



# Uncertainty Quantification in Simulations of Reactive Flows

## Part 3: Sampling & Quadrature

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**Moments** of a quantity of interest are **integrals** in the probability space defined by the uncertain variables!

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**No randomness** is introduced! but convergence is exponential (cfr. MC)

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- ▶ Another avenue is to use these methods in conjunction with polynomial chaos approaches
- ▶ Reminder: in polynomial chaos (stochastic Galerkin) the solution is expressed as a spectral expansion of the *uncertain* variable(s):  $\xi \in \Omega$  as:

$$u(x, t, \xi) = \sum_{i=0}^P \underbrace{u_i(x, t)}_{\text{deterministic}} \underbrace{\psi_i(\xi)}_{\text{stochastic}}$$

and this expansion is **inserted** in the governing PDE!

# Non-intrusive Polynomial Chaos

- ▶ **idea** apply the Galerkin procedure directly to the formula:

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- ▶ Steps:

- ▶ multiply by  $\psi_k(\xi)$
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- ▶ repeat for each  $k = 0, 1, \dots, P$

- ▶ The result is

$$\int_{\Omega} u(x, t, \xi) \psi_k(\xi) d\xi = \int_{\Omega} \sum_{i=0}^P u_i(x, t) \psi_i(\xi) \psi_k(\xi) d\xi$$

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- ▶ The orthogonality condition  $\langle \psi_i \psi_k \rangle = \delta_{ik} h_k$  leads to:

$$\int_{\Omega} u(x, t, \xi) \psi_k(\xi) d\xi = u_k(x, t) h_k$$

where  $h_k$  is a known constant

# Non-intrusive Polynomial Chaos

- ▶ The conclusion is that we can compute the **coefficients** of the polynomial chaos expansion

$$u(x, t, \xi) = \sum_{i=0}^P u_i(x, t) \psi_i(\xi)$$

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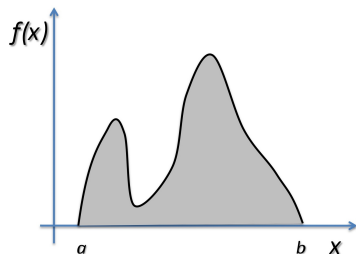
$$u_k(x, t) = \frac{1}{h_k} \int_{\Omega} u(x, t, \xi) \psi_k(\xi) d\xi \quad k = 0, 1, \dots, P$$

- ▶ Every numerical integration method (Monte Carlo, LHS, quadrature) can be used and only require few (?) evaluations of the solution  $u(x, t, \xi)$  of the **original problem**.



# Numerical Integration

- ▶ Recall ordinary numerical integration:



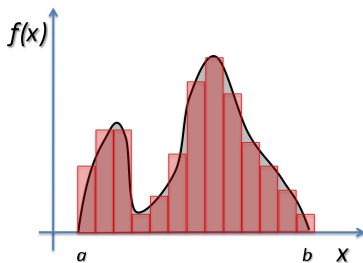
Problem: Compute the integral of  $f(x)$  over the interval  $[a : b]$ .

# Numerical Integration

- ▶ Evaluate the function at  $N$  regular interval  $\Delta x = (b - a)/N$
- ▶ **Midpoint rule** (direct summation)

$$A = \sum_{i=1}^N f(x_i) \Delta x = \frac{b-a}{N} \sum_{i=1}^n f(x_i)$$

with  $x_i = a + (i - 0.5)\Delta x$  are the *abscissas*



# Numerical Integration

## d-dimensional case

- ▶ Function defined on a  $d$  – dimensional interval  
( $[a_1 : b_1], [a_2 : b_2], \dots, [a_d : b_d]$ )
- ▶ The integral becomes

$$V^{d+1} = \frac{(b_1 - a_1)(b_2 - a_2) \cdots (b_d - a_d)}{N_1 N_2 \cdots N_d} \sum_{i_1=1}^{N_1} \sum_{i_2=1}^{N_2} \cdots \sum_{i_d=1}^{N_d} f(x_i)$$

with  $x_i = (x_{i_1}, x_{i_2}, \dots, x_{i_d})$

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- ▶ We can write the integral more compactly:

