Comparing different interpolation methods on two-dimensional test functions

Thomas Mühlenstädt, Sonja Kuhnt

TU Dortmund

ENBIS EMSE, St. Etienne

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Institut für Mathematische Statistik und industrielle Anwendungen

Statistische Modellbildung

Computer experiments

Simulation model for real world phenomena *Fang et al. (2006)*

- Deterministic
- Computational expensive

Needed: Easy to calculate surrogate

Setting:

- Design $D = \{\vec{x}_1, \ldots, \vec{x}_n\}, \vec{x}_i = (x_{i,1}, x_{i,2})$.
- One-dimensional output $y_1, \ldots, y_n$
- $y_i = f(\vec{x}_i)$, f unknown

Multivariate interpolation

Treated approaches:

- Kriging (Gaussian Random Fields)
- Thin plate spline (*TPS*)
- Natural neighbor interpolation (*NNI*)
- Kernel interpolation (*KI*)

Kriging

Santner et al. (2003)

$$Y(\vec{x}_i) = g_\beta(\vec{x}_i) + Z(\vec{x}_i), 1 \leq i \leq n,$$

- $g_\beta(\vec{x}_i)$ regression part (here: $g_\beta = \beta \in \mathbb{R}$)
- $Z(\vec{x}) \sim (0, \sigma^2)$ normally distributed
- $Z(\vec{x}_1)$ and $Z(\vec{x}_2), \vec{x}_1 \neq \vec{x}_2$ explicitly dependent:

$$cor_\theta(Z(\vec{x}_1), Z(\vec{x}_2)) \to 1 \text{ for } \vec{x}_1 \to \vec{x}_2$$

Kriging

$$cor(Z(\vec{x}_i), Z(\vec{x}_{i'})) = \exp\left(-\sum_{d=1}^{2} \theta_i \left|x_{i,d} - x_{i',d}\right|^2\right)$$

- Estimation of parameters β, θ, σ^2: REML
- Optimization of Log-likelihood: by *R* command `optim` for 50 different initial values

Thin plate spline (*TPS*)

- Generalization of cubic splines *Micula (2002)*
- Solves the following optimization problem:

  Search f^*, such that $I(f)$ is minimized
  in a suitable functional space
  under the constraint of interpolation

$$I(f) = \int_{\mathbb{R}^2} \left(\frac{\partial^2 f(\vec{x})}{\partial x_1^2} \right)^2 + 2 \left(\frac{\partial^2 f(\vec{x})}{\partial x_1 \partial x_2} \right)^2 + \left(\frac{\partial^2 f(\vec{x})}{\partial x_2^2} \right)^2 d\vec{x}$$

Thin plate spline (*TPS*)

- Can be solved explicitly:

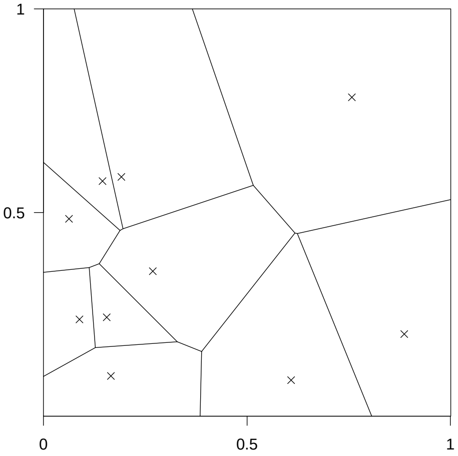
$$f^*(\vec{x}) = \sum_{i=1}^{n} \lambda_i \phi(\|\vec{x} - \vec{x}_i\|_2) + \lambda_{n+1} + \lambda_{n+2} x_1 + \lambda_{n+3} x_2$$

- $\phi(r) = r^2 log(r)$
- Computation $\lambda_1, \ldots, \lambda_{n+3}$: system of linear equations

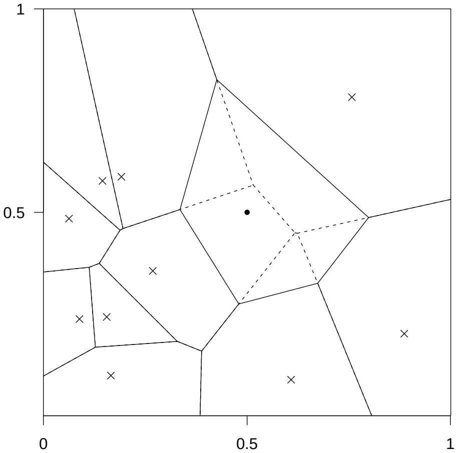
Natural neighbor interpolation (*NNI*)

