Surrogate Modeling Applications

Introduction to Multidisciplinary Design Optimization
May 2014

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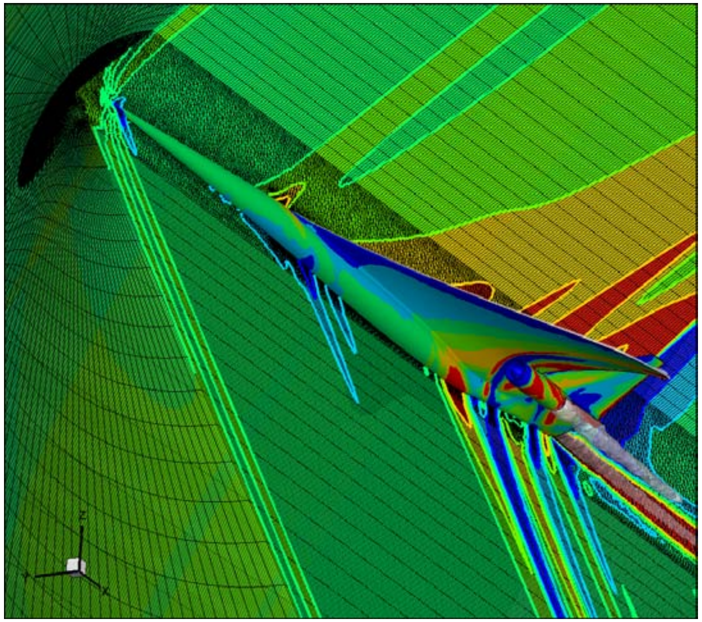
Optimal Shape Design

Goal: Improve aircraft performance by iteratively changing an aerodynamic shape

Common Approaches:

- Local Optimizers:
  - Gradient Based Algorithms
- Global Optimizers:
  - Genetic Algorithms
  - Particle Swarm Algorithms
- Surrogate Based Optimizers:
  - Gaussian Process Regression



Gaussian Process Regression

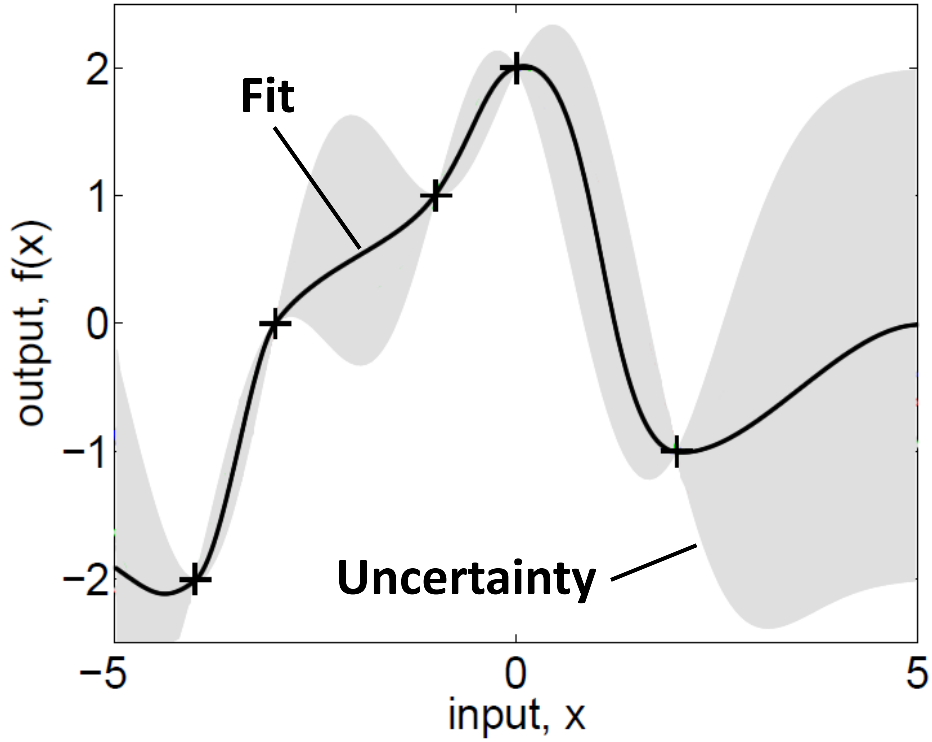
For Response Surface Modeling

Strengths

+ Non-parametric
+ Uncertainty of Fit
+ Gradient Information

Challenges

– Hyperparameter Tuning
– Numerical Stability
– Computational Cost
– High Dimensionality



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Gaussian Process Regression

A multivariate normal distribution with zero mean …

$$\begin{bmatrix} f_p \\ f_k^* \end{bmatrix} \sim \mathcal{N}\left(0, \begin{bmatrix} k(x_p, x_q) & k(x_p, x_j^*) \\ k(x_k^*, x_q) & k(x_k^*, x_j^*) \end{bmatrix}\right)$$

$$\{\, f_i(x_i) \,|\, i = 1, ..., n \,\} \;,\; \{\, f_t^*(x_t^*) \,|\, t = 1, ..., m \,\}$$

… Conditioned with the known data …

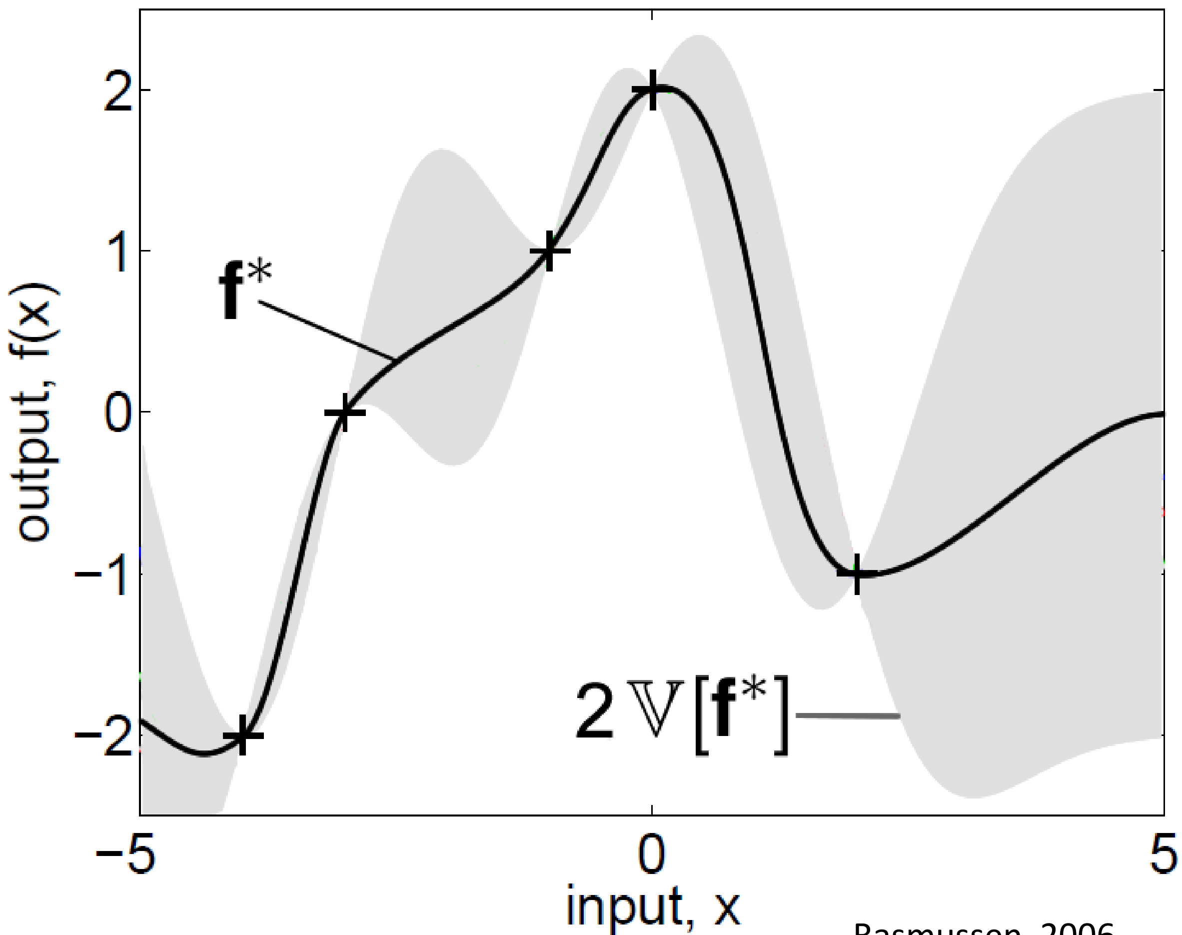
$$f|x^*, x, f \sim \mathcal{N}\left(f^*, \mathbb{V}[f^*]\right)$$

… Yields a system of linear equations
that estimates an unknown function value

$$f_k^* = k(x_k^*, x_q)\, k(x_p, x_q)^{-1}\, f_p$$

$$\mathbb{V}[f_k^*] = \left(k(x_k^*, x_j^*) \;-\; k(x_k^*, x_q)\, k(x_p, x_q)^{-1}\, k(x_p, x_j^*)\right)_k$$

Gaussian Process Regression



Rasmussen, 2006

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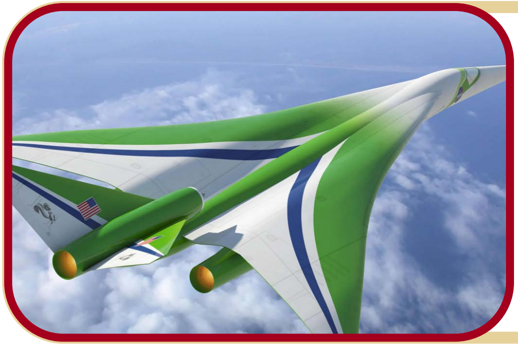
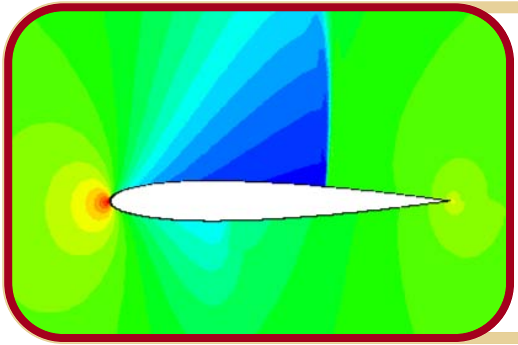
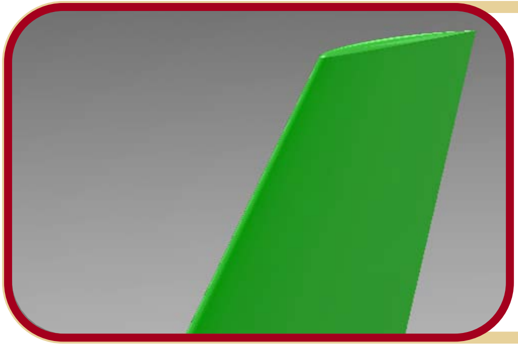
Outline



Gradient Enhanced Response Surfaces



Managing Gradient Inaccuracies



Managing High Dimensional Spaces

Response Surface Methodologies for Low-Boom Supersonic Aircraft Design using Equivalent Area Distributions

AIAA MDAO 2012

Trent Lukaczyk
Francisco Palacios
Juan Alonso

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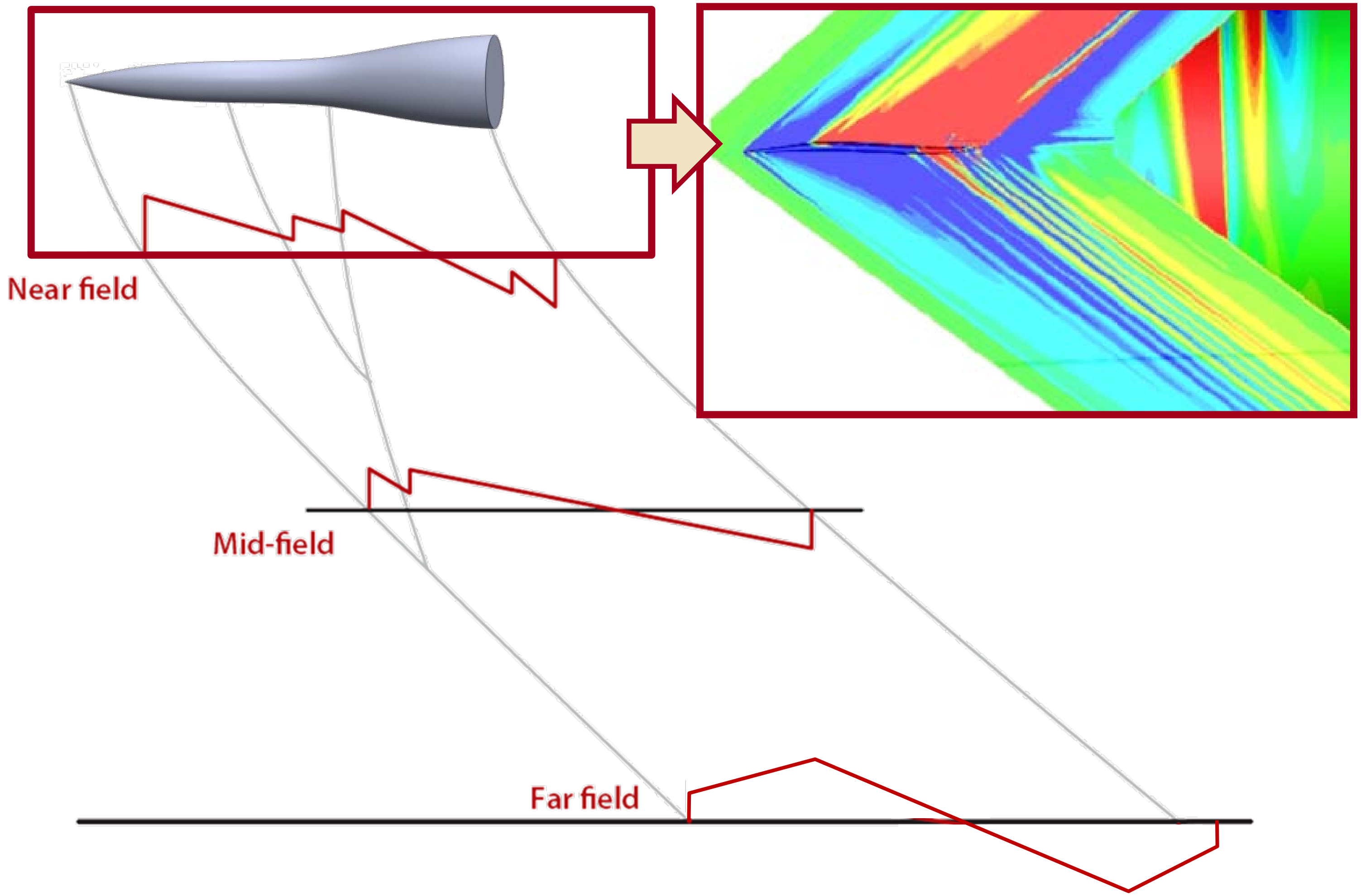
Motivation

N+2 Supersonic Passenger Jet Concept

Cruise:
Ma 1.6 – 1.8
Sonic Boom:
65-70 PLdB
Fuel Efficiency:
3 pax-mi/lbs fuel
Range:
4000 nmi
Payload:
35-70 pax

➢ **Reduce Boom Noise, Reduce Drag, Maintain Lift**

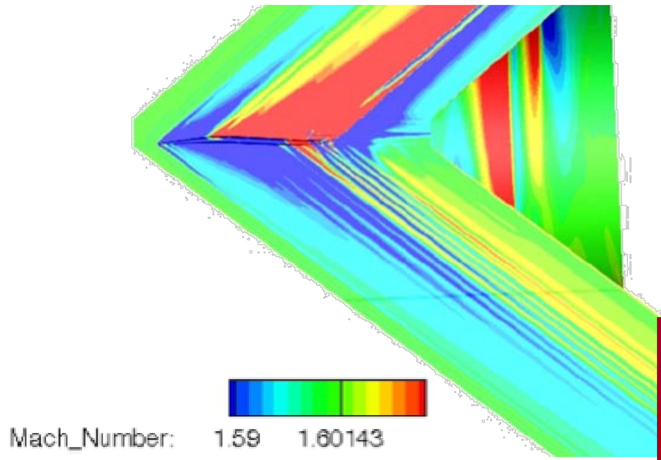
Sonic Boom Shaping



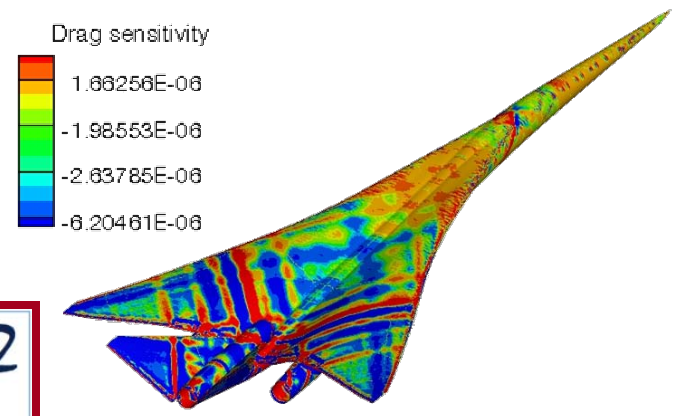
➢ **CFD-based equivalent area inverse design**

Computational Tools

Direct Solver

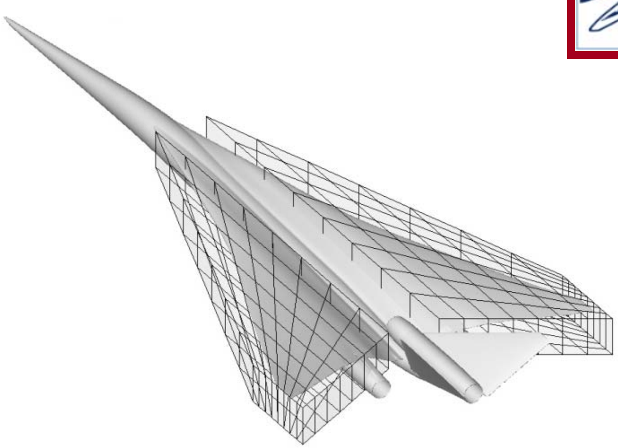


Adjoint Solver



SU2
STANFORD UNIVERSITY
Unstructured Code

Mesh Deformation

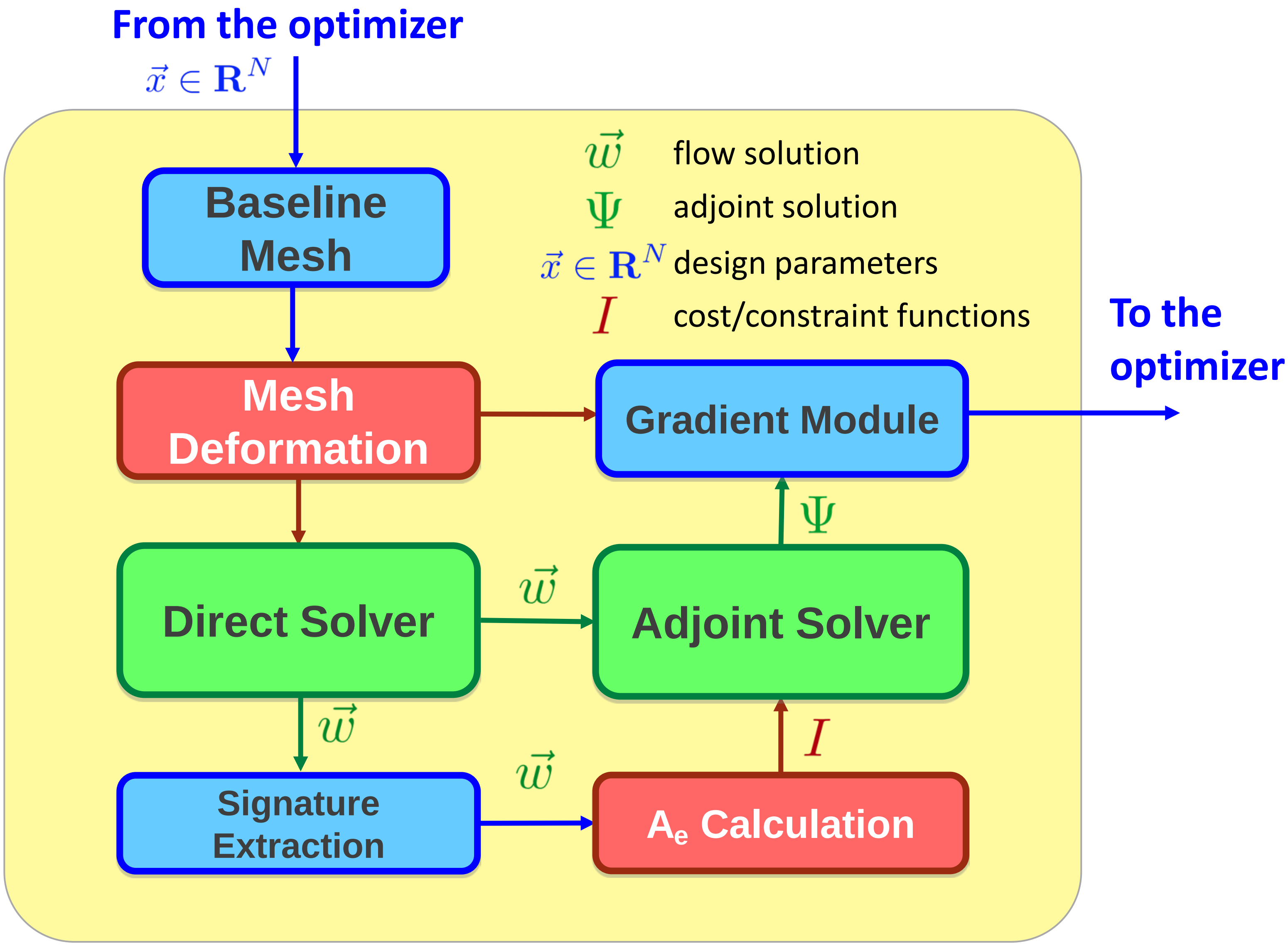


And More

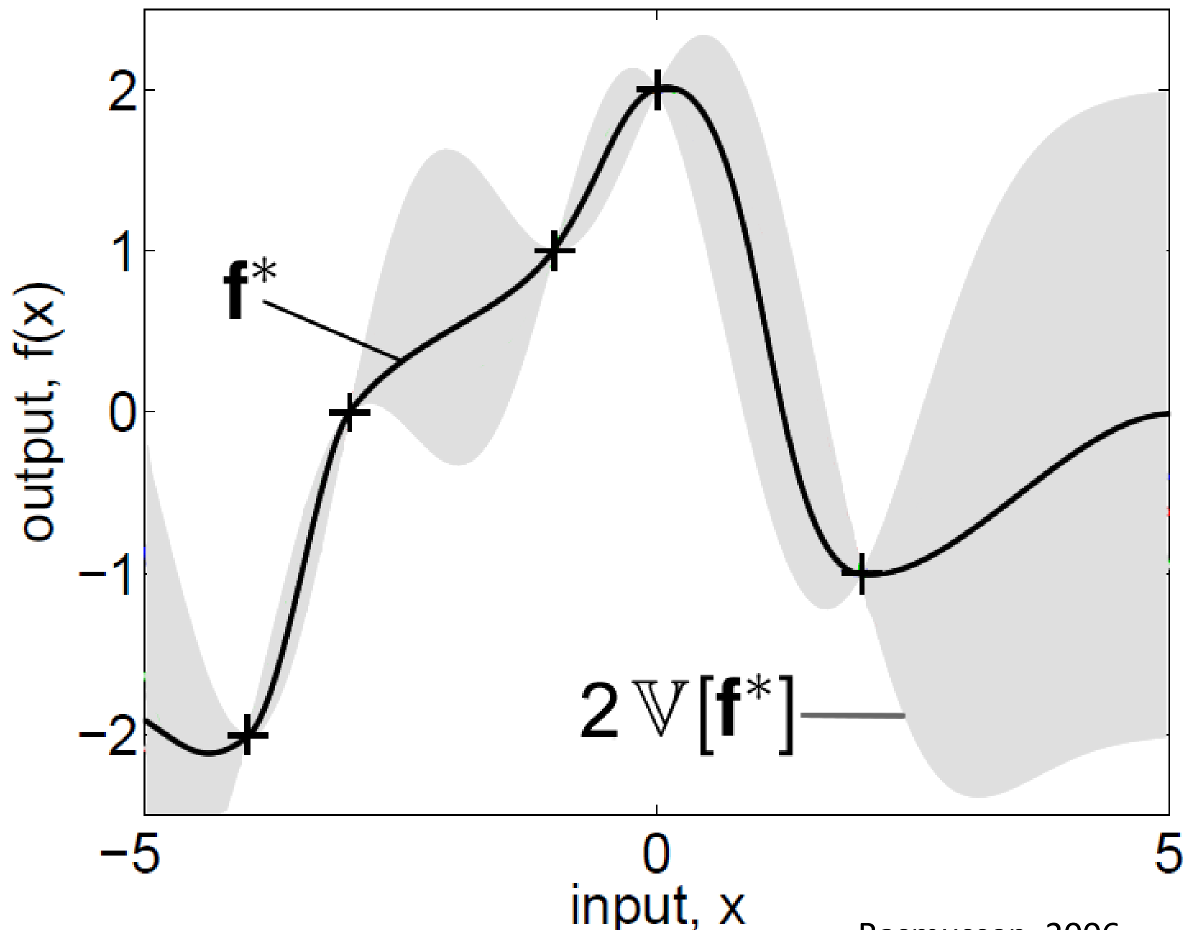
- Gradient Projection
- Python Wrappers
- Under active development by the Aerospace Design Lab

http://su2.stanford.edu

Gradient Based Design Procedure



Gaussian Process Regression



Rasmussen, 2006

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Kernel Function

$$k(x_p, x_q) = k(p, q) = \theta_1^2 \exp\left(-\frac{1}{2\theta_2^2}\sum_{z=1}^{d}(p_z - q_z)^2\right)$$

$$\{p_i, q_i, \frac{\partial}{\partial x_i} \mid i = 1, ..., d\}$$

$$\log p(f_p|x_p, \theta_h) = -\frac{1}{2} f_p^\top [\sigma]^{-1} f_p - \frac{1}{2}\log|[\sigma]| - \frac{n}{2}\log\, 2\pi$$

Gradients

$$k\left(\frac{\partial p}{\partial x_v}, q\right) = \left.\frac{\partial k(p,q)}{\partial x_v}\right|_q$$

$$k\left(p, \frac{\partial q}{\partial x_w}\right) = \left.\frac{\partial k(p,q)}{\partial x_w}\right|_p$$

$$k\left(\frac{\partial p}{\partial x_v}, \frac{\partial q}{\partial x_w}\right) = \left.\frac{\partial}{\partial x_w}\left(\left.\frac{\partial k(p,q)}{\partial x_v}\right|_q\right)\right|_p$$

$$k(p,q) \rightarrow \begin{bmatrix} k(p,q) & k\left(p, \frac{\partial q}{\partial x_w}\right) \\ k\left(\frac{\partial p}{\partial x_v}, q\right) & k\left(\frac{\partial p}{\partial x_v}, \frac{\partial q}{\partial x_w}\right) \end{bmatrix} \qquad f_p \rightarrow \begin{bmatrix} f_p \\ \frac{\partial f_p}{\partial x_d} \end{bmatrix}$$

Noise Models

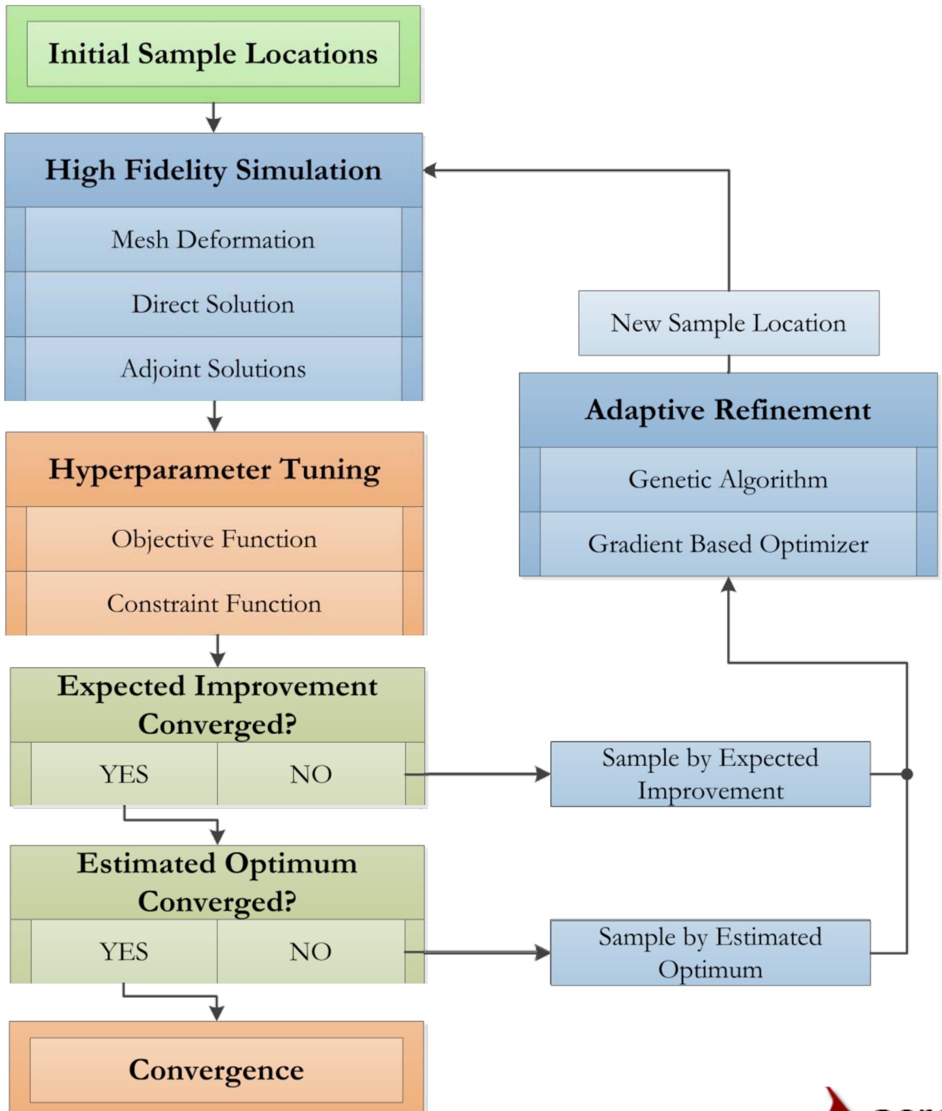
$$f_N^*(x) = f^*(x) + \epsilon$$

$$[k] \rightarrow [k] + [k_N]$$

$$[k_N] = \begin{bmatrix} \theta_3^2 I_{n',n'} & 0_{n',m'} \\ 0_{m',n'} & \theta_4^2 I_{m',m'} \end{bmatrix}$$

$$n' = n(1+d)$$
$$m' = m(1+d)$$

Our Approach to SBO



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Our Approach to SBO

- Optimize one objective with constraints
- Two Adaptive Refinement Criteria
  1. Modified expected improvement
  2. Estimated optimum
- Computational Cost
  - Scale data and assume isotropic variation
  - Condense hyperparameter space to four variables
- Numerical Stability
  - Constrain noise hyperparameters to maintain a minimum amount of noise

Hyperparameter Selection

Hyp.	Description
θ_1	Nominal Variance
θ_2	Length Scale
θ_3	Noise in Objective Function
θ_4	Noise in Gradients

- Maximize marginal likelihood

$$\log p(f_p|x_p,\theta_h) = -\frac{1}{2} f_p^\top [\sigma(\theta_i)]^{-1} f_p - \frac{1}{2}\log|[\sigma(\theta_i)]| - \frac{n}{2}\log 2\pi$$

- Becomes expensive in higher dimensions
  - requires inversion of (1+d)n x (1+d)n matrix at every evaluation

Hyperparameter Selection

Hyp.	Description
θ_1	Nominal Variance
θ_2	Length Scale
θ_3	Noise in Objective Function
θ_4	Noise in Gradients

- There could potentially be one length scale and one gradient noise parameter per dimension
- Scale data and assume isotropy to reduce computational expense

Hyperparameter Selection

Hyp.	Description
Θ_1	Nominal Variance
Θ_2	Length Scale
Θ_3	Noise in Objective Function
Θ_4	Noise in Gradients

To improve numerical stability and robustness:

Constraint	Motivation
$\Theta_3/\Theta_1 < 1\text{e-}1$	Avoid interpreting data as noise
$\Theta_3/\Theta_1 > 1\text{e-}8$	Maintain well conditioned numerics
$\mathrm{rcond}([\sigma]) > 1\text{e-}10$	Maintain well conditioned numerics
$\Theta_3 < \Theta_4$	Honor function value before gradient

Our Approach to SBO

- Optimize one objective with constraints
- Two Adaptive Refinement Criteria
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Modified Expected Improvement

Traditional expected improvement ...

$$\begin{aligned} \mathrm{E}\left[I(x)\right] &= \mathrm{E}\left[\max(f_{\min} - F, 0)\right] \\ &= (f_{\min} - f^*)\Phi\left(\frac{f_{\min}-f^*}{s^*}\right) + s^*\phi\left(\frac{f_{\min}-f^*}{s^*}\right) \end{aligned}$$

Condition by probability of constraint feasibility ...

$$\mathrm{P}[c(x) < 0] = \phi\left(\frac{c^*}{s_c^*}\right)$$

Avoid boundaries of the design space ...

$$\mathrm{B}(x) = 1 - \exp\left(-\frac{1}{2}\min\left(\frac{x_k - x_k^l}{b_k^2}, \frac{x_k^u - x_k}{b_k^2}, k = 1, ..., d\right)\right)$$

Combine to yield an infill sampling criteria ...

$$ISC_1(x) = \mathrm{E}\left[I(x)\right] \cdot \mathrm{P}[c(x) < 0] \cdot \mathrm{B}(x)$$
$$x_{new} = x \,|\, \max\left(ISC_1(x)\right)$$