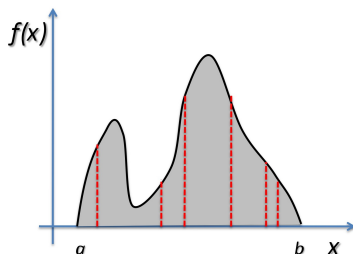
$$V^{d+1} = V^d \frac{\sum_{i_1=1}^{N_1} \sum_{i_2=1}^{N_2} \cdots \sum_{i_d=1}^{N_d} f(x_i)}{N}$$

with  $N = N_1 N_2 \cdots N_d$  the total number of points where the function is evaluated

# Monte Carlo Integration

- ▶ Pick  $N$  random  $d$ -dimensional vectors  $x_i = (x_{i_1}, x_{i_2}, \dots, x_{i_d})$  (the  $x_{i_j}$  are independent uniform random numbers)
- ▶ The desired volume is

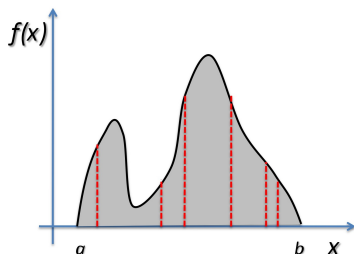
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Compare to: 
$$V^{d+1} = V^d \frac{\sum_{i_1=1}^{N_1} \sum_{i_2=1}^{N_2} \cdots \sum_{i_d=1}^{N_d} f(x_i)}{N}$$

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# Monte Carlo Integration

- ▶ The difference between mid-point integration and MC is the replacement of  $d$  nested sums with one, and the random choice of the abscissas.
- ▶ In **1D** there is not much difference and indeed using high-order integration (e.g. Simpson rule) the conventional integration can be quite accurate and efficient
- ▶ In **Multi D** the conventional integration becomes cumbersome and expensive.
  - ▶ Assume  $N_j = 5$  for all  $j$  (this is a low value!), for  $d = 10$ , we need  $5^{10}$  points to get a reasonable answer

# MC versus Conventional Integration

## Classical example

Compute the volume of a (hyper-) sphere in  $d$  dimensions

- ▶ Conventional integration:  $N_j = 20$  for all  $j \rightarrow V_{NI}$
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d	sec	$V_{NI}/V_e$	sec	$V_{MC}/V_e$
2	0.00	1.0034	0.01	1.0006
3	0.00	0.9964	0.07	1.0002
4	0.00	0.9934	0.08	0.9996
5	0.02	0.9951	0.10	1.0028
6	0.30	0.9956	0.13	1.0012
7	5.02	0.9885	0.15	0.9968
8	89.9	0.9755	0.17	0.9973
9	1320	1.0307	0.20	1.0062

# Monte Carlo method

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Monte Carlo integration **error** is unbiased and can be estimated as:

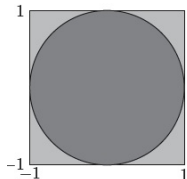
$$\int f dV = V \langle f \rangle \pm \alpha V \sqrt{\frac{1}{N} (\langle f^2 \rangle - \langle f \rangle^2)}$$

Larger  $\alpha$  imply broader confidence that the *true* value is included in the error bar.

# Monte Carlo method

Computing  $\pi$

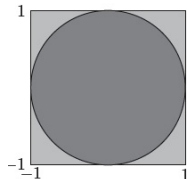
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$$P(\sqrt{x^2 + y^2} < R) = \frac{A_{circle}}{A_{square}} = \frac{\pi}{4}$$



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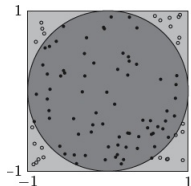
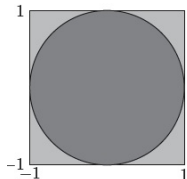
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- ▶ Consider  $N$  independent rain drops and count the ones falling within the circle (rejection)



# Monte Carlo method

## Computing $\pi$

- ▶  $p = P(\sqrt{x^2 + y^2} < R) \approx \frac{N_{in}}{N}$  and  $p = \frac{A_{circle}}{A_{square}} = \frac{\pi}{4}$
- ▶ We can estimate  $\bar{\pi} \approx 4 \frac{N_{in}}{N}$ 
  - ▶ Assume  $N = 100$
  - ▶ **a result** is  $N_{in} = 77$
  - ▶  $\bar{\pi} = 4N_{in}/N = 3.08$  (a fairly bad estimate...)

