Intrinsic Kriging and Prior Information

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Part One: Kriging

- named after D.G. Krige (1951)
- classical theory – (Matheron, 1963)
- intrinsic theory – (Matheron, 1973)
- well-established in Geostatistics
- connections with time-series prediction
- also known under the name of Gaussian processes

Objective: predict system output from observed data using black-box modelling

System modeled by a random process $F(\mathbf{x})$

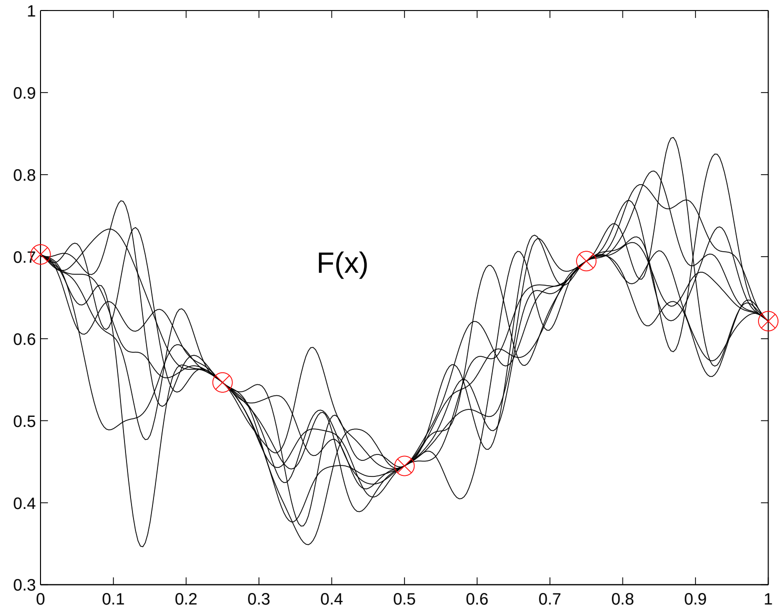


Figure 1: Conditional simulations of $F(x)$ given $F(x_i)$

Linear prediction on $\mathcal{H}_S = \text{vect}\{F(\mathbf{x}_1), \cdots, F(\mathbf{x}_n)\}$

$$\hat{F}(\mathbf{x}) = \sum_{i=1}^{n} \lambda_{i,\mathbf{x}} F(\mathbf{x}_i), \tag{1}$$

Best linear prediction

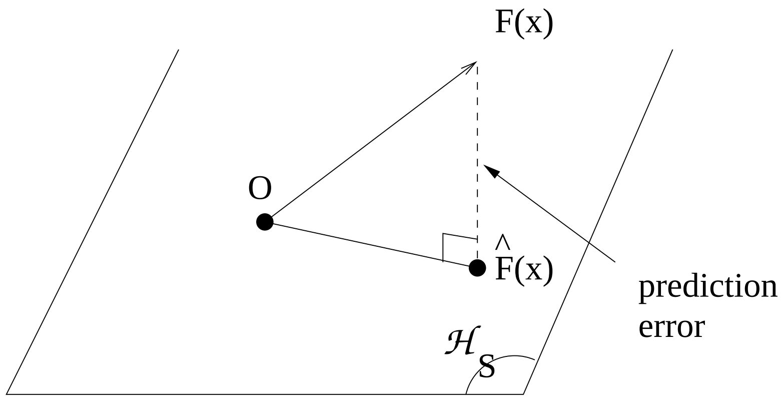


Figure 2: Orthogonal projection

Three points of view, one structure

(Assume $\mathsf{E}F(\mathbf{x}) = 0$)

1. $F(\mathbf{x})$ generates a Hilbert space $\mathcal{H}$, whose elements are limits of linear combinations

$$\sum_{i=1}^{n} \lambda_{i,\mathbf{x}} F(\mathbf{x}_i) \tag{2}$$

$\mathcal{H}$ endowed with scalar product

$$(F(\mathbf{x}), F(\mathbf{y}))_{\mathcal{H}} = \mathsf{E}[F(\mathbf{x})F(\mathbf{y})] = k(\mathbf{x}, \mathbf{y})$$

2. Define the finite support measure

$$\lambda = \sum_{i=1}^{n} \lambda_{i,\mathbf{x}} \delta_{\mathbf{x}_i} \tag{3}$$

The set of these measures generates another Hilbert space Λ

– Λ can be identified to $\mathcal{H}$

– inherits the scalar product of $\mathcal{H}$

$$(\lambda, \mu)_\Lambda = \sum_{i,j} \lambda_i k(\mathbf{x}_i, \mathbf{x}_j) \mu_j \tag{4}$$

3. Λ can also be viewed as the dual of an *rkhs*, or a *feature space* $\mathcal{F}$ in SVM theory.

