A Multivariate Interpolation and Regression Enhanced Kriging Surrogate Model

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Outline

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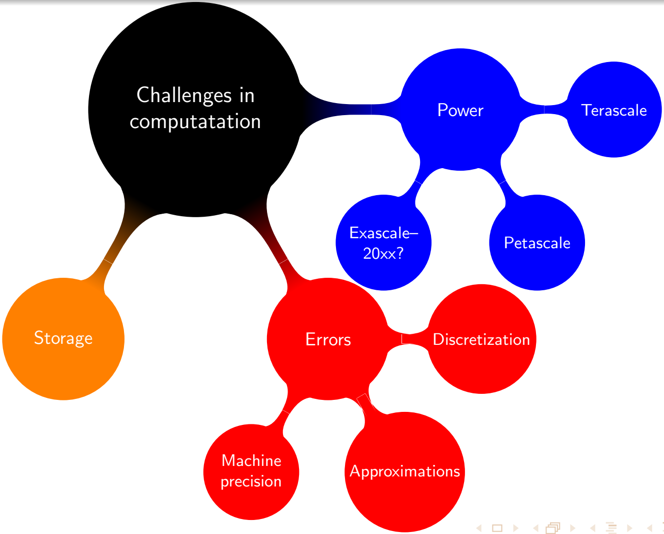
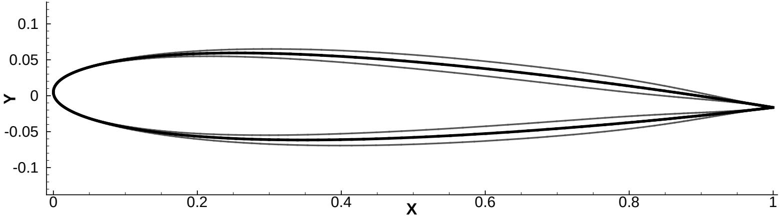
Introduction and Motivation I

- **Analysis:**
  - Theoretical
  - Experimental
  - Computational
- **Advancements:**
  - Hardware (processor speed, multi-core systems)
  - Software (parallel programming)
  - Algorithms and other tools (sophisticated methods)

Introduction and Motivation II



Introduction and Motivation III

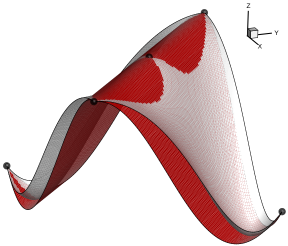


Optimization:

- Many design iterations – can be very expensive
- Highly coupled with several disciplines
- Time consuming to do physical testing and infeasibility

Introduction and Motivation IV

- **How to alleviate computational burden?**
  - Surrogate models / Meta models/ Response surfaces



Surrogate Model

Approximation of the exact function using interpolation and/or extrapolation

Introduction and Motivation V

Active Research

- **Enhance the existing surrogates**
  - Training point selection
  - Higher order information (gradients & Hessian)
  - Variable-fidelity (multi-fidelity)

Introduction and Motivation V

Active Research

- **Enhance the existing surrogates**
  - Training point selection
  - Higher order information (gradients & Hessian)
  - Variable-fidelity (multi-fidelity)
- **Develop new surrogates**
  - Robust & versatile

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Training Point Selection

Domain based sampling

- Monte-Carlo
- Latin Hypercube
- Delaunay Triangulation

Training Point Selection

Domain based sampling

- Monte-Carlo
- Latin Hypercube
- Delaunay Triangulation

Response based (adaptive)

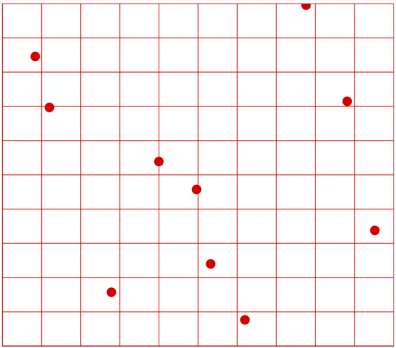
- Distance / Function values / Gradients / Physics