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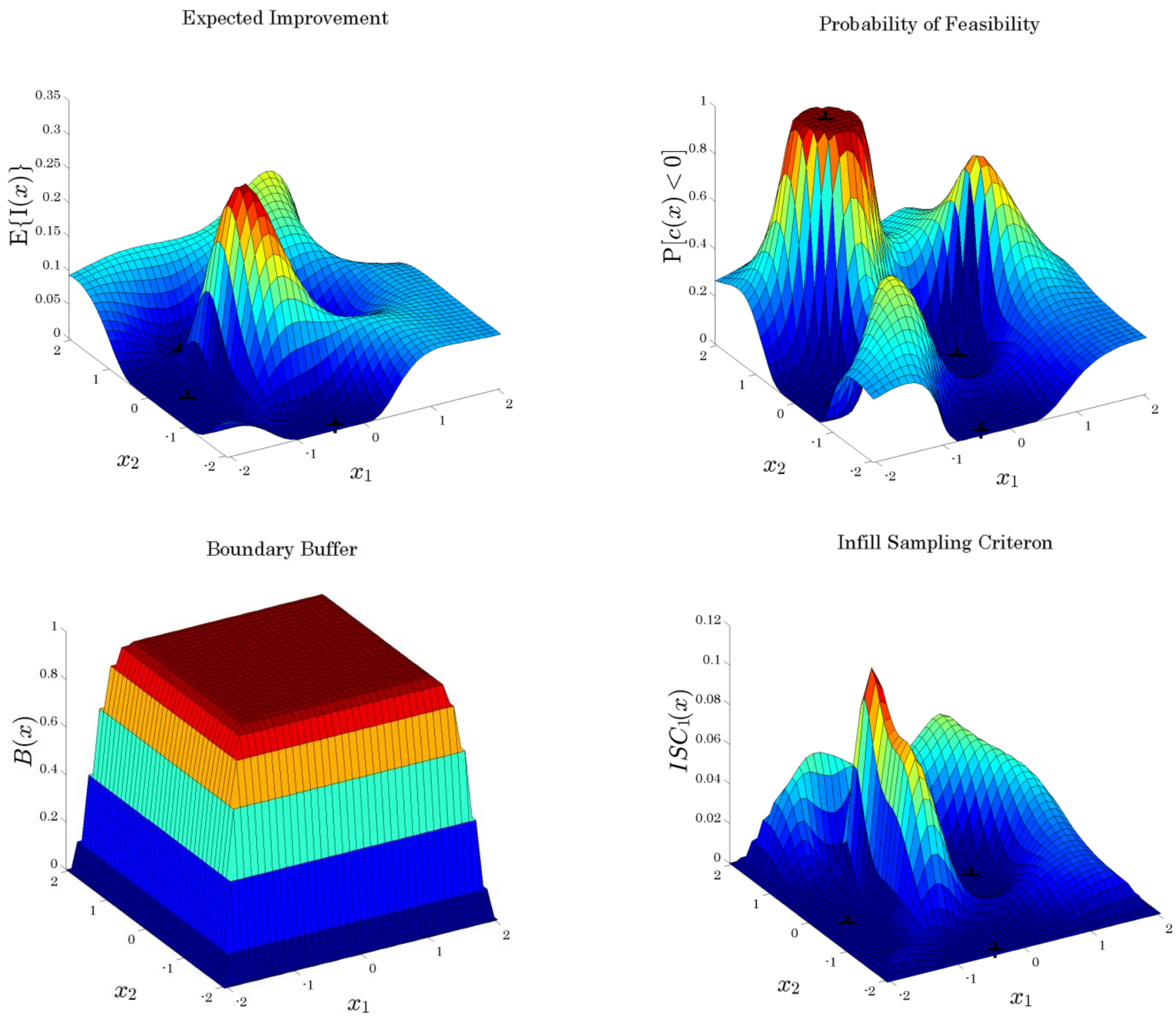
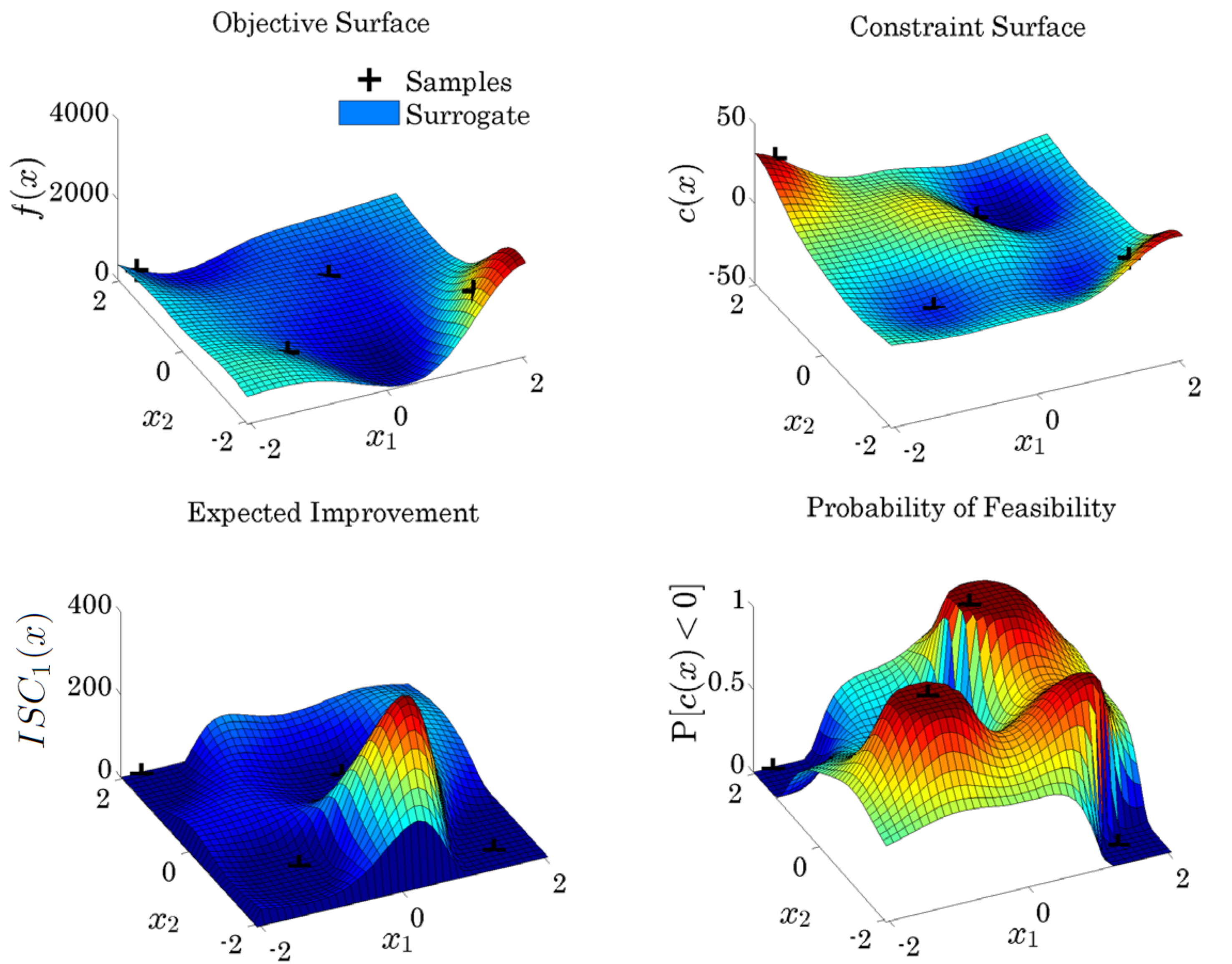
Modified Expected Improvement

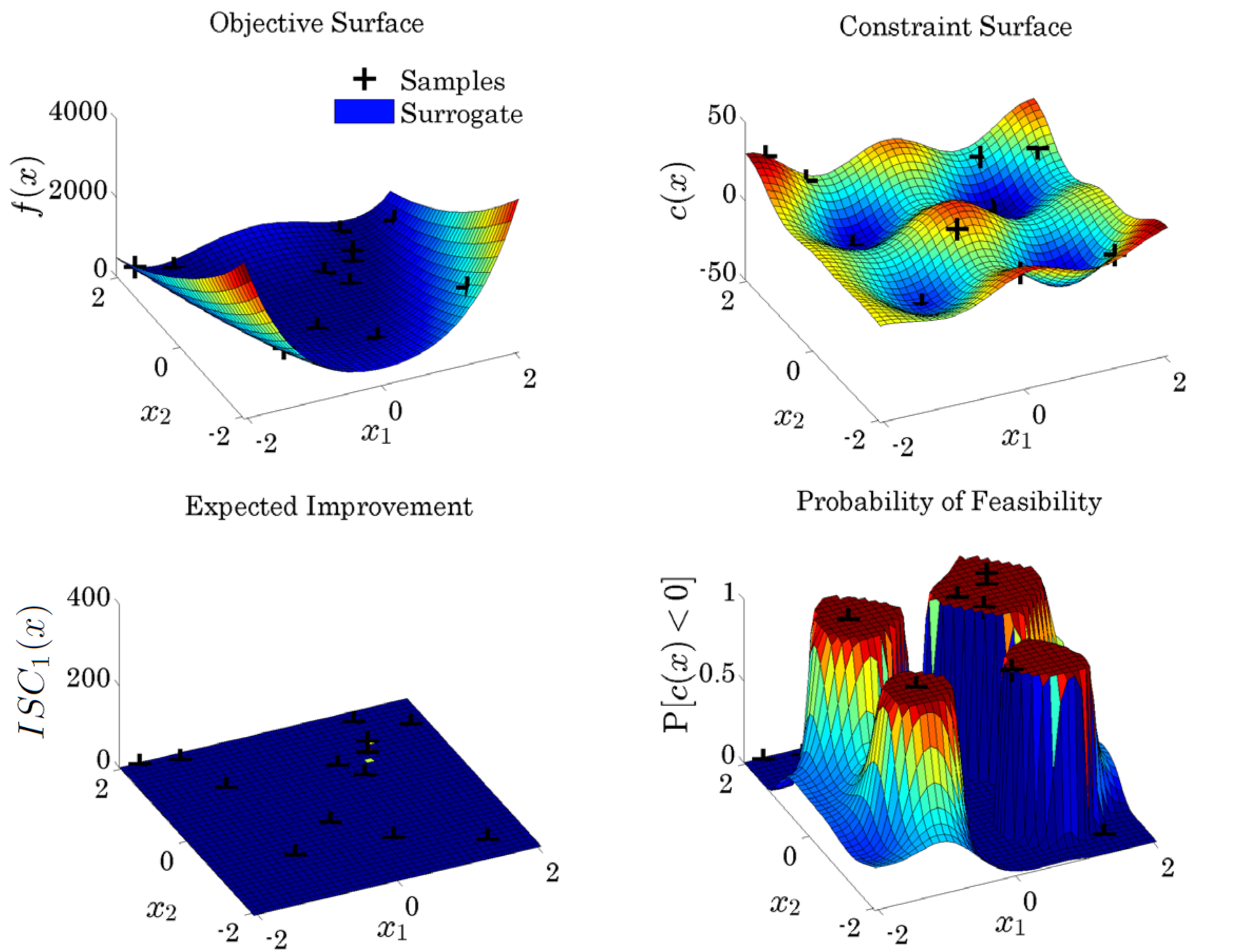
$$ISC_1(x) = \mathrm{E}\left[I(x)\right] \cdot \mathrm{P}[c(x) < 0] \cdot \mathrm{B}(x)$$



Example Refinement



Example Refinement



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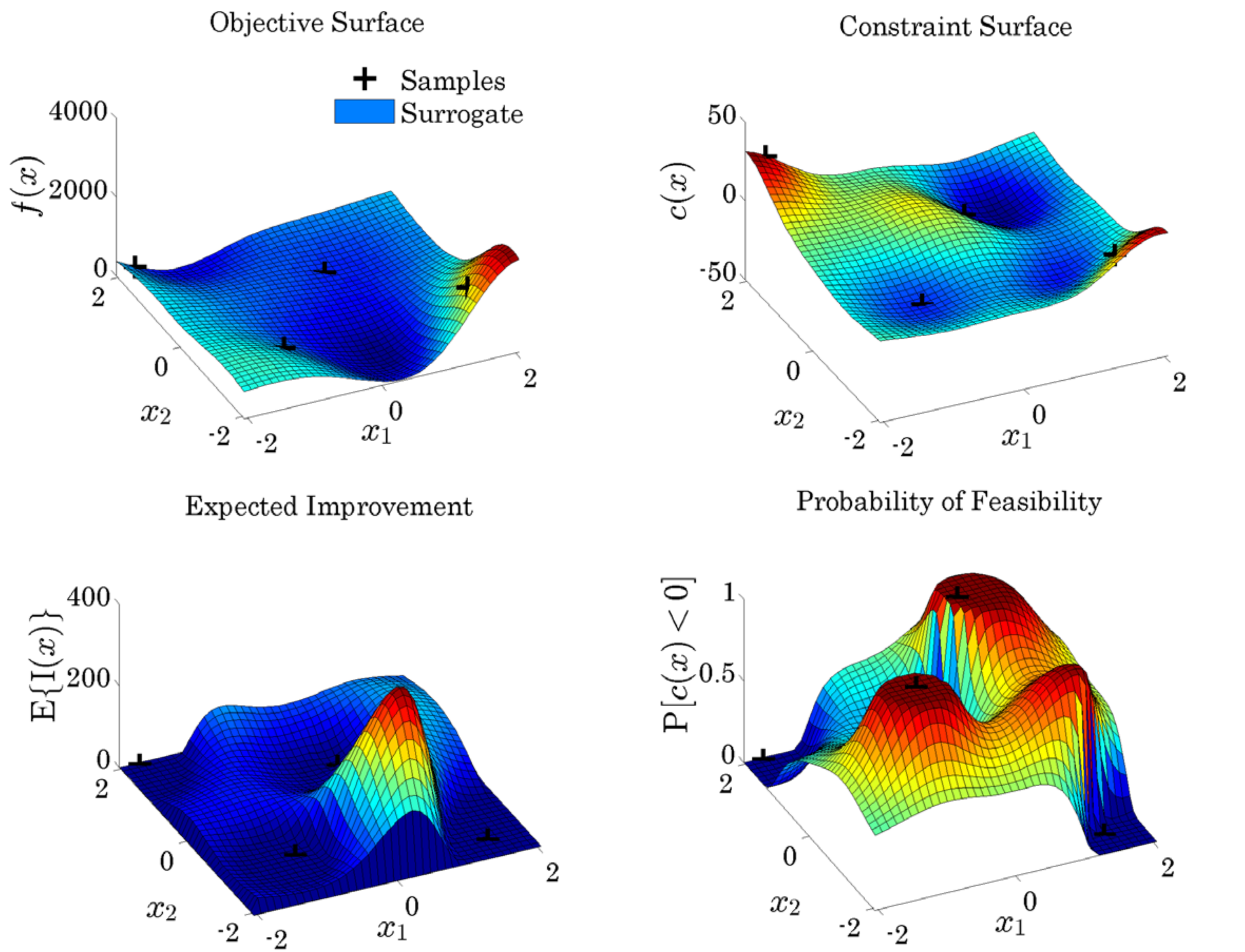
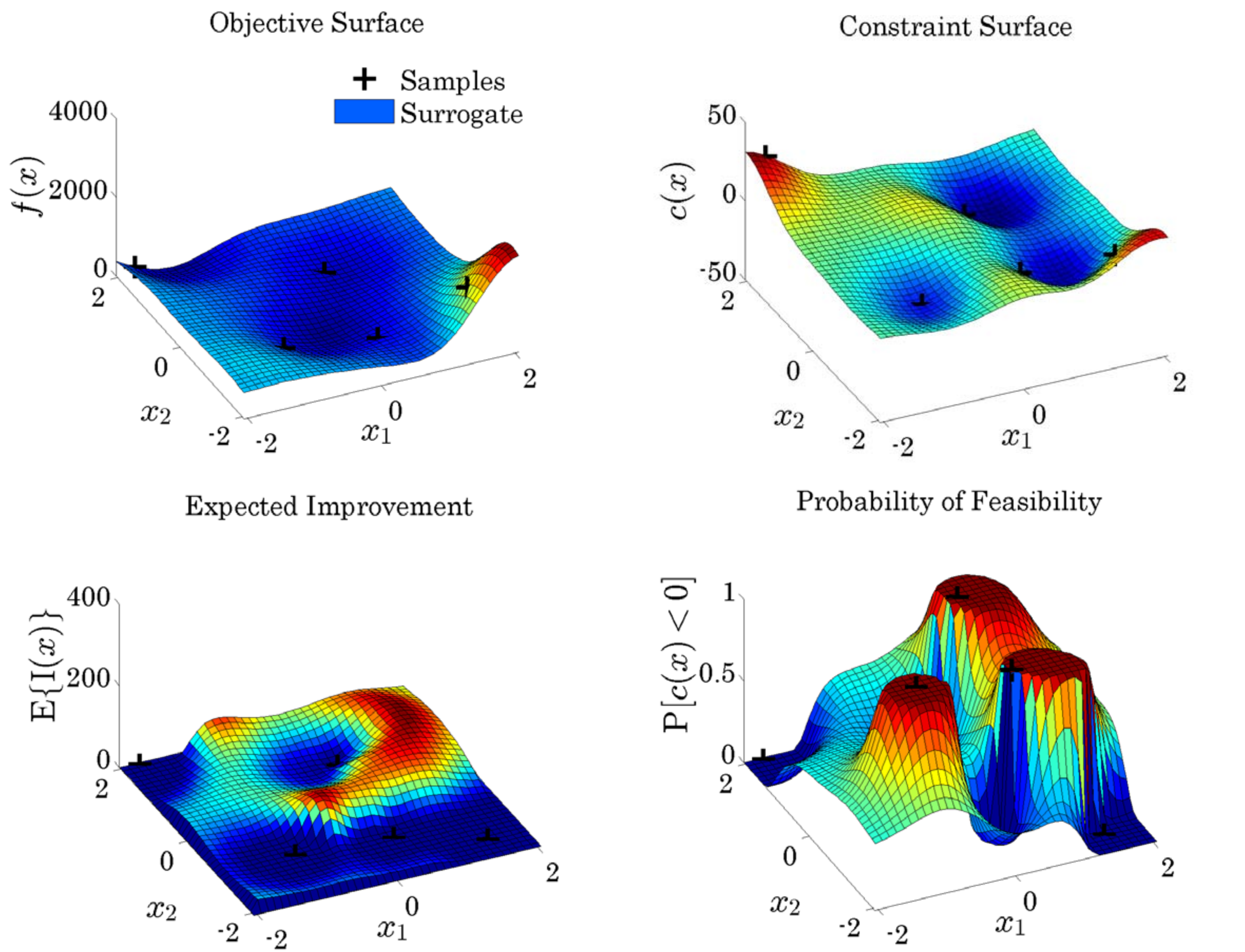
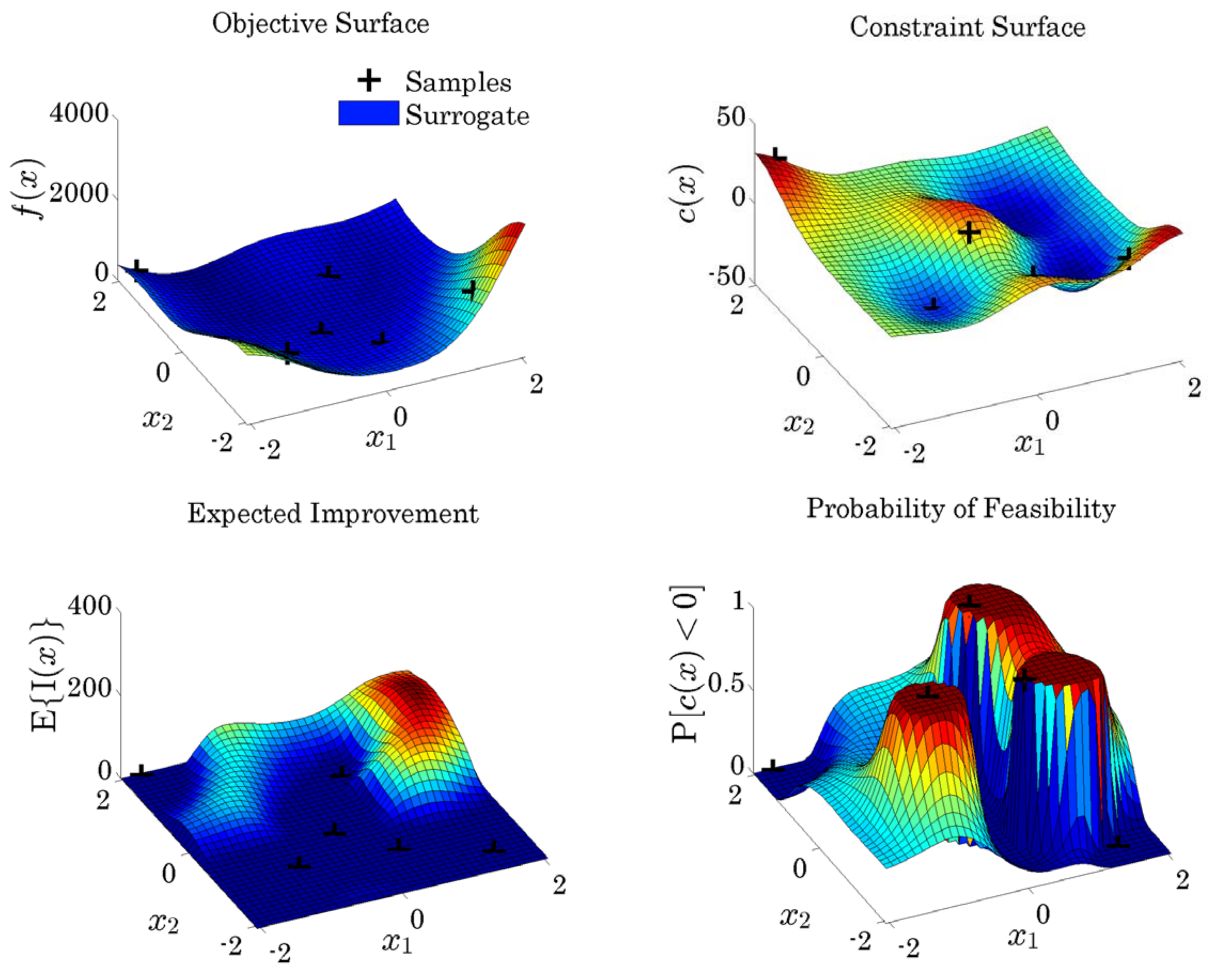

Objective Surface
Samples
Surrogate
4000
2000
0
$f(x)$
2
0
-2
x_2
-2
0
2
x_1
Constraint Surface
50
0
-50
$c(x)$
2
0
-2
x_2
-2
0
2
x_1
Expected Improvement
400
200
0
$E\{I(x)\}$
2
0
-2
x_2
-2
0
2
x_1
Probability of Feasibility
1
0.5
0
$P[c(x) < 0]$
2
0
-2
x_2
-2
0
2
x_1

N_Samples = 5


Objective Surface
Samples
Surrogate
4000
2000
0
f(x)
2
0
-2
x2
-2
0
2
x1
Constraint Surface
50
0
-50
c(x)
2
0
-2
x2
-2
0
2
x1
Expected Improvement
400
200
0
E{I(x)}
2
0
-2
x2
-2
0
2
x1
Probability of Feasibility
1
0.5
0
P[c(x) < 0]
2
0
-2
x2
-2
0
2
x1

N_Samples = 6


Objective Surface
Samples
Surrogate
4000
2000
0
$f(x)$
2
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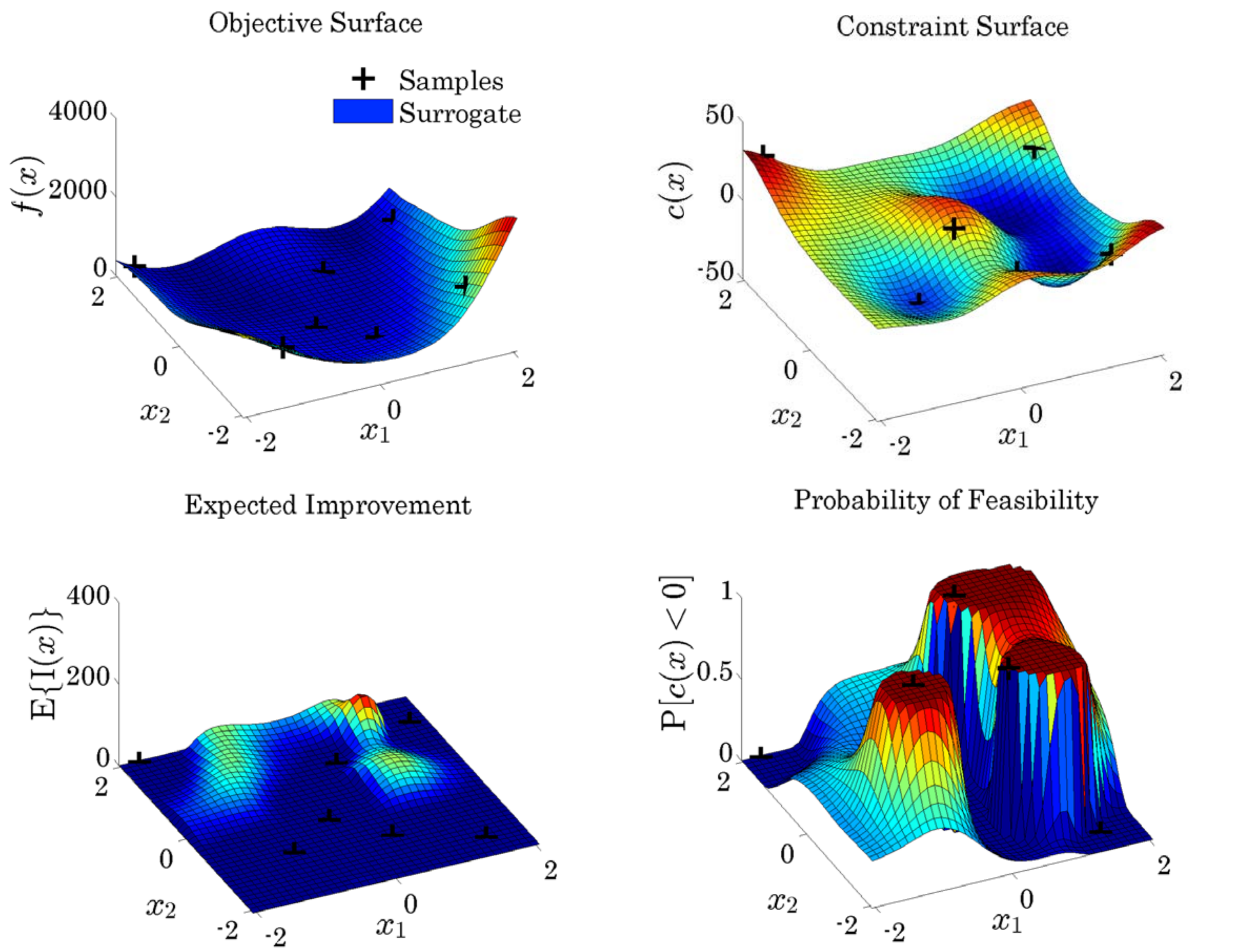
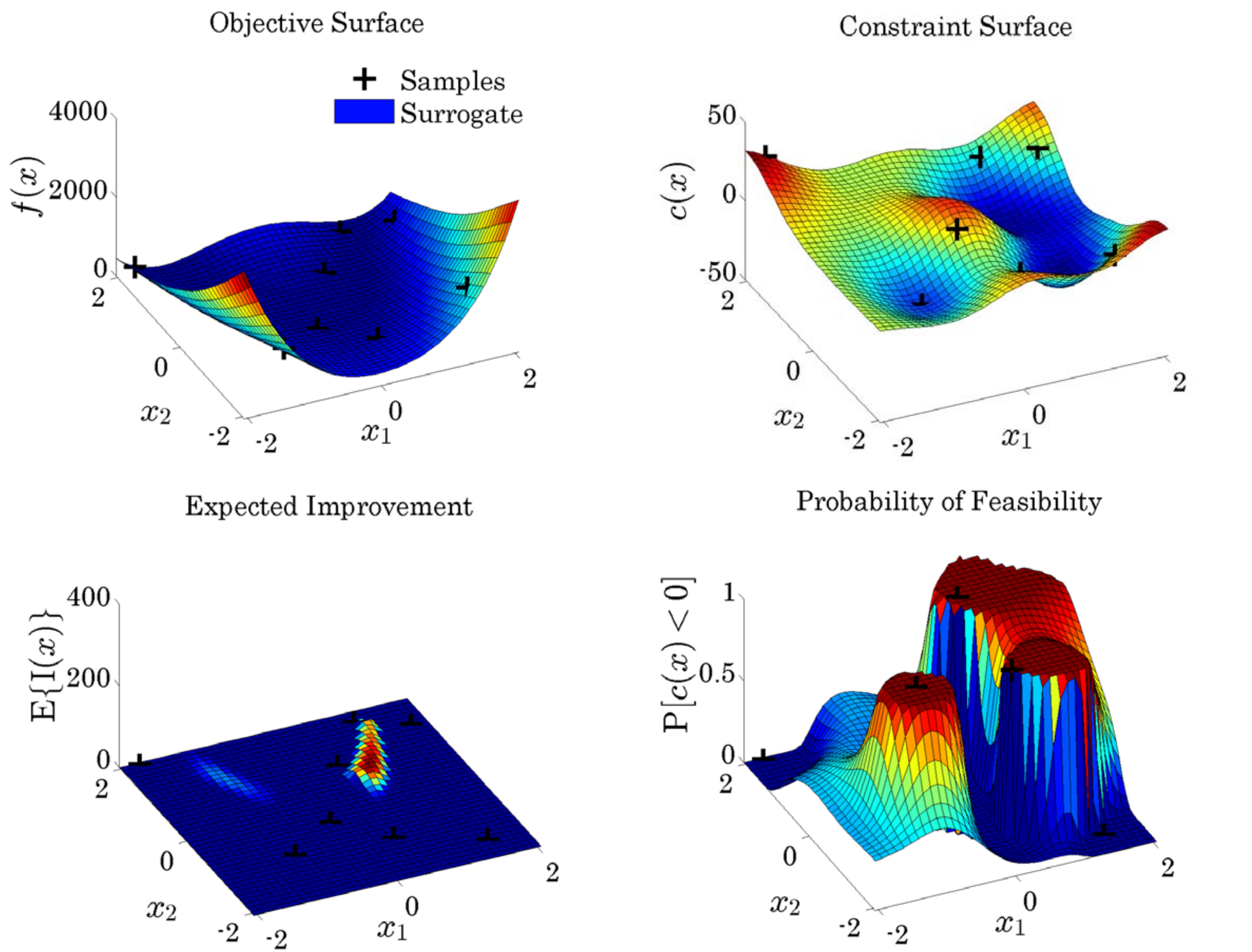
-2
x_2
-2
0
2
x_1
Constraint Surface
50
0
-50
$c(x)$
2
0
-2
x_2
-2
0
2
x_1
Expected Improvement
400
200
0
$\mathrm{E}\{\mathrm{I}(x)\}$
2
0
-2
x_2
-2
0
2
x_1
Probability of Feasibility
1
0.5
0
$\mathrm{P}[c(x) < 0]$
2
0
-2
x_2
-2
0
2
x_1

N_Samples = 7



Objective Surface
Samples
Surrogate
4000
2000
0
$f(x)$
2
0
x_2
-2
-2
x_1
0
2
Constraint Surface
50
0
-50
$c(x)$
2
0
x_2
-2
-2
x_1
0
2
Expected Improvement
400
200
0
$\mathrm{E}\{\mathrm{I}(x)\}$
2
0
x_2
-2
-2
x_1
0
2
Probability of Feasibility
1
0.5
0
$\mathrm{P}[c(x) < 0]$
2
0
x_2
-2
-2
x_1
0
2

N_Samples = 8


Objective Surface
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$f(x)$
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$c(x)$
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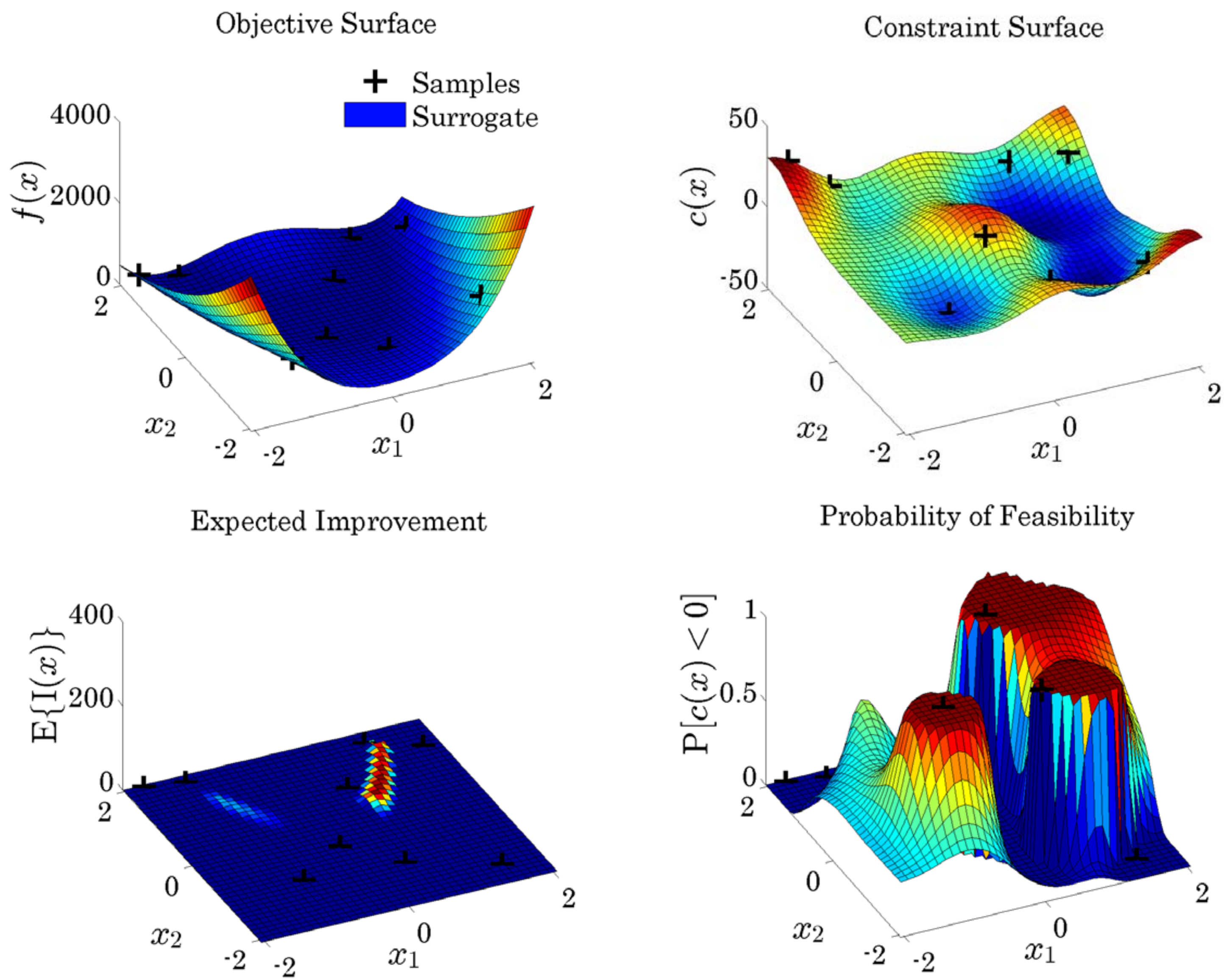
x_2
-2
-2
0
x_1
2
Expected Improvement
400
200
0
$\mathrm{E}\{\mathrm{I}(x)\}$
2
0
x_2
-2
-2
0
x_1
2
Probability of Feasibility
1
0.5
0
$\mathrm{P}[c(x) < 0]$
2
0
x_2
-2
-2
0
x_1
2