- Weighted mean of the y-values *Sibson (1980)*
- Strictly local method
- Uses the Voronoi diagramm for weighting

Natural neighbor interpolation (*NNI*)



Natural neighbor interpolation (*NNI*)

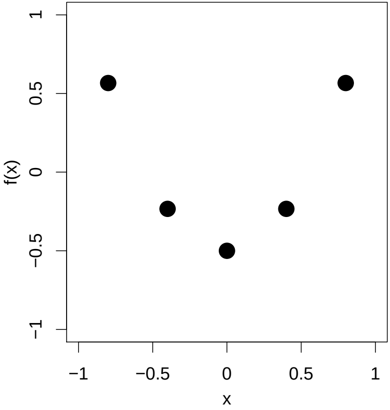


Kernel interpolation (*KI*)

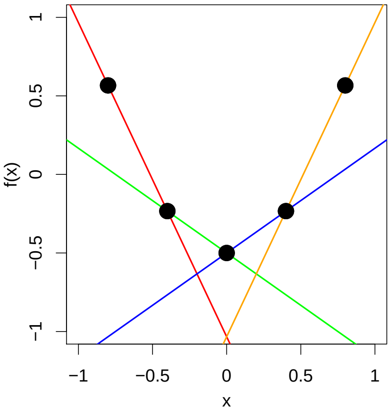
- Weight locally fitted linear functions under the constraint of interpolation *Mühlenstädt and Kuhnt (2009)*
- Split up the convex hull of the design into simplices S_j (Delaunay triangulation)
- Fit a linear function $\hat{y}_j(x)$ to each simplex S_j
- Weight the linear functions:

$$\frac{\sum_{j=1}^{N} g_j(\vec{x})\hat{y}_j(\vec{x})}{\sum_{j=1}^{N} g_j(\vec{x})}, \quad g_j(\vec{x}) = \frac{1}{\prod_{i=0}^{2} \|\vec{x}_i^j - \vec{x}\|_2^2}$$

Kernel interpolation (*KI*)



Kernel interpolation (*KI*)



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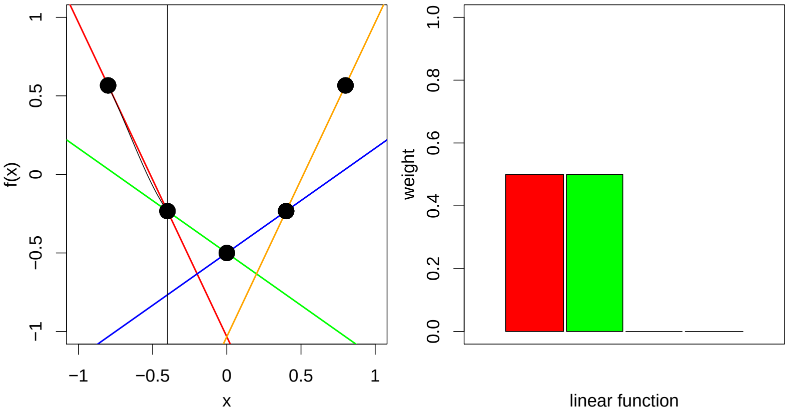

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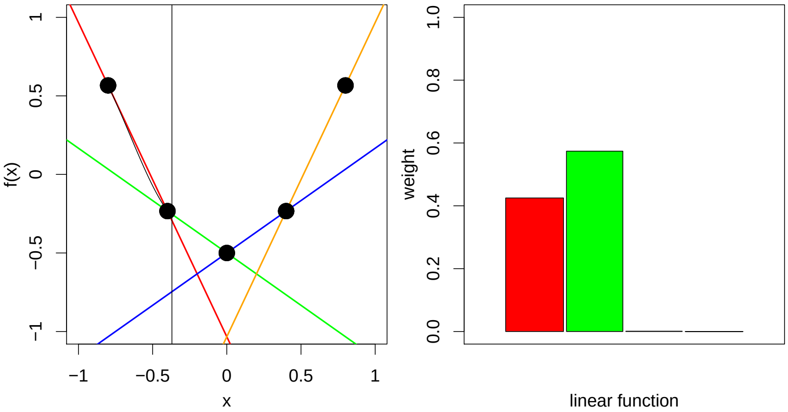