Monte-Carlo Sampling

Monte-Carlo

- Random number generator
- Very simple to program
- No control over locations

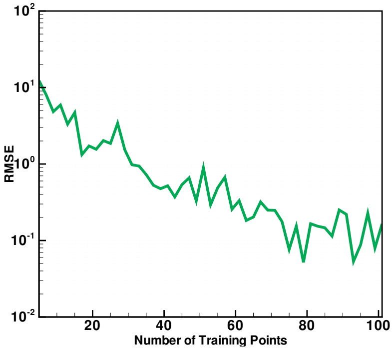
Latin Hypercube Sampling



Latin Hypercube

- McKay - while designing computer experiments
- Equal probability
- N^M bins in the design space
- No two points lie in the same bin

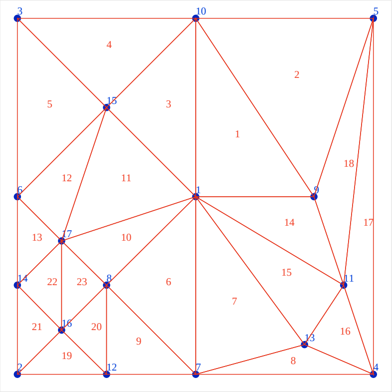
Latin Hypercube Sampling



Typical convergence history

- Random fluctuations
- Each data point is expensive to obtain
- Waste of computational time
- Need for monotonicity

Delaunay Triangulation



Delaunay Triangulation

- Geometrical method
- Split into hyper triangles
- Poor scaling to higher dimensions

Kriging Surrogate

- Originated in geological statistics
- Predicts the function by stochastic processes
- Highly non-linear and multi-modal functions
- The basic formulation of Kriging is given as,

$$\tilde{f}(x) = \mu + Z(x)$$

  $\rightarrow$ μ models the mean behavior

  $\rightarrow$ $Z(x)$ models the local variations using a Gaussian process
- Variants:
  - Direct: Gradient/Hessian terms are included in the formulation (correlation between func-grad, func-Hess, grad-grad, etc.)
  - Indirect: Same formulation as original Kriging but additional samples are created by using gradient/Hessian information

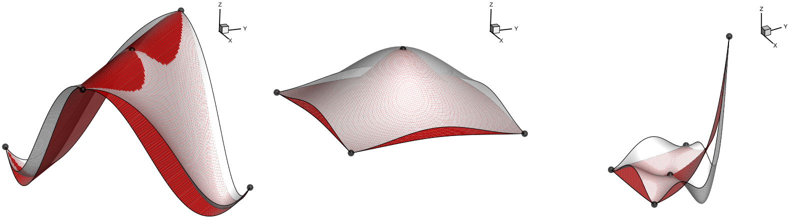
Multivariate Interpolation and Regression

- Based on Taylor series expansion
- Mathematically,

$$\tilde{f} = \sum_{i=1}^{N_v} a_{vi}(x) f(x_{vi}) + \sum_{i=1}^{N_g} a_{gi}(x) \nabla f(x_{gi})$$

  - N_v, N_g is the number of function and func-grad data points
  - a_{vi} and a_{gi} are the basis functions
  - f and ∇f are the function f and gradient values
- **Tunable parameters:** Taylor order n and others

Analytic Test Functions

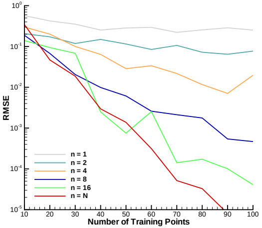


Cos   Runge   Exponential

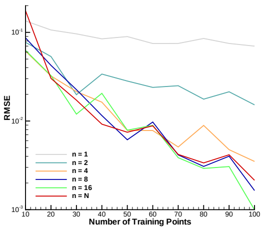
Analytic test functions on hypercube $[-2, 2]^M$

1. Cosine: $f_1(x_1, \ldots, x_M) = \cos(x_1 + \ldots + x_M)$
2. Runge: $f_2(x_1, \ldots, x_M) = \frac{1}{1+x_1^2+\ldots+x_M^2}$
3. Exponential: $f_3(x_1, \ldots, x_M) = e^{(x_1+\ldots+x_M)}$

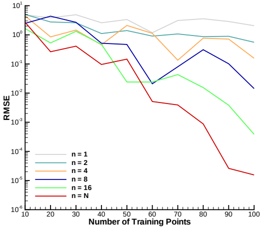
Effect of Taylor order (2D)



