data via training
- Artificial Neural Networks can be trained to
  - store, recognise, and associatively retrieve patterns;
  - filter noise from measurement data;
  - estimate functions of unknown analytical form.

Learning Approaches

- Supervised learning
  - Inputs and the corresponding known target output values are available form the training set;
  - ANN output is computed for each set of inputs presented to ANN;
  - ANN output is compared with the target value;
  - ANN weights are updated to minimise error measure between the ANN output and the target output.

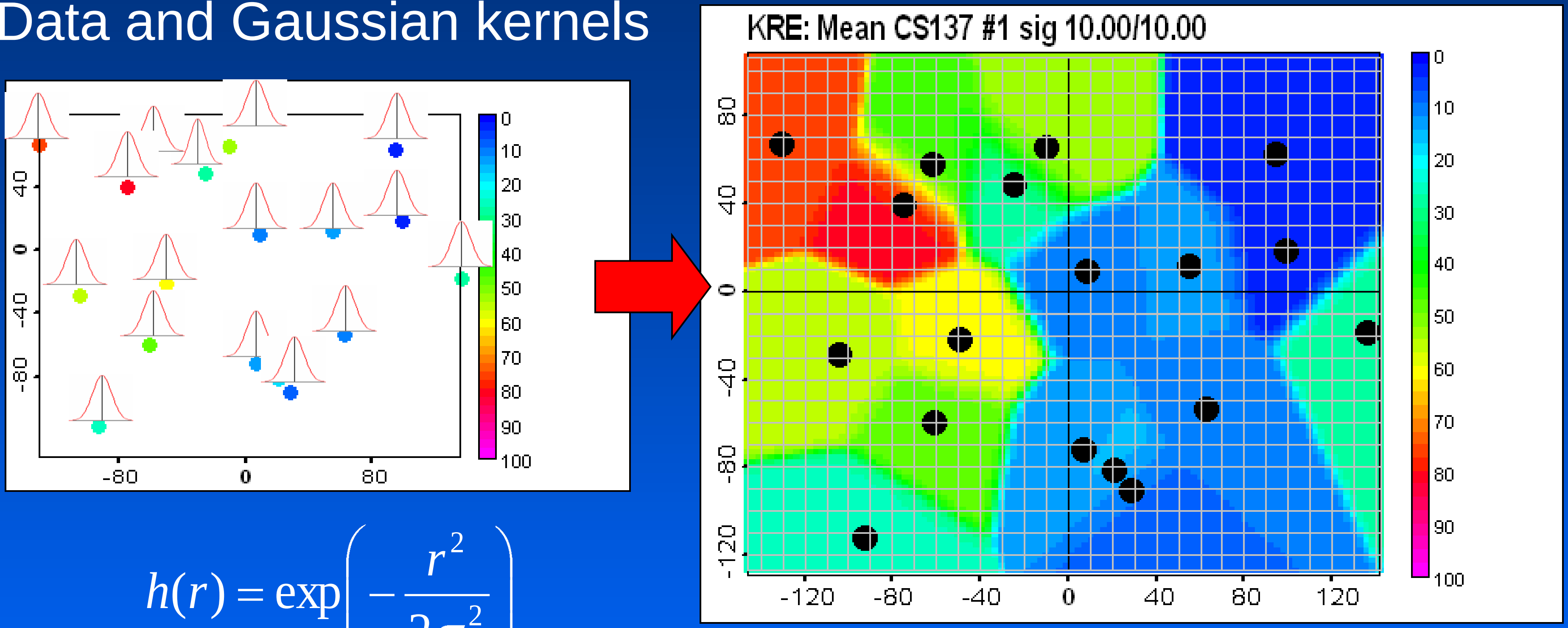
- Unsupervised learning
  - A set of inputs is presented to the network with no target outputs
  - Inputs are assumed to belong to several classes and the ANN output is an identification of the class to which its input belongs.
  - Competitive learning rule may be used: a “winner-takes-all”

Learning Approahes

- Semi-supervised learning
  - Use labelled and unlabeled data for training and prediction
- Active Learning
  - Interaction between User and learning machine
  - Update the training data set with particular new samples
- Reinforcement Learning
  - Learn how to act given an observation
- Transduction
  - Predict new outputs based on training data and new inputs

General Regression Neural Network (GRNN)

Data and Gaussian kernels

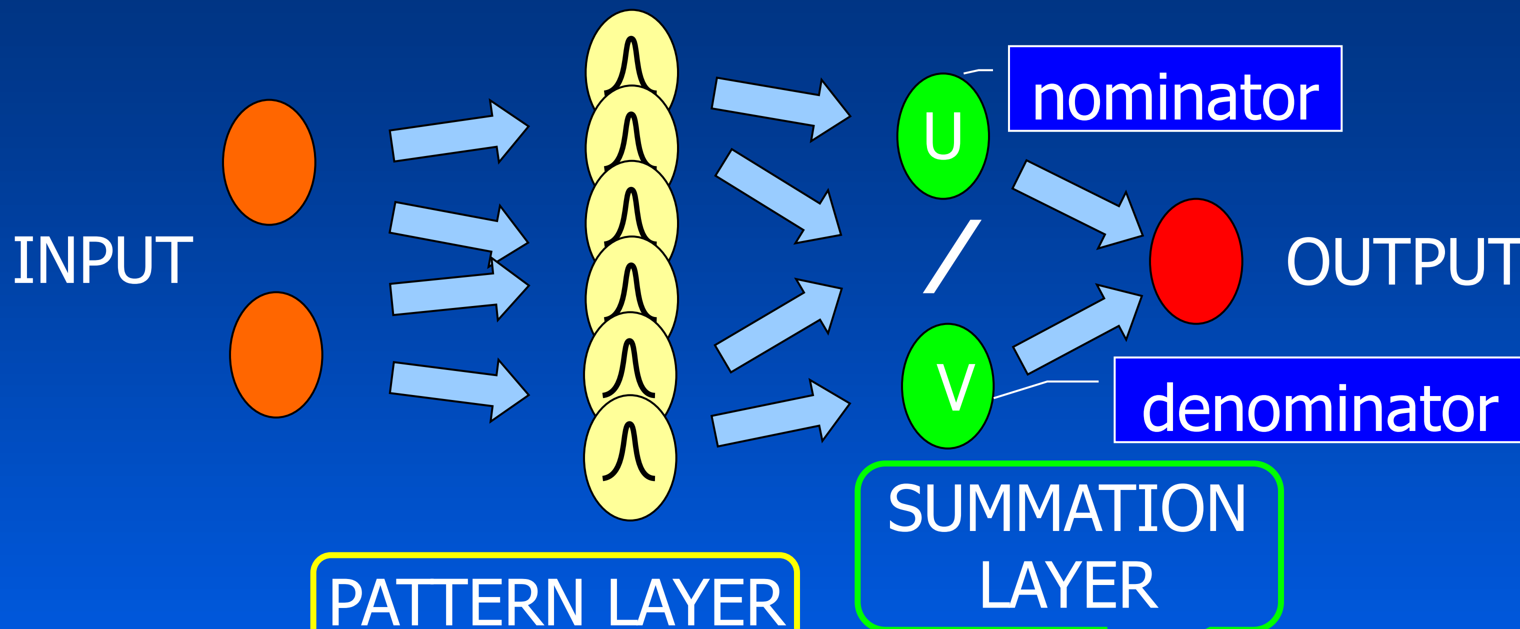


$$h(r) = \exp\left(-\frac{r^2}{2\sigma^2} \right)$$

Kernel smoothing parameter: $\overleftrightarrow{\sigma}=10$

How to choose the kernel width σ? – Cross-validation

General Regression Neural Network (GRNN)



Pattern layer consists of N kernels – one for every available data point

Signal from pattern units:

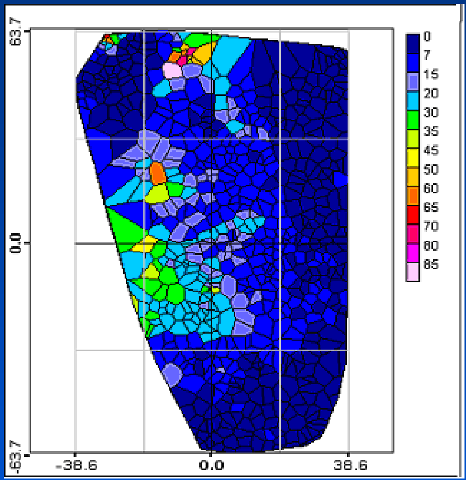
$$U = \sum_{i=1}^{N} Z_i \exp\left(-r_i^2 / 2\sigma^2\right)$$

Weights:

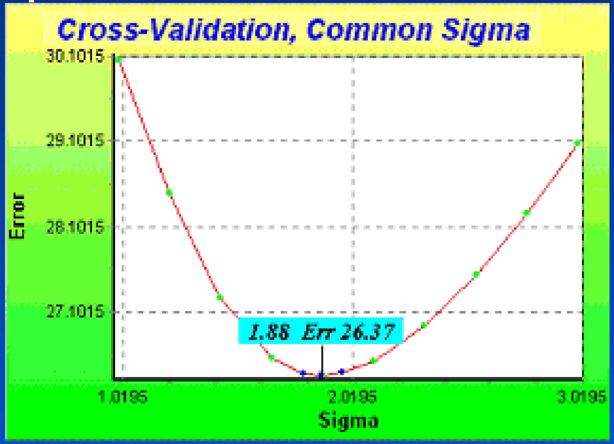
$$V = \sum_{i=1}^{N} \exp\left(-r_i^2 / 2\sigma^2\right)$$