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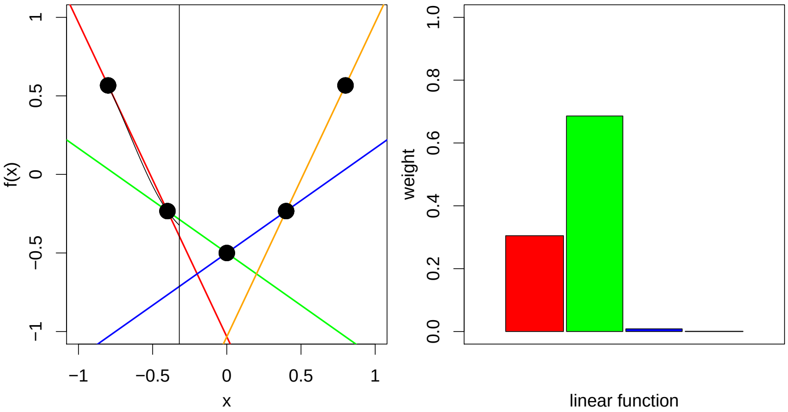

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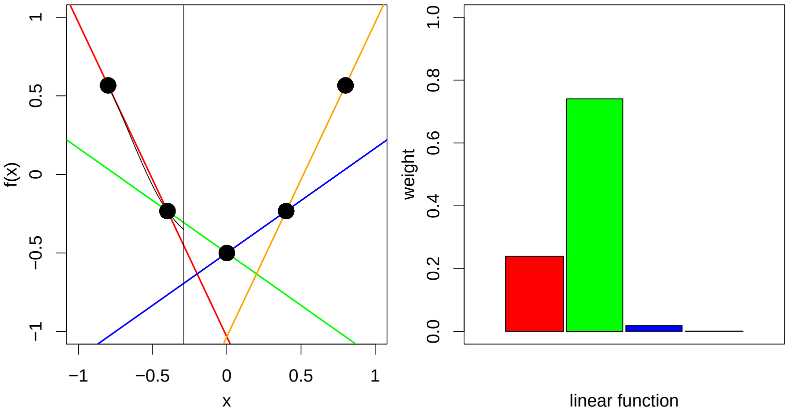

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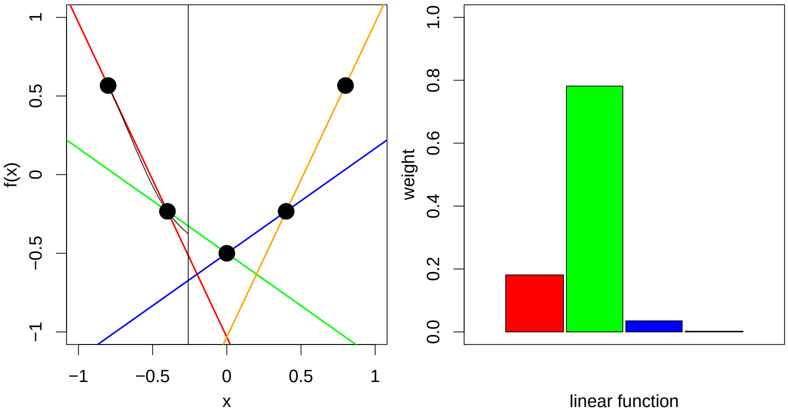

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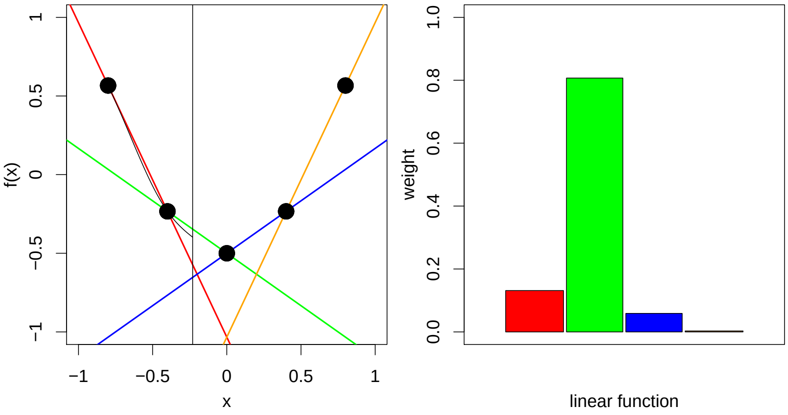

