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Kriging Metamodels for Simulation Optimization

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Part 1: Expected Improvement (EI)/ Efficient Global Optimization (EGO)

Classic reference: Jones, Schonlau, Welch ('98)
- Deterministic simulation (CAE), Kriging

Problem: Plug-in estimates for predictor variance

Solution: Parametric bootstrapping
- Origin: Den Hertog, Kleijnen, Siem (2006)

Empirical results: four test functions (Hartmann)
- # dimensions: 1, 2, 3, 6
- Bootstrap: faster (first 3 functions) or tie

Future research: *constrained* & *random* outputs

EI / EGO: details

Local vs. *global* optima

Exploration vs. exploitation; see Fu (2007)

Expensive simulation: Kriging *meta*model

Deterministic vs. *random* simulation;

see Frazier, Powell, Dayanik (2009), Ankenman, Nelson, Staum (2010)

Predictor variance depends on unknown correlations $\theta(j) \longrightarrow$ estimate $\theta(j)$

$\sigma^2(x) = 0$ if $x = x(i)$ ($i = 1, \ldots, n$) ("old" data)

EI / EGO: more details

EI / EGO *algorithm* for unconstrained minimization:

1. Find $w^o = \min[w(i)]$ ($i = 1, \ldots, n$)
2. *EI*($\boldsymbol{x}$) = E[$w^o - y(\boldsymbol{x}) \mid y(\boldsymbol{x}) < w^o$] with $y(\boldsymbol{x}) \sim N(\hat{y}, s^2)$
3. Find maximizer $\boldsymbol{x}^o$ of *EI*($\boldsymbol{x}$) in candidate set
4. Simulate $\boldsymbol{x}^o$; refit Kriging; return to 1 until $EI \approx 0$

Sub 2: *Bootstrap* estimator s^{2*}:

1. Original I/O ($\boldsymbol{X}$, $\boldsymbol{w}$) gives original $\hat{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\mu}}$
2. Sample $(w^*(1), \ldots, w^*(n+1))'$ from $N(\hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\theta}})$
3. Squared Error $SE = [w^*(n+1) - y^*\{\boldsymbol{x}(n+1)\}]^2$
4. Repeat 2 & 3, B times: $s^{2*} = [\Sigma_b SE(b)] / (B - 1)$

Part 2: Robust optimization

Taguchi's worldview:

Decision inputs (e.g., order quantity)

Environmental inputs (e.g., demand rate)

Example: EOQ

Classic optimization: known demand rate a

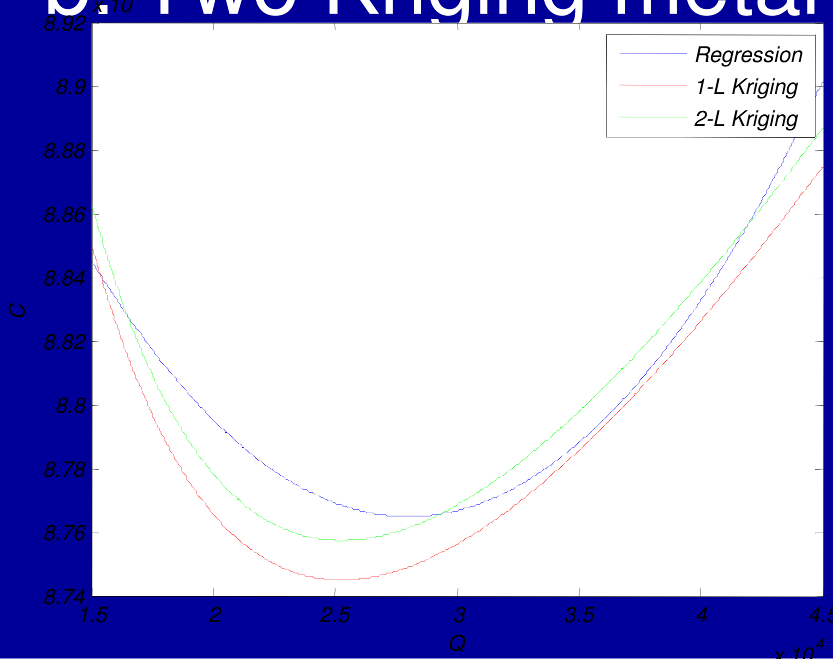
Robust optimization: $a \sim N(\mu, \sigma)$

