

SAND2016-3697PE

# Compressed sensing and its role in designing aircraft nozzles in the presence of uncertainty

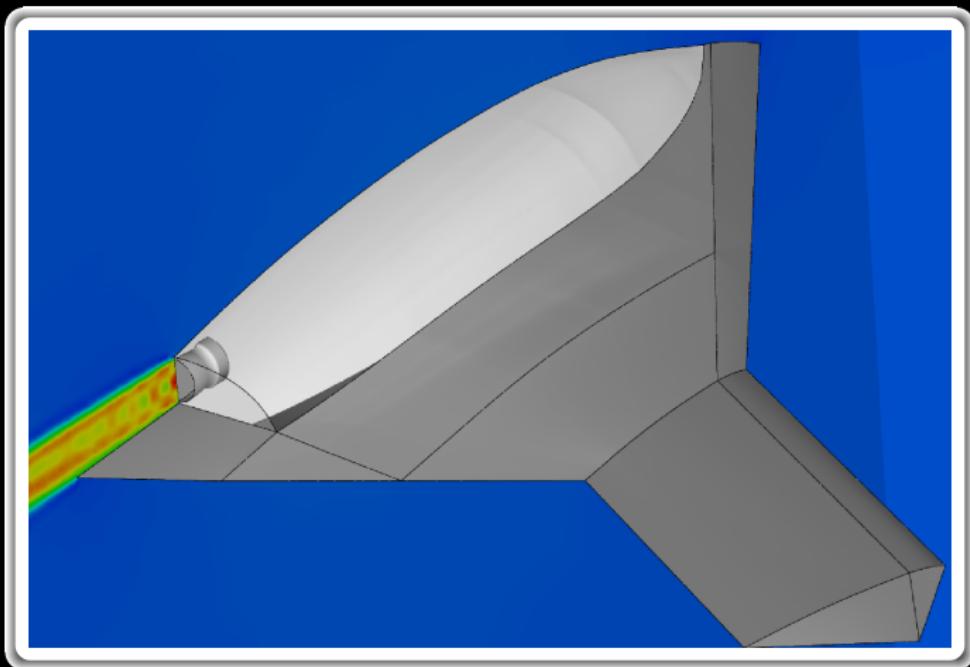
John D. Jakeman

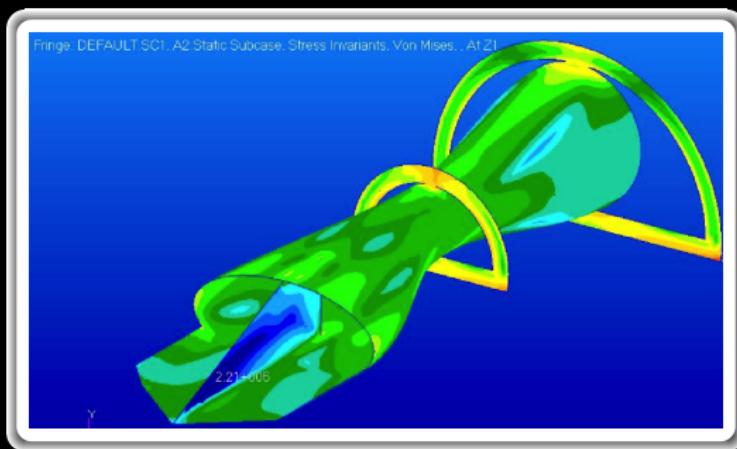
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Sandia National Laboratories is a multi program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Goal: design nozzle propulsion systems of advanced aircraft that optimize aerodynamic performance, thermal and pressure loads, and fatigue





## Problem Characteristics

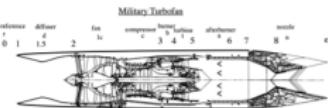
Nonlinear governing equations

Computationally expensive simulations

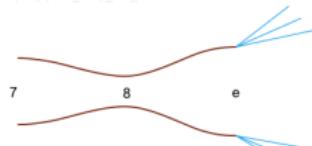
Large number of design variable

Many sources of uncertainty

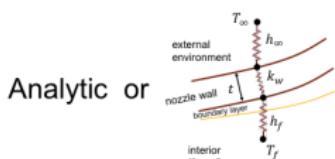
Large number of uncertain variables



1-D engine model



Ideal and non-ideal nozzle aero

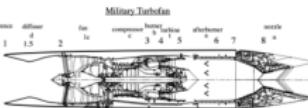


1-D Heat Transfer

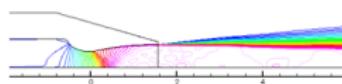
$$\sigma(x) = P(x) \frac{D(x)}{2t(x)}$$

Simplified hoop stresses

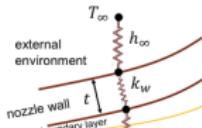
Low-fidelity model



1-D engine model



Axisymmetric RANS nozzle aero

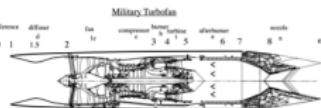


1-D Heat Transfer

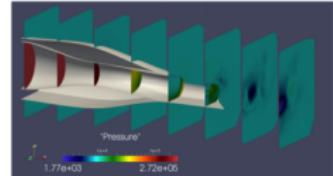


Coarse FEM structural model

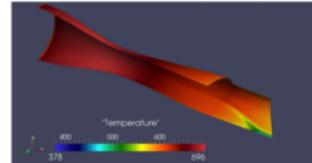
Medium-fidelity model



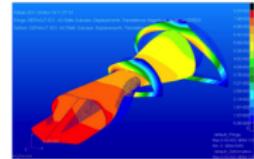
1-D engine model



RANS nozzle aerodynamics



Conjugate heat transfer



FEM structural model

High-fidelity model

# Design is expensive

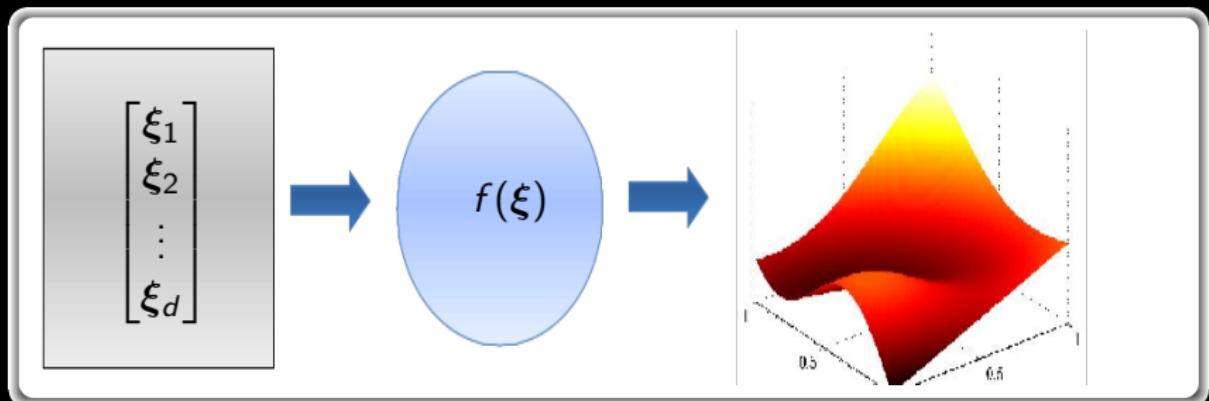
Optimization involves many evaluations of  
model and gradient