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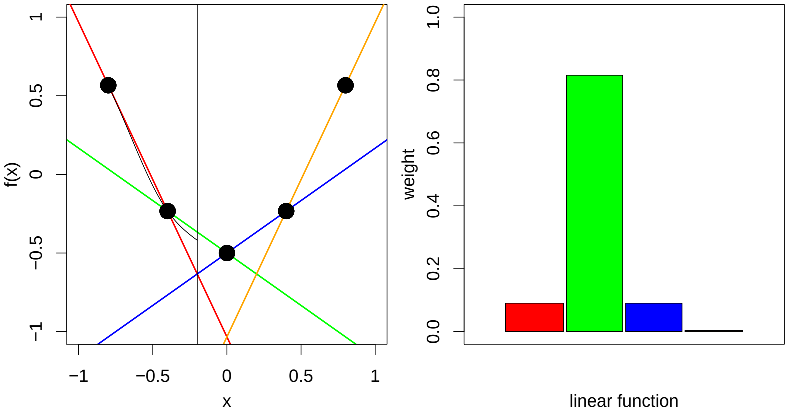

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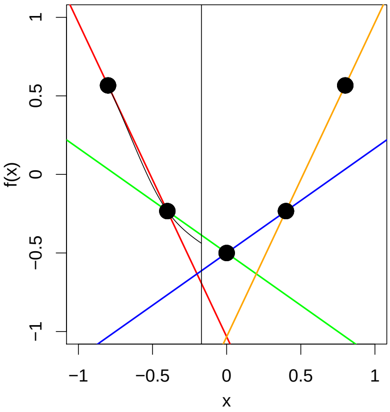

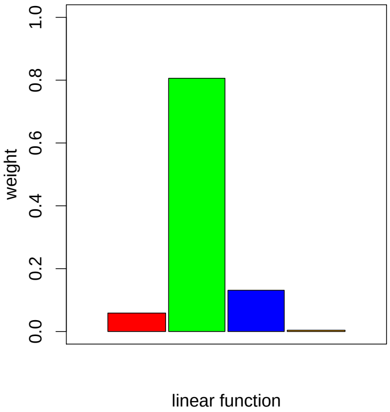

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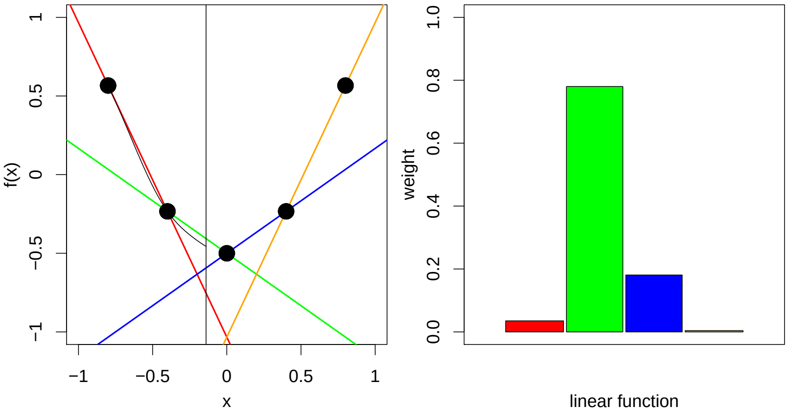

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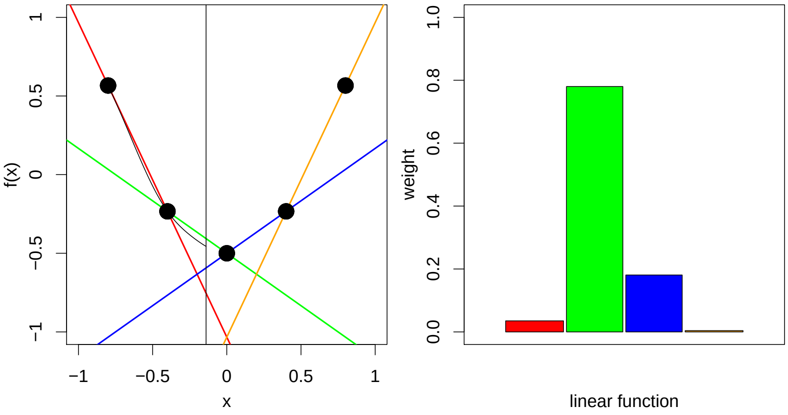