Cosine



Runge

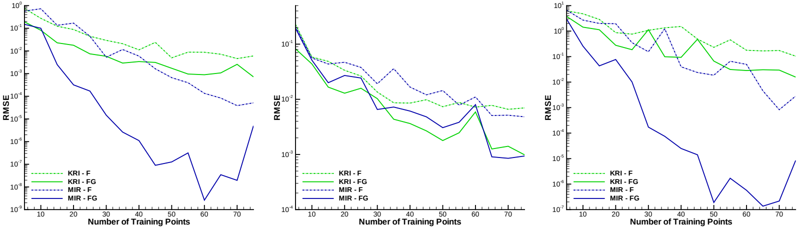


Exponential

Remarks:

- Higher *n* can corrupt the solution as well
- Higher *n* mandates more computational time
- Choice of an optimum Taylor order: tedious task

Original Kriging vs. MIR in two dimensions



Cosine | Runge | Exponential

Remarks:

- **Advantage:** Accuracy, convergence rate
- **Disadvantage:** Computationally intensive, tunable params.

Choice of local and global surrogate

	Kriging	MIR

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Computational time	Less	Very high

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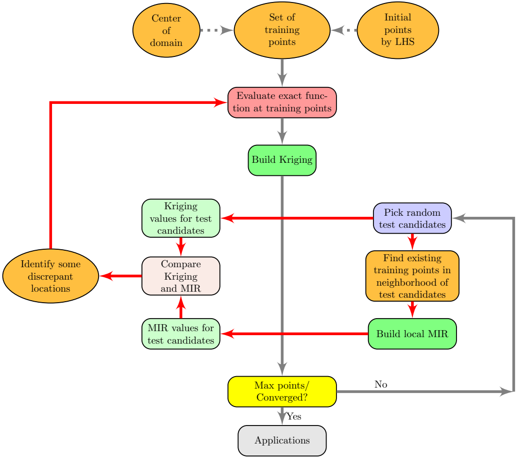
Our theme: Use MIR to guide global Kriging

Adaptive Training Point Selection



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Conclusion

- **Summary:**
  - Made use of local surrogate for training point selection
  - Applied to multi-dimensional test functions
  - Showed improvement for monotonic convergence behavior
  - Showed Variable-fidelity results
- **Future Work:**
  - Where to use gradient information?
  - How to use variable-fidelity data efficiently?
- **Potential Applications:**
  - Aerospace design & optimization
  - Uncertainty quantification
  - Aerodynamic databases

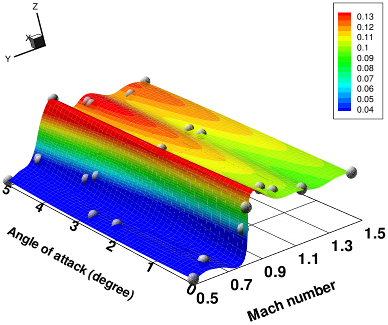
Acknowledgments

1. Wataru Yamazaki – Kriging surrogate
2. Qiqi Wang – MIR source code

Selected Bibliography

Any Questions?

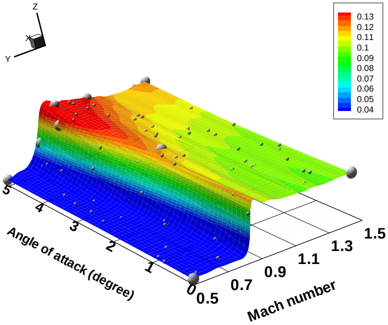
Kriging Drag Database - High Fidelity Model



Kriging Drag Database

- 25 Euler evaluations
- Fine mesh $19,548$ elements
- Adaptive sampling strategy
- Not computationally expensive
- Nicely captures transonic behavior

