東北大学 流体科学研究所
Institute of Fluid Science, Tohoku University

不確かさの定量的評価のための効果的手法の開発

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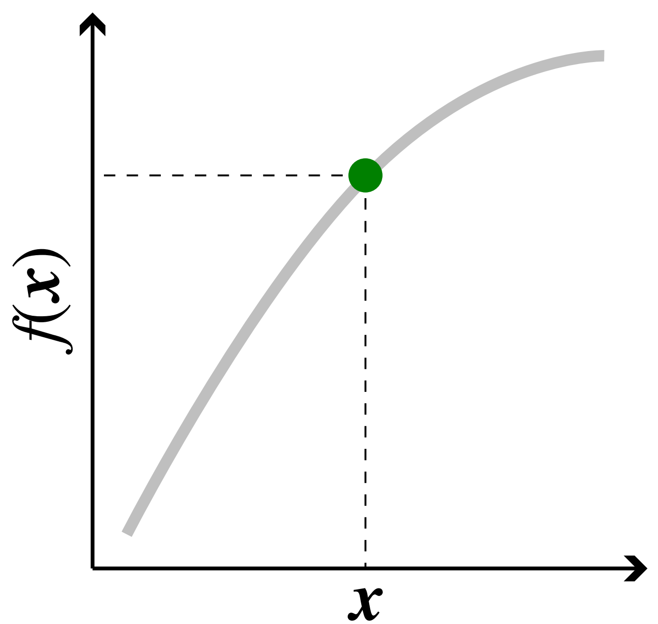
日本機械学会計算力学部門　第7回設計情報学研究会，軽井沢，*2015年1月23日*

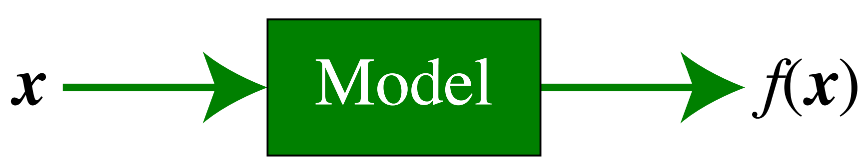
Outline

- ✓ **Fundamentals of Uncertainty Quantification**
- ✓ Research Topics
  - ● Polynomial Chaos Expansion with Order Adjustment
    - ✳ Prof. Shigeru Obayashi (Tohoku Univ.)
    - ✳ Mr. Akihiro Inoue (Tohoku Univ.)
    - ✳ JAXA/NSRG
  - ● Dynamic Adaptive Sampling based on Kriging Surrogate Model
    - ✳ Dr. Soshi Kawai (JAXA/ISAS)
    - ✳ Prof. Juan J. Alonso (Stanford Univ.)
- ✓ Summary

Uncertainty Quantification (UQ)

Science of quantitative characterization and reduction of uncertainties in applications [wikipedia.org]





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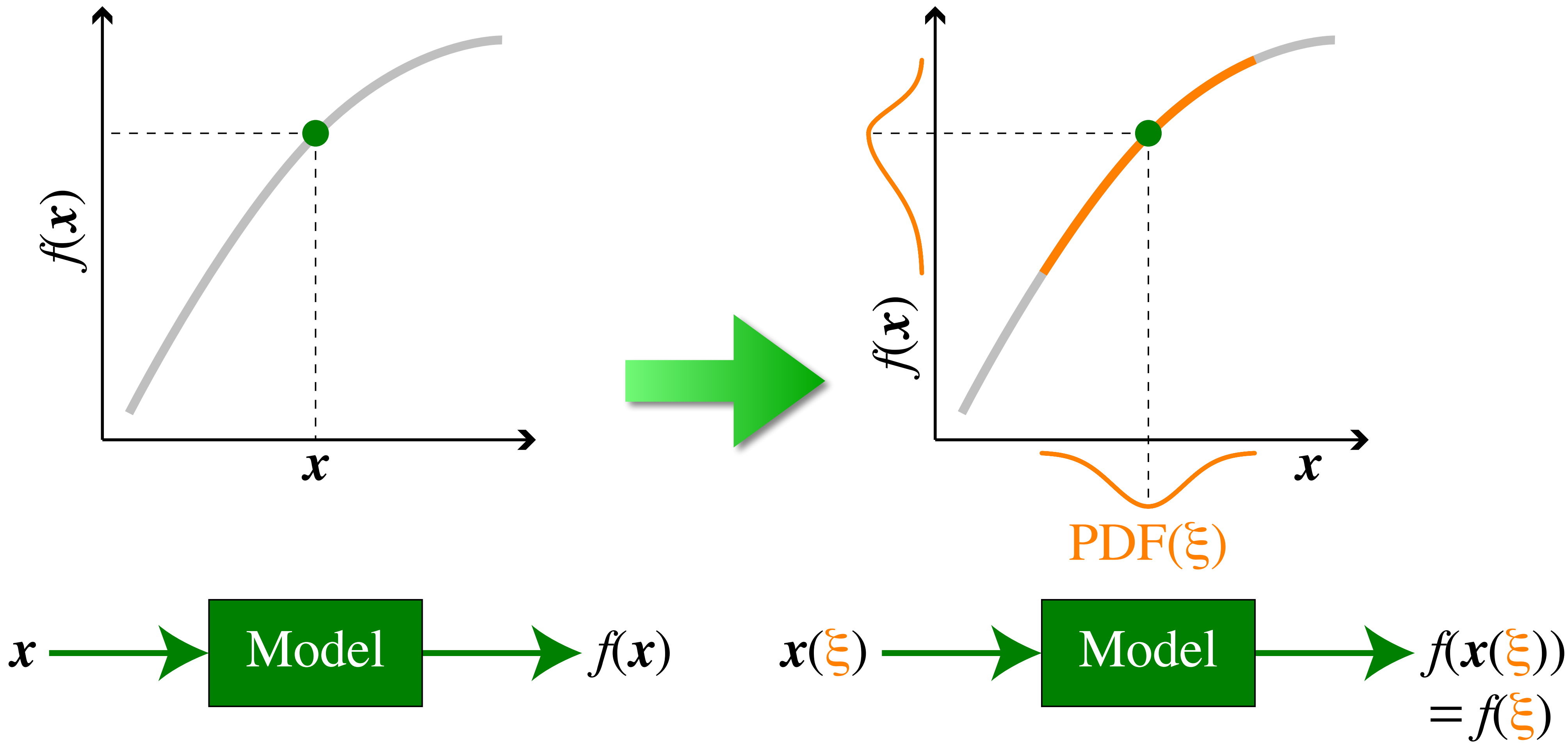


CFD Challenges

Vision 2030 "Where we believe CFD should go"

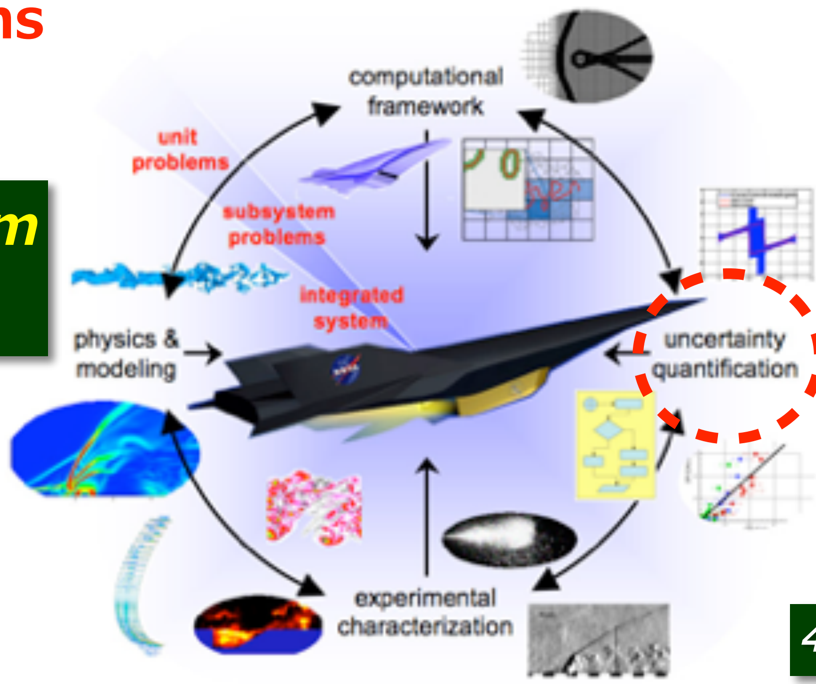
[Andersen 2012]

- Accurate prediction of boundary layer transition
- Improved RANS model for efficient complex flow analysis
- Accurate prediction recovery, dynamic distortion, and swirl patterns at the Aerodynamic Interface Plane (AIP) for propulsion integration
- Accurate prediction of shock-boundary layer in presence of corner flows
- An advanced turbulence model within a single framework for accurate unsteady flow phenomena
- Efficient and robust mesh adaptation for complex configurations
- **Error estimation and uncertainty predictions**
- Multidisciplinary analysis (aeroelasticity, etc.)

Predictive Science Academic Alliance Program (PSSAP)

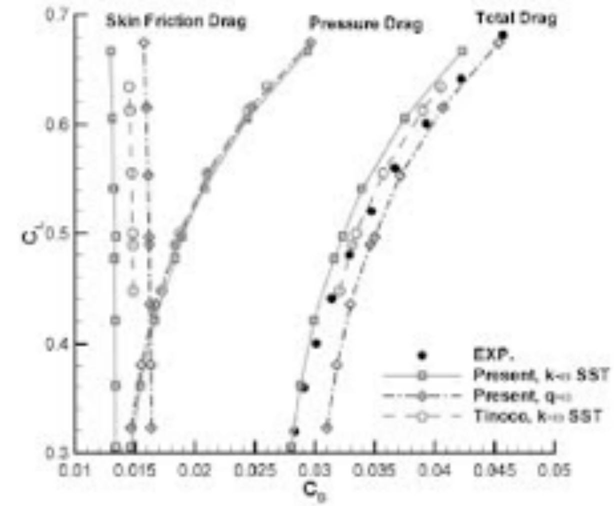
[pssap.stanford.edu]

Predictive Simulations of Multi-Physics Flow Phenomena, with Application to Integrated Hypersonic Systems

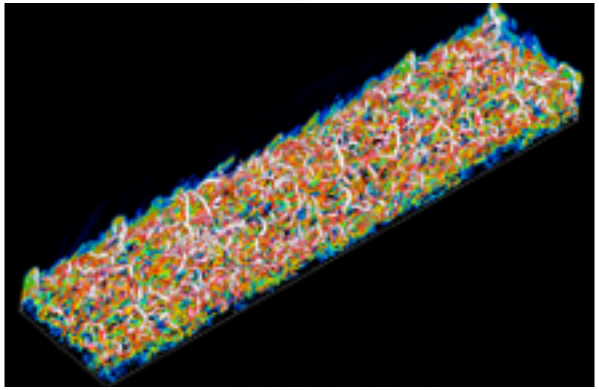


Contributions of UQ

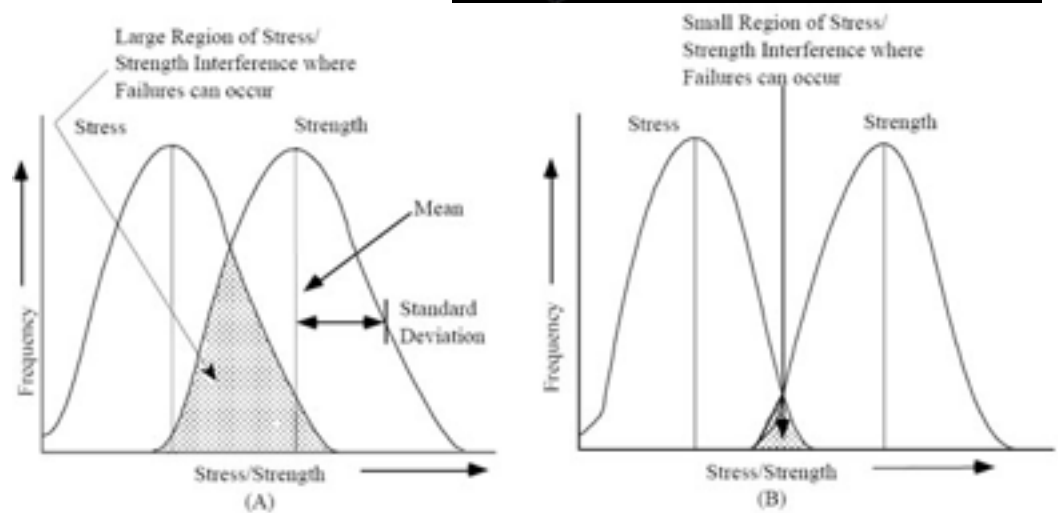
✓ Simulation
- Assist verification and validation
- Make perfect models



✓ Physics
- Understand complex phenomena
- Find exact principles



✓ Design
- Evaluate robustness
- Ensure reliability

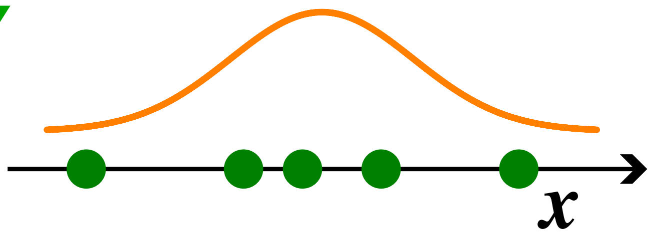


Types of Uncertainty

✓ Aleatory (Irreducible) Uncertainty

- Inherent variation associated with the system under consideration
- Defined in a probabilistic framework

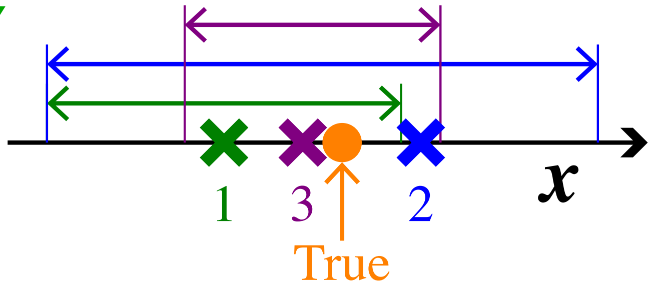
→ Material properties, operating conditions, manufacturing tolerances, ...



✓ Epistemic (Reducible) Uncertainty

- Lack of knowledge or information in any phase or activity of the modeling process
- Involves a single but unknown true value

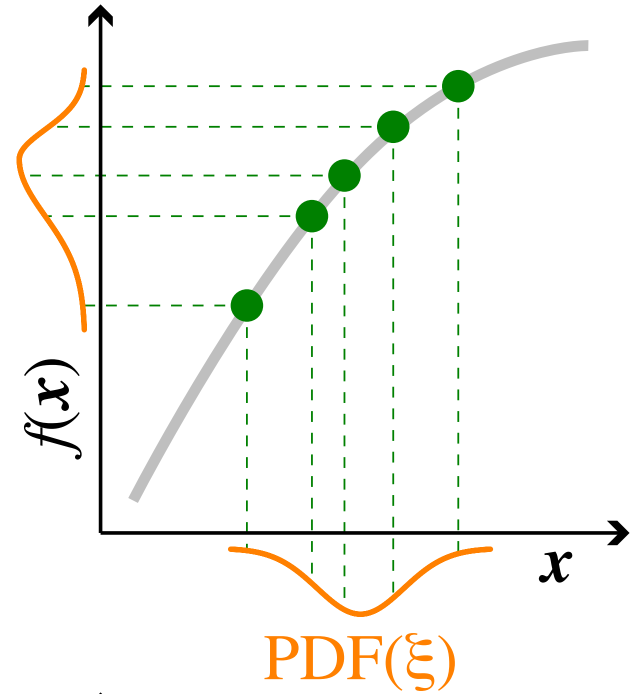
→ Turbulence models, chemical process models, ...



Types of Uncertainty Propagation

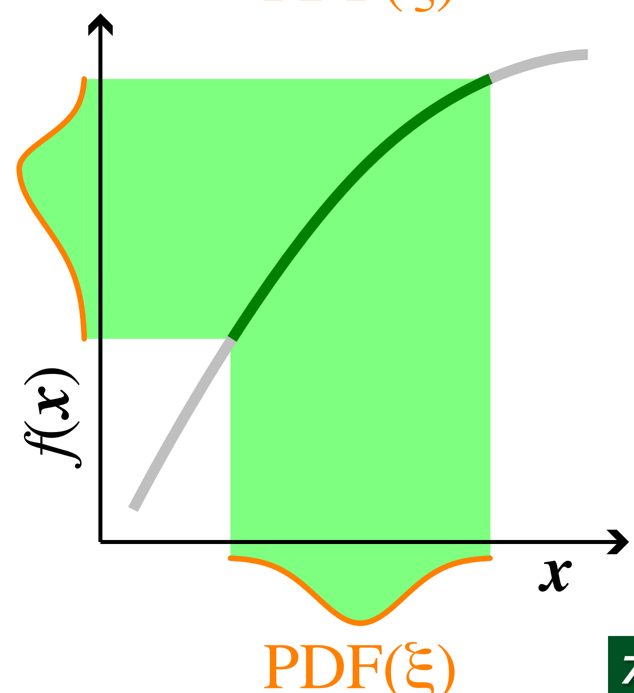
✓ Non-Intrusive Methods

- Only require (multiple) solutions of the original (deterministic) model
- Treat the model as a black box
- Less efficient to compute



✓ Intrusive Methods

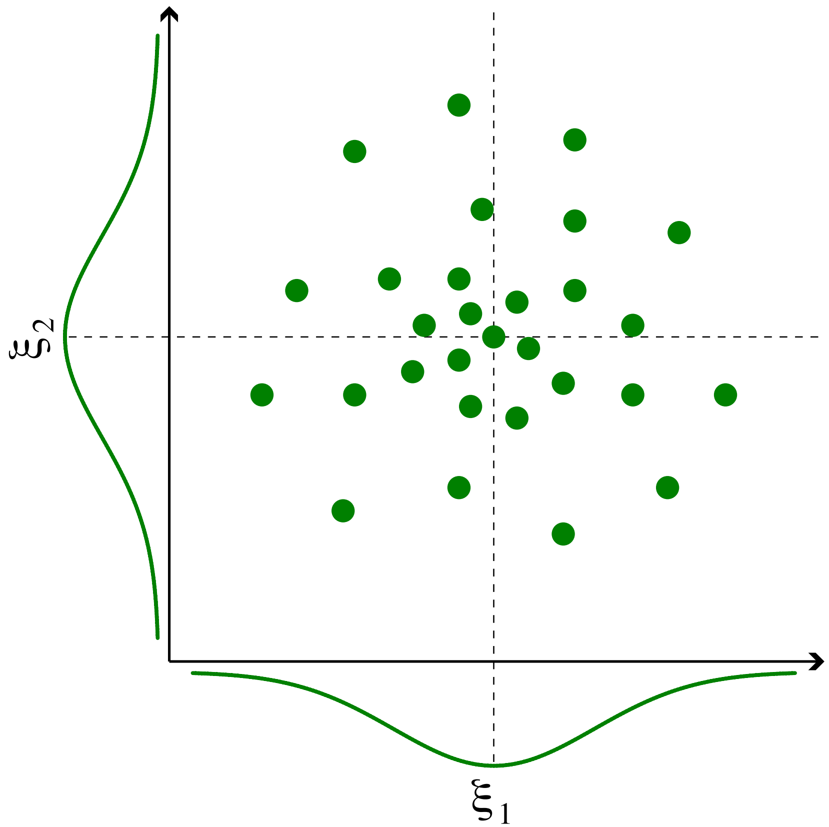
- Require the formulation and solution of a stochastic version of the original model
- Need to know the mathematical structure of the model
- More efficient to compute



Sampling Methods

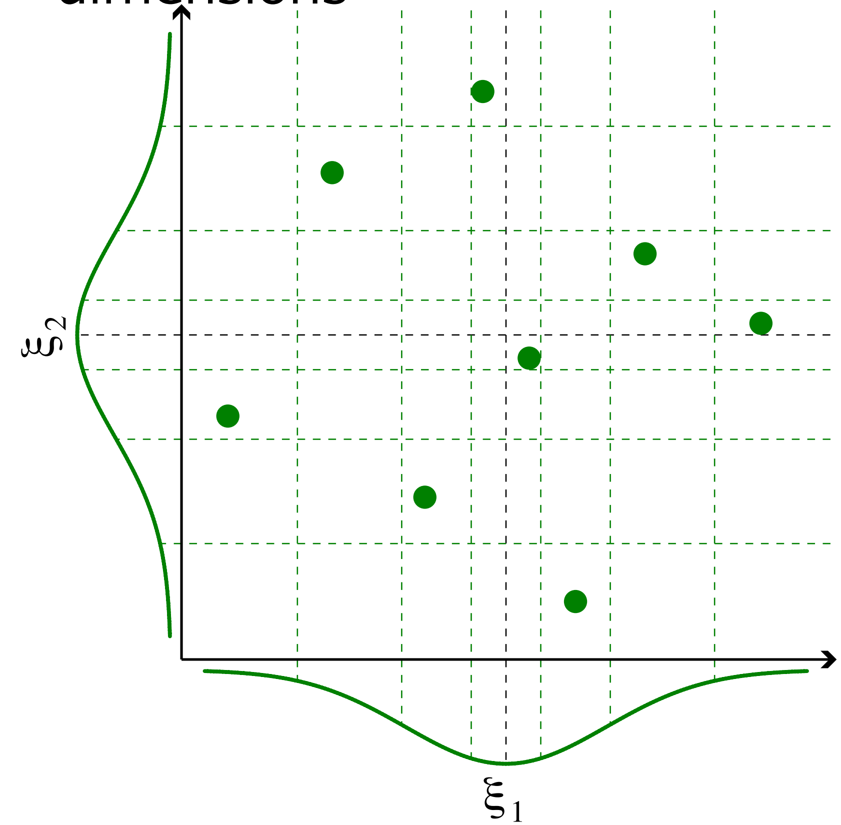
✓ Monte Carlo (MC)

Samples all points randomly



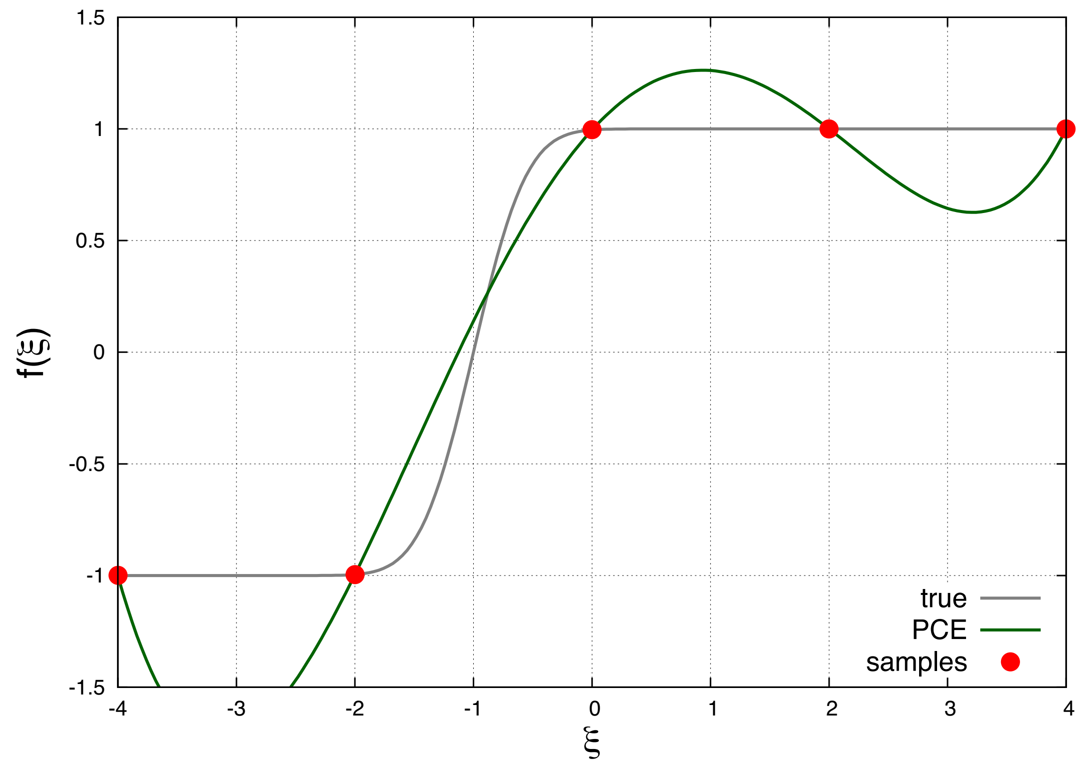
✓ Latin Hypercube Sampling (LHS) [Mckay *et al.* 1979]

- Samples a point in each equi-probability partition randomly
- Does not allow overlapping partitions to be sampled for all dimensions



Approximation Methods

$$f(\xi) \simeq \sum_{i=1}^{P} \alpha_i \phi_i(\xi)$$



✓ *Polynomial Chaos Expansion (PCE)* [Xiu & Karniadakis 2002]

- Approximates as a linear combination of orthogonal polynomials
- Estimates coefficients for known orthogonal polynomials

✓ *Stochastic Collocation (SC)* [Xiu & Hesthaven 2005]

- Approximates as a linear combination of interpolation polynomials
- Forms interpolation functions for known coefficients

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Point Collocation Rules for PCE

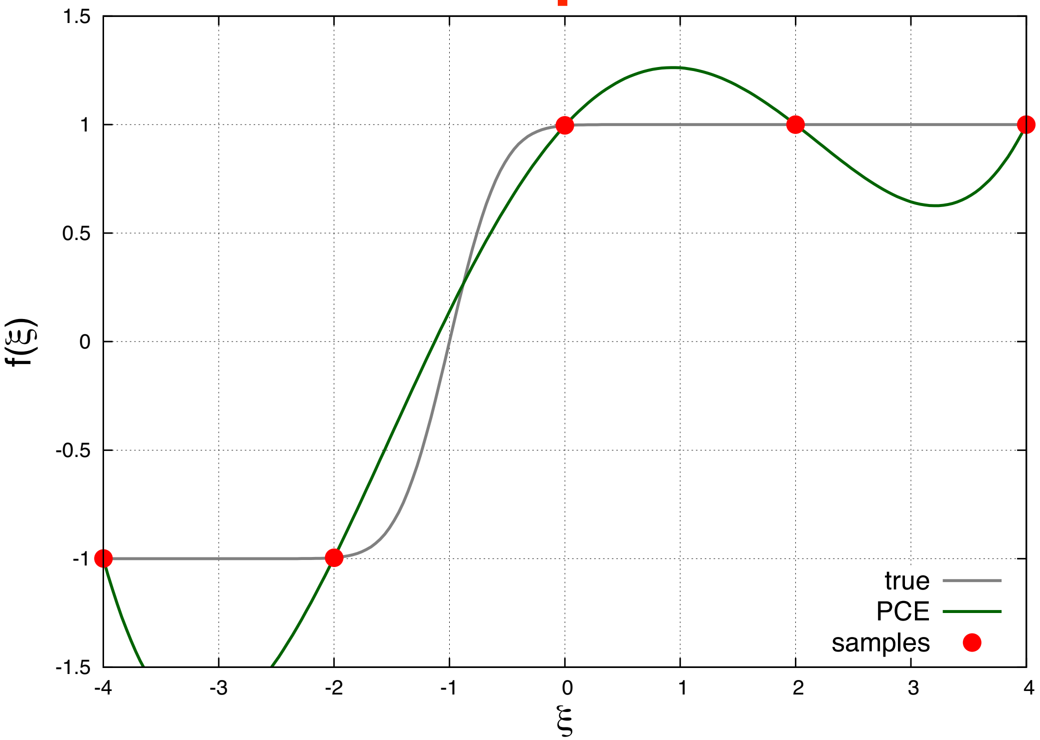
✓ Space Filling

- Reuses the previous samples efficiently
- May induce oscillations as the polynomial order increases (Runge's Phenomenon)

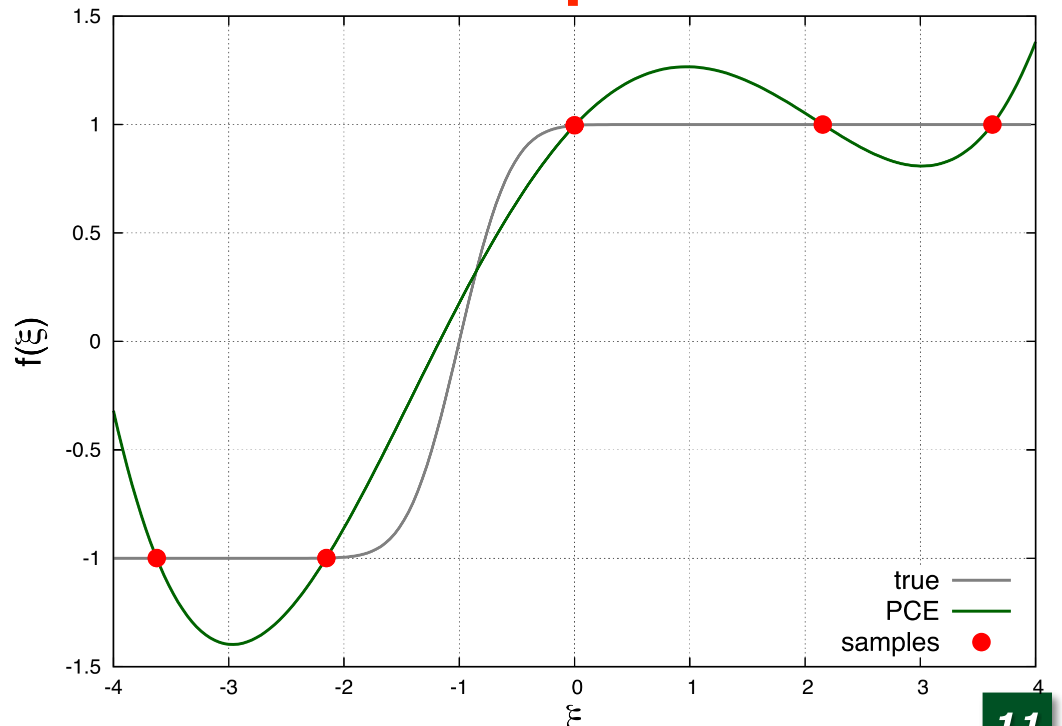
✓ Gauss Quadrature

- Achieves accurate adaptation without oscillations
- Restricts samples to unique locations

5 samples



5 samples



Point Collocation Rules for PCE

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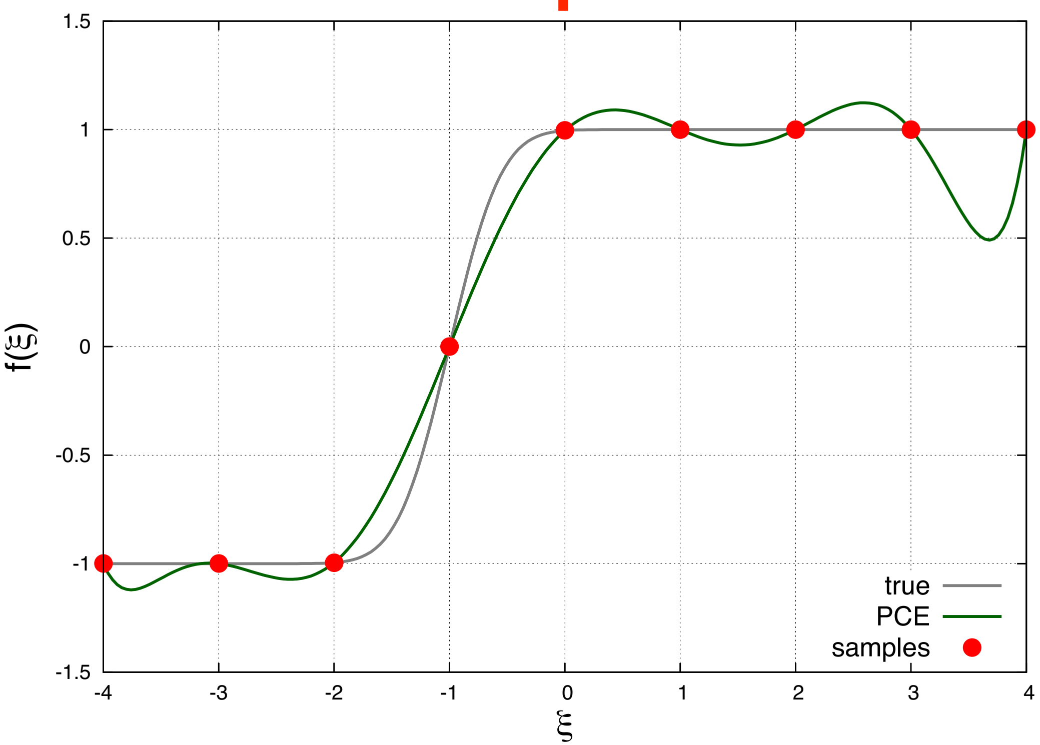
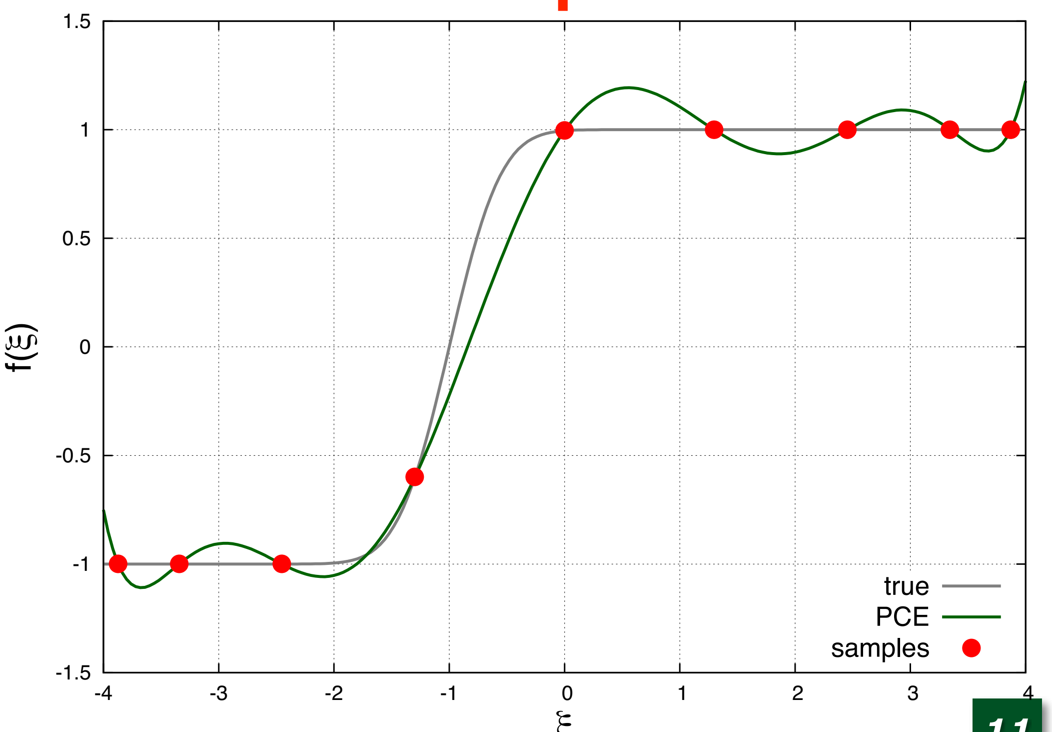
9 samples



9 samples



Point Collocation Rules for PCE

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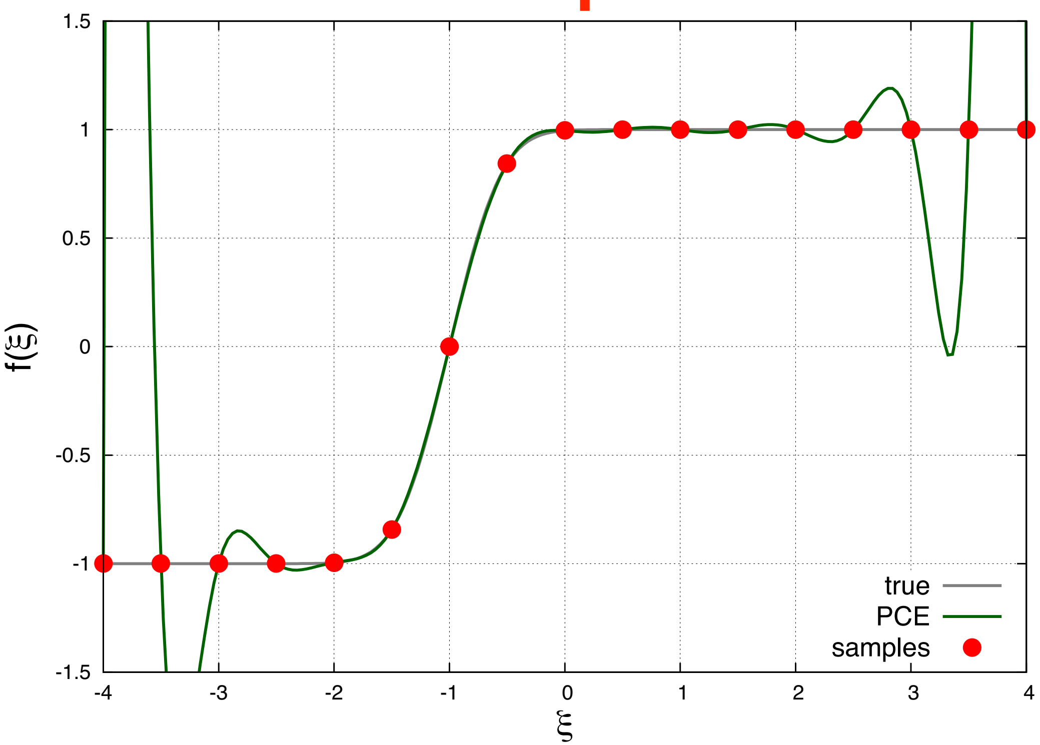
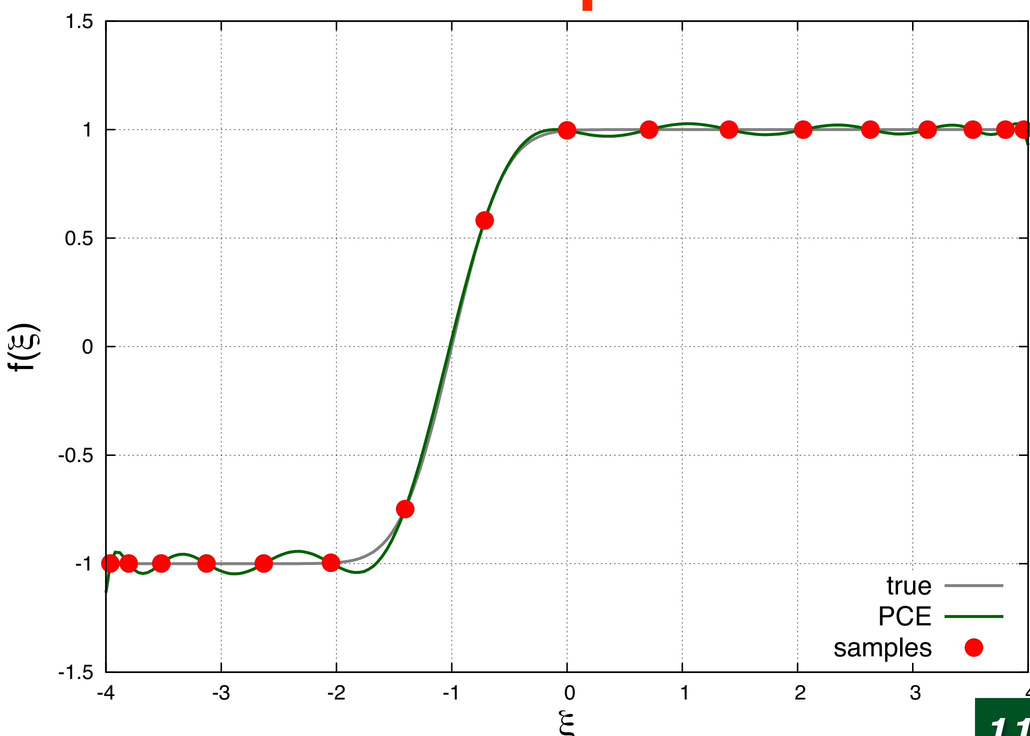
17 samples



17 samples



Research Objectives

✓ Propose PCE with order adjustment for effective UQ

- Criteria to adjust the polynomial order and the number of samples

✓ Test the proposed PCE with order adjustment compared with MC

- Analytic functions
- Sonic boom analysis

Polynomial Chaos Expansion (PCE)

$$f(\boldsymbol{\xi}) \simeq \hat{f}(\boldsymbol{\xi}) = \sum_{i=1}^{P} \alpha_i \phi_i(\boldsymbol{\xi})$$

where $P = \dfrac{(n+p)!}{n!p!}$

n: **# dimensions in $\boldsymbol{\xi}$**

p: **Polynomial order**

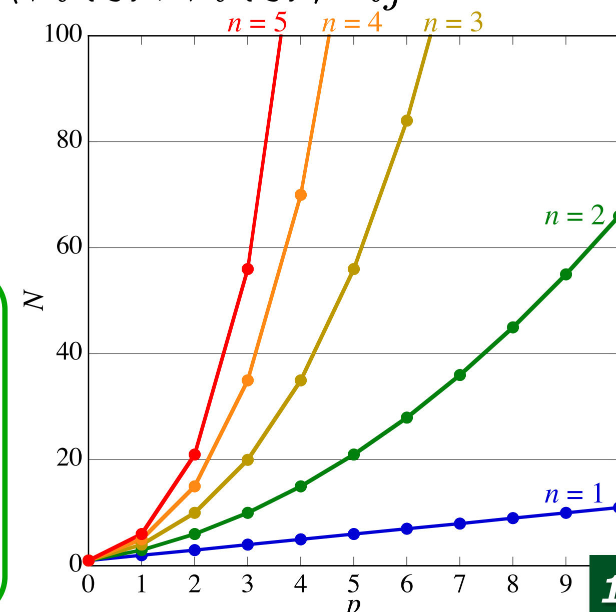
Input uncertainty PDF($\boldsymbol{\xi}$)	Polynomial $\phi_i(\boldsymbol{\xi})$
Uniform	Legendre
Normal	Hermite
Gamma	Laguerre
Beta	Jacobi

$$\langle \phi_i(\boldsymbol{\xi}), \phi_j(\boldsymbol{\xi}) \rangle = \int_{-\infty}^{\infty} \phi_i(\boldsymbol{\xi}) \phi_j(\boldsymbol{\xi}) \mathrm{PDF}(\boldsymbol{\xi}) \mathrm{d}\boldsymbol{\xi} = \langle \phi_i(\boldsymbol{\xi}), \phi_i(\boldsymbol{\xi}) \rangle \delta_{ij}$$

$\alpha_1, \alpha_2, \cdots, \alpha_P$ obtained from N ($\geq P$) samples

$$f(\boldsymbol{\xi}^{(j)}) = \sum_{i=1}^{P} \alpha_i \phi_i(\boldsymbol{\xi}^{(j)})$$

$$(j = 1, 2, \cdots, N)$$



$$\mu_f = \mathrm{E}[f(\boldsymbol{\xi})] \simeq \alpha_1$$

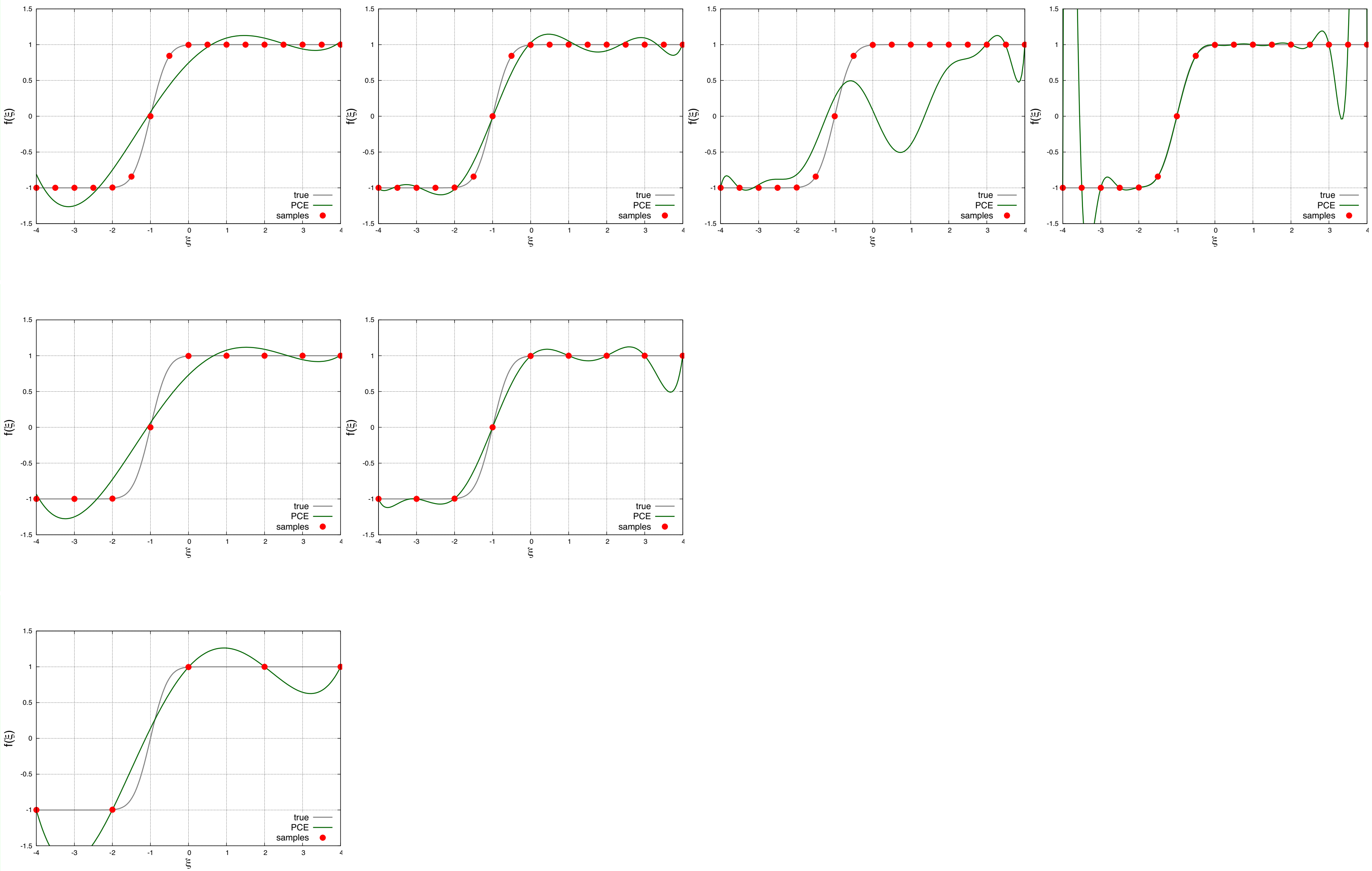
$${\sigma_f}^2 = \mathrm{Var}[f(\boldsymbol{\xi})] \simeq \sum_{i=2}^{P} {\alpha_i}^2 \langle \phi_i(\boldsymbol{\xi}), \phi_i(\boldsymbol{\xi}) \rangle$$

PCE Examples

$N = 17$

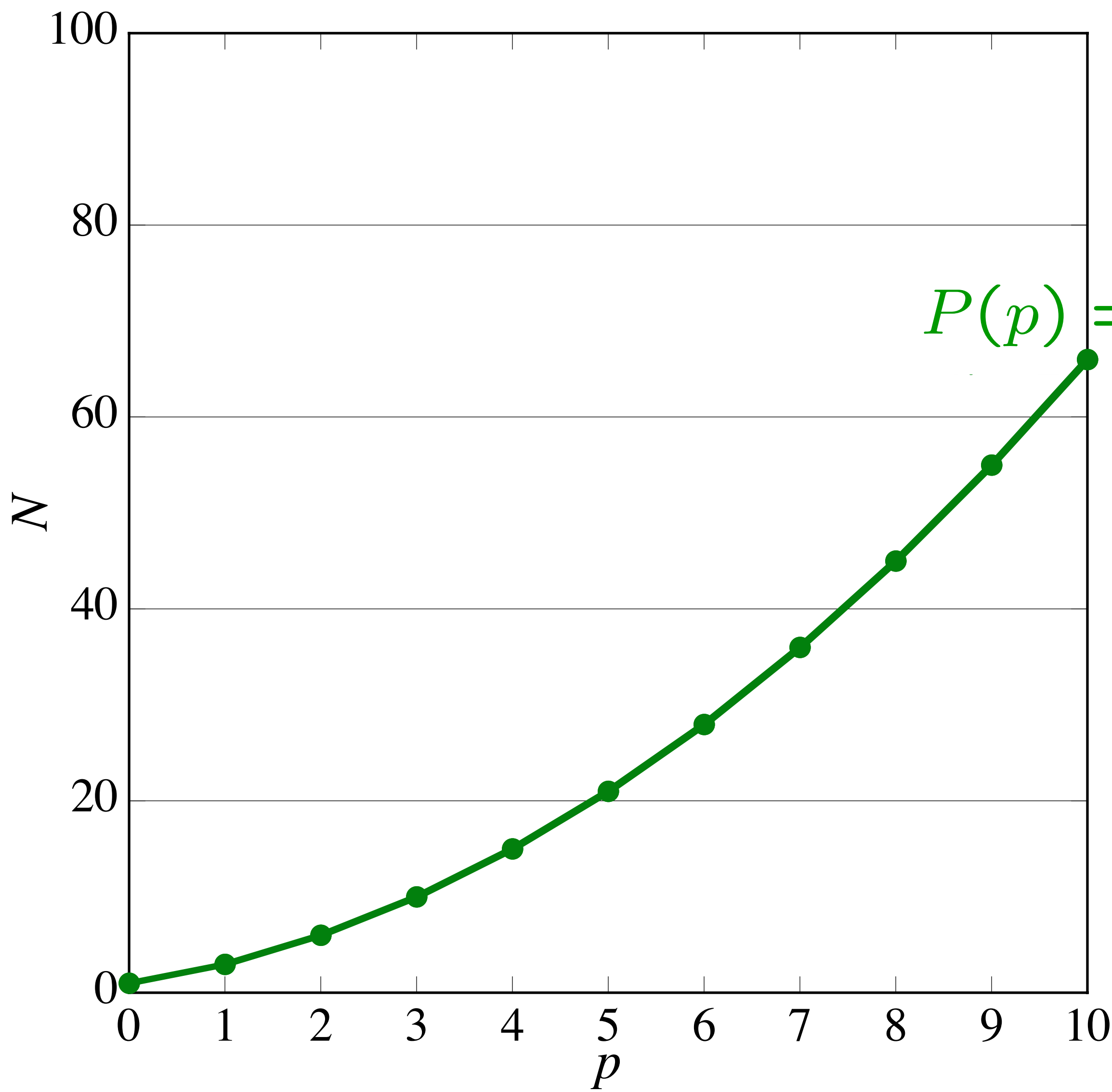
$N = 9$

$N = 5$



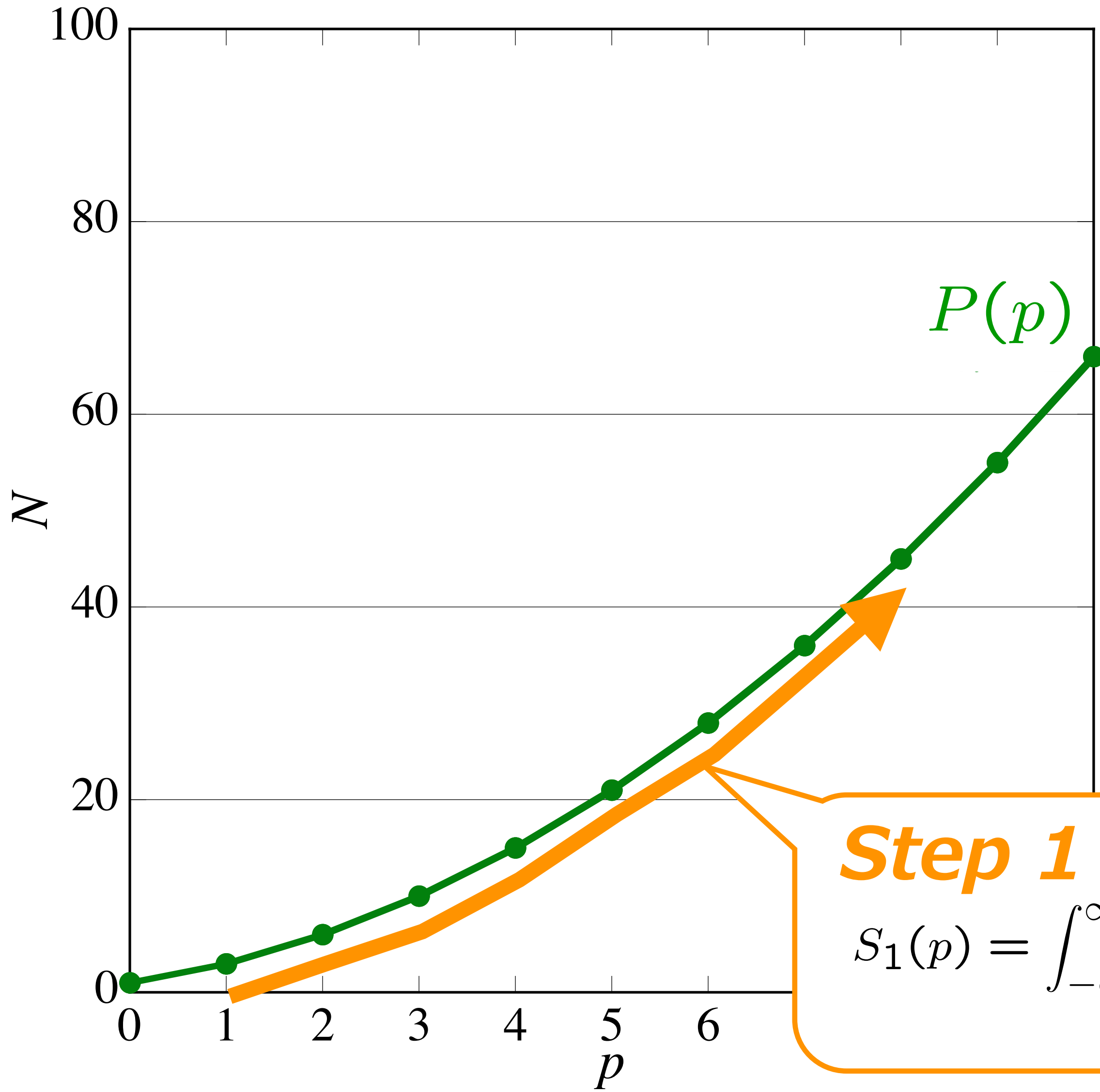
$p = 4$ | $p = 8$ | $p = 12$ | $p = 16$

Adjustment Strategy for PCE



$$P(p) = \frac{(n+p)!}{n!p!}$$

Adjustment Strategy for PCE

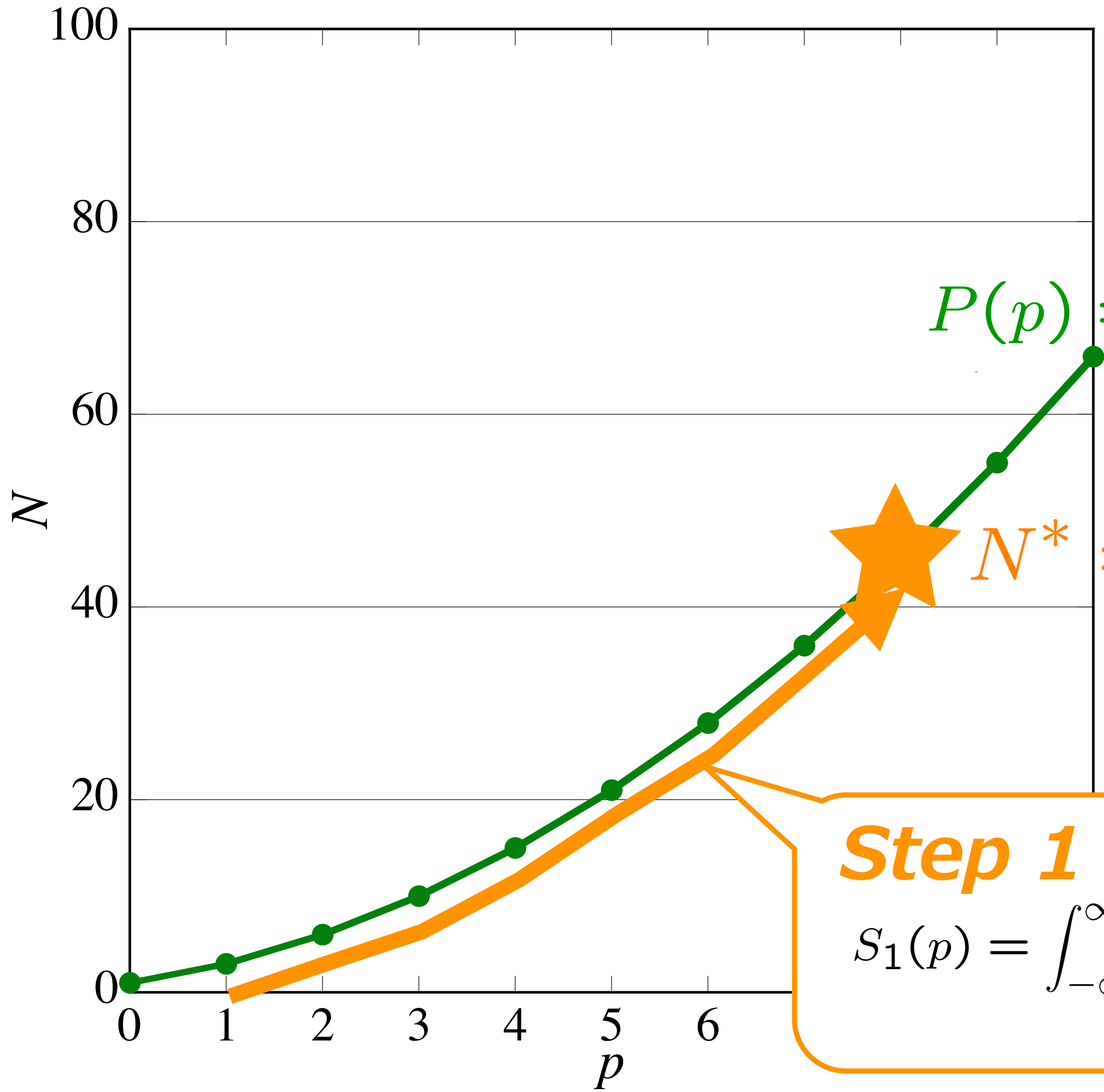


$$P(p) = \frac{(n+p)!}{n!p!}$$

Step 1 adjusts **# samples**

$$S_1(p) = \int_{-\infty}^{\infty} |\hat{f}(\boldsymbol{\xi}|p, P(p)) - \hat{f}(\boldsymbol{\xi}|p-1, P(p-1))| \times \mathrm{PDF}(\boldsymbol{\xi}) d\boldsymbol{\xi}$$

Adjustment Strategy for PCE



$$P(p) = \frac{(n+p)!}{n!p!}$$

$$N^* = P(p^*)$$

Step 1 adjusts **# samples**

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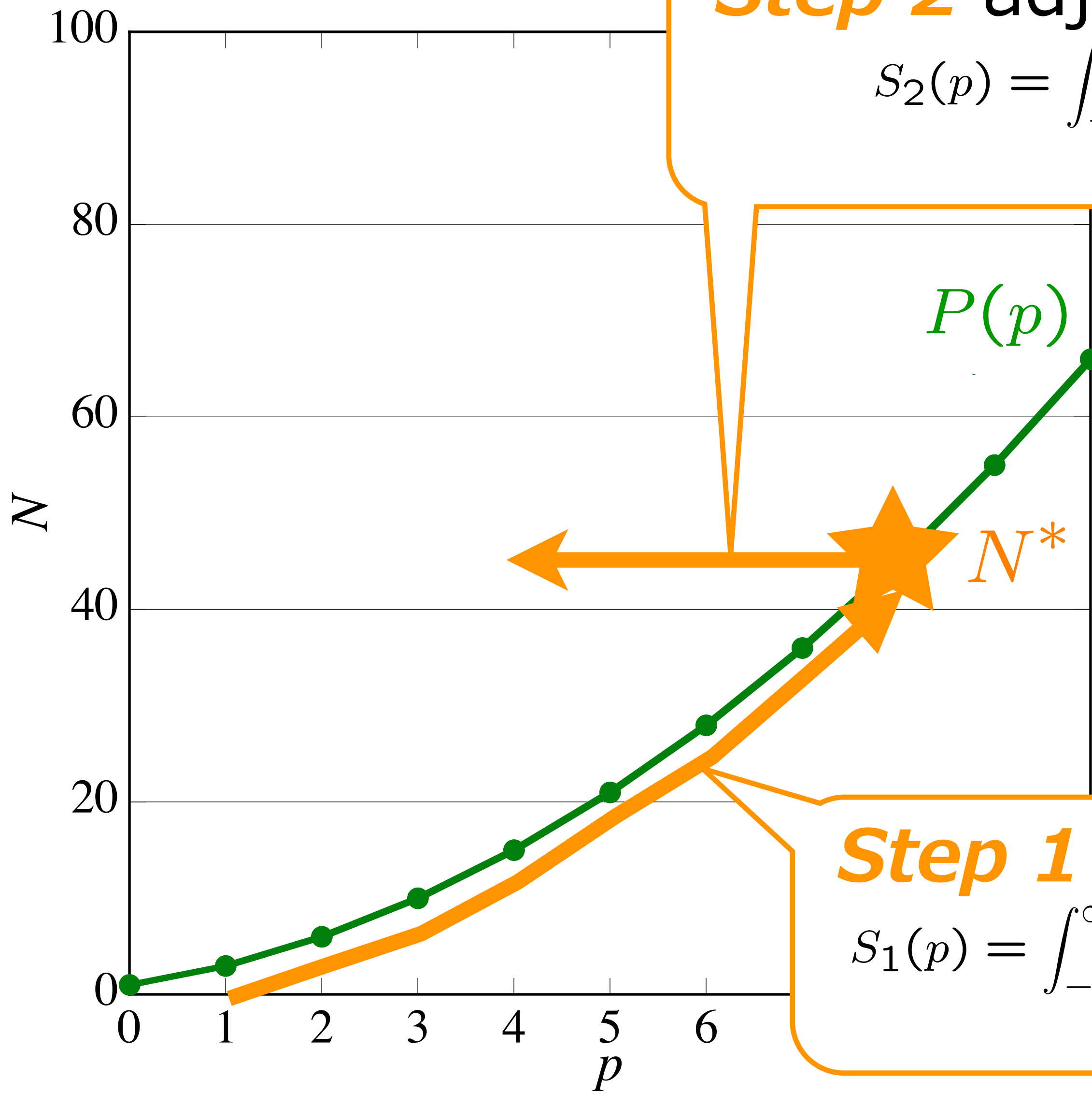

Step 2 adjusts **polynomial order**

$$S_2(p) = \int_{-\infty}^{\infty} |\hat{f}(\boldsymbol{\xi}|p, N^*) - \hat{f}(\boldsymbol{\xi}|p-1, N^*)| \times \mathrm{PDF}(\boldsymbol{\xi}) d\boldsymbol{\xi}$$

Step 1 adjusts **# samples**

$$S_1(p) = \int_{-\infty}^{\infty} |\hat{f}(\boldsymbol{\xi}|p, P(p)) - \hat{f}(\boldsymbol{\xi}|p-1, P(p-1))| \times \mathrm{PDF}(\boldsymbol{\xi}) d\boldsymbol{\xi}$$

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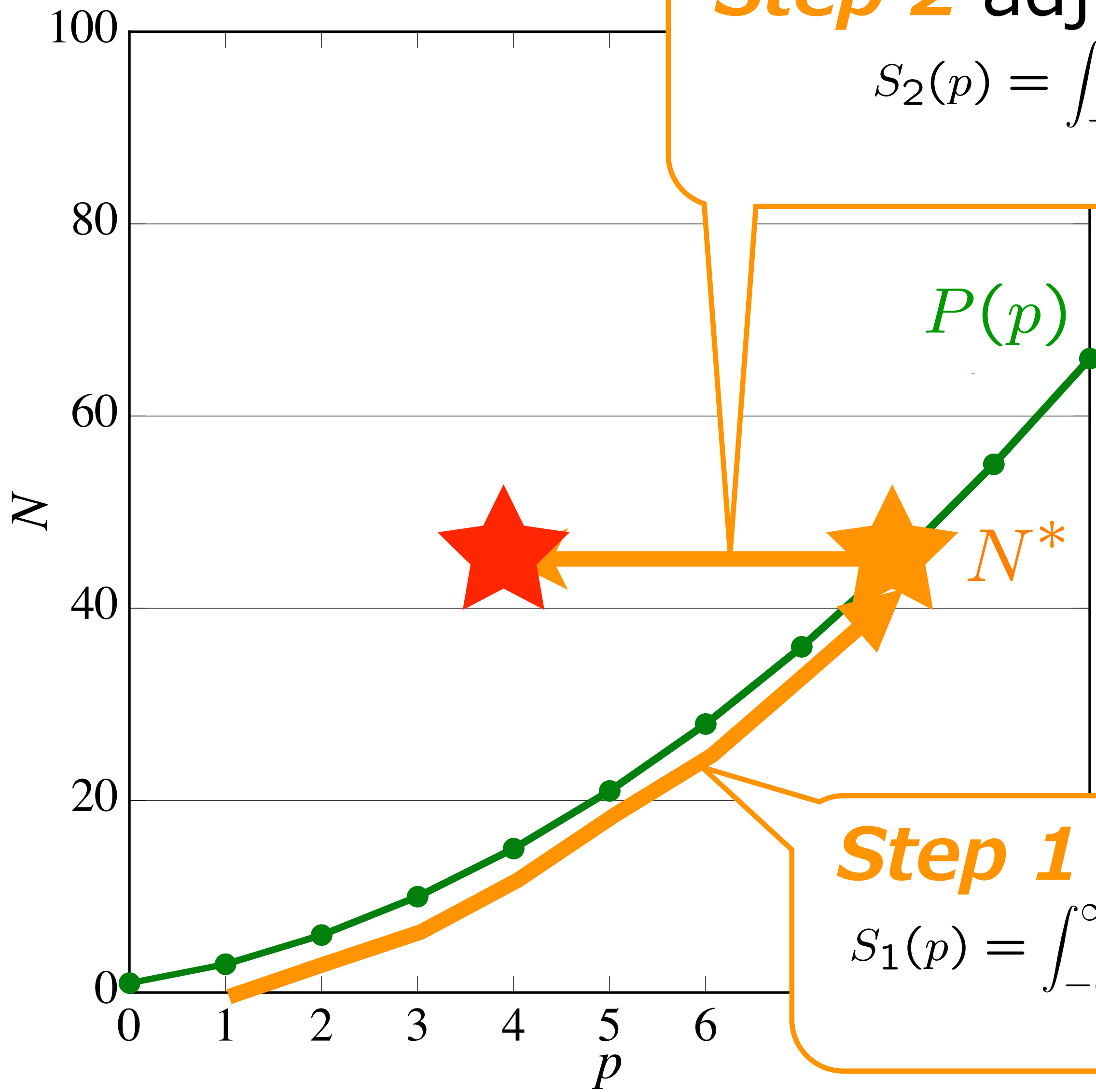

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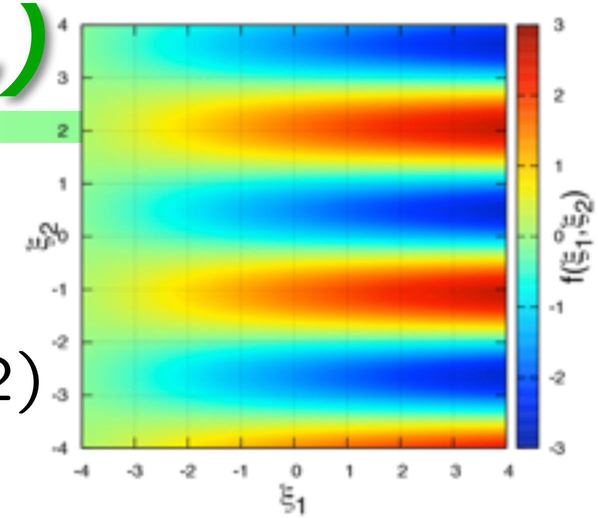
Step 1 adjusts **# samples**

$$S_1(p) = \int_{-\infty}^{\infty} |\hat{f}(\boldsymbol{\xi}|p, P(p)) - \hat{f}(\boldsymbol{\xi}|p-1, P(p-1))| \times \mathrm{PDF}(\boldsymbol{\xi}) d\boldsymbol{\xi}$$

Numerical Tests (2D Func.)

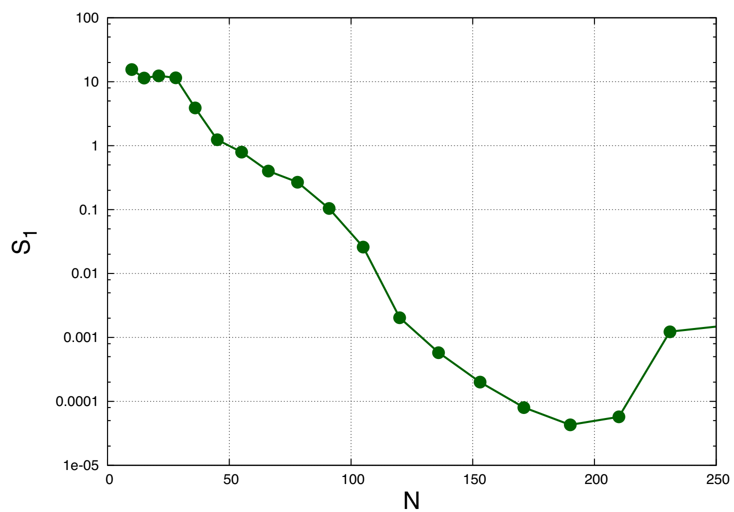


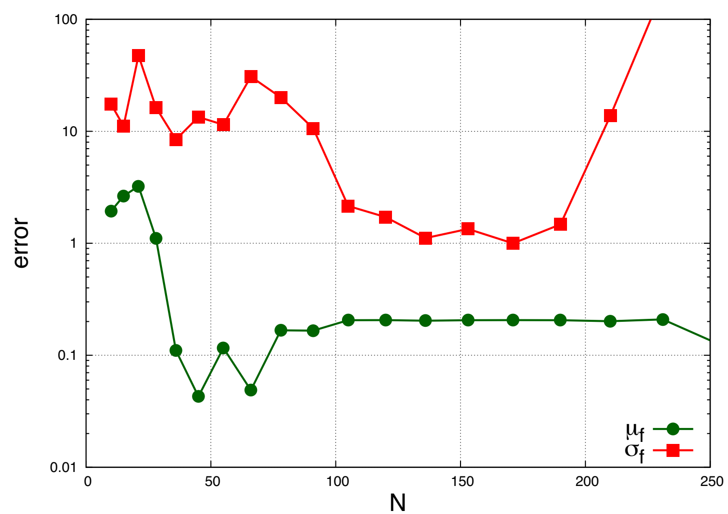
$$f(x_1,x_2) = \ln\left(1+{x_1}^2\right)\sin 5x_2$$

$$\text{where}\quad x_i = 2 + 0.4\xi_i$$

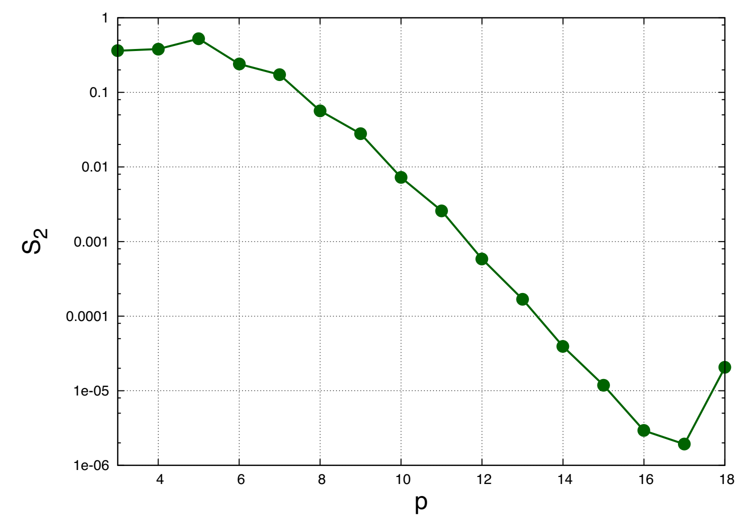
$$\xi_i \sim \mathrm{Norm}(0,1) \qquad (i=1,2)$$

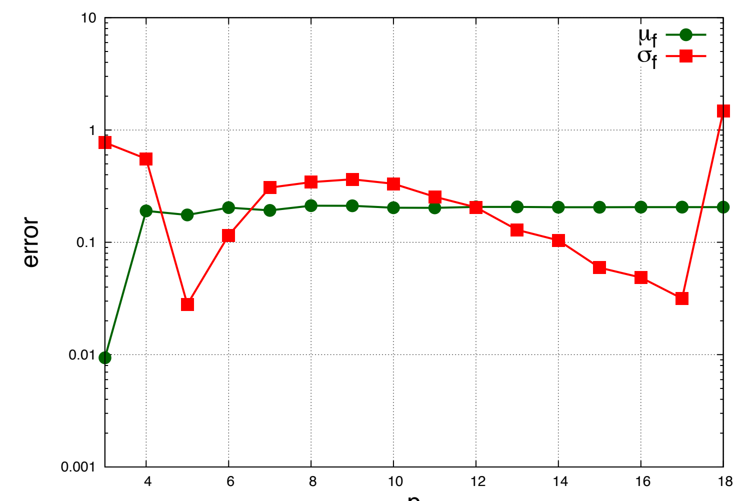
✓ Step 1





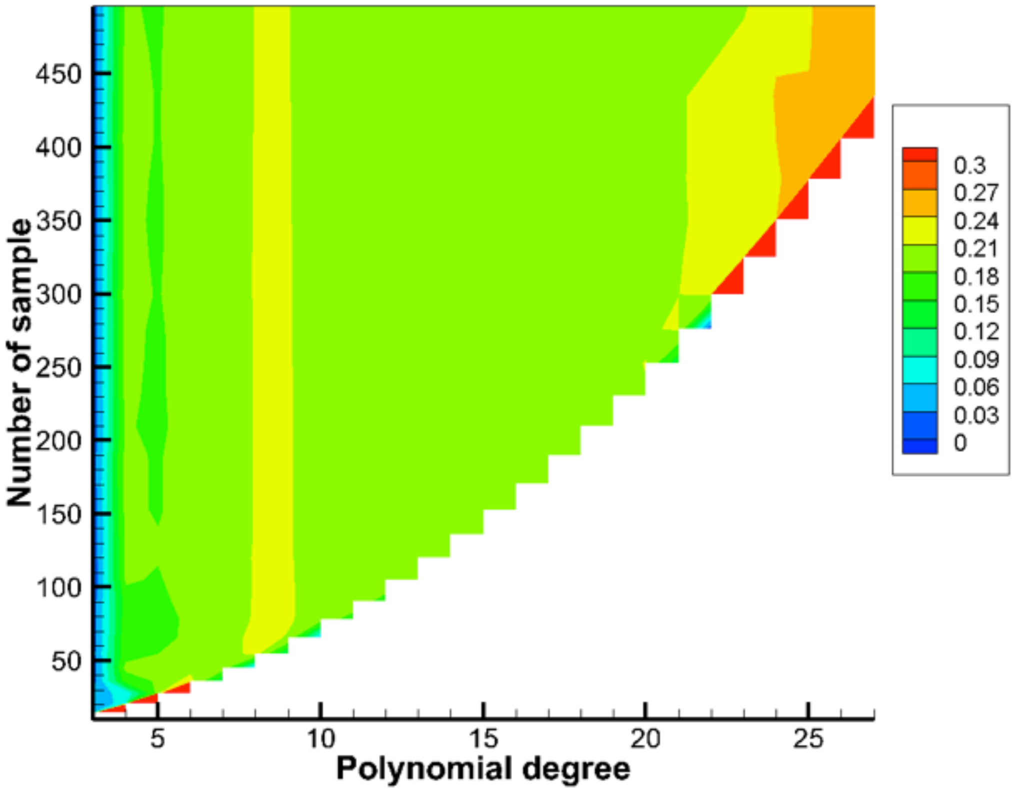
✓ Step 2



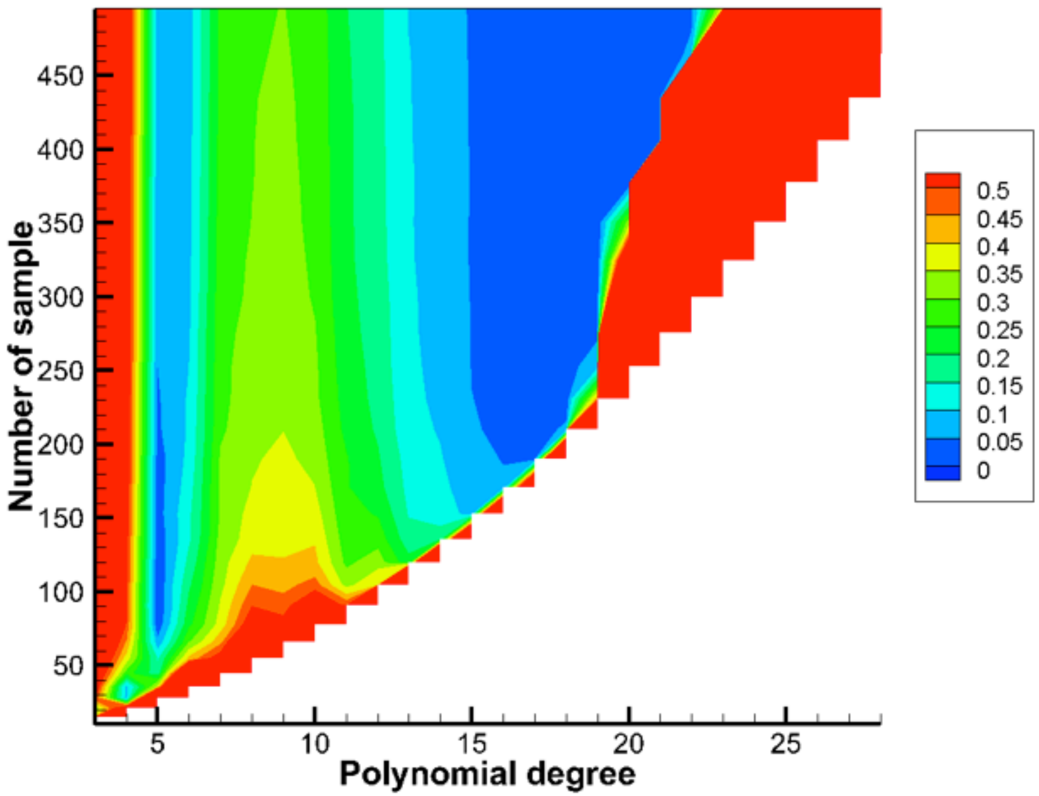


Numerical Tests (2D Func.)

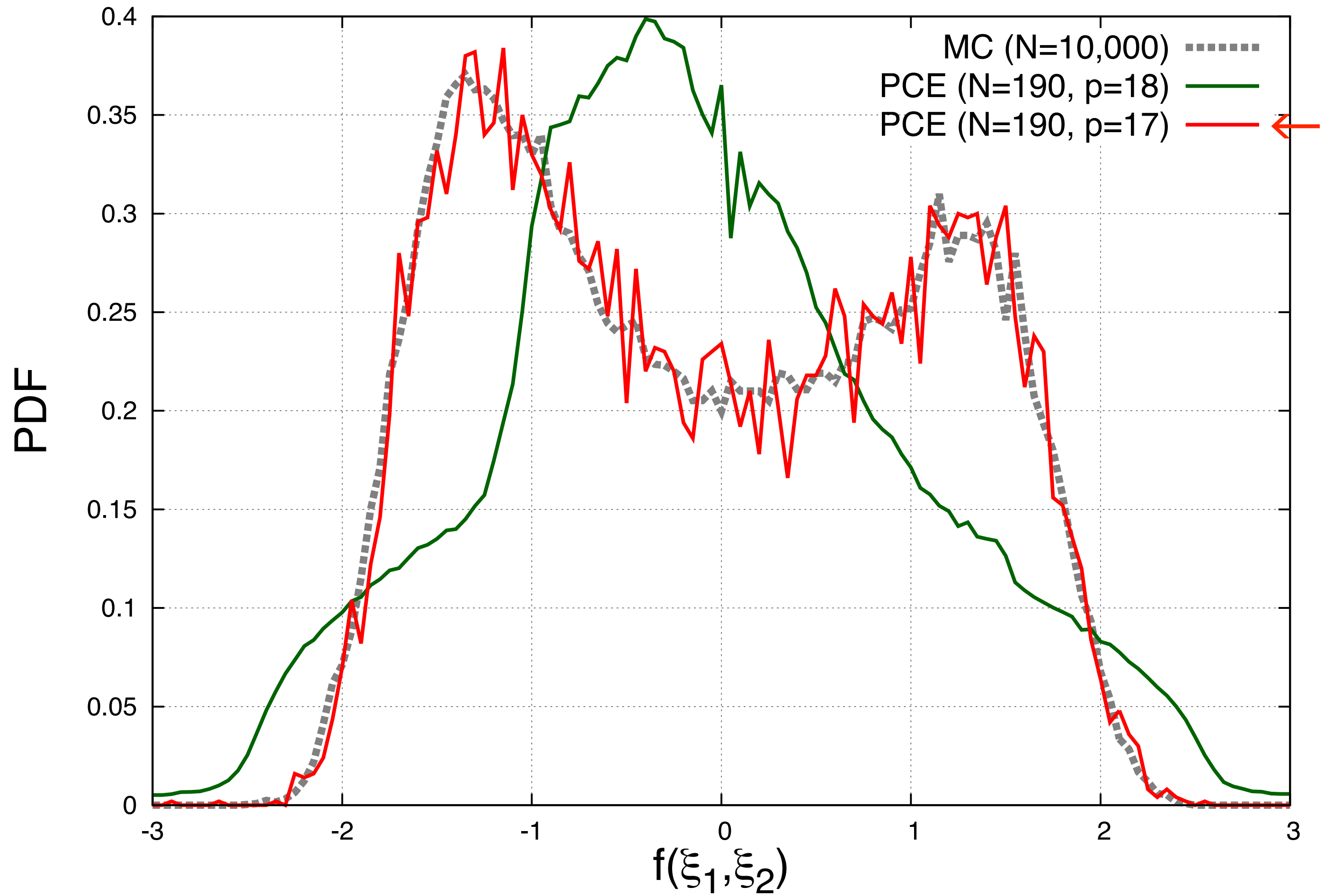
Error in μ_f



Error in σ_f



Numerical Tests (2D Func.)



← after adjustment

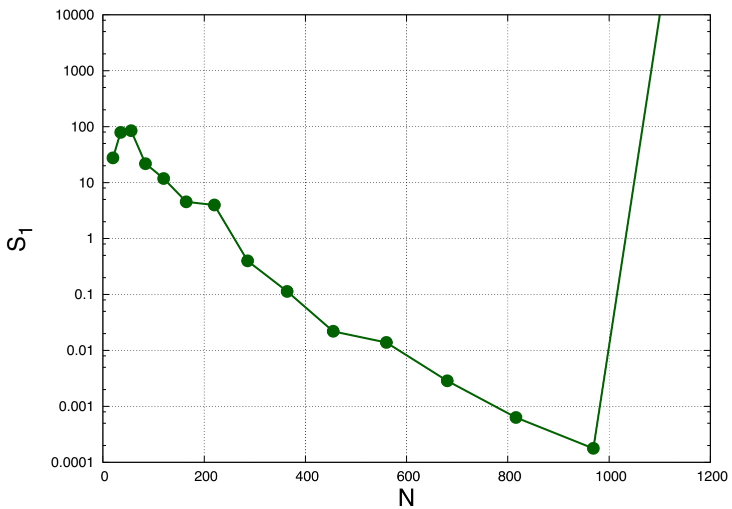
Numerical Tests (3D Func.)

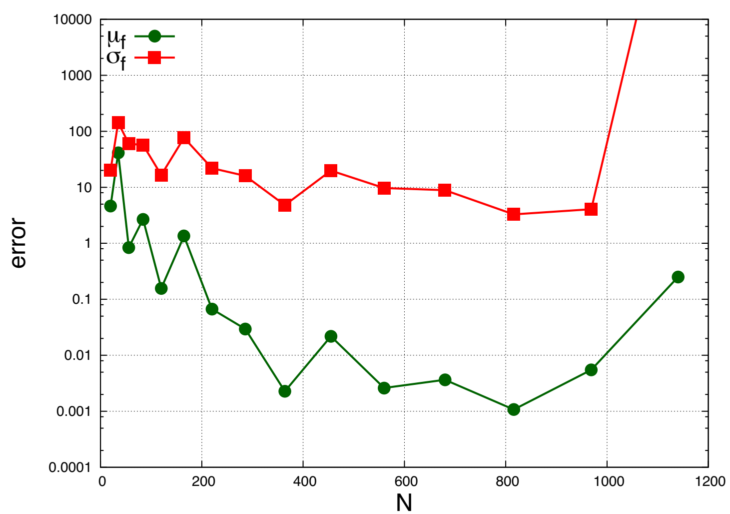
$$f(x_1, x_2, x_3) = \ln\left(1 + {x_1}^2\right) \sin 5x_2 \sin x_3$$

$$\text{where} \quad x_i = 2 + 0.4\xi_i$$

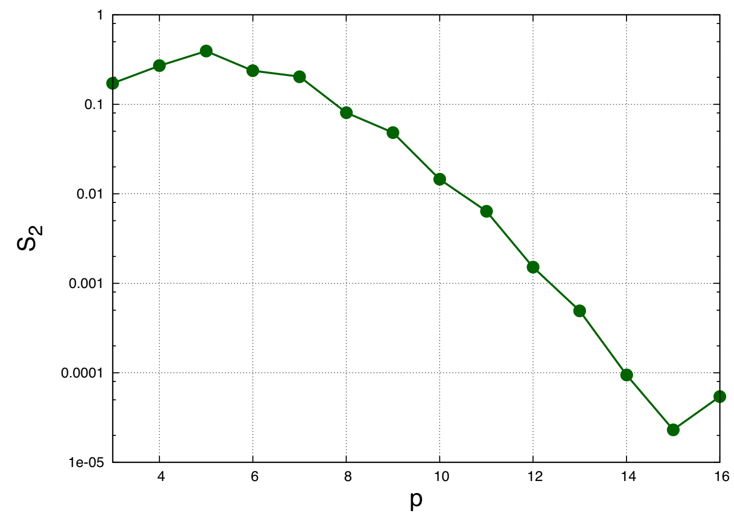
$$\xi_i \sim \mathrm{Norm}(0,1) \qquad (i = 1, 2, 3)$$

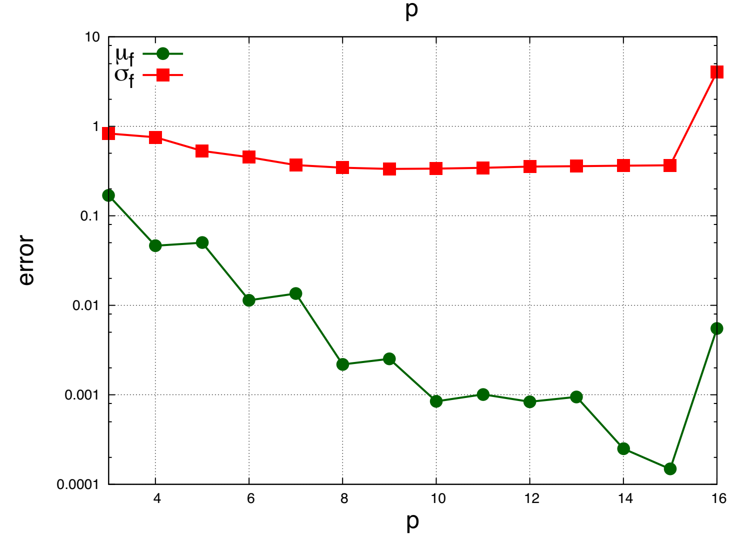
✓Step 1



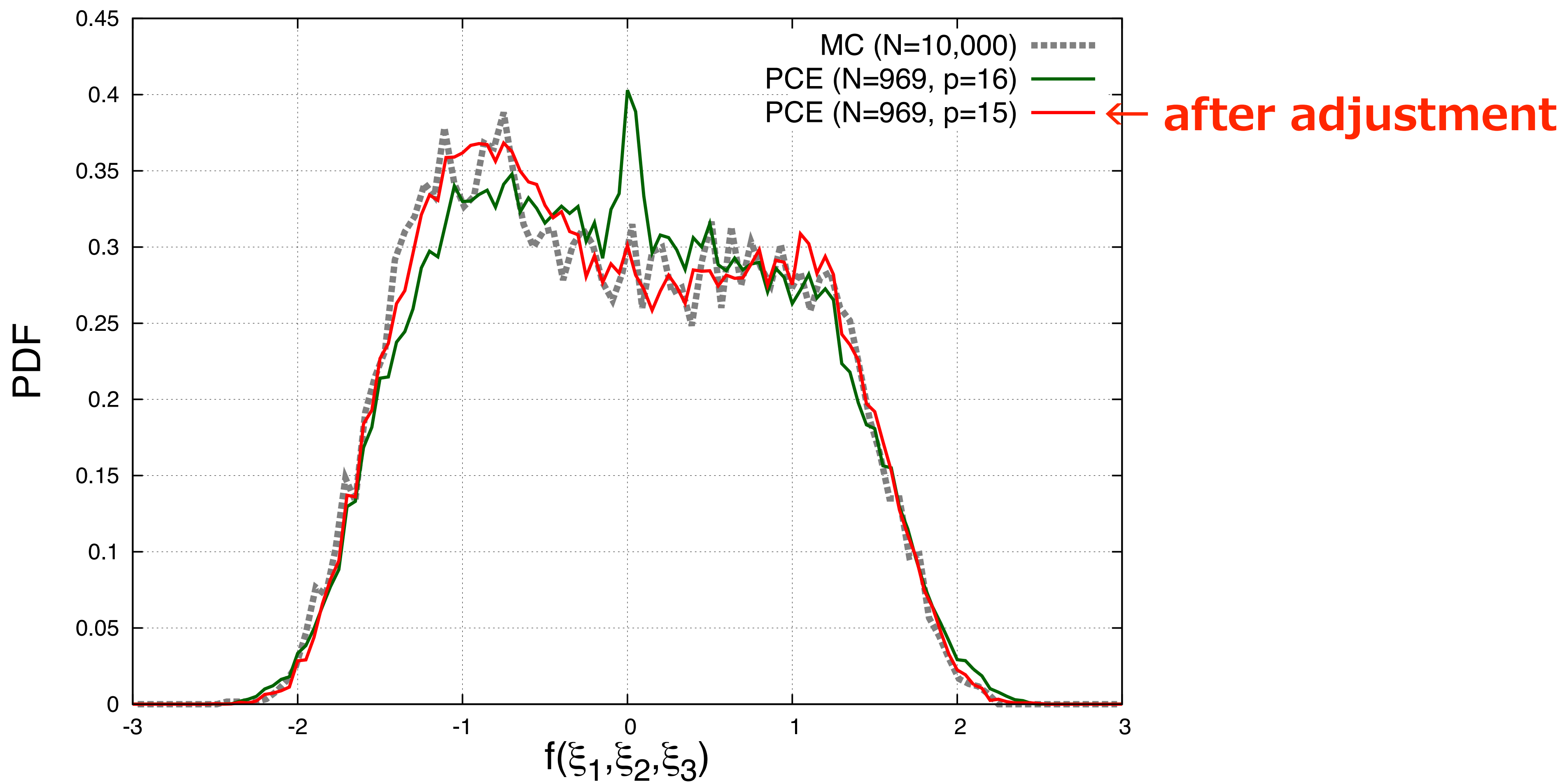


✓Step 2





Numerical Tests (3D Func.)



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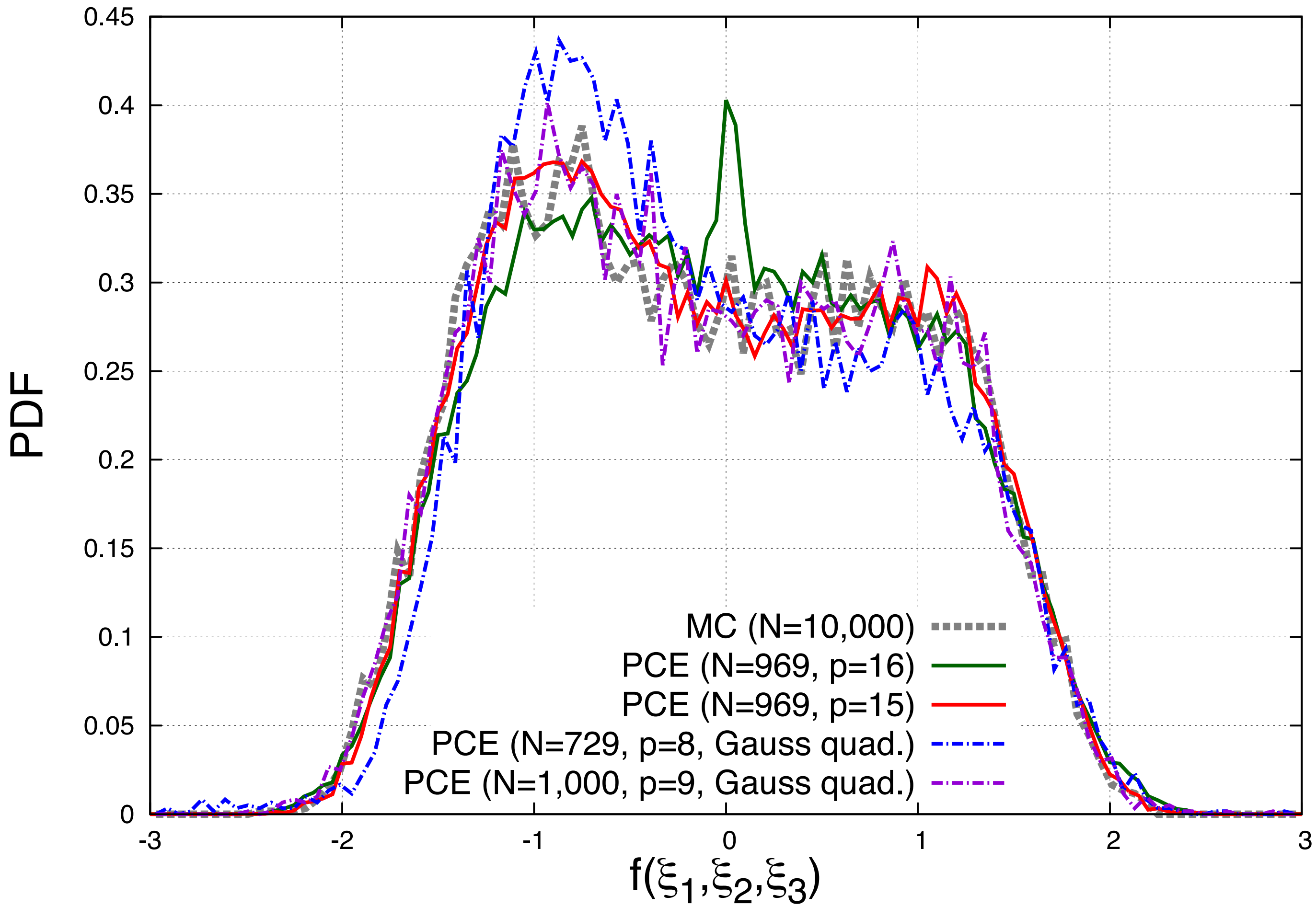
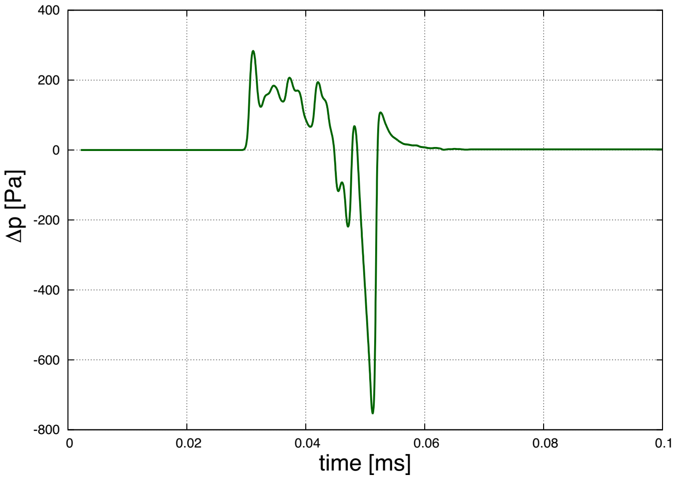
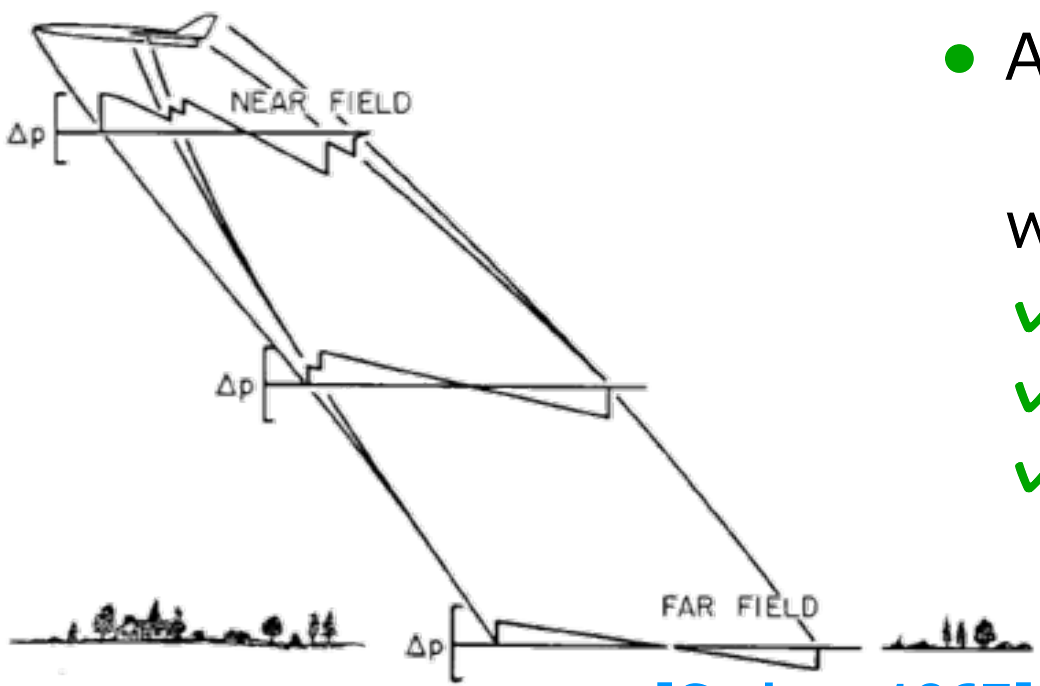


Application (Sonic Boom)



- D-SEND#2 model

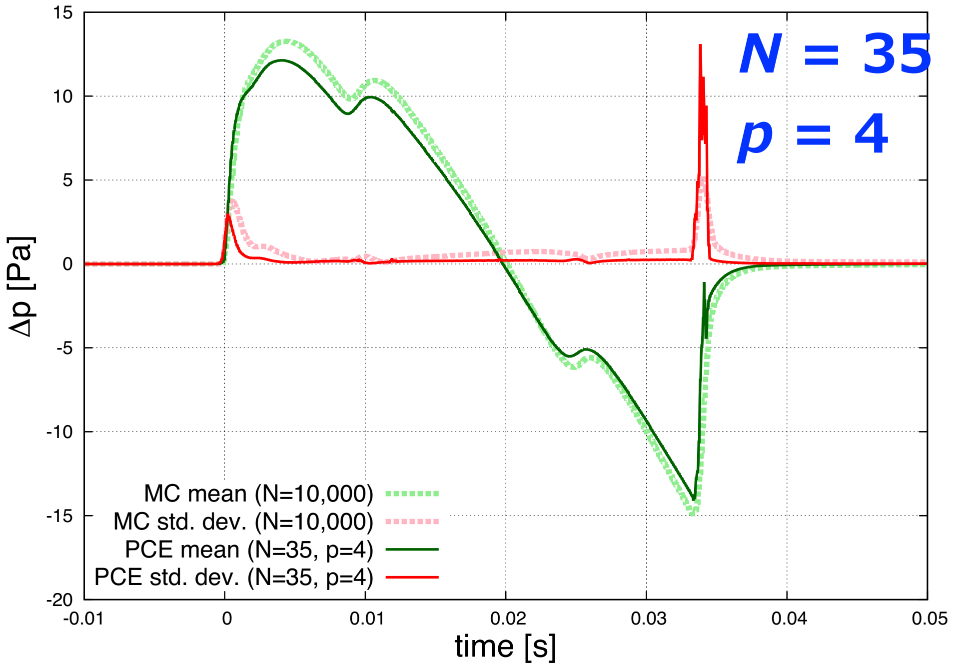
Altitude [m]	8000
Mach #	1.3
Path angle [deg]	-50

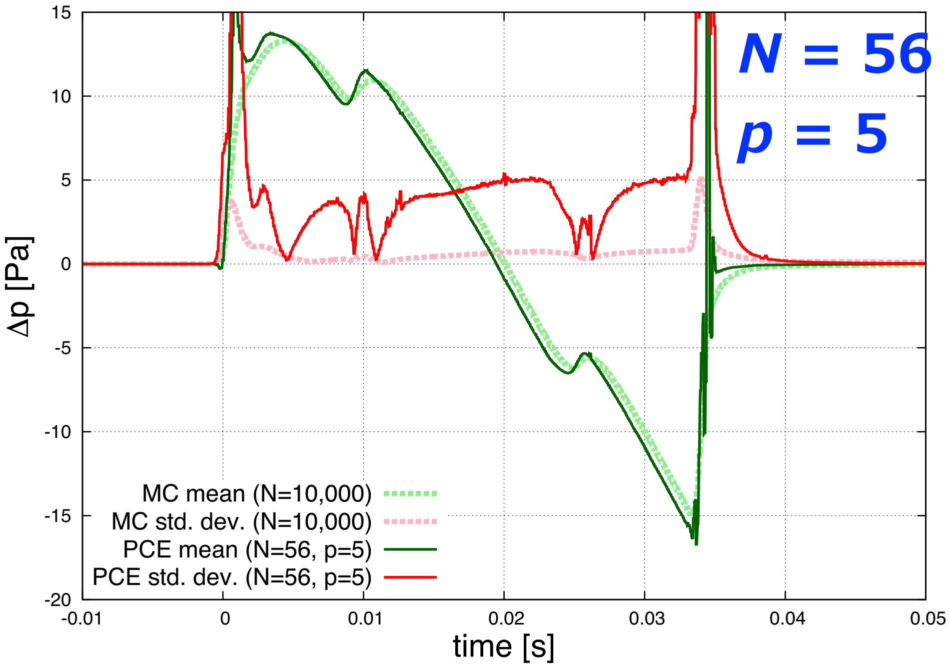


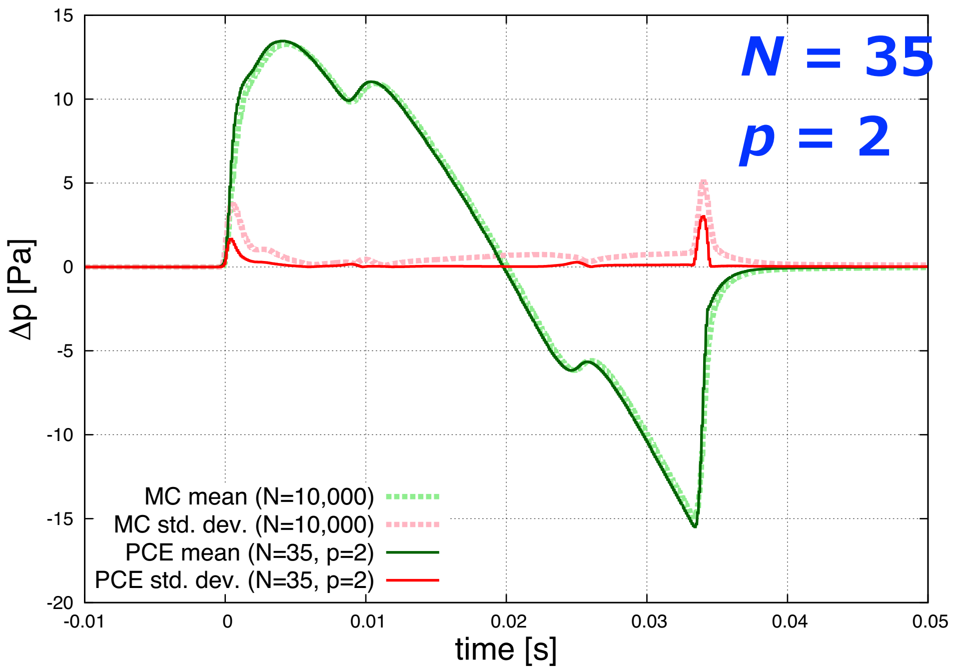
[Carlson 1967]

- Augmented Burgers equation [Cleveland and Blackstock 1996] with atmospheric uncertainties
  - ✓Temperature
  - ✓Humidity
  - ✓Wind velocity

Application (Sonic Boom)







← after adjustment

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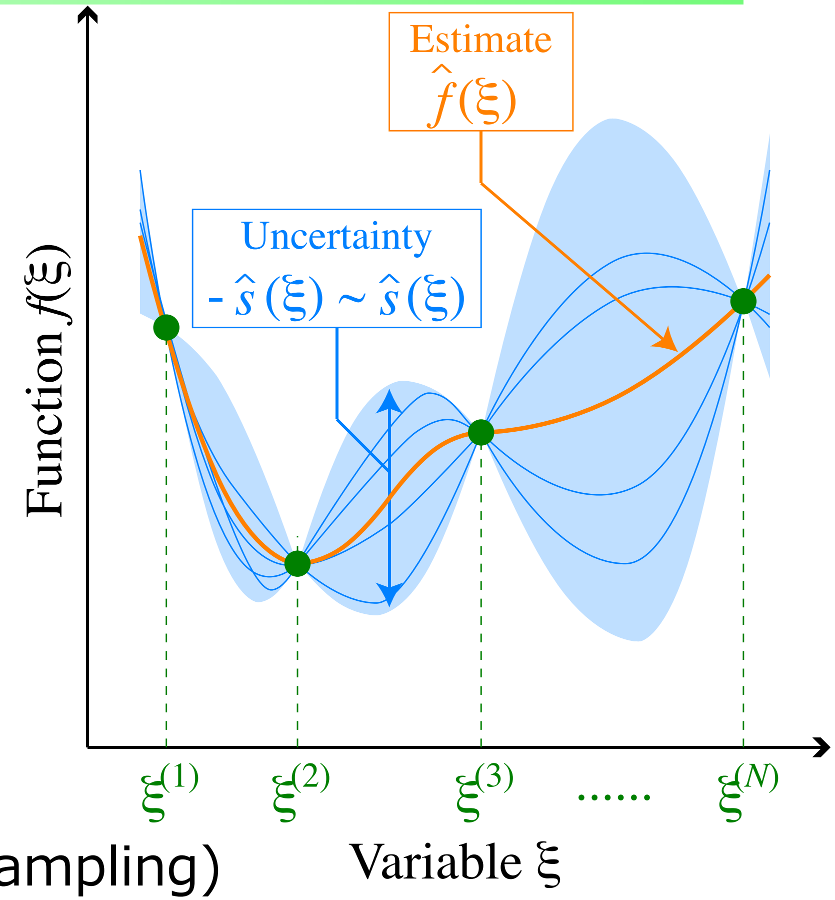
Kriging-Based Methods

✓ Kriging Surrogate Model

[Sacks *et al.* 1989]

- Based on the Bayesian statistics
- Adapts well to non-linear functions
- Estimates not only the function values but also their fit uncertainties



[Yamazaki 2013]

Inferior to a classical PCE (without adaptive sampling)

[Dwight and Han 2009]

Adaptive sampling based the fit uncertainty in the Kriging predictor and the PDF of input parameter uncertainties

[Bilionis and Zabaras 2012]

Adaptive refinement based on the fit uncertainty predicted by the Gaussian process regression

Research Objectives

✓ Propose a new dynamic adaptive sampling method based on

- **fit uncertainty**
- **gradient**

estimated by the Kriging surrogate model

✓ Test this method in

- Analytic functions
- CFD of a transonic airfoil

↓

Accurate and efficient non-intrusive UQ

Kriging Surrogate Model

Deterministic $f(\boldsymbol{\xi})$

Realization

Stochastic $F(\boldsymbol{\xi}) = \mu + Z(\boldsymbol{\xi})$

where

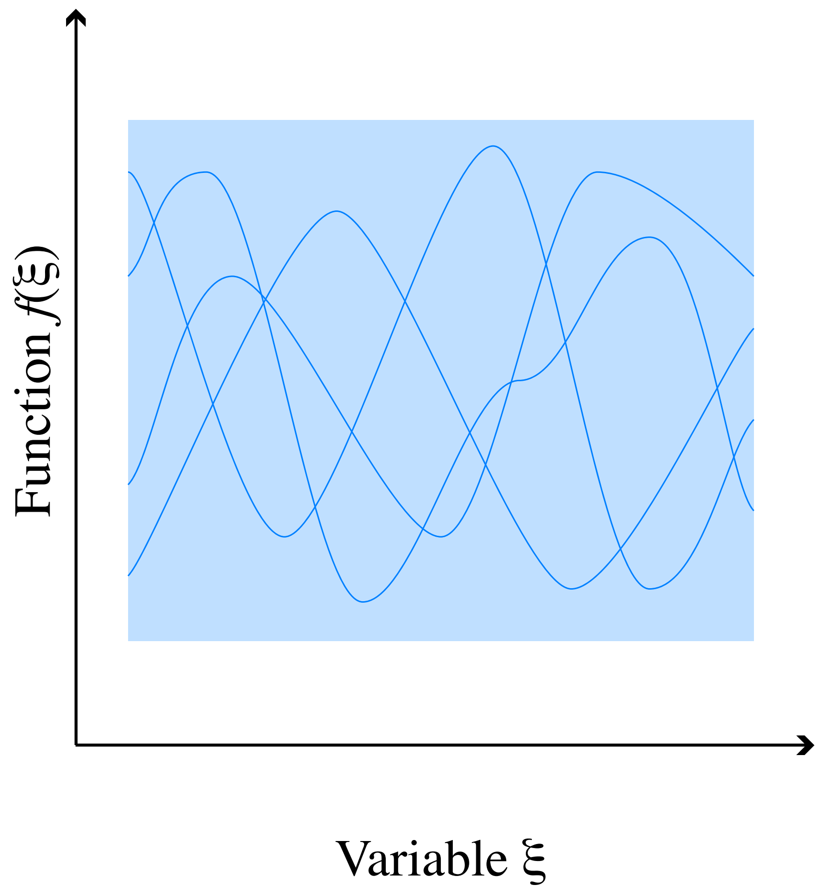
$$\mathrm{E}[Z(\boldsymbol{\xi})] = 0$$

$$\mathrm{Cov}[Z(\boldsymbol{\xi}), Z(\boldsymbol{\xi}')] = \sigma^2 k(\boldsymbol{\xi}, \boldsymbol{\xi}')$$

Correlation function (kernel)

- Depends on $|\boldsymbol{h}| = |\boldsymbol{\xi} - \boldsymbol{\xi}'|$
- With a set of constants $\boldsymbol{\Theta}$ ***(hyperparameters)***

Prior distribution



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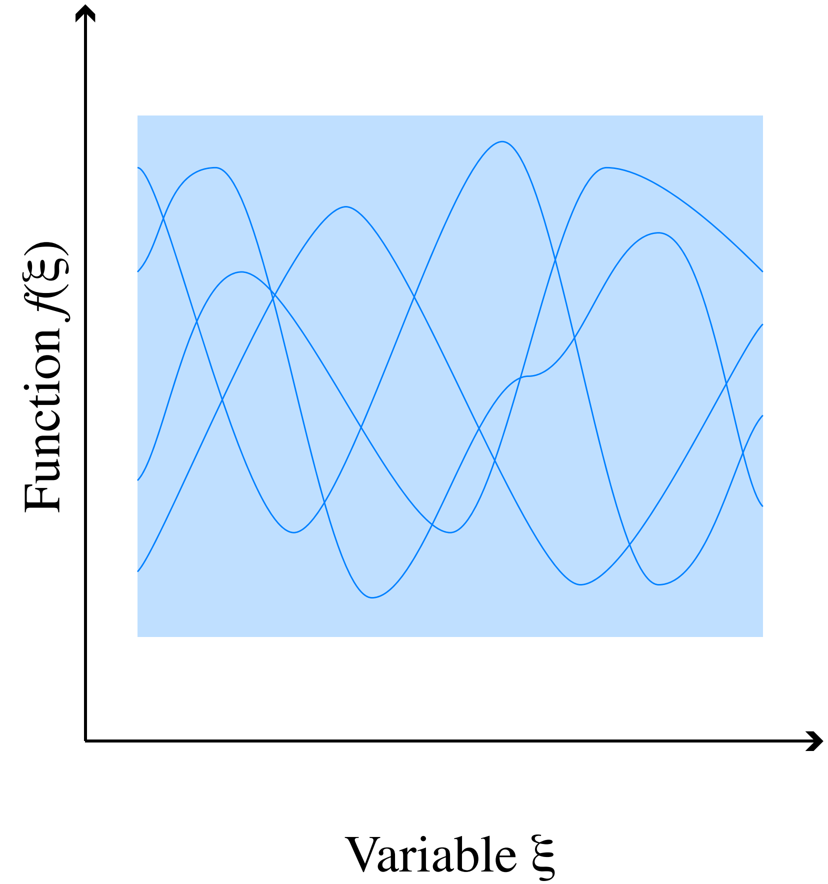


Determined by the ***maximum likelihood estimation***

Kriging Surrogate Model (cont.)

N samples $f(\boldsymbol{\xi}^{(i)}) = F(\boldsymbol{\xi}^{(i)})$

$(i = 1, 2, \cdots, N)$

Likelihood function

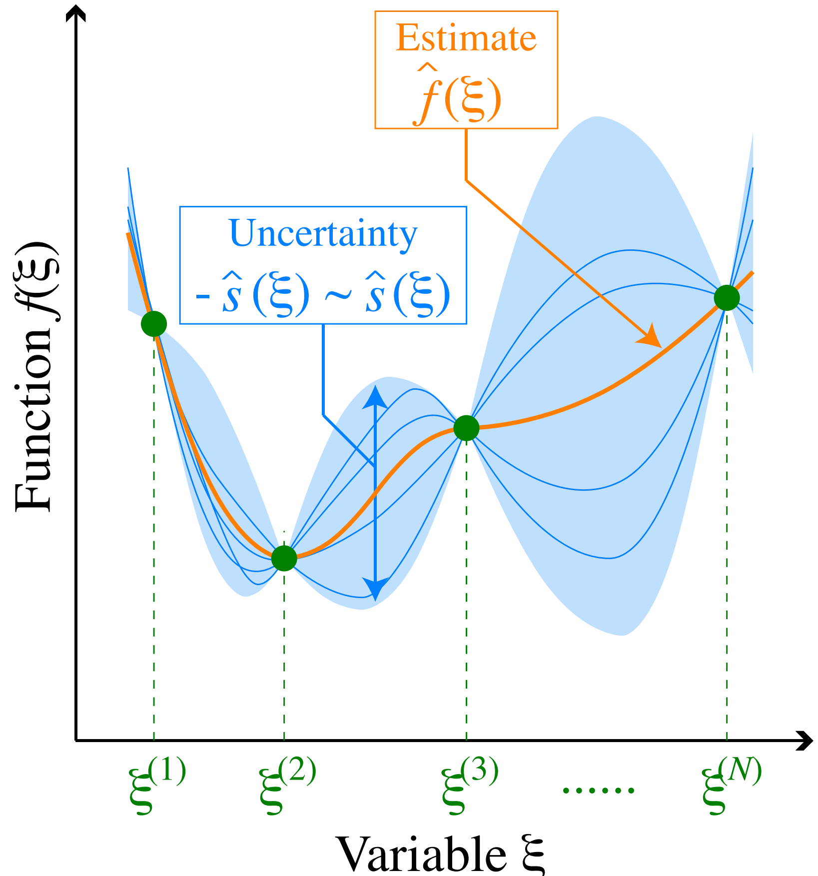
$$Ln(\mu, \sigma^2, \Theta) = -\frac{N}{2}\ln(2\pi) - \frac{N}{2}\ln\sigma^2 - \frac{1}{2}\ln|\boldsymbol{R}| - \frac{(\boldsymbol{f} - \mathbf{1}\mu)^\top \boldsymbol{R}^{-1}(\boldsymbol{f} - \mathbf{1}\mu)}{2\sigma^2}$$

Maximization

$$\hat{\mu} = \frac{\mathbf{1}^\top \boldsymbol{R}^{-1}\boldsymbol{f}}{\mathbf{1}^\top \boldsymbol{R}^{-1}\mathbf{1}}$$

$$\hat{\sigma}^2 = \frac{(\boldsymbol{f} - \mathbf{1}\hat{\mu})^\top \boldsymbol{R}^{-1}(\boldsymbol{f} - \mathbf{1}\hat{\mu})}{N}$$

Posterior distribution



Best linear unbiased predictor

$$\hat{f}(\boldsymbol{\xi}) = \hat{\mu} + \boldsymbol{r}^\top(\boldsymbol{\xi})\boldsymbol{R}^{-1}(\boldsymbol{f} - \mathbf{1}\hat{\mu})$$

$$\hat{s}^2(\boldsymbol{\xi}) = \hat{\sigma}^2\left[1 - \boldsymbol{r}^\top(\boldsymbol{\xi})\boldsymbol{R}^{-1}\boldsymbol{r}(\boldsymbol{\xi}) + \frac{\left(1 - \mathbf{1}^\top \boldsymbol{R}^{-1}\boldsymbol{r}(\boldsymbol{\xi})\right)^2}{\mathbf{1}^\top \boldsymbol{R}^{-1}\mathbf{1}}\right]$$

where

$R_{ij} = k(\boldsymbol{\xi}^{(i)}, \boldsymbol{\xi}^{(j)})$

$r_i(\boldsymbol{\xi}) = k(\boldsymbol{\xi}, \boldsymbol{\xi}^{(i)})$

Correlation Functions

$$k(\boldsymbol{\xi}, \boldsymbol{\xi}') = \prod_{k=1}^{n} k(\xi_k, {\xi_k}')$$

For $h_k = \xi_k - {\xi_k}'$

✓ Gaussian correlation

$$k(\xi_k, {\xi_k}') = \exp\left(-\theta_k |h_k|^2\right)$$

where $\theta_k \geq 0$ (*n* hyperparameters)

✓ Cubic correlation

$$k(\xi_k, {\xi_k}') = \begin{cases} 1 - 6|h_k|^2/{\theta_k}^2 + 6|h_k|^3/{\theta_k}^3, & \text{if } |h_k| \leq \theta_k/2 \\ 2\left(1 - |h_k|/\theta_k\right)^3, & \text{if } \theta_k/2 < |h_k| \leq \theta_k \\ 0, & \text{if } \theta_k < |h_k| \end{cases}$$

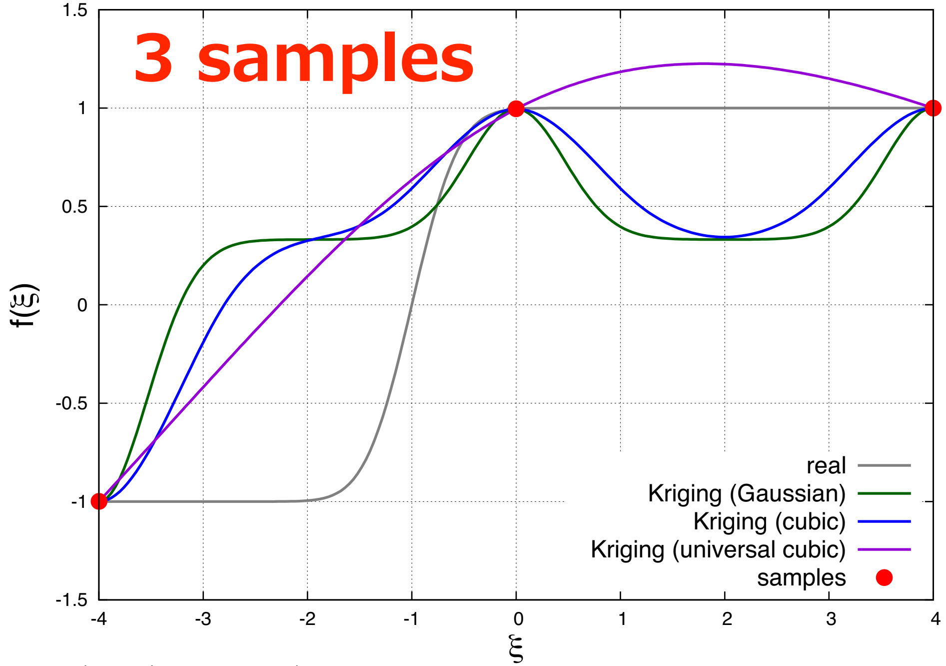
where $\theta_k > 0$ (*n* hyperparameters)

✓ Universal cubic correlation

$$k(\xi_k, {\xi_k}') = 1 - \frac{3\left(1-\rho_k\right)}{2+\gamma_k}|h_k|^2 + \frac{\left(1-\rho_k\right)\left(1-\gamma_k\right)}{2+\gamma_k}|h_k|^3$$

where $0 \leq \rho_k \leq 1, \quad 0 \leq \gamma_k \leq 1, \quad \rho_k \geq \dfrac{5{\gamma_k}^2 + 8\gamma_k - 1}{{\gamma_k}^2 + 4\gamma_k + 7}$

(2*n* hyperparameters)



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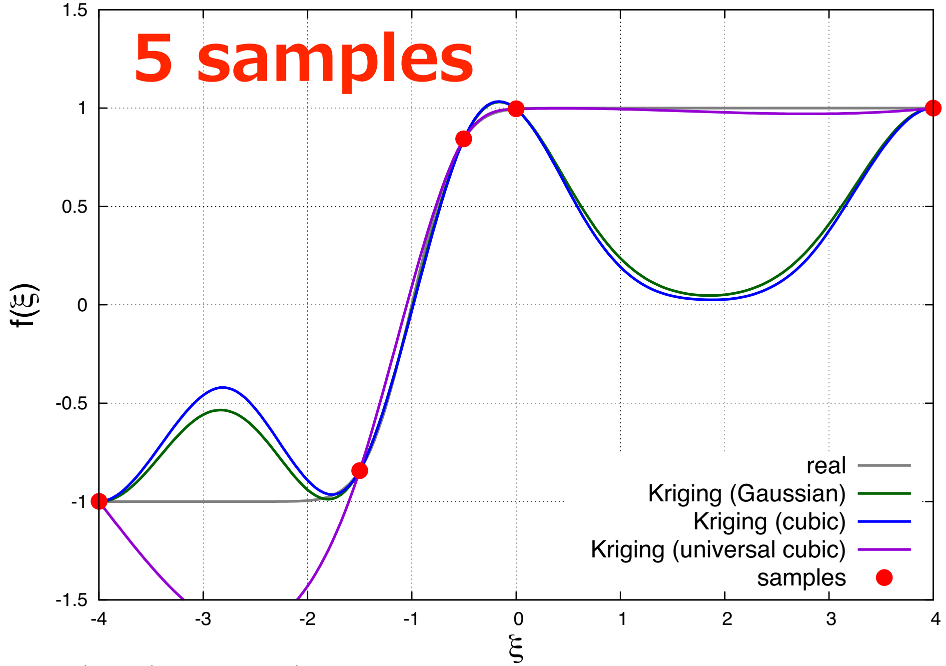

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(2*n* hyperparameters)

Dynamic Adaptive Sampling

✓ Criterion 1 [Dwight and Han 2009]

$$\mathrm{Crit}(\xi) = \hat{s}(\xi) \times \mathrm{PDF}(\xi)$$

✓ Criterion 2

$$\mathrm{Crit}(\xi) = \left| \frac{\partial \hat{f}(\xi)}{\partial \xi} \right| \times \mathrm{PDF}(\xi)$$

✓ Criterion 3

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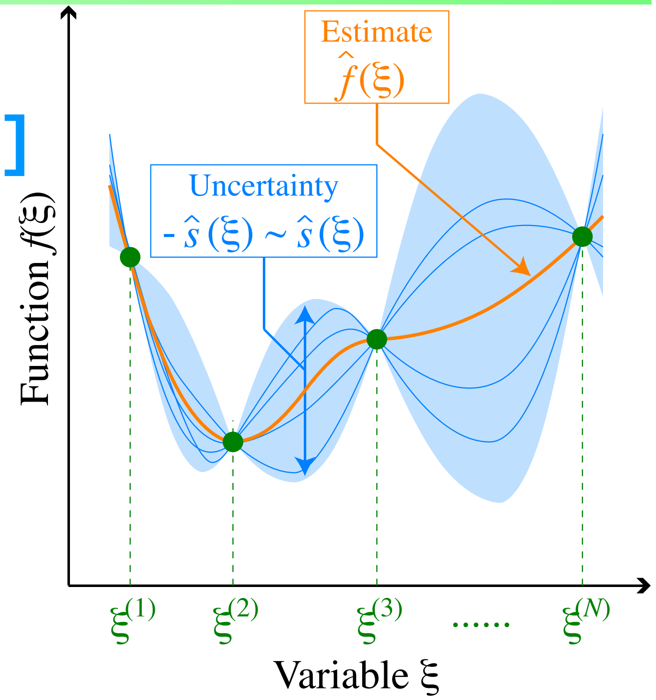

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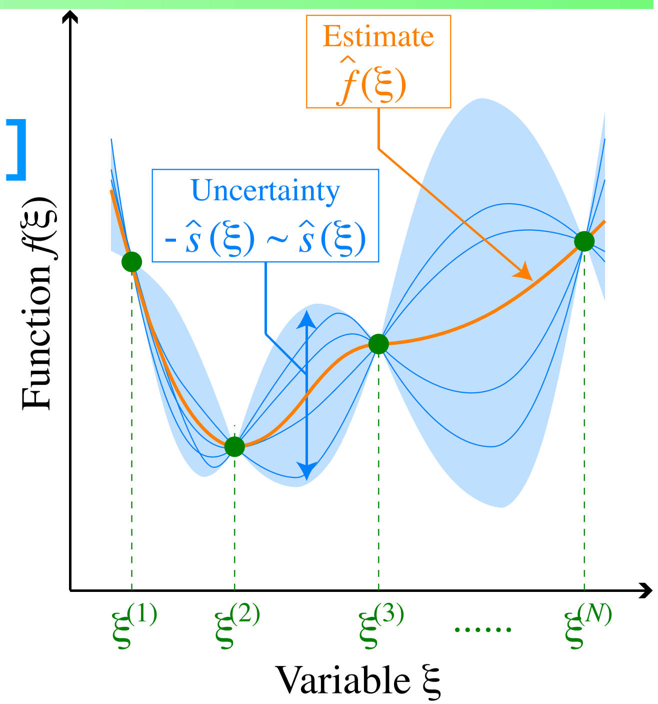
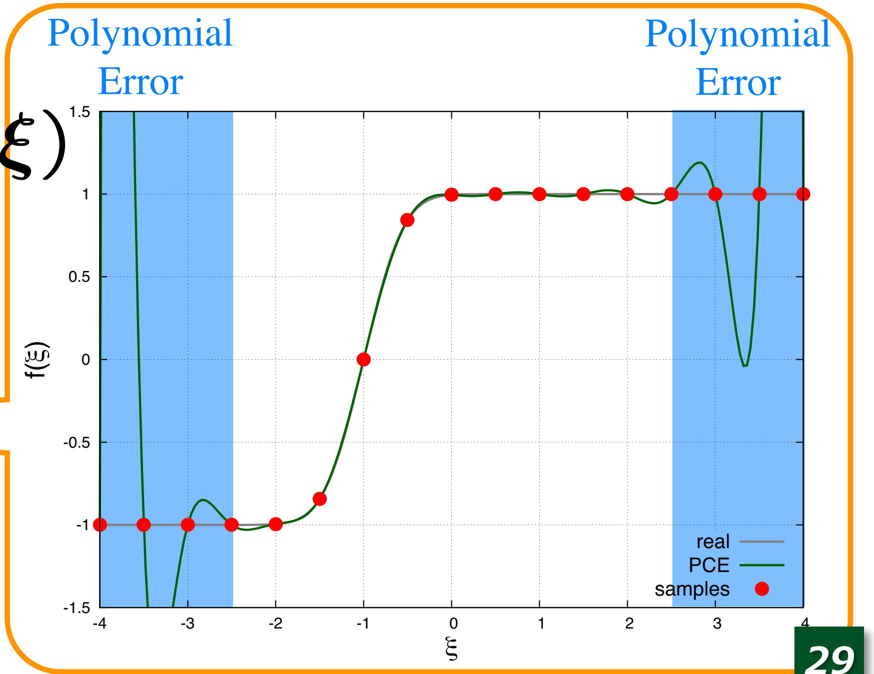
✓ **Criterion 3**

$$\mathrm{Crit}(\xi) = \left| \frac{\partial \hat{f}(\xi)}{\partial \xi} \right| \times \hat{s}(\xi) \times \mathrm{PDF}(\xi)$$

$= 0$

in smooth regions





Dynamic Adaptive Sampling (cont.)

✓ *Criterion 4* **(proposed)**

$$\mathrm{Crit}(\boldsymbol{\xi}) = \left(\boxed{\left| \frac{\partial \widehat{f}(\boldsymbol{\xi})}{\partial \boldsymbol{\xi}} \right|} \times \Delta\xi + D_{\widehat{f}}(\boldsymbol{\xi}) \right) \times \boxed{\widehat{s}(\boldsymbol{\xi})} \times \mathrm{PDF}(\boldsymbol{\xi})$$

Dynamic Adaptive Sampling (cont.)

✓ Criterion 4 (proposed)

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$$D_{\hat{f}}(\boldsymbol{\xi}) = \left| \hat{f}(\boldsymbol{\xi}) - \hat{f}_{\mathrm{pre}}(\boldsymbol{\xi}) \right|$$

Current (N samps.)

Previous (N-1 samps.)

Dynamic Adaptive Sampling (cont.)

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$$\Delta\xi = \min_{i=1,2,\cdots,N} |\boldsymbol{\xi} - \boldsymbol{\xi}^{(i)}|$$

$$D_{\widehat{f}}(\boldsymbol{\xi}) = |\widehat{f}(\boldsymbol{\xi}) - \widehat{f}_{\mathrm{pre}}(\boldsymbol{\xi})|$$

Current (N samps.)

Previous (N-1 samps.)

Summary of Sampling Criteria

✓ ***Criterion 1*** **[Dwight and Han 2009]**

considers only **fit uncertainty**

✓ ***Criterion 2***

considers only **gradient**

✓ ***Criterion 3***

considers both **fit uncertainty** & **gradient**

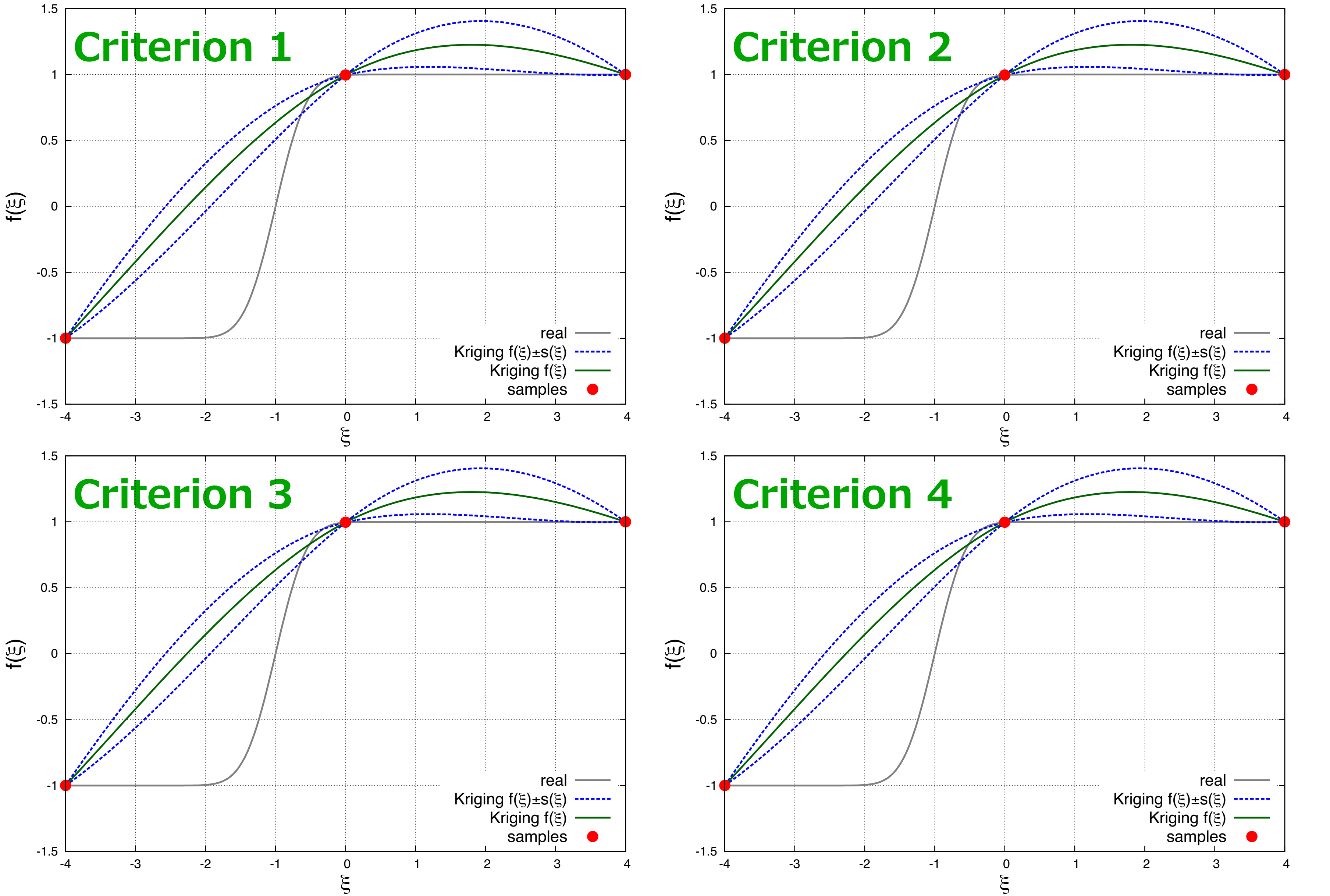
✓ ***Criterion 4*** **(proposed)**

adds an extra **error-estimate term** in criterion 3

Numerical Tests (1D Funcs.)

3 samples (evenly distributed)

$$f(\xi) = \mathrm{erf}\left[2\left(\xi + 1\right)\right]$$
$$\xi \sim \mathrm{Unif}(-4, 4)$$



Numerical Tests (1D Funcs.)

4 samples

$$f(\xi) = \mathrm{erf}\left[2\left(\xi + 1\right)\right]$$
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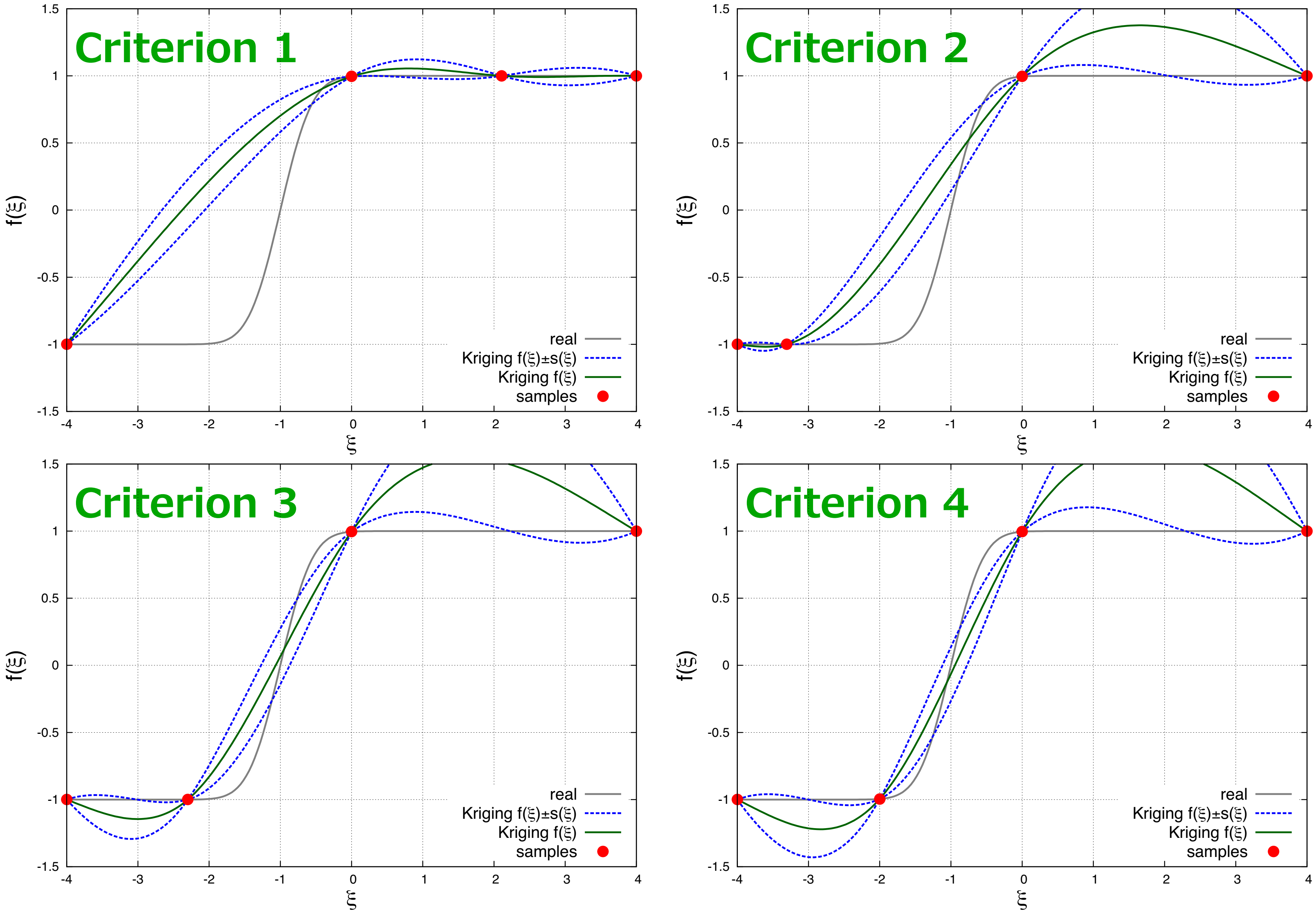

Numerical Tests (1D Funcs.)

5 samples

$$f(\xi) = \mathrm{erf}\left[2\left(\xi + 1\right)\right]$$

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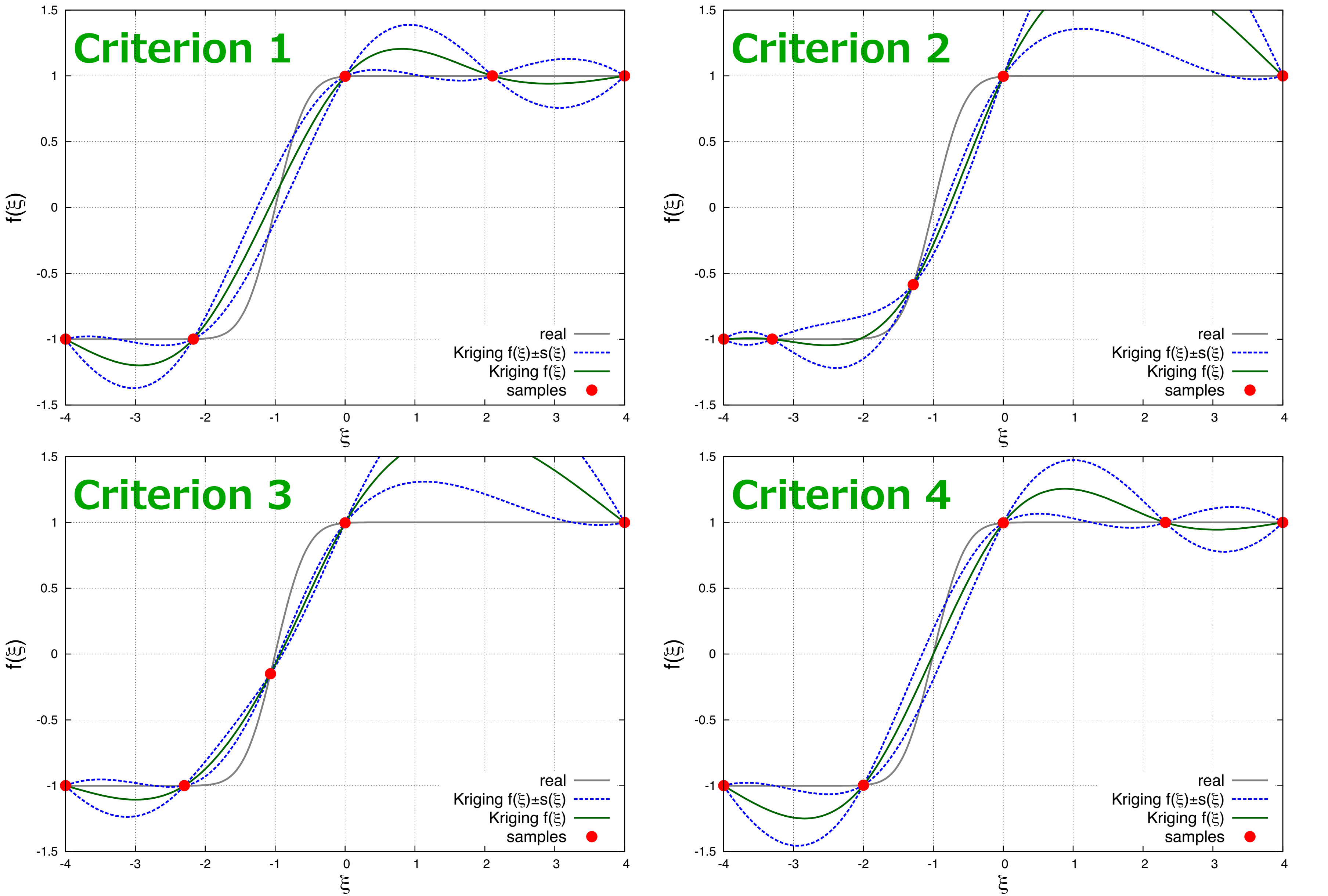

Numerical Tests (1D Funcs.)

6 samples

$$f(\xi) = \mathrm{erf}\left[2\left(\xi + 1\right)\right]$$
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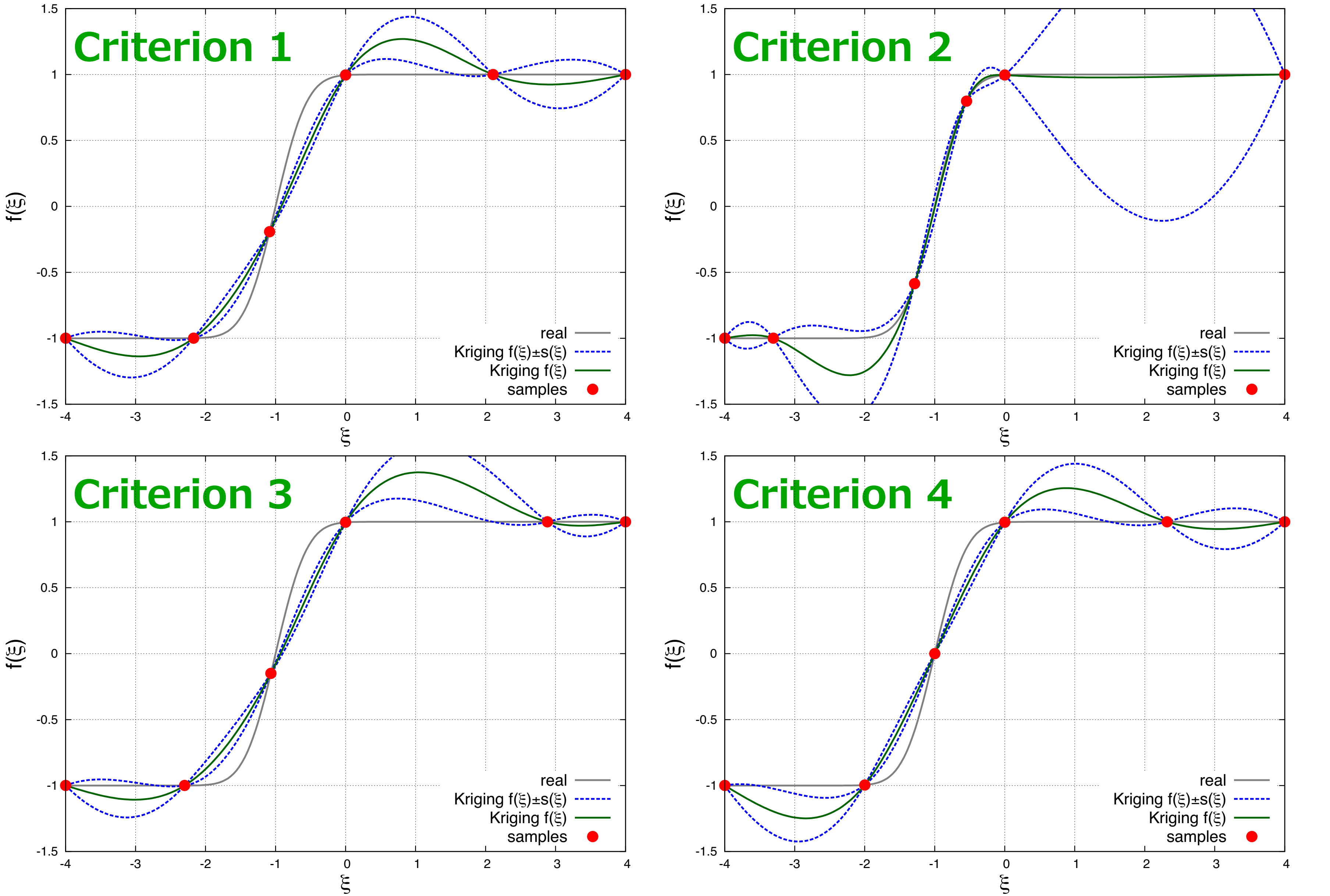

Numerical Tests (1D Funcs.)

7 samples

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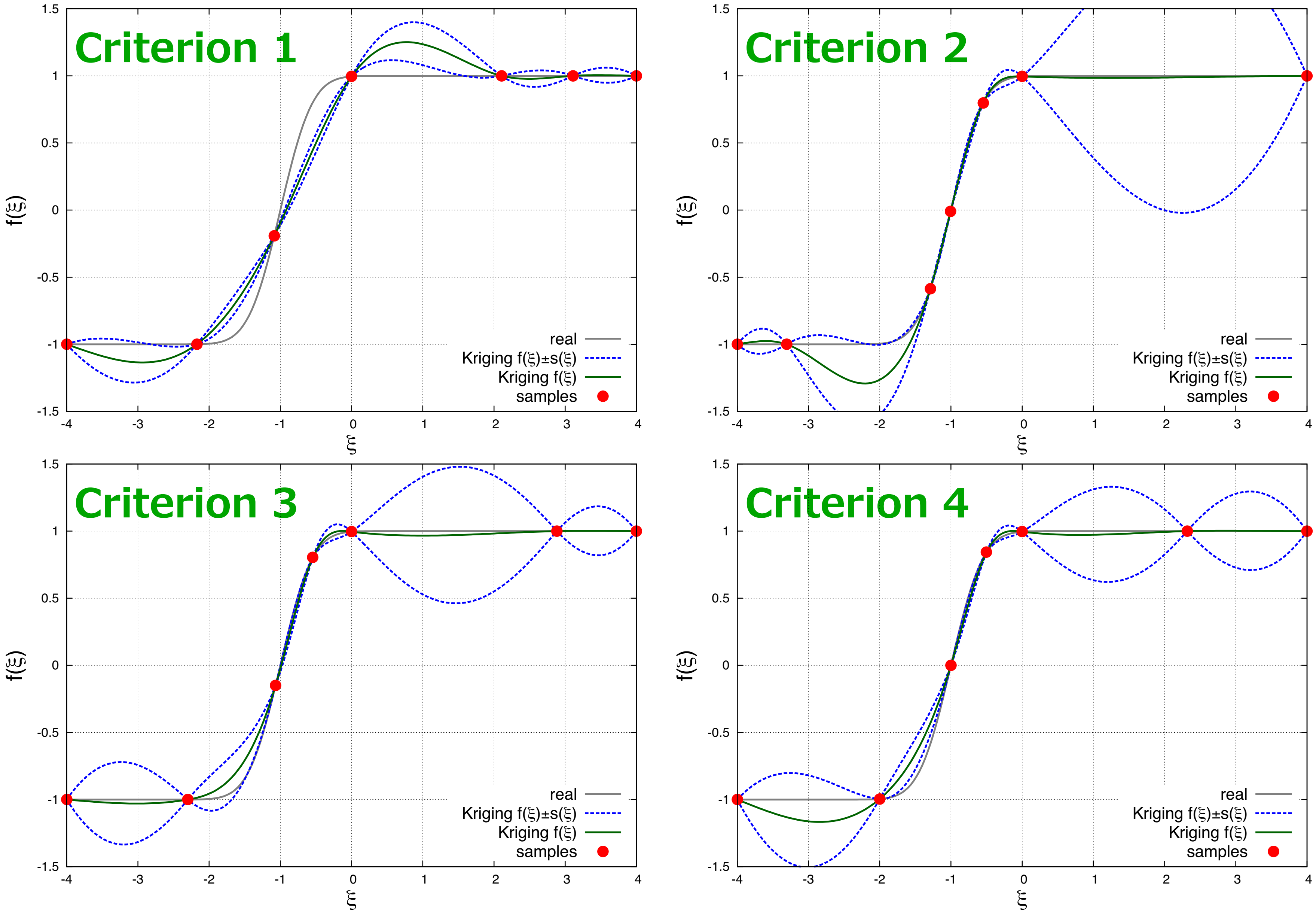

Numerical Tests (1D Funcs.)

8 samples

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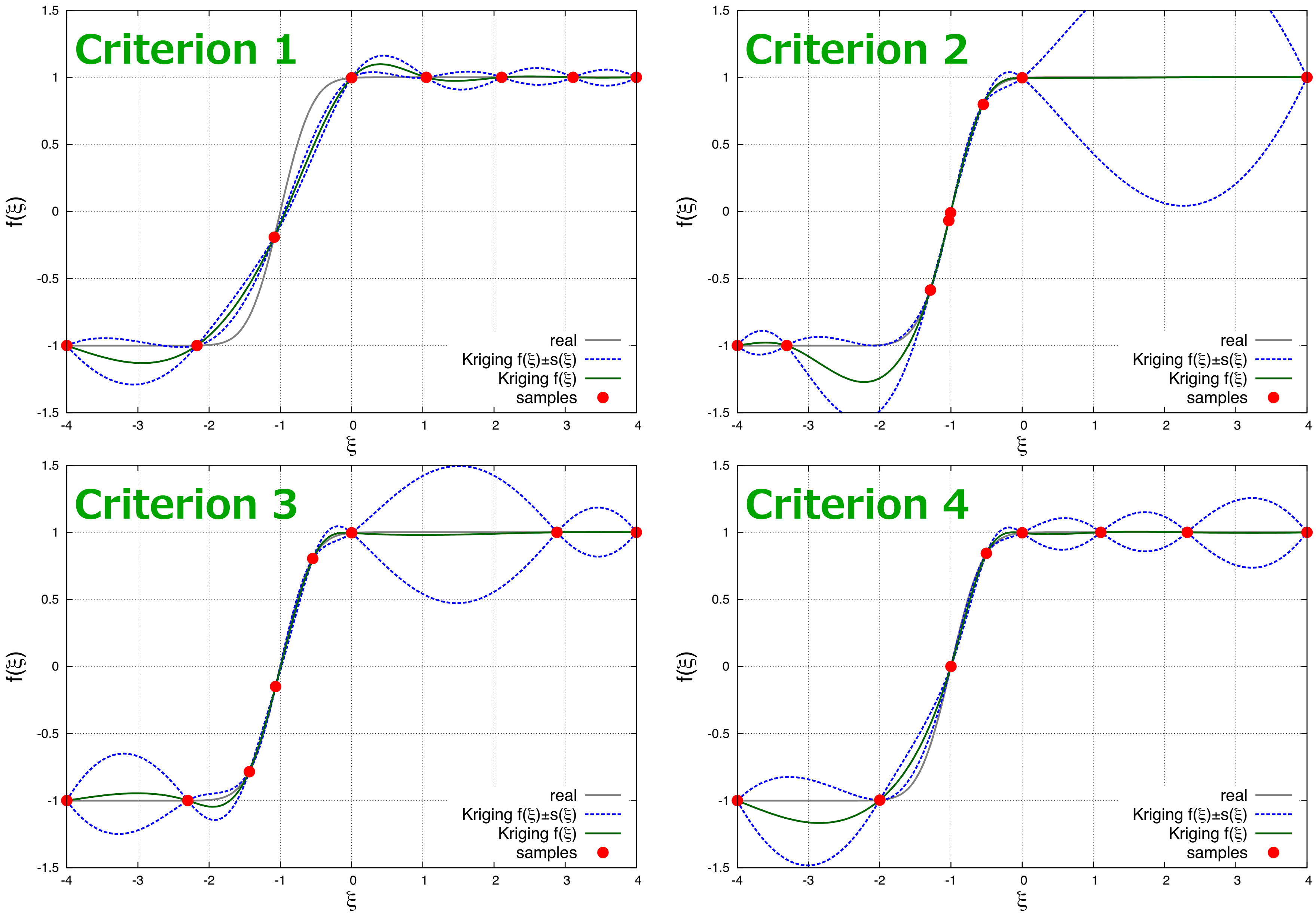

Numerical Tests (1D Funcs.)

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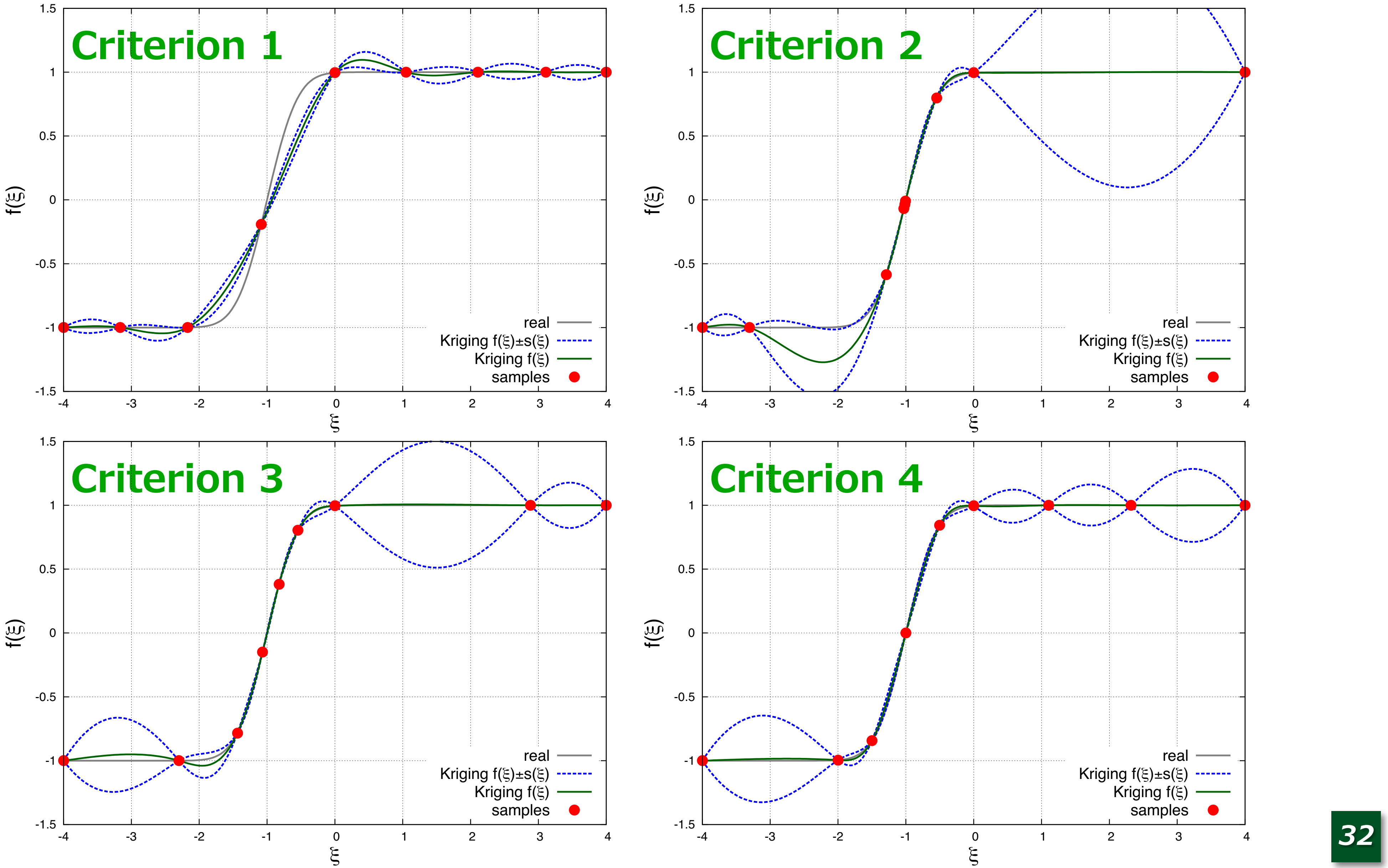

Numerical Tests (1D Funcs.)

10 samples

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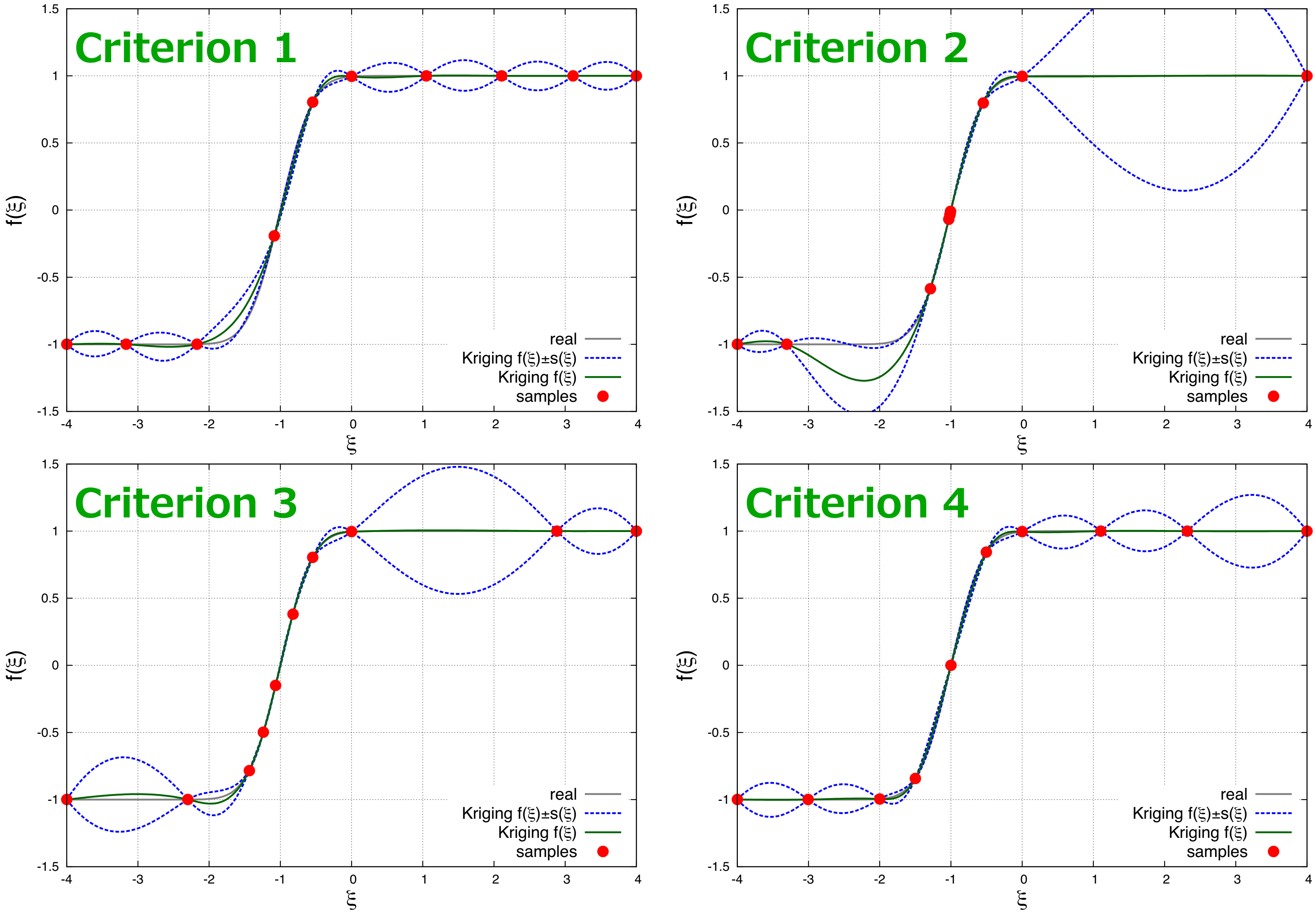
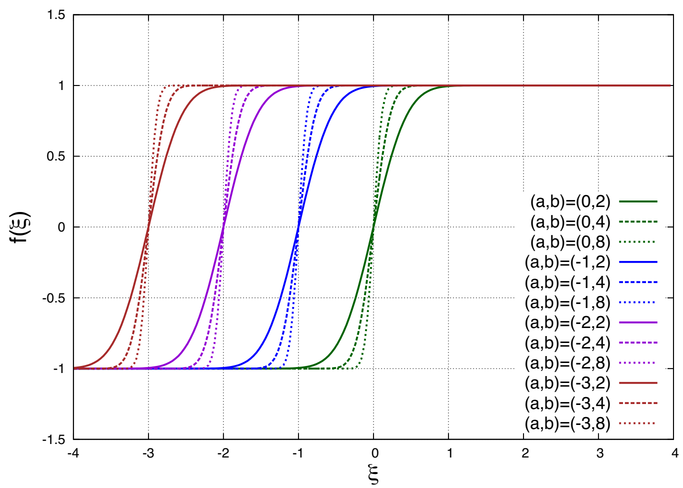


Numerical Tests (1D Funcs.)

Averaged on **30 trials from 3 initial samples (randomly generated)**
in **all cases (4 pos x 3 grad)**



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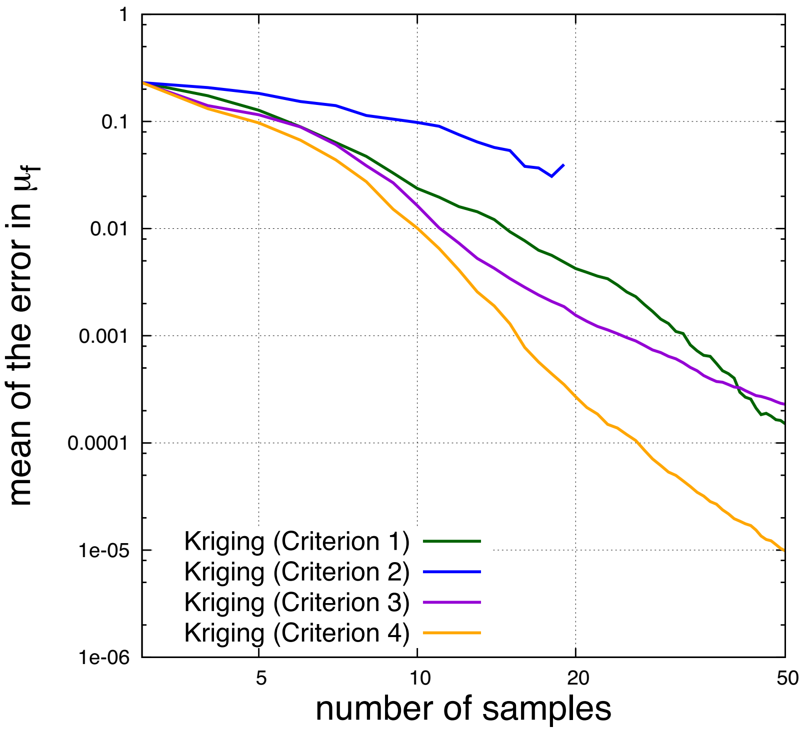

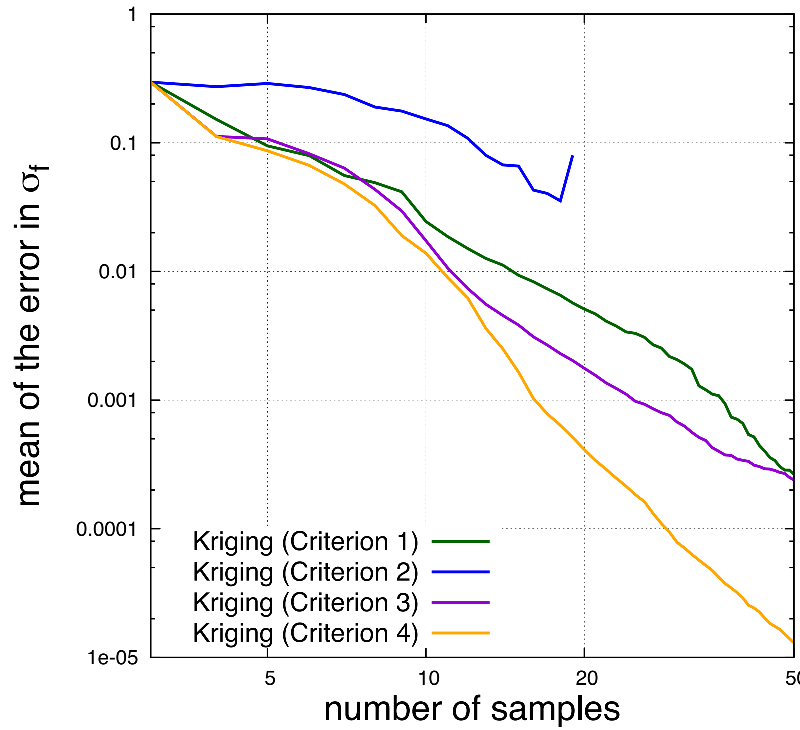

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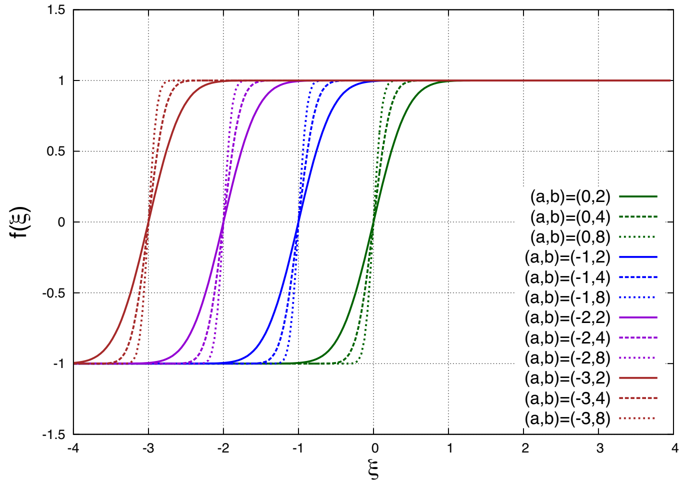

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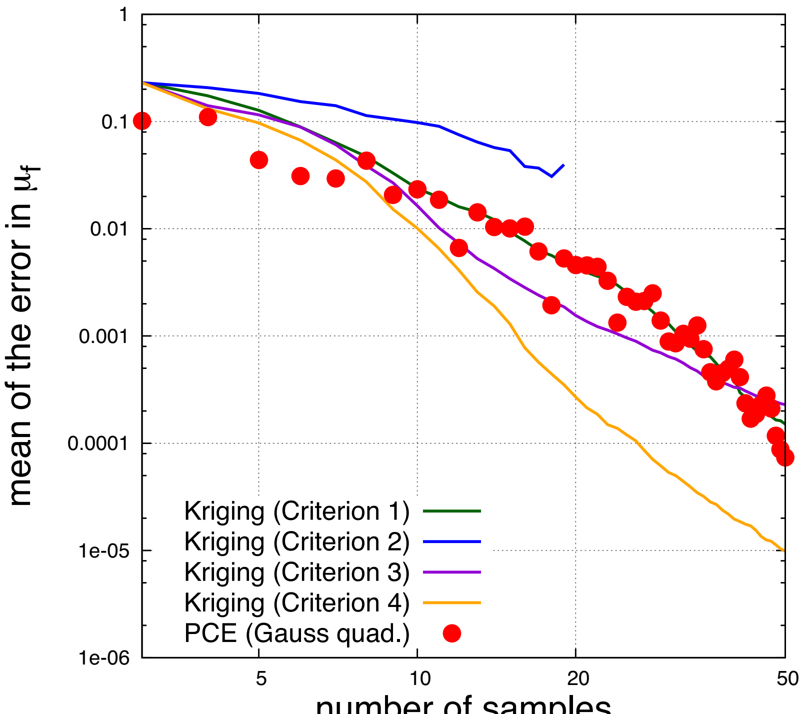
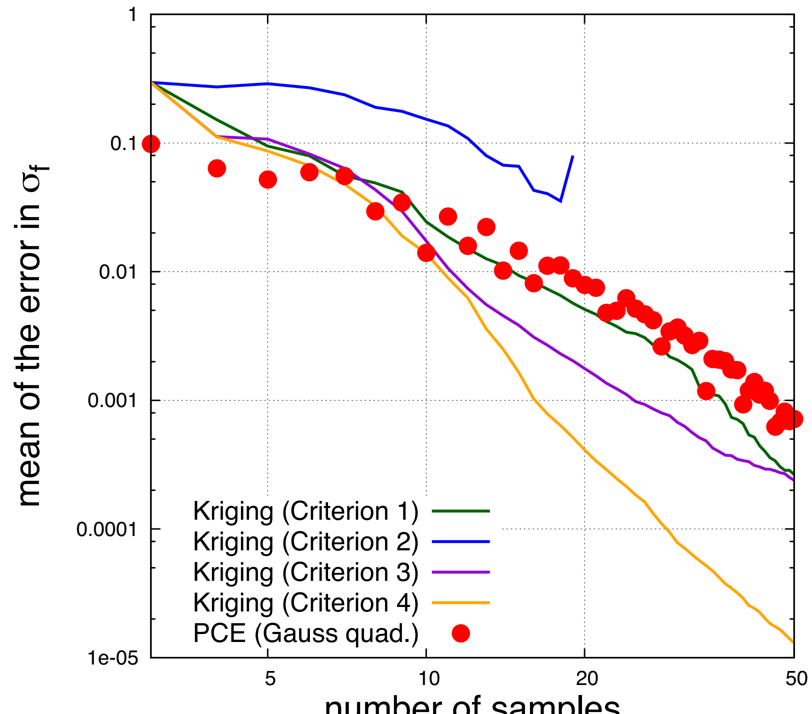
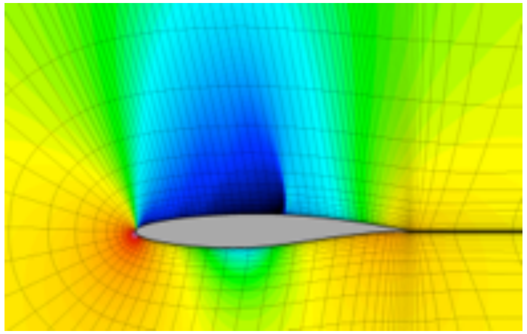
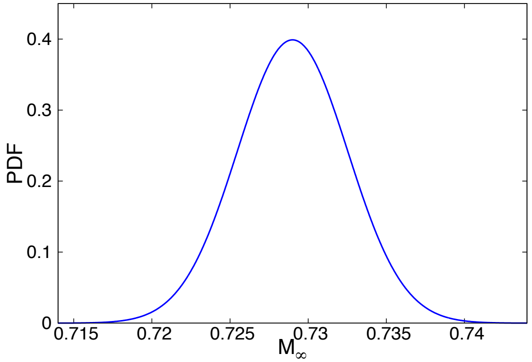




Application (Transonic Airfoil)



$M_\infty = 0.729$



$\sigma_M = 0.005$

- 2D RANS (Baldwin-Lomax)
- $Re_c = 6.5 \times 10^6$
- $\alpha = 2.31$
- MC (10,000 pts.)

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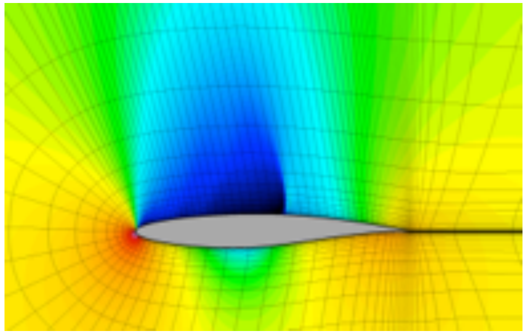

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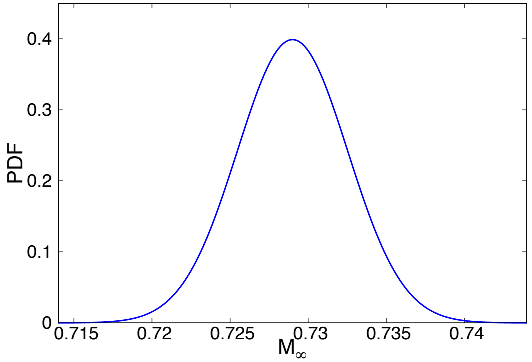

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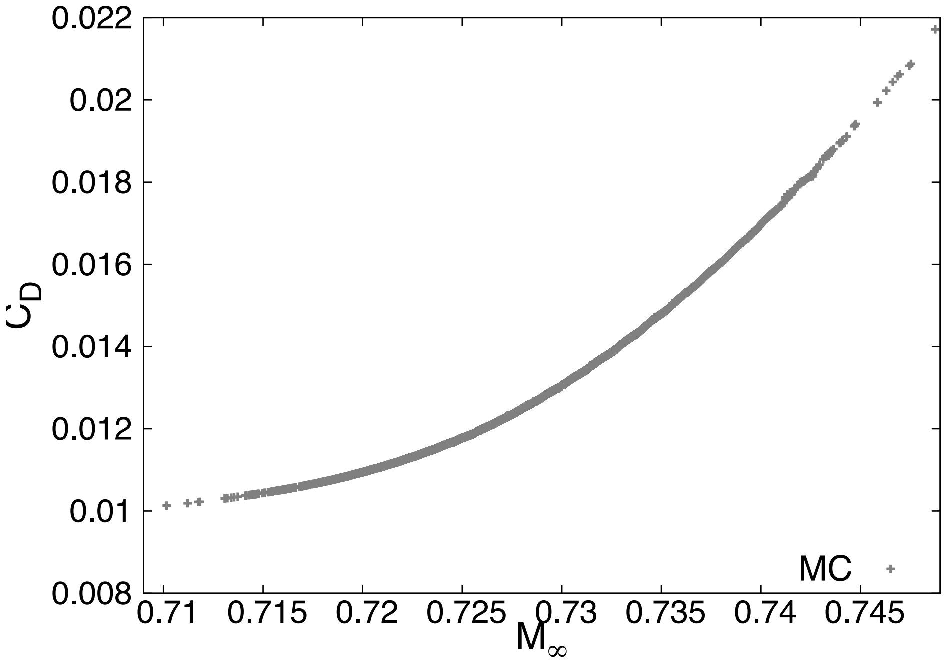

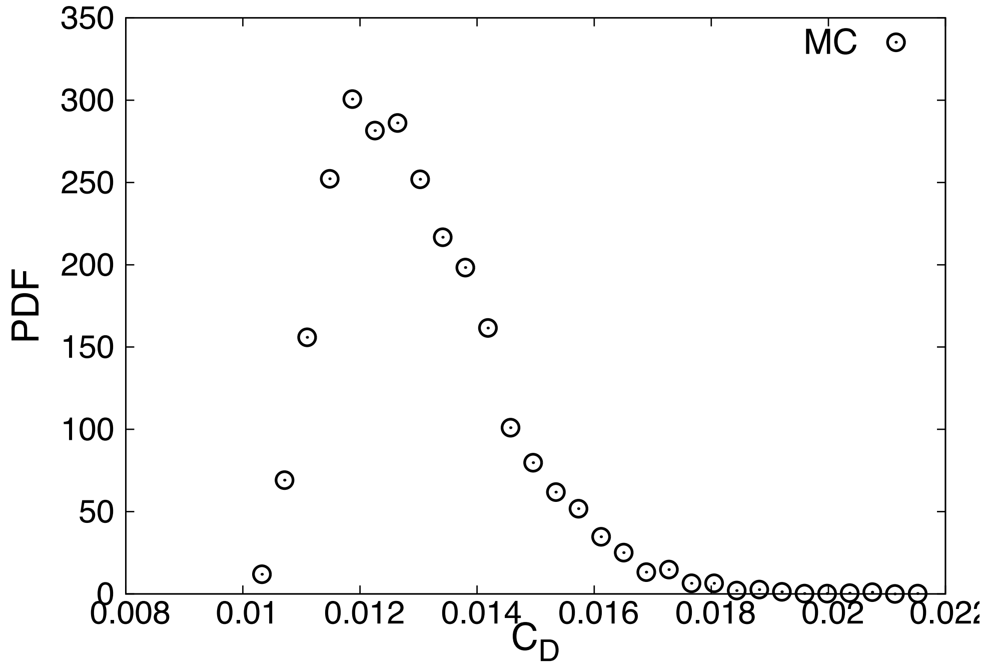

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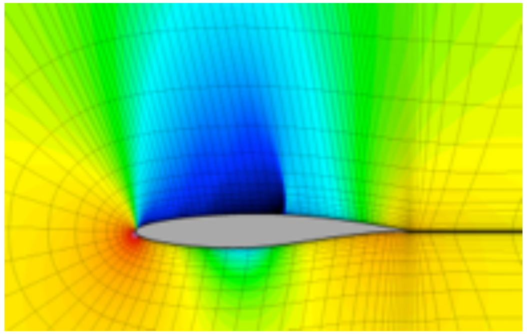

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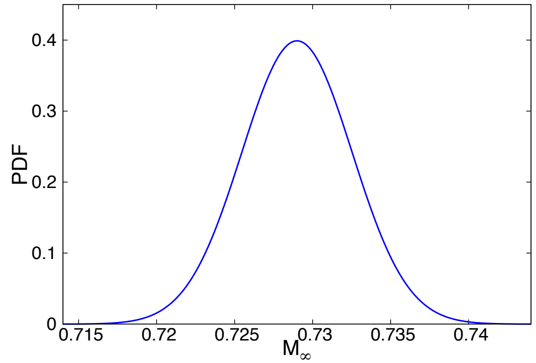

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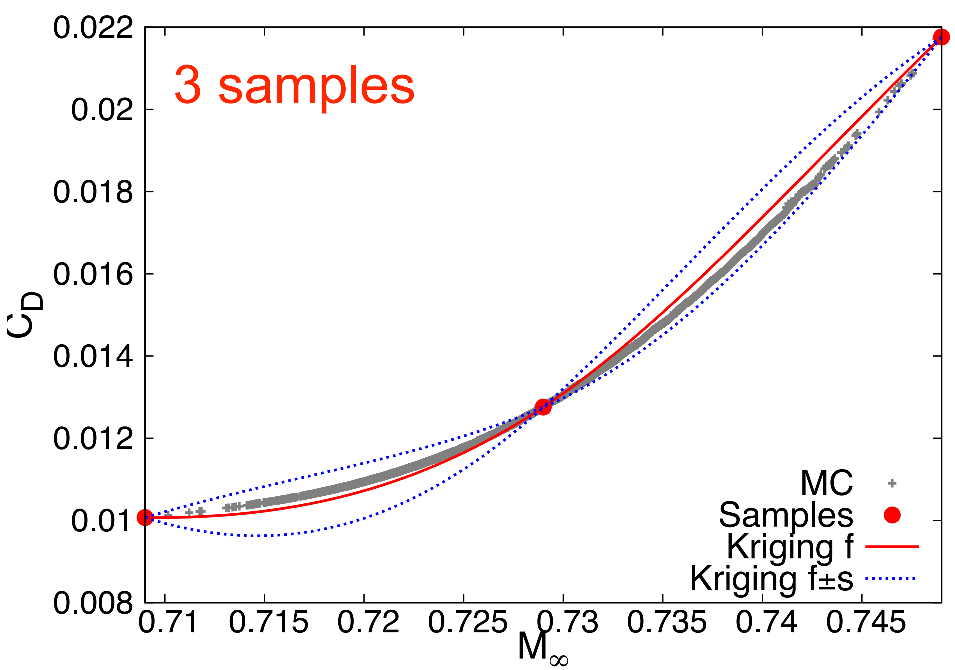

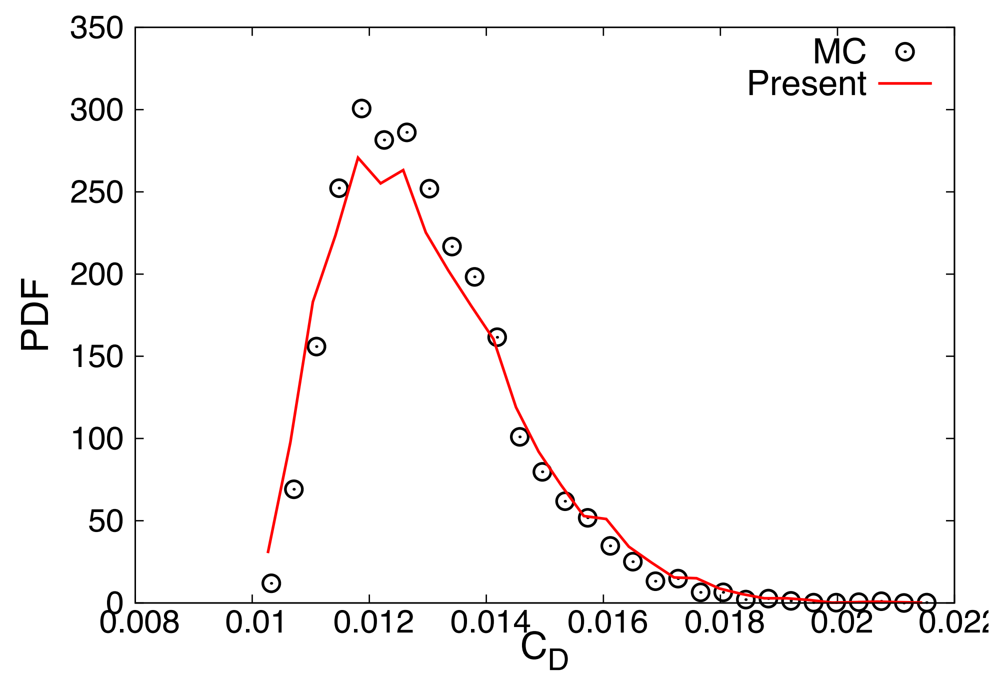

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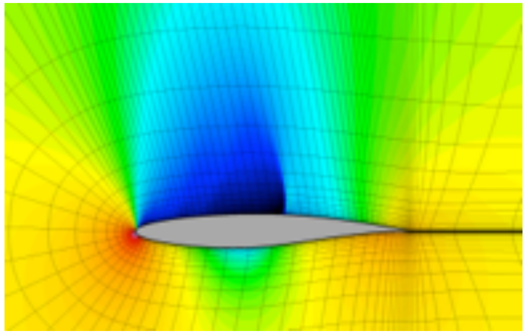

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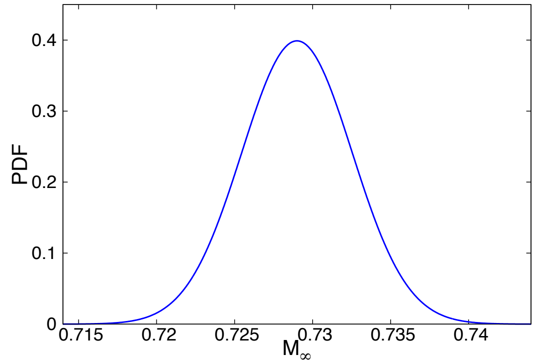

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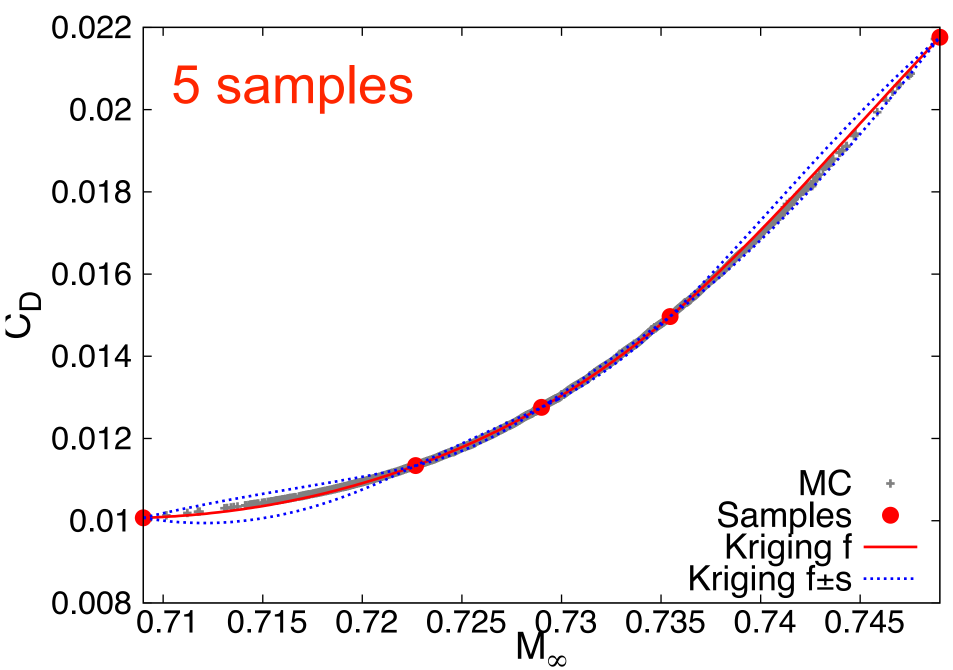

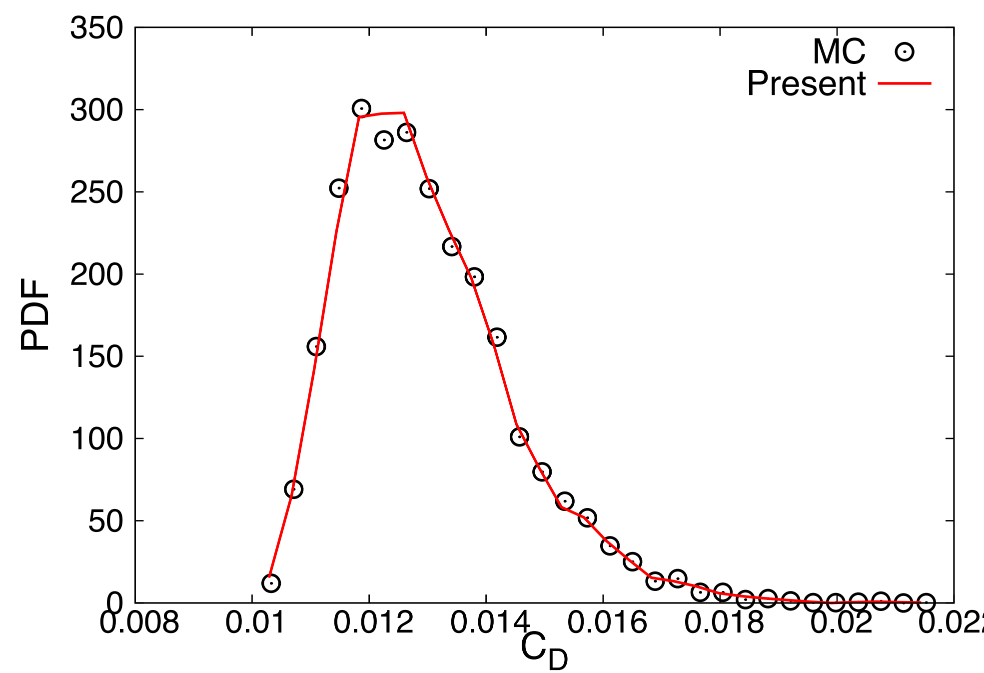

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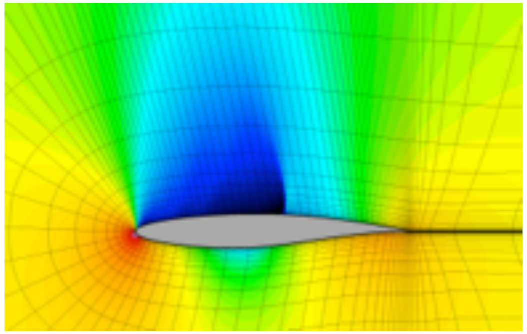

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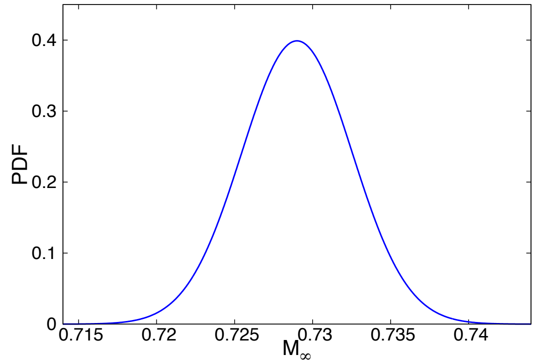

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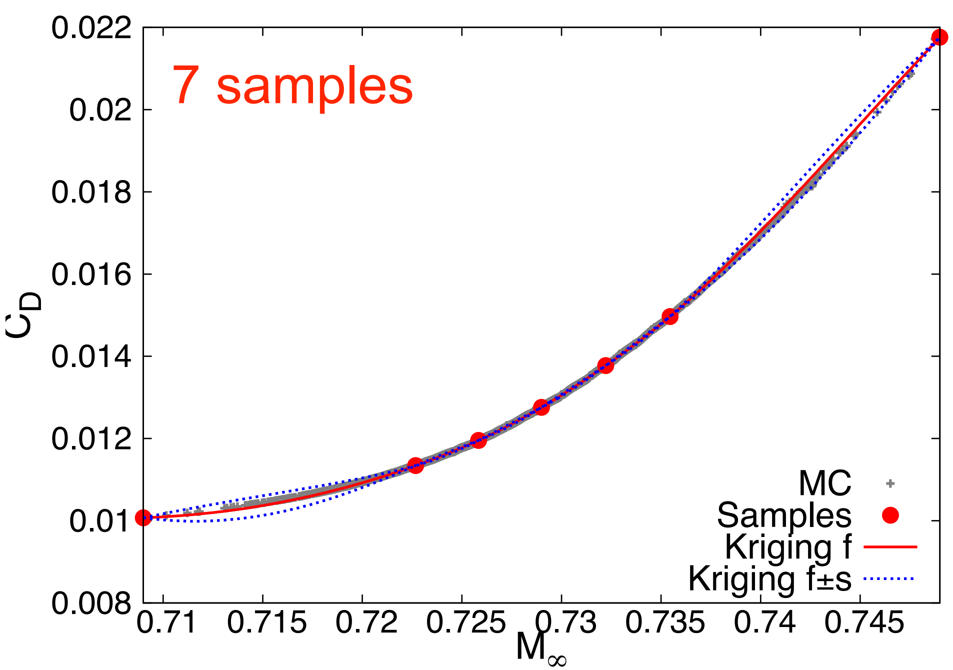

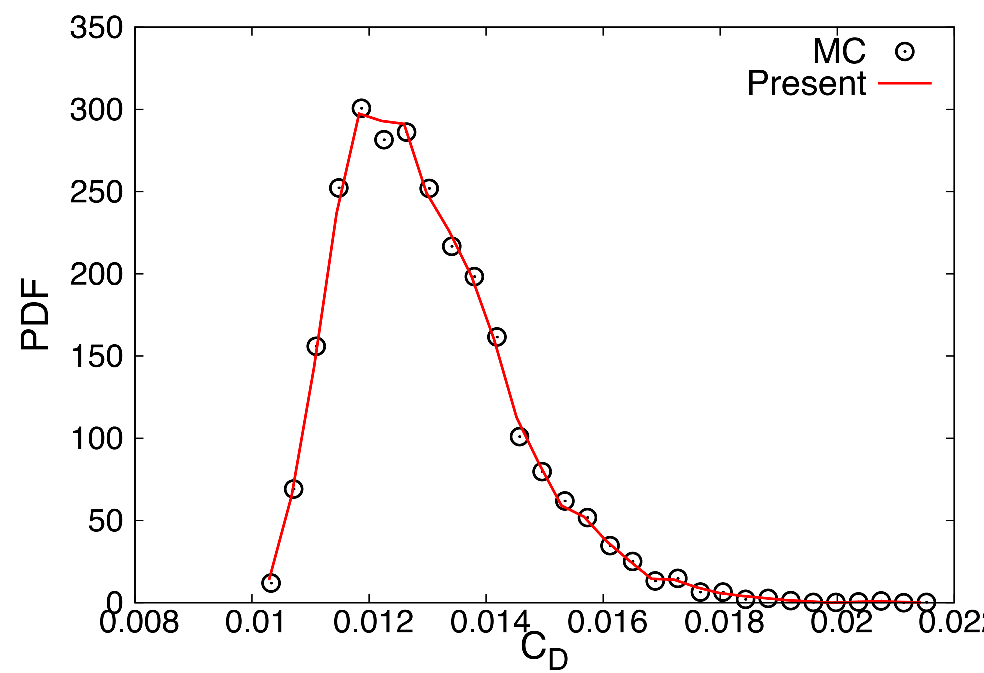

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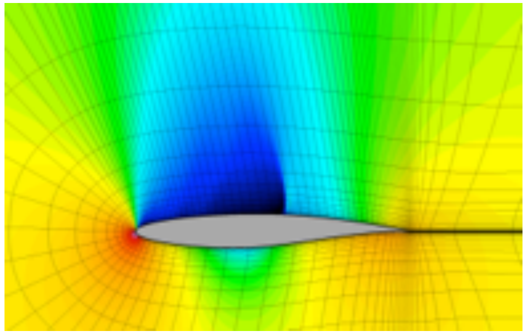

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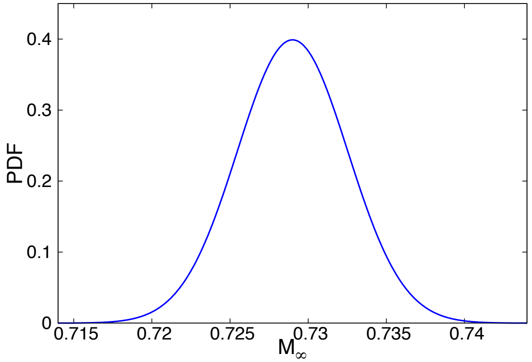

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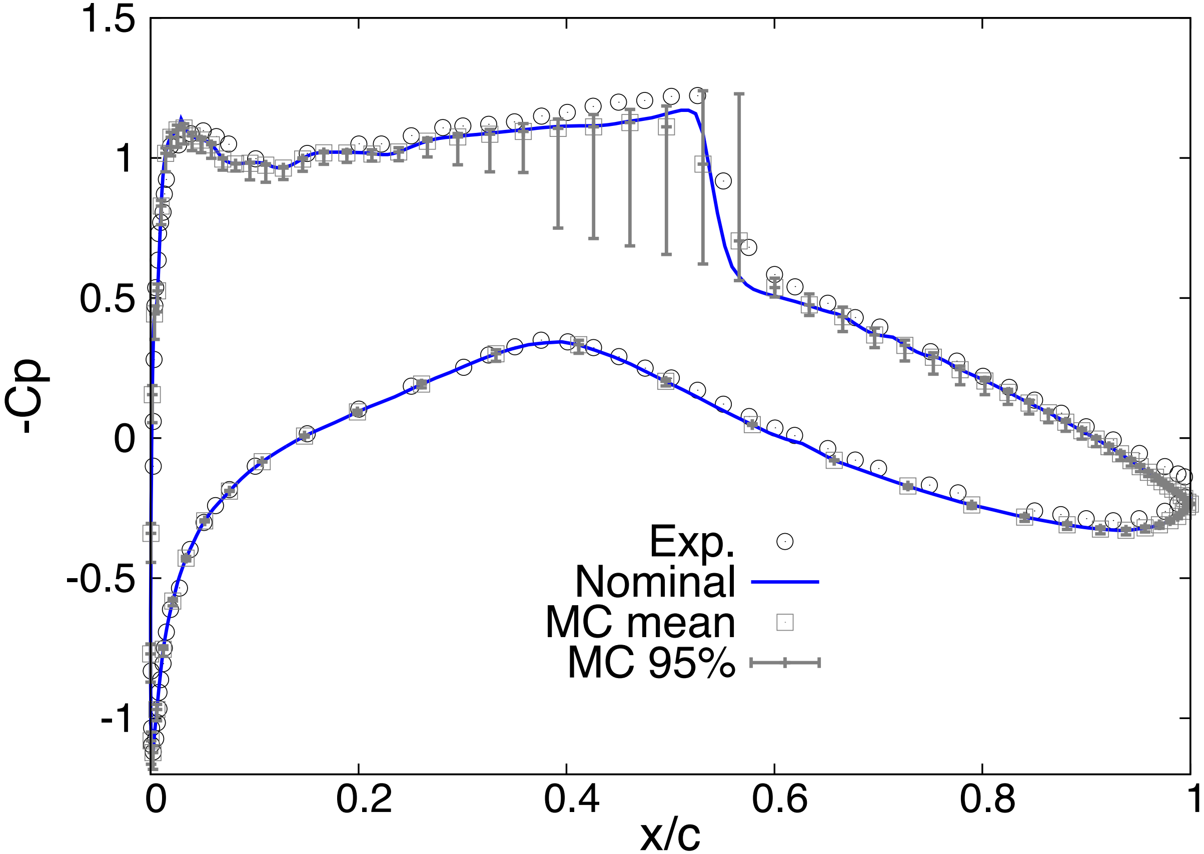
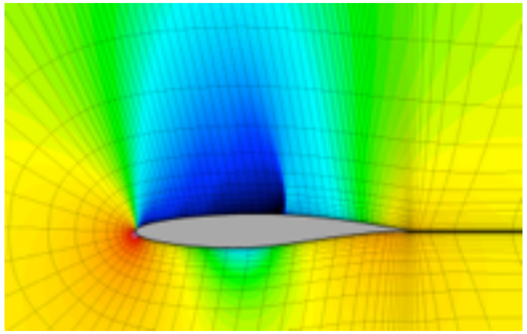


Application (Transonic Airfoil)



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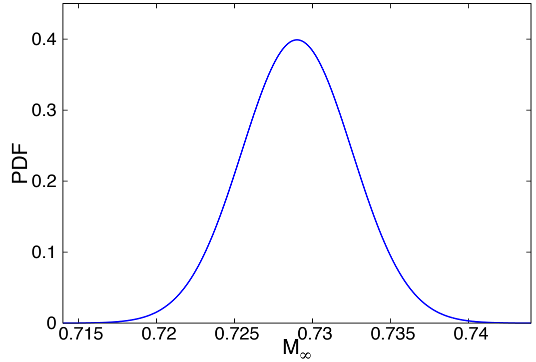

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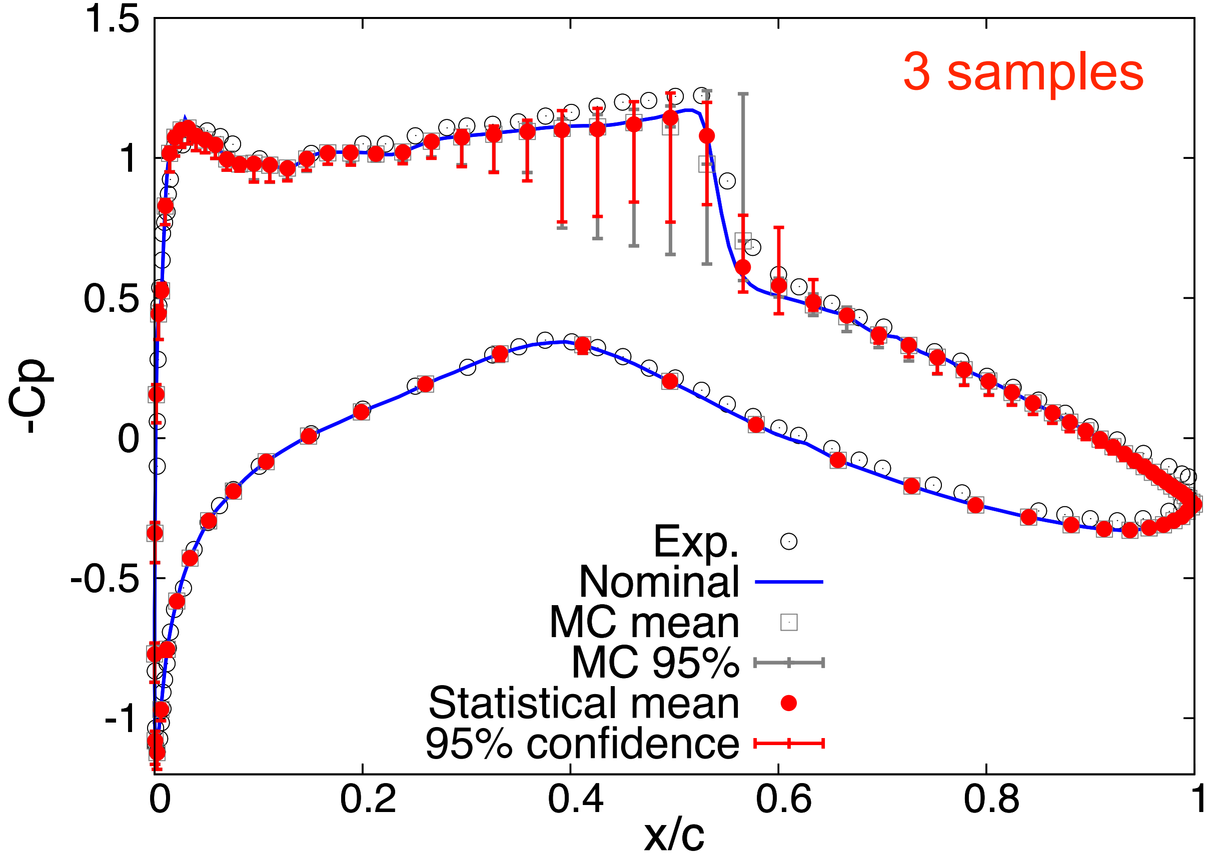

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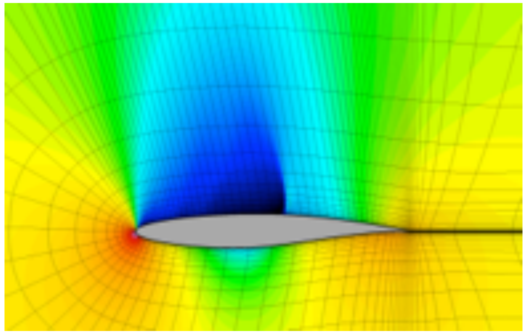

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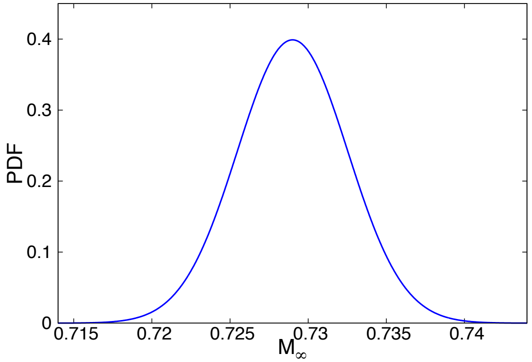

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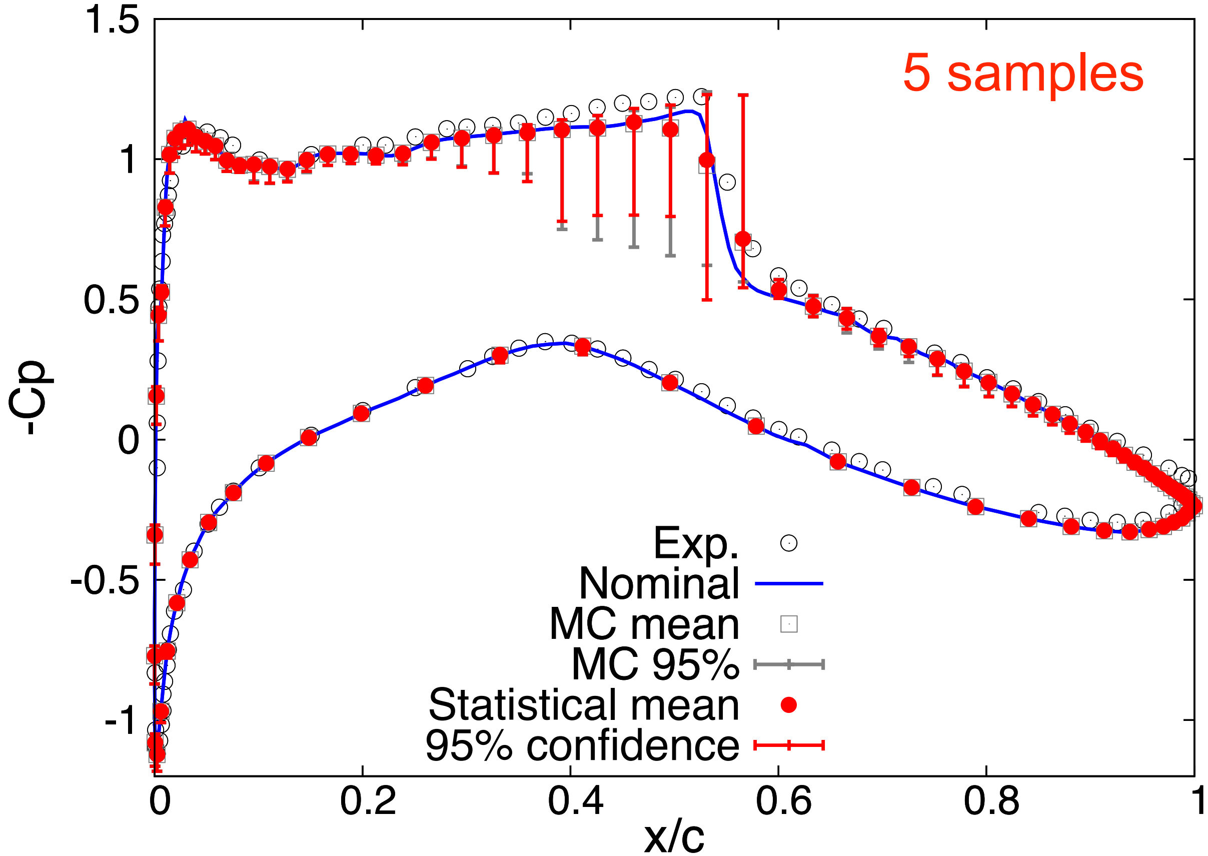

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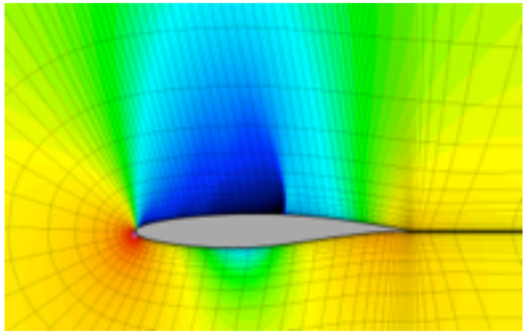

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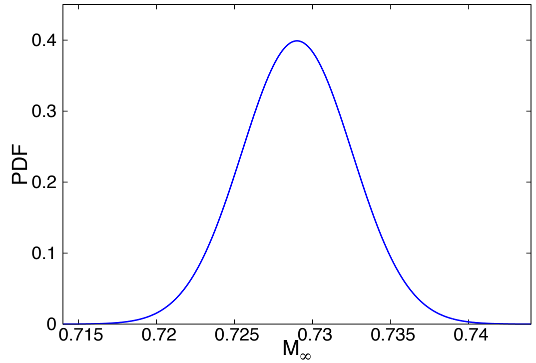

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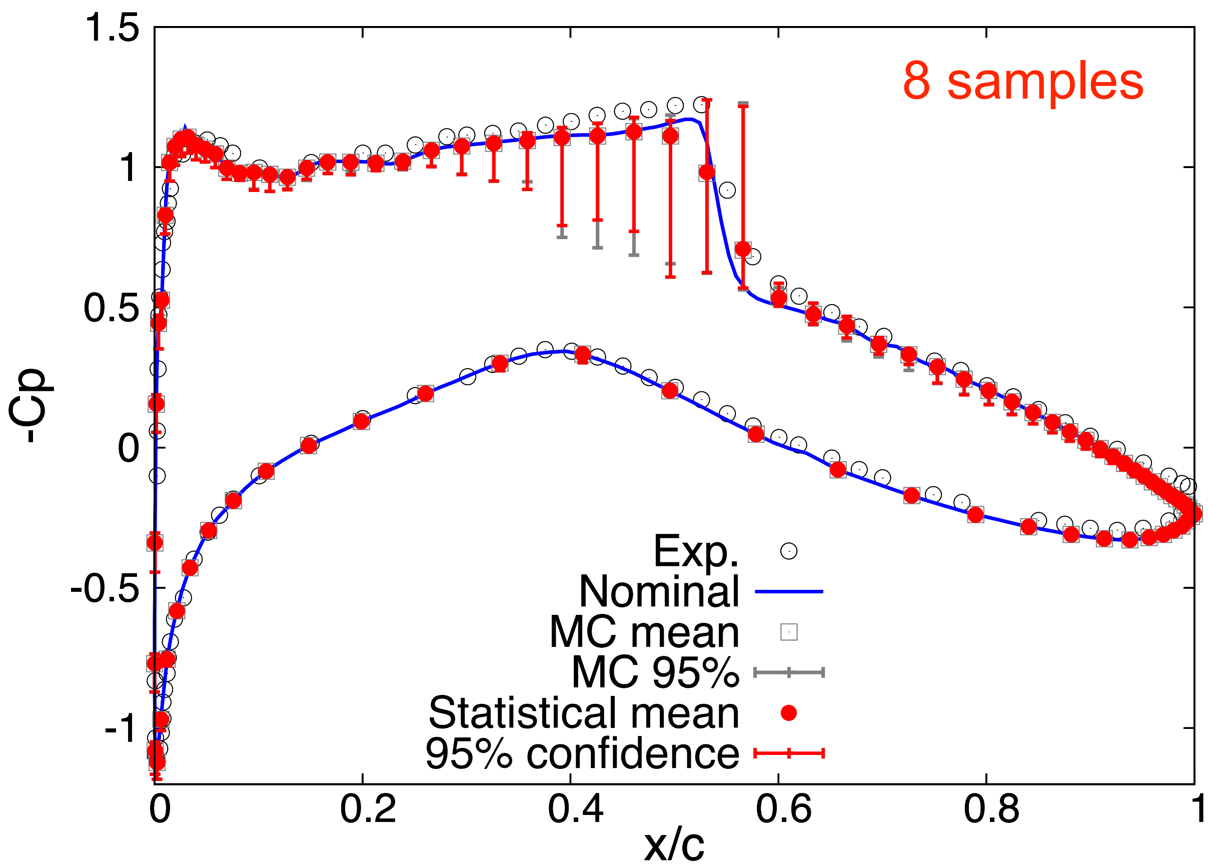

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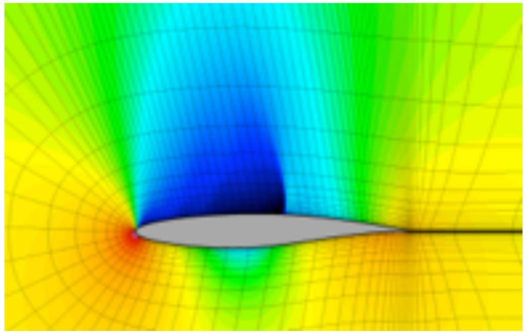

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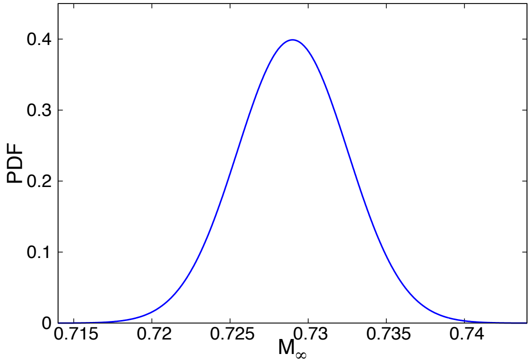

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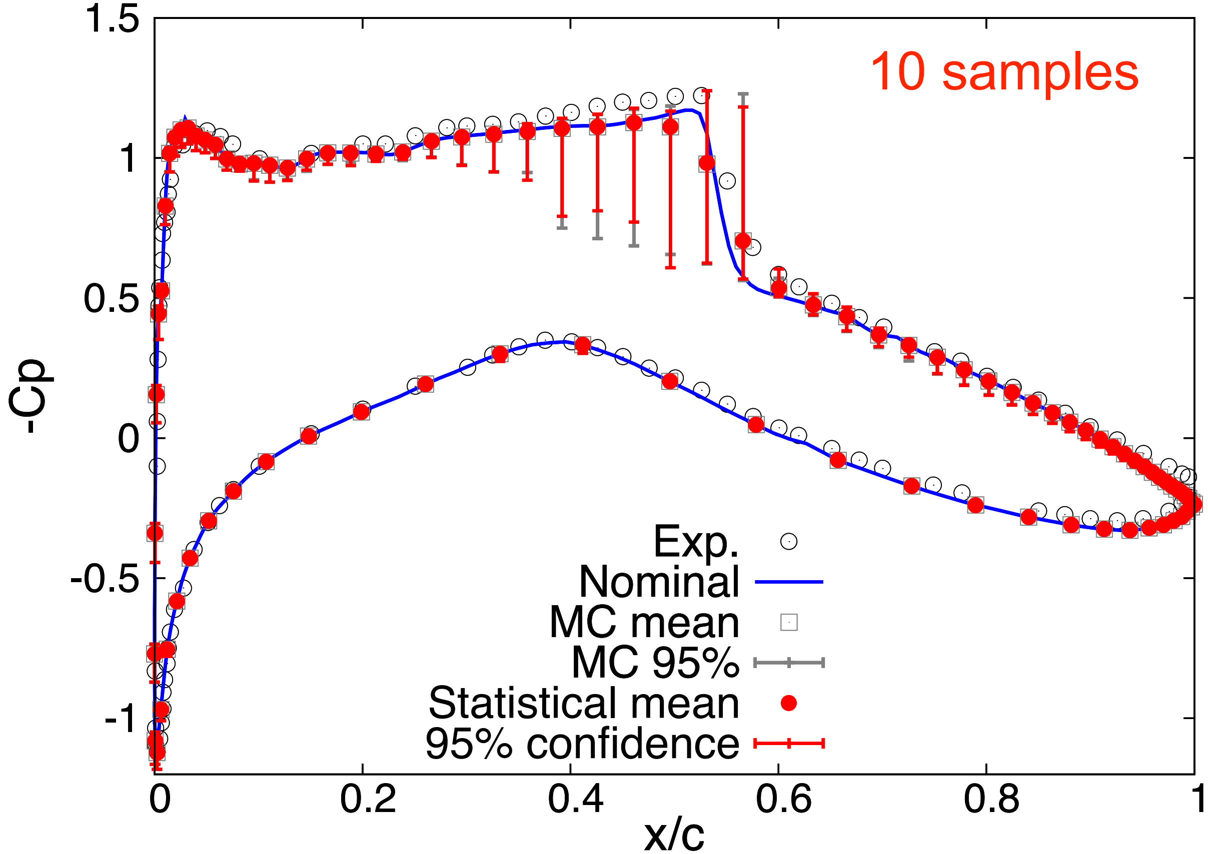

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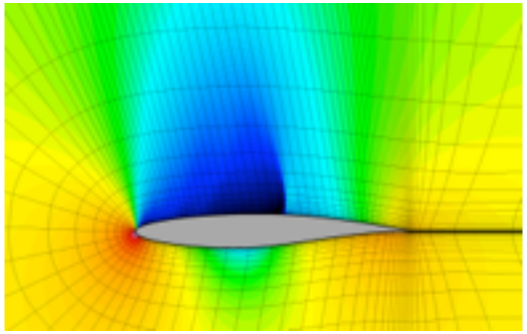

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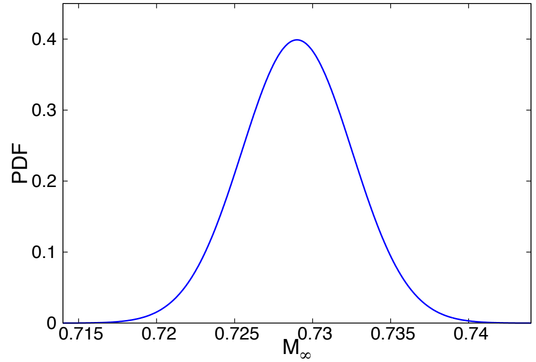

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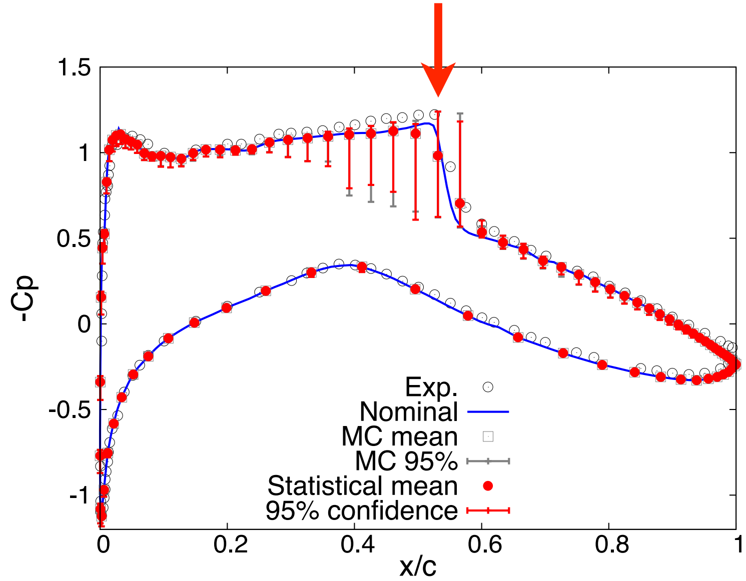

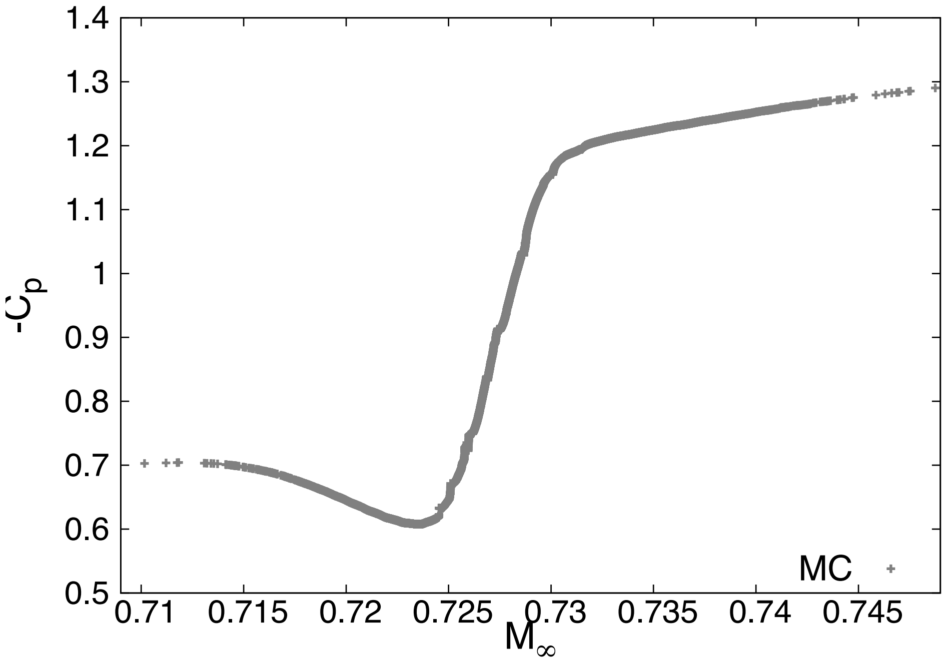

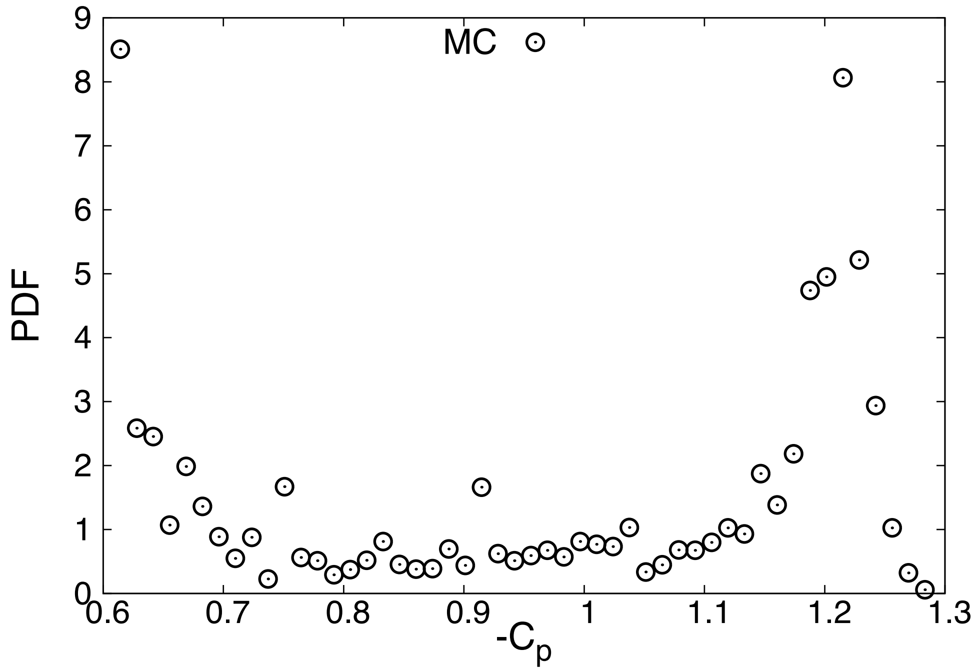

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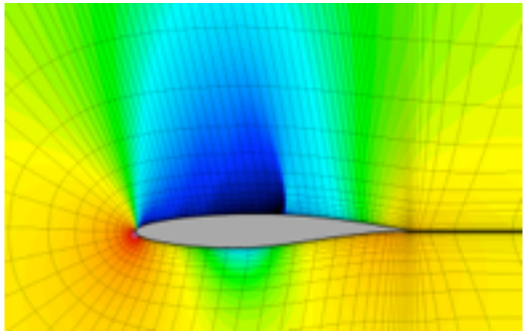

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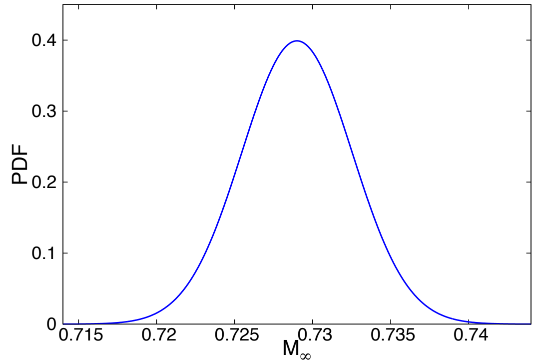

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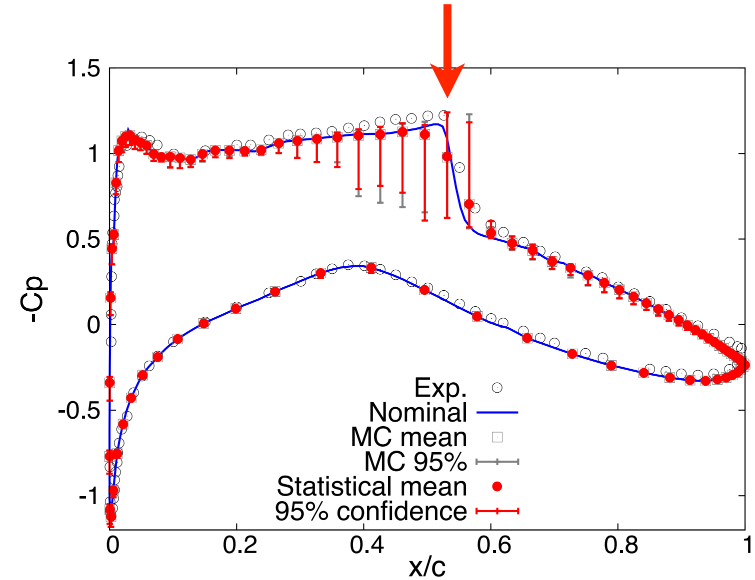

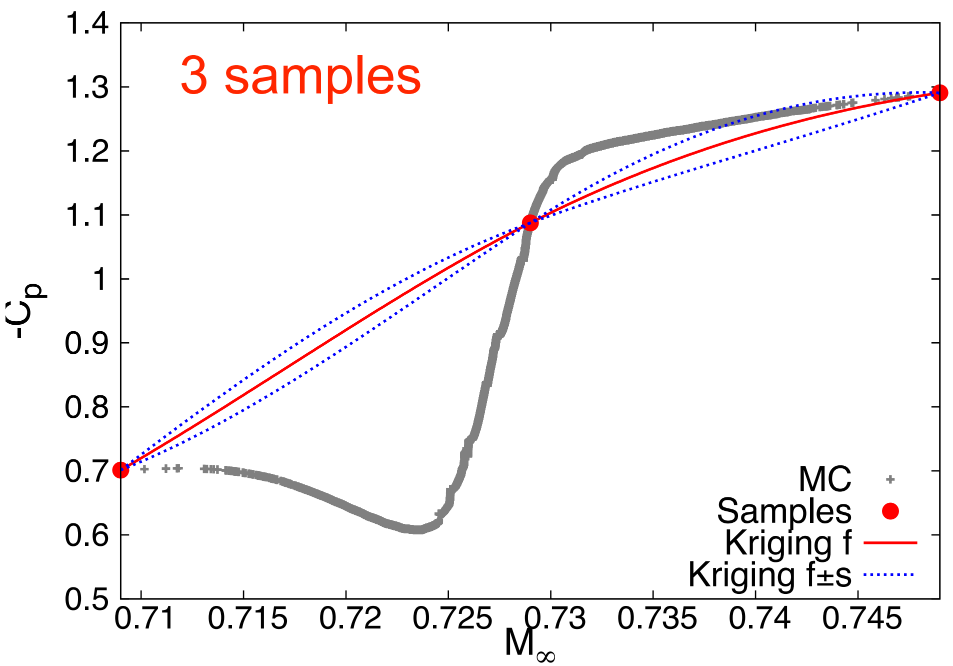

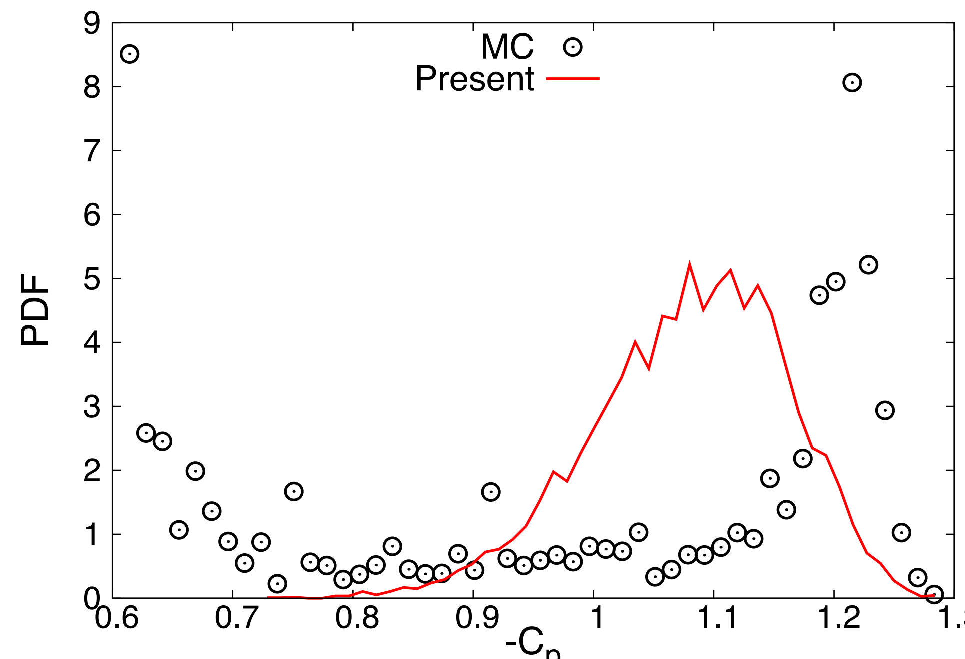

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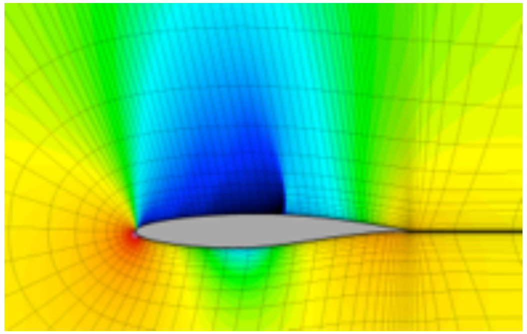

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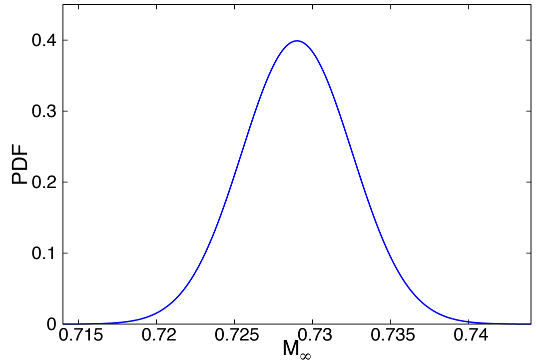

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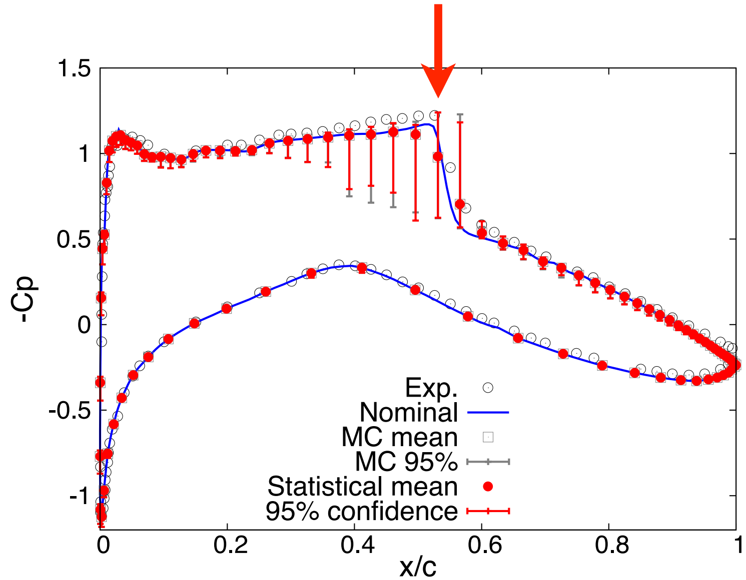

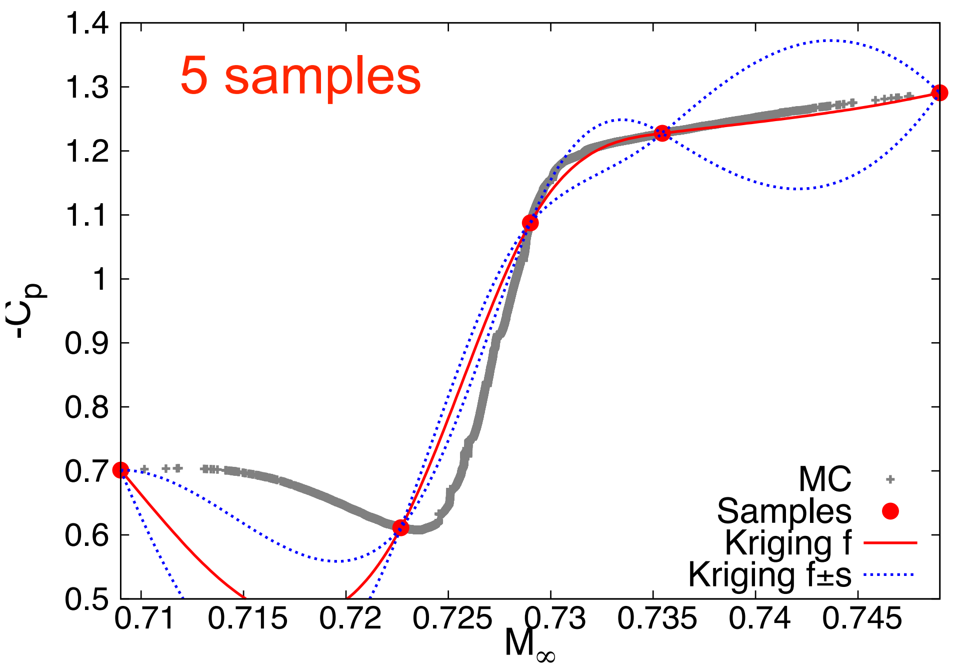

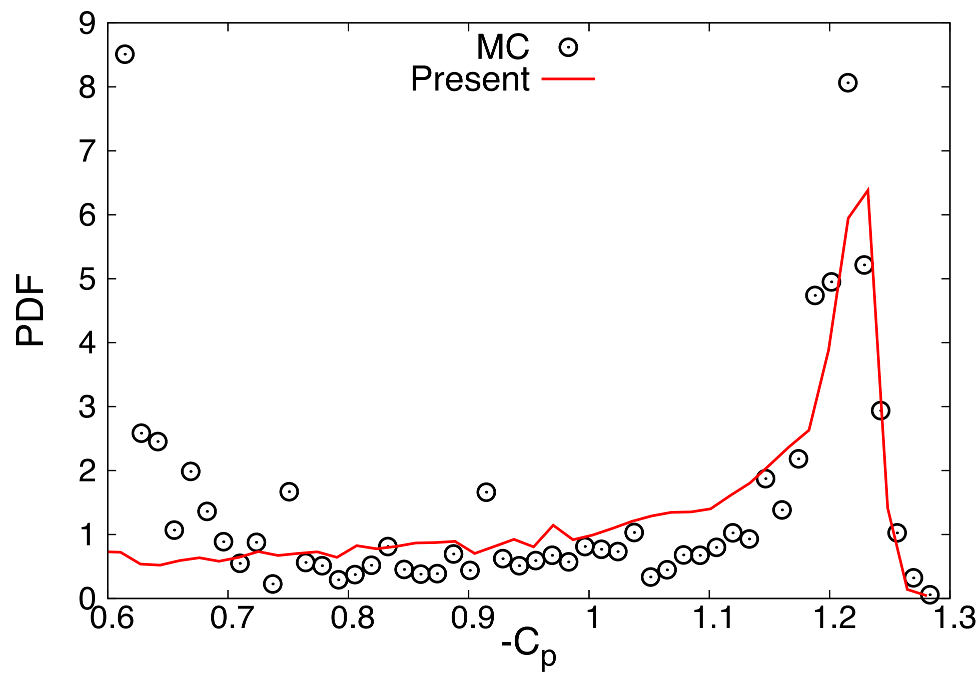

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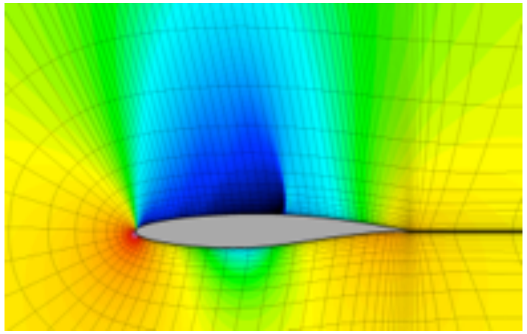

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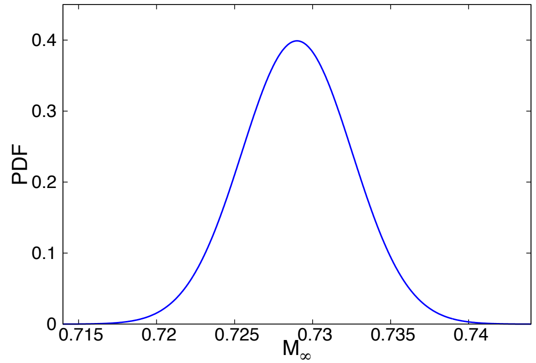

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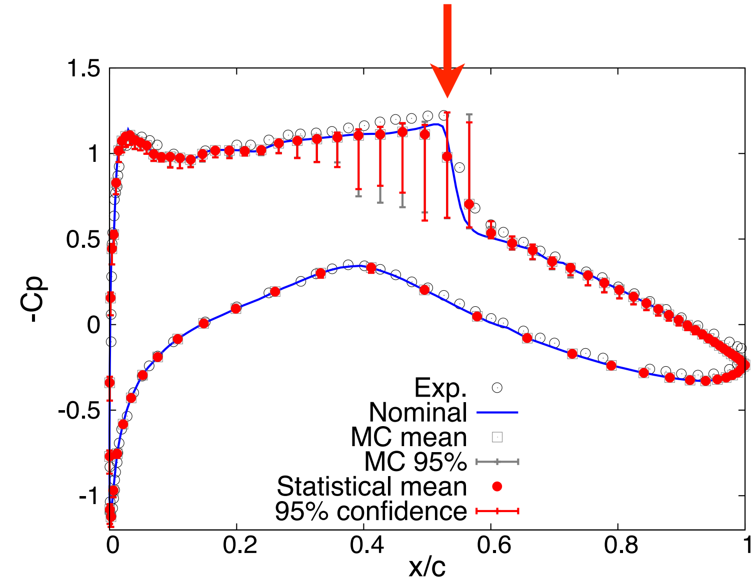

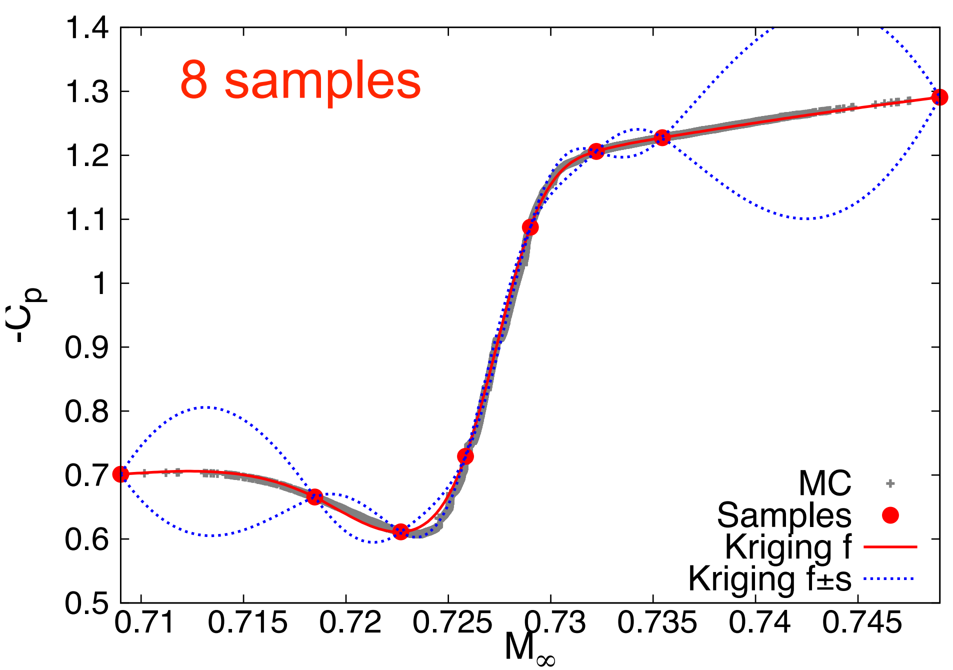

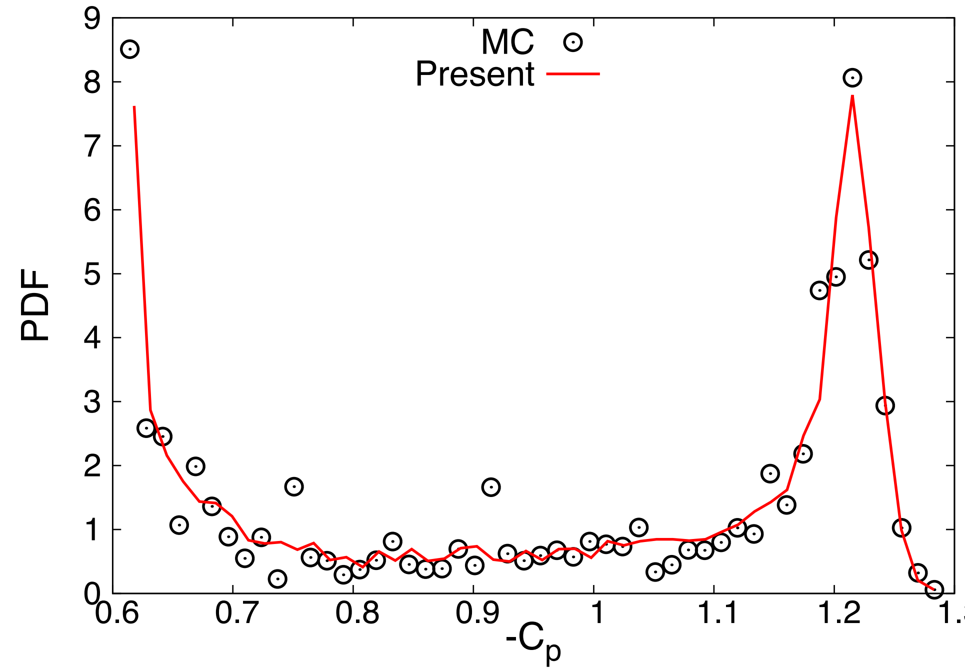

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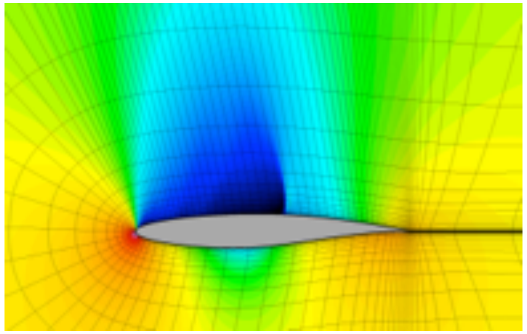

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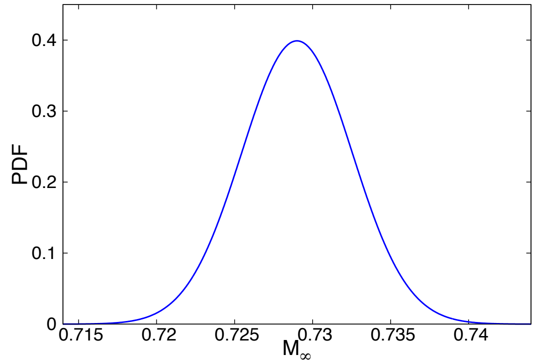

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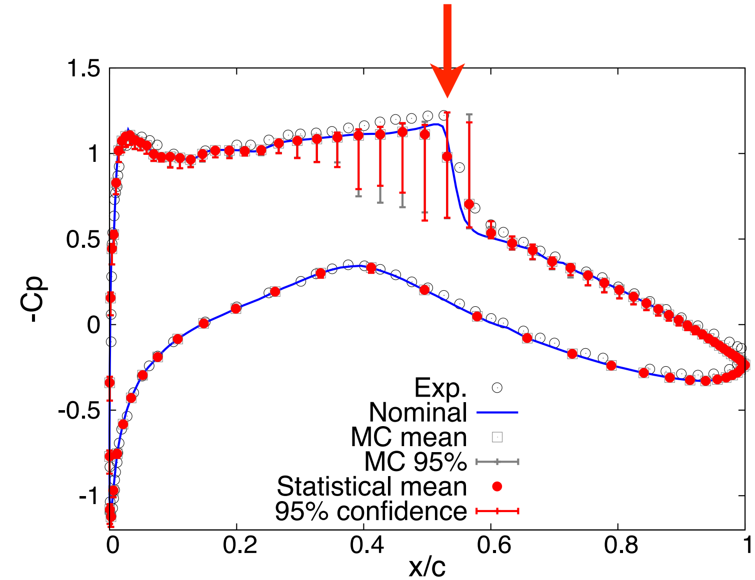

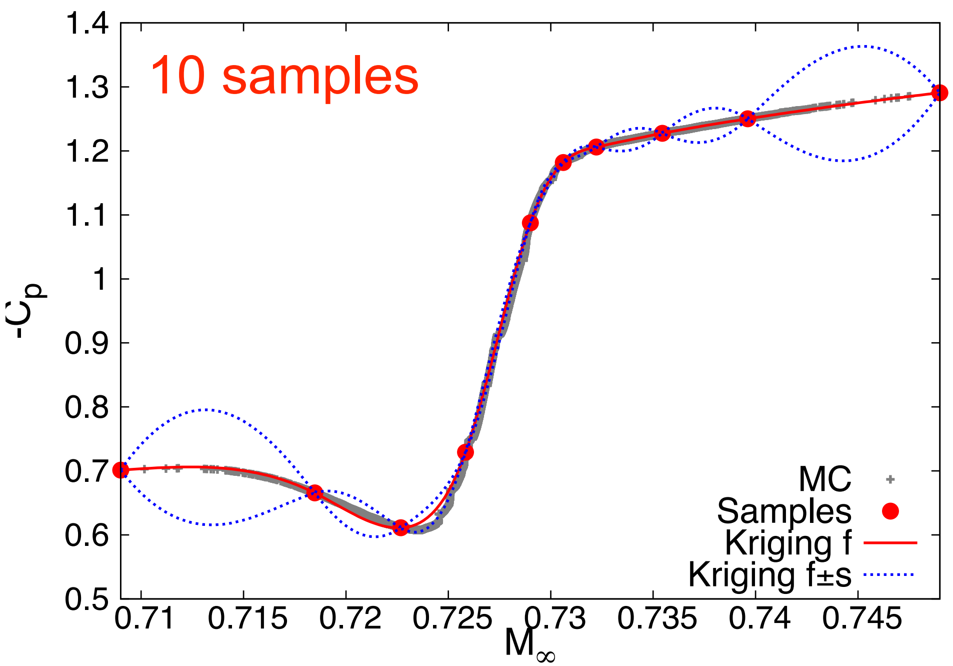

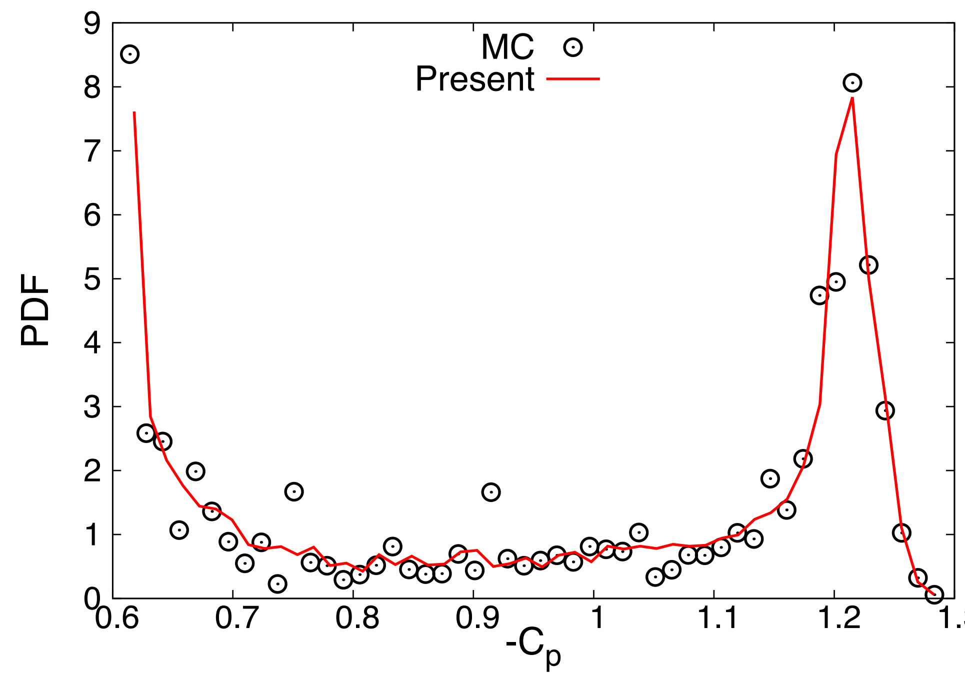

Outline

- ✓ Fundamentals of Uncertainty Quantification
- ✓ Research Topics
  - Polynomial Chaos Expansion with Order Adjustment
    - ✳ Prof. Shigeru Obayashi (Tohoku Univ.)
    - ✳ Mr. Akihiro Inoue (Tohoku Univ.)
    - ✳ JAXA/NSRG
  - Dynamic Adaptive Sampling based on Kriging Surrogate Model
    - ✳ Dr. Soshi Kawai (JAXA/ISAS)
    - ✳ Prof. Juan J. Alonso (Stanford Univ.)
- ✓ **Summary**

Summary

- UQ is expected to contribute to the fields of simulation, physics, design, etc., but still has technical issues to be considered
- PCE can be well tuned through the order adjustment based on appropriate measures
- Kriging-based dynamic adaptive sampling can make UQ with discontinuity more effective

Acknowledgments

JSPS 独立行政法人 日本学術振興会
Japan Society for the Promotion of Science

- Young Researcher Overseas Visits Program for Vitalizing Brain Circulation
- Grant-in-Aid for Young Scientists (A)

JAXA 宇宙航空研究開発機構
Japan Aerospace Exploration Agency

- International Top Young Fellowship Program