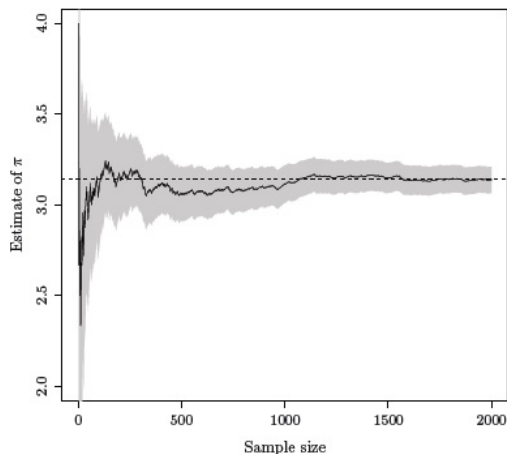
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  - ▶ The *Law of Large Numbers* guarantees that this estimate converges to  $\pi$  as  $N \rightarrow \infty$

# Monte Carlo method

Computing  $\pi$  - Convergence of the estimate



The Central Limit Theorem gives an estimate for the variance  
— and therefore of the error in the estimate

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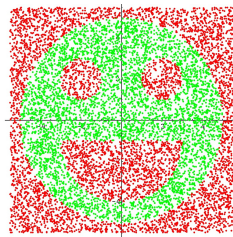
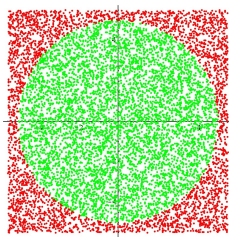
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- ▶ **It is general**





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- ▶ Need to cheat ...
  - ▶ Importance sampling
  - ▶ Control variate
  - ▶ Latin Hypercube
  - ▶ Quasi Monte Carlo
  - ▶ ...

# Latin Hypercube Sampling, LHS

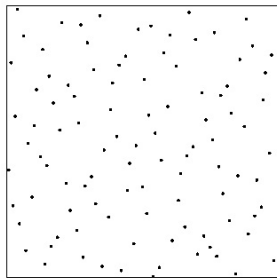
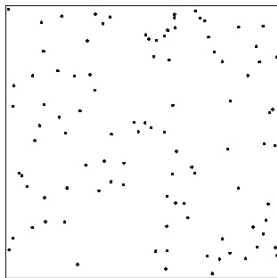
Also *stratified MC* or *constrained MC*

- ▶ Assume we have a  $d$ -dimensional input vector  $y$
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- ▶ In LHS the realizations  $y^i$  are chosen in a different way...



# LHS

## Simple example

- ▶ Consider a 2D problem ( $d = 2$ ) and assume we want to generate  $N = 5$  LHS samples with  $y_1$  a Gaussian r.v. and  $y_2$  a Uniform r.v.

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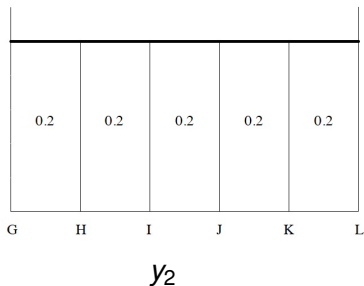
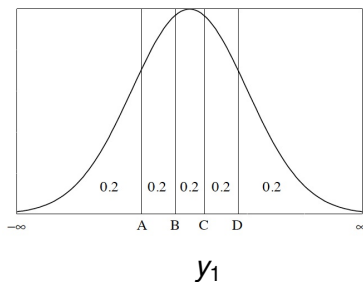
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consider  $d$  random permutations of the first  $N$  integers and  
associate the result with each input variable interval.

