Stacking designs: designing multi-fidelity computer experiment with target predictive accuracy

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Outline

Multi-Fidelity Simulations

- Computer models have been widely adopted to understand a real-world feature, phenomenon or event.
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  - (intermediate-fidelity simulation)

Motivated Example: Finite Element Simulations

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- **Input**: $\mathbf{x} = (x_1, x_2) = (\text{pressure}, \text{suction})$
- **Output**: $f(\mathbf{x})$: average of thermal stress
- e.g., $\mathbf{x} = (0.23, 0.71)$

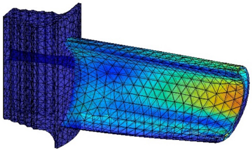

Figure: *average of thermal stress* $f(0.23, 0.71) = 10.5$

Multi-Fidelity Simulations via Mesh Configuration

less accurate but cheaper accurate but expensive

$\mathbf{x} = (0.50, 0.50)$

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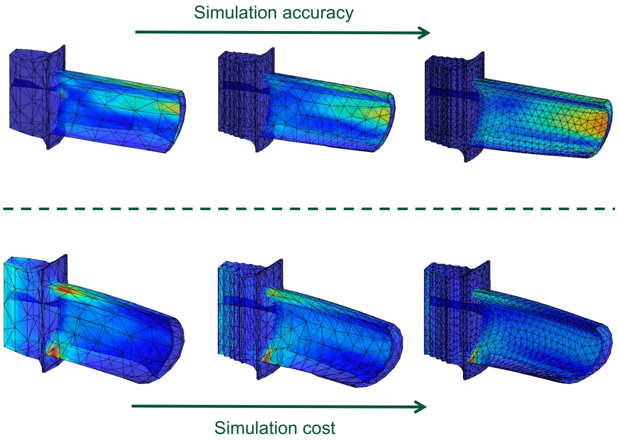

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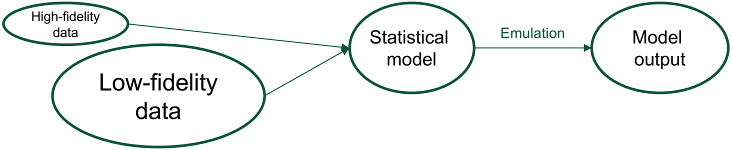
  - maximize the accuracy of model predictions,
  - while minimizing the cost associated with the simulations?
  - A cheaper statistical model emulating the model output based on the simulations with multiple fidelities
  - Often called emulator or surrogate model



Notation

fidelity level	1		2		3
output	$f_1(\mathbf{x})$		$f_2(\mathbf{x})$		$f_3(\mathbf{x})$
mesh size	h_1	$>$	h_2	$>$	h_3
cost	C_1	$<$	C_2	$<$	C_3

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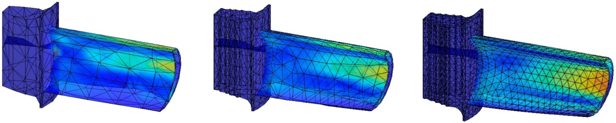

Existing Methods

- Modeling:
  - Co-kriging (Kennedy and O'Hagan, 2000, and many others)

$$f_l(\mathbf{x}) = \rho_{l-1} f_{l-1}(\mathbf{x}) + Z_{l-1}(\mathbf{x}), \quad l = 2, \ldots, L$$

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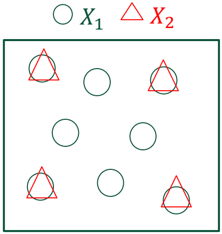
  - Non-stationary GP (Tuo, Wu and Yu, 2014): emulate $f_\infty(\mathbf{x})$ as $h_\infty \to 0$

- Experimental Design: Nested space-filling design (Qian, Ai, and Wu, 2009, and many others)

$$X_L \subseteq X_{L-1} \subseteq \cdots \subseteq X_1$$



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Multi-Level Interpolator

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- Idea: with $f_0(\mathbf{x}) = 0$

$$f_L(\mathbf{x}) = (f_1(\mathbf{x}) - f_0(\mathbf{x})) + (f_2(\mathbf{x}) - f_1(\mathbf{x})) + \cdots + (f_L(\mathbf{x}) - f_{L-1}(\mathbf{x}))$$