N_Samples = 9



Objective Surface
Samples
Surrogate
4000
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0
f(x)
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x2
-2
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Expected Improvement
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E{I(x)}
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-2
x2
-2
0
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x1
Probability of Feasibility
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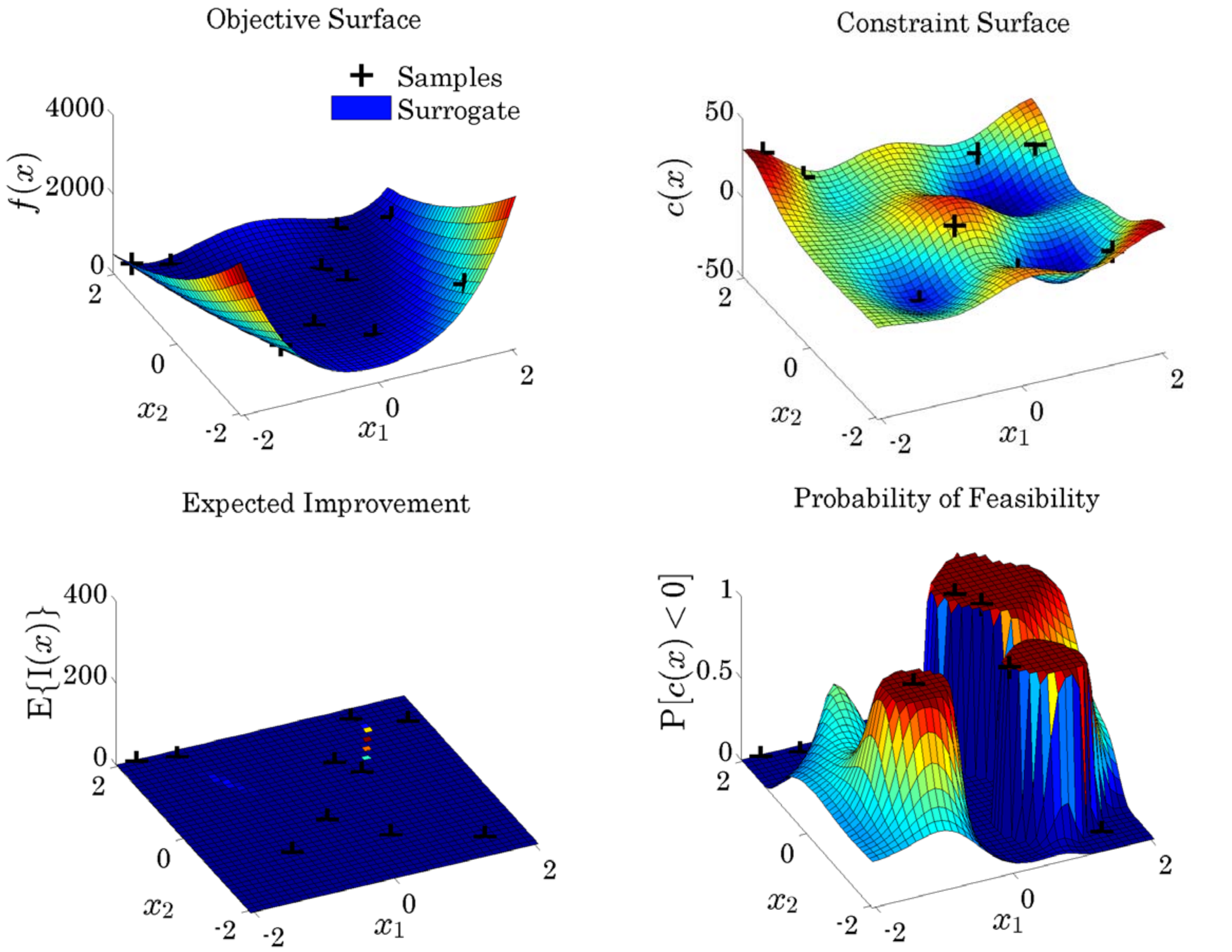
0.5
0
P[c(x) < 0]
2
0
-2
x2
-2
0
2
x1

N_Samples = 10


Objective Surface
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$f(x)$
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x_1
Expected Improvement
$\mathrm{E}\{\mathrm{I}(x)\}$
400
200
0
2
0
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x_2
-2
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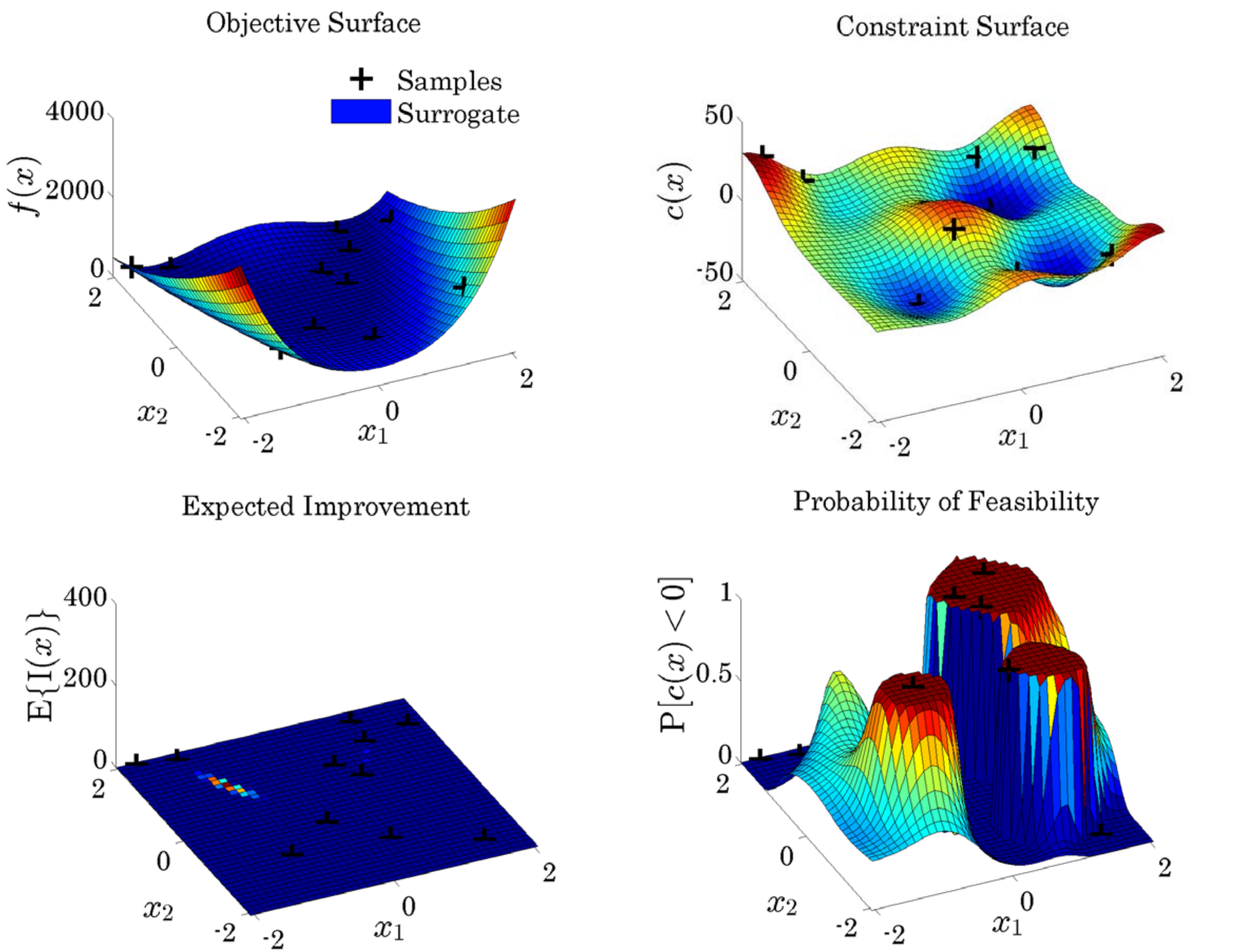
2
x_1
Probability of Feasibility
$\mathrm{P}[c(x) < 0]$
1
0.5
0
2
0
-2
x_2
-2
0
2
x_1

N_Samples = 11


Objective Surface
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x_2
x_1
Expected Improvement
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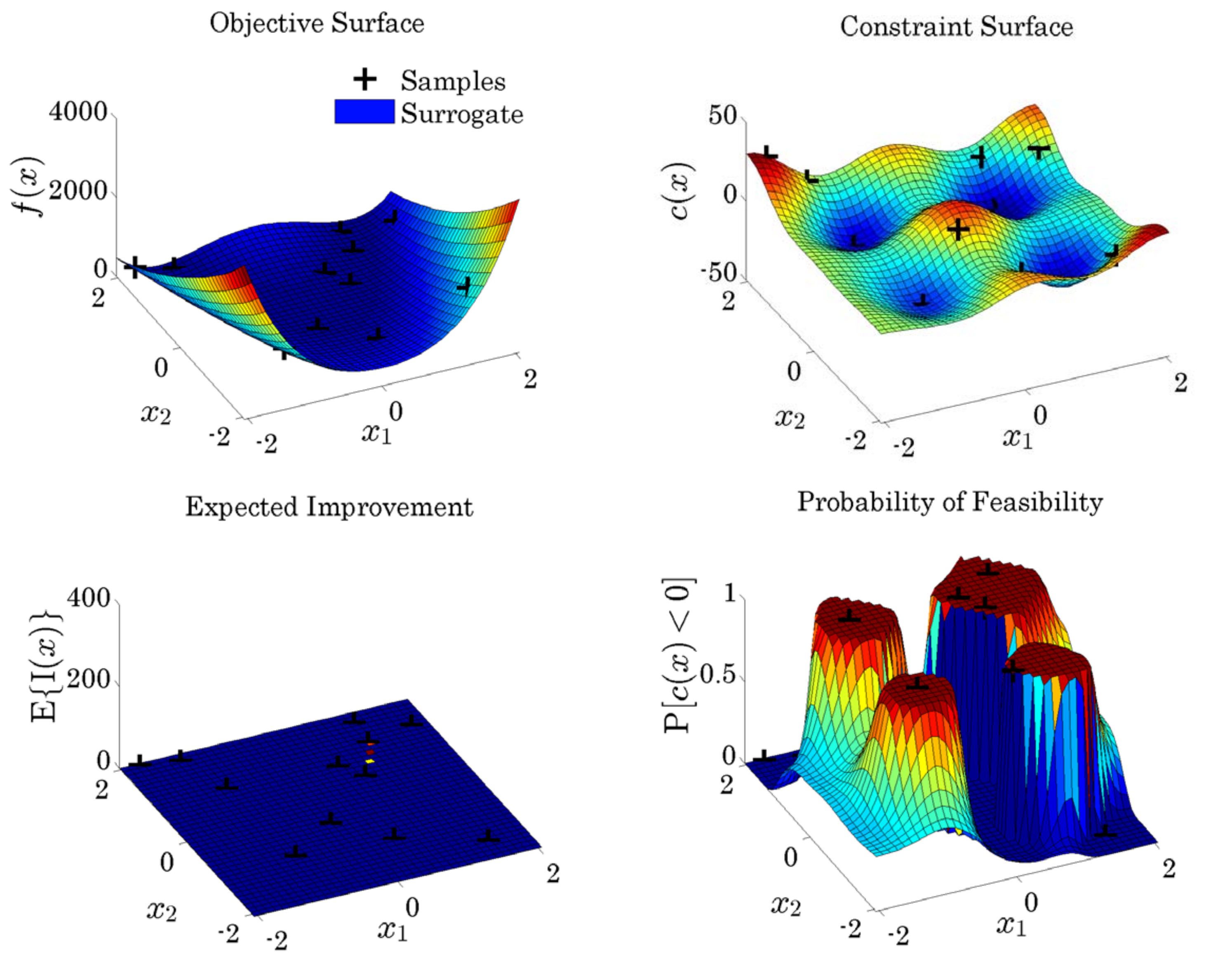
$\mathrm{E}\{\mathrm{I}(x)\}$
x_2
x_1
Probability of Feasibility
1
0.5
0
$\mathrm{P}[c(x) < 0]$
x_2
x_1

N_Samples = 12



Objective Surface
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$f(x)$
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x_2
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x_2
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-2
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x_1
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Expected Improvement
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$E\{I(x)\}$
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x_2
-2
-2
0
x_1
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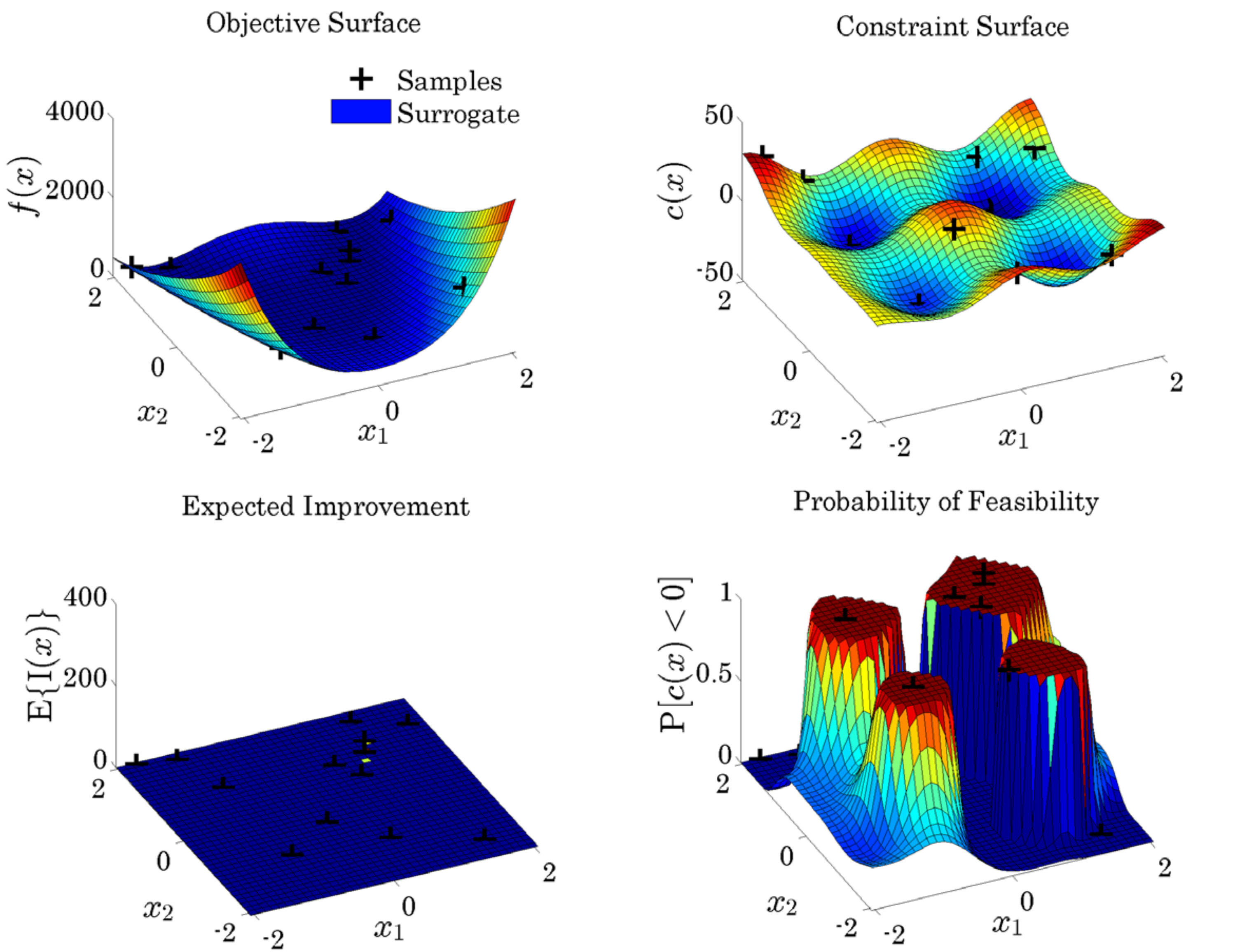
Probability of Feasibility
1
0.5
0
$P[c(x) < 0]$
2
0
x_2
-2
-2
0
x_1
2

N_Samples = 13



Objective Surface
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Surrogate
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$f(x)$
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E{I(x)}
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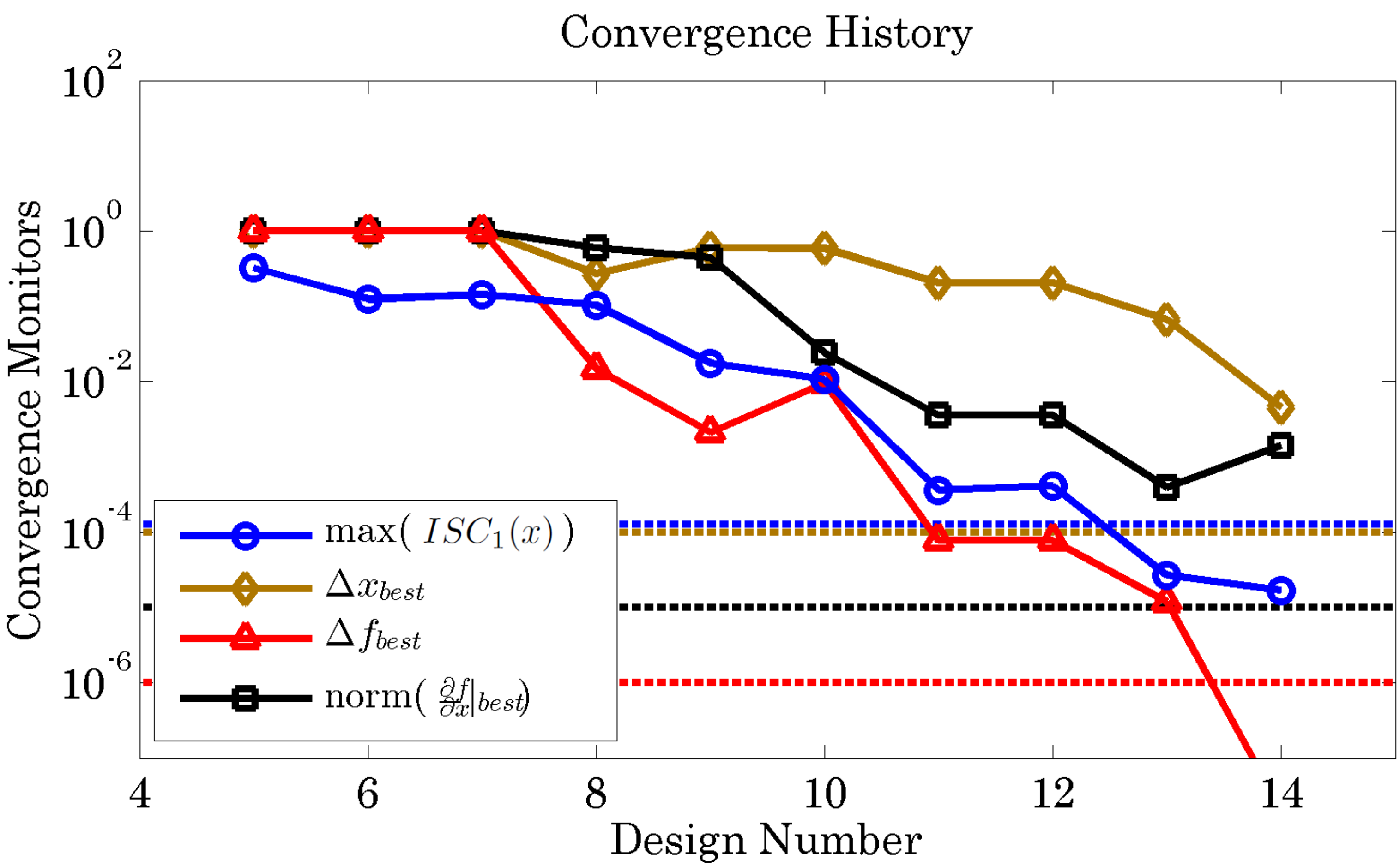
x_1



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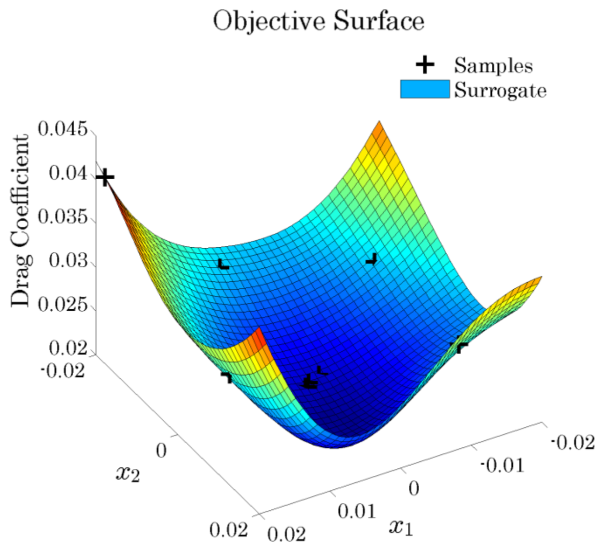
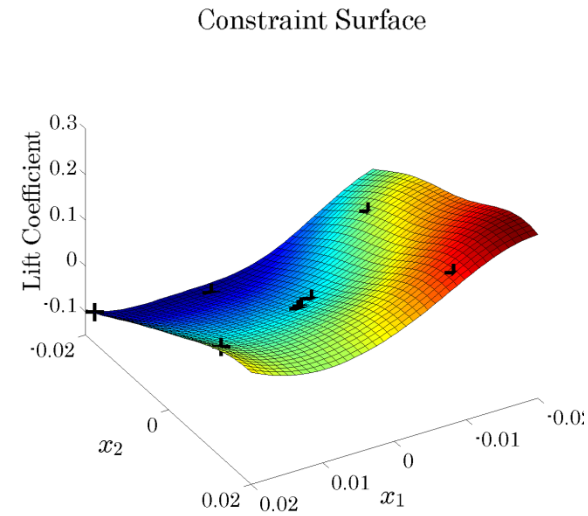
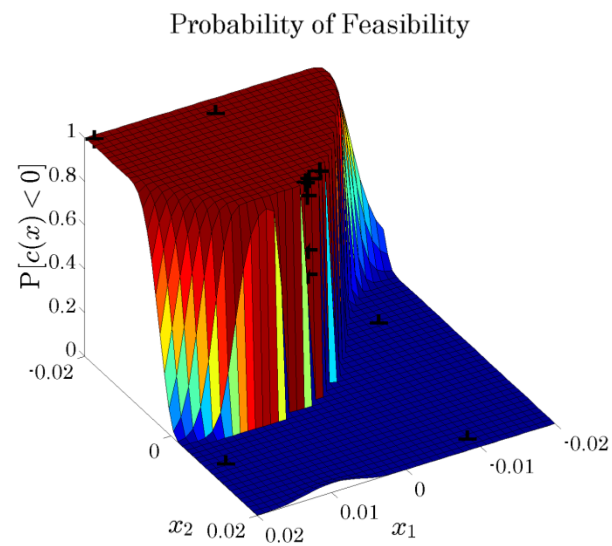
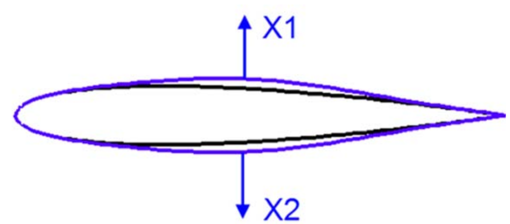
NACA 0012 Example









2 Hicks-Hinne bump functions

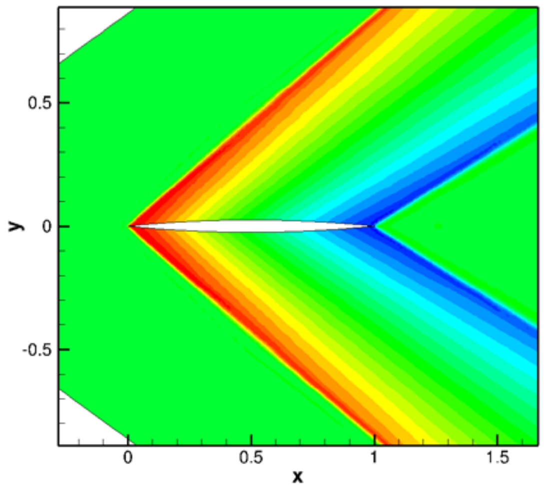
Minimize drag

Maintain CL > 0.328

Ma 0.3, 1.25° AoA

Parabolic Airfoil Example

- 5% Thick parabolic airfoil
- 10 Hicks-Hinne bump functions
- Minimize drag
- Maintain equivalent area
  - Allowed 5% constraint violation
  - Sampled 2 chord-lengths below
- Ma 1.7, 0° AoA



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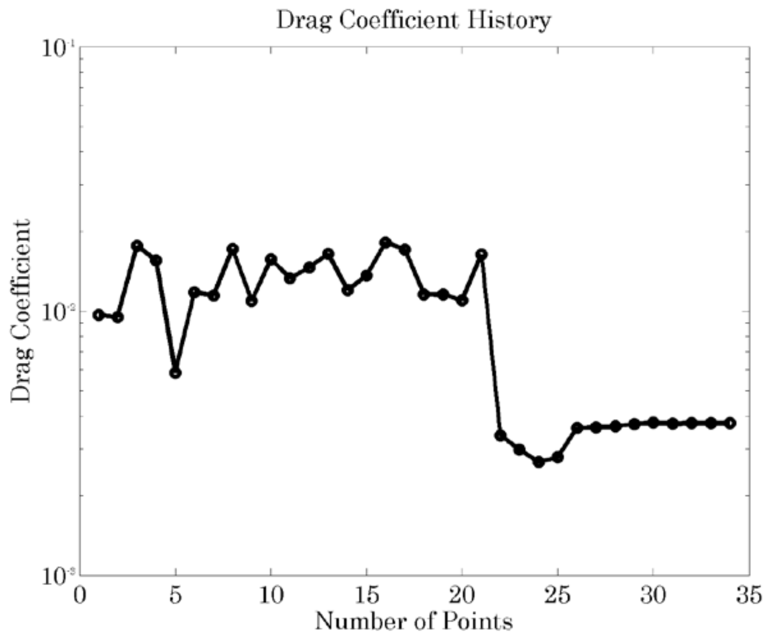
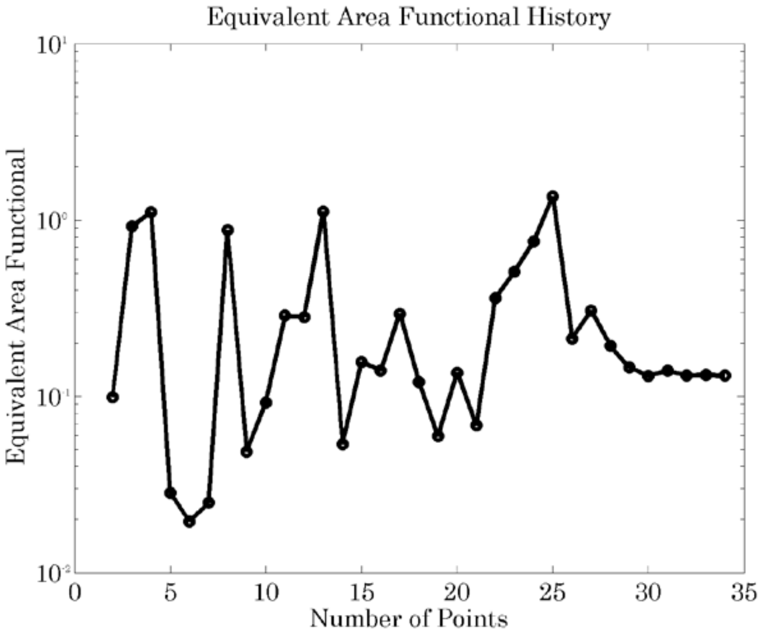
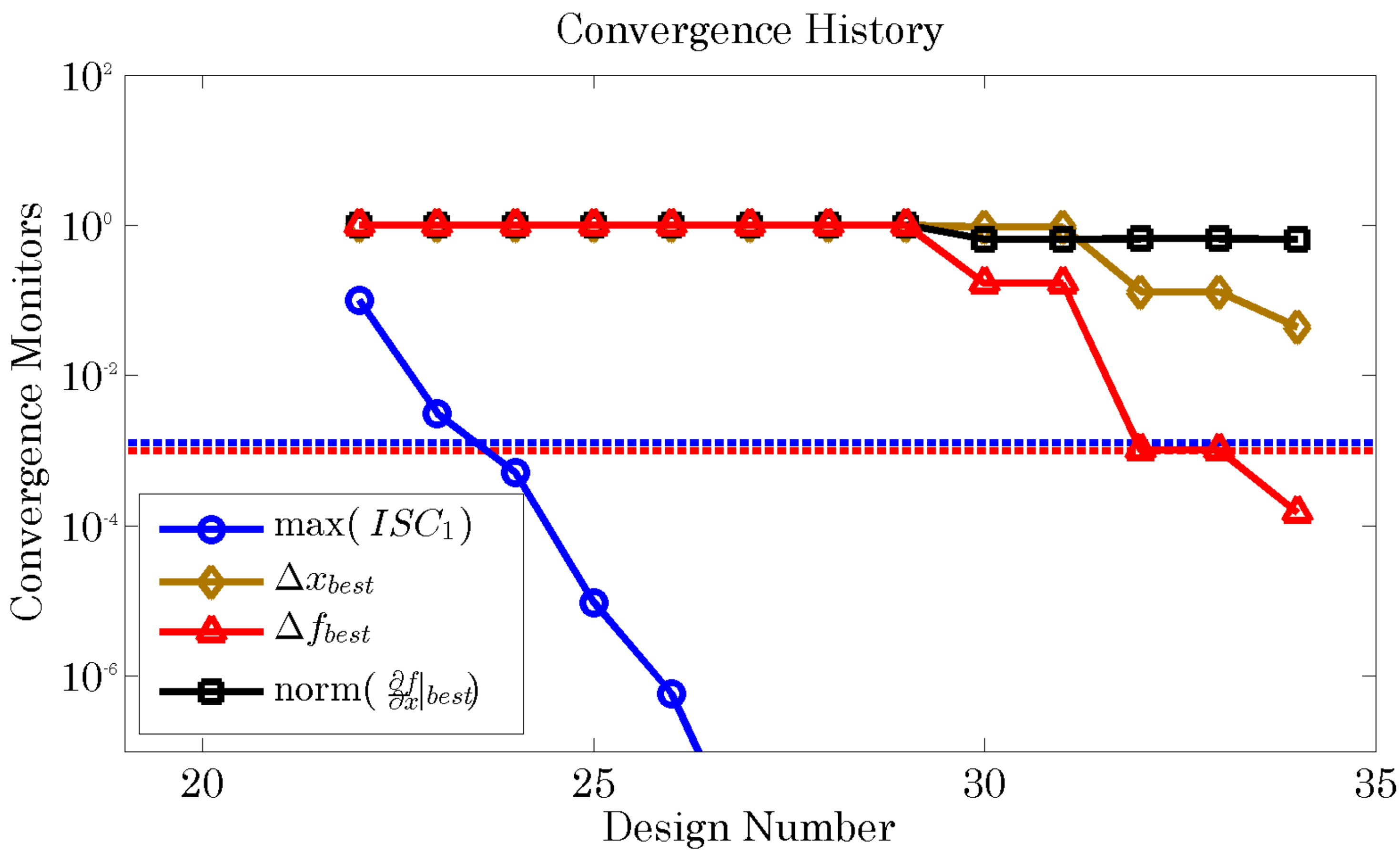
Parabolic Airfoil Example





Parabolic Airfoil Example



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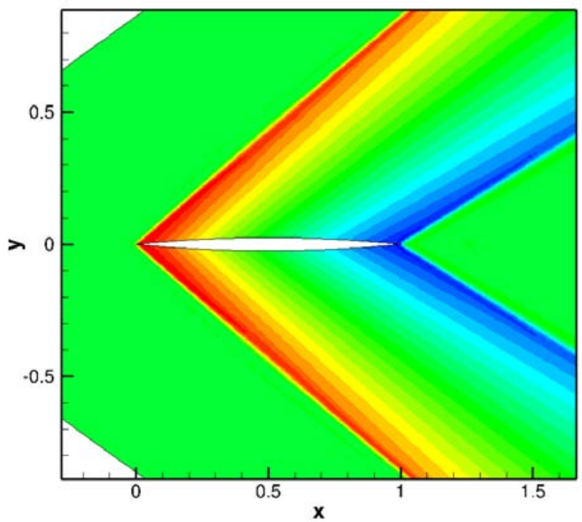
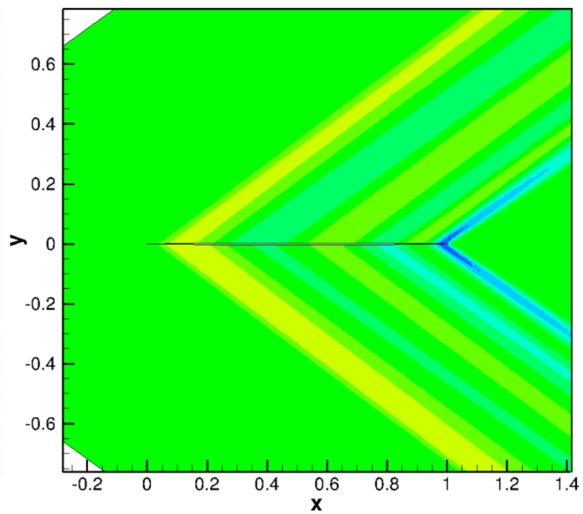
Parabolic Airfoil Example

Baseline



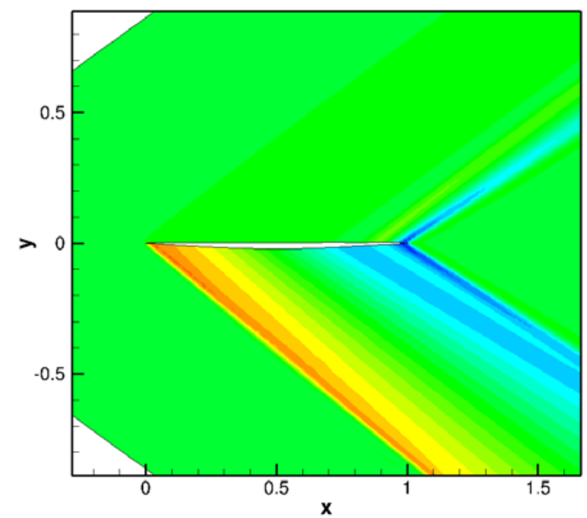
Cd = 0.00965

Unconstrained

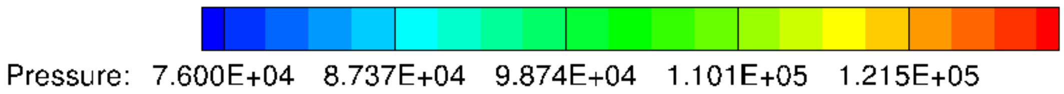


Cd = 0.00029

Constrained



Cd = 0.00376



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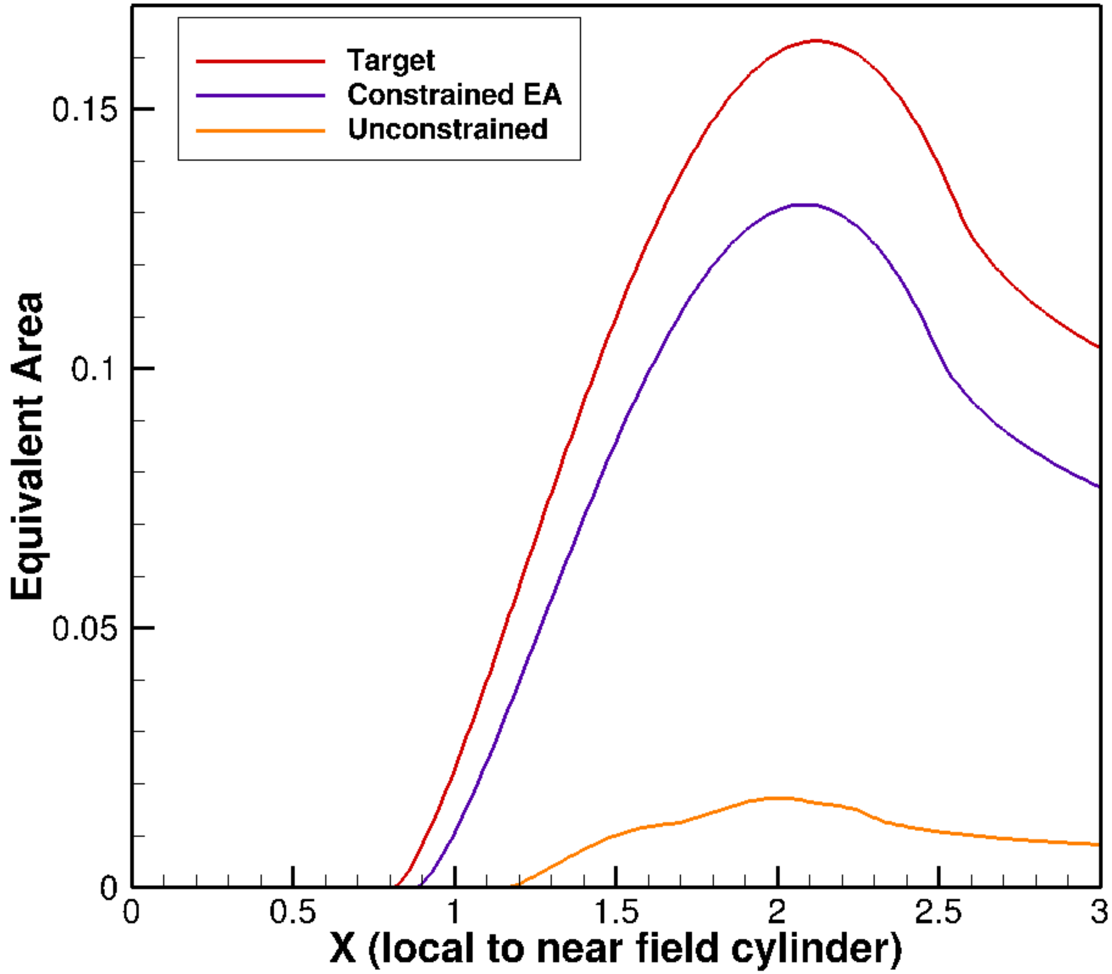
Parabolic Airfoil Example



