

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

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Outline

1 Introduction

- Multi-fidelity data
- Finite Element Simulations

2 Stacking Design

- ML Interpolator
- Error Analysis
- Stacking design with target predictive accuracy

3 Real Application

4 Cost Complexity Theorem

5 Conclusion

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)

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Motivated Example: Finite Element Simulations

- Thermal stress of jet engine turbine blade can be analyzed through a static structural **computer model**.
- The model can be *numerically* solved via **finite element method**.
- **Input:** $\mathbf{x} = (x_1, x_2) = (\text{pressure}, \text{suction})$
- **Output:** $f(\mathbf{x})$: average of thermal stress
- e.g., $\mathbf{x} = (0.23, 0.71)$

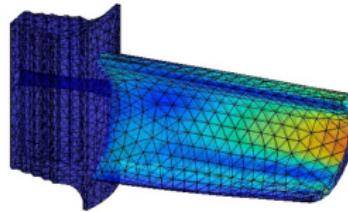
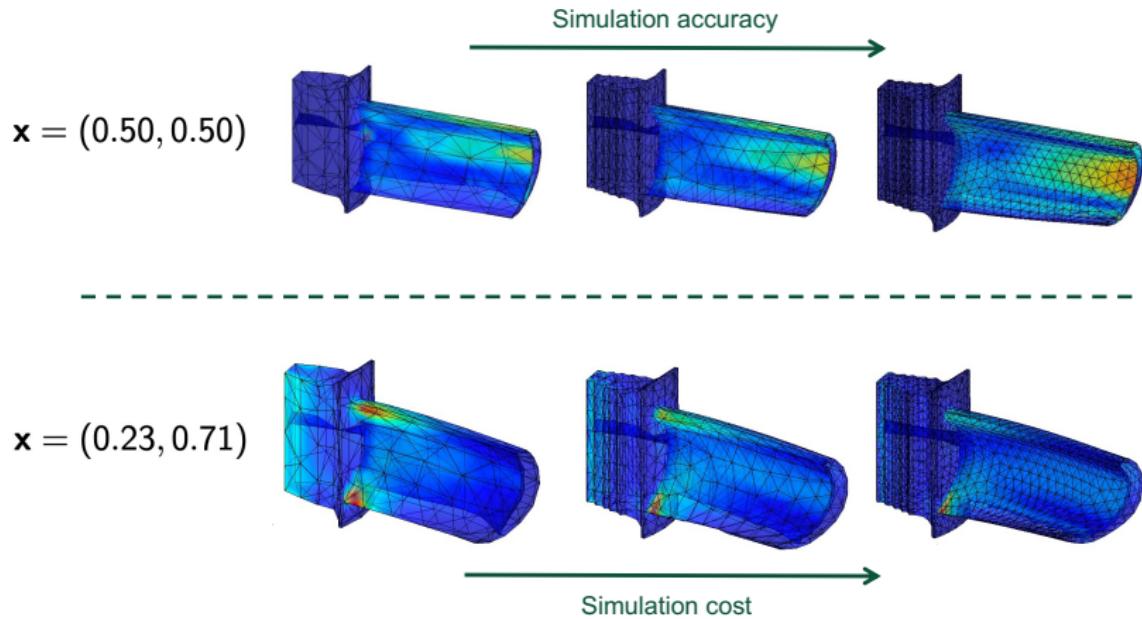