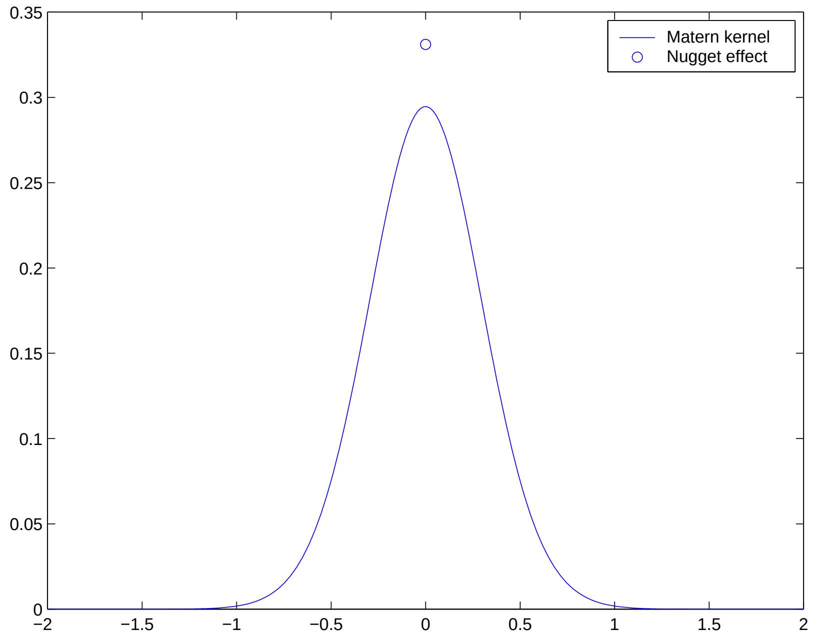
The covariance $k(\mathbf{x}, \mathbf{y})$ is the reproducing kernel of $\mathcal{F}$

$\mathcal{F}$ and $\mathcal{H}$ share the same structure.

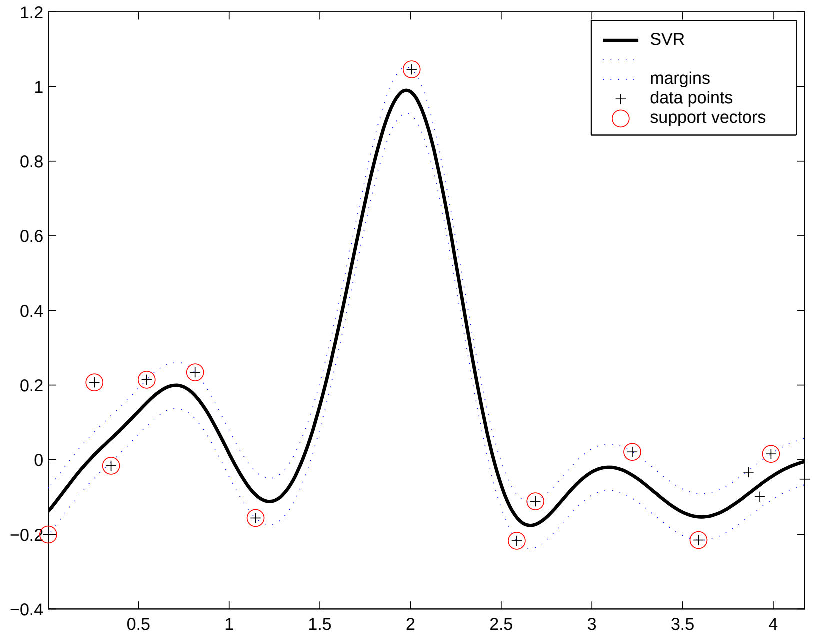
$\Rightarrow$ Kriging can be used to build SVM

Example

Kriging lore



applied in SVR



Regularization and intrinsic Kriging

Regularization minimizes

$$\underbrace{||\hat{f}||^2_{\mathcal{F}}}_{\text{smoothness}} \quad + \quad \underbrace{C\sum_i l(\hat{f}(\mathbf{x}_i) - f_{\mathbf{x}_i})}_{\text{data fidelity}} \tag{5}$$

- Strongly connected with Kriging (Wahba and Kimeldorf, 1970) and (Matheron, 1981)
- Intrinsic Kriging (I.K.) facilitates incorporation of prior knowledge
- In I.K., $||.||_{\mathcal{F}}$ replaced by a seminorm $\Rightarrow$ null-space N of the seminorm not regularized $\rightarrow$ N should correspond to prior information (Smola et al., 1999).