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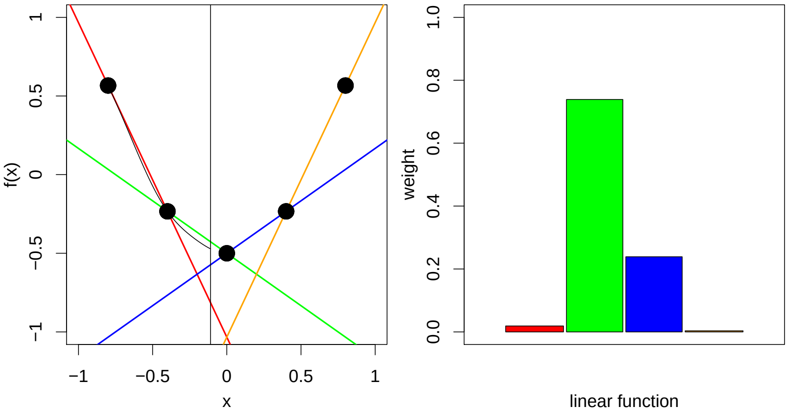

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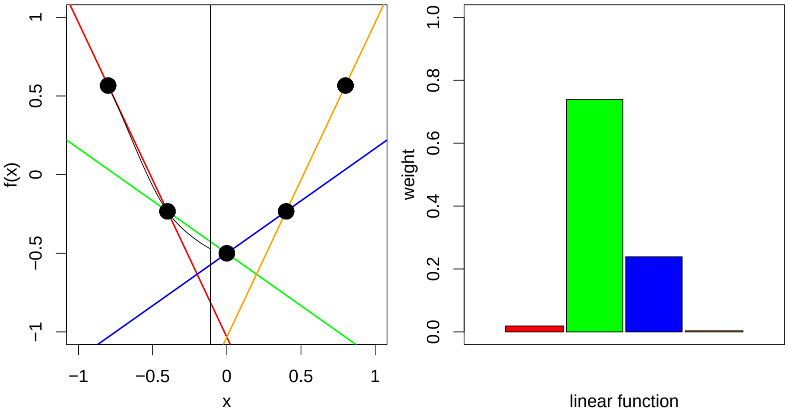

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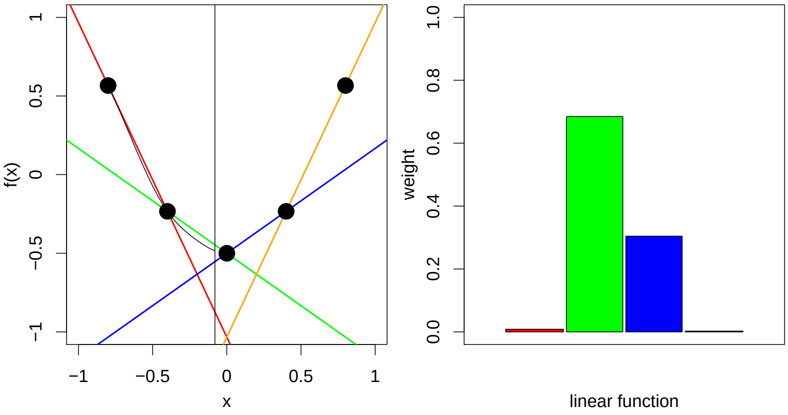

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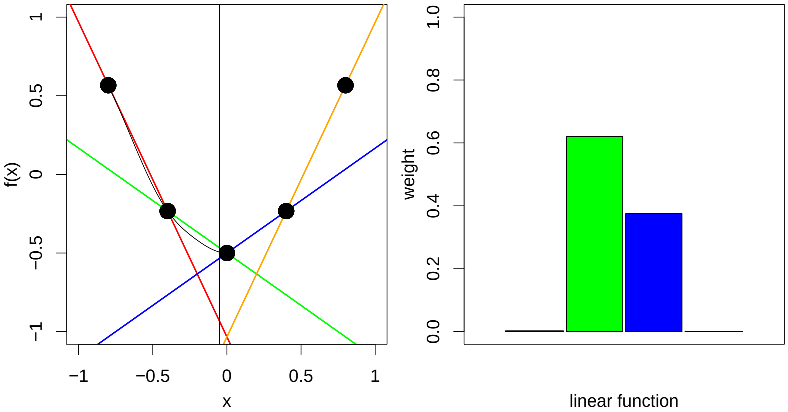