Figure: *average of thermal stress* $f(0.23, 0.71) = 10.5$

Multi-Fidelity Simulations via Mesh Configuration

less accurate but cheaper

accurate but expensive



Statistical Emulation

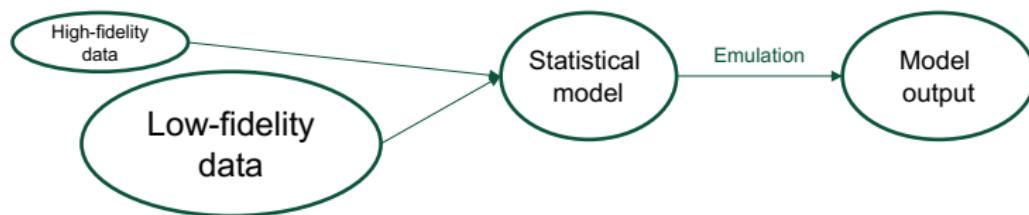
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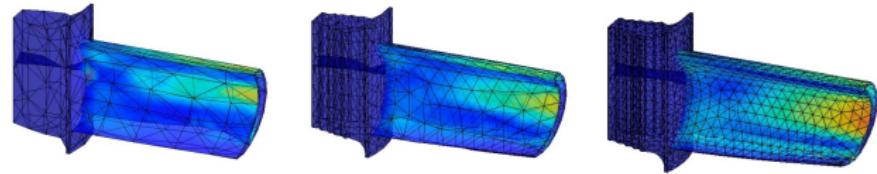
- Can we leverage both low- and high-fidelity simulations in order to
 - maximize the accuracy of model predictions,
 - while minimizing the cost associated with the simulations?
- A cheaper statistical model **emulating** the model output based on the simulations with multiple fidelities
- Often called **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

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



Existing Methods

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

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

where both $f_{l-1}(\mathbf{x})$ and $Z_{l-1}(\mathbf{x})$ have Gaussian Process (GP) priors.

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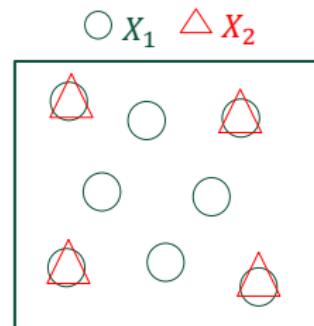
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- Non-stationary GP (Tuo, Wu and Yu, 2014): emulate $f_\infty(\mathbf{x})$ as $h_\infty \rightarrow 0$

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

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



Questions

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

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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

$$\Phi_I(\mathbf{x}, \mathbf{x}') = \phi_I(\|\theta_I \odot (\mathbf{x} - \mathbf{x}')\|_2)$$

with

$$\phi_I(r) = \frac{\sigma_I^2}{\Gamma(\nu_I)2^{\nu_I-1}}(2\sqrt{\nu_I}r)_I^\nu B_{\nu_I}(2\sqrt{\nu_I}r),$$

- ν_I : smoothness parameter
- θ_I : lengthscale 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 $Z_I(\mathbf{x})$ follows a Gaussian process (GP) prior.

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- Alternatively, one can assume $Z_I(\mathbf{x})$ 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 ($\rho_I = 1$)

Error Analysis of ML Interpolator

- ML Interpolator $\hat{f}_L(\mathbf{x}) = \hat{Z}_1(\mathbf{x}) + \hat{Z}_2(\mathbf{x}) + \dots + \hat{Z}_L(\mathbf{x})$
- 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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$$\|f_\infty - f_L\| < \frac{\epsilon}{2}$$



determine L

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



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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- 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

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

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

Sample size determination n_l

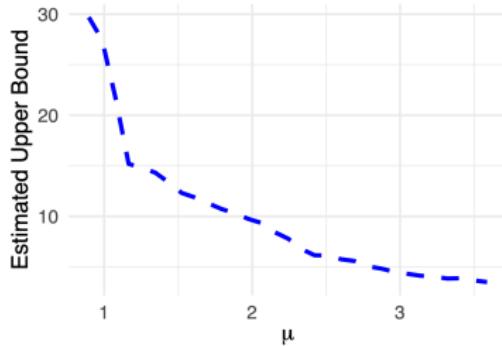
$$\|f_L - \hat{f}_L\| < \sum_{l=1}^L \|P_l\| \|f_l - f_{l-1}\|_{\mathcal{N}_{\Phi_l}(\Omega)} < \epsilon/2$$