GRNN Mapping

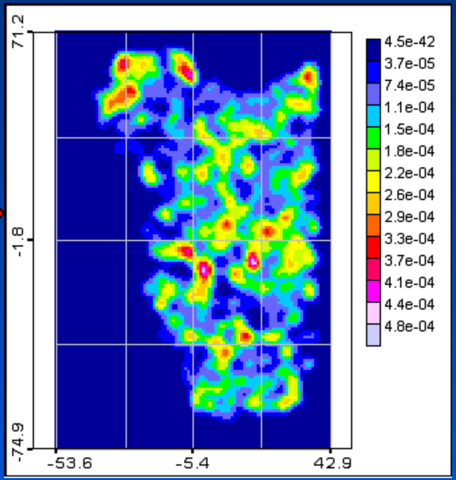
Data



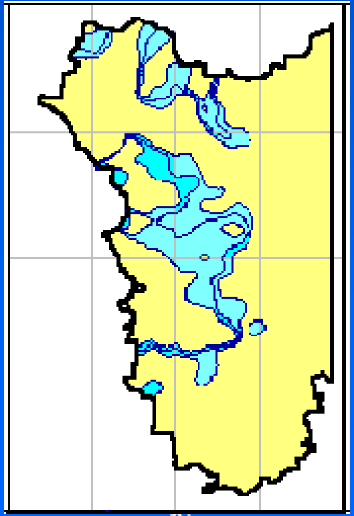
Optimise kernel width σ



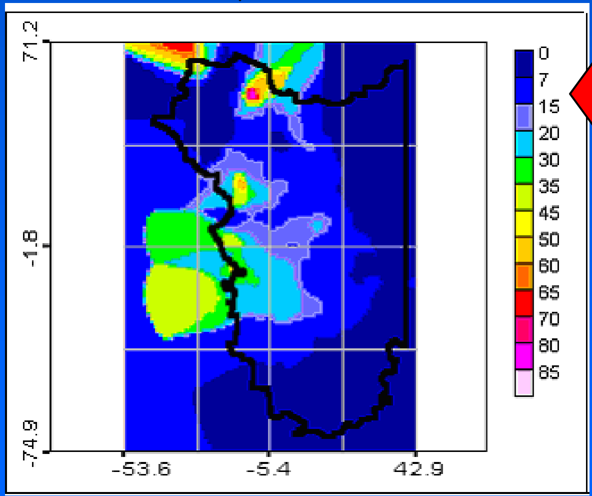
Kernel density



residual estimation



Thick contours



GRNN estimate

Uncertainty Quantification

Chernobyl radioactive soil contamination

M.Kanevski, V.Timonin

Uncertainty Modelling Questions

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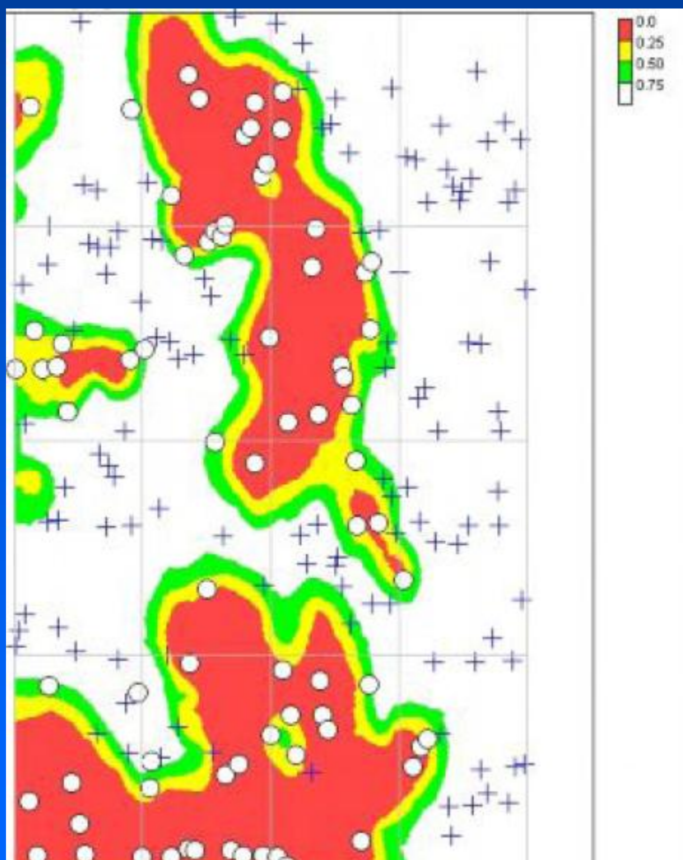
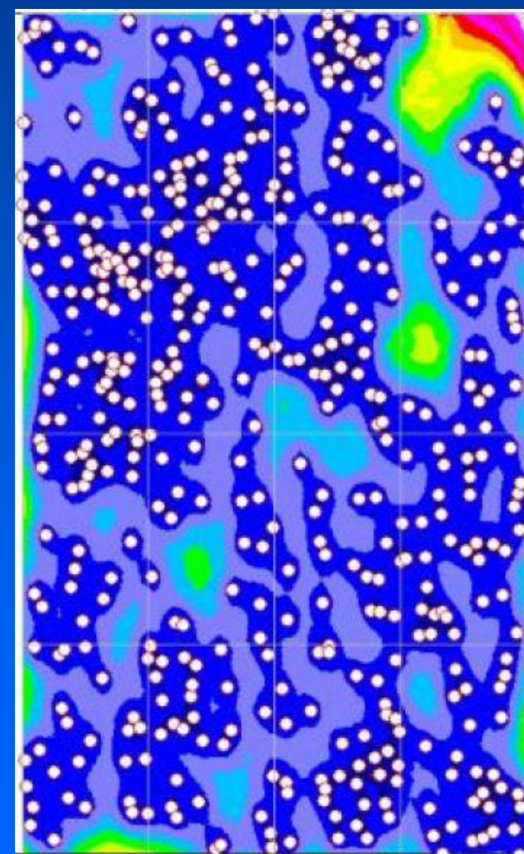
Probabilistic Prediction with Indicator Kriging

Probability to be below a level based on local cdf



Indicator kriging variance



○ data locations

Kriging variance is unconditional:

- depends on data density
- does not reflect function value

Chernobyl radioactive soil contamination

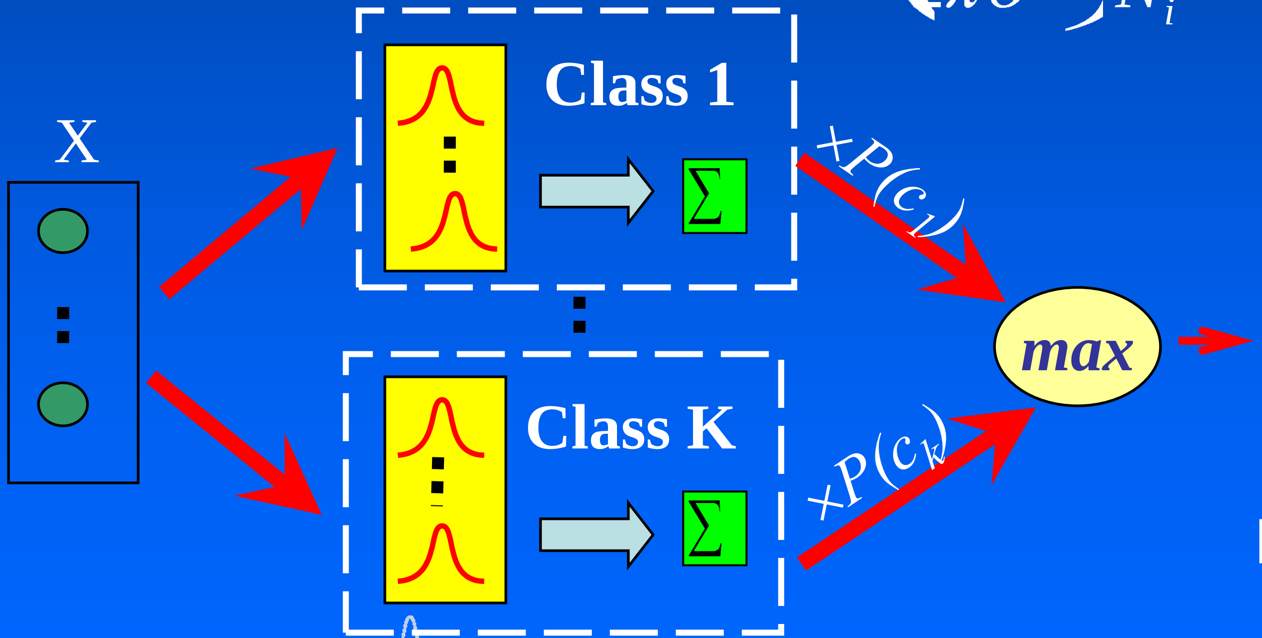
Probabilistic Neural Network (PNN)

Classification model based on maximum posterior decision rule:

$$C(x) = \{c_1, \ldots, c_K\} \arg\max_{c_i} P(c_i)\,p(x|c_i)$$

Class probability density kernel estimator:

$$p(x|c_i) = \frac{1}{(2\pi\sigma^2)^{\frac{n}{2}} N_i} \sum_{n=1}^{N_i} \exp\left(\frac{-\left\| x - x_i^{(n)} \right\|^2}{2\sigma^2} \right)$$

