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

Chih-Li Sung

Department of Statistics and Probability
Michigan State University

Joint work with Wenjia Wang (HKUST(GZ)), Yi Ji, Tao Tang, and Dr. Simon Mak (Duke)

UMass Amherst, April 17, 2024

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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- 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., $\mathbf{x} = (0.23, 0.71)$

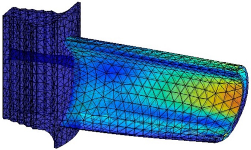

Figure: *average of thermal stress* $f(0.23, 0.71) = 10.5$

Multi-Fidelity Simulations via Mesh Configuration

less accurate but cheaper — accurate but expensive

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

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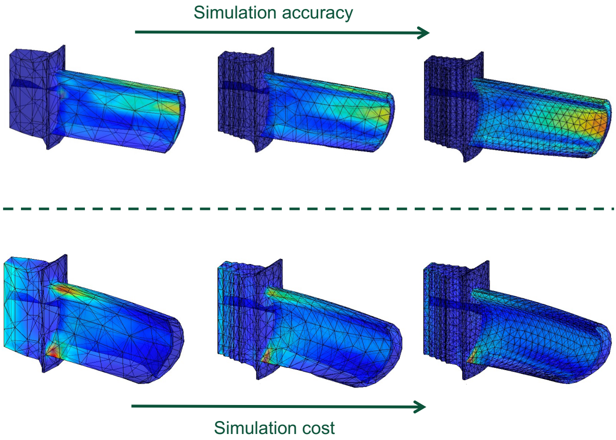

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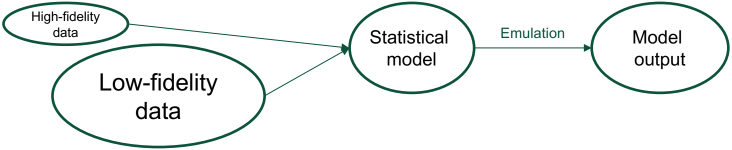
  - maximize the accuracy of model predictions,
  - while minimizing the cost associated with the simulations?
  - A cheaper statistical model emulating the model output based on the simulations with multiple fidelities
  - Often called emulator or surrogate model



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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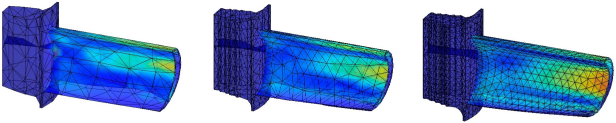

Existing Methods

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

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

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

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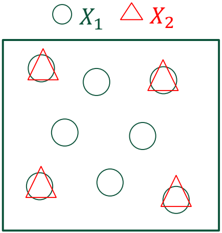
  - Non-stationary GP (Tuo, Wu and Yu, 2014): emulate $f_\infty(\mathbf{x})$ as $h_\infty \to 0$

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

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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

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

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
- θ_l: lengthscale parameter
- σ_l^2: scalar parameter
- 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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$$|f_\infty(\mathbf{x}) - \hat{f}_L(\mathbf{x})| \leq \underbrace{|f_\infty(\mathbf{x}) - f_L(\mathbf{x})|}_{\text{simulation error}} + \underbrace{|f_L(\mathbf{x}) - \hat{f}_L(\mathbf{x})|}_{\text{emulation error}}.$$

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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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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

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

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

Sample size determination n_l

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

- $P_l(\mathbf{x})$ 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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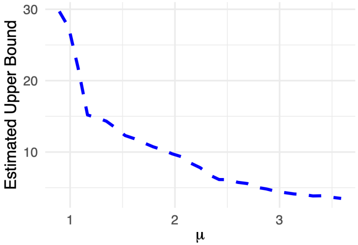

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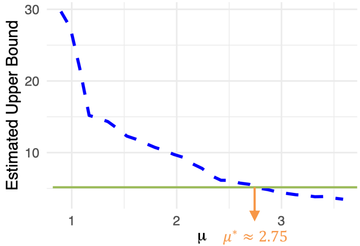

Questions

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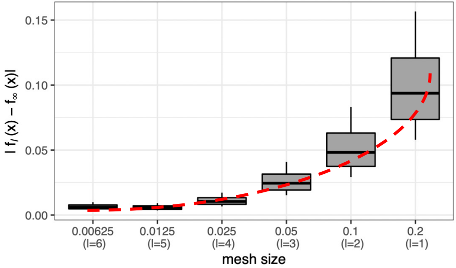
Control simulation error $\|f_\infty - f_L\|$

Error Rate of finite element simulations

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

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

Recall h_L is the mesh size.