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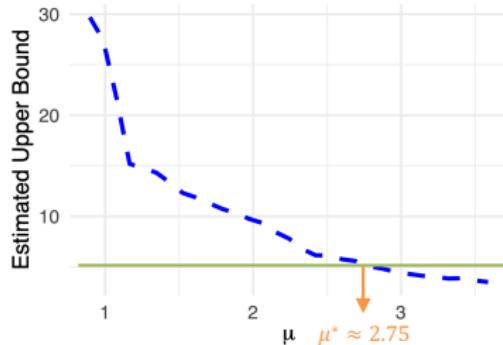
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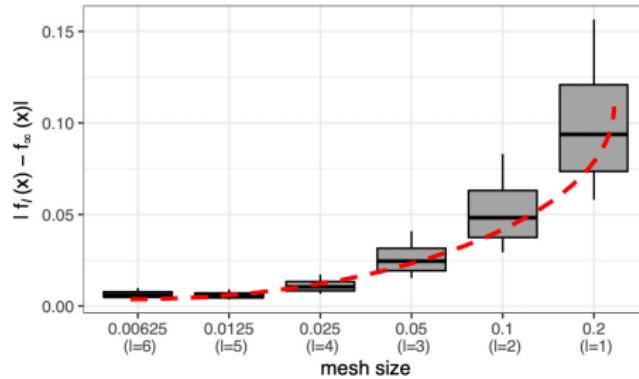
Control simulation error $\|f_\infty - f_L\|$

Error Rate of finite element simulations

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

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

Recall h_L is the mesh size.



Determine the fidelity level L

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- One can show that

$$\|f_\infty - f_L\| = \frac{\|f_L - f_{L-1}\|}{2^\alpha - 1},$$

assuming that the terms of order $\xi_L^{\alpha+1}$ and higher can be neglected.

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- $\|f_L - f_{L-1}\|$ can be approximated by $\|\hat{Z}_L\|$.
- 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)

$$\hat{\alpha} = \frac{1}{L-2} \sum_{l=3}^L \sum_{\mathbf{x} \in X_l} \frac{\log \left(\left| \frac{f_{l-1}(\mathbf{x}) - f_{l-2}(\mathbf{x})}{f_l(\mathbf{x}) - f_{l-1}(\mathbf{x})} \right| \right)}{n_l \log 2}.$$

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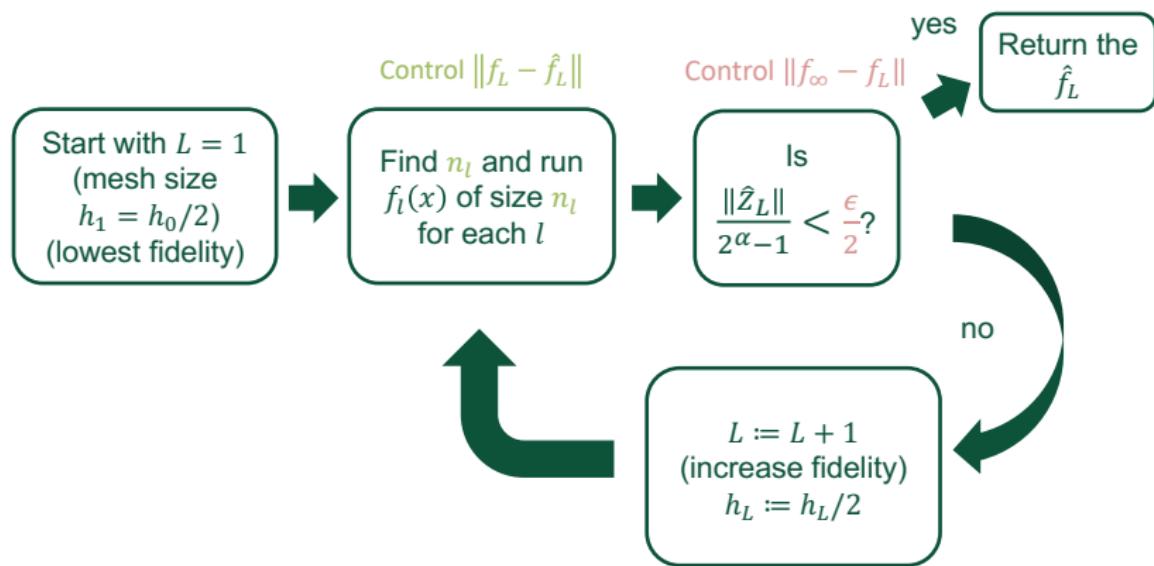
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Stacking design with error upper bound ϵ

