**Kriging interpolation in simulation: a survey**

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**Outline**

Goal of Kriging: Interpolation
- Our focus: Interpolation for "expensive" simulations
  - Kriging: History, applications, basics
  - Kriging versus regression analysis
  - Application domain: Deterministic simulations in CAE
    - Random simulation: Just started!
  - Fractional factorials (regression) versus space filling (e.g., LHS)
  - Novel design: Our customized, sequential design
    (using cross-validation & bootstrapping)

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**Kriging interpolation: History**

- Danie Krige: Method to determine ore-grades (1950s)
- Predictions based on sample
- Assumption: The closer the input data, the more positively correlated their outputs
- Georges Mathéron: Covariance function (1962)
  - Assumption: Second-order stationary
    - Constant mean: \( \mu \)
    - Covariances of outputs depend only on distances between inputs:
      \[
      \text{cov}(Y(x_1), Y(x_2)) = C(x_1 - x_2)
      \]

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**Kriging interpolation: Applications**

- **Origin:** Geostatistics (Krige/Mathéron 1951)
  - Examples: Ore bodies (coal), air pollution (CO\(_2\)), …
- **Later:** Deterministic simulation (Sacks et al. 1989)
  - Examples: Computer chips, TV monitors, air planes, …
- **Now:** Random simulation (Van Beers and Kleijnen, *EJOR*, in press)
  - Examples: Queueing, inventory systems, …

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**Kriging interpolation: Basics (1)**

- Kriging predictor: Weighted linear combination of \( n \) 'old' (observed) outputs
  \[
  \hat{Y}(x) = \sum_{i=1}^{n} \lambda_i \cdot Y(x_i)
  \]
- Weights \( \lambda_i \): Function of distance \( d \) between \( n \) 'old' inputs and 'new' input \( x \)
- Statistical dependence: Example \( C(d) = \sigma^2 \cdot \exp(-\theta \cdot |d|) \)
  - The closer the inputs, the higher the weights of their outputs
  - Note: If 'new' input = 'old' input, then weight = 1 (i.e., exact interpolator)
  - Different 'new' inputs \( \Rightarrow \) different weights for 'old' inputs

**Example correlation function**

\[
\text{cov}(Y(x + d), Y(x)) = 13.94 \times \exp(-3.9 \times |d|)
\]
**Kriging interpolation: Basics (2)**

- **BLUE criterion for \( \lambda \)**: 
  \[
  \lambda = \min \left\{ \text{MSE}(\hat{Y}(x)) \right\} = \min \left\{ \text{MSE}(E[\hat{Y}(x)]) \right\}
  \]
  – Best: Minimum variance
  – Unbiased: Exact interpolator

- Result: Optimal weights
  \[
  \lambda = \left( \gamma + \frac{1}{\lambda} \right) \gamma
  \]
  \( \gamma \): covariances between new output and \( n \) old outputs
  \( \Gamma \): covariances between \( n \) old outputs

See software
DACE/Matlab by Lophaven, Nielsen, and Søndergaard (2002)

**Kriging versus regression**

Example: Kleijnen & van Beers (WP, 2004): M/M/1 waiting times

**Standard designs for Kriging**

Design & analysis: ‘Chicken & egg’
  - Classic: Polynomial regression & fractional factorials (\( 2^{k-p} \) designs)
  - Random simulation: Replicate ‘enough’ to show signal/noise
  - Strategy versus tactics: Precision \( \delta \) and CRN

Kriging uses the averages per input

Design: LHS (flexible \( n \), for any \( k \))

Example (see figure): \( k = 2; n = 4 \) \( n \) values per input

**Customized Sequential DOE**

Seven steps:
1. Select a pilot design
2. Simulate a small number of replicates, per ‘point’ of pilot design (CRN)
3. Add replicates, until specified precision is obtained
4. Select candidate inputs, and predict their outputs via Kriging
5. Bootstrap the replicates; predict candidate outputs; quantify prediction uncertainty; Bootstrap variances
6. Find ‘winning’ candidate, simulate, and add to I/O data
7. Sequentialize: Repeat steps 4 through 6, until stopping criterion is reached