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

assuming that the terms of order $h_L^{\alpha+1}$ 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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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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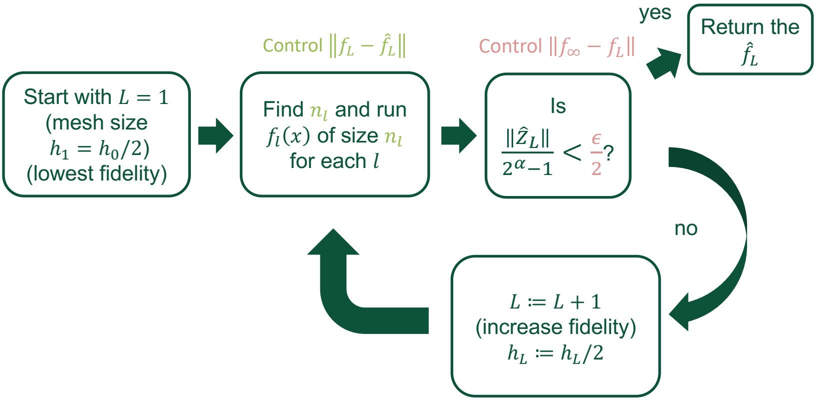
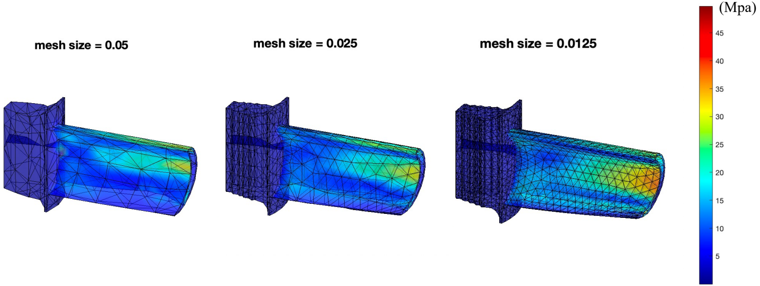


Prediction Uncertainty

- 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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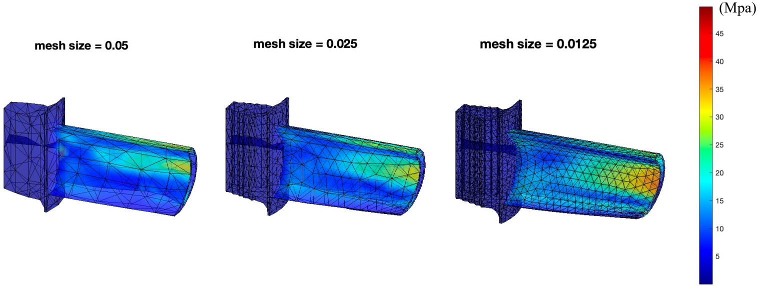

- **Input**: $\mathbf{x} = (x_1, x_2) = (\text{pressure}, \text{suction})$
- **Output**: $f(\mathbf{x})$: average of thermal stress
- **Test data**: Simulations with mesh size $h \approx 0$ at 20 uniform test input locations are conducted to examine the performance

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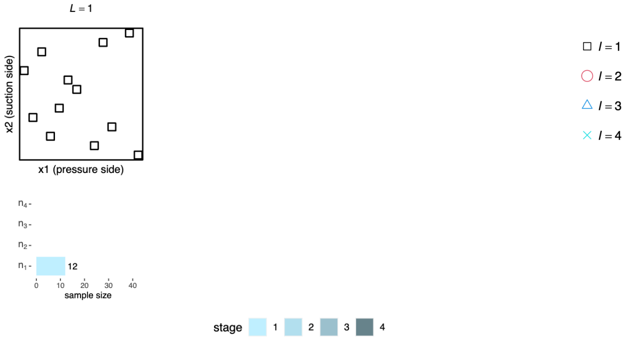