- **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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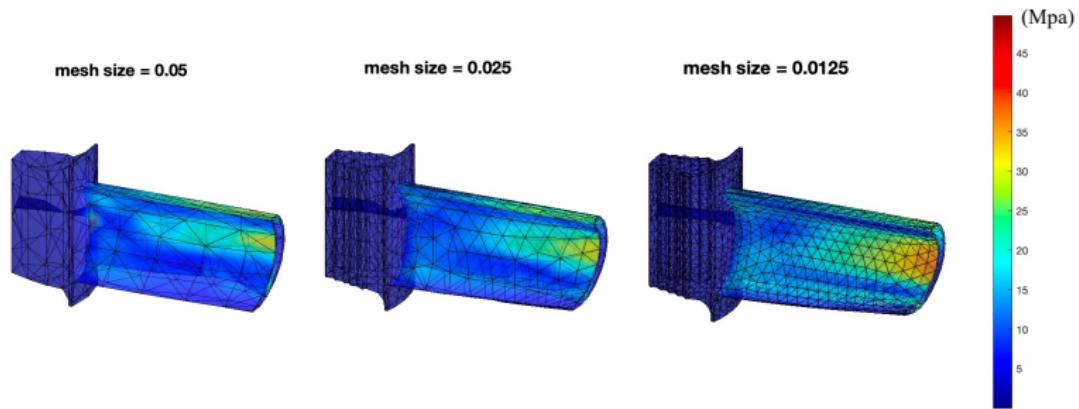


Prediction Uncertainty

- An approximated pointwise error interval of $f_\infty(\mathbf{x})$ can be constructed as

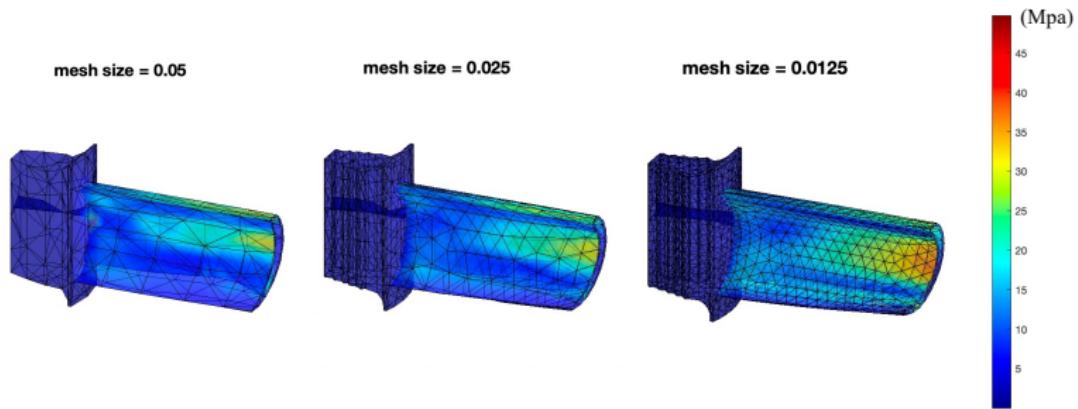
$$\hat{f}_L(\mathbf{x}) \pm \left(\frac{|\hat{Z}_L(\mathbf{x})|}{2^\alpha - 1} + \sum_{l=1}^L P_l(\mathbf{x})(Z_l(X_l)^T \Phi_l(X_l, X_l)^{-1} Z_l(X_l))^{1/2} \right).$$