**Step 1: Pilot design**

- Start with small number of input combinations: \( n_x = 5 \)
- Choose these combinations space filling: e.g. maximin design: •
- In our M/M/1 example: \( x_i \in \{0.1, 0.3, 0.5, 0.7, 0.9\} \)

**Step 2: IID replicates**

Analysis method: Renewal process for M/M/1
(Replicated runs for terminating (x, S) inventory simulation)
Step 2: Replicates (continued)
- Simulate \( m_0 = 10 \) IID replicates \( (y) \) per input \( x \)
- Common Random Numbers (CRN) across \( n \) input values
- \( y_x = \frac{1}{n} \sum_{i=1}^{n} y_{x_i} \) (illustrates variability; not bootstrapped! See Step 5)

Step 3: Add replicates for precision
- Add replicates, one at a time, until desired precision:
- Estimate \( E(y(x)) \) with relative error \( \delta = 0.15 \)
- \( \bar{y} = \frac{\sum_{i=1}^{m_0} y_{x_i}}{m_0} \)

Step 4: Candidates
Select space-filling candidate input combinations:
- \( x'_g = \frac{x_g + x_{g+1}}{2} \) \( (g = 1, \ldots, n-1) \)

Step 5: Bootstrap variance (continued)
Measure prediction uncertainty
Bootstrap variance per candidate input combination:
- \( \text{vär}(\hat{y}_g^*) = \frac{1}{B-1} \sum_{b=1}^{B} (\hat{y}_{g,b}^* - \bar{y}_g^*)^2 \)

Step 6: Find ‘winner’
- Winner: Candidate with biggest bootstrap prediction variance \( \nu = \arg \max_{\nu \in \{1, \ldots, B\}} \left\{ \text{vär}(\hat{y}_g^*) \right\} \)
- Add selected \( x'_g \) input to ‘old’ design
- Simulate – with CRN – with this new input \( x'_g \)
- Repeat tactics: Renewal analysis, precision \( \delta \)
Step 7: Sequentialize

Repeat steps 4 through 6, until stopping criterion is reached:
- Computer budget exhausted
- Time expired
- Kriging metamodel ‘acceptable’
- We: Fix $n$ and precision $\delta$ (see $n$ in LHS)

Example: M/M/1

- True I/O function $E(y) = x/(1-x)$
- Sequentialized, customized design with stopping criterion $n = 15$
- Tactics: $\delta = 15\%$; CRN

\[ y = \frac{x}{1-x} \]

Example: LHS versus Customized Design

Same $n = 15$, same precision $\delta = 0.15$, and CRN:

Example: M/M/1 example: Test set

- Compare both designs at new $x'$ \in \{0.1125, 0.1375, ..., 0.8875\}; see figure below
- Calculate Corrected EIMSE: $C^{*} = \frac{1}{n} \sum_{i=1}^{n} \left( \hat{y}(x') - E[y(x')] \right)^2$
  with $C =$ total number LHS replicates / total number CD replicates; see next figure

M/M/1 example: Different $n$ and seeds

CEIMSE $\times 10^3$

\[ CEIMSE_{\times 10^3} \]
**M/M/1 example: Different n and seeds**

![Graph showing MaxMSE x 10^2 for different seeds and n values](image)

**Example: (s, S) inventory**

- Law & Kelton (2000, p. 651): Terminating after 120 months
- Law & Kelton: 2nd order polynomial regression predictor, estimated from 4x4 points (n = 16) with m = 5 replicates
- We: Kriging predictor, estimated from same 4x4 points with m = 5
- True output (costs) estimated thru m = 10 replicates of 21x20 points
- Smaller prediction errors
- Next: Customized sequential design versus LHS with fixed sample size

**Conclusions & further research**

Conclusion: Customized sequential design predicts better than LHS, with same number of replicates

Future research:
- Kriging is an exact interpolation method; drop this constraint for random simulation?
- Optimization through Kriging