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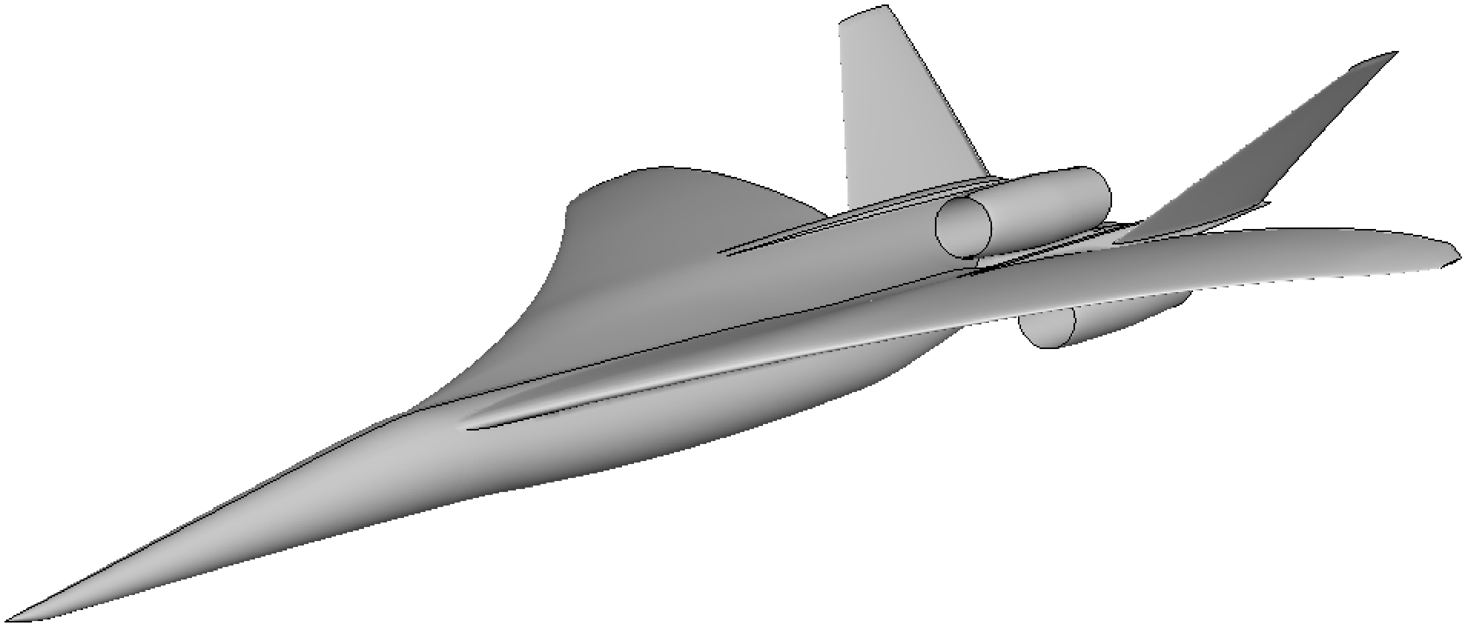
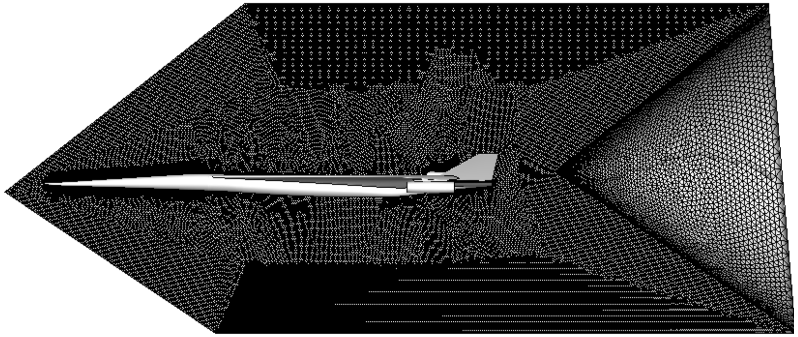
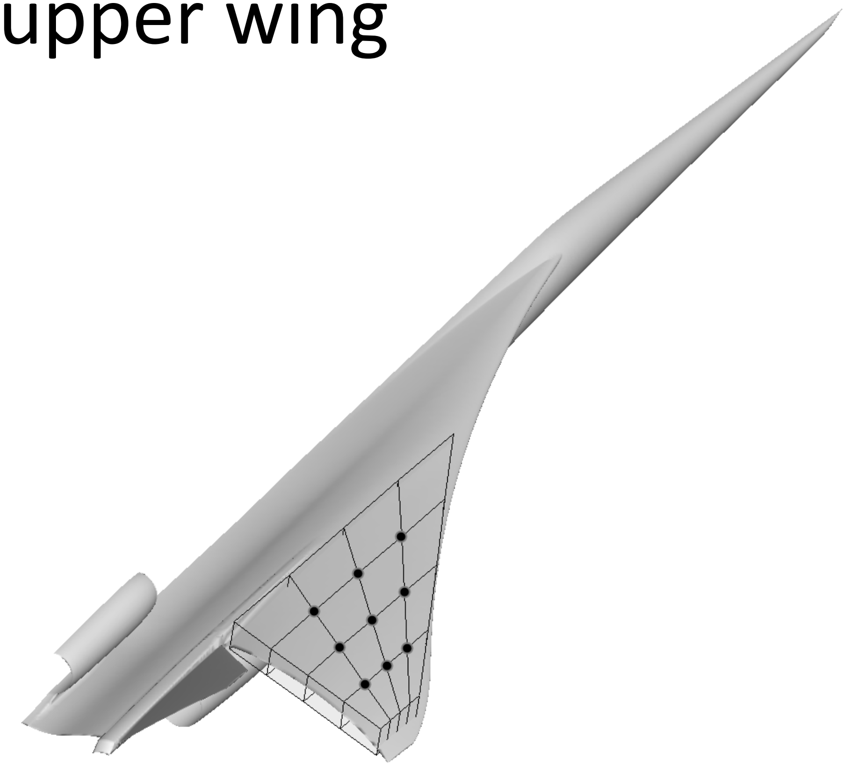
N+2 Geometry



N+2 Drag Example

- 1.3 million node drag mesh
- 9 FFD contol points on upper wing
- Ma 1.7, 2.1° AoA





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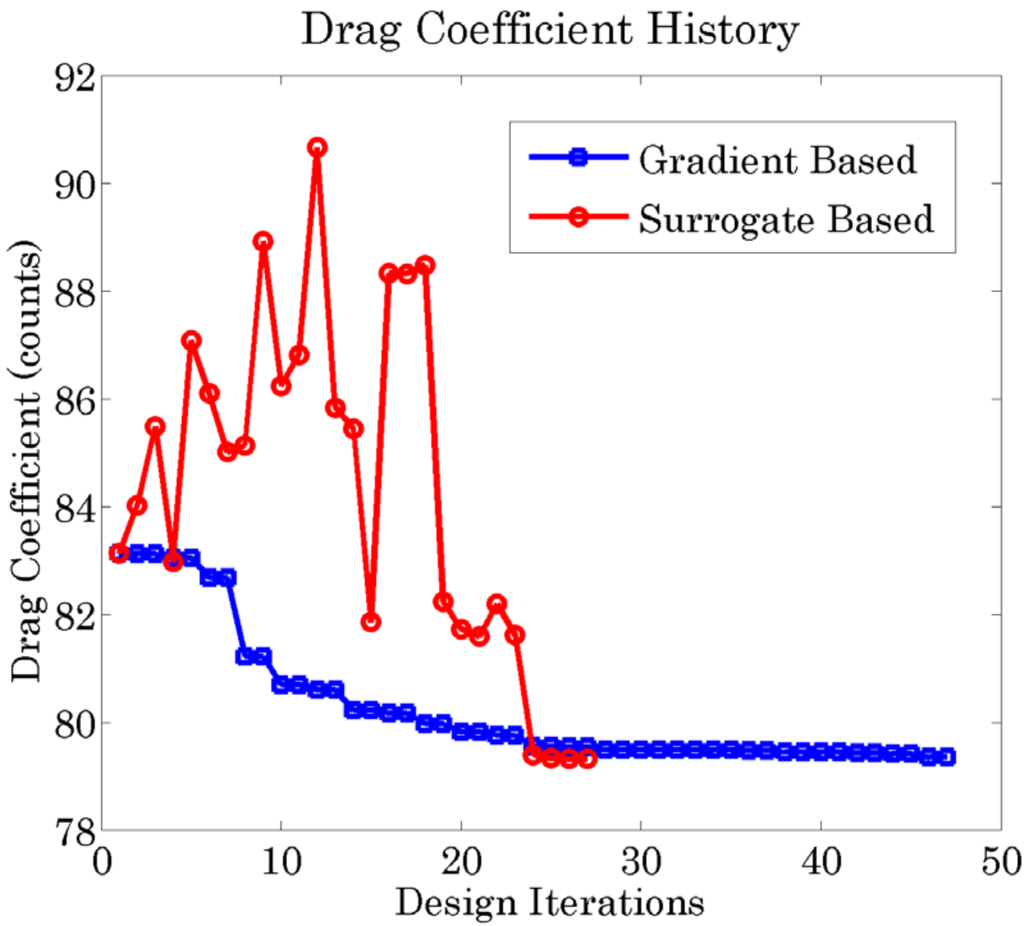
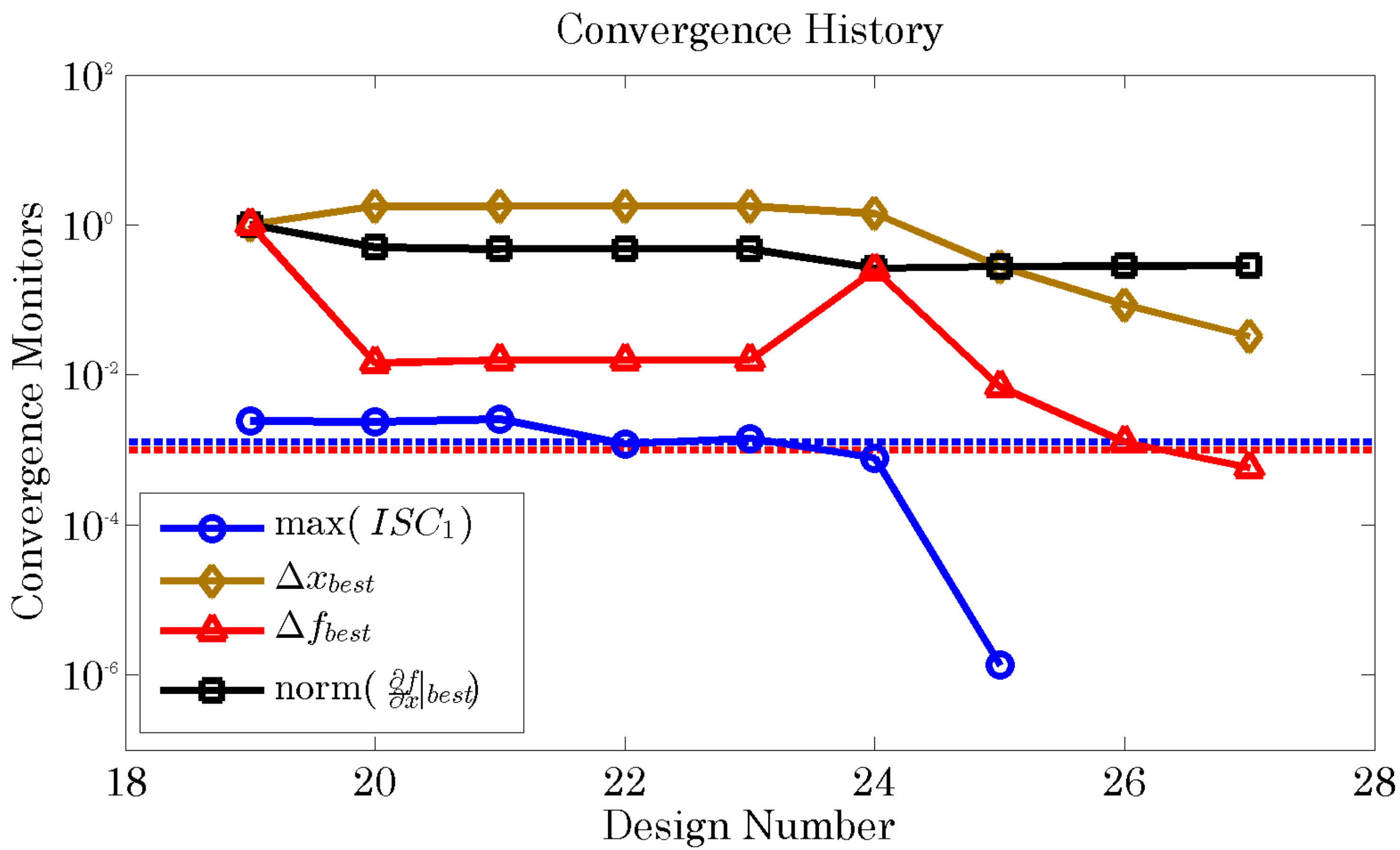
N+2 Drag Example



Method	Improvement	Iterations
SBO	4.59%	27
GBO	4.55%	47

N+2 Drag Example



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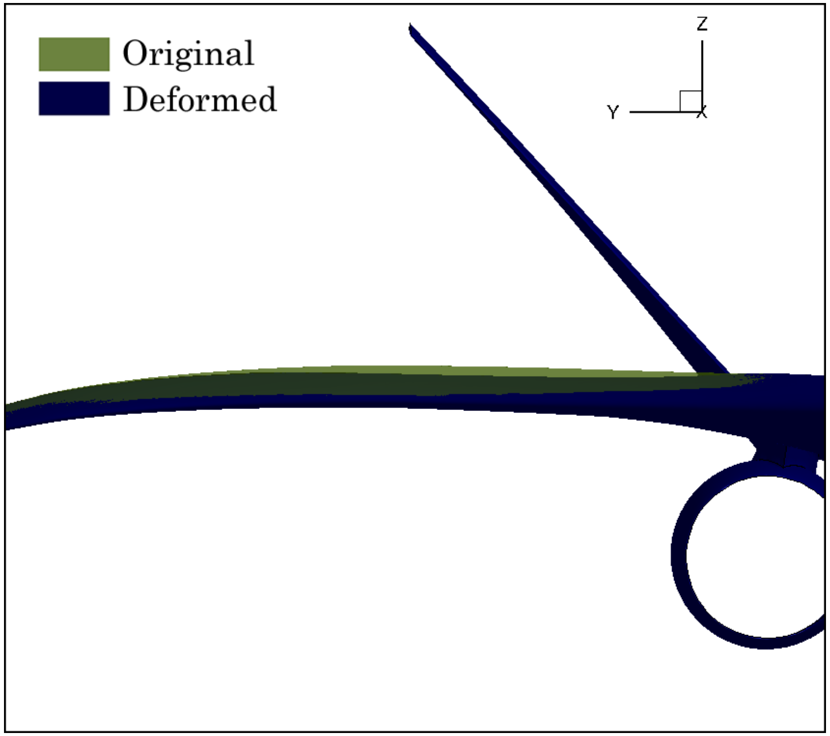
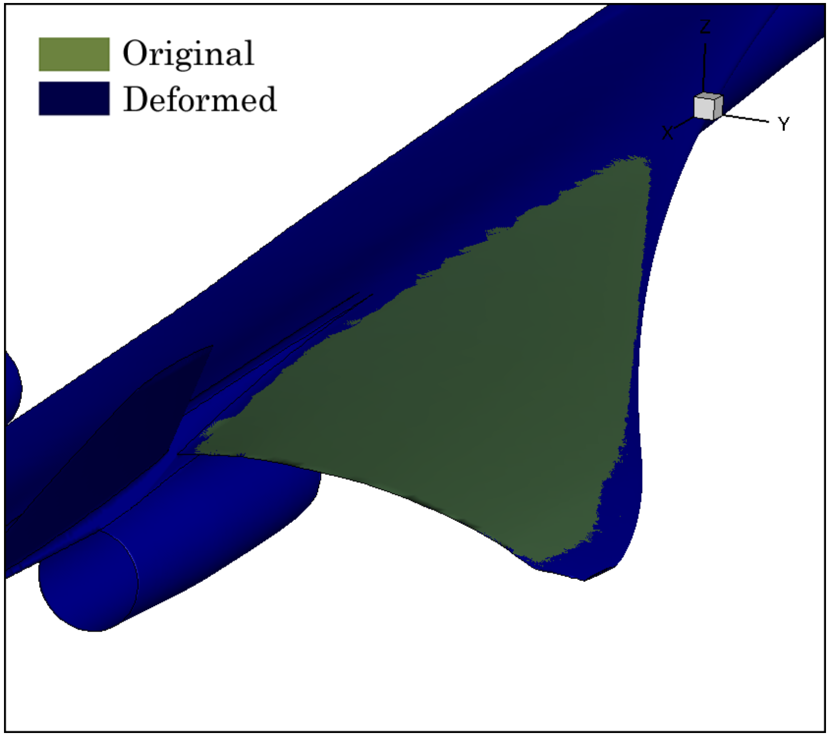
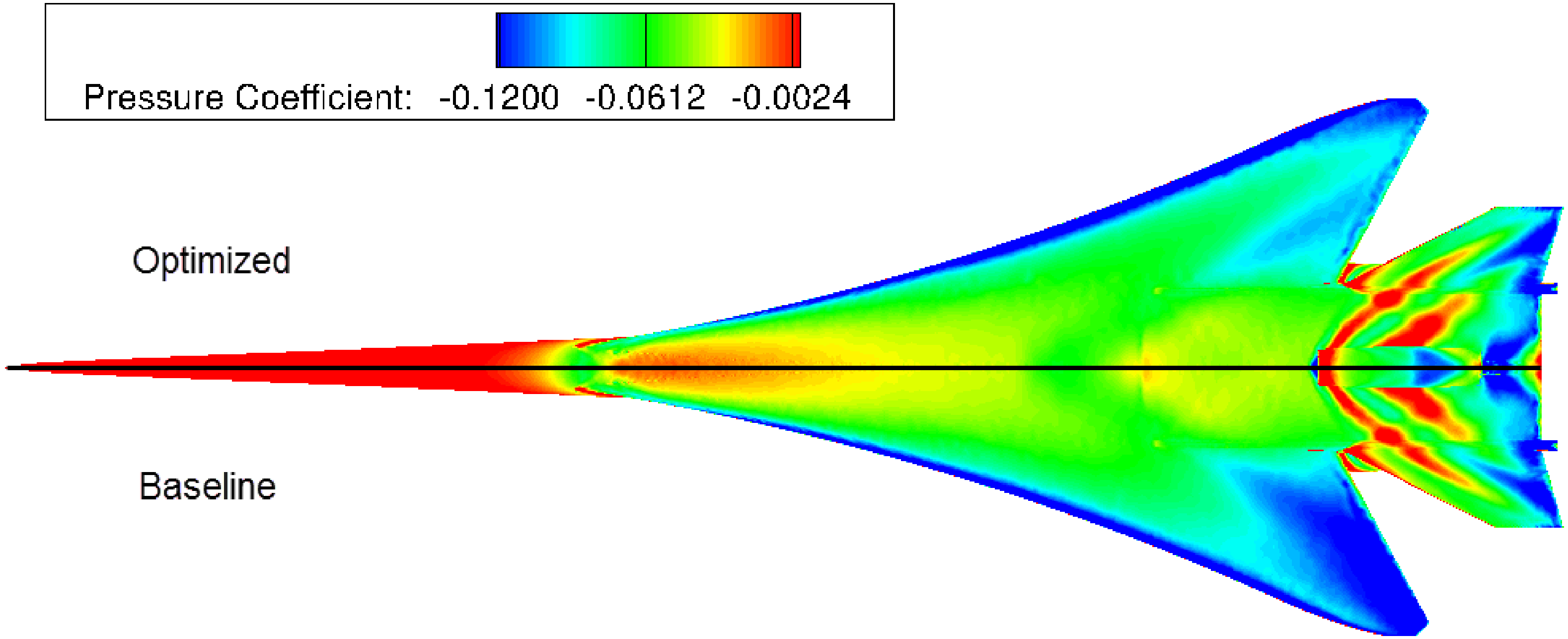
N+2 Drag Example





N+2 Drag Example



Our Approach to SBO

- Optimize one objective with constraints
- Two Adaptive Refinement Criteria
  1. Modified expected improvement
  2. Estimated optimum
- Computational Cost
  - Scale data and assume isotropic variation
  - Condense hyperparameter space to four variables
- Numerical Stability
  - Constrain noise hyperparameters to maintain a minimum amount of noise

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Questions?

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Managing Gradient Inaccuracies

while Enhancing Optimal Shape Design Methods

Trent Lukaczyk, Francisco Palacios, Juan J. Alonso
Department of Aeronautics & Astronautics
Stanford University

51st AIAA Aerospace Sciences Meeting
Grapevine, TX
January 10, 2013

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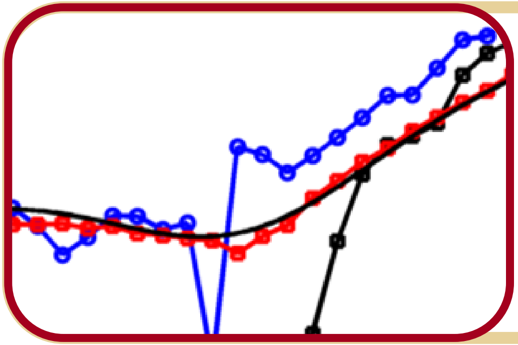
Motivation

N+2 Supersonic Passenger Jet Concept

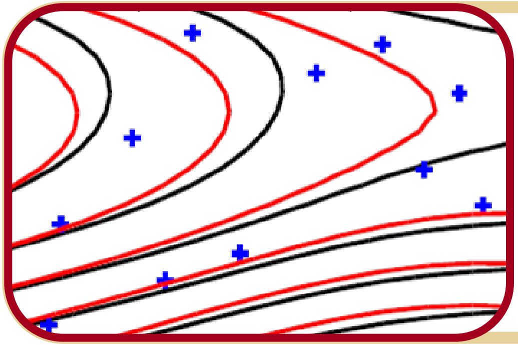
LOCKHEED MARTIN

NASA

Outline



Gradient Accuracy Evaluation

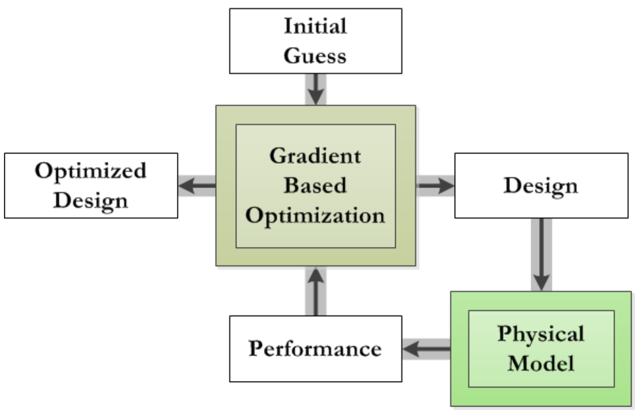


Noise-Tolerant Response Surfaces

BACKGROUND

Optimization Approaches

Gradient-Based Optimization (GBO)



Lambe and Martins, 2012.

SciPy SLSQP
Kraft, 1994

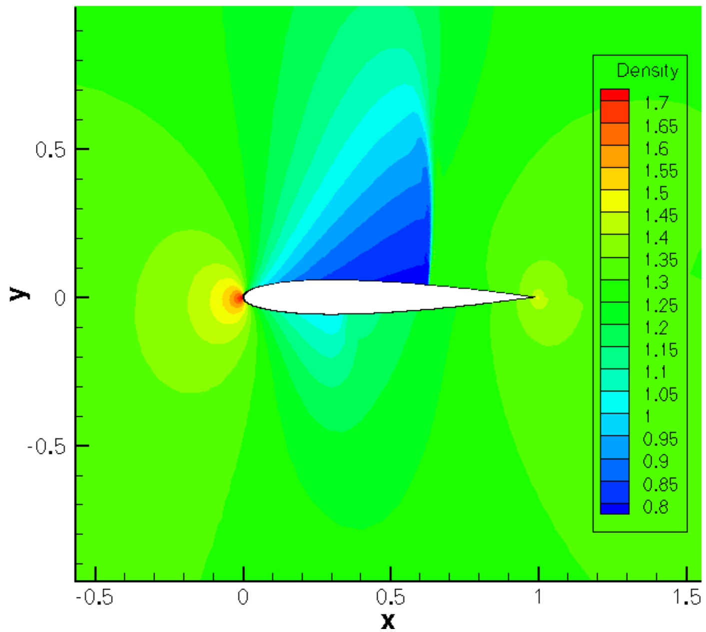
Surrogate-Based Optimization (SBO)

In-house geGPR
Lukaczyk, 2012

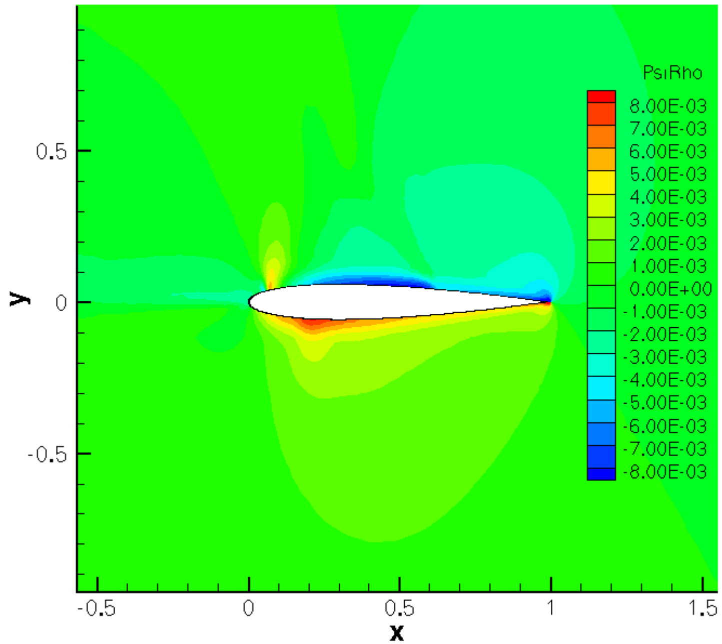
NACA 0012 Test Problem

- NACA 0012, Ma=0.8, AoA=1.25^{o}
- Euler second order
- Surface based continuous adjoint formulation
- Converged 10 orders of magnitude
- Hicks-Henne bump function design variables

Contours of Density



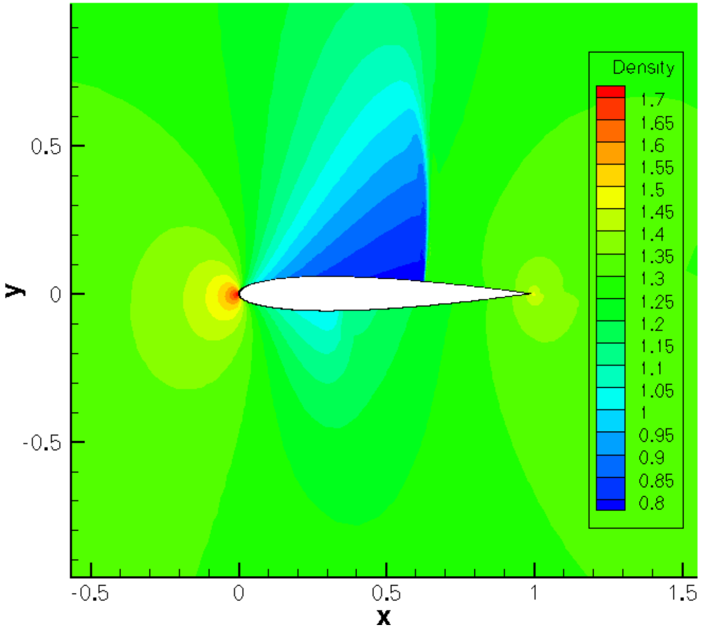
Contours of Drag Adjoint Density



NACA 0012 Test Problem

Minimize drag while maintaining a minimum lift and pitching moment

Contours of Density



$$\text{Min.} \quad C_D(x)$$
$$x \in R^n$$
$$\text{s.t.} \quad C_L(x) > 0.3282$$
$$C_{MZ}(x) > 0.0341$$

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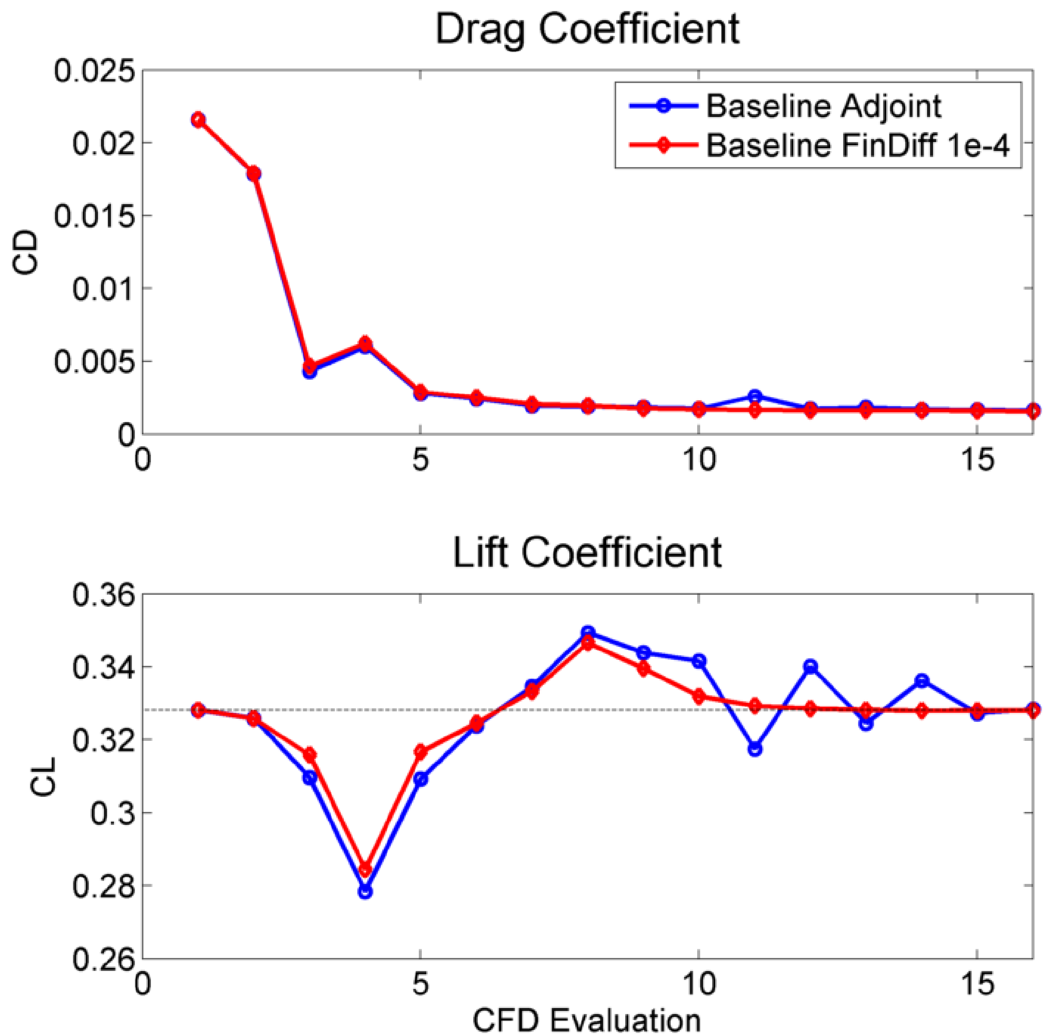
GBO Convergence Issues



- Baseline grid
- Adjoint and finite difference gradients
- 10 Hicks-Henne Bumps
- Plotting all CFD evaluations, including sub-iterations
- Performance set back loosely indicative of inaccurate update to Hessian

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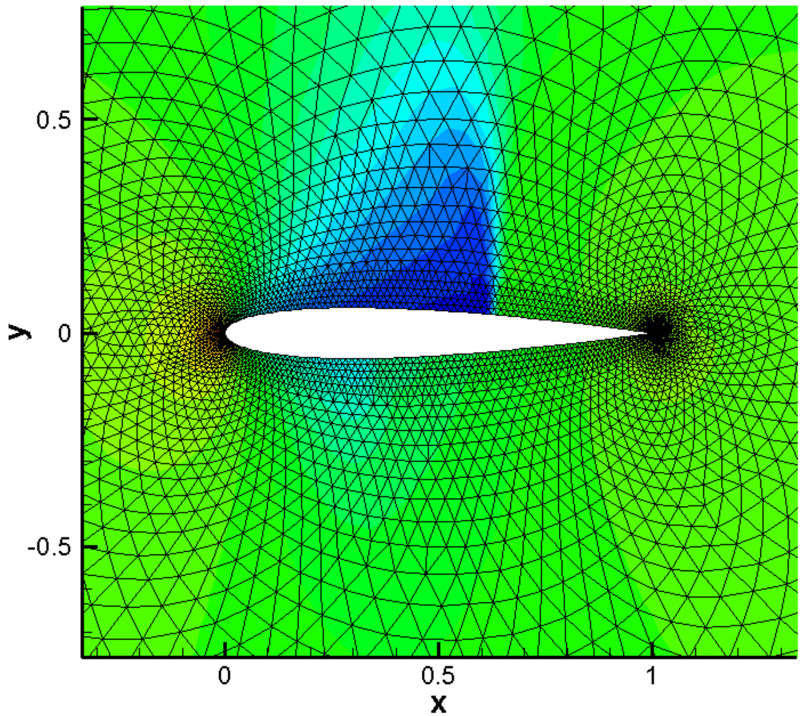
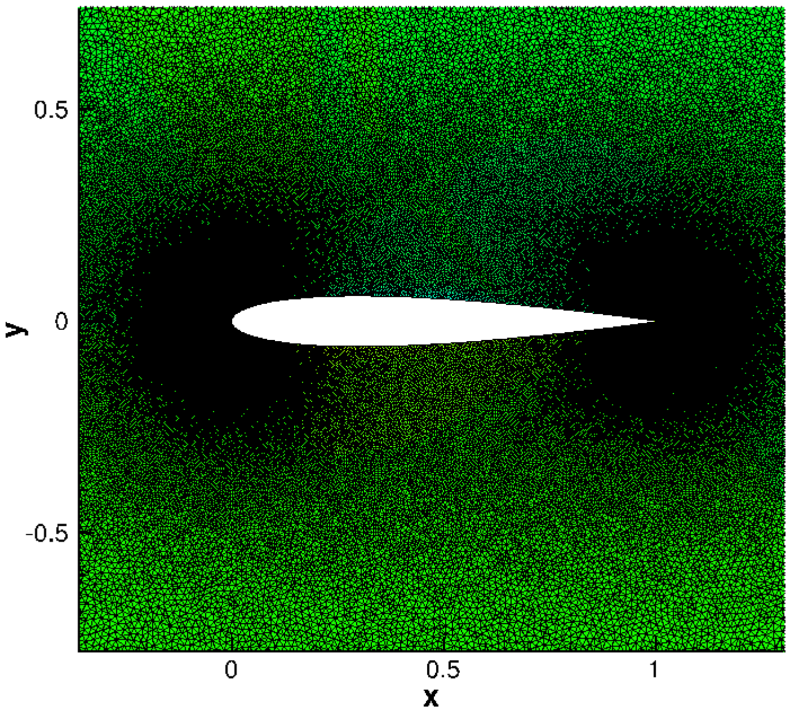
Mesh Adaptation