Revisit motivated example



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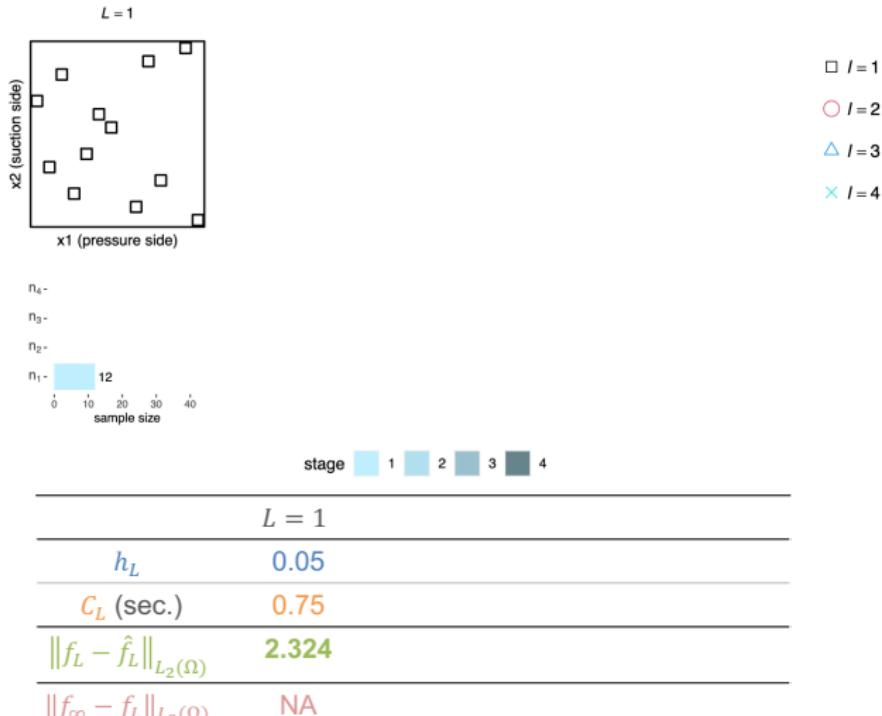
- **Input:** $\mathbf{x} = (x_1, x_2) = (\text{pressure}, \text{suction})$
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- **Test data:** Simulations with mesh size $h \approx 0$ at 20 uniform test input locations are conducted to examine the performance