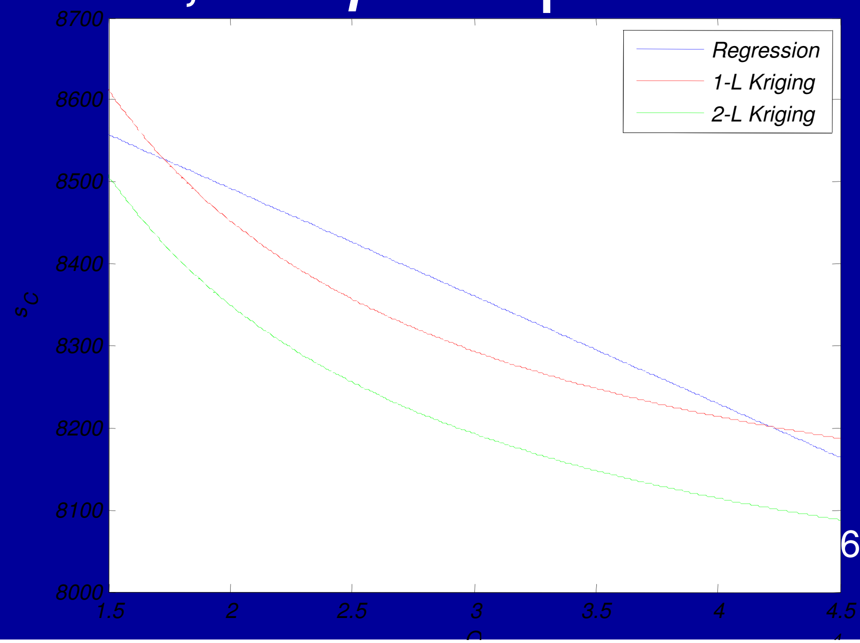
Goal: minimize expected cost E(C)

Constraint: keep standard dev. σ(C) below T

Methodology for robust opt.

1. *Design*: Cross
   CCD for decision inputs *d*
   LHS for environmental inputs *e*
2. *Metamodel*:
   a. Regress: $y = \beta 0 + \beta' d + d' B d + \gamma' e + d' \Delta e + \varepsilon$
   b. Two Kriging metamodels, for μ resp. σ

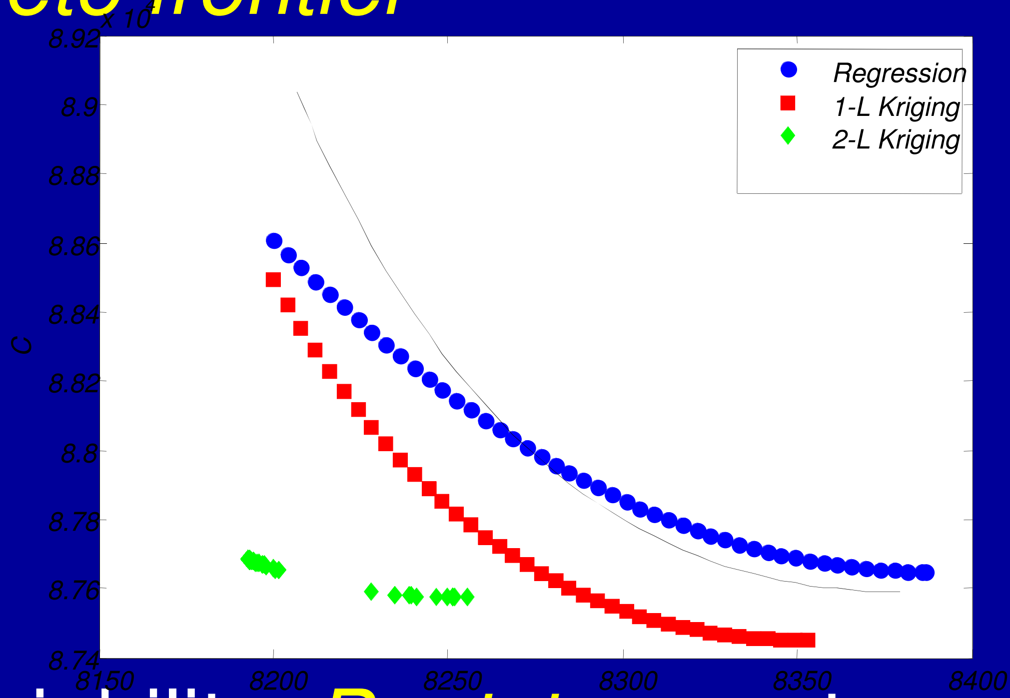




Methodology continued

3. Min μ s.t. $\sigma \leq T$: *Mathematical Programming*

4. Vary *T*: *Pareto frontier*



5. Quantify variability: *Bootstrap* metamodel

Future research: Random (*s*, *S*) & constraints