Coarse Baseline



10.2K Cells

Isotropically Refined



200.1K Cells

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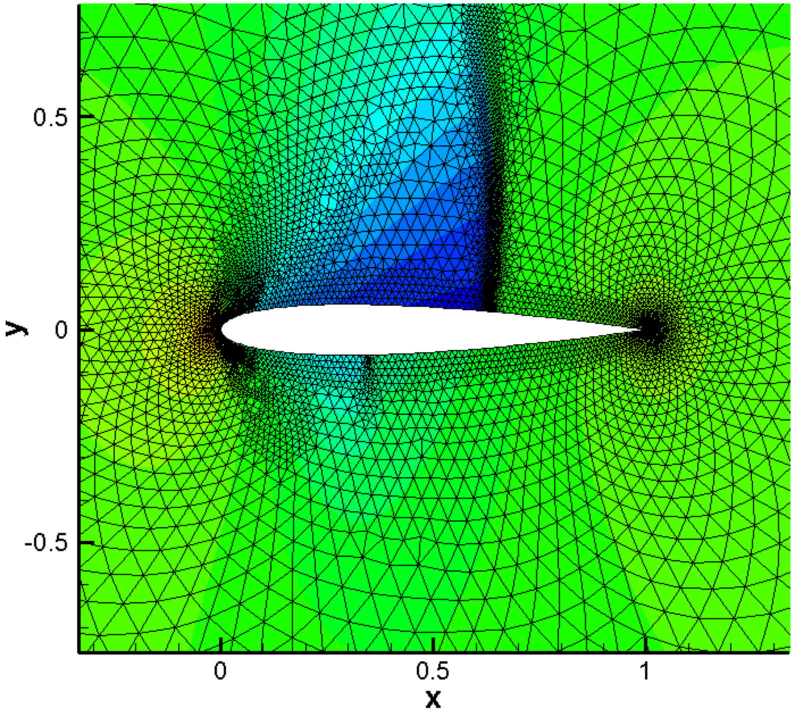
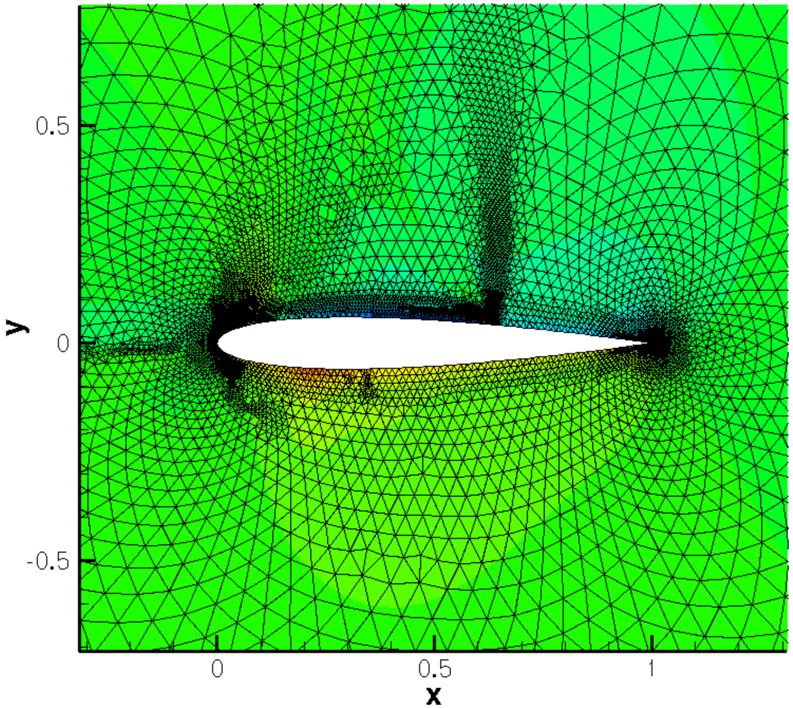
Mesh Adaptation

Direct Adapted



16.4K Cells

Adjoint Adapted



25.7K Cells

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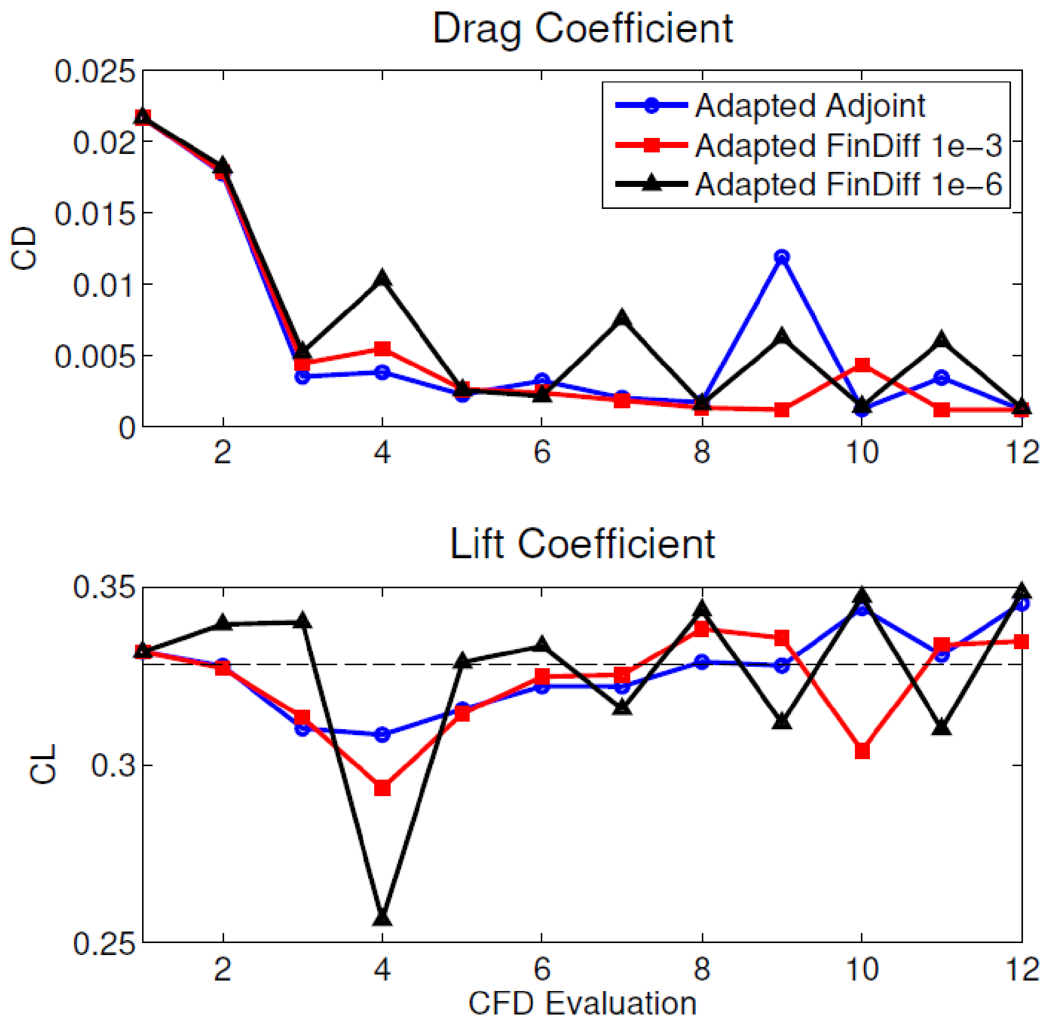
GBO Convergence Issues



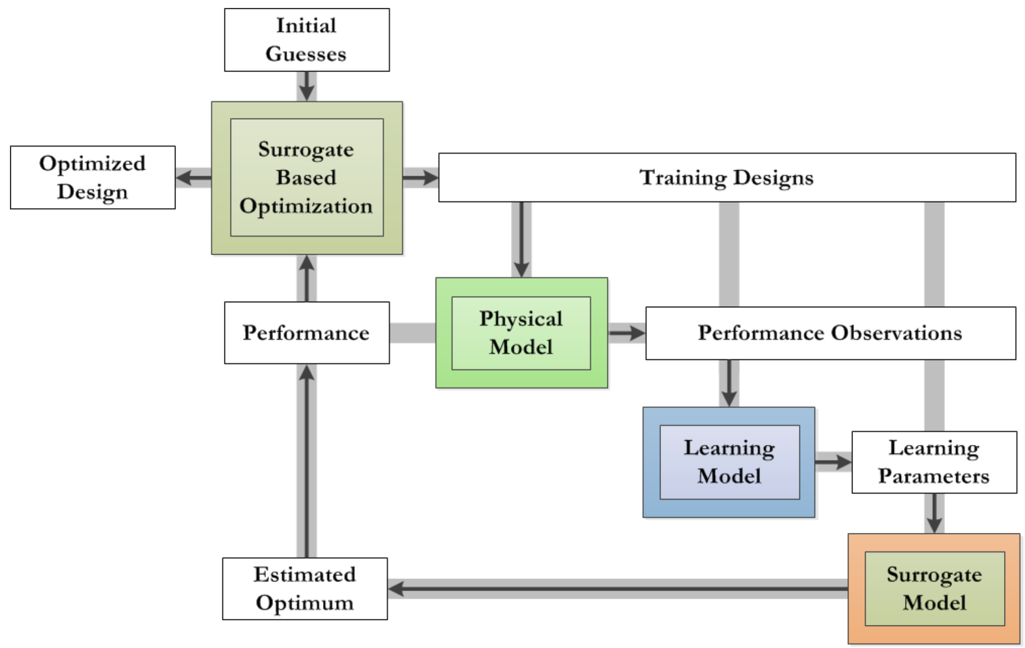
- Adaptation with different gradient approaches
- Adjoint suffers from poor sub-iterations near optimum
- Clear dependence of problem on finite difference step
- Larger step appears more robust to changes in discretization

Optimization Approaches

Gradient-Based Optimization (GBO)

Lambe and Martins, 2012.

Surrogate-Based Optimization (SBO)



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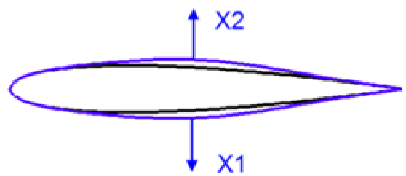
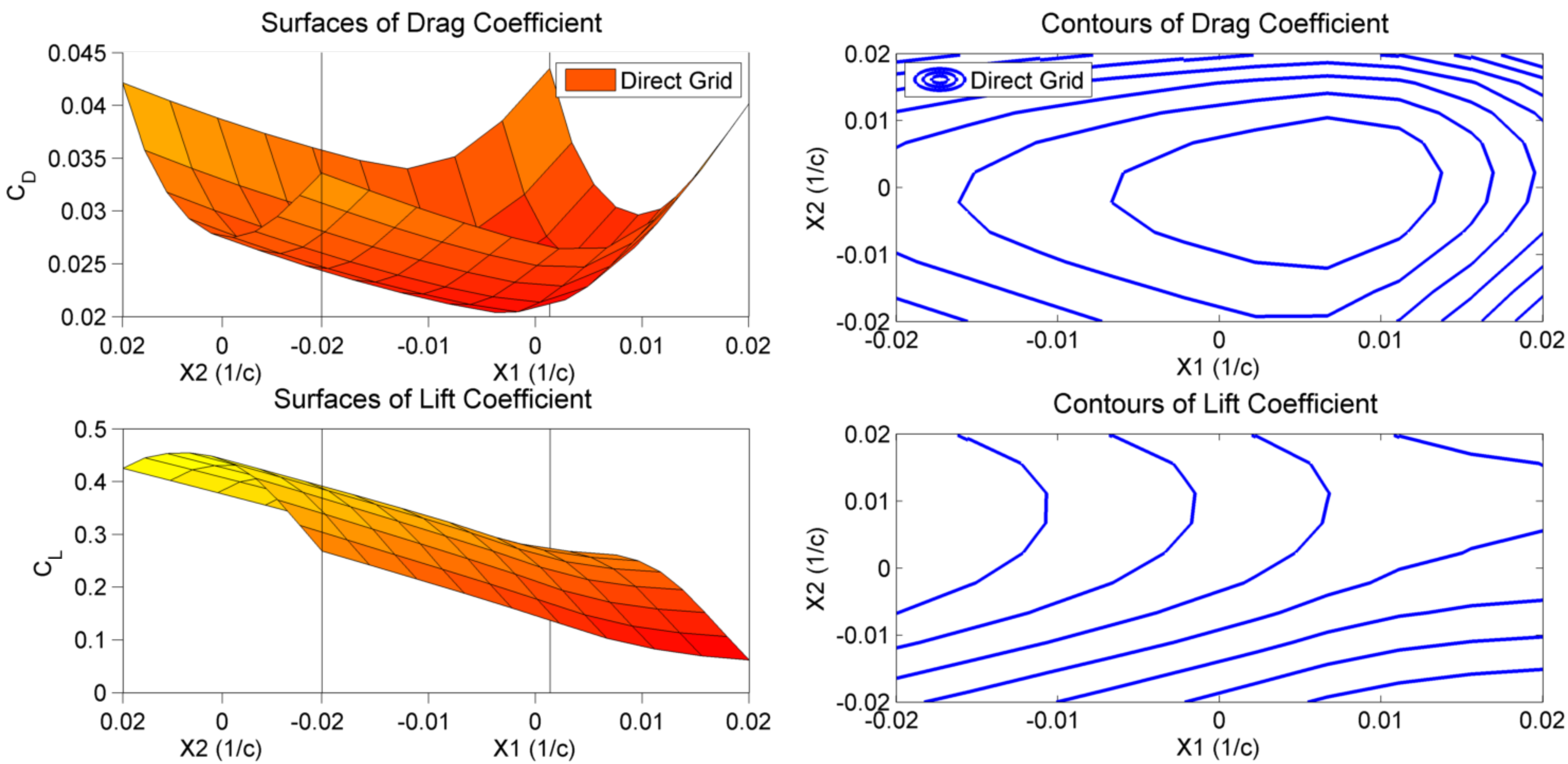
RSM Generation Issues

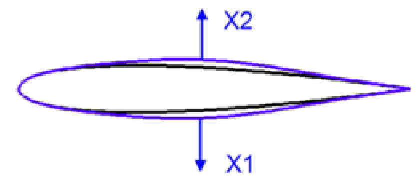
- RSM enhanced with Adjoint Gradients
- Two Hicks-Henne Bump Functions
- 10x10 grid of simulations

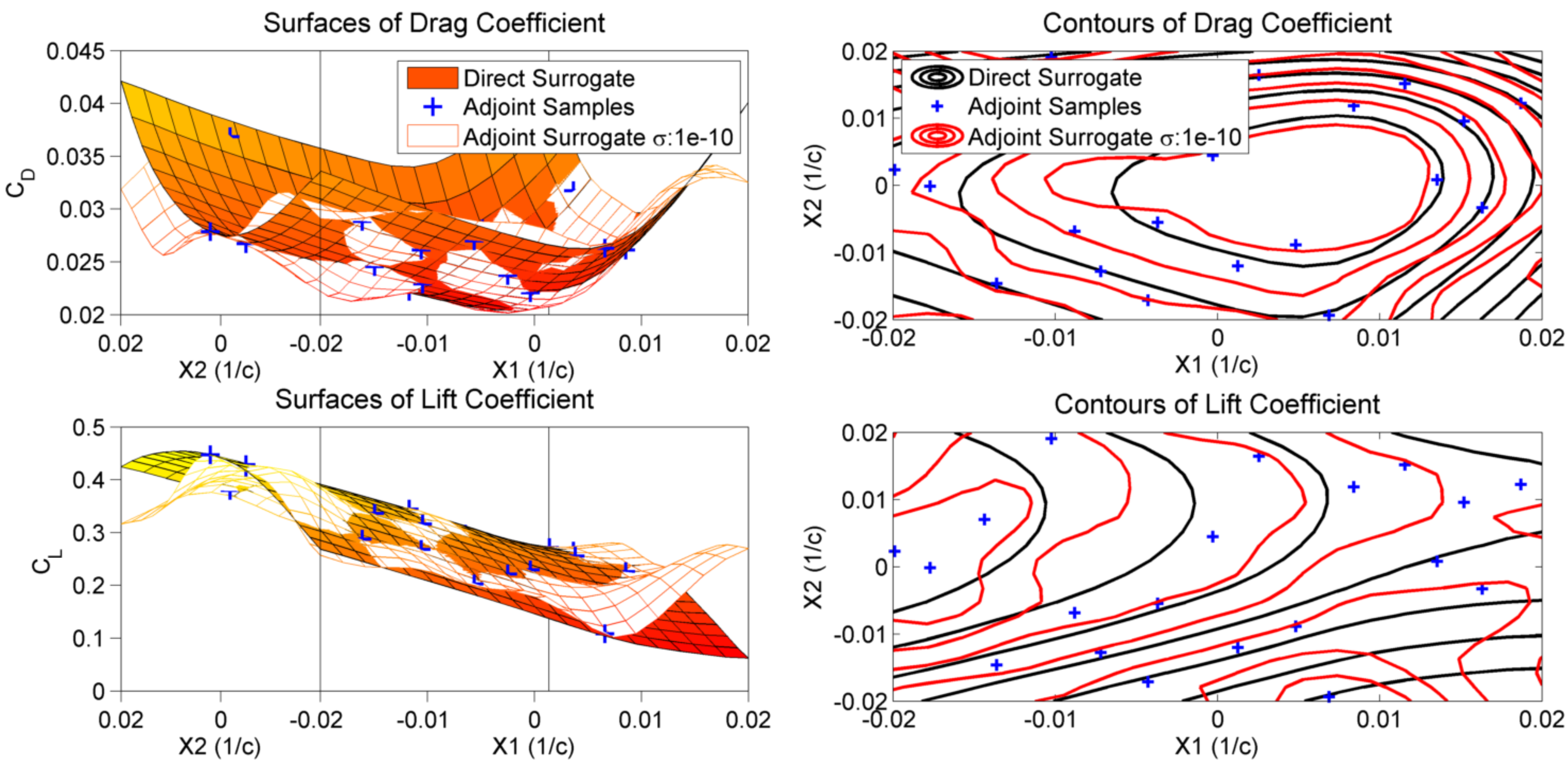




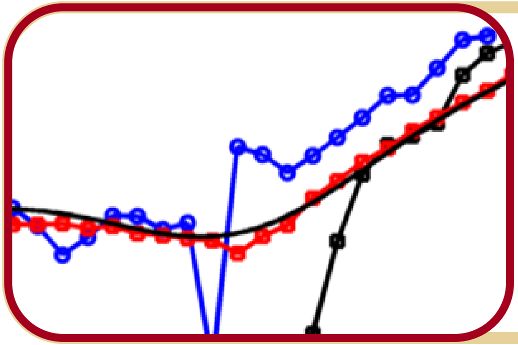
RSM Generation Issues

- RSM enhanced with Adjoint Gradients
- Two Hicks-Henne Bump Functions
- LHC sampled simulations

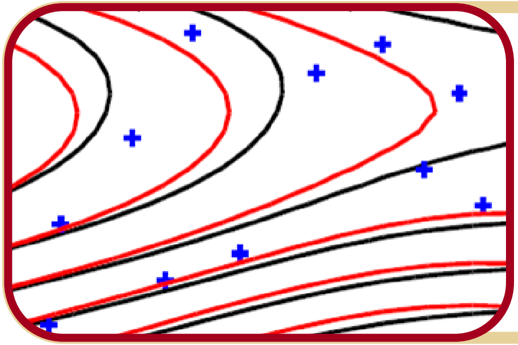




Outline

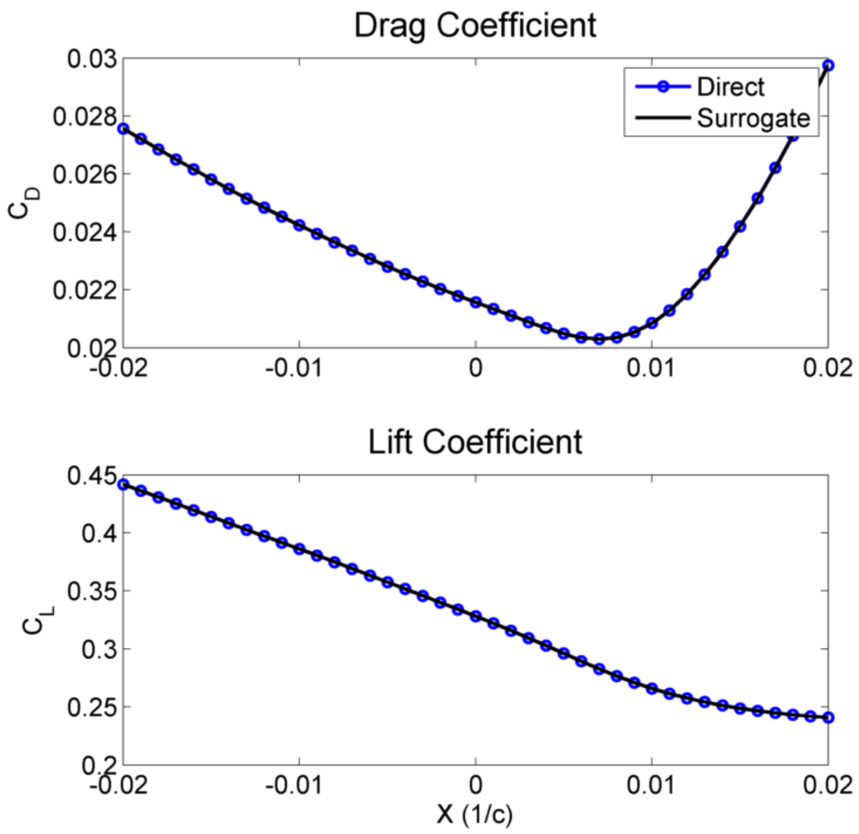


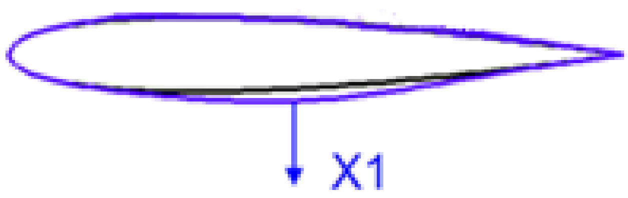
Gradient Accuracy Evaluation



Noise-Tolerant Response Surfaces

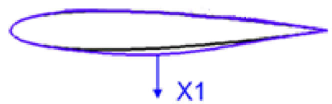
Reference Gradient



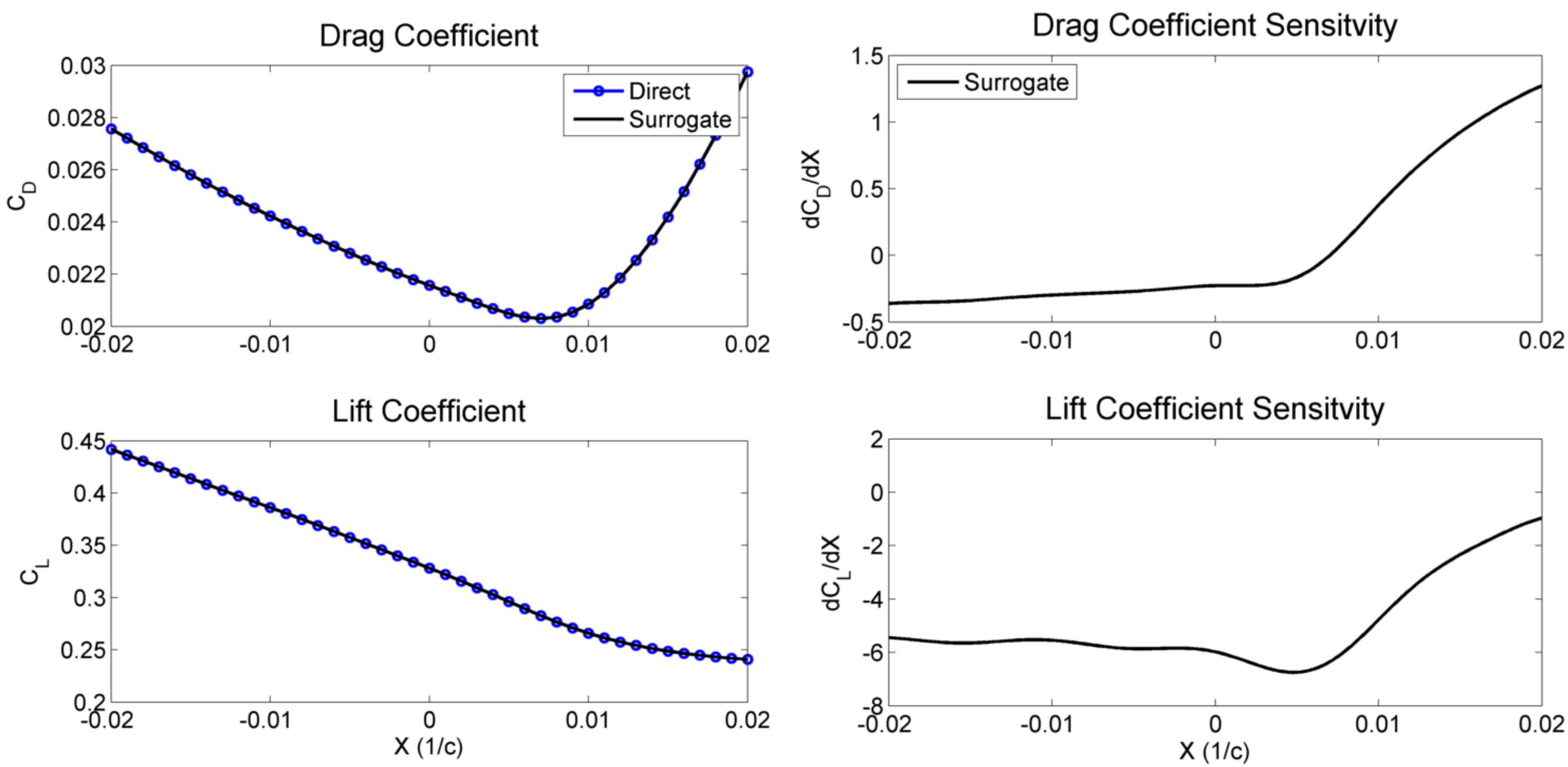


- NACA 0012 Test Case
- One Hicks-Henne Bump Function
- 41 Evaluations in X ϵ [-0.02 , 0.02]

Reference Gradient



(One Hicks-Henne Bump Function)



- RSM with only direct data used to estimate reference gradient

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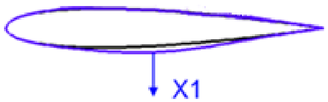
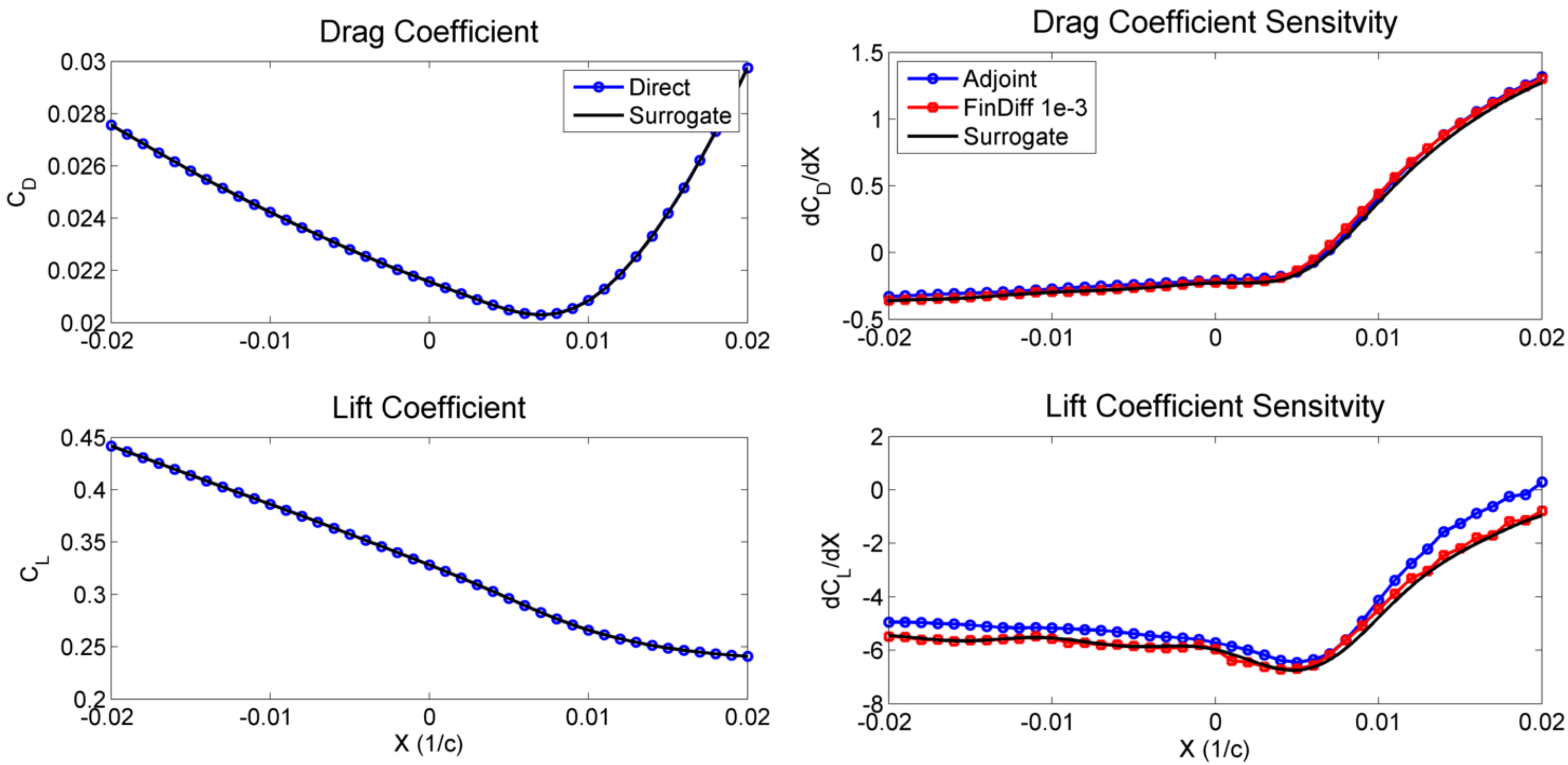
Baseline Mesh Gradients



(One Hicks-Henne Bump Function)



- Adjoint gradients show bias errors, Finite difference gradients show noise

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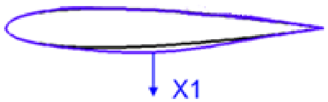
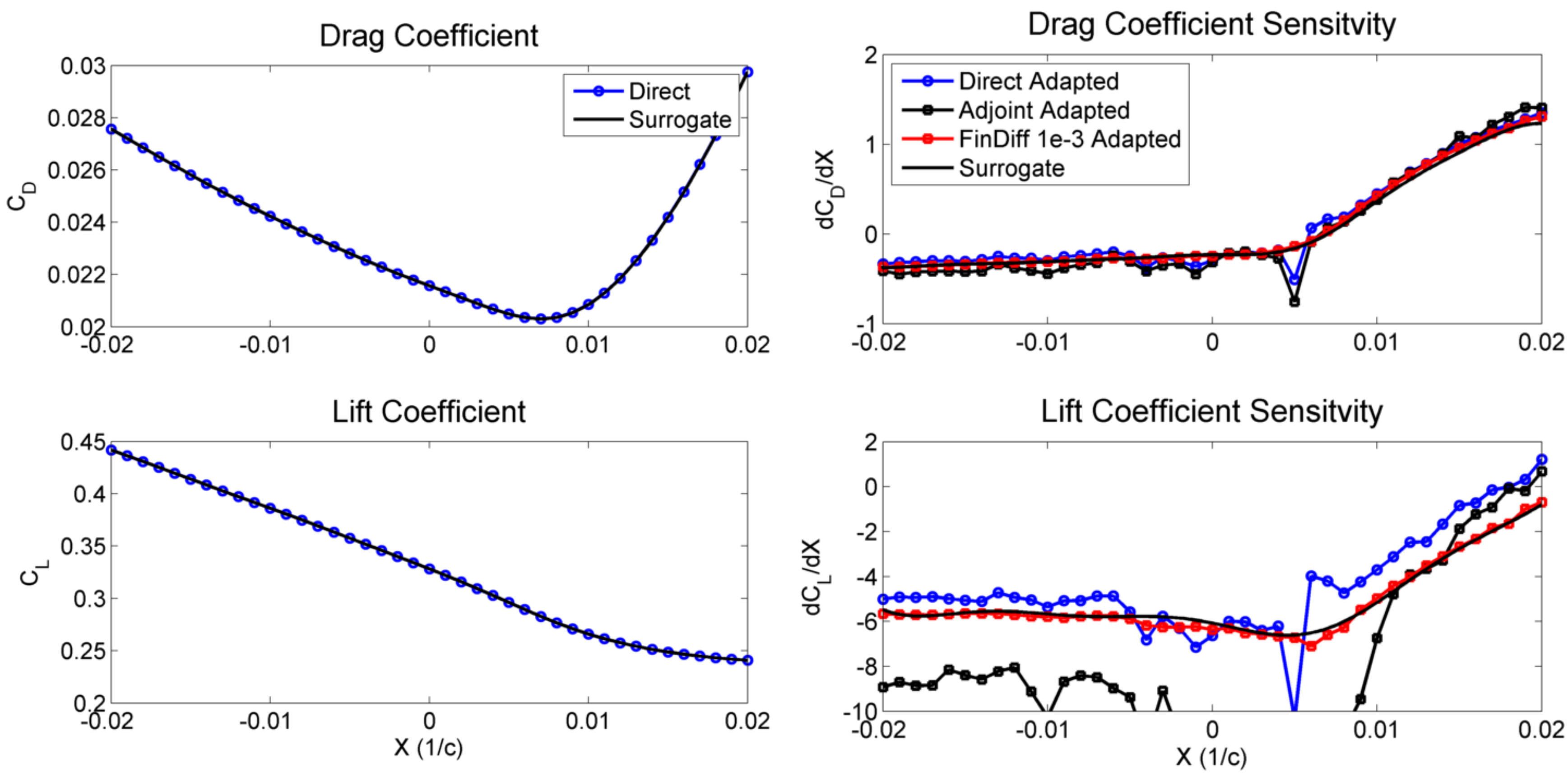
Adapted Mesh Gradients



(One Hicks-Henne Bump Function)