	$L=1$
h_L	0.05
C_L (sec.)	0.75
$\|f_L - \hat{f}_L\|_{L_2(\Omega)}$	**2.324**
$\|f_\infty - f_L\|_{L_2(\Omega)}$	NA

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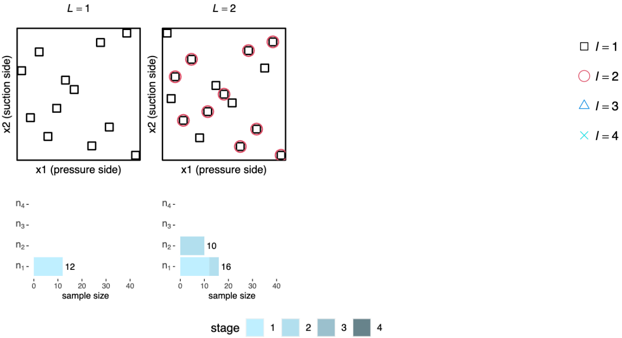

	$L=1$	$L=2$
h_L	0.05	0.025
C_L (sec.)	0.75	1.07
$\|f_L - \hat{f}_L\|_{L_2(\Omega)}$	2.324	2.408
$\|f_\infty - f_L\|_{L_2(\Omega)}$	NA	NA

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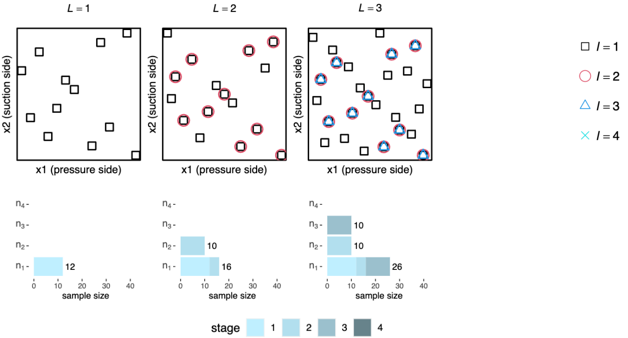

	$L=1$	$L=2$	$L=3$
h_L	0.05	0.025	0.0125
C_L (sec.)	0.75	1.07	2.13
$\|f_L - \hat{f}_L\|_{L_2(\Omega)}$	**2.324**	**2.408**	**2.481**
$\|f_\infty - f_L\|_{L_2(\Omega)}$	NA	NA	2.969

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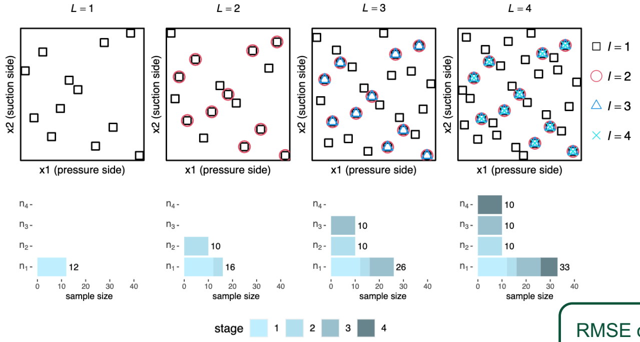

	$L=1$	$L=2$	$L=3$	$L=4$	
h_L	0.05	0.025	0.0125	0.00625	
C_L (sec.)	0.75	1.07	2.13	11.51	
$\|f_L - \hat{f}_L\|_{L_2(\Omega)}$	**2.324**	**2.408**	**2.481**	**2.491**	$< \frac{\epsilon}{2}$
$\|f_\infty - f_L\|_{L_2(\Omega)}$	NA	NA	2.969	**0.956**	$< \frac{\epsilon}{2}$