- Assume the data is nested $X_L \subseteq X_{L-1} \subseteq \cdots \subseteq X_1$

Multi-Level Interpolator

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- ML Interpolator:

$$\hat{f}_L(\mathbf{x}) = \hat{Z}_1(\mathbf{x}) + \hat{Z}_2(\mathbf{x}) + \cdots + \hat{Z}_L(\mathbf{x}).$$

Matérn kernel

Assumption: Matérn kernel Φ

$$\Phi_l(\mathbf{x},\mathbf{x}') = \phi_l(\|\theta_l(\mathbf{x}-\mathbf{x}')\|_2)$$

with

$$\phi_l(r) = \frac{\sigma_l^2}{\Gamma(\nu_l)2^{\nu_l-1}}(2\sqrt{\nu_l}r)_l^{\nu}B_{\nu_l}(2\sqrt{\nu_l}r),$$

- ν_l: smoothness parameter
- θ_l: lengthscale parameter
- σ_l^2: scalar parameter
- B_ν: the modified Bessel function of the second kind

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- ν_l: smoothness parameter
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- B_ν: the modified Bessel function of the second kind
- Parameters can be estimated via either CV or MLE (by a GP assumption)

Note of ML Interpolator

- Alternatively, one can assume $Z_l(\mathbf{x})$ follows a Gaussian process (GP) prior.

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- Alternatively, one can assume $Z_l(\mathbf{x})$ follows a Gaussian process (GP) prior.
- The posterior mean is equivalent to the ML Interpolator $\hat{f}_L(\mathbf{x})$.
- Can be viewed as a special case of Kennedy and O'Hagan (2000) model ($\rho_l = 1$)

Error Analysis of ML Interpolator

- ML Interpolator $\hat{f}_L(\mathbf{x}) = \hat{Z}_1(\mathbf{x}) + \hat{Z}_2(\mathbf{x}) + \cdots + \hat{Z}_L(\mathbf{x})$
- Recall our goal is to emulate $f_\infty(\mathbf{x})$

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- Recall our goal is to emulate $f_\infty(\mathbf{x})$

$$|f_\infty(\mathbf{x}) - \hat{f}_L(\mathbf{x})| \leq \underbrace{|f_\infty(\mathbf{x}) - f_L(\mathbf{x})|}_{\text{simulation error}} + \underbrace{|f_L(\mathbf{x}) - \hat{f}_L(\mathbf{x})|}_{\text{emulation error}}.$$

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$\|f_\infty - f_L\| < \frac{\epsilon}{2}$ $\|f_L - \hat{f}_L\| < \frac{\epsilon}{2}$

$\Downarrow$ $\Downarrow$

determine L determine sample sizes n_l

Stacking Design

Control emulation error $\|f_L - \hat{f}_L\|$

Proposition 1: Emulation error

Suppose that

- the input space is d-dimensional and is bounded and convex,
- X_l is **quasi-uniform** with sample size n_l,

Then,

$$|f_L(\mathbf{x}) - \hat{f}_L(\mathbf{x})| \leq c \sum_{l=1}^{L} \|\theta_l\|_2^{\nu_l} n_l^{-\nu_l/d} \|f_l - f_{l-1}\|_{\mathcal{N}_{\Phi_l}(\Omega)},$$

where $\| \cdot |||_{\mathcal{N}_{\Phi_l}(\Omega)}$ is the RKHS norm.

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where $\|\cdot\||\|_{\mathcal{N}_{\Phi_l}(\Omega)}$ is the RKHS norm.

- Denote $q_X = \min_{1 \leq j \neq k \leq n} \|\mathbf{x}_j - \mathbf{x}_k\|/2$ and $h_{X,\Omega}$ as the fill distance.
- A design $\mathbf{X}_n$ satisfying $h_{X,\Omega}/q_X \leq C$ for some constant C is called a **quasi-uniform** design.