- Finite difference gradients are more robust to changes in discretization

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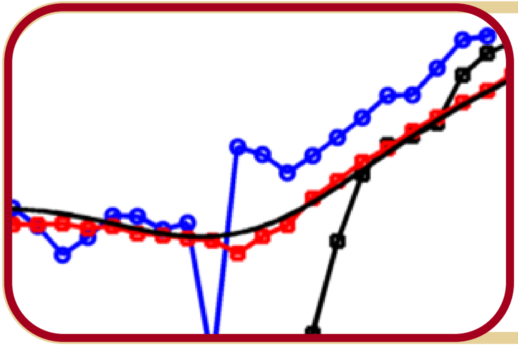
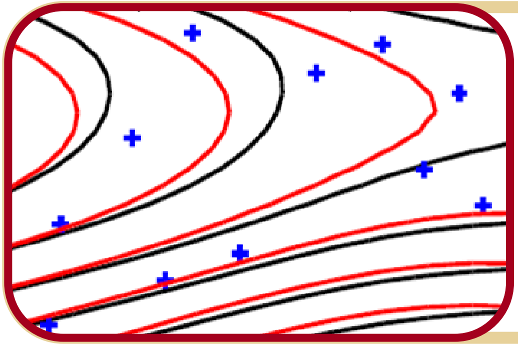
Outline



Gradient Accuracy Evaluation



Noise-Tolerant Response Surfaces

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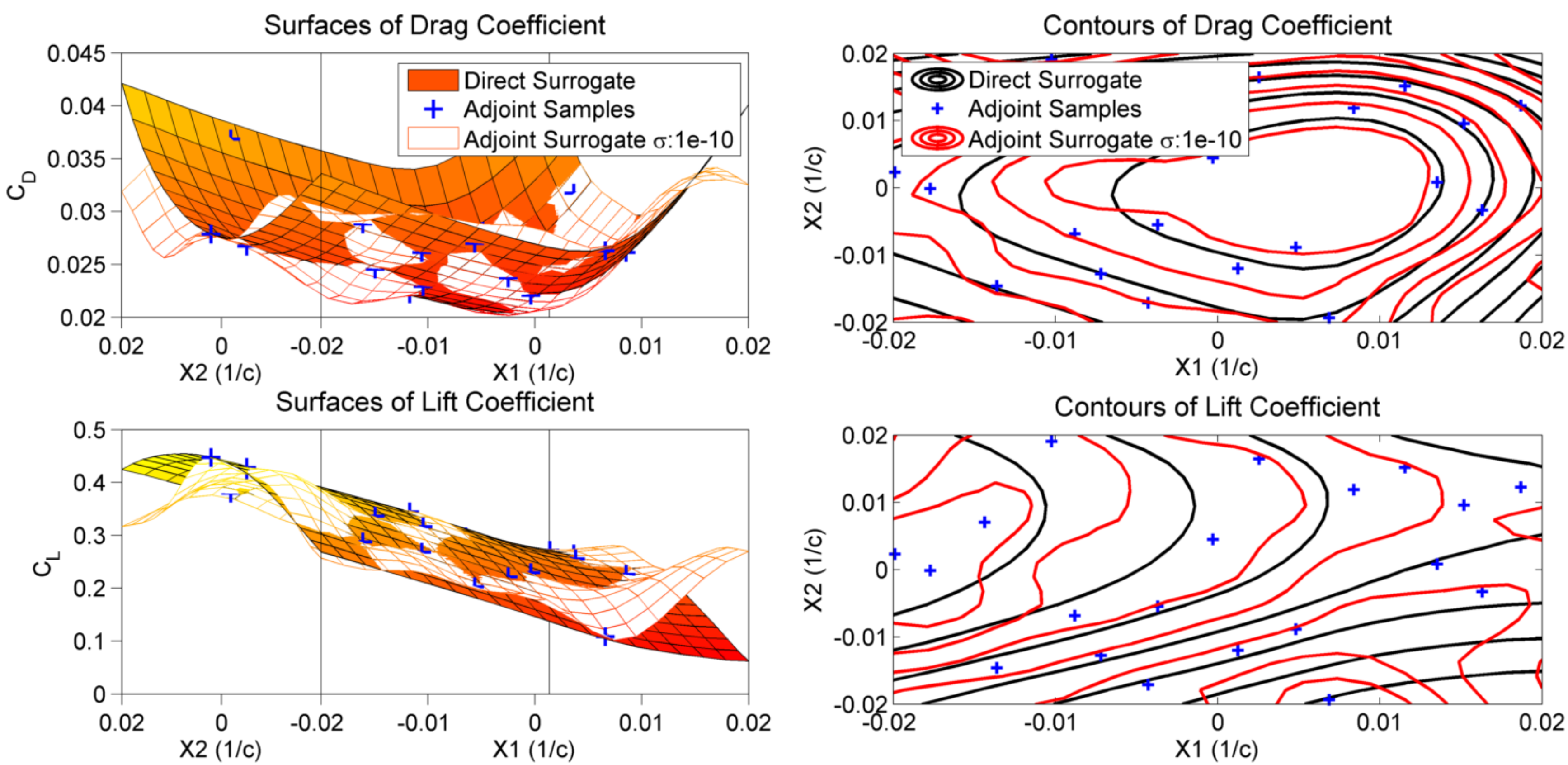
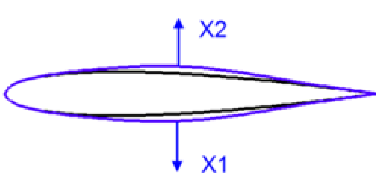
RSM Generation Issues

Adjoint Gradients



Mean Errors: Lift Objective: 5.5%; Lift Gradient: 50.8%; Drag Objective: 4.8%; Drag Gradient: 12.8%



(Two Hicks-Henne Bump Functions)

geGPR Formulation

The GPR derivation yields a system of linear equations that estimates an unknown function value …

$$f_k^* = k(x_k^*, x_q)\, k(x_p, x_q)^{-1}\, f_p$$

To include gradient information, we use the derivatives of the correlation model…

$$k\left(\frac{\partial p}{\partial x_v}, q\right) = \left.\frac{\partial k(p,q)}{\partial x_v}\right|_q$$

$$k\left(p, \frac{\partial q}{\partial x_w}\right) = \left.\frac{\partial k(p,q)}{\partial x_w}\right|_p$$

$$k\left(\frac{\partial p}{\partial x_v}, \frac{\partial q}{\partial x_w}\right) = \left.\frac{\partial}{\partial x_w}\left(\left.\frac{\partial k(p,q)}{\partial x_v}\right|_q\right)\right|_p$$

This assumes an exact correlation between function and gradient!

Rasmussen, 2006

geGPR with Noise Models

Including a model of independent Gaussian noise …

$$f_N^*(x) = f^*(x) + \epsilon$$

… requires us to update our correlation model …

$$[k] \rightarrow [k] + [k_N]$$

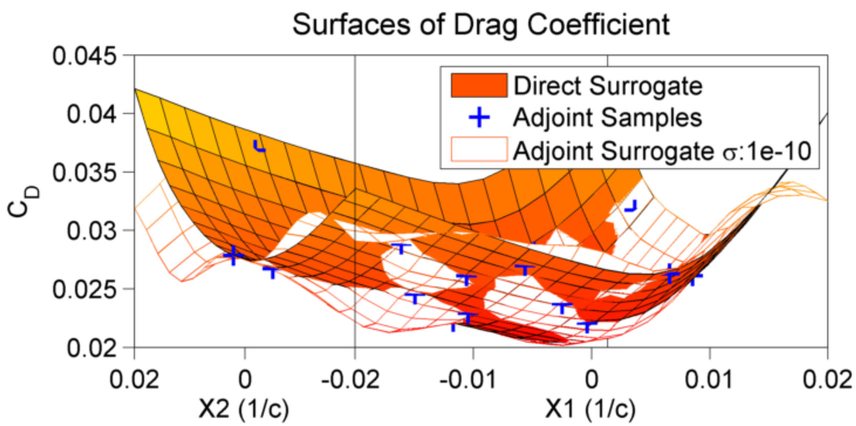
$$[k_N] = \begin{bmatrix} \theta_3^2 I_{n',n'} & 0_{n',m'} \\ 0_{m',n'} & \theta_4^2 I_{m',m'} \end{bmatrix} \quad \begin{matrix} n' = n(1+d) \\ m' = m(1+d) \end{matrix}$$

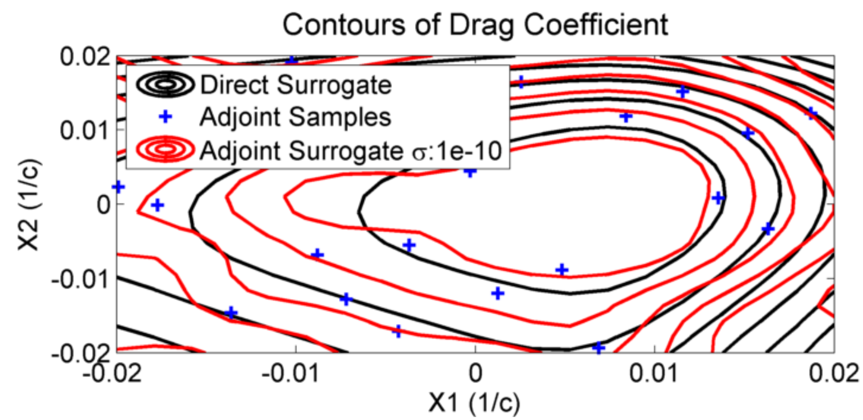
… which adds two parameters that control the amount of deviation from functions and gradients.

Rasmussen, 2006

RSM Generation Issues

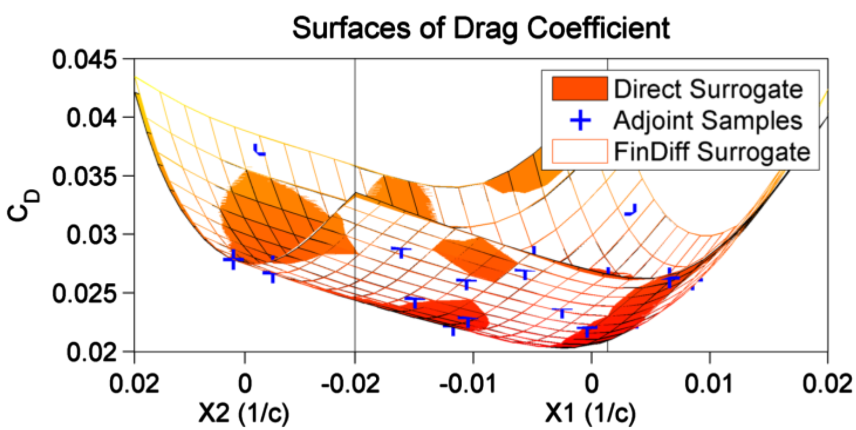
Adjoint Gradients, No Noise

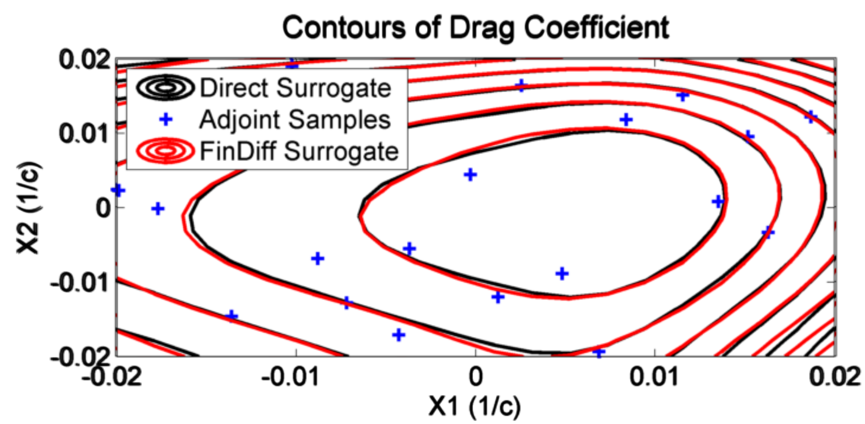




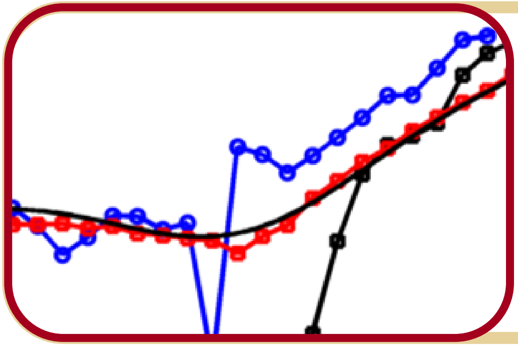
Finite Difference Gradients (Step:1e-3)

Adjoint Gradients, $\theta_{3,4}$=1e-3

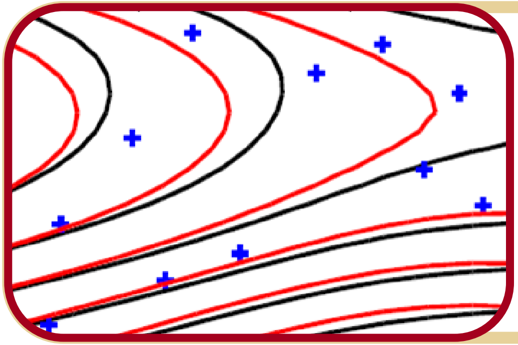




Outline



Gradient Accuracy Evaluation



Noise-Tolerant Response Surfaces

Motivation

Active Subspaces for Shape Optimization

Trent Lukaczyk, Francisco Palacios, Juan J. Alonso
Department of Aeronautics & Astronautics
Stanford University

Paul G. Constantine
Department of Applied Mathematics and Statistics
Colorado School of Mines

52st AIAA Aerospace Sciences Meeting
National Harbor, MD
January 16, 2014

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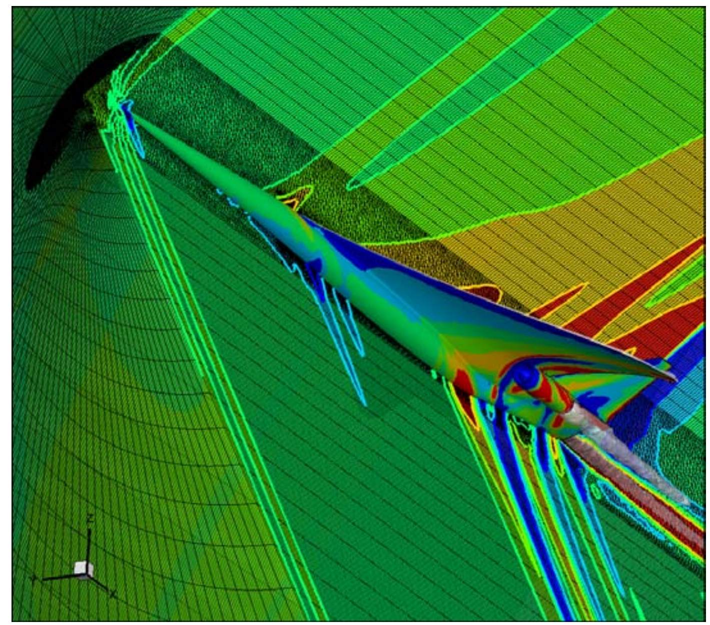
Optimal Shape Design

Goal: Improve aircraft performance by iteratively changing an aerodynamic shape

Common Approaches:

- Local Optimizers:
  - Gradient Based Algorithms
- Global Optimizers:
  - Genetic Algorithms
  - Particle Swarm Algorithms
- Surrogate Based Optimizers:
  - Gaussian Process Regression



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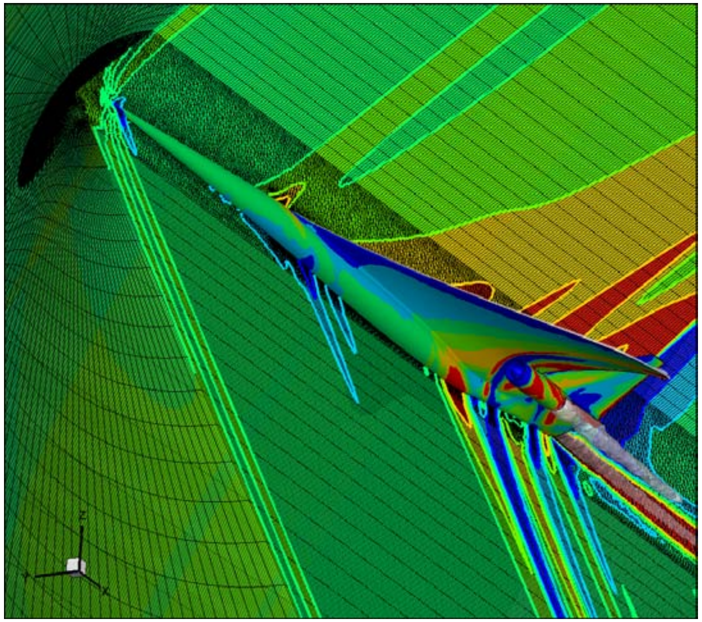
Curse of Dimensionality

Problem: Realistic shape design problems require order-100+ design variables

Common Challenges:

- Local Optimizers:
  - Locked in local minima
- Global Optimizers:
  - Tens of thousands of design evaluations
- Surrogate Based Optimizers:
  - **Not predictive above ~10 design variables**



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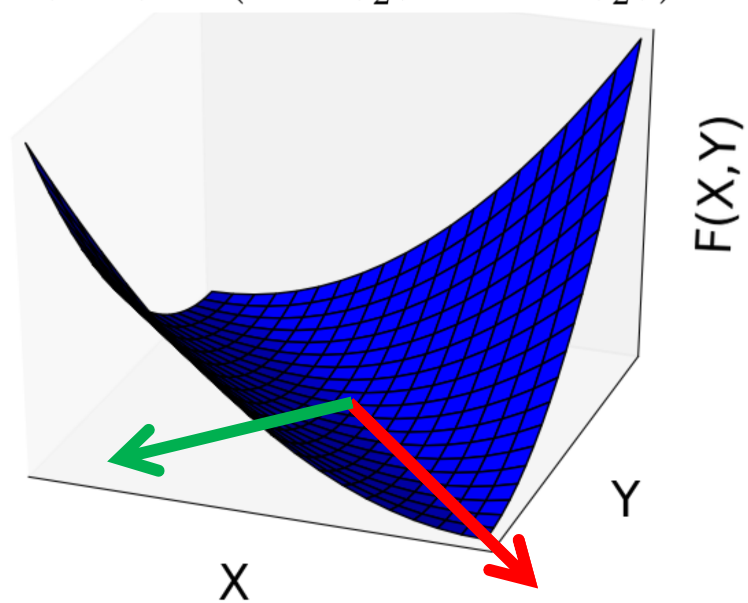
Dimensionality Reduction

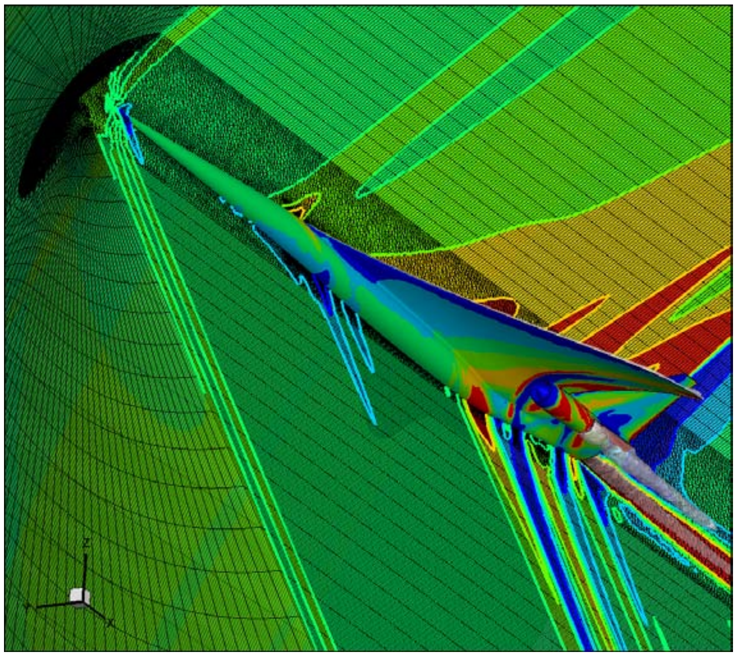
Solution: Exploit redundant variables and global trends to estimate objectives in a smaller subspace

Example:

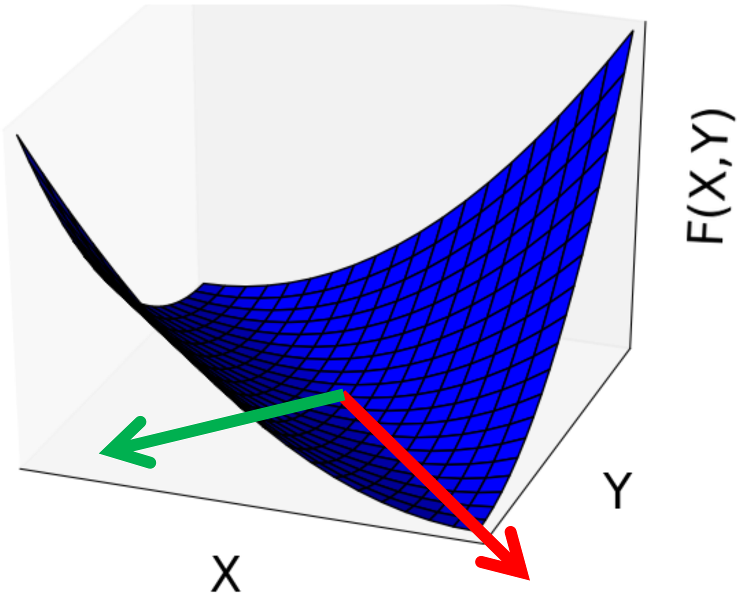
$$f(\mathbf{x}, \mathbf{y}) = \left(\mathbf{x}\sin(\tfrac{\pi}{2}) + \mathbf{y}\cos(\tfrac{\pi}{2})\right)^2$$



Fundamental Assumption



$$f(\mathbf{x},\mathbf{y}) = \left(\mathbf{x}\sin(\tfrac{\pi}{2}) + \mathbf{y}\cos(\tfrac{\pi}{2})\right)^2$$



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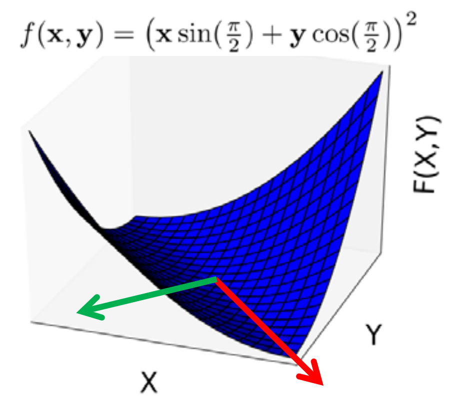
ACTIVE SUBSPACE

Active Subspace

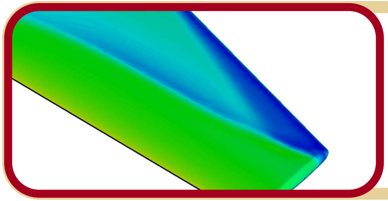
"A low-dimensional subspace of the inputs that captures global trends of the objective"

- Works by finding eigenvectors of objective **gradients**
- Comparable to Principal Components Analysis
  - PCA: reduce **output** space dimension
  - Active Subspace: reduce **input** space dimension



Constantine, P. G., Dow, E., and Wang, Q., "Active subspace methods in theory and practice: applications to kriging surfaces," 2013.

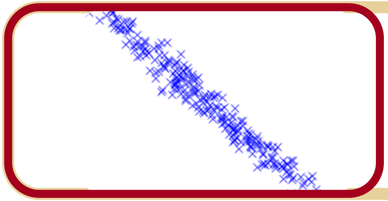
Active Subspace Based Design



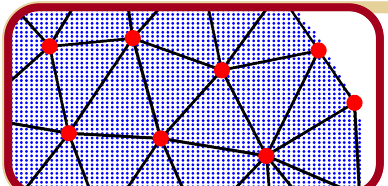
Design Space Sampling

$$W \Lambda W^T$$

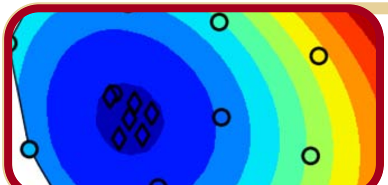
Eigenvalue Decomposition



Project into Active Subspace



Resample in Active Subspace



Apply Surrogate Model

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Active Subspace Construction

With a set of design samples, estimate the covariance matrix of the objective's gradients:

$$\boldsymbol{C} \approx \frac{1}{M}\sum_{i=1}^{M} \nabla_{\mathbf{x}} f_i \, \nabla_{\mathbf{x}} f_i^T$$

Decompose the matrix into eigenvalues and eigenvectors:

$$\boldsymbol{C} = \boldsymbol{W}\Lambda\boldsymbol{W}^T$$

Sort these by decreasing eigenvalue, and partition them into an active space *U* and inactive space *V:*

$$\boldsymbol{W} = \begin{bmatrix}\boldsymbol{U} & \boldsymbol{V}\end{bmatrix} \quad \Lambda = \begin{bmatrix}\Lambda_1 & \\ & \Lambda_2\end{bmatrix}$$

The columns of *U* define the active subspace, and designs can be projected using the forward map:

$$\mathbf{y} = \boldsymbol{U}^\top \mathbf{x}$$

MAPPING

Mapping

Full space

high dimension

$$\mathbf{x} \in \mathcal{X}$$

Forward map

$$\mathbf{y} = \boldsymbol{U}^\top \mathbf{x}$$

One y for each x

Inverse map

???

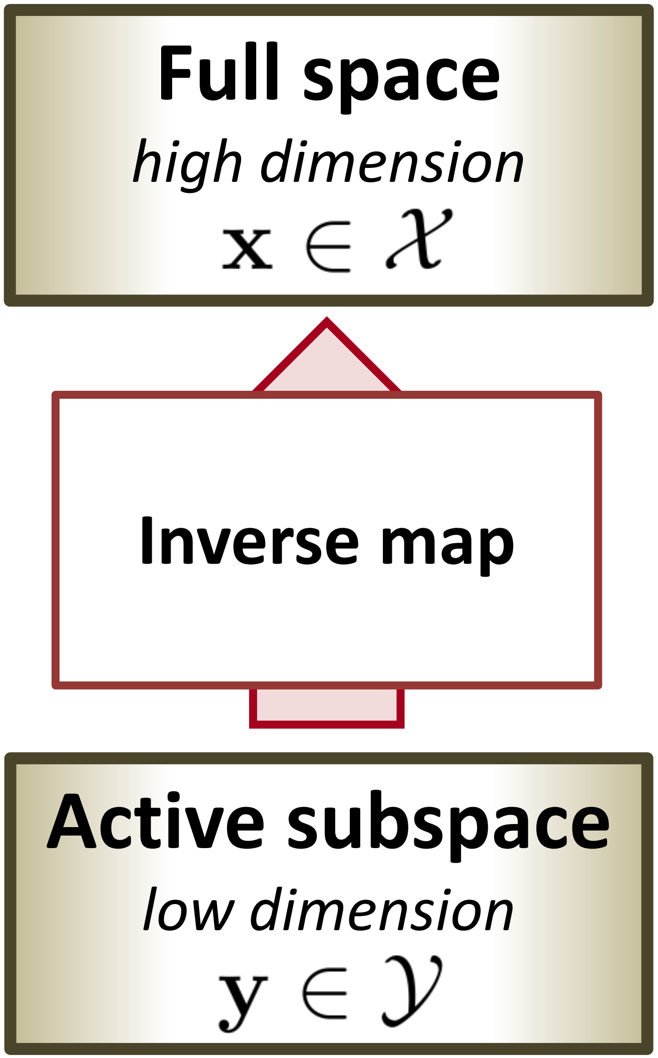
Many x for each y

Active subspace

low dimension

$$\mathbf{y} \in \mathcal{Y}$$

Inverse Mapping



- A simple injection

$$\mathbf{y} = \boldsymbol{U}^T \mathbf{x}$$

Pseudo inverse
(orthogonal basis)

$$\mathbf{x} = \boldsymbol{U} \mathbf{y} + \mathbf{x}_0$$

➢ May not be bounded in the full space

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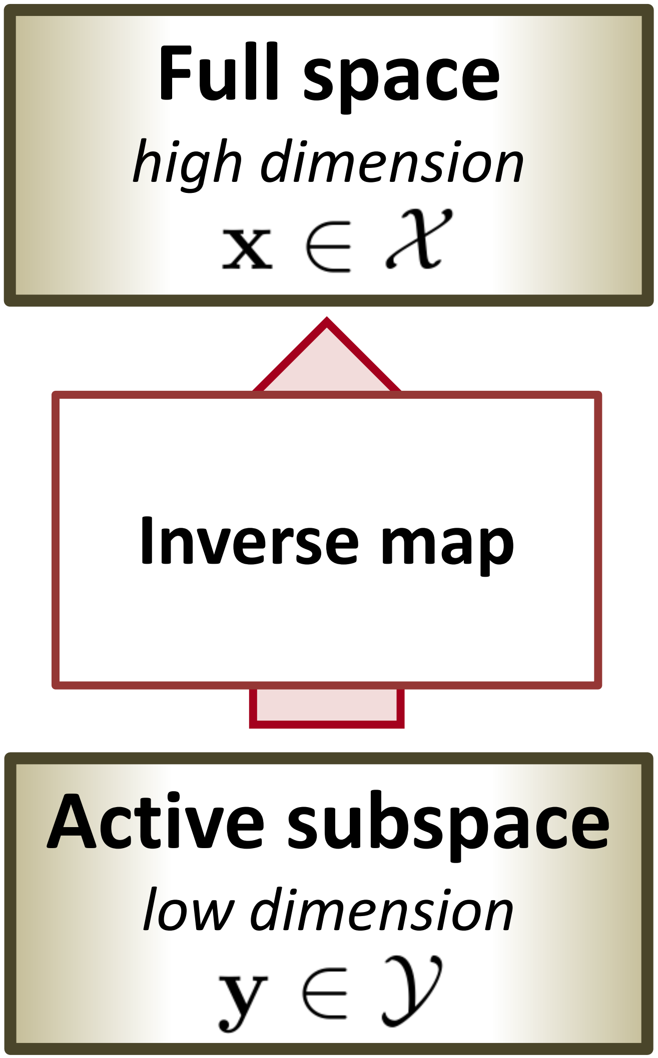
Inverse Mapping



- Bounded injection

$$\begin{array}{ll} \text{given} & \mathbf{y} = \mathbf{y}_{select} \\ \underset{\mathbf{x}}{\text{minimize}} & \mathbf{0}^\top \mathbf{x} \quad \text{(a dummy function)} \\ \text{subject to} & lb_i < \mathbf{x}_i < ub_i \\ & \mathbf{y} = \boldsymbol{U}^T \mathbf{x} \\ \text{yield} & \mathbf{x} \end{array}$$

➢ Solvable by linear program

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Inverse Mapping

- Advanced Mappings

Example:

$$
\begin{aligned}
\text{given} \quad & \mathbf{y}_a = \mathbf{y}_{select} \\
& f_a(\mathbf{x}) \approx g_a(\mathbf{y}_a) \\
& f_b(\mathbf{x}) \approx g_b(\mathbf{y}_b) \\
& \mathbf{y}_a = \boldsymbol{U}_a^T \mathbf{x}, \; \boldsymbol{U}_a \in \mathcal{R}_{m \times k_a} \\
& \mathbf{y}_b = \boldsymbol{U}_b^T \mathbf{x}, \; \boldsymbol{U}_b \in \mathcal{R}_{m \times k_b} \\
\underset{\mathbf{x}}{\text{minimize}} \quad & 0, \; \text{(a dummy function)} \\
\text{subject to} \quad & lb_i < \mathbf{x}_i < ub_i, \; i \in \{0, ..., m\} \\
& \mathbf{y}_a = \boldsymbol{U}_a^T \mathbf{x} \\
& g_b(\boldsymbol{U}_b \mathbf{x}) \leq c \\
\text{yield} \quad & \mathbf{x}
\end{aligned}
$$

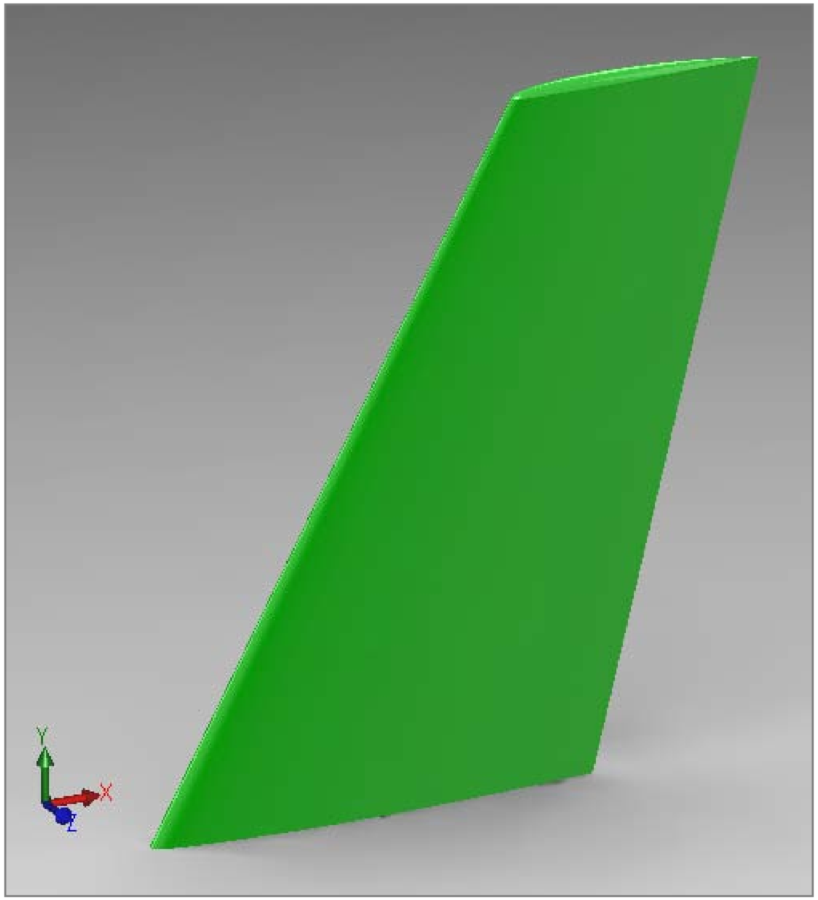
- $f_a(\mathbf{x}) \approx g_a(\mathbf{y}_a)$ — Drag Surrogate
- $f_b(\mathbf{x}) \approx g_b(\mathbf{y}_b)$ — Lift Surrogate
- $\mathbf{y}_a = \boldsymbol{U}_a^T \mathbf{x}$ — Drag Subspace
- $\mathbf{y}_b = \boldsymbol{U}_b^T \mathbf{x}$ — Lift Subspace
- $g_b(\boldsymbol{U}_b \mathbf{x}) \leq c$ — Lift Constraint

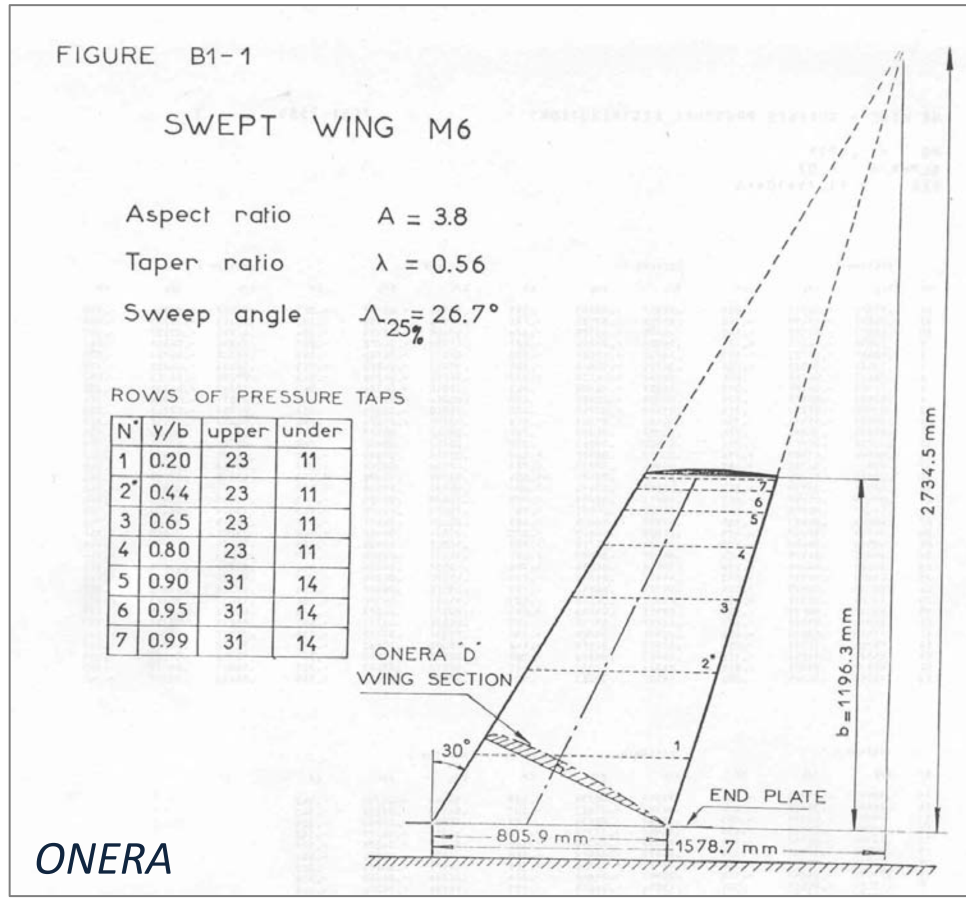
➢ Construct one subspace for each objective

DESIGN PROBLEM

ONERA M6 Geometry

A Standard Test Case for Transonic Fixed Wings





Schmitt, V. and F. Charpin, "Pressure Distributions on the ONERA-M6-Wing at Transonic Mach Numbers," *Experimental Data Base for Computer Program Assessment.* Report of the Fluid Dynamics Panel Working Group 04, AGARD AR 138, May 1979.