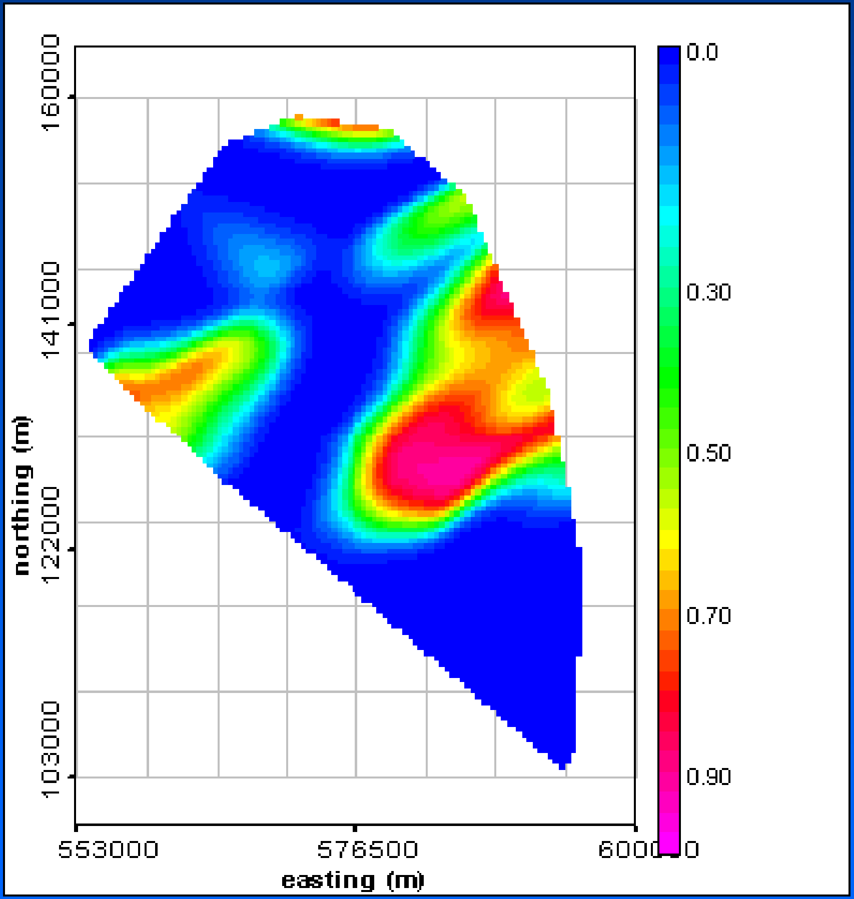


$$P(x|c_i) = \frac{P(c_i)\,p(x|c_i)}{\sum_{k-1}^{K} P(c_k)\,p(x|c_k)}$$

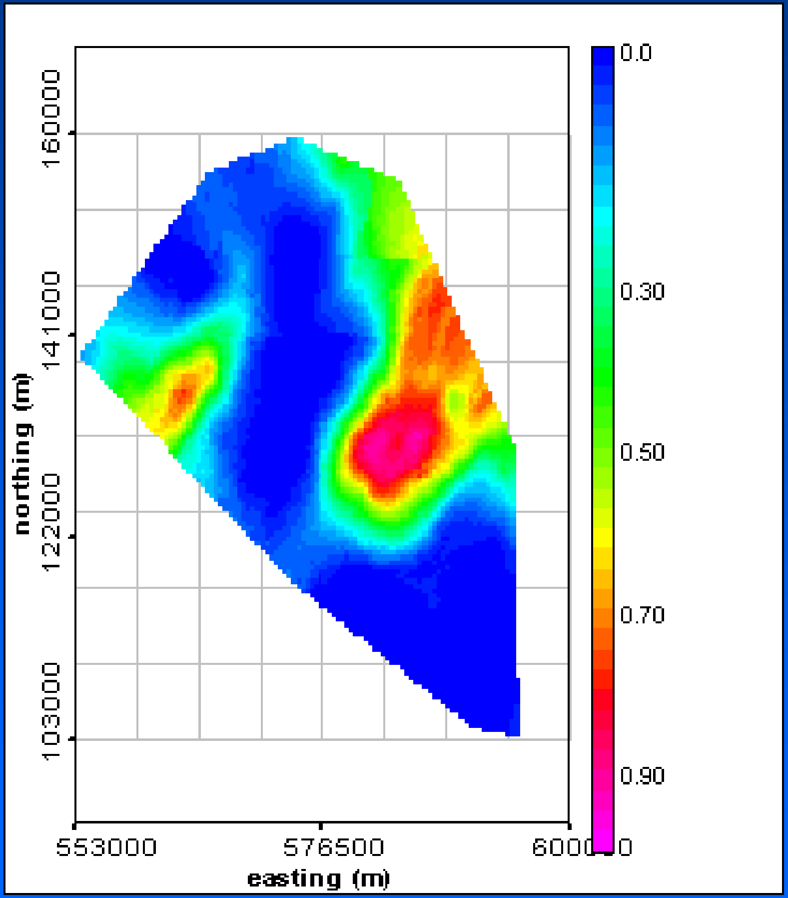
Posterior probability to belong to class *i*:

Probability Class Predictions

PNN prediction



Indicator kriging prediction



Probability of Ringold lower mud presence

Kansvski et.al, Characterization of Hydrogeologic Systems with Machine Learning Algorithms and Geostatistical Models, 2001

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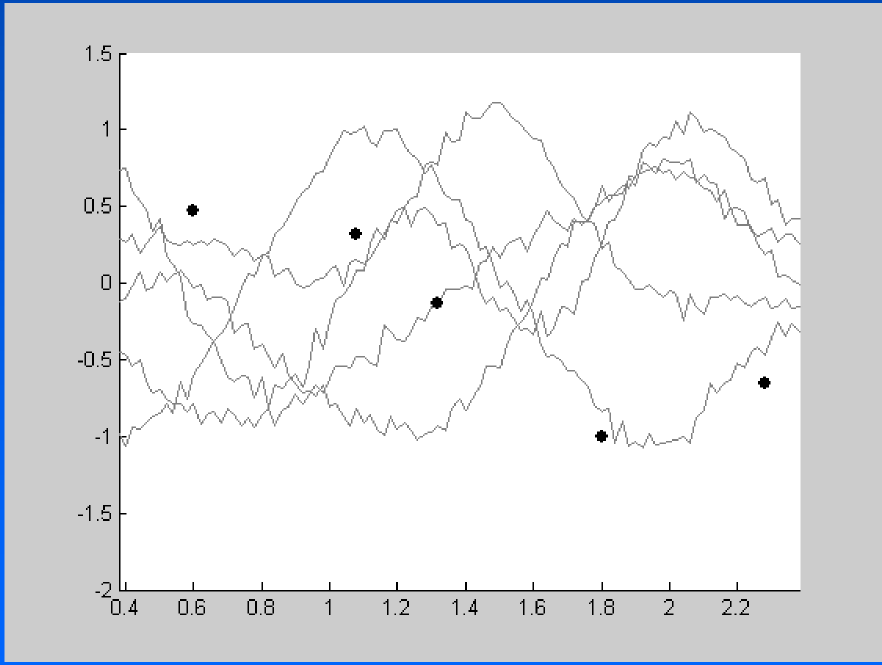
Geostatistical Simulations

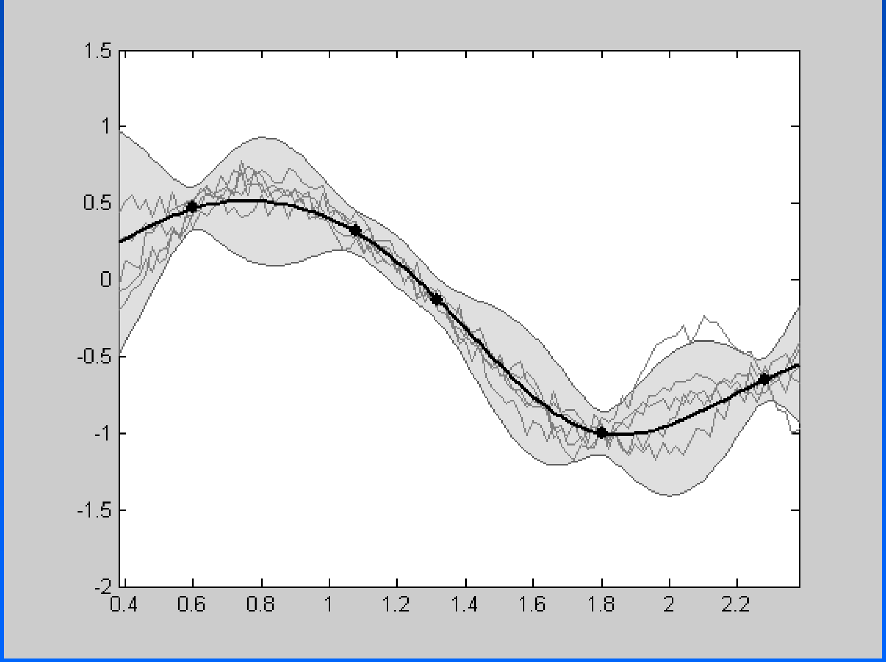
Kriging estimates vs. stochastic simulations:

- Stochastic realisations describe variability and local uncertainty

Unconditional

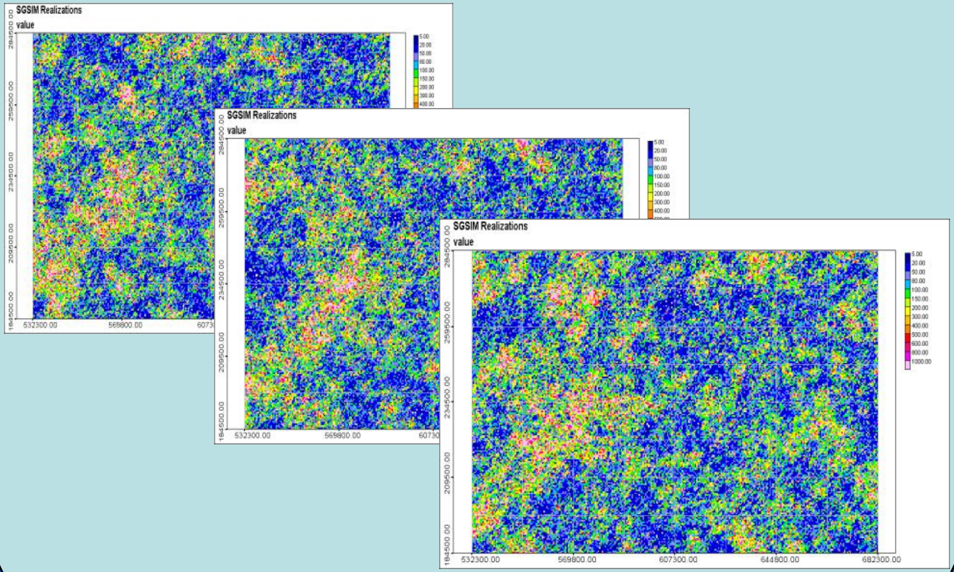


Conditional



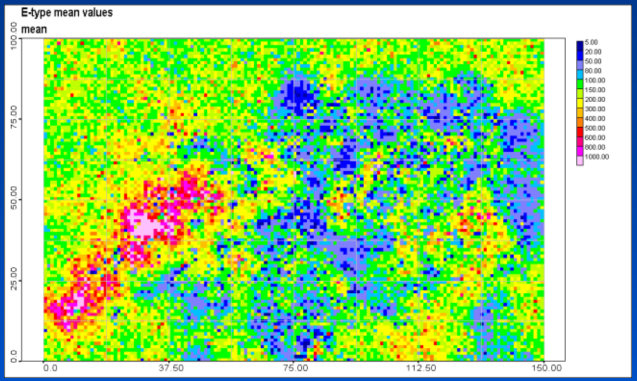
Stochastic Realisations

Multiple realisations

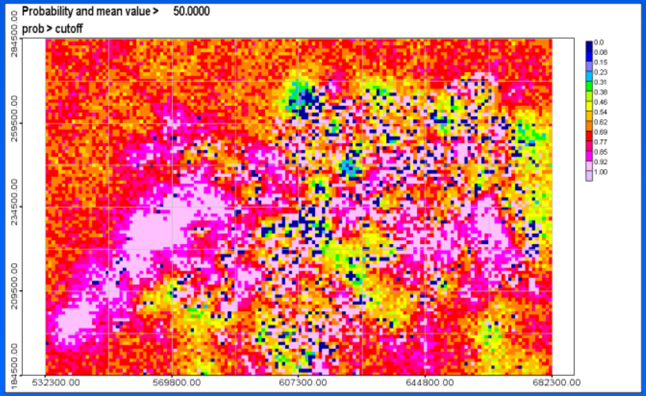


averaging

E-type estimate



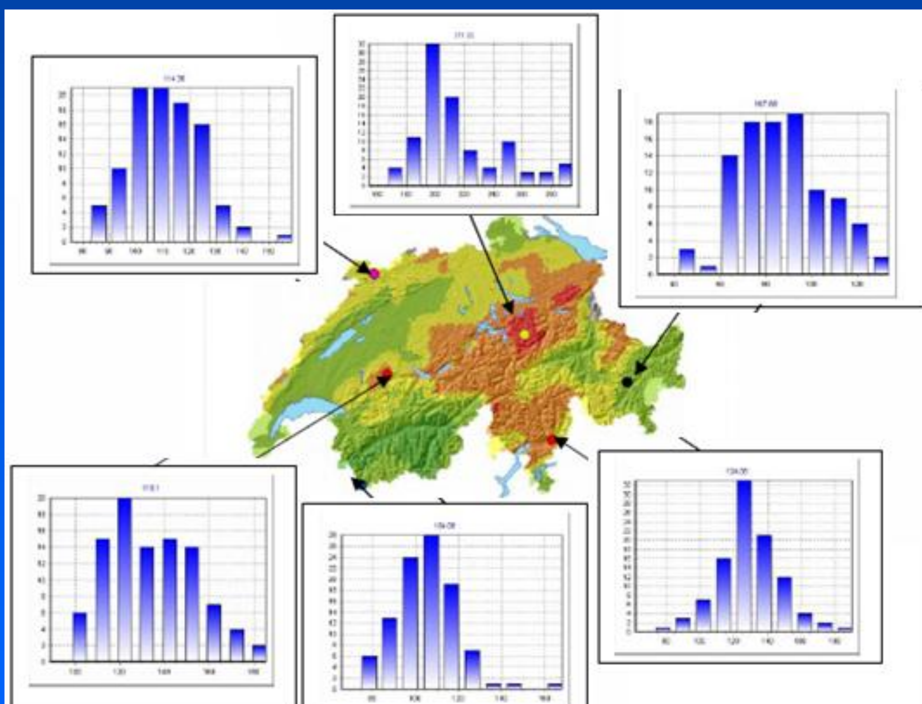
Probability above a level



Demyanov et al., Indoor Radon Risk Assessment with Geostatistics and Artificial Neural Networks, Geostatistics 2000

Stochastic Variability

Local distributions based on multiple realisations



Variance of a set of stochastic realisations is conditional to the functional value unlike kriging variance

Monthly precipitation, Switzerland

Bayesian Maximum Entropy

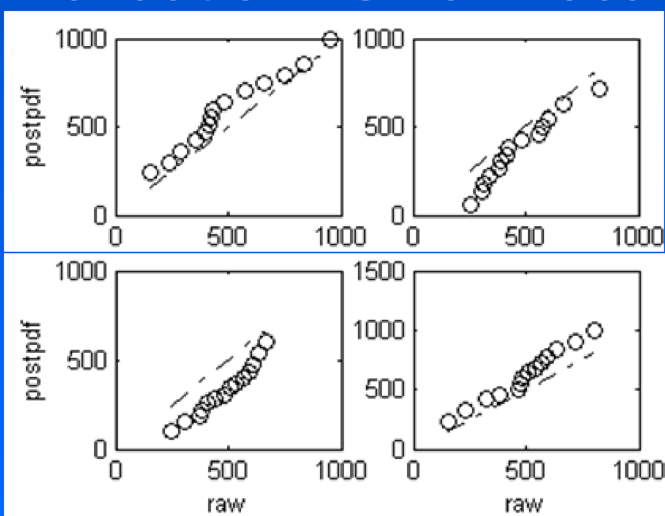
Epistemic principle – information is maximised subject to available general knowledge

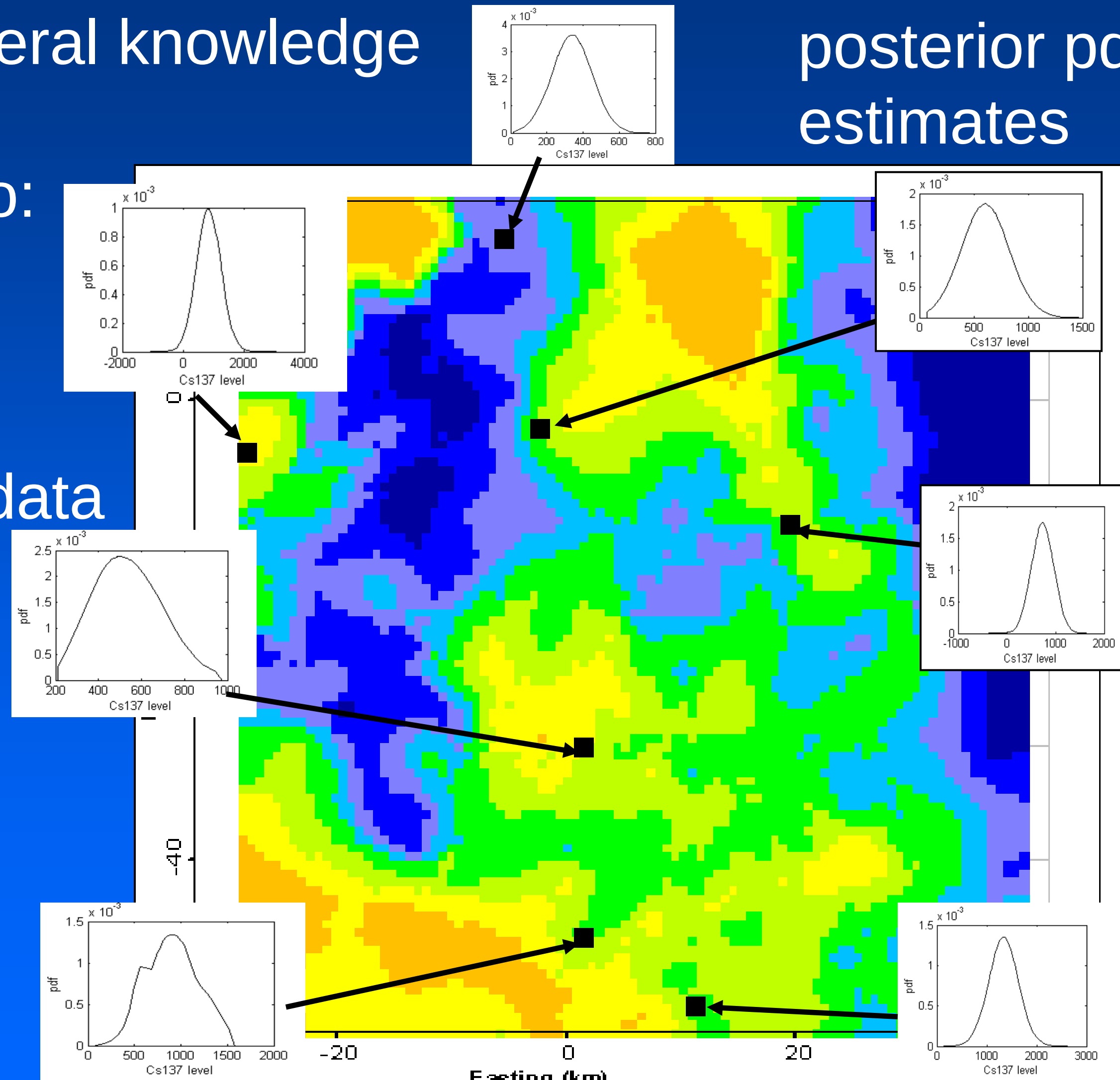
posterior pdf estimates

Bayesian conditioning to:

- Hard data
- Soft data

Validation vs. raw local data





E.Savelieva, et.al. BME-based uncertainty assessment of Chernobyl fallout, Geoderma,2005

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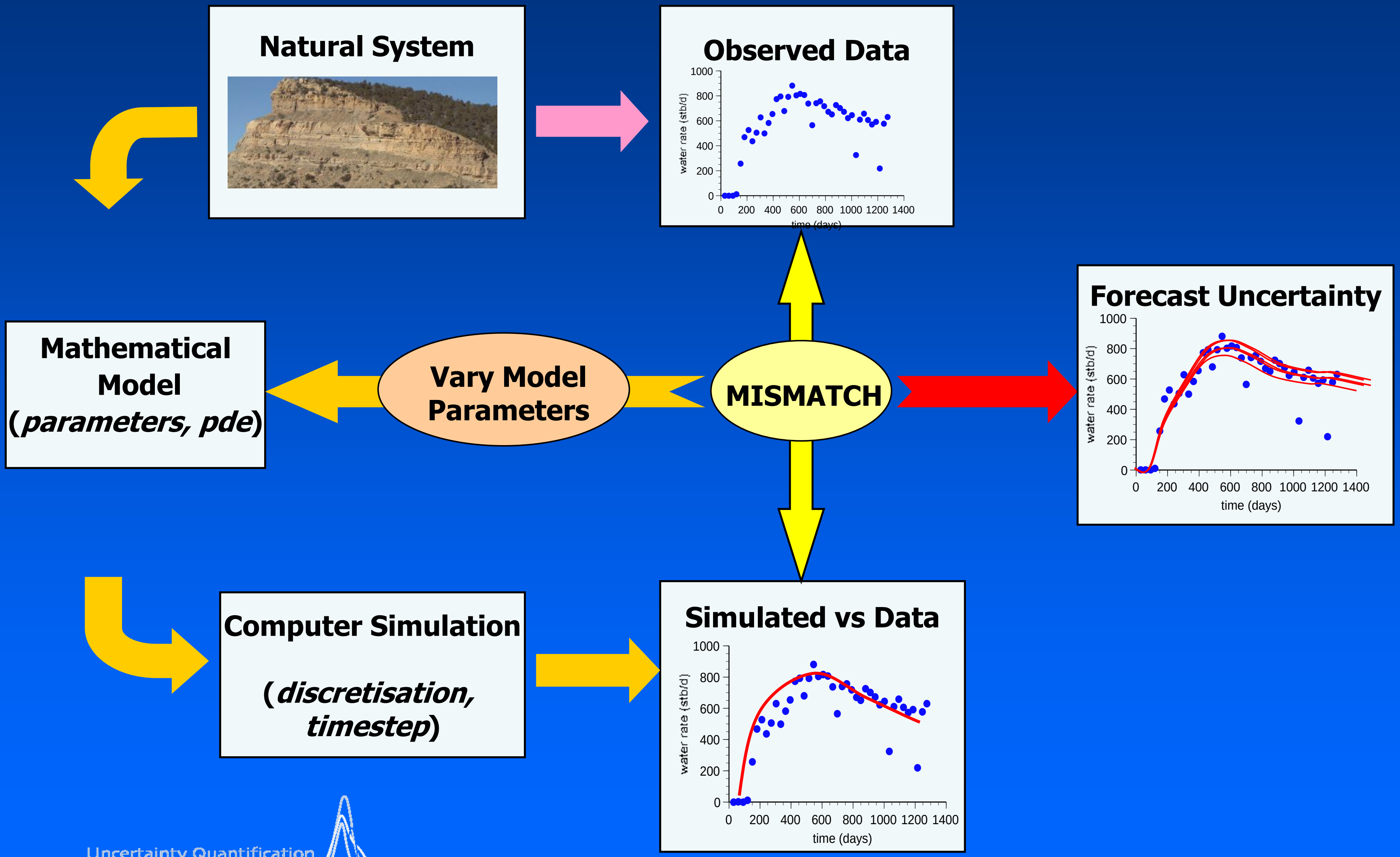
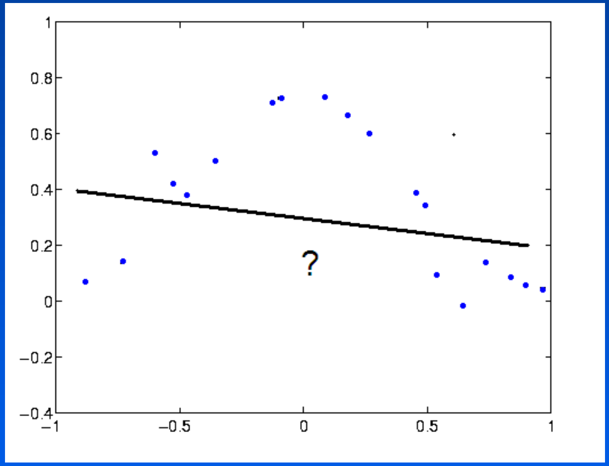
Uncertainty Quantification Framework

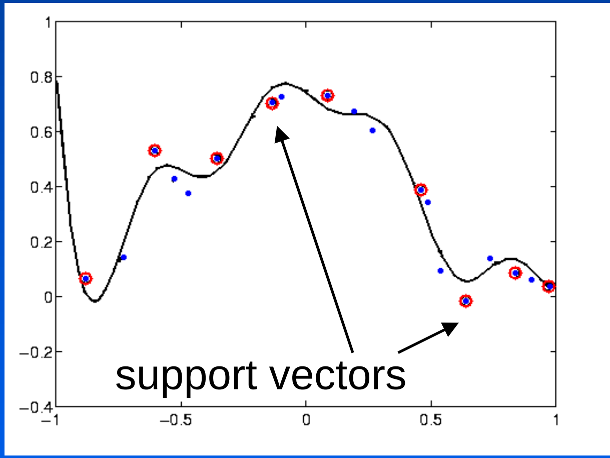


Support Vector Regression (SVR)

Linear regression in hyperspace

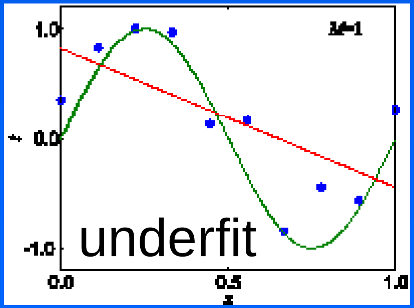
Kernel trick projects data into sufficiently high dimensional space: $f(x) = wx + b \longrightarrow f(x) = \sum_{i=1}^{L} y_i \alpha_i K(x, x_i) + b$