For prediction by I.K., error of prediction required to be be orthogonal to N.

- Define $\Lambda' \subset \Lambda$ such that $\Lambda' \perp N$ (more rigourously $\Lambda' = \{\lambda, \langle \lambda, g \rangle_{\mathcal{F}^*,\mathcal{F}} = 0 \quad \forall g \in N\}$).
- Λ' corresponds to $\mathcal{H}' \subset \mathcal{H}$, with $\mathcal{H}' \perp N$.
- Thus, in I.K. prediction error required to be in $\mathcal{H}'$.

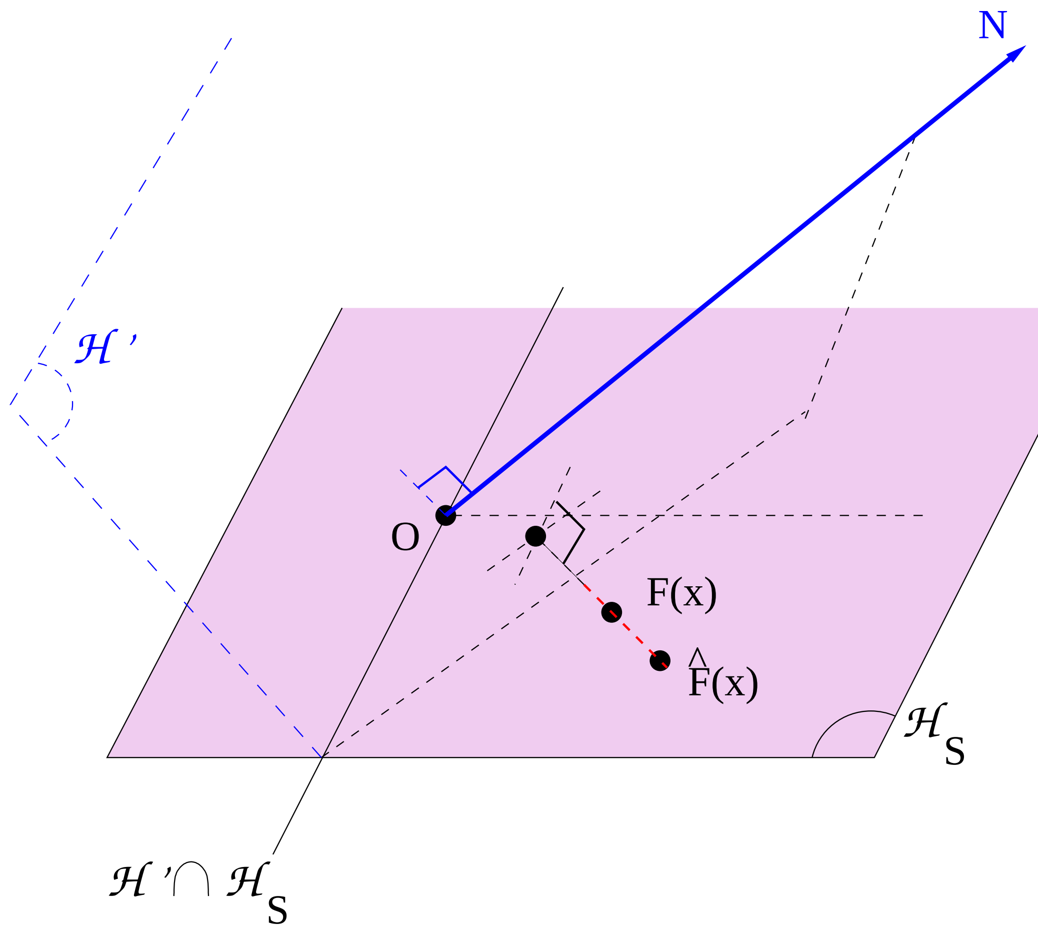


Figure 3: Best approximation given $\hat{F}(\mathbf{x}) - F(\mathbf{x}) \perp N$

Simple example of I.K.