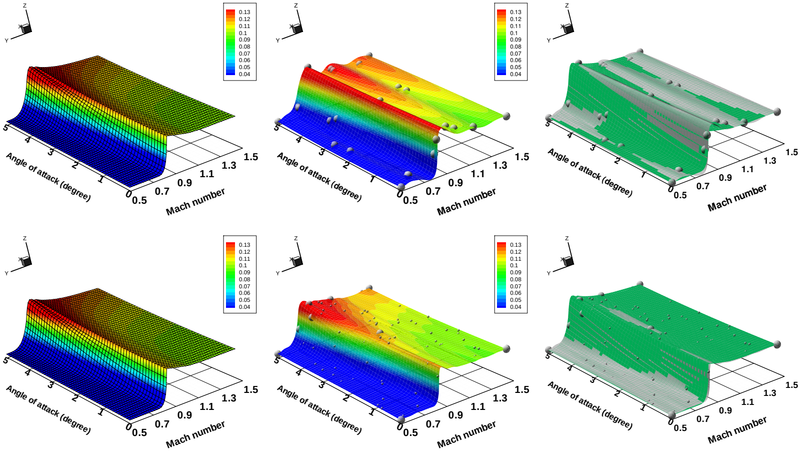
Kriging Drag Database - Variable Fidelity Model



Variable Fidelity

- 9 High fid. training points adaptively
- Fine mesh 19,548 elements
- 64 Low fid. training points via LHS
- Coarse mesh 4,433 elements

Drag Database



Euler | Our Kriging | Both combined

Direct Kriging

- Gradient/Hessian terms are included in the formulation
  - Function value estimated using a linear combination of function, gradient and Hessian values
  - Minimize mean-squared-error (MSE) between exact and estimated function value
  - Final form of the gradient/Hessian enhanced direct Cokriging:

$$\hat{\mathcal{J}}(D) = \mu + r^T(D)R^{-1}(Y - \mu I)$$

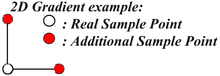
where

$\mu = (I^T R^{-1} I)^{-1}(I^T R^{-1} Y)$	constant mean term
R	correlation matrix between samples
$Y = \left(\mathcal{J}(D_1), \ldots, \left.\frac{d\mathcal{J}}{dD}\right\|_{D_1}, \ldots, \left.\frac{d^2\mathcal{J}}{dD^2}\right\|_{D_1}, \ldots \right)$	vector of sample point information
$r(D)$	correlation between D and samples

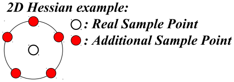
  - Determine required derivatives of correlation function (up to fourth order) with automatic differentiation

Indirect Kriging

- Additional samples are created by using gradient and Hessian information



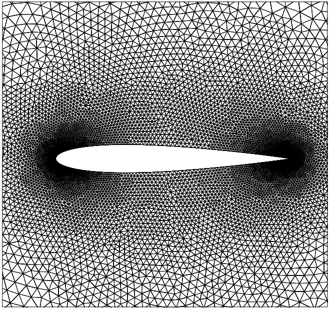
$$\mathcal{J}_{add} = \mathcal{J}(D_i) + \left.\frac{d\mathcal{J}}{dD}\right|_{D_i} \Delta D$$



$$\mathcal{J}_{add} = \mathcal{J}(D_i) + \left.\frac{d\mathcal{J}}{dD}\right|_{D_i} \Delta D + \frac{1}{2}\Delta D^T \left.\frac{d^2\mathcal{J}}{dD^2}\right|_{D_i} \Delta D$$

  - Major parameters: distance between real and additional points ΔD and number of additional points per real sample point
  - Worse R matrix conditioning with smaller distances and larger number of additional points
    $\rightarrow$ Severe trade-offs for these parameters

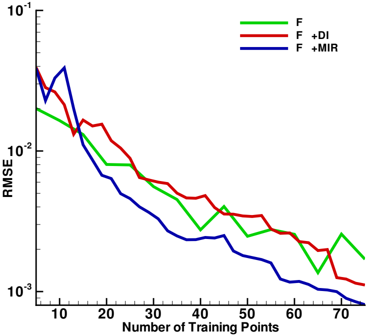
Test Case



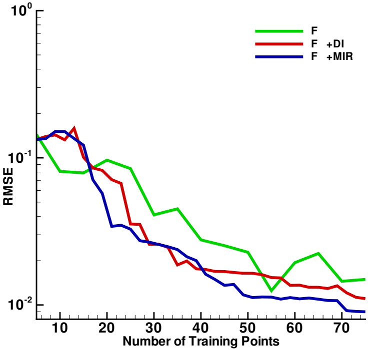
Problem Setup

- NACA0012 airfoil
- Eulerian flow solver
- Cell-centered second-order accurate finite-volume approach
- $0.5 < M < 1.5$ and $0^\circ < \alpha < 5^\circ$
- Fine mesh $19,548$ elements
- Coarse mesh $4,433$ elements