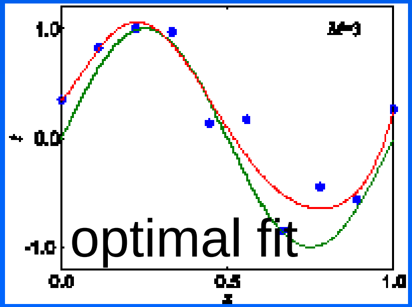


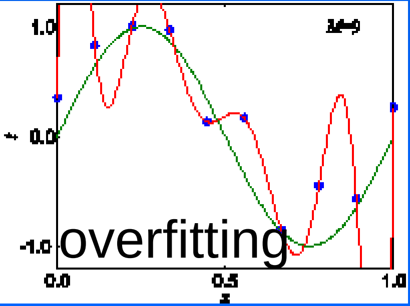


Complexity control with training errors

- data
- model
- truth

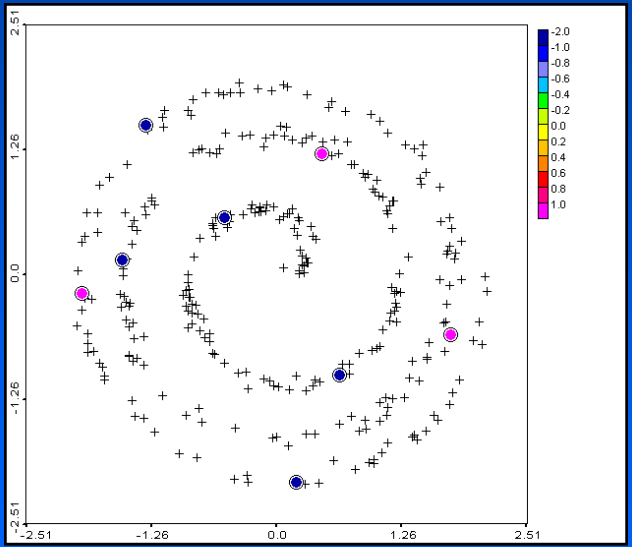




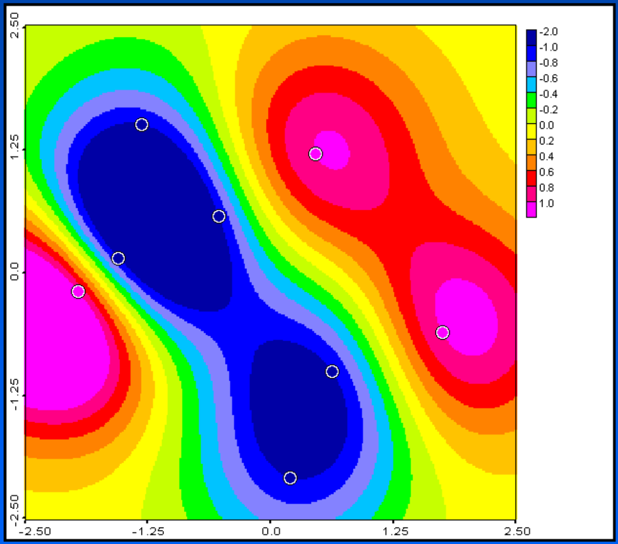


Semi-supervised SVR Model

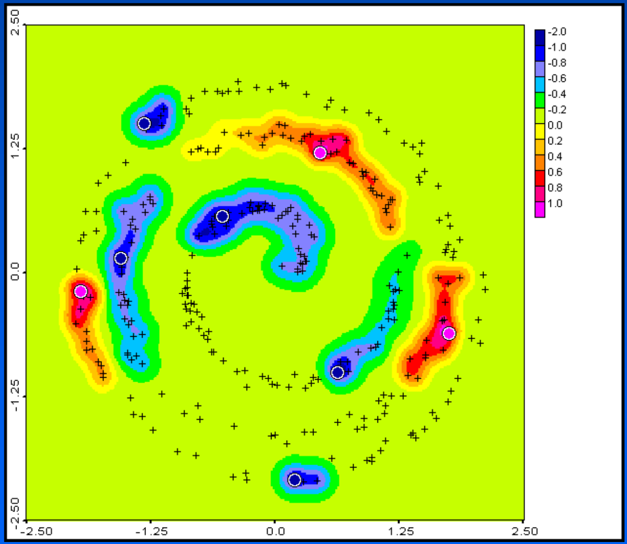
- Incorporate prior knowledge as graphs in input space
- Kernel function enforces continuity along the graph model – manifold – obtained from the prior information



Spiral manifold represented by unlabelled points (+)

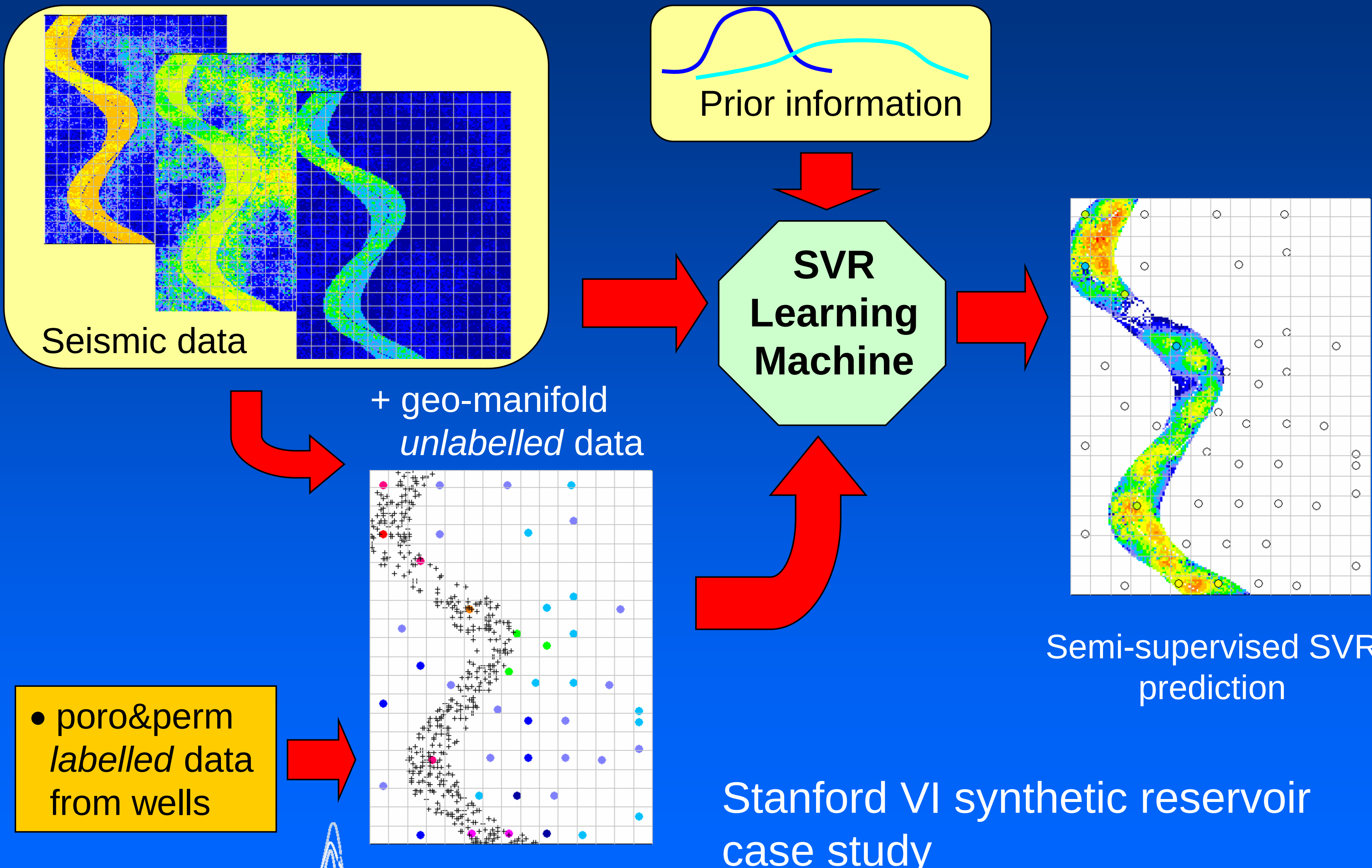


Conventional regression estimate based on labelled data only (●)