Revisit motivated example

- We wish $\|f_\infty - \hat{f}_L\|_{L_2(\Omega)} < \epsilon = 5$

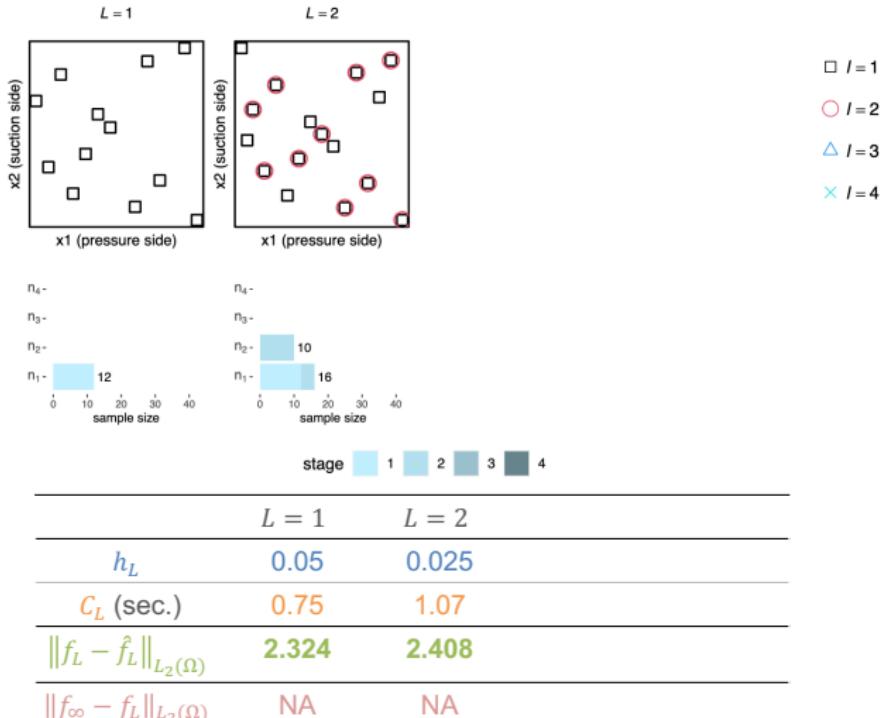
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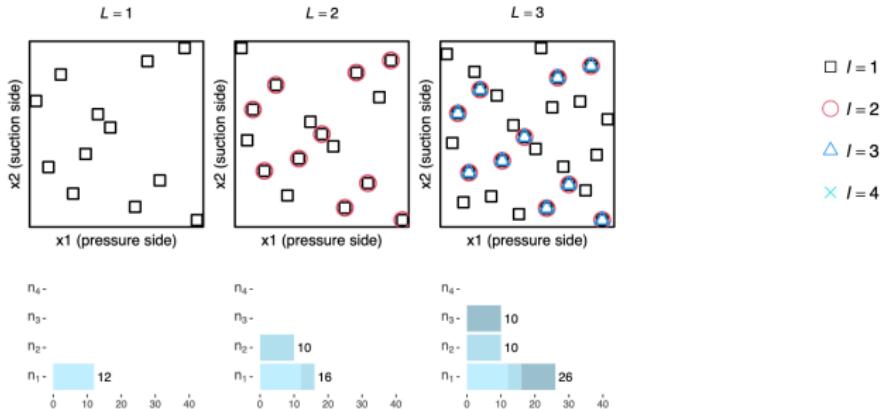
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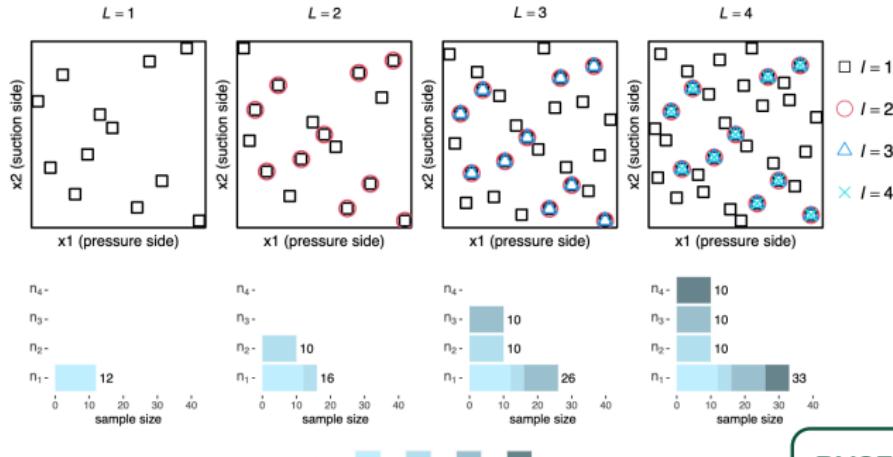


stage 1 2 3 4

	$L = 1$	$L = 2$	$L = 3$
h_L	0.05	0.025	0.0125
C_L (sec.)	0.75	1.07	2.13
$\ f_L - \hat{f}_L\ _{L_2(\Omega)}$	2.324	2.408	2.481
$\ f_\infty - f_L\ _{L_2(\Omega)}$	NA	NA	2.969