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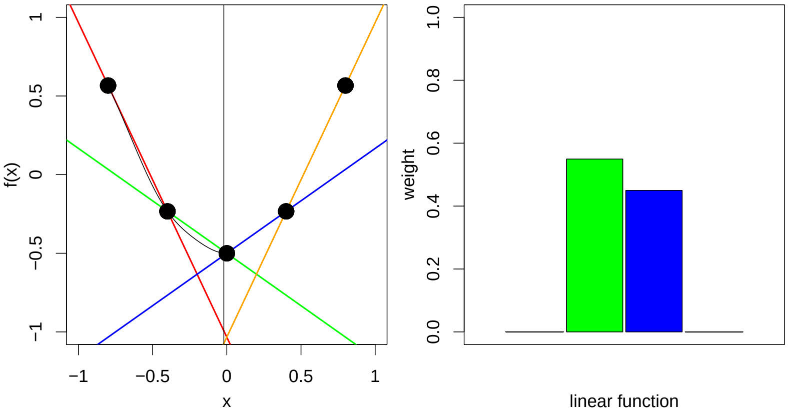

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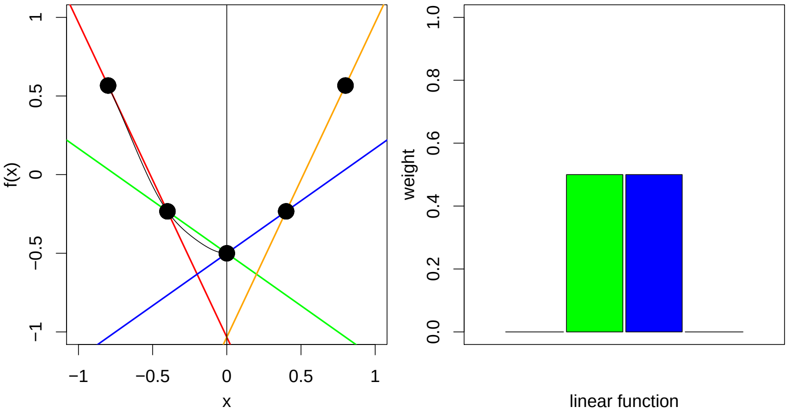


Kernel interpolation (*KI*)

Properties of the Kernel interpolation:

- Continuous
- Differentiable (also at observation points)
- Able to predict outside of observation range
- Exactly reproduces linear functions

Comparison of interpolation methods

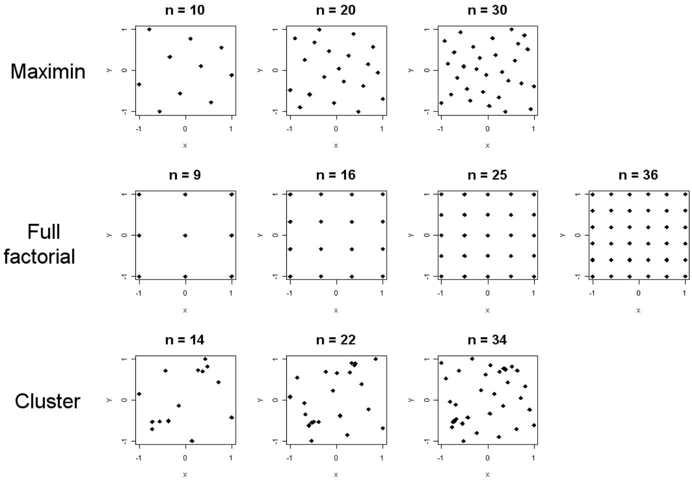
Which interpolation method should be used?

- 5 analytical 2-dim. examples
- Aim: high prediction power
- Prediction power: root mean square error (RMSE)
- Different experimental designs

Designs for computer experiments

- Difference to 'standard' DoE: no random error
- Example for a 'good' space filling designs: maximin latin hypercube design *Fang et al. (2006)*
- Also often encountered: factorial designs
- For sequential procedures: designs with clusters

Used Designs



Root Mean square error($RMSE$)

- Criterium for comparing different predictions:

$$RMSE(y, \hat{y}, \vec{r}_1, \ldots, \vec{r}_m) := \sqrt{\frac{1}{m}\sum_{i=1}^{m}(y(\vec{r}_i) - \hat{y}(\vec{r}_i))^2}$$

- $\vec{r}_1, \ldots, \vec{r}_m$ points in the design space
- $\vec{r}_1, \ldots, \vec{r}_m$ 10000 points of a Sobol' Uniform Sequence