Semi-supervised regression estimation follows the smoothness along the graph

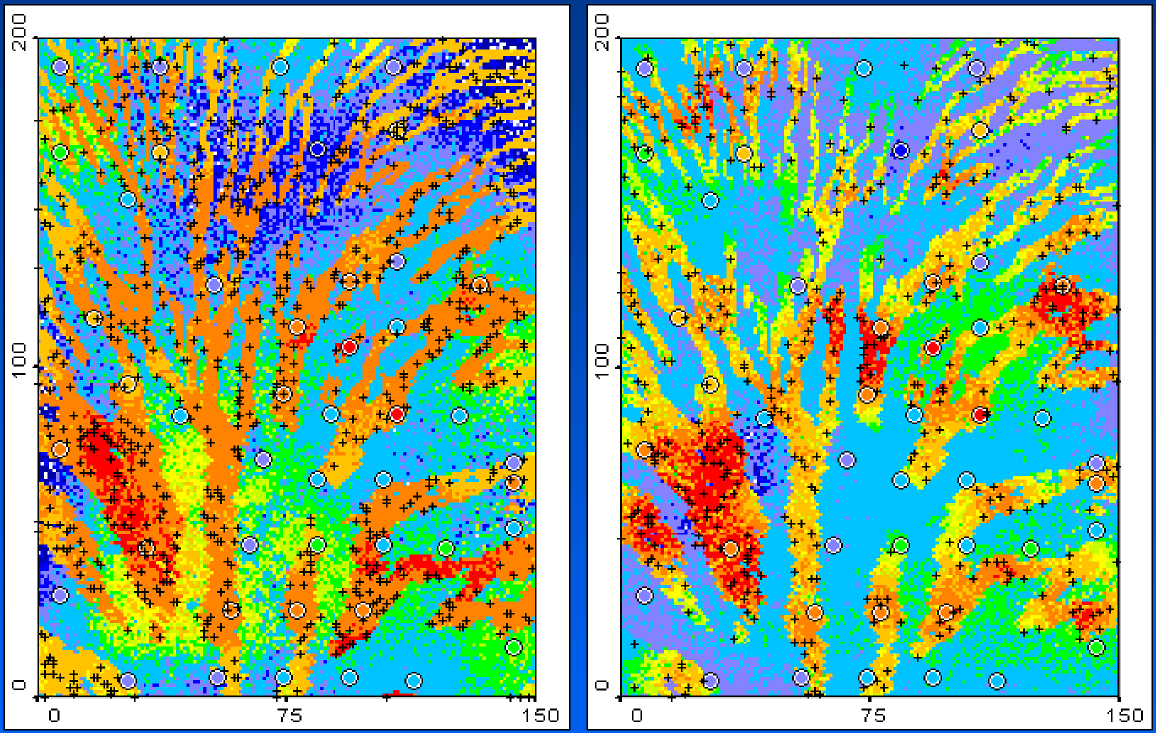
Semi-supervised SVR Reservoir Geomodel



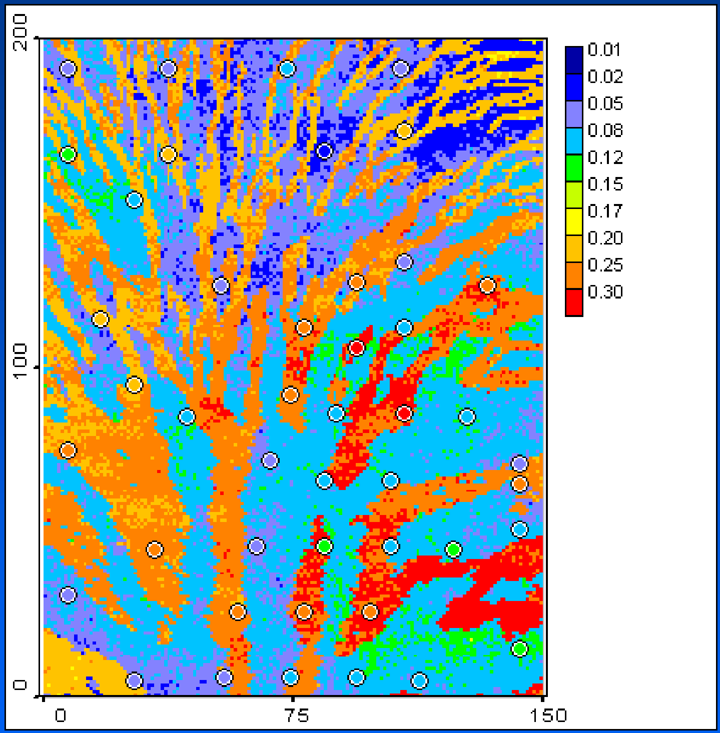
V. Demyanov, et.al. Geomodelling of a Fluvial System with Semi-Supervised Support Vector Regression, Geostatistics Congress, 2008

Multiple Realisations vs Truth case

Multiple good fitting porosity models



Truth case porosity



labelled (hard) data

\+ unlabelled data

- The river delta front structure is preserved
- Data conditioning
- Local spatial variability

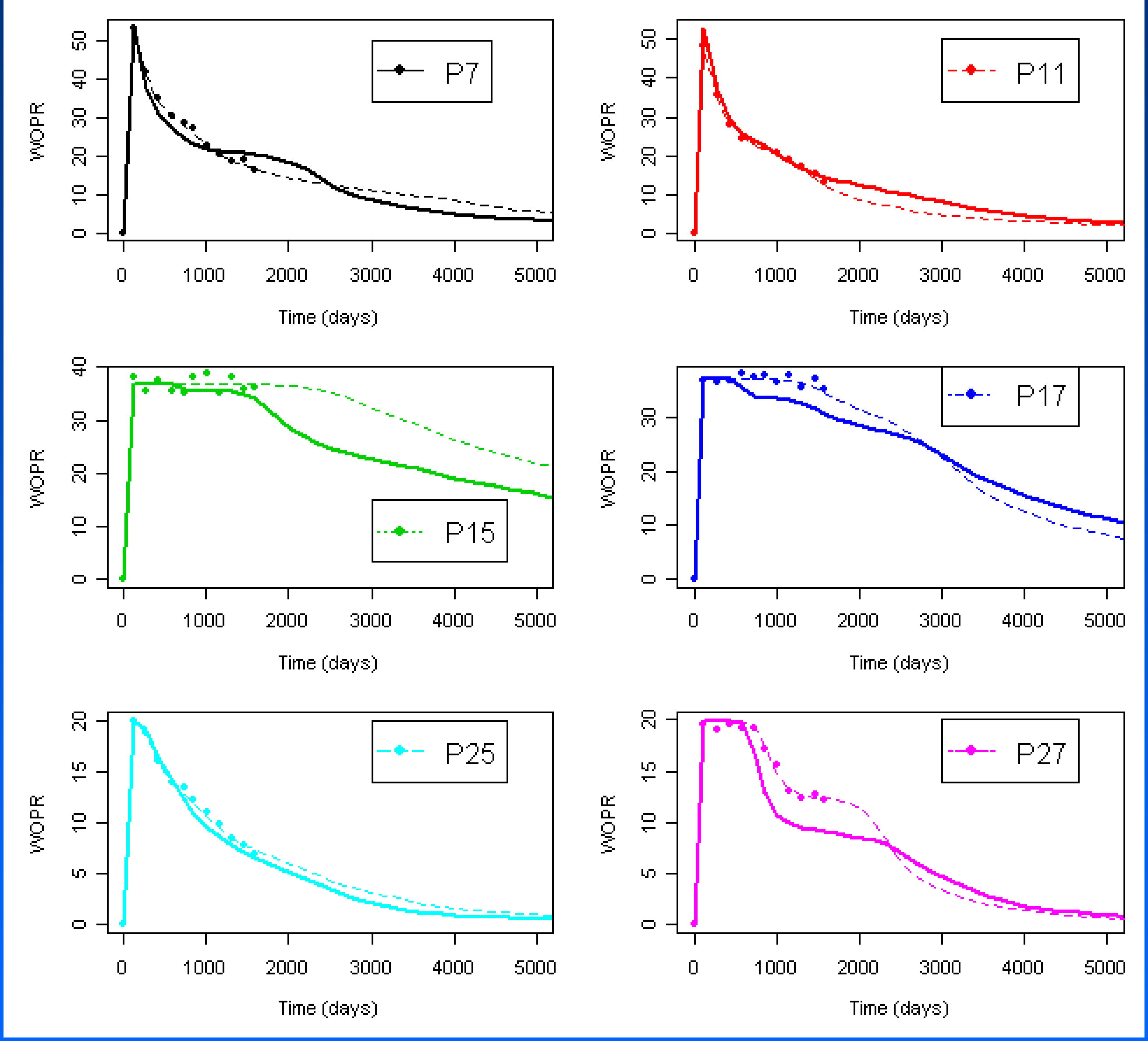
Model Forecast: Production Profiles

Oil production from 6 largest producing wells:

Past history data (truth case + noise)

— Fitted model

- - Truth case



Forecast with Uncertainty

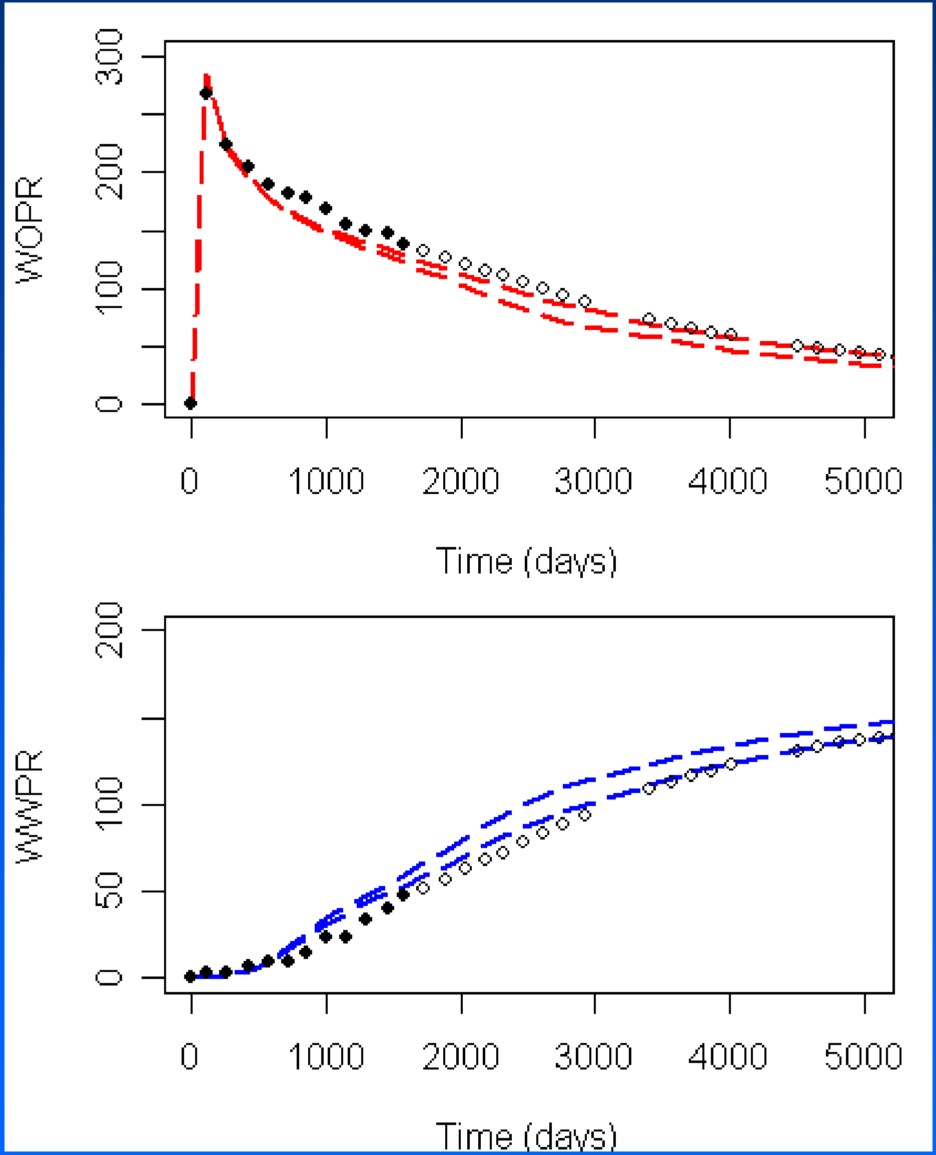
Confidence P10/P90 interval for production forecast based on multiple models

Total oil and water production profiles:

Past history data (truth case + noise)