ONERA M6 Problem

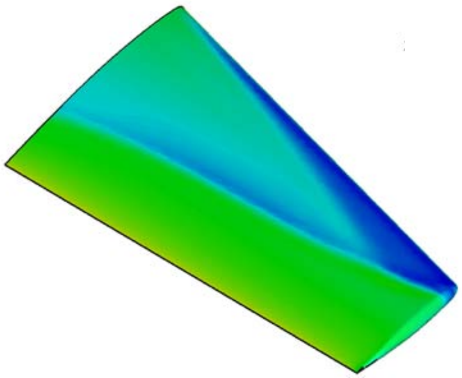
Simulation Conditions

$$\text{Ma} = 0.8395$$
$$\text{AoA} = 3.06^\circ$$
$$\text{Euler Equations}$$

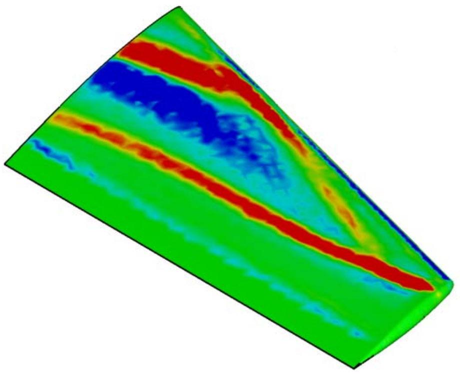
Optimization Problem

$$\begin{aligned} \underset{\mathbf{x}}{\text{minimize}} \quad & C_D(\mathbf{x}) \\ \text{subject to} \quad & C_L(\mathbf{x}) \geq 0.2864 \\ & lb_i < \mathbf{x}_i < ub_i, \; i \in \{0, ..., m\}, \\ & \mathbf{x} \in \mathbb{R}^m \end{aligned}$$

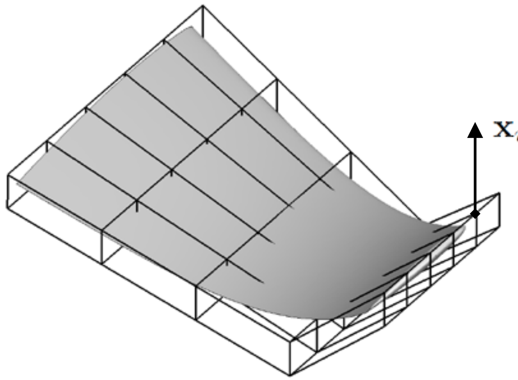
Direct Solution



Adjoint Solution



Mesh Deformation



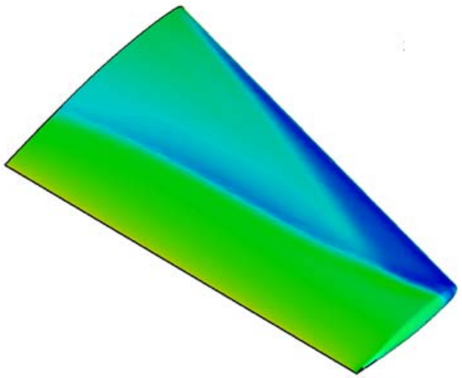
ONERA M6 Problem

http://su2.stanford.edu

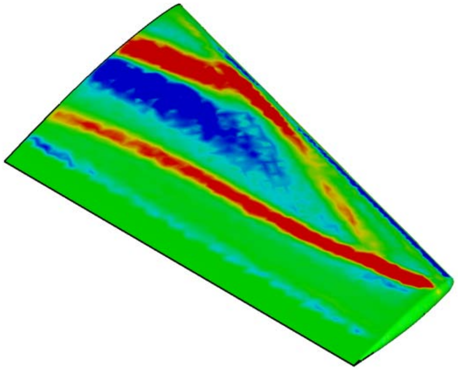
Open Source and Actively Developed
by the Aerospace Design Lab

The Open-Source CFD Code

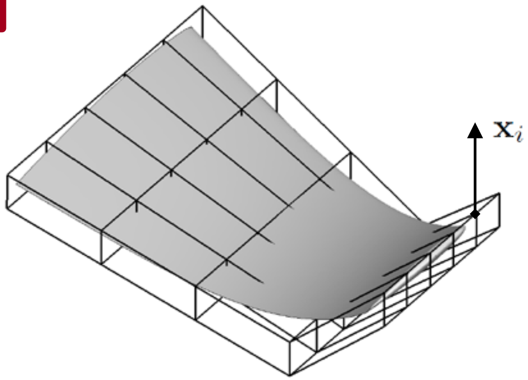
Direct Solution



Adjoint Solution



Mesh Deformation

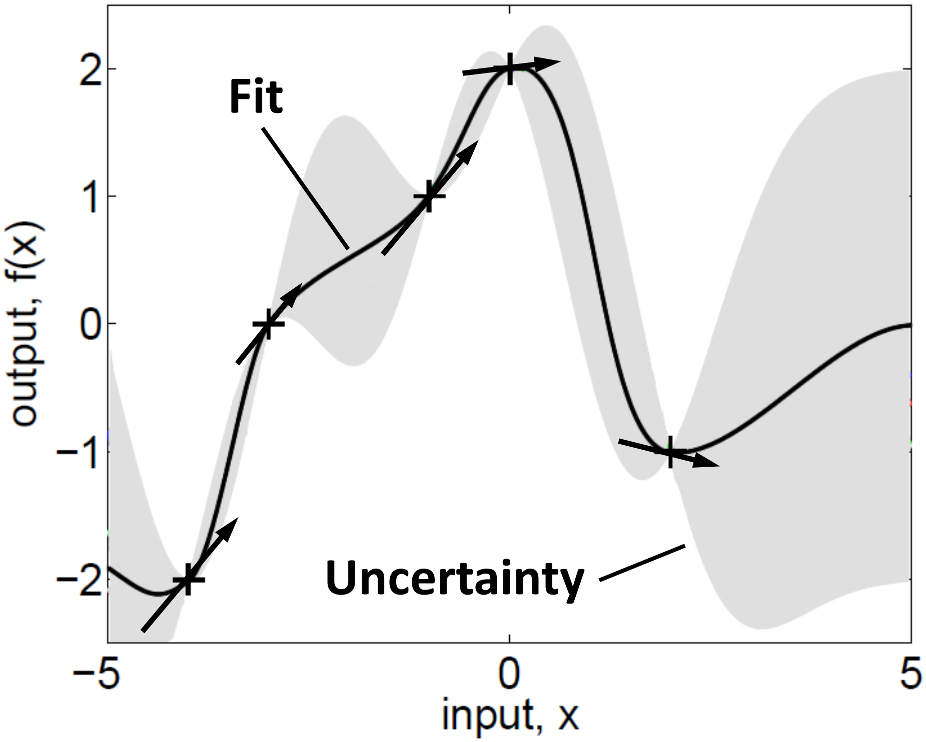


Gaussian Process Regression

for Surrogate Based Optimization

Important Attributes

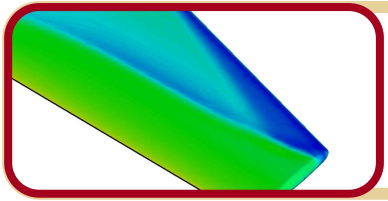
+ Non-parametric
+ Uncertainty of Fit Available
+ Can Model Noisy Data
+ Gradient Information
- Struggles with D>10



Trent Lukaczyk, T. , Palacios, F., and Alonso, J. J., "Managing Gradient Inaccuracies while Enhancing Response Surface Models," 51st AIAA Aerospace Sciences Meeting and Exhibit, Grapevine, TX, January 2013.

DESIGN EXPLORATION

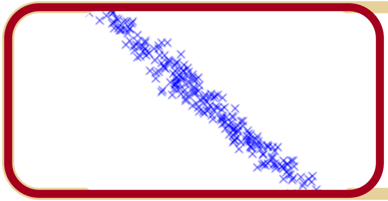
Active Subspace Construction



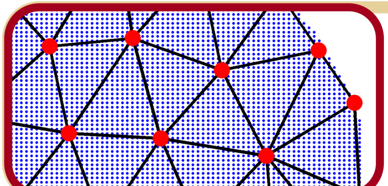
Design Space Sampling

$$W \Lambda W^T$$

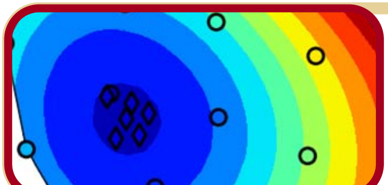
Eigenvalue Decomposition



Project into Active Subspace

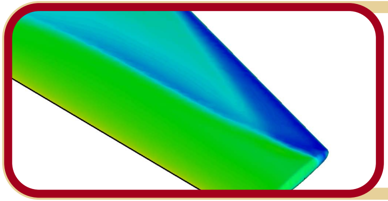


Resample in Active Subspace



Apply Surrogate Model

Active Subspace Construction



Design Space Sampling

$$W \Lambda W^T$$

Eigenvalue Decomposition

Project into Active Subspace

Resample in Active Subspace

Apply Surrogate Model

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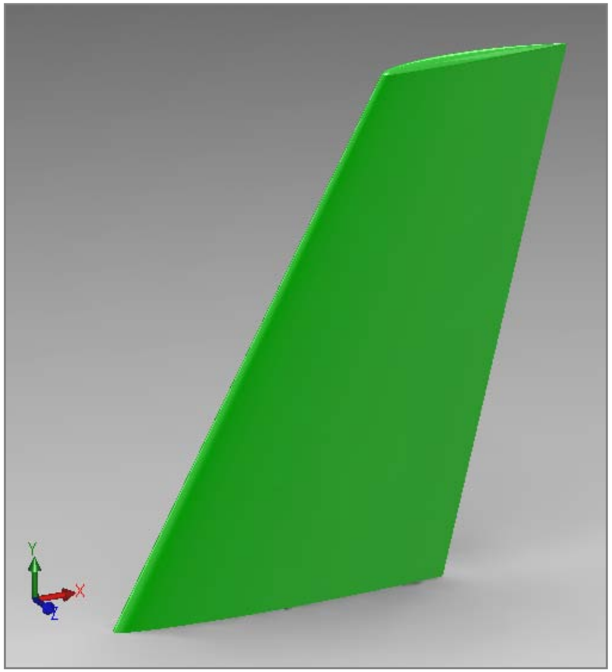
Design of Experiments

ONERA-M6 Wing Test Case

- **50 FFD control points** with motion in z-direction
- **Latin Hypercube Sampling**
  300 Samples in bounding box
  $x_i \in [-0.05, 0.05]$, $i = \{1,\ldots,50\}$
- **CFD evaluations** for Direct Flow, Drag Adjoint, Lift Adjoint



➢ High performance computing can exploit parallel sampling

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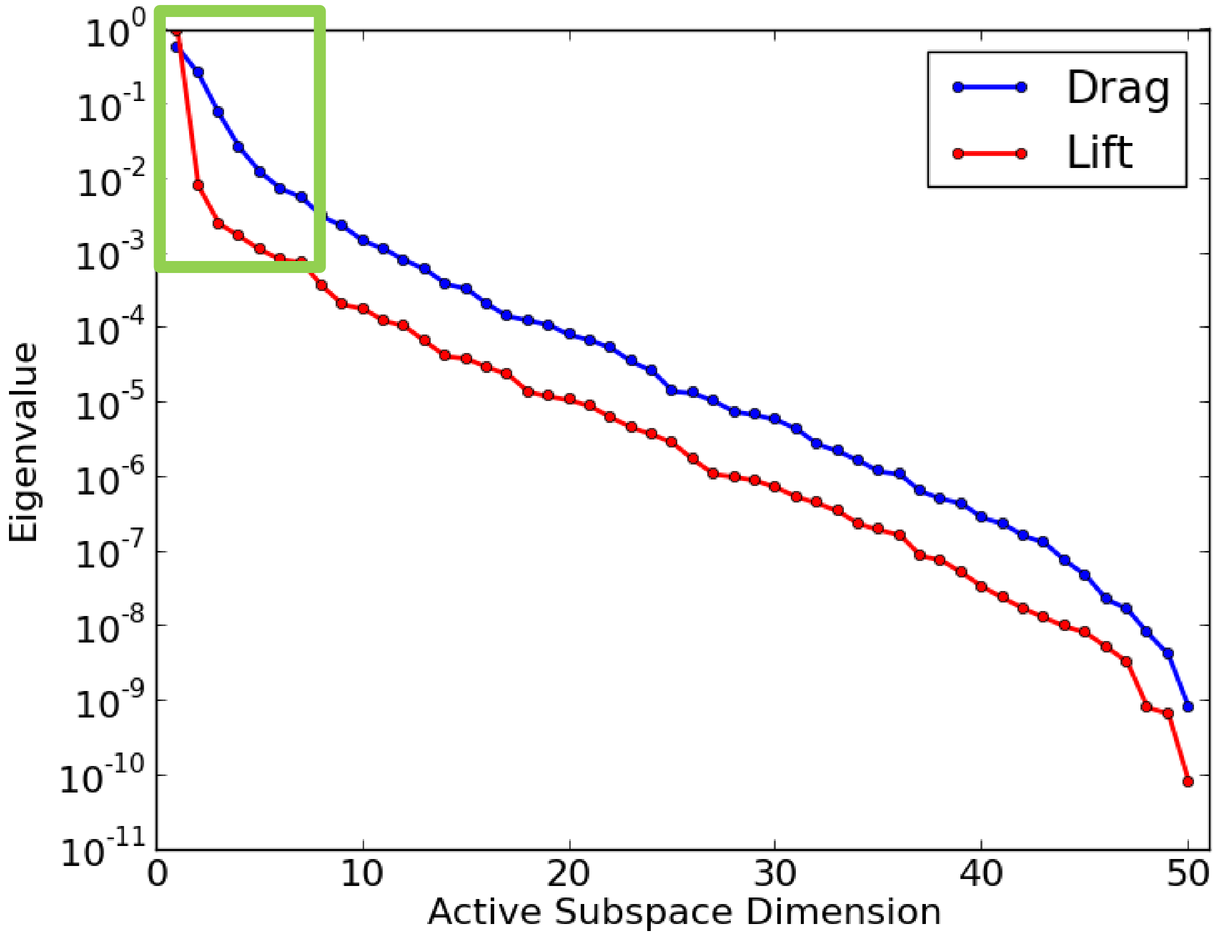
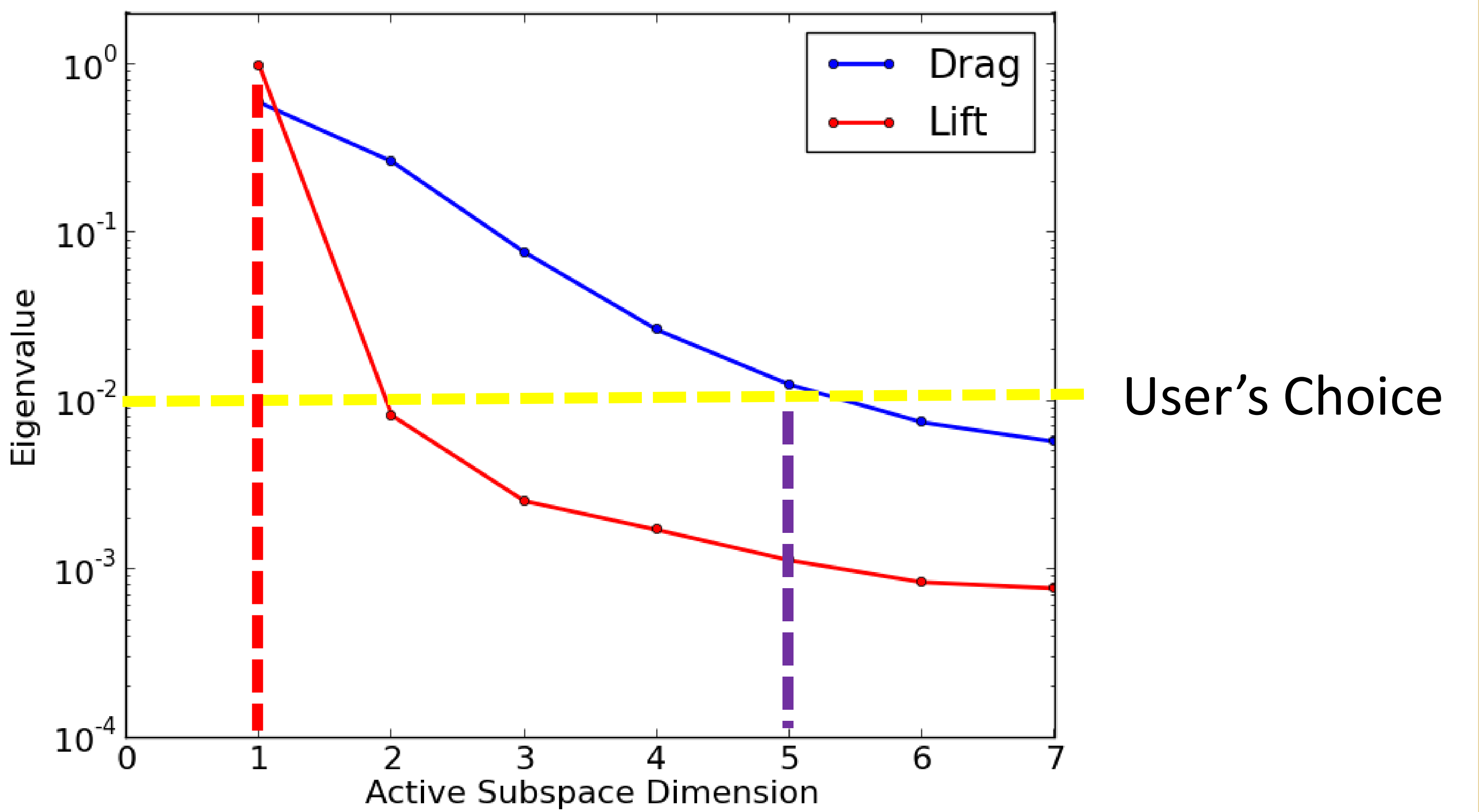
Eigenvalue Decay



Selecting Subspace Dimension



➢ **Choose 1-D Lift, and 5-D Drag**

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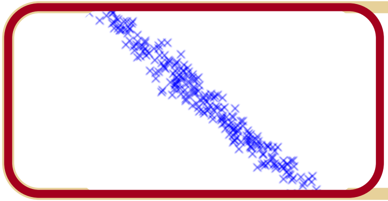
Active Subspace Construction

Design Space Sampling

$W \Lambda W^T$

Eigenvalue Decomposition



Project into Active Subspace

Resample in Active Subspace

Apply Surrogate Model

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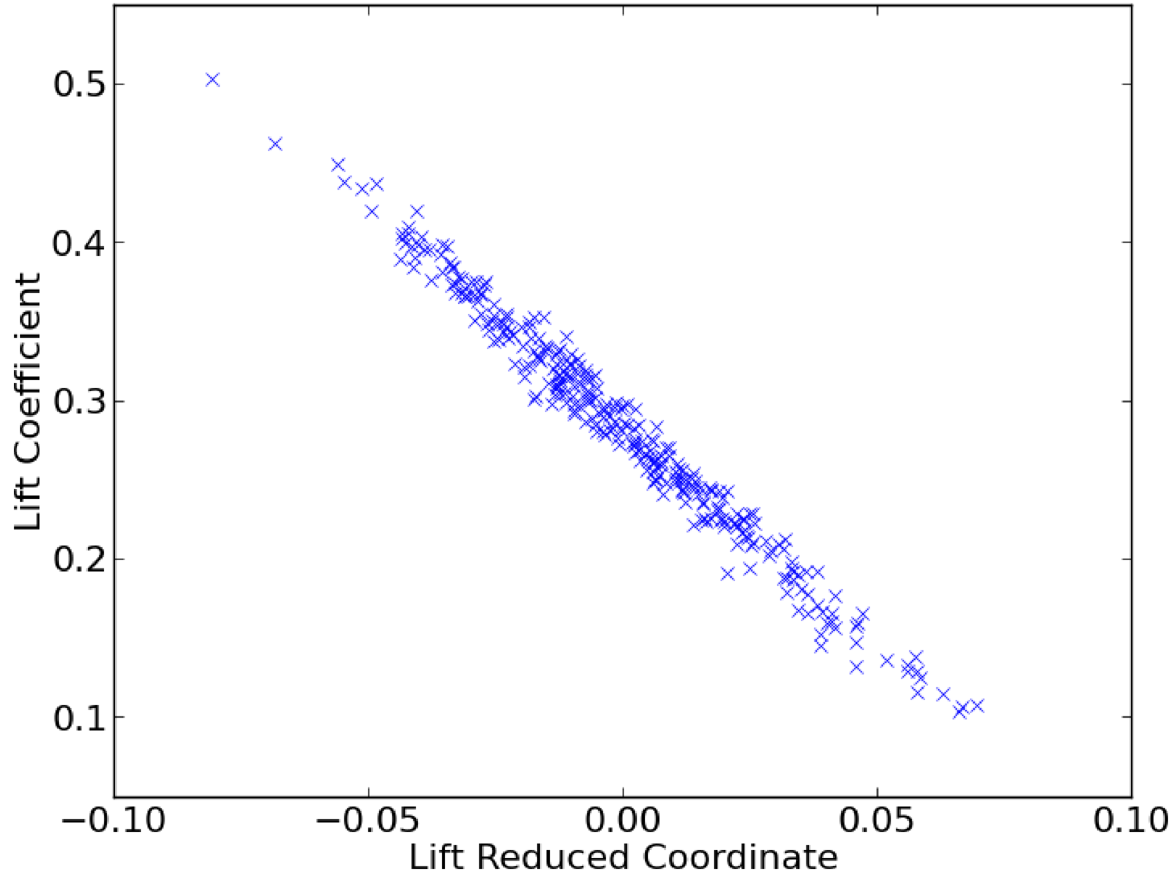
Project into Active Subspace

Lift Coefficient in 1-D



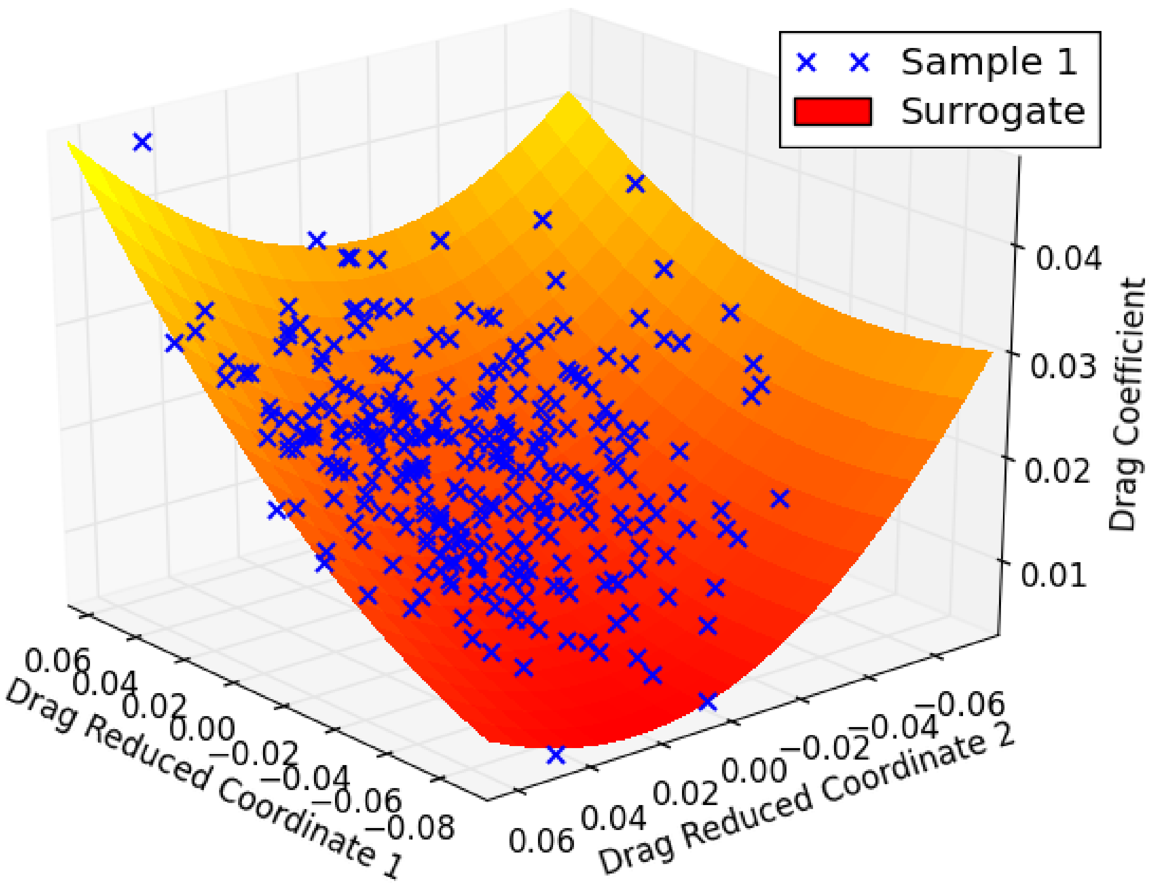
$$\mathbf{y} = U^{\top}\mathbf{x}$$

Dim.	Training Error
1	2.6%
2	2.3%
3	2.2%
4	2.1%

➢ **Lift collapses into 1-D with a linear trend**

Project into Active Subspace

Drag Coefficient in 2-D



Dim.	Training Error
1	8.3%
2	5.1%
…	…
5	2.9%
6	2.5%

➢ **Model in 5-D, Explore in 2-D**

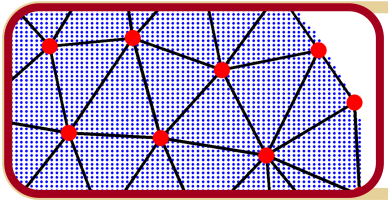
Active Subspace Construction

Design Space Sampling

$W \Lambda W^T$

Eigenvalue Decomposition

Project into Active Subspace



Resample in Active Subspace

Apply Surrogate Model

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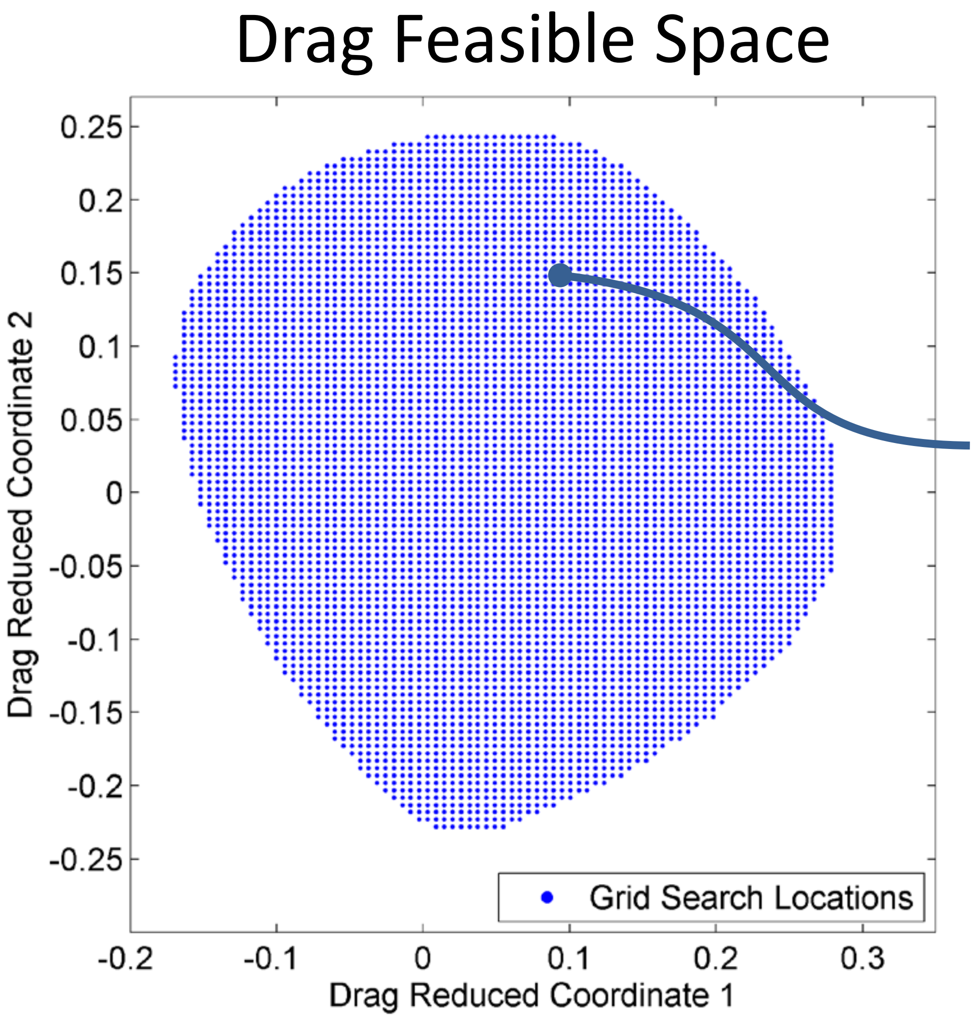
Resampling for Surrogates



Construct a Feasibility Hull

An n-dimensional polygon which bounds the feasible space for this design problem.

For each grid sample, at least one point in the full space:

1. Projects to the given point in the drag active subspace.
2. Is contained in the full-space bounding hyper-cube.
3. Has a lift, estimated in the lift active subspace, that is feasible.

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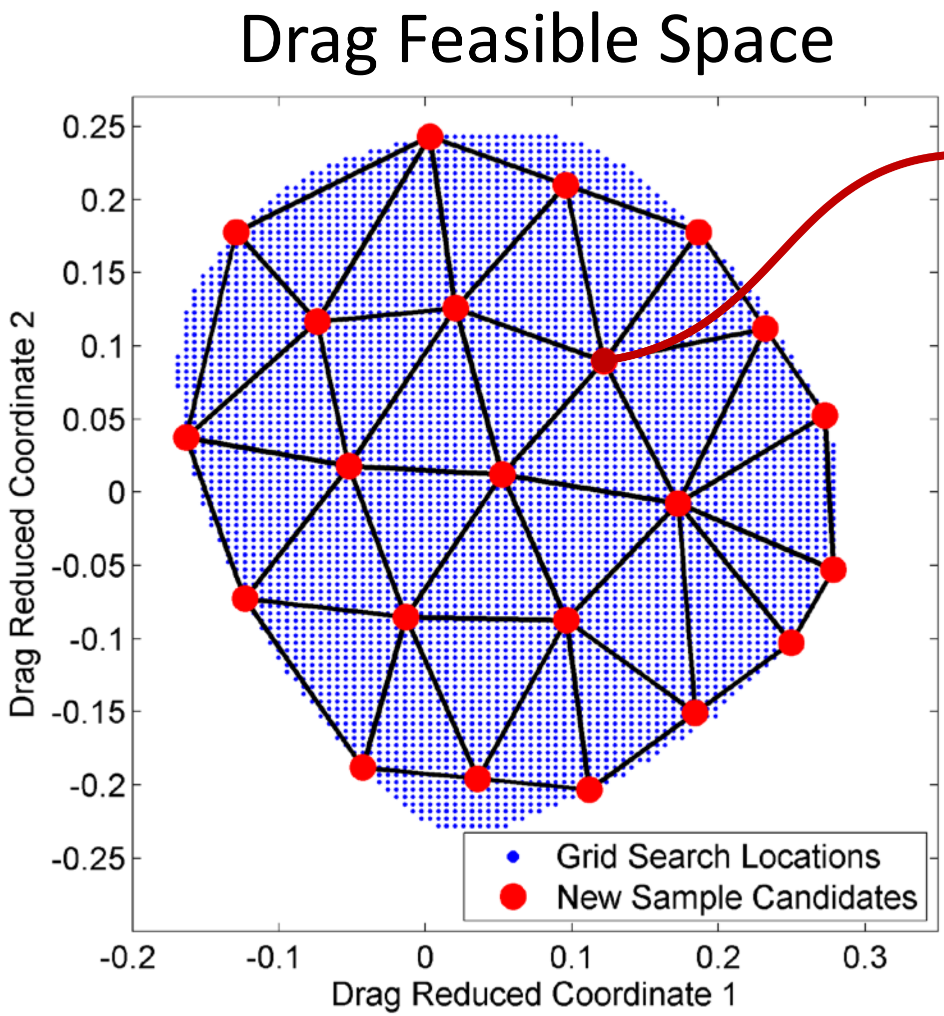
Resampling for Surrogates



Coarsen the sample grid with a mesh

Inject these points into the full space

Evaluate with CFD (only the direct solution)

Active Subspace Construction

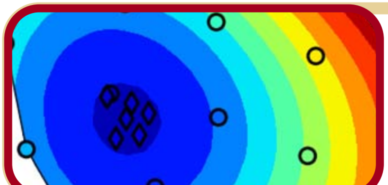
Design Space Sampling

$$W \Lambda W^T$$

Eigenvalue Decomposition

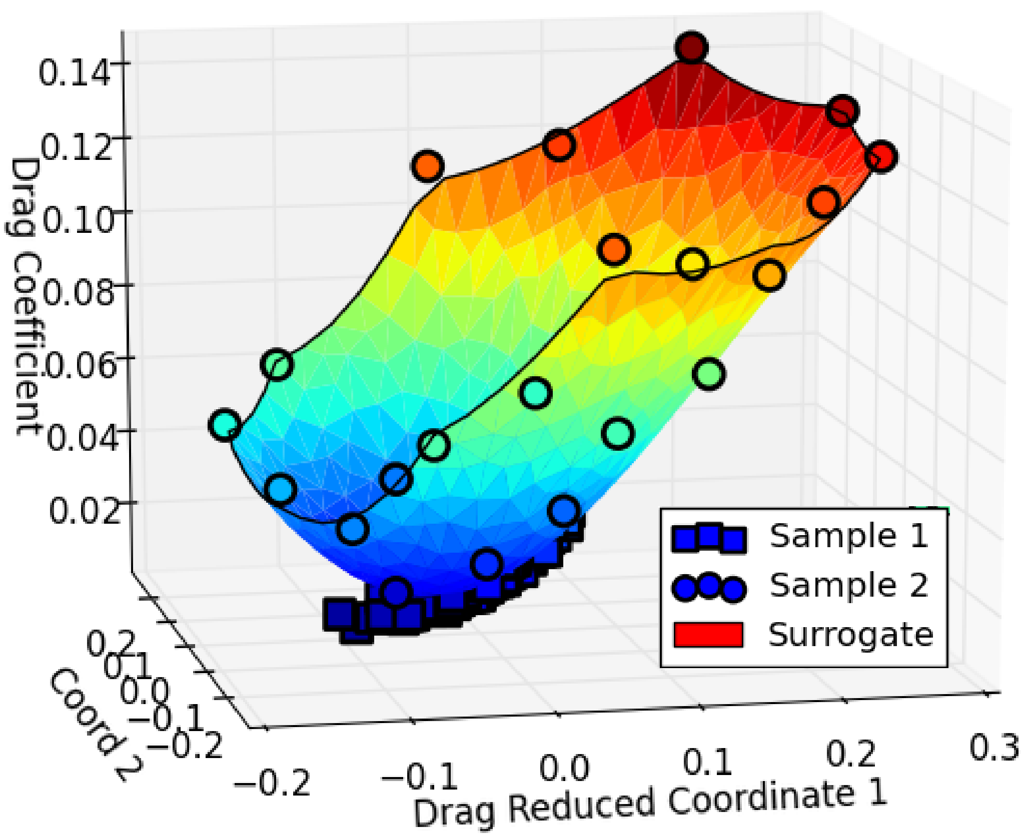
Project into Active Subspace

Resample in Active Subspace



Apply Surrogate Model

Final Surrogate Model



- **Sample 1**: used to find the active subspace
- **Sample 2**: used to produce a surrogate model
- Each point on the surrogate should have a feasible lift, and a minimum drag for that location

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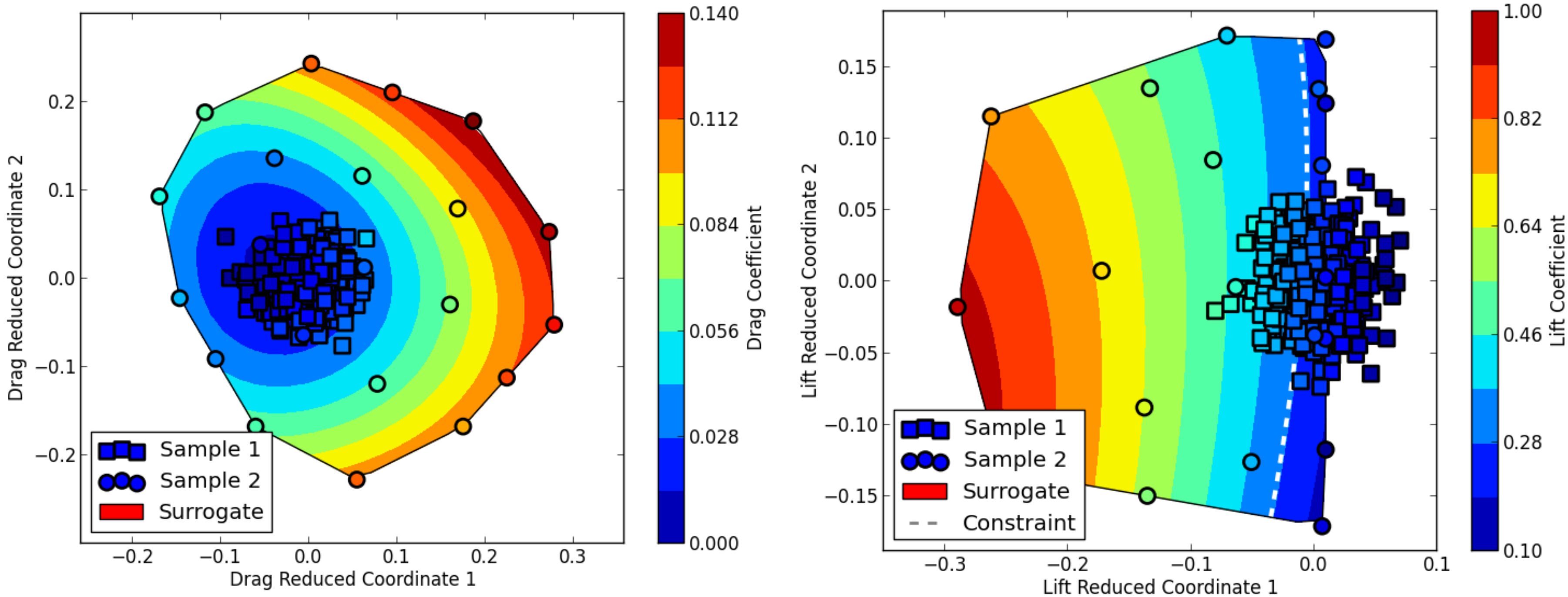
Constrained Design Exploration

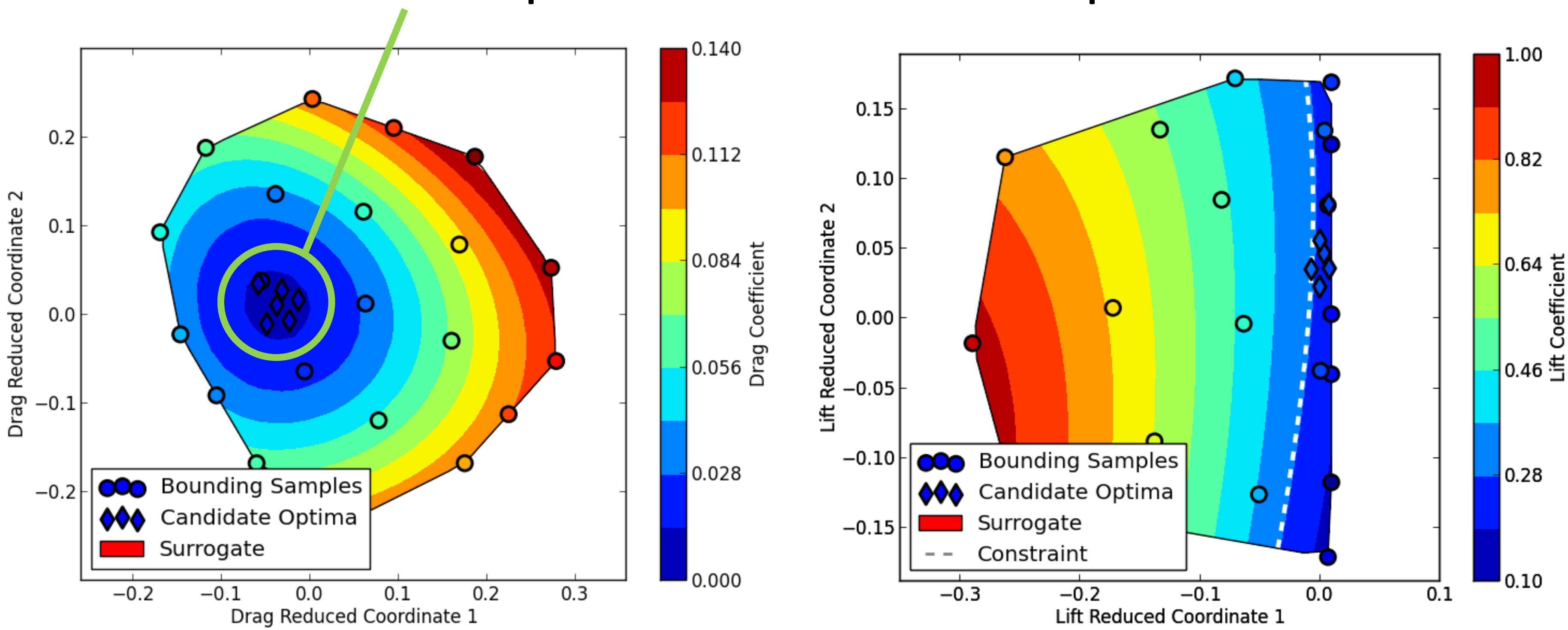


- Two active-space variables for drag, GPR surrogate
- Identifies feasible region in drag space, given lift constraint
  - ➢ **Surrogate can be used to estimate optimal designs**

OPTIMIZATION RESULTS

Constrained Optimization

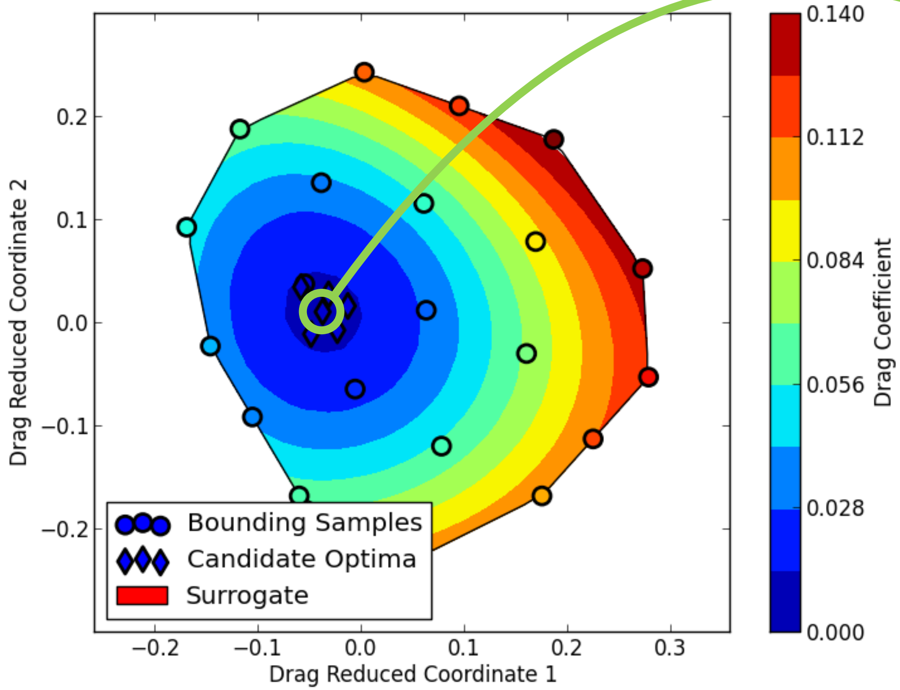
New samples near estimated optimum

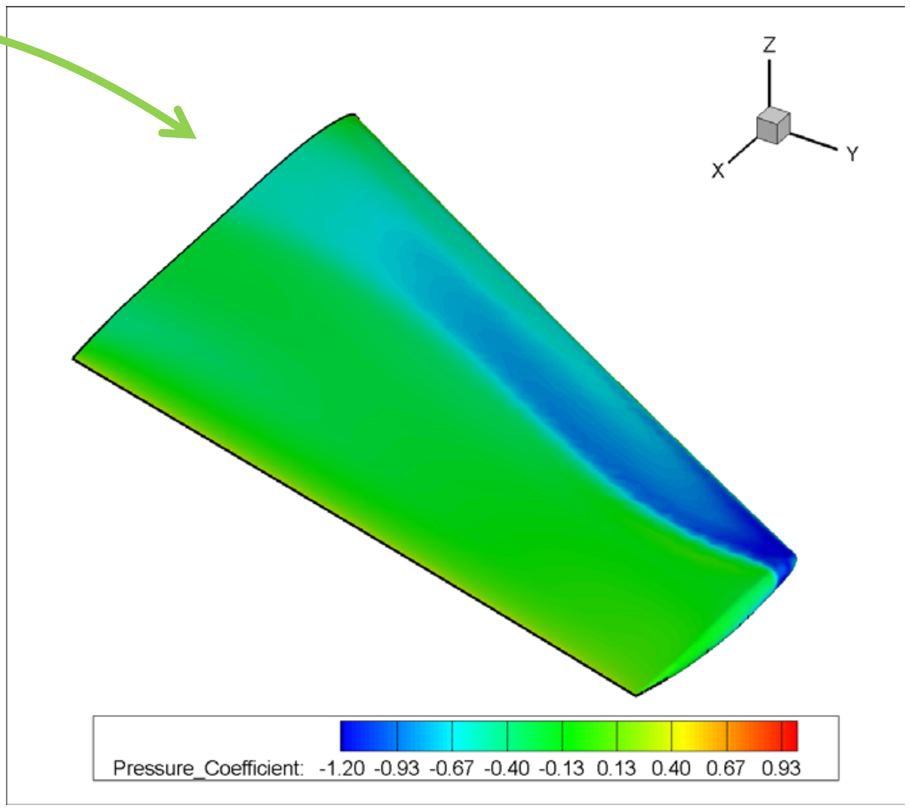


- ➢ **Surrogate model predicts optimum in 2-D**
- ➢ **Locations are injected into 50-D**

Constrained Optimization

The Predicted Optimum

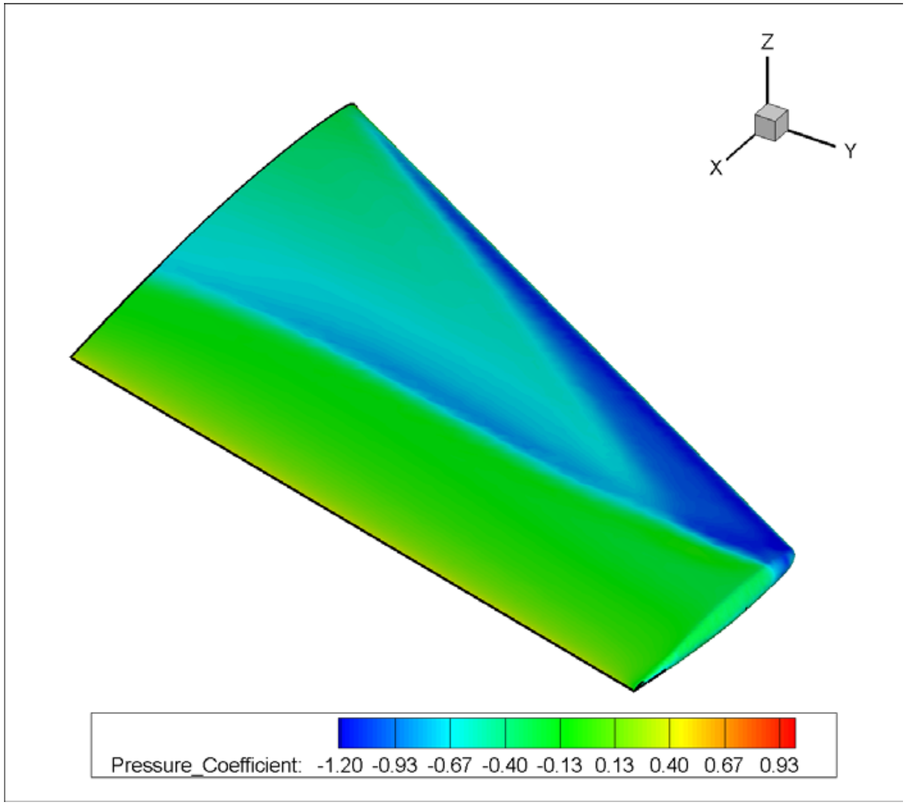




$$C_D = 0.0101,\ C_L = 0.2786$$

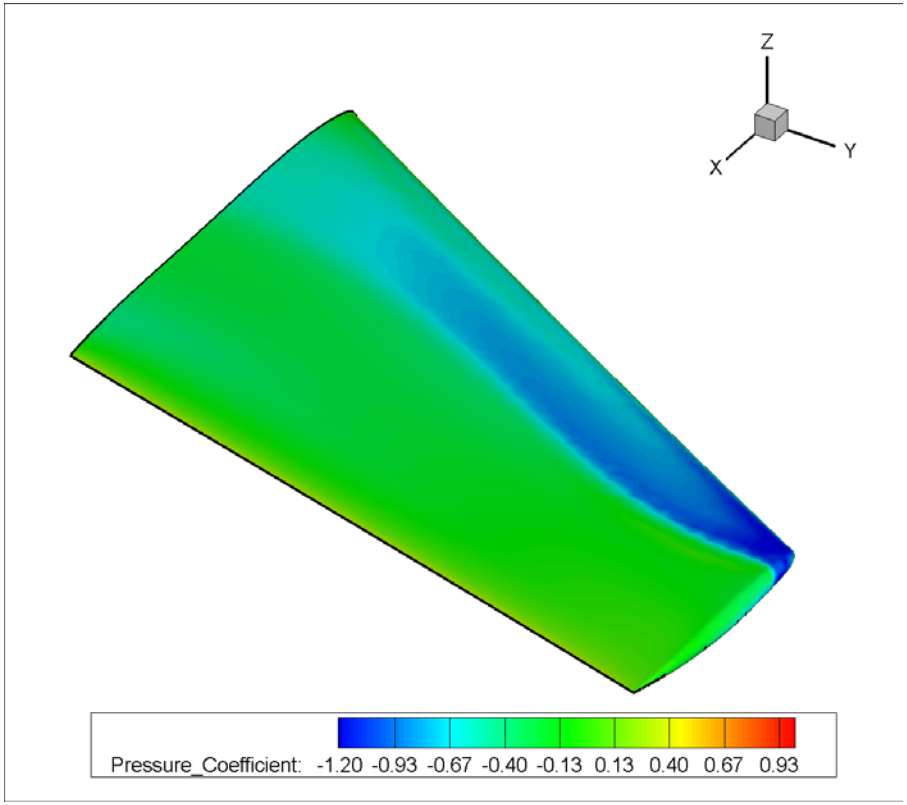
Constrained Optimization

Baseline Design



$C_D = 0.0118,\ C_L = 0.2864$

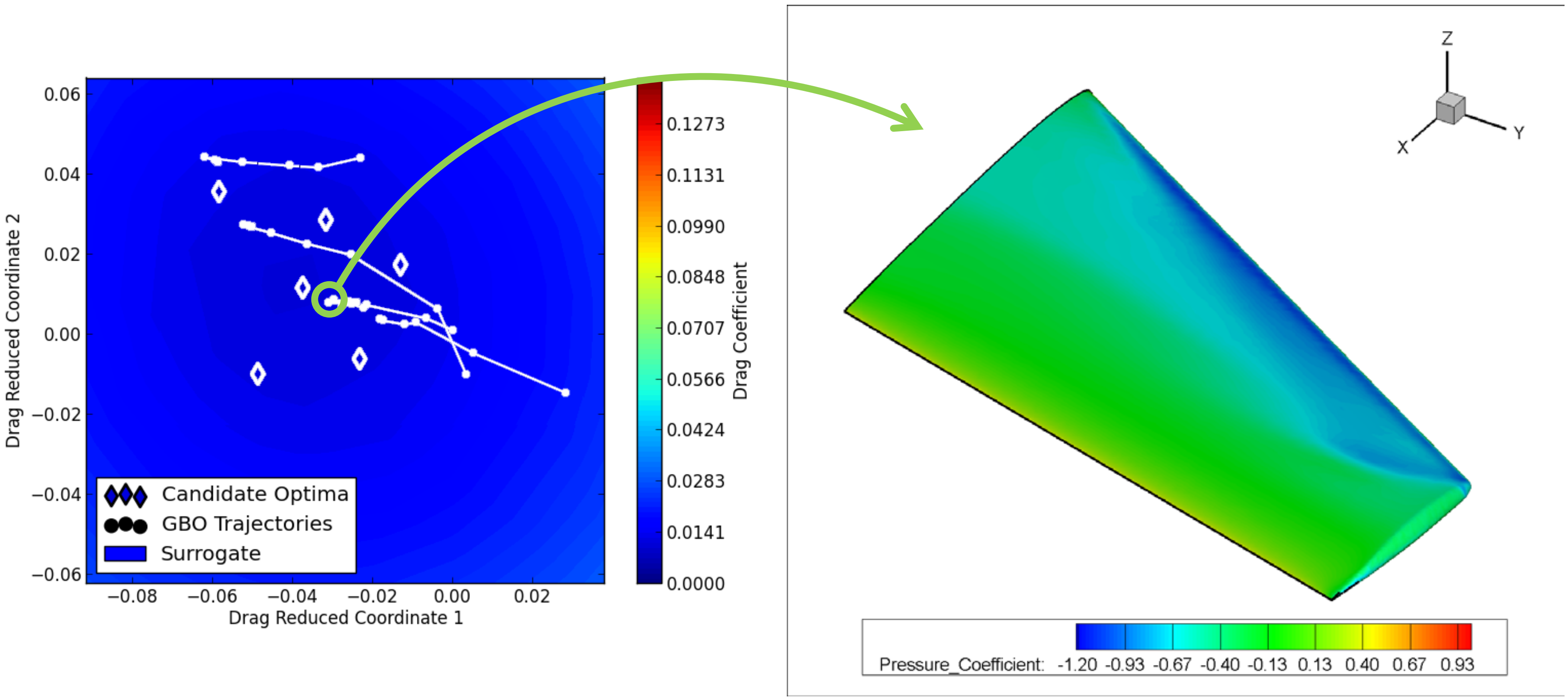
Active Subspace Optimum



$C_D = 0.0101,\ C_L = 0.2786$

- **14.4% Drag Reduction, 2.7% Lift Reduction**

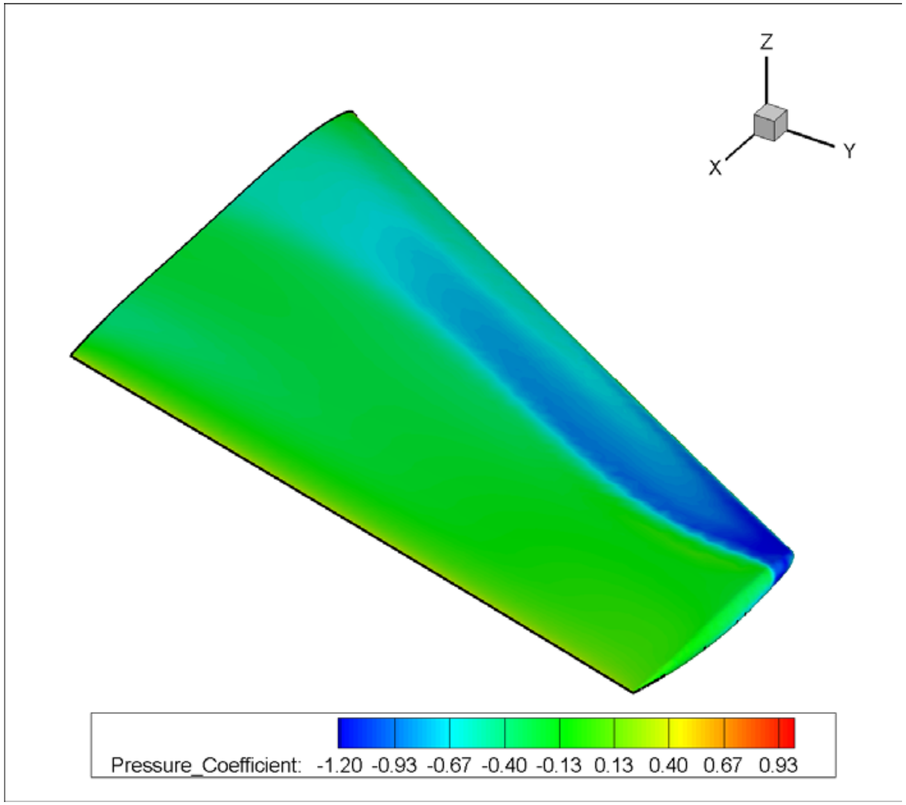
A Gradient-Based Optimum



$C_D = 0.0089,\ C_L = 0.2868$

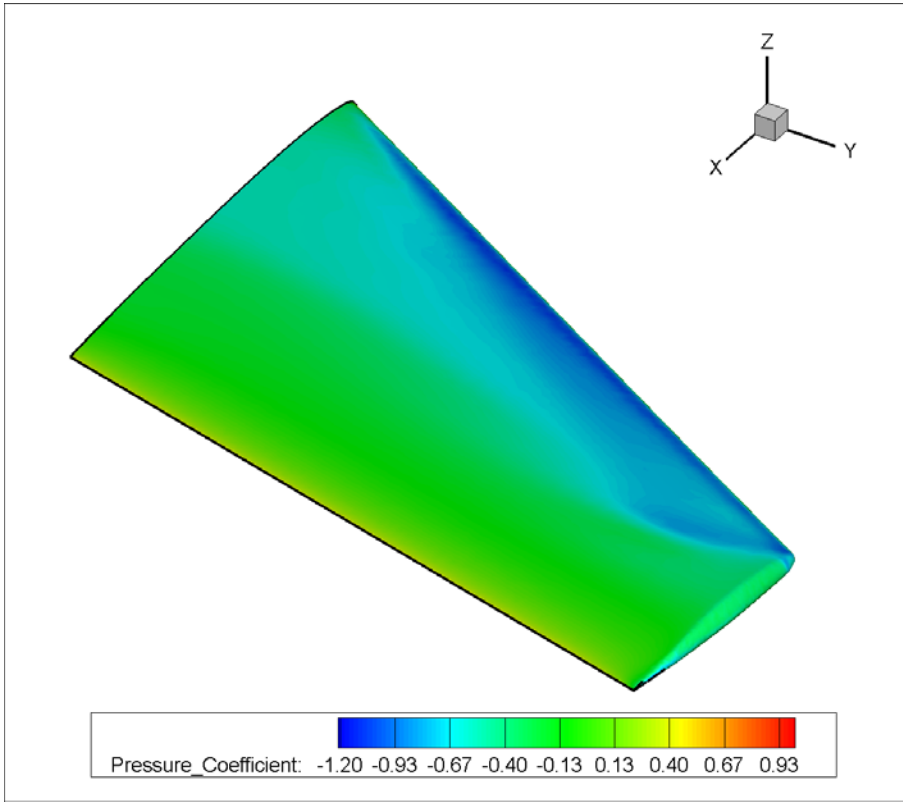
Compared to GBO

Active Subspace Optimum



$C_D = 0.0101,\ C_L = 0.2786$

Gradient Based Optimum



$C_D = 0.0089,\ C_L = 0.2868$

- **GBO still out-performs locally**

Cost

Active Subspace

Step	Flow + Adjoint Evaluations
Initial Sample	300 x 3
Active Subspace Resample	22
Optimum Samples	5
Total	**925**

Gradient Based

Step	Flow + Adjoint Evaluations
GBO Start 1	56
GBO Start 2	28
GBO Start 3	41
GBO Start 4	34
Total	**159**

Summary

Active Subspaces

Mapping

Design Problem

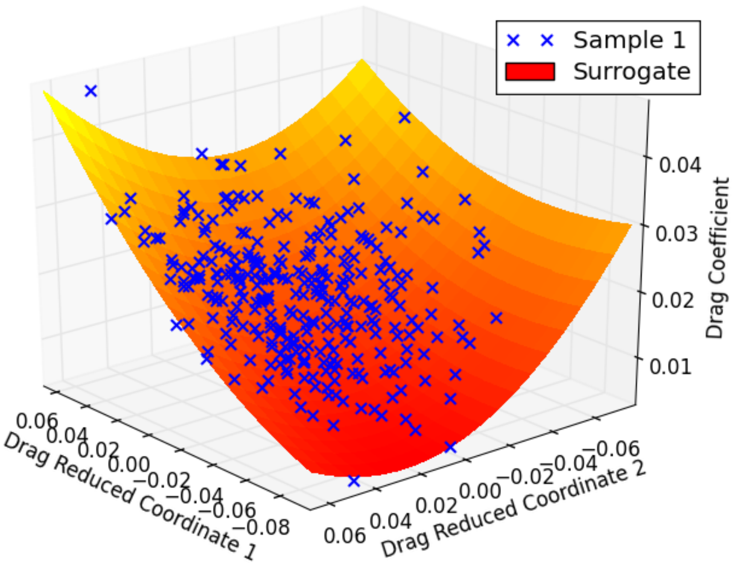
Design Exploration

Optimization Results

Conclusions

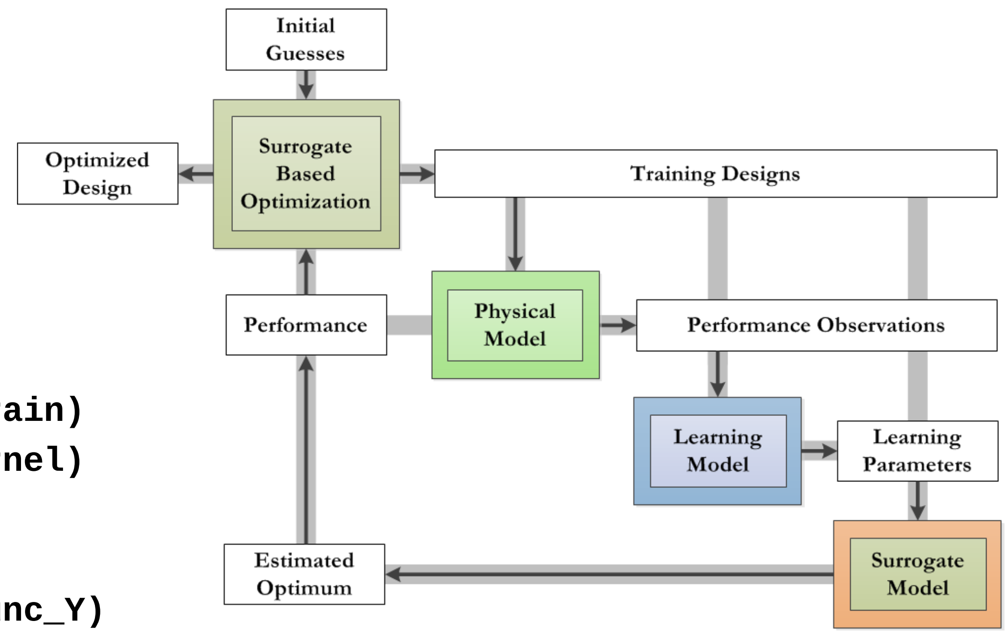
- Addresses problems faced while using surrogate models in dimensions greater than order ten
- Enables design exploration in low dimension and visualization in two dimensions
- Novel approach to mapping between coupled subspaces of a design problem

Surrogate Modeling Tools



VyPy

github.com/aerialhedgehog/VyPy




```
# Objective
Y,DY = Rosenbrock_Function(X)
Train  = VyPy.Training(XB,X,Y,DY)
Kernel = VyPy.Kernels.Gaussian(Train)
Model_Y = VyPy.Modeling(Train,Kernel)

# Efficient Global Optimization
Sample = VyPy.Sampling(Model_Y,Func_Y)
Sample.Optimize()
```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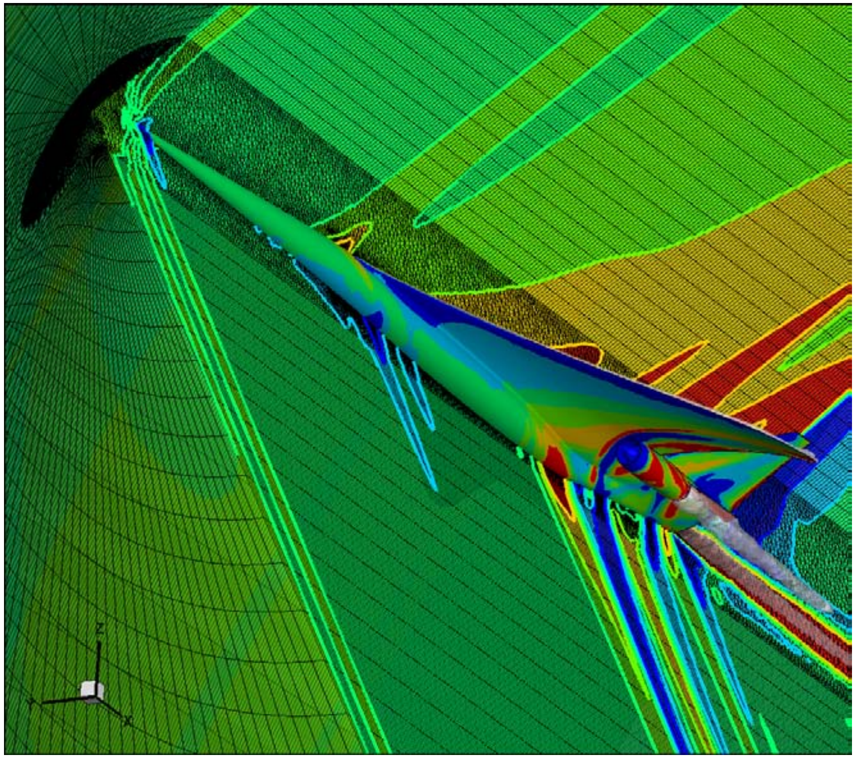
Ongoing Work

- Complex design problems (sonic boom)
- Poorly behaved objectives
- Mode visualization



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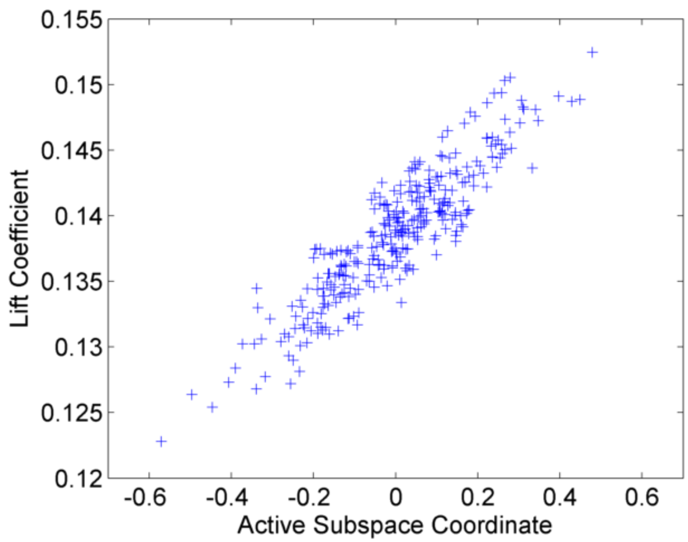
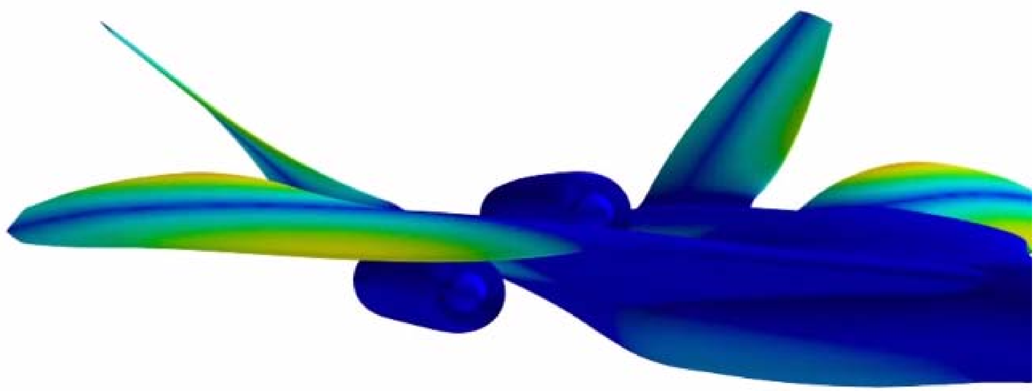
Ongoing Work

Active Subspace Mode Visualization





➢ **To provide design insight**

aerospace**design**lab

Questions?

Thank You!

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