Convergence History

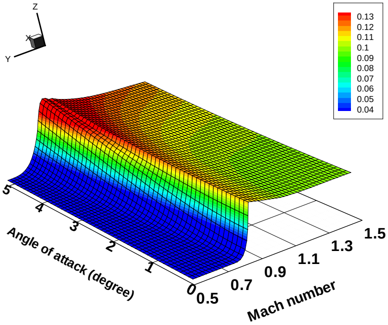


Drag



Lift

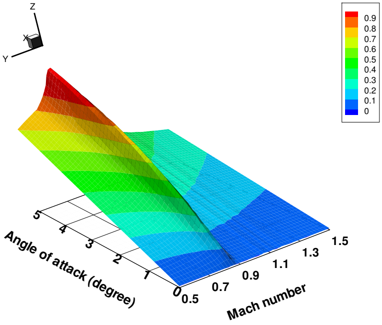
Exact Drag Database



Exact Drag Database

- Solves Euler Equations (Inviscid)
- Cartesian mesh - α vs. M
- 2601 nodes
- Computationally expensive

Exact Lift Database



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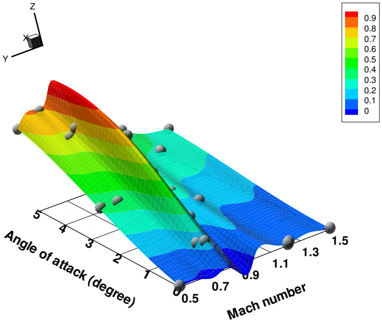
Kriging Lift Database - High Fidelity Model



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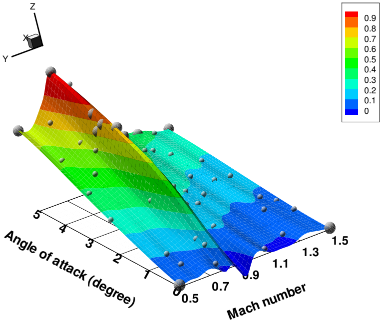
Kriging Lift Database - Variable Fidelity Model



Variable Fidelity

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- 40 Low fid. training points via LHS
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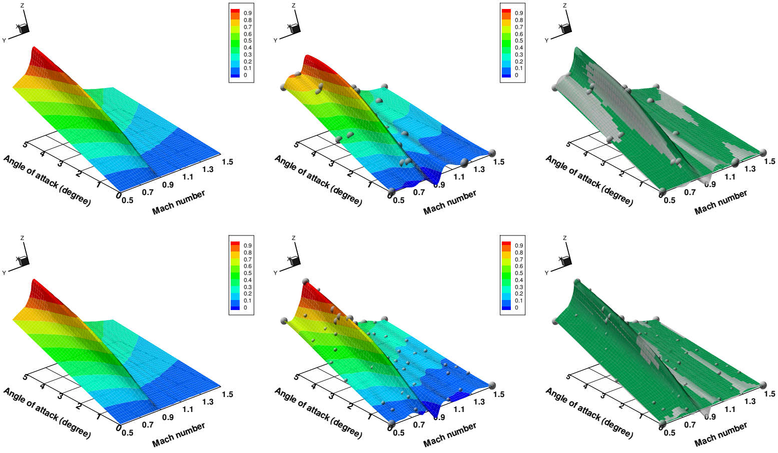
Lift Database



Euler | Our Kriging | Both combined

Observations

RMSE comparisons for Kriging models

RMSE	High-fidelity	Variable-fidelity

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RMSE comparisons for Kriging models

RMSE	High-fidelity	Variable-fidelity
Drag Coefficient	0.45868×10^{-2}	0.38118×10^{-2}

Observations

RMSE comparisons for Kriging models

RMSE	High-fidelity	Variable-fidelity
Drag Coefficient	0.45868×10^{-2}	0.38118×10^{-2}
Lift Coefficient	0.32746×10^{-1}	0.27735×10^{-1}