Assume variance of $F(\mathbf{x}_1) - F(\mathbf{x}_2)$ is stationary, *i.e.*,

$$\mathsf{Var}(F(\mathbf{x}_1) - F(\mathbf{x}_2)) = 2\gamma(||\mathbf{x}_1 - \mathbf{x}_2||) = 2\gamma(h) \tag{6}$$

Then

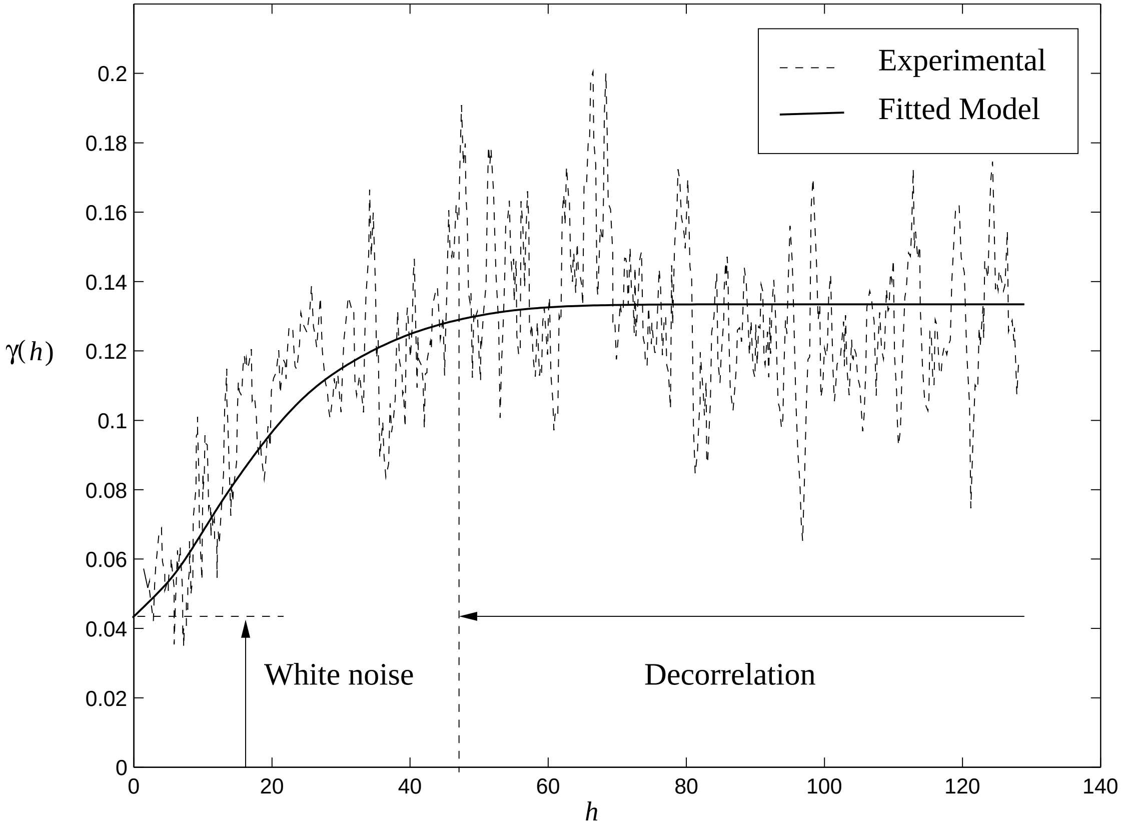
- $\gamma(h)$ called variogram
- Nullspace N made of constant functions

Canonical decomposition:

$$F(\mathbf{x}) = G(\mathbf{x}) + b \text{ with } \mathsf{E}G(\mathbf{x}) = 0 \tag{7}$$