Sample size determination n_l

- Sample size n_l can be determined by minimizing the error bound and the total cost by the method of Lagrange multipliers

$$\sum_{l=1}^{L} \|\theta_l\|_2^{\nu_l} n_l^{-\nu_l/d} \|f_l - f_{l-1}\|_{\mathcal{N}_{\Phi_l}(\Omega)} + \lambda \sum_{l=1}^{L} n_l C_l,$$

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which gives

$$n_l = \mu \left(\frac{\|\theta_l\|^{\nu_l}}{C_l} \|f_l - f_{l-1}\|_{\mathcal{N}_{\Phi_l}(\Omega)} \right)^{d/(\nu_l+d)}$$

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- Find μ such that $\|f_L - \hat{f}_L\| < \epsilon/2$

Sample size determination n_l

$$\|f_L - \hat{f}_L\| < \sum_{l=1}^{L} \|P_l\| \|f_l - f_{l-1}\|_{\mathcal{N}_{\Phi_l(\Omega)}} < \epsilon/2$$

- $P_l(\mathbf{x})$ is a *power function*
- $\|f_l - f_{l-1}\|_{\mathcal{N}_{\Phi_l(\Omega)}}$ can be estimated by $\|\hat{Z}_l\|_{\mathcal{N}_{\Phi_l(\Omega)}}$

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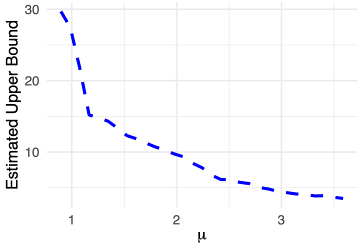

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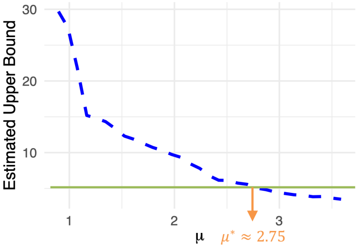

Questions

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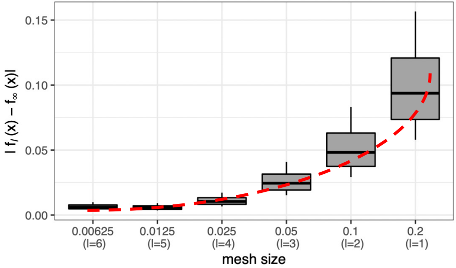
Control simulation error $\|f_\infty - f_L\|$

Error Rate of finite element simulations

(Brenner and Scott, 2007, Tuo, Wu and Yu, 2014) Under some regularity conditions, for a constant $\alpha \in \mathbb{N}$,

$$|f_\infty(\mathbf{x}) - f_L(\mathbf{x})| < ch_L^\alpha.$$

Recall h_L is the mesh size.



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- Find L that ensures $\frac{\|\hat{Z}_L\|}{2^\alpha - 1} \leq \epsilon/2$

Determination of α

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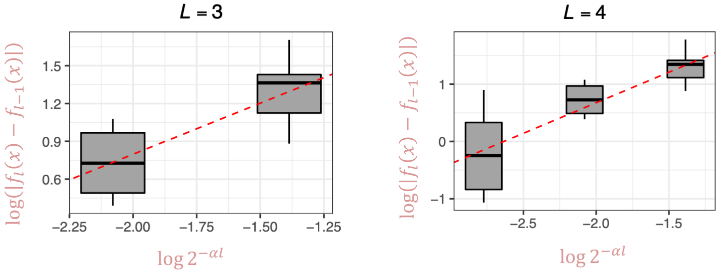
- Alternatively, it can be determined by collected data (can be done only when $L \geq 3$) (details omitted)



$$\hat{\alpha} \approx 1$$

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Stacking design with error upper bound ϵ

- **Idea:** Start with low-fidelity simulations and sequentially increase the fidelity level until $\frac{\|\hat{Z}_L\|}{2^\alpha - 1} \leq \epsilon/2$.