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RMSE of \hat{f}_4
= 1.60

	$L = 1$	$L = 2$	$L = 3$	$L = 4$
h_L	0.05	0.025	0.0125	0.00625
C_L (sec.)	0.75	1.07	2.13	11.51
$\ \hat{f}_L - f_L\ _{L_2(\Omega)}$	2.324	2.408	2.481	2.491
$\ f_\infty - f_L\ _{L_2(\Omega)}$	NA	NA	2.969	0.956

$$< \frac{\epsilon}{2}$$

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

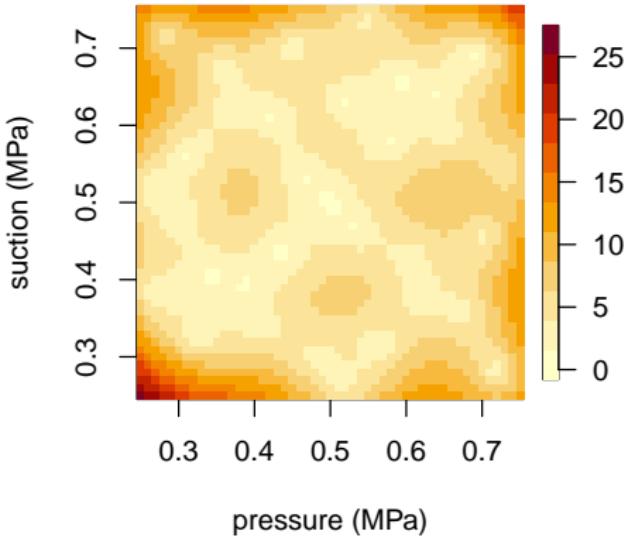
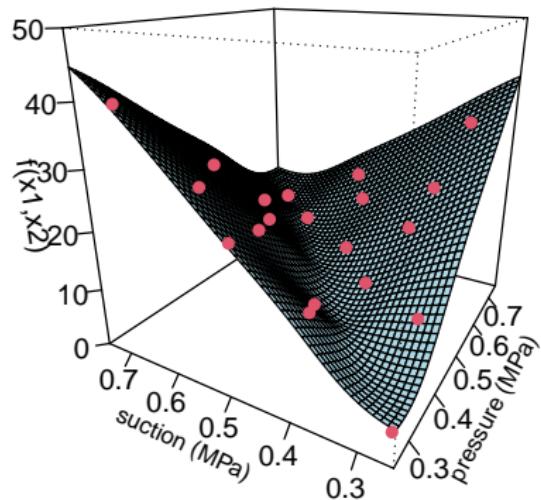


Figure: (left) $\hat{f}_4(\mathbf{x})$ and true test points (red dots); (right) pointwise error bounds

Cost complexity theorem

Theorem

Suppose that

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

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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

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

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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

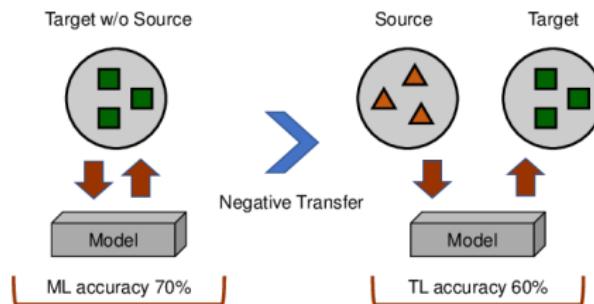
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Single-fidelity vs Multi-fidelity

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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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Under some regularity conditions, it follows that

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

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

$$C_H \leq c_h \epsilon^{-\frac{\beta}{\alpha} - \frac{d}{2\nu}}.$$

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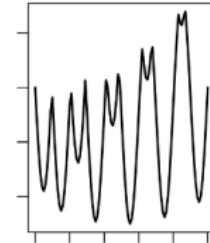
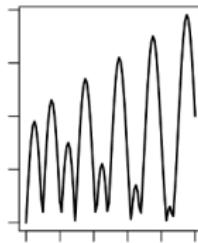
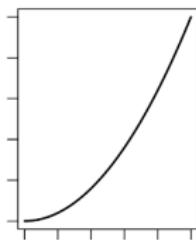
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$$f_{\text{high}}(x) = f_{\text{low}}(x) + (f_{\text{high}}(x) - f_{\text{low}}(x))$$



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

 Cornell University

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

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

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. A multi-level reproducing kernel Hilbert space (RKHS) interpolator is first introduced to build the emulator, under which 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 interpolator, 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 conventional RKHS interpolator 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.

Subjects: Methodology (stat.ME); Applications (stat.AP)

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