I.K. is a semi-parametric formulation of Kriging

Example of variogram

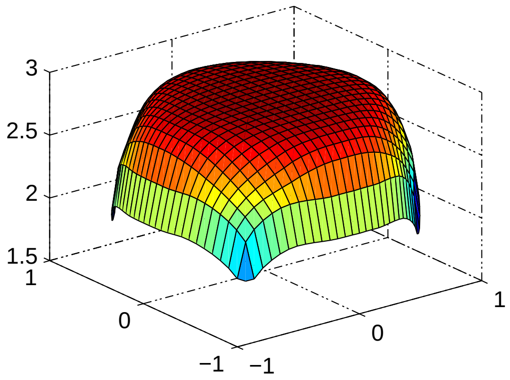


Part Two: Incorporating prior information

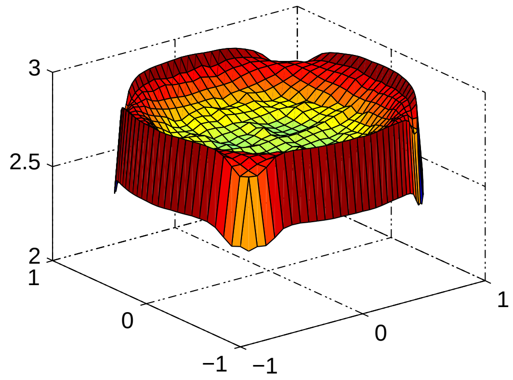
Application to flow measurement

collaboration with Services des Mesures Supélec

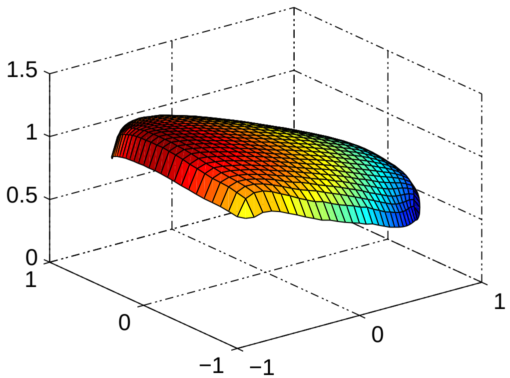
- Estimation of flow in a pipe from punctual observations of speed of fluid;
- Desired performance: relative error $< 1\%$;
- Many fluid speed profiles have been simulated, for different types of pipes.



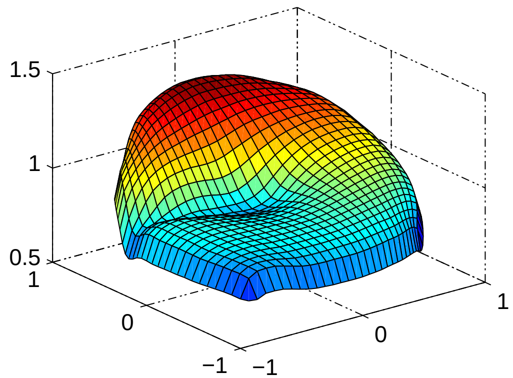
(A)



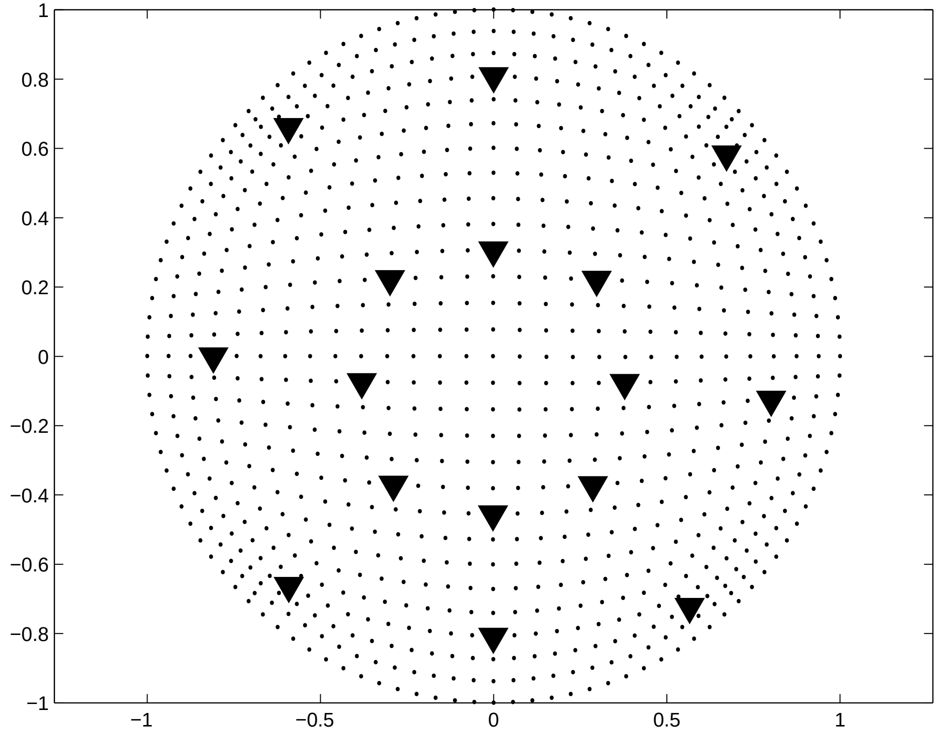
(B)