Implementation aspects

- Easy: Thin plate spline
- Acceptable:
  - Kriging
  - Kernel interpolation (if Delaunay triangulation is available)
- Difficult: Natural neighbor interpolation (Calculation of the Voronoi diagram constrained to design space)

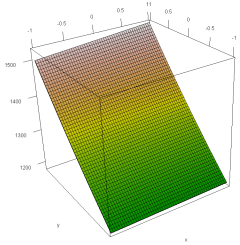
Computation times

Design	*TPS*	*KI*	Kriging	*NNI*
D_{10}^{Mm}	10	15	13 - 22	839
D_{20}^{Mm}	13	27	69 - 162	1536
D_{30}^{Mm}	15	39	178 - 448	2239

- Computation times in seconds
- For 10000 prediction points
- Based on the maximin latin hypercube designs

Die force

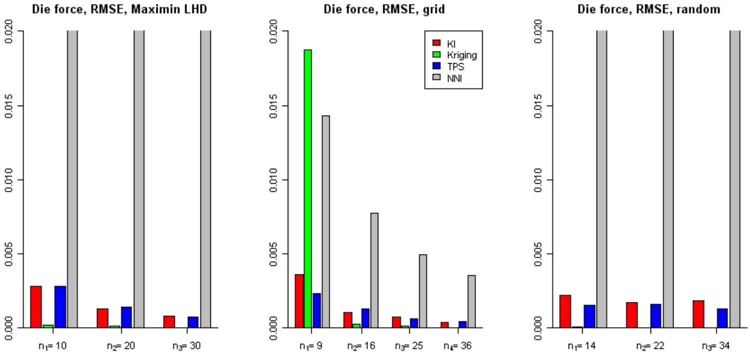
- Model for the effective die force in sheet metal forming processes depending on friction and blankholder force
- Nearly linear in one variable



$$f(\vec{x}) = 0.9996(1090.91 + 4x_1x_2)\exp\left(x_1\frac{\pi}{2}\right),$$

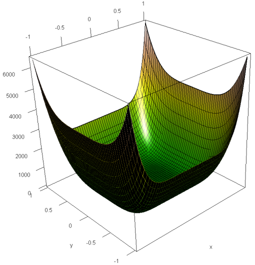
$$D = [0.05, 0.2] \times [5, 30]$$

Die force


Die force, RMSE, Maximin LHD
0.000
0.005
0.010
0.015
0.020
n_1= 10
n_2= 20
n_3= 30
Die force, RMSE, grid
KI
Kriging
TPS
NNI
n_1= 9
n_2= 16
n_3= 25
n_4= 36
Die force, RMSE, random
n_1= 14
n_2= 22
n_3= 34

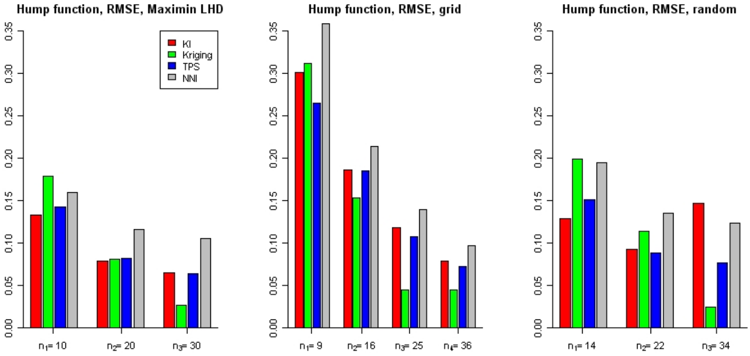
Hump function

- Standard example from optimization literature
- Extreme values on boundary



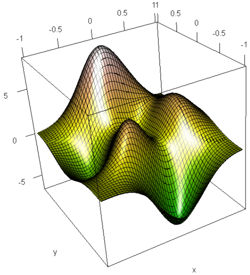
$$f(x,y) = 1.0316 + 4x^2 - 2.1x^4 + \frac{1}{3}x^6 + xy - 4y^2 + 4y^4,$$
$$D = [-5,5]^2$$