Validation truth case forecast data

– – P10/P90 production forecast confidence bounds



Uncertainty Quantification

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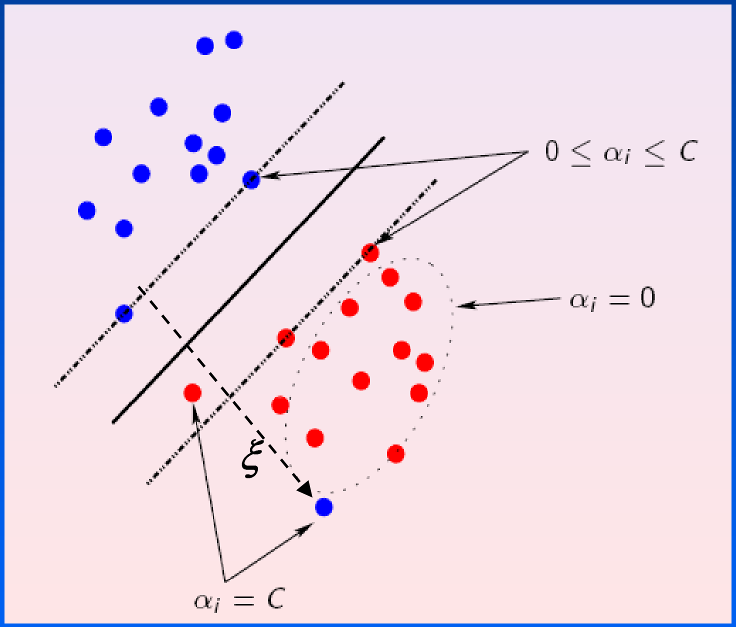
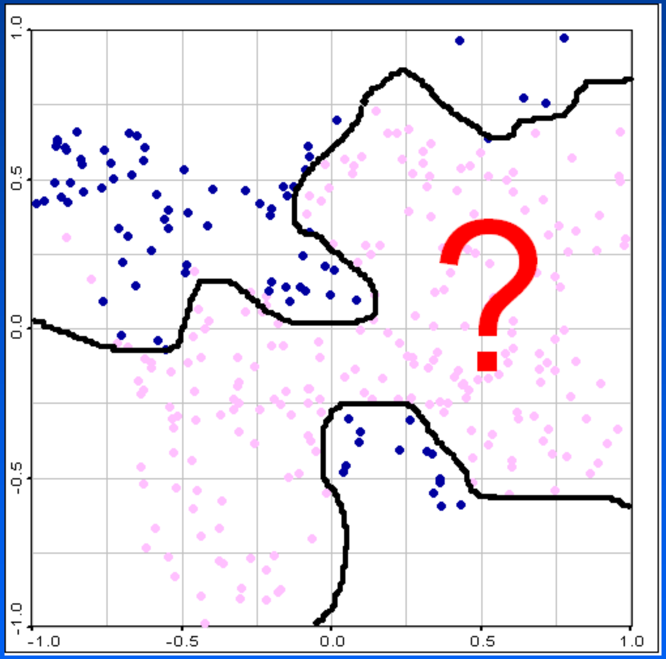
Monitoring Optimisation

- Monitoring Network
- Classification problem
- SVM classification model



- Find locations for additional measurements to refine the current model



Support Vectors (SVs): $0 < \alpha_i < C$

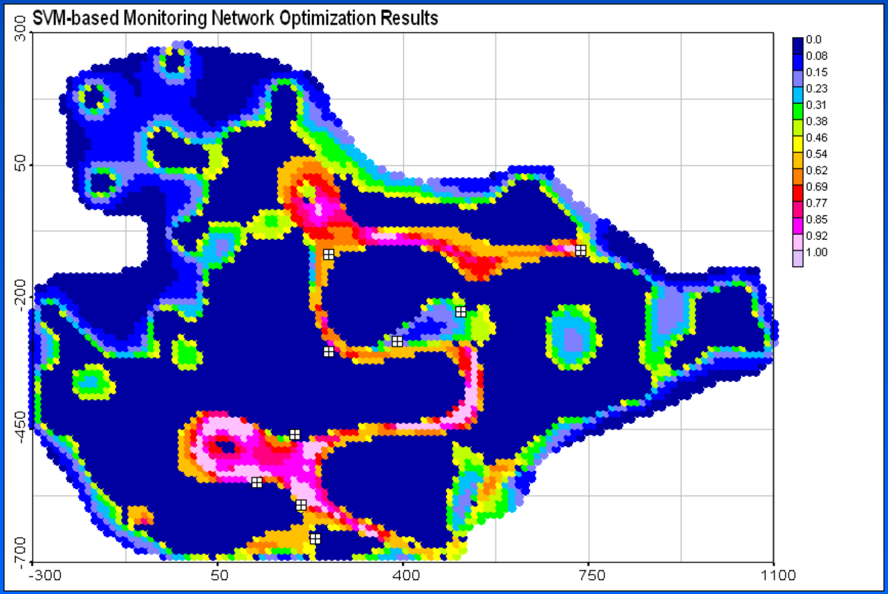
- only SVs contribute to maximum margin solution.
- SVs are the closest samples to the decision boundary

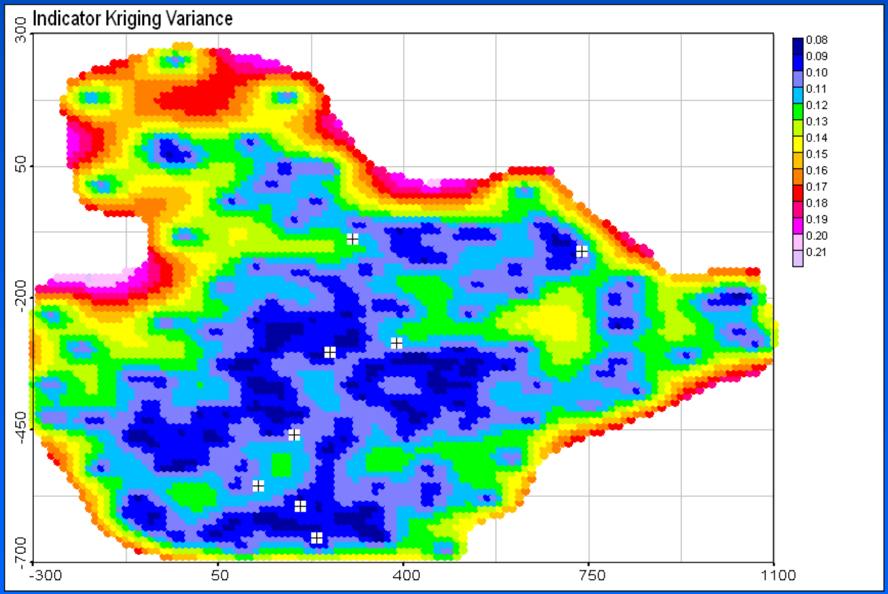
Active Learning with Support Vectors

- Sample decision boundary to label most uncertain locations
- Minimize cross-validation error for misclassifications

SV-based importance measure
- task-oriented result
- follows classification model

Kriging variance
- improves network topology only





A. Pozdnoukhov, M. Kanevski, Monitoring Network Optimisation for Spatial Data Classification Using Support Vector Machines. International Journal of Environment and Pollution, 2005

Summary

- Approaches for spatial uncertainty modelling
  - Geostatistics
  - Machine Learning
  - Combination of both
- Need for stochastic models for adequate uncertainty description
- Bayesian approach handles uncertainty of the model definitions and data uncertainty
- Uncertainty modelling for sampling optimisation

Acknowledgement

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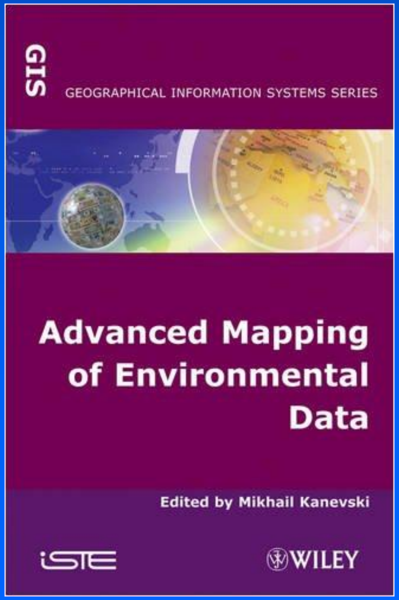
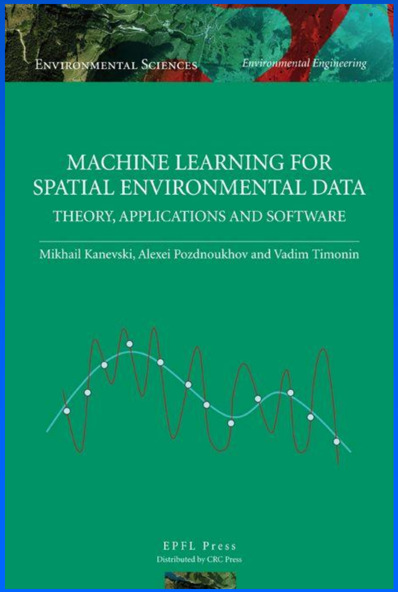
- G. Christakos, San-Diego State University
- E. Savelieva, Nuclear Safety Institute, Moscow





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3. Demyanov V., Pozdnoukhov A., Kanevski M., Christie M. (2008) *Geomodelling of a Fluvial System with Semi-Supervised Support Vector Regression*, Proceedings of the VII International Geostatistics Congress, pp. 627-636, GECAMIN, Chile.
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