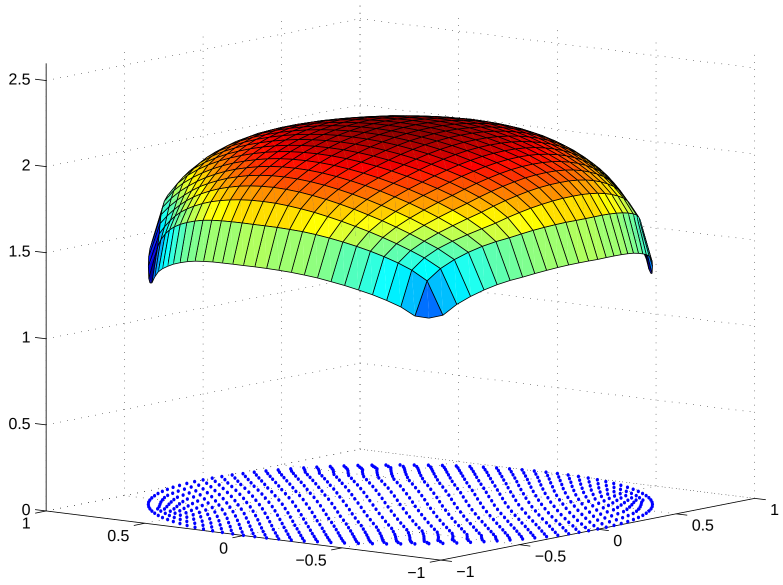
(C)



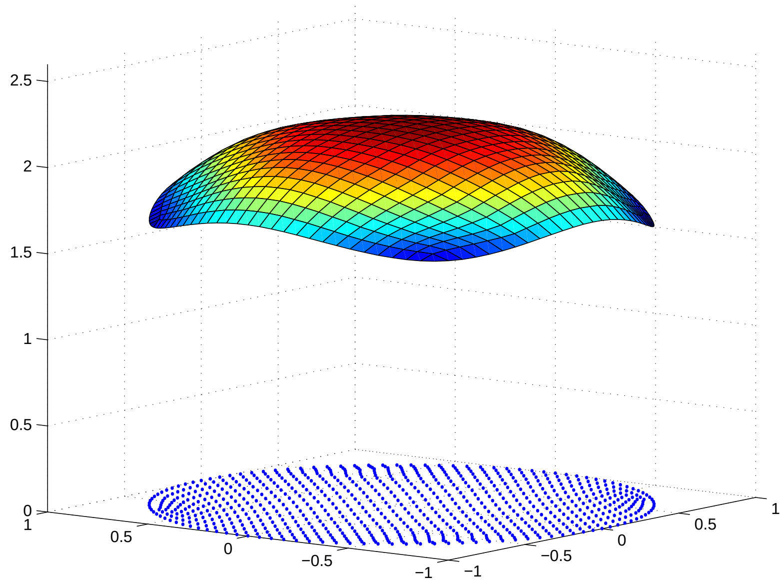
(D)


1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1
−1
−0.5
0
0.5
1

Direct estimation of speed profile is not sufficient.