Hump function



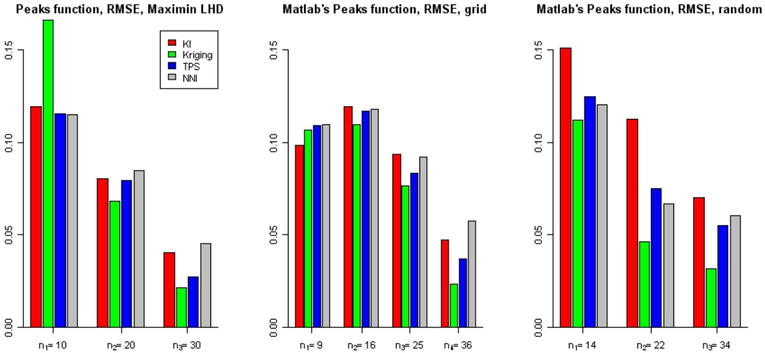
Matlabs peaks function

- Good example for a hilly contour



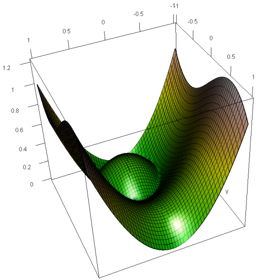
$$
\begin{aligned}
f(\vec{x}) =& 3(1 - x_1)^2 \exp\left(-x_1^2 - (x_2+1)^2\right) - \\
& 10\left(\frac{x_1}{5} - x_1^3 - x_2^5\right)\exp\left(-x_1^2 - x_2^2\right) - \\
& \frac{1}{3}\exp\left(-(x_1+1)^2 - x_2^2\right), \quad D = [-2,2]^2
\end{aligned}
$$

Matlabs peaks function



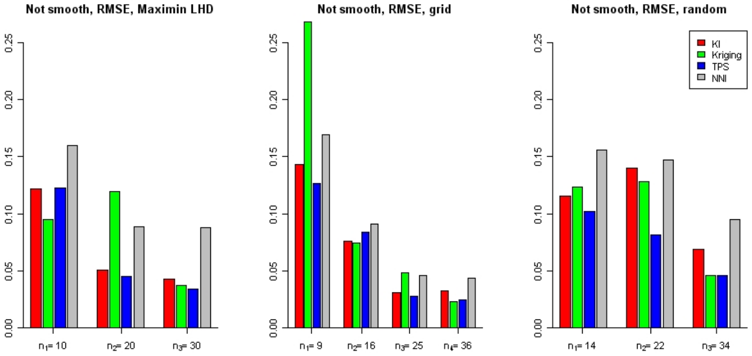
Not smooth

- Assumption of smoothness often unrealistic
- Continuous but not differentiable



$$f(x, y) = |x^2 + \sin(0.5\pi y) - y|, \qquad D = [0, 1]^2.$$

Not smooth


Not smooth, RMSE, Maximin LHD
0.00
0.05
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n1= 10
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Not smooth, RMSE, random
KI
Kriging
TPS
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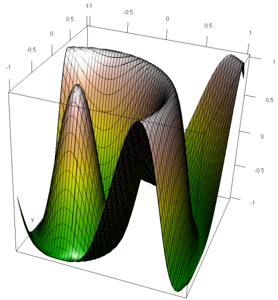
Sibson's function

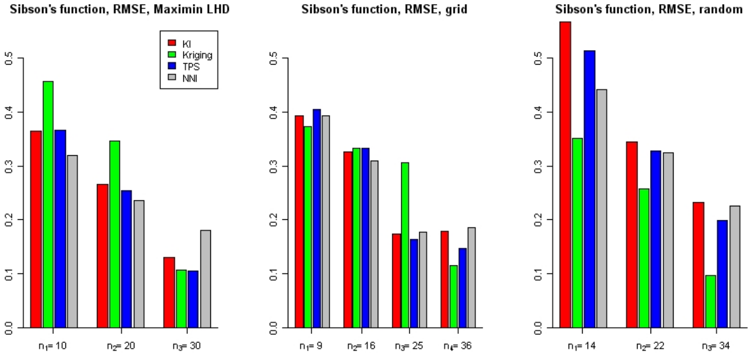
- Proposed by Sibson (1980) for illustrating *NNI*
- High complexity for size of sample



$$f(\vec{x}) = cos\left(4\pi\sqrt{(x_1 - 0.25)^2 + (x_2 - 0.25)^2}\right),$$

$$D = [0,1]^2$$

Sibson's function



Summary

- No overall winner
- Decision depends on design
- Kriging often very efficient, especially for higher sample sizes, designs with clusters
- *KI* and *TPS* good for small sample sizes
- *NNI* not recommendable

Literatur

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