Permutation #1: (3, 1, 5, 2, 4)

Permutation #2: (2, 4, 1, 3, 5)

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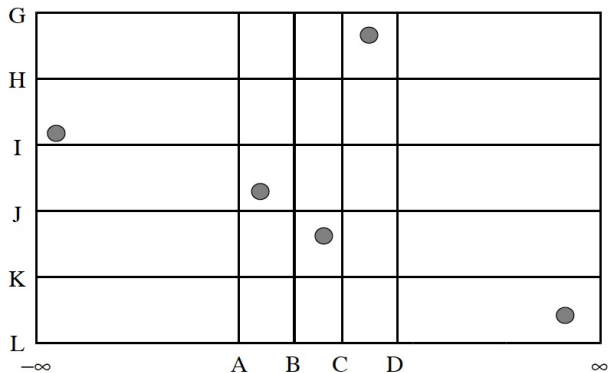
- ▶ The  $N$  input vectors  $y^j$  are then

Realization	$y_1$	$y_2$
1	3	2
2	1	4
3	5	1
4	2	3
5	4	5

# LHS

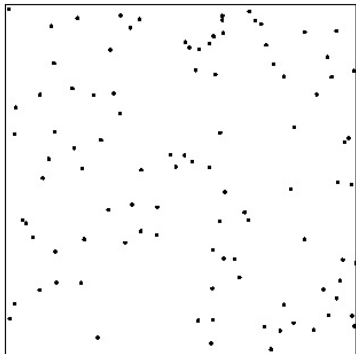
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These are the resulting realizations

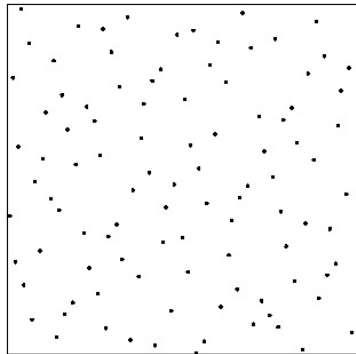


# MC vs. LHS

Qualitative differences...suggestive of better coverage in LHS



Monte Carlo



LHS

# LHS properties

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  - ▶ Convergence is typically faster (lower variance of the estimate for equal  $N$ )
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  - ▶ *Optimal* coverage of the marginals → equi-probability partitions
- ▶ Disadvantages w.r.t. MC
  - ▶ LHS has a history
  - ▶ Need to run exactly  $N$  samples
  - ▶ It is possible (but not straightforward) to control the correlations between input variables by modifying the *pairing* step [Iman & Conover, 1992]

# LHS properties

- ▶ Advantages w.r.t. MC
  - ▶ Convergence is typically faster (lower variance of the estimate for equal  $N$ )
  - ▶ *Optimal* coverage of the marginals → equi-probability partitions
- ▶ Disadvantages w.r.t. MC
  - ▶ LHS has a history
  - ▶ Need to run exactly  $N$  samples
  - ▶ It is possible (but not straightforward) to control the correlations between input variables by modifying the *pairing* step [Iman & Conover, 1992]

Remains the **Method of choice** for a number of engineering applications...



## Concluding...

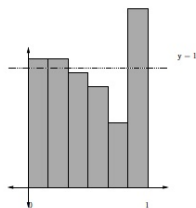
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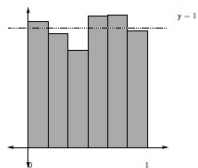
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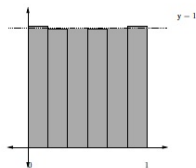
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$N = 100$



$N = 5000$



$N = 100000$

# Sampling Methods

- ▶ Sample the **random** *input parameter vector* according to its probability distributions
- ▶ Perform a sequence of independent simulations
- ▶ Compute statistics of the quantity of interest

# Sampling Methods

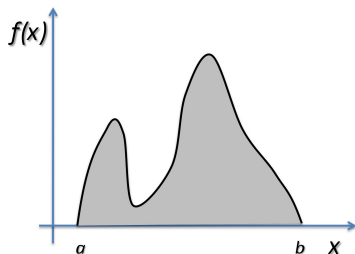
- ▶ Sample the **random** *input parameter vector* according to its probability distributions
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- ▶ Compute statistics of the quantity of interest

Now we will introduce an alternative way of computing the output statistics **without** random sampling!