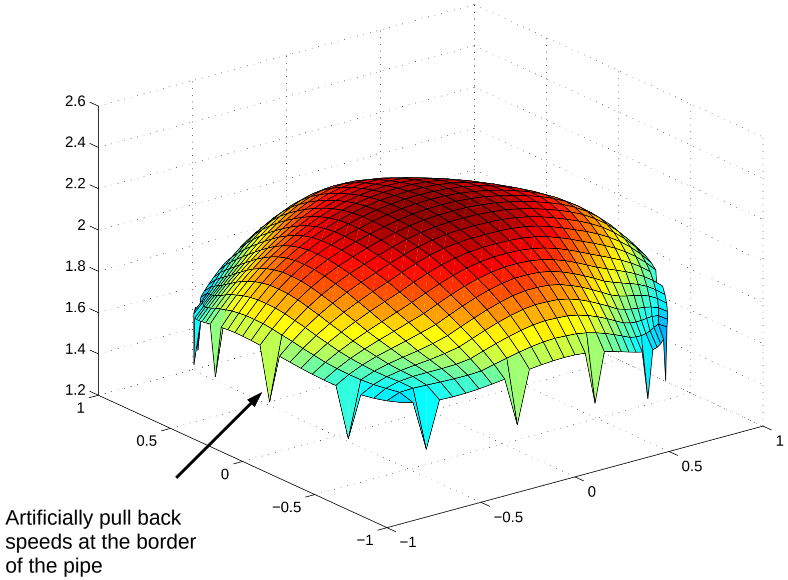


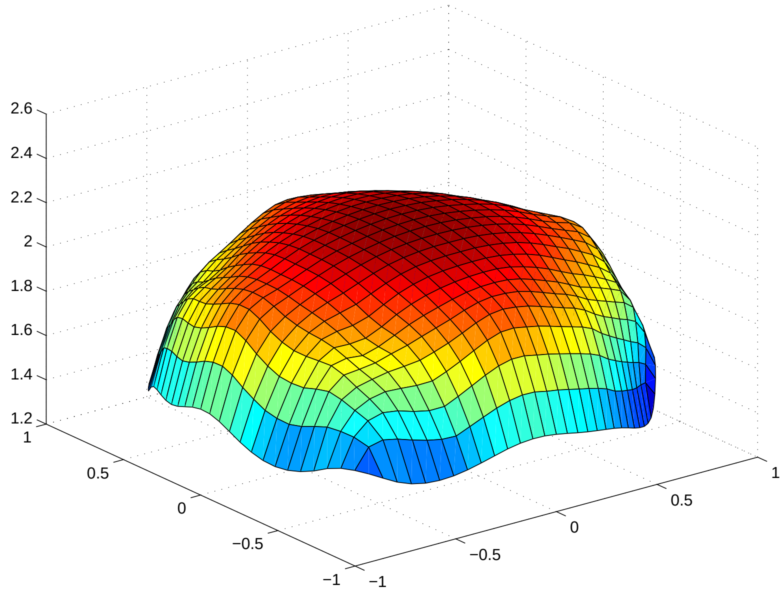
Actual profile



Predicted profile

First idea: artificially add the trend





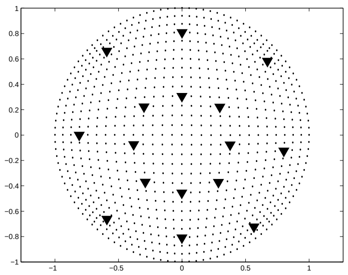
Including prior information via I.K.

Principle:

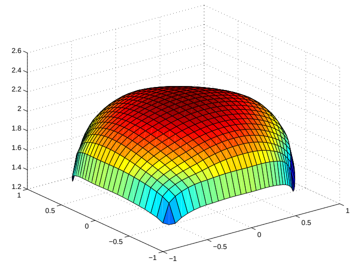
- Add new factors $\mathbf{x}^*$ corresponding to prior information. For instance, at each position $\mathbf{x}$ of the cross section of the pipe, add a scalar factor x^* indicating nominal speed there.
- For prior knowledge to be preserved by regularization it should be introduced in the nullspace N. This is done under the form

$$\mathbf{x}, \mathbf{x}^* \mapsto \mathbf{a}^\top \mathbf{x}^* + \mathbf{b} \tag{8}$$

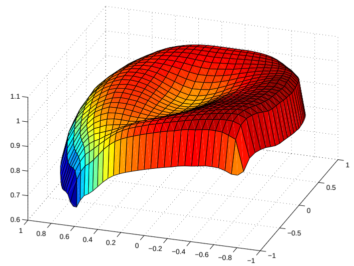
- $\mathbf{a}$ estimated by I.K. Prediction error orthogonal to $\mathbf{x}^*$.