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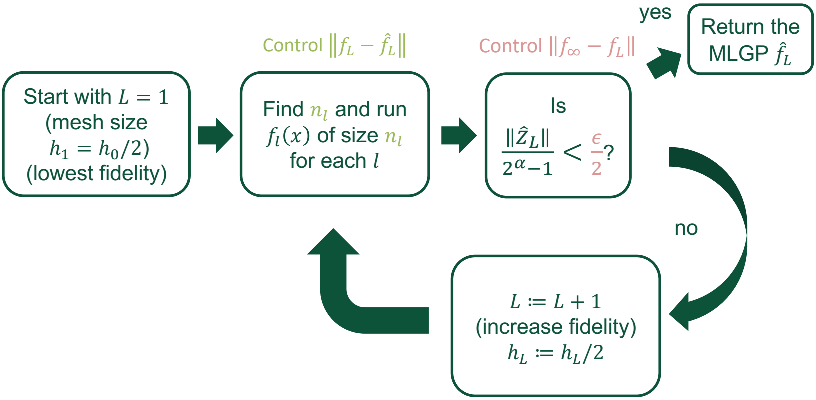
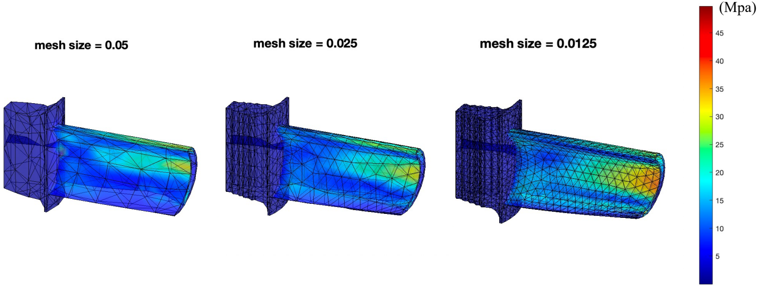


Revisit motivated example



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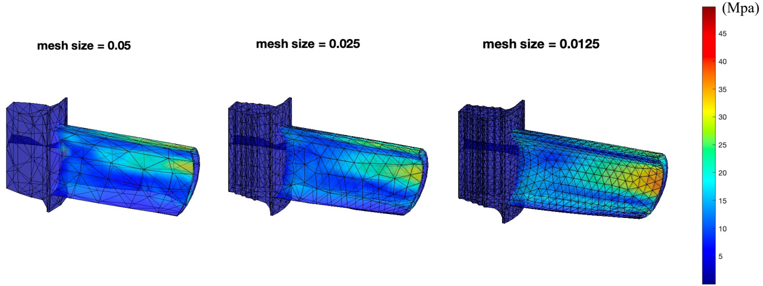

- **Input**: $\mathbf{x} = (x_1, x_2) = (\text{pressure}, \text{suction})$
- **Output**: $f(\mathbf{x})$: average of thermal stress
- **Test data**: Simulations with mesh size $h \approx 0$ at 20 uniform test input locations are conducted to examine the performance

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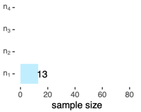

	$L=1$
h_L	0.05
C_L (sec.)	0.62
$\|f_L - \hat{f}_L\|_{L_2(\Omega)}$	**2.411**
$\|f_\infty - f_L\|_{L_2(\Omega)}$	NA

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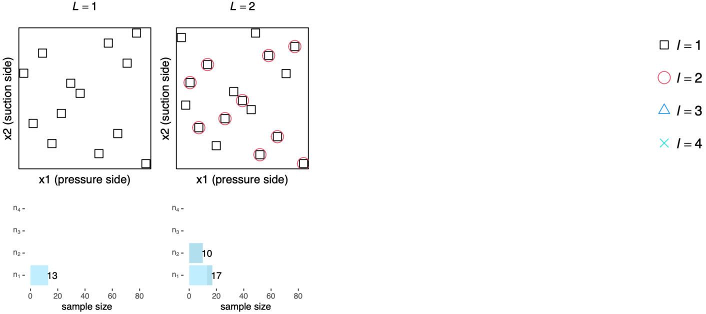

	$L=1$	$L=2$
h_L	0.05	0.025
C_L (sec.)	0.62	1.03
$\|f_L - \hat{f}_L\|_{L_2(\Omega)}$	**2.411**	**2.407**
$\|f_\infty - f_L\|_{L_2(\Omega)}$	NA	NA