RMSE of $\hat{f}_4$ $= 1.60$

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

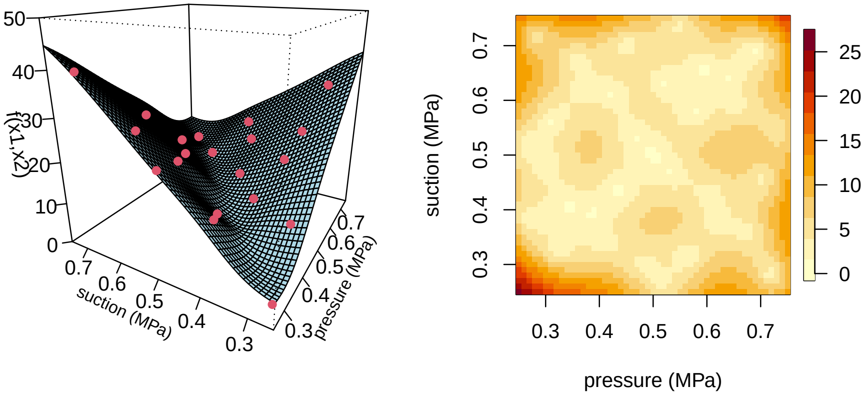

Figure: *(left)* $\hat{f}_4(\mathbf{x})$ *and true test points (red dots); (right) pointwise error bounds*

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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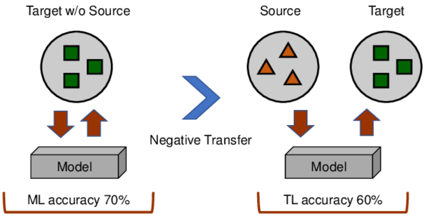
- Negative transfer?



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

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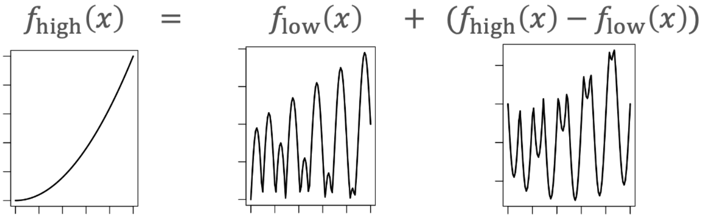


Questions

- 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

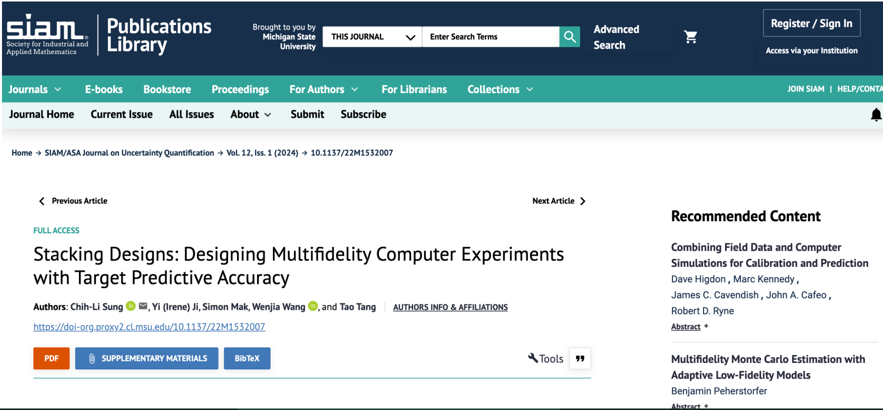
Conclusion

- Stacking design for multi-fidelity simulations with desired accuracy
  - Sample determination
  - Mesh size determination

- Cost complexity
  - Budget allocation
  - Comparison with single fidelity simulation

Reference

- **Sung, C.-L.**, Ji, Y., Mak, S., Wang, W., & Tang, T. (2024). Stacking Designs: Designing Multifidelity Computer Experiments with Target Predictive Accuracy. *SIAM/ASA Journal on Uncertainty Quantification*, 12(1), 157-181.



Thank You!

Thank NSF DMS 2113407 for supporting this work.

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