At each step of the design we must quantify  
certain statistics of uncertainty

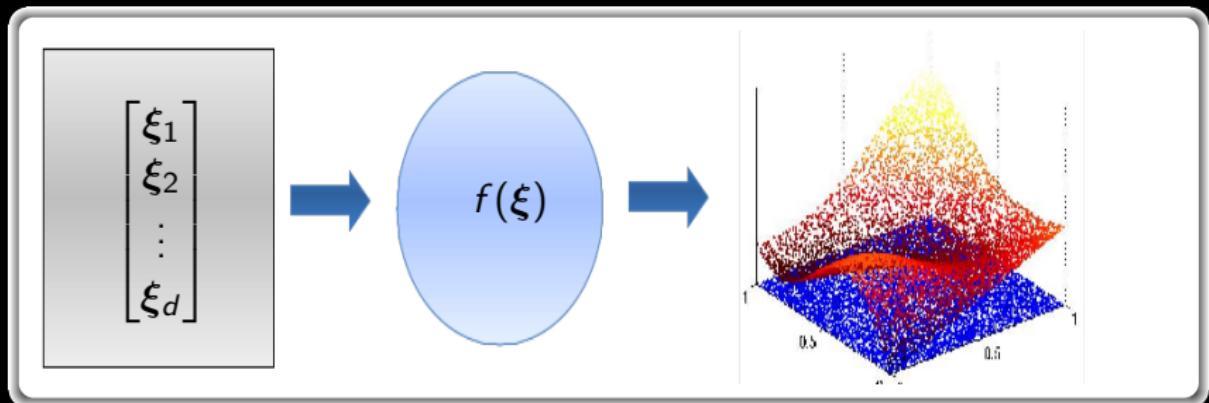
# A fundamental challenge facing UQ

Can we capture the salient features of a high-fidelity, high-dimensional model from limited simulation data

Given distributions on the input data we can calculate statistical moments, distributions, etc. of the QOIs

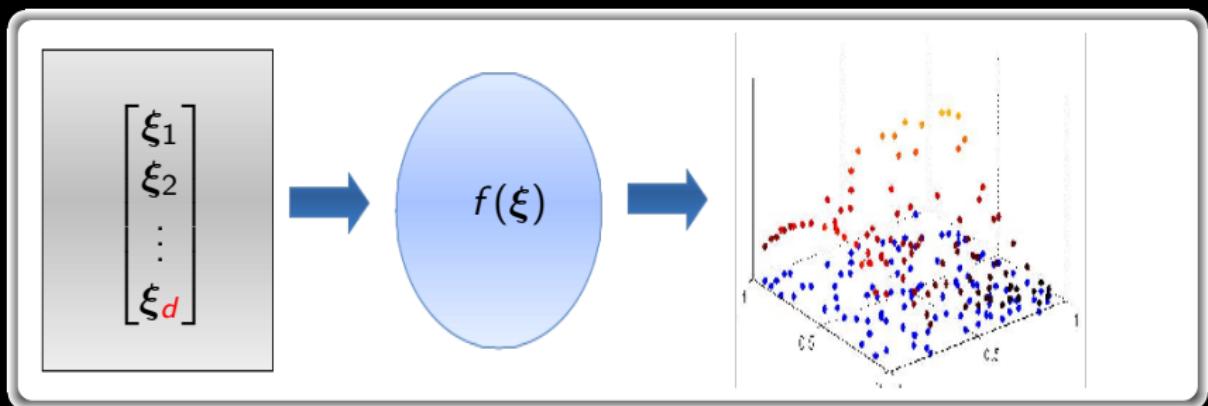


We usually must sample from the input distributions to calculate statistics



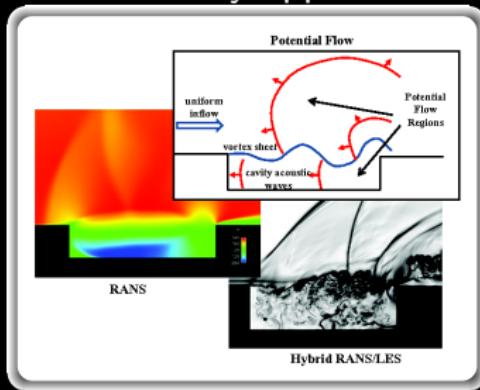
BUT...

Simulation models are computationally and financially expensive

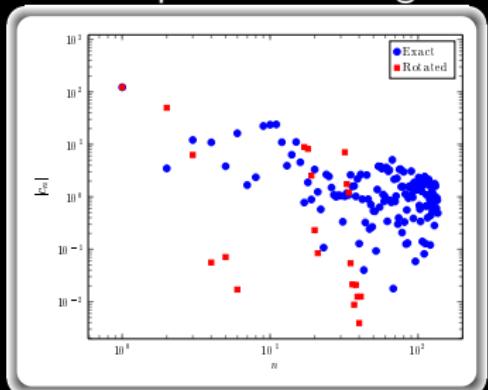


# What are we doing to address these challenges?

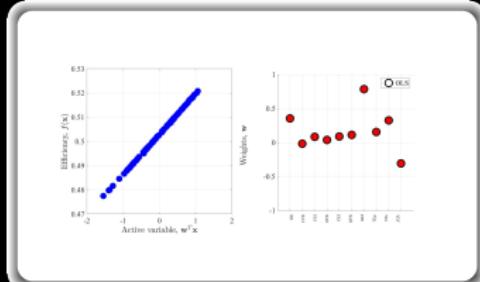
## Multifidelity approaches



## Compressed sensing



## Dimension reduction



Today I will focus on compressed sensing

# Polynomial Chaos Expansions (PCE)

Multidimensional approximation of  $f(\xi)$  with finite variance

$$f(\xi) \approx f_{\Lambda}(\xi) = \sum_{\lambda \in \Lambda} \alpha_{\lambda} \phi_{\lambda}(\xi), \quad \lambda = (\lambda_1, \dots, \lambda_d)$$

Orthonormal basis

$$(\phi_i(\xi), \phi_j(\xi)) = \int_{I_{\xi}} \phi_i(\xi) \phi_j(\xi) w(\xi) = \delta_{ij}$$

Assume ordering  $n = 1, \dots, N$  assigned to elements of  $\Lambda$

Askey scheme

Normal	Hermite $He_n(x)$	$e^{\frac{-x^2}{2}}$	$[-\infty, \infty]$
Uniform	Legendre $P_n(x)$	$\frac{1}{2}$	$[-1, 1]$

# Why are PCE useful?

calculate moments and Sobol indices

$$\mu = \alpha_0, \quad \sigma^2 = \sum_{\lambda \in \Lambda} \alpha_{\lambda}^2$$

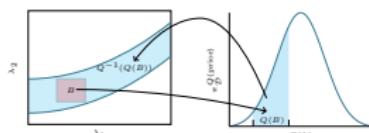
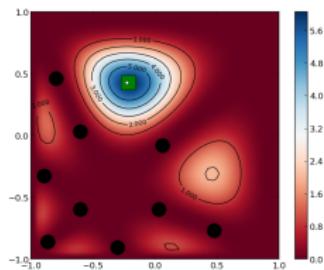
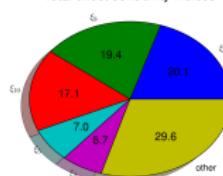
Tailor sampling to density

Weighted Leja sequences.

Surrogate for sampling methods

Computing PDFs, CDFs,  
probability of rare events,  
posterior-densities, etc.

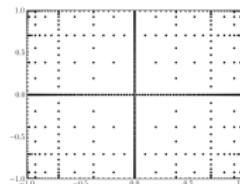
Total effect sensitivity indices



# How can we calculate PCE coefficients

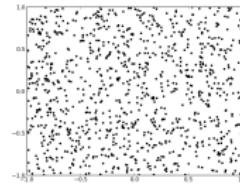
Pseudo spectral projection

$$\alpha_{\lambda} = \int_{I_{\xi}} f(\xi) \phi_{\lambda}(\xi) d\rho(\xi)$$



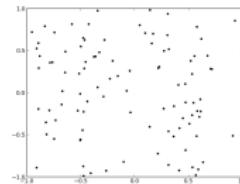
Least squares

$$\arg \min_{\alpha} \|f(\xi_m) - f_{\Lambda}(\xi_m)\|_2$$



Compressed sensing

$$\arg \min_{\alpha} \|\alpha\|_1 \text{ s.t. } \|f(\xi_m) - f_{\Lambda}(\xi_m)\|_2 \leq \varepsilon$$



# What does compressed sensing do?

Compressed sensing attempts to find a sparse solution that is a “good” approximation of the observational data

A sparse solution

$$s = \#\{\lambda : |\alpha_\lambda| > 0\}$$

Typical “Good” approximation

$$\|f(\xi_m) - f_\Lambda(\xi_m)\|_2 \leq \varepsilon$$

Why do we care about sparsity?

## Why do we care about sparsity?

Occam's razor — “when faced with many possible ways to represent a signal, the simplest choice is the best one.”

Why do we care about sparsity?

“KISS”

# Why do we care about sparsity?

The number of samples required grows  
LINEARLY with dimension

# Compressed Sensing

Generate  $M$  model runs

$$\Xi_M = \{\xi_1, \dots, \xi_M\}, \quad \mathbf{f} = (f(\xi_1), \dots, f(\xi_M))^T$$

We want 'good' solution to

$$\begin{bmatrix} f(\xi_1) \\ f(\xi_2) \\ \vdots \\ f(\xi_M) \end{bmatrix} = \begin{bmatrix} \phi_1(\xi_1) & \phi_2(\xi_1) & \dots & \phi_N(\xi_1) \\ \phi_1(\xi_2) & \phi_2(\xi_2) & \dots & \phi_N(\xi_2) \\ \vdots & \vdots & & \vdots \\ \phi_1(\xi_M) & \phi_2(\xi_M) & \dots & \phi_N(\xi_M) \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_N \end{bmatrix} + \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_M \end{bmatrix}$$

# Sparse solutions

A sparse solution

$$s = \#\{\lambda : |\alpha_\lambda| > 0\}$$

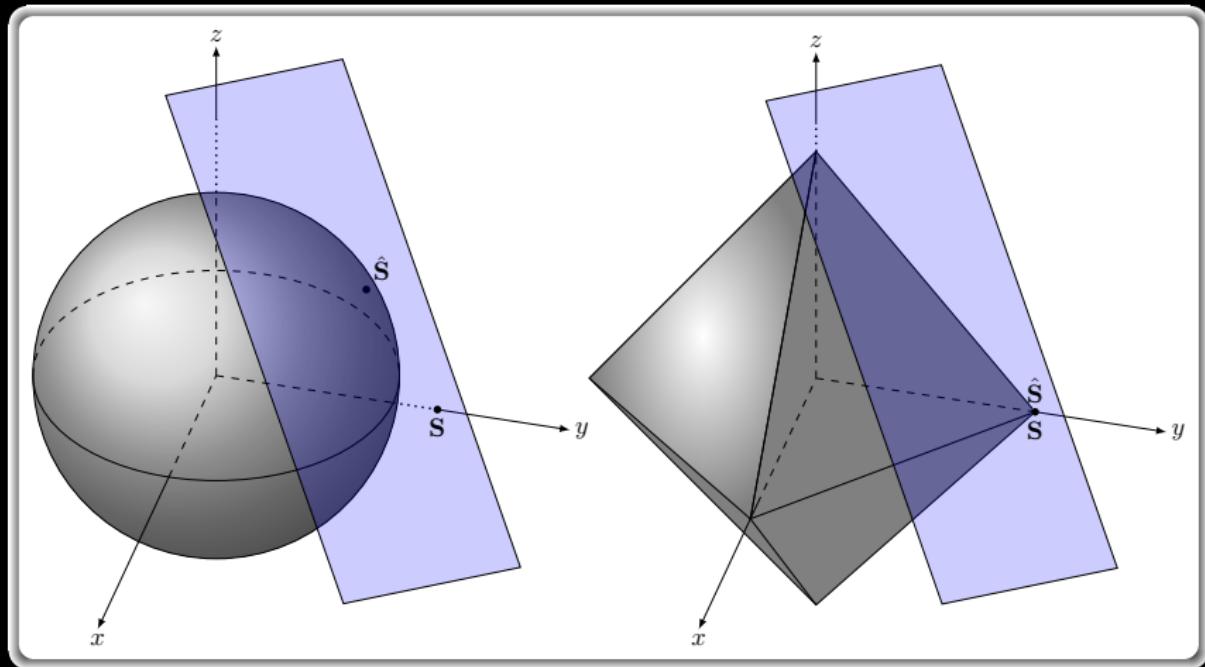
$\ell_0$ -minimization (NP HARD)

$$\arg \min_{\alpha} \|\alpha\|_0 \text{ s.t. } \|f(\Xi_M) - f_\Lambda(\Xi_M)\|_2 \leq \varepsilon$$

$\ell_1$ -minimization

$$\arg \min_{\alpha} \|\alpha\|_1 \text{ s.t. } \|f(\Xi_M) - f_\Lambda(\Xi_M)\|_2 \leq \varepsilon$$

# Why does $\ell_1$ -minimization produce a sparse solution



# How well does compressed sensing work?

## $\ell_2$ -minimization

$$M \geq N \log(N) = dn^d \log(n)$$

## $\ell_1$ -minimization

$$M \geq s \log^3(s) \log(N)L = ds \log^3(s) \log(n)L$$



Are PCE representations of models  
usually sparse?

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usually sparse?

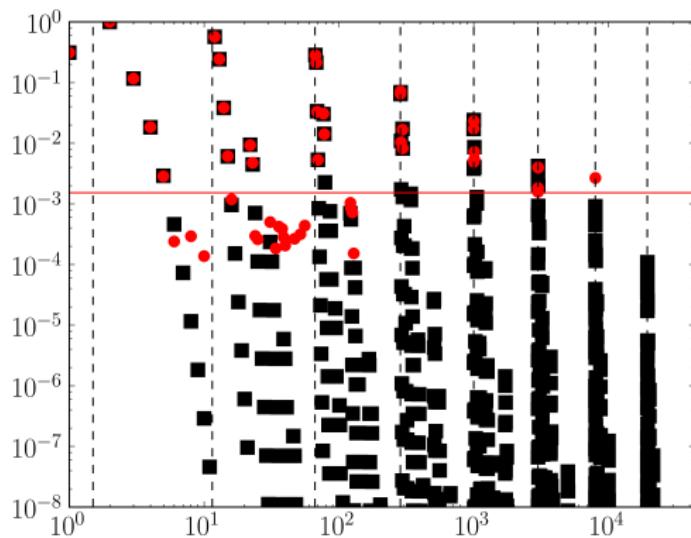
NO

But...

# Are PCE representations of models usually sparse?

PCE are compressible

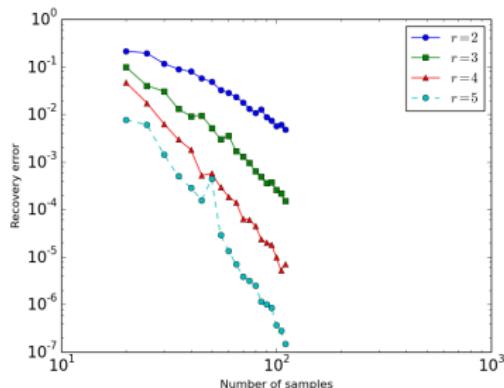
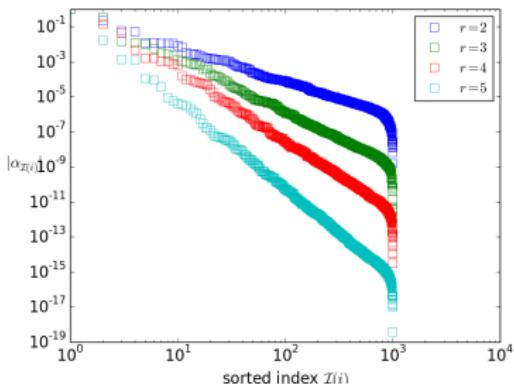
$$s = \#\{\lambda : |\alpha_\lambda| > \tau\}$$



# How well does CS apply to compressible signals?

## Compressible signals

$$|\alpha_{\mathcal{I}(i)}| \leq Ci^{-r}$$



## Recent contributions

- ▶ Reweighting
- ▶ Adaptive basis selection
- ▶ Change of measure

$$\boldsymbol{\alpha}^* = \arg \min_{\boldsymbol{\alpha}} \|\boldsymbol{\alpha}\|_1 \quad \text{such that} \quad \|\mathbf{W}\Phi\boldsymbol{\alpha} - \mathbf{W}\mathbf{f}\|_2 \leq \varepsilon$$

# Requirements for finding a sparse solution

Small mutual coherence  $\mu$

$$\mu(\Phi) = \max_{1 < j < k \leq N} \frac{|\tilde{\phi}_j^T \tilde{\phi}_k|}{\|\tilde{\phi}_j\|_2 \|\tilde{\phi}_k\|_2}$$

Small RIP constant  $\delta_s$

$$(1 - \delta_s) \|\alpha_s\|_2^2 \leq \|\Phi \alpha_s\|_2^2 \leq (1 + \delta_s) \|\alpha_s\|_2^2$$

$$\Phi = \left( \begin{array}{cccc} \dots & \boxed{\phi_{\lambda_j}(\xi_1)} & \dots & \boxed{\phi_{\lambda_k}(\xi_1)} & \dots \\ \dots & \boxed{\phi_{\lambda_j}(\xi_2)} & \dots & \boxed{\phi_{\lambda_k}(\xi_2)} & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & \boxed{\phi_{\lambda_j}(\xi_M)} & \dots & \boxed{\phi_{\lambda_k}(\xi_M)} & \dots \end{array} \right)$$

$\underbrace{\tilde{\phi}_j}_{\tilde{\phi}_k}$

## Theorem: RIP bound for Orthonormal Systems [Rahut and Ward 2010]

Consider the orthonormal system  $\{\phi_j, j \in [N]\}$  with

$$\sup_{\xi \in D, j \in [N]} \|\phi_j\|_\infty \leq K$$

and the matrix  $\Phi \in \mathbb{R}^{M \times N}$  with entries formed by i.i.d. samples drawn from  $w$ . If

$$M \geq C\delta^{-2}K^2s \log^3(s) \log(N),$$

then with probability at least  $1 - N^{-\gamma \log^3(s)}$  the restricted isometry constant  $\delta_s$  of  $\frac{1}{\sqrt{M}}\Phi$  satisfies  $\delta_s \leq \delta$  for universal constants  $C, \gamma > 0$

# Change of measure

Enforce small coherence parameter

Scale basis functions by  $\sqrt{W}$  so that

$$L = K^2 = O(1)$$

This can be achieved using the Chirstoffel function

Maintain orthogonality

We can no longer sample from  $w(\xi)$  but must instead sample from the biased density

$$w(\xi)/W(\xi)$$

The corresponding measure of this density is the equilibrium measure  $\mu$  where  $w/W \approx d\mu$

## The Christoffel function

$$W_\Lambda(\xi) = \frac{N}{\sum_{n=1}^N \phi_n^2(\xi)}$$

### Properties

- ▶ Generates bounded orthonormal system
- ▶  $w/W \rightarrow d\mu$ , as  $n \rightarrow \infty$

$$R_{kl} = \int_{I_\xi} \phi_k(\xi) \phi_l(\xi) W_\Lambda(\xi) d\mu, \quad 0 \leq j, k \leq N$$

**R**  $\rightarrow$  **I**, as  $N \rightarrow \infty$

## Theorem [Nevai et. al. 1994]

$$\max_{\xi \in [-1, 1]} \frac{N\phi_N^2(\xi)}{\sum_{k=0}^N \phi_k^2(\xi)} \leq \frac{4N(2 + \sqrt{\alpha^2 + \beta^2})}{2N + \alpha + \beta + 2} = K$$

## [Levin and Lubinsky 1994]

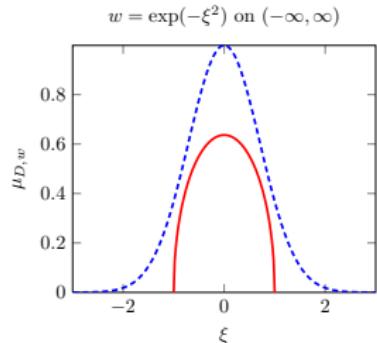
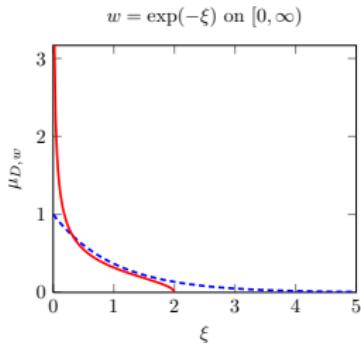
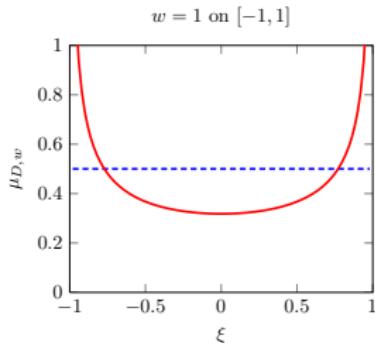
Similar more complicated bounds are known for unbounded variables with weight functions of the form

$$w(x) = \exp(-|\xi|^\alpha), \quad \alpha \geq 1$$

## The equilibrium measure

Given  $I_\xi$  and  $w$ , we will be concerned with  $\mu$

- ▶  $\mu$  is a unique probability measure
- ▶  $\mu$  has compact support (even if  $I_\xi$  does not)
- ▶ With  $d = 1$ ,  $\mu$  coincides with the weighted potential-theoretic equilibrium measure (e.g., “Chebyshev-like” on 1D intervals)



## Equilibrium sampling: Normal

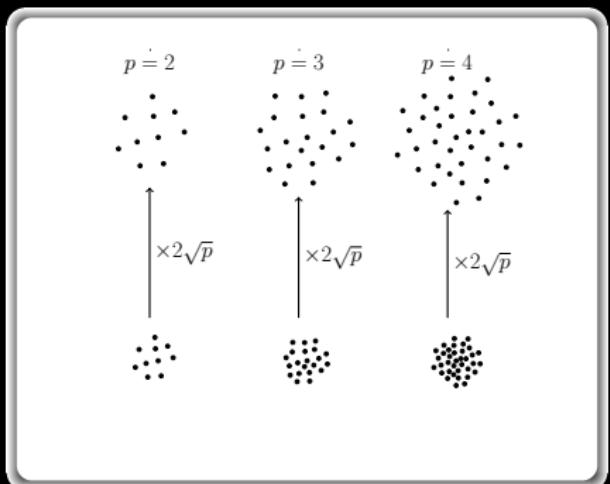
Let  $z_i \sim N(0, 1)$  and  $u \in [0, 1]$  with PDF  
 $w(u) = (1 - u^2)^{d/2} u^{d-1}$

$$\mathbf{y} = \frac{\mathbf{z}}{\|\mathbf{z}\|_2} u, \quad \xi = \mathbf{y} 2\sqrt{p}$$

## Equilibrium sampling: all bounded variables

Let  $z_i \sim U[0, 1]$

$$\xi = \cos(\mathbf{z}\pi)$$



# Motivation for the equilibrium measure

## $\ell_1$ -minimization

Allows one to bound weighted polynomials.

## Regression

Ensures that the stability of the condition number can be achieved using only log-linear, i.e.  $M = N \log N$ .

## Interpolation

It is necessary to sample from the equilibrium measure to obtain a 'good' Lebesgue constant.

## Theorem: [Jakeman et al.]

Suppose that  $M$  sampling points  $(\xi^{(1)}, \dots, \xi^{(M)})$  are drawn iid according to the equilibrium measure density  $v_n$  and the diagonal matrix  $\mathbf{W}$  with entries given by  $W_{ii} = W_\Lambda(\xi^{(i)})$ . Assume that the number of samples satisfies

$$M \geq L(n) \left\| \mathbf{R}^{-1/2} \right\|_1^2 s \log^3(s) \log(N),$$

where  $\mathbf{R}$  measures the deviation from orthogonality. Then the coefficient vector  $\mathbf{R}^{1/2}\alpha$  is recoverable by solving the inequality-constrained  $\ell^1$ -minimization problem

$$\mathbf{R}^{1/2}\alpha^* = \arg \min_{\alpha} \|\mathbf{R}^{1/2}\alpha\|_1 \quad \text{such that} \quad \|\sqrt{\mathbf{W}}\Phi\alpha - \sqrt{\mathbf{W}}\mathbf{f}\|_2 \leq \varepsilon$$

and the error in  $\alpha^*$  satisfies

$$\|\alpha - \alpha^*\|_2 \leq \frac{C_1 \sigma_{s,1}(\mathbf{R}^{1/2}\alpha)}{\sqrt{s \lambda_{\min}(\mathbf{R})}} + C_2 \frac{\varepsilon}{\sqrt{\lambda_{\min}(\mathbf{R})}}$$

$$\|\alpha - \alpha^*\|_1 \leq D_1 \sigma_{s,1}(\mathbf{R}^{1/2}\alpha) \left\| \mathbf{R}^{-1/2} \right\|_1 + D_2 \sqrt{s} \left\| \mathbf{R}^{-1/2} \right\|_1 \varepsilon$$

## Theorem: [Jakeman et al.]

$L(n)$  has the following behavior:

1. There is a constant  $C = C(\alpha, \beta)$  such that uniformly in  $n \geq 1$ ,

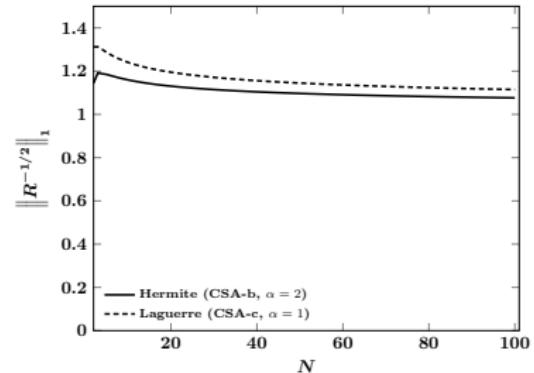
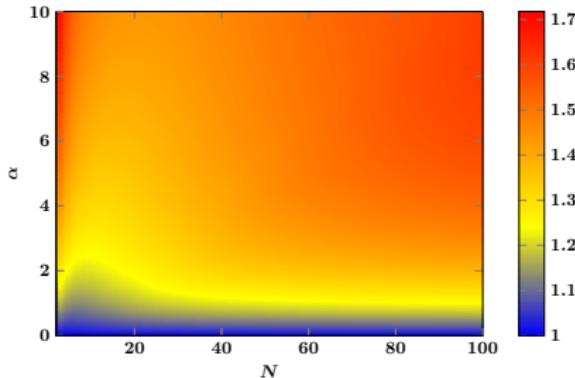
$$L(n) \leq C.$$

2. There is a constant  $C = C(\alpha)$  such that uniformly in  $n \geq 1$ ,

$$L(n) \leq Cn^{\max\{1/\alpha, 2/3\}} = \begin{cases} Cn^{2/3}, & \alpha \geq \frac{3}{2} \\ Cn^{1/\alpha}, & 1 < \alpha < \frac{3}{2} \end{cases}$$

3. There is a constant  $C = C(\alpha)$  such that uniformly in  $n \geq 1$ ,

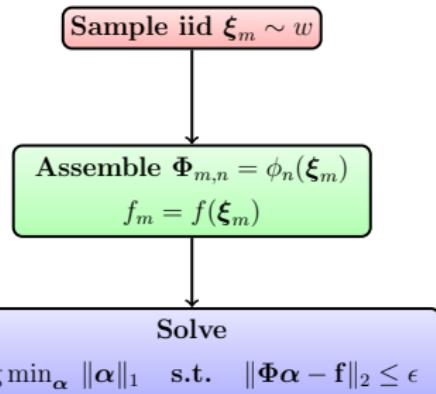
$$L(n) \leq Cn^{\max\{1/2\alpha, 2/3\}} = \begin{cases} Cn^{2/3}, & \alpha \geq \frac{3}{4} \\ Cn^{1/2\alpha}, & \frac{1}{2} < \alpha < \frac{3}{4} \end{cases}$$



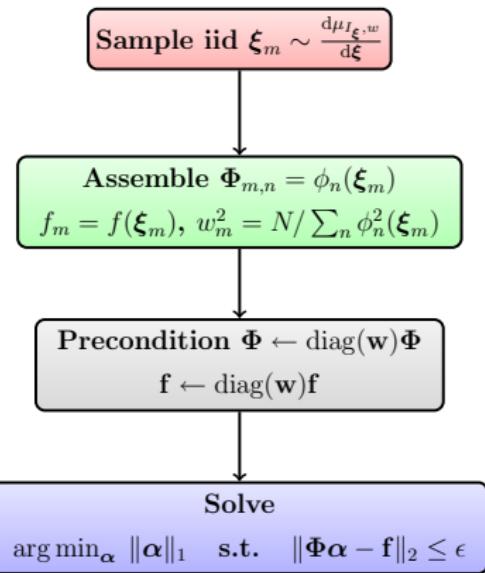
Left:  $\|\mathbf{R}^{-1/2}\|_1$  for Jacobi polynomials  $\alpha = \beta$ .

Right:  $\|\mathbf{R}^{-1/2}\|_1$  for Hermite polynomials with  $w = \exp(-x^2)$  on  $\mathbb{R}$ , and Laguerre polynomials with  $w = \exp(-x)$  on  $[0, \infty)$ .

### Standard $\ell_1$ -minimization



### Christoffel Sparse Approximation (CSA)



## Manufactured solutions

- ▶ Generate  $s$ -sparse vectors  $\alpha$ 
  - ▶ Index of each non-zero entries chosen  
 $i = 1, \dots, s \sim U(1, N)$  without replacement
  - ▶ Value of each non-zero entry  $\alpha_i \sim N(0, 1)$
- ▶ Use Basis Pursuit to recover coefficients  $\alpha^*$  from noiseless data  $f(\xi_m) = \sum_{n=1}^N \alpha_n \phi_n(\xi)$ 
  - ▶ Generate samples from  $w$  and  $\rho_{I_\xi, w}$
- ▶ Recovery successful if  $\|\alpha - \alpha^*\|_2 / \|\alpha\|_2 \leq 0.01$
- ▶ Measure probability of recovery using 100 trials

# Alternative pre-conditioning schemes

## Beta

Let  $z_i \sim U(0, 1)$

$$\xi = \cos(\pi z), \quad w_{m,m} = \prod_{i=1}^d (1 - \xi_i^2)^{1/4} \sqrt{w(\xi)}$$

## Gaussian

Let  $z_i \sim N(0, 1)$  and  $u \sim U[0, 1]$

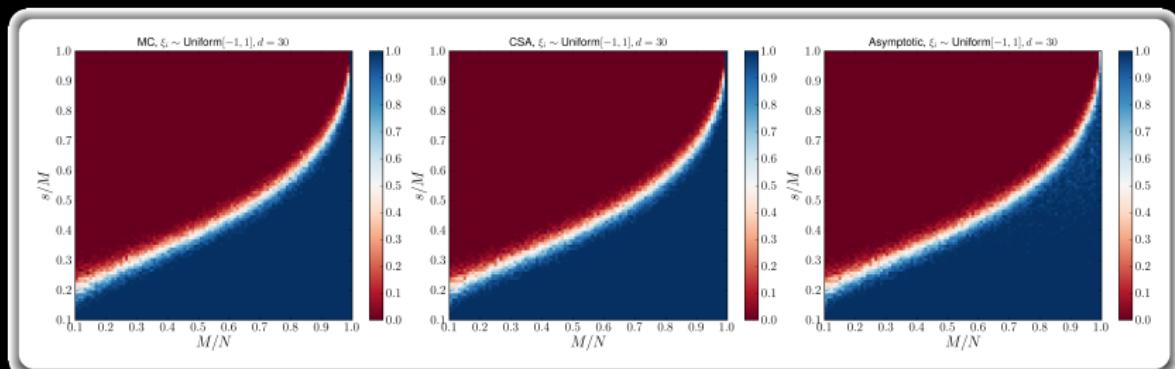
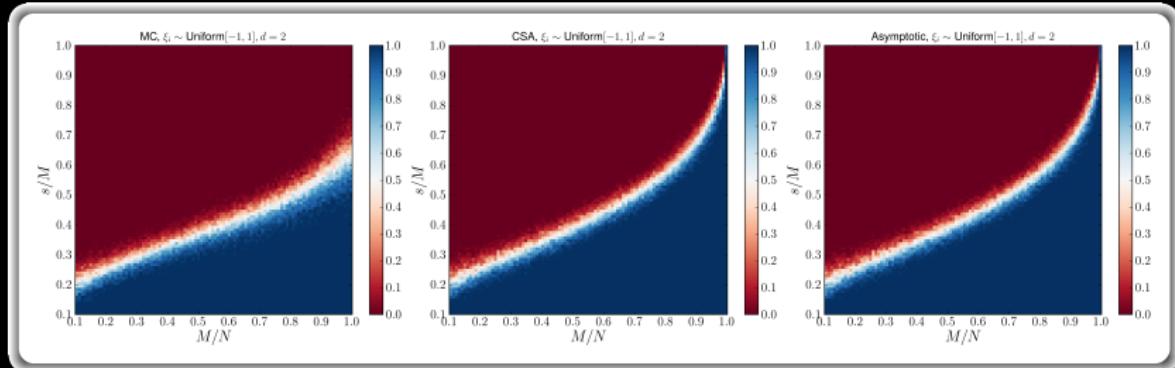
$$\mathbf{y} = \frac{\mathbf{z}}{\|\mathbf{z}\|_2} u^{1/d}, \quad \xi = \mathbf{y} \sqrt{2} \sqrt{2p+1}$$

$$w_{m,m} = \exp(-\|\xi\|_2^2/4)$$

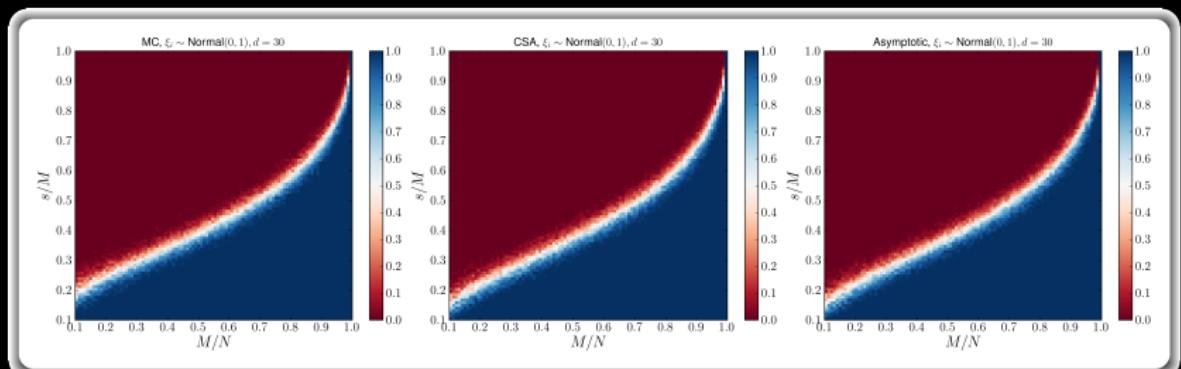
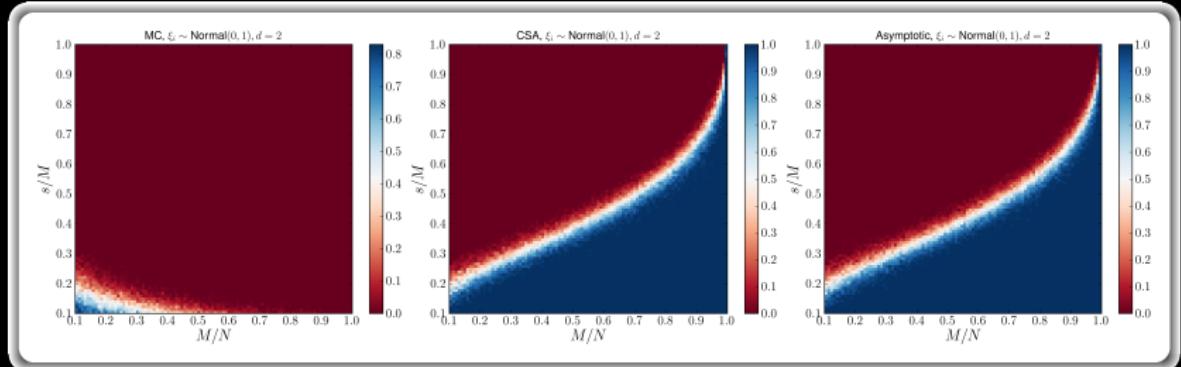
- ▶ Asymptotic sampling:  $\mathbf{y}$  are uniformly sampled in the unit ball.
- ▶ Equilibrium sampling:  $\mathbf{y}$  are concentrated towards the center of the unit ball.

Special mention: coherence optimal sampling based upon MCMC. (Hampton and Doostan 2015)

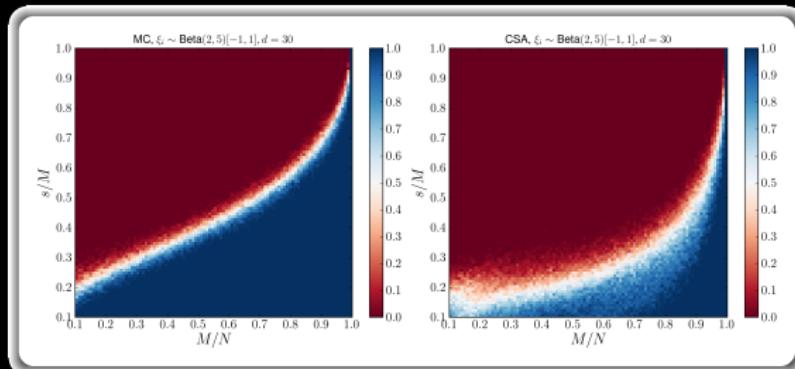
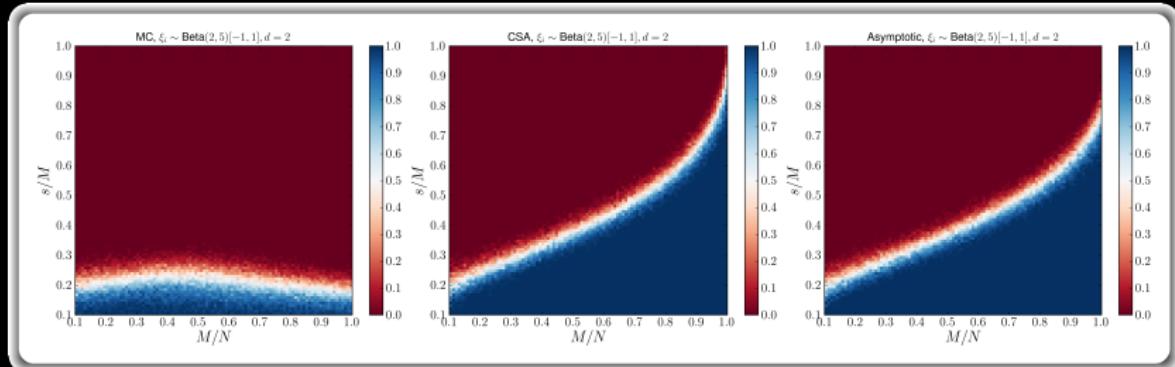
# Uniform Variables ( $d=2,30$ )



# Normal Variables (d=2,30)



# Beta(2,5) Variables ( $d=2,30$ )



## Approximating an Elliptic PDE

We want to approximate  $q(\xi) = u(1/2, \xi)$  where

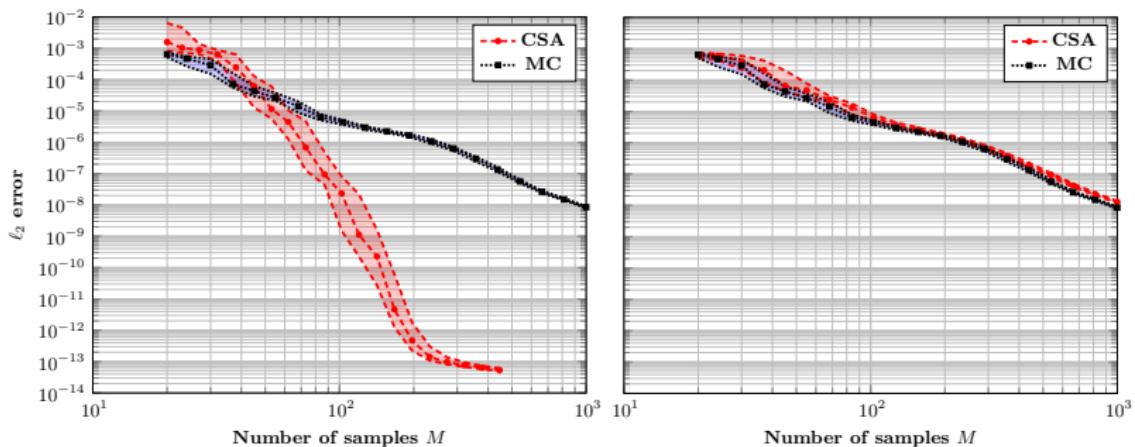
$$\begin{aligned} -\frac{d}{dx} \left[ a(x, \xi) \frac{du}{dx}(x, \xi) \right] &= 1 \quad (x, \xi) \in (0, 1) \times I_\xi \\ u(0, \xi) &= u(1, \xi) = 0 \end{aligned}$$

with diffusivity  $\log(a(x, \xi)) = \bar{a} + \sigma_a \sum_{k=1}^d \sqrt{\lambda_k} \varphi_k(x) \xi_k$ , where

$\{\lambda_k\}_{k=1}^d$  and  $\{\varphi_k(x)\}_{k=1}^d$  are determined by  $C_a(x_1, x_2) = \exp \left[ -\frac{(x_1 - x_2)^2}{l_c^2} \right]$

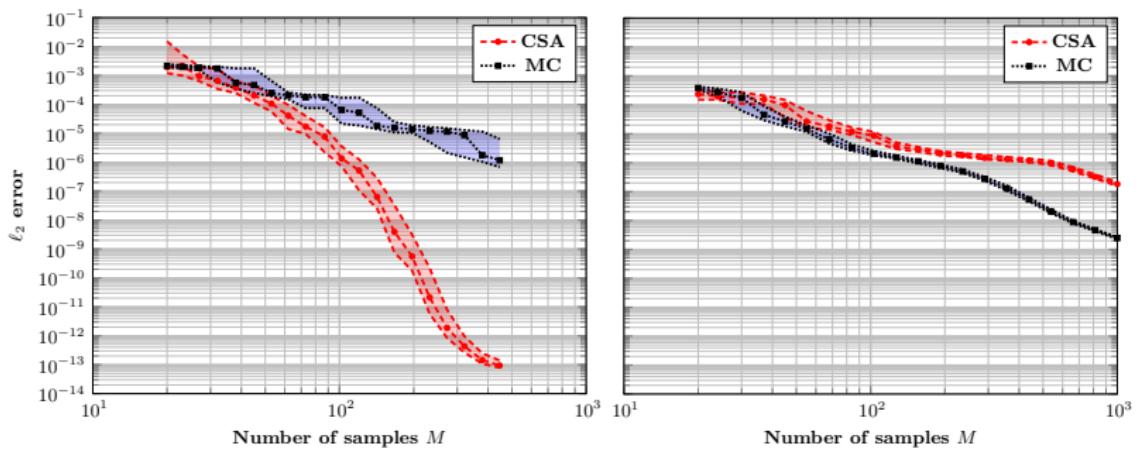
- ▶ Compute PCE using Basis Pursuit (Least Angle Regression)
- ▶ Measure accuracy in PCE approximation  $q_\Lambda$  by computing  $M_{\text{test}}^{-1/2} \|q - q_\Lambda\|_{\ell_2(w)}$  using  $M_{\text{test}} = 10000$  samples from  $w(\xi)$ .
- ▶ Measure mean error using 20 trials

# Effect of dimension on performance of CSA



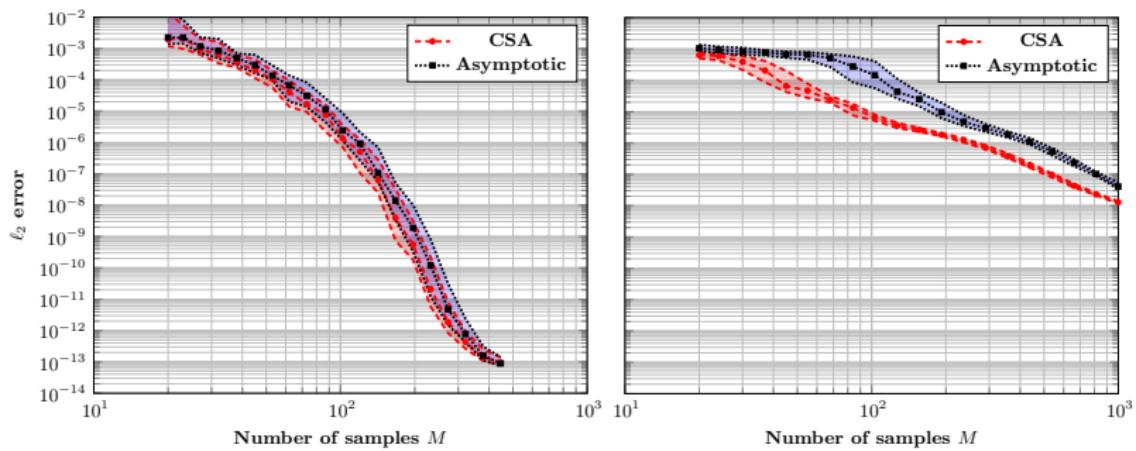
(Left) 30th degree Legendre polynomial in 2 dimensions. (Right) 4th degree Legendre polynomial in 20 dimensions

# Effect of dimension on performance of CSA



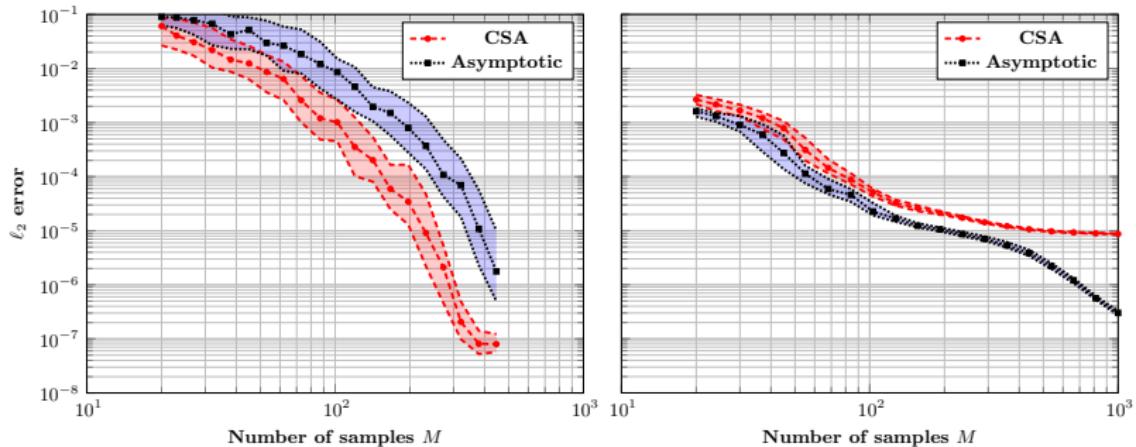
(Left) 30th degree Jacobi polynomial in 2 dimensions. (Right) 4th degree Jacobi polynomial in 20 dimensions

# CSA vs. asymptotic method



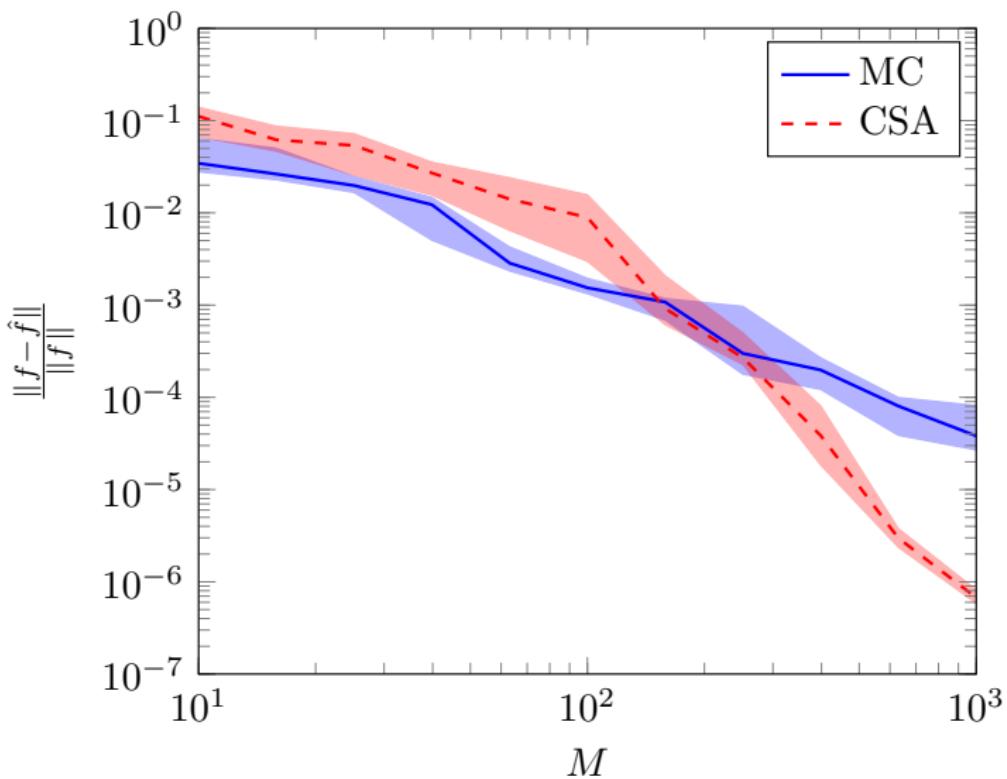
(left)  $d = 2$  Jacobi approximation and (right)  $d = 20$  Legendre approximation.

# CSA vs. asymptotic method



(left)  $d = 2$  and (right)  $d = 20$  Hermite approximation.

# Applying CSA to the nozzle problem



## Applying CSA to the nozzle problem