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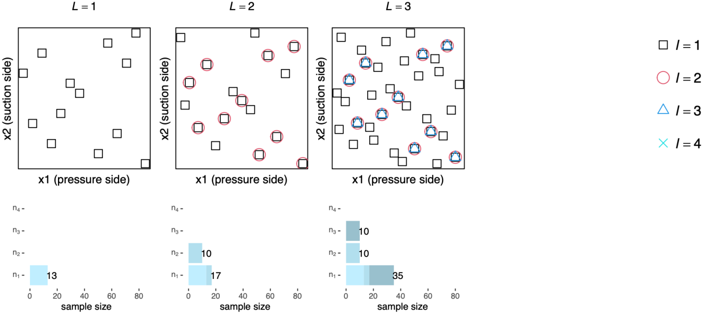

	$L=1$	$L=2$	$L=3$
h_L	0.05	0.025	0.0125
C_L (sec.)	0.62	1.03	2.28
$\|f_L - \hat{f}_L\|_{L_2(\Omega)}$	**2.411**	**2.407**	**2.445**
$\|f_\infty - f_L\|_{L_2(\Omega)}$	NA	NA	2.943

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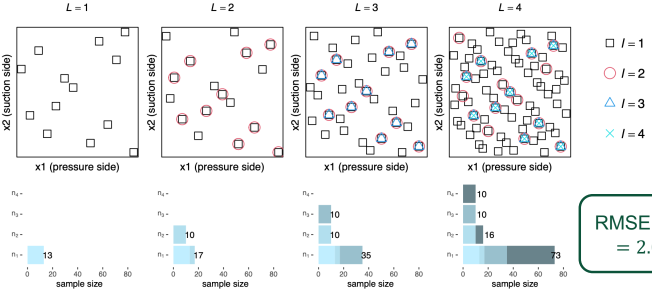
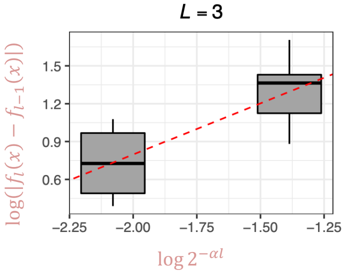


RMSE of $\hat{f}_4$
$= 2.01$

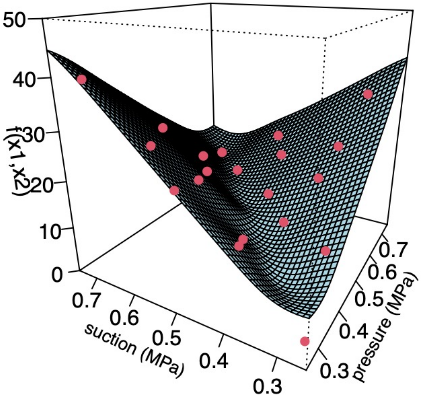
	$L = 1$	$L = 2$	$L = 3$	$L = 4$	
h_L	0.05	0.025	0.0125	0.00625	
C_L (sec.)	0.62	1.03	2.28	12.58	
$\|f_L - \hat{f}_L\|_{L_2(\Omega)}$	**2.411**	**2.407**	**2.445**	**2.48**	$< \frac{\epsilon}{2}$
$\|f_\infty - f_L\|_{L_2(\Omega)}$	NA	NA	2.943	**0.974**	$< \frac{\epsilon}{2}$

Determination of α



$$\hat{\alpha} \approx 1$$

Visualize $\hat{f}_L(\mathbf{x})$



Cost complexity theorem

Theorem

Suppose that

- $\nu := \nu_1 = \cdots = \nu_L$
- $|f_\infty(\mathbf{x}) - f_l(\mathbf{x})| < c_1 2^{-\alpha l}$
- $C_l < c_2 2^{\beta l}$

Cost complexity theorem

Theorem

Suppose that

- $\nu := \nu_1 = \cdots = \nu_L$
- $|f_\infty(\mathbf{x}) - f_l(\mathbf{x})| < c_1 2^{-\alpha l}$
- $C_l < c_2 2^{\beta l}$