# Numerical Integration

The basic idea is to use *advanced* numerical integration techniques

- ▶ Recall **numerical quadrature**:



Problem: Compute the integral of  $f(x)$  over the interval  $[a : b]$ .

# Numerical integration

Express integrals as a *finite, weighted sum*

$$\int_a^b f(\xi) d\xi \approx \sum_{i=1}^N w_i f(\xi_i)$$

- ▶ Examples: midpoint, trapezoidal, Simpson rules
- ▶ Remark: all use equispaced abscissas  $\xi_i \in [a : b]$  (Newton-Cotes)

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What are the abscissas  $\xi_i$  and the weights  $w_i$ ?

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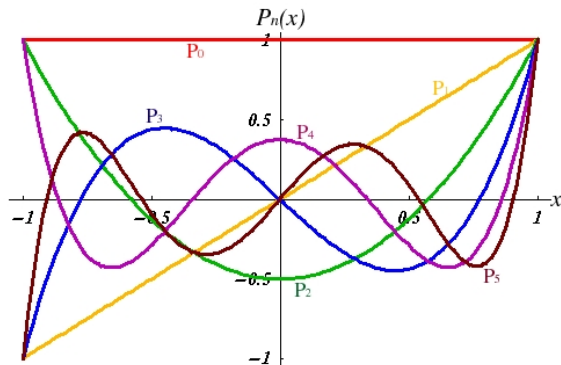
Abscissas: impose  $p_N(\xi) = 0 \rightarrow \xi_1, \dots, \xi_N$

The **weights** are the integrals of the Lagrange interpolating polynomials passing through the abscissas

$$w_i = \int_{-1}^1 L_{i,N}(\xi) d\xi \quad \text{with} \quad L_{i,N}(\xi) = \prod_{\substack{k=1 \\ k \neq i}}^N \frac{\xi - \xi_k}{\xi_i - \xi_k}$$

# Legendre-Gauss quadrature

## Legendre Polynomials



$$(n+1)P_{n+1}(\xi) = (2n+1)\xi P_n(\xi) - nP_{n-1}(\xi) \quad \text{Three-term recurrence}$$

$$\int_{-1}^1 P_j(x)P_i(x)dx = \frac{2}{2n+1}\delta_{ij} \quad \text{Orthogonality}$$

# Legendre-Gauss quadrature

Both the abscissas and the weights are tabulated and can be computed in several ways

For example:

```
function I = gauss(f,n)                % (n+1)-pt Gauss quadrature
beta = .5/sqrt(1-(2*(1:n))^(-2));      % 3-term recurrence coeffs
T = diag(beta,1) + diag(beta,-1);     % Jacobi matrix
[V,D] = eig(T);                       % eigenvalue decomposition
x = diag(D); [x,i] = sort(x);          % nodes (= Legendre points)
w = 2*V(1,i)^2;                       % weights
I = w*feval(f,x);                     % the integral
```

The command `gauss(cos,6)` yields **1.68294196961579**  
which is correct to double precision [Trefethen, 2008]

# Advanced Concepts



# Beyond Uniform rvs

## Gaussian rvs

What do we do if the input variables are not distributed as uniform r.v.?

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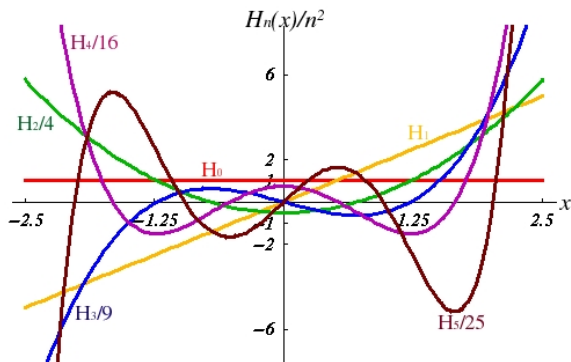
Consider  $y$  distributed as a  $N(0, 1)$ , we can build orthogonal polynomials w.r.t. to a Gaussian measure as:

$$\int_{-\infty}^{\infty} p_j(x)p_i(x)e^{-x^2} dx = C_i\delta_{ij}$$

**Hermite polynomials** for normal r.v. play the same role as Legendre polynomials for uniform r.v.s!

# Hermite-Gauss quadrature

## Hermite Polynomials



$$H_{n+1}(\xi) = 2\xi H_n(\xi) - 2nH_{n-1}(\xi) \quad \text{Three-term recurrence}$$

$$\int_{-\infty}^{\infty} H_j(x)H_i(x)e^{-x^2} dx = 2^i i! \sqrt{\pi} \delta_{ij} \quad \text{Orthogonality}$$

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We can use Legendre or Hermite polynomials, can we do even more?

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Distribution	pdf	Polynomials	Weights	Support
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Gaussian	$(1/\sqrt{2\pi})e^{(-x^2/2)}$	Hermite	$e^{(-x^2/2)}$	$[-\infty : \infty]$
Exponential	$e^{-x}$	Laguerre	$e^{-x}$	$[0 : \infty]$
Beta	$\frac{(1-x)^\alpha(1+x)^\beta}{B(\alpha,\beta)}$	Jacobi	$(1-x)^\alpha(1+x)^\beta$	$[-1 : 1]$

Table: Some polynomials in the Askey family

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1. Szego (1939). Orthogonal Polynomials - American Mathematical Society.
2. Schoutens (2000). Stochastic Processes and Orthogonal Polynomial - Springer.
3. Gram-Schmidt Procedure



# Nested rules

## The choice of abscissas

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Two extensions are possible

- ▶ **Gauss-Kronrod** rules
- ▶ **Clenshaw-Curtis** rules: express the integrand using Chebyshev polynomials (lower polynomial exactness)

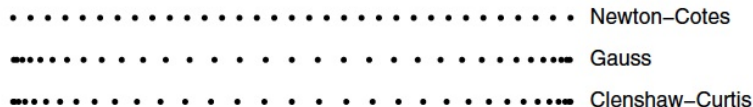


Figure: 32 abscissas in  $[-1 : 1]$

# Clenshaw-Curtis vs. Gauss

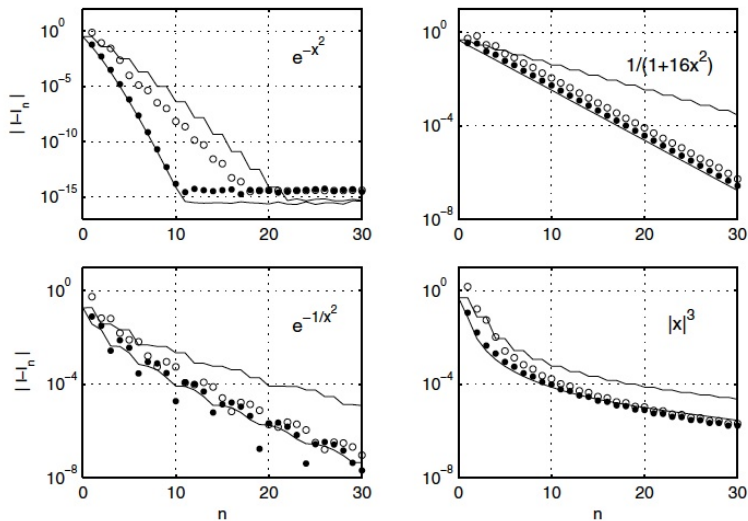


Figure: Black: Gauss, White: CC [Trefethen, 2008]

# Why Nested rules?

Assume you have a budget of  $N = 9$  computations.

- ▶ With 9 **Gauss abscissas** (Legendre), we can obtain an estimate of the statistics of the solution which would be exact if the solution is a polynomial of degree  $\leq 2N - 1 = 17$

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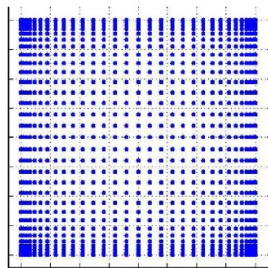
- ▶ With 9 **Gauss abscissas** (Legendre), we can obtain an estimate of the statistics of the solution which would be exact if the solution is a polynomial of degree  $\leq 2N - 1 = 17$
- ▶ With **Clenshaw-Curtis** we can obtain again an estimate (only exact for polynomials of degree  $\leq N = 9$ ).  
On the other hand, with the same computations ( $N = 9$  abscissas) we can also estimate the solution statistics corresponding to  $N = 5$  and  $N = 3 \rightarrow$  **error estimate**.

# Multi-dimensional rules

## Tensor Product

The extension of the previous 1D rules (Gauss or CC) is straightforward

- ▶ The abscissas are tensor products of the quadrature points in 1D
- ▶ The weights are the products of the 1D weights

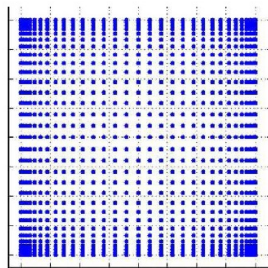


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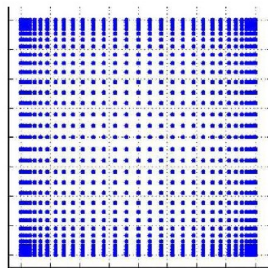
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- ▶ The number of function evaluations increases as  $N^d$   
→ **curse of dimensionality**
- ▶ **Remark:** This is valid **ONLY** if the uncertain variables are independent (because the joint PDF becomes the product of the marginals)!



# Extension of the Stochastic Collocation Methodology

- ▶ Stochastic Collocation is a very simple and powerful alternative to MC sampling
- ▶ Several limitations remain:
  - ▶ High-Dimensionality
  - ▶ Non-Smooth Responses
  - ▶ General Correlated/Dependent Inputs

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- ▶ Various extensions have attempted to address these issues:
  - ▶ Multi-dimensional constructions: Sparse Grids
  - ▶ Global vs. Local Basis: Multi-element methods and Simplex Stochastic Collocation
  - ▶ Adaptive Quadrature
  - ▶ Different Choice of Basis (non-polynomials): Wavelets, Pade'

# Multi-dimensional Extensions

## Sparse Grids - Smolyak Grids

Smolyak idea is to **sparsify** the construction of quadrature grids

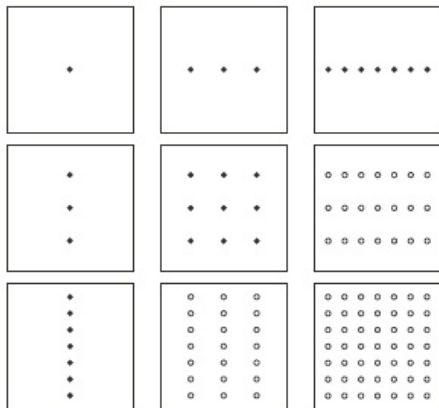


Figure: Sequence of grids used in 2D by a nested rule

# Multi-dimensional Extensions

## Sparse Grids - Smolyak Grids

The *nominal* accuracy can be preserved with much less points

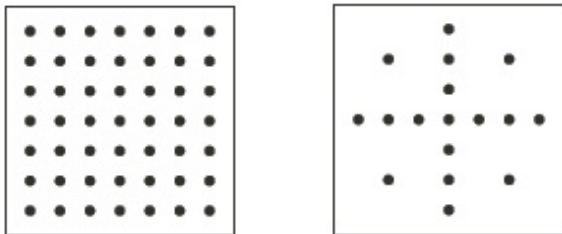


Figure: From Tensor grid to Sparse grid in 2D

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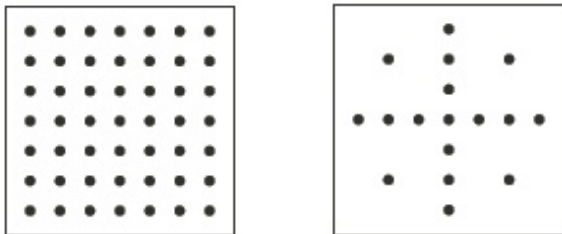