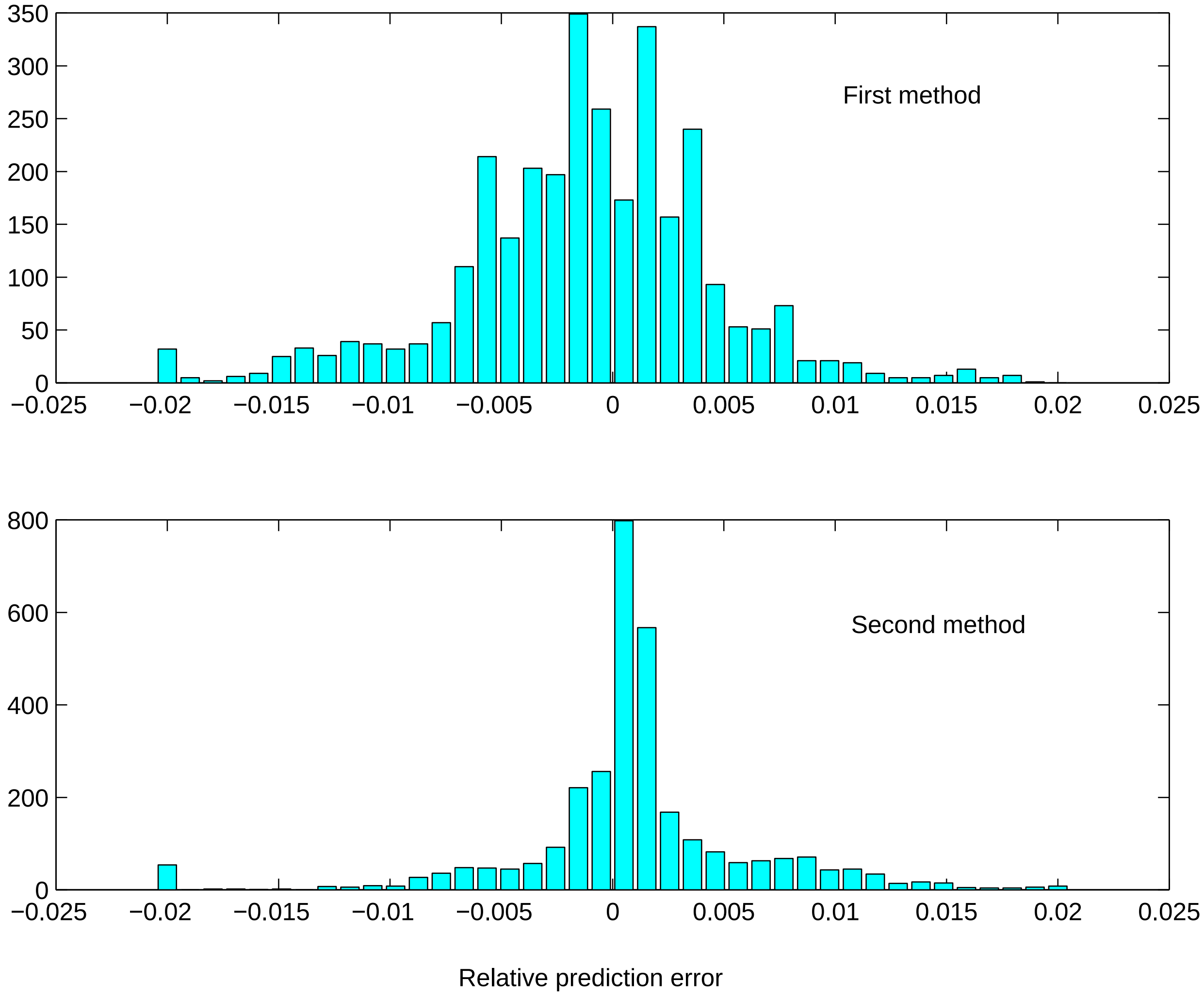
$+$



$\longrightarrow$



observations	prior knowkedge	estimation
$f(\mathbf{x}_i)$	x^*	$\hat{f}(\mathbf{x}, x^*)$


First method
Second method
Relative prediction error
350
300
250
200
150
100
50
0
800
600
400
200
−0.025
−0.02
−0.015
−0.01
−0.005
0.005
0.01
0.015
0.02
0.025

Conclusions

- including prior knowledge in black-box modelling made easy via a semi-parametric approach
- good results obtained in a real application
- I.K. theory allows to interpret regularization methods (Splines, RBF, SVR) in a probabilistic framework
- interpretation of a kernel as the covariance of a random process helps choosing a kernel for a given application

References

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