Under some regularity conditions, it follows that

$$|f_\infty(\mathbf{x}) - \hat{f}_L(\mathbf{x})| < \epsilon,$$

with a **total computational cost** C_{tot} bounded by

$$C_{\mathrm{tot}} \leq \begin{cases} c_3 \epsilon^{-\frac{d}{\nu}}, & \frac{\alpha}{\beta} > \frac{2\nu}{d}, \\ c_3 \epsilon^{-\frac{d}{\nu}} \log(\epsilon^{-1})^{1+\frac{d}{\nu}}, & \frac{\alpha}{\beta} = \frac{2\nu}{d}, \\ c_3 \epsilon^{-\frac{d}{\nu}-\frac{2\beta\nu-\alpha d}{2\alpha(\nu+d)}}, & \frac{\alpha}{\beta} < \frac{2\nu}{d}. \end{cases}$$

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$\frac{\alpha}{\beta}$	$\frac{2\nu}{d}$
simulation error reduction over the rate computational cost as fidelity increases	the rate of convergence of RKHS interpolator as sample size increases

Single-fidelity vs Multi-fidelity

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- Independent kriging vs co-kriging?

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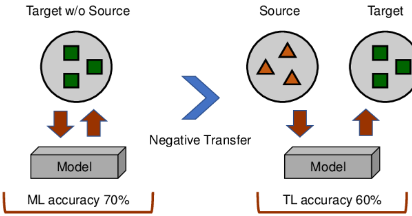
- Independent kriging vs co-kriging?
- Negative transfer?



Zhang et al. (2021) A Survey on Negative Transfer. *IEEE Transactions on Neural Networks and Learning Systems*

Complexity of single-fidelity interpolator

Corollary

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with a **total computational cost** C_H bounded by

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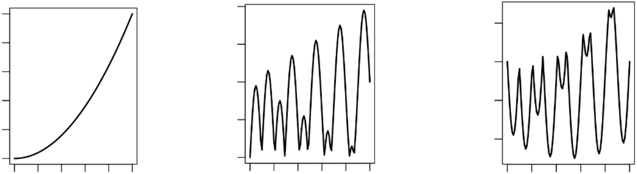
$$f_{\text{high}}(x) = f_{\text{low}}(x) + (f_{\text{high}}(x) - f_{\text{low}}(x))$$



Questions

- Q1: Sample size of each level? n_l
- Q2: How many fidelity levels? L
- Q3: Mesh size/density specification? $h_l = h_0 2^{-l}$
- Q4: Is it better than single-fidelity simulation? In some cases, yes

Conclusion

- Stacking design for multi-fidelity simulations with desired accuracy
  - Sample determination
  - Mesh size determination
- Cost complexity
  - Budget allocation
  - Comparison with single fidelity simulation

Arxiv

Statistics > Methodology

[Submitted on 1 Nov 2022 (v1), last revised 22 Jun 2023 (this version, v2)]

Stacking designs: designing multi-fidelity experiments with target predictive accuracy

Chih-Li Sung, Yi Ji, Tao Tang, Simon Mak

In an era where scientific experiments can be very costly, multi-fidelity emulators provide a useful tool for cost-efficient predictive scientific computing. For scientific applications, the experimenter is often limited by a tight computational budget, and thus wishes to (i) maximize predictive power of the multi-fidelity emulator via a careful design of experiments, and (ii) ensure this model achieves a desired error tolerance with some notion of confidence. Existing design methods, however, do not jointly tackle objectives (i) and (ii). We propose a novel stacking design approach that addresses both goals. Using a recently proposed multi-level Gaussian process emulator model, our stacking design provides a sequential approach for designing multi-fidelity runs such that a desired prediction error of $\epsilon > 0$ is met under regularity assumptions. We then prove a novel cost complexity theorem that, under this multi-level Gaussian process emulator, establishes a bound on the computation cost (for training data simulation) needed to achieve a prediction bound of ϵ. This result provides novel insights on conditions under which the proposed multi-fidelity approach improves upon a standard Gaussian process emulator which relies on a single fidelity level. Finally, we demonstrate the effectiveness of stacking designs in a suite of simulation experiments and an application to finite element analysis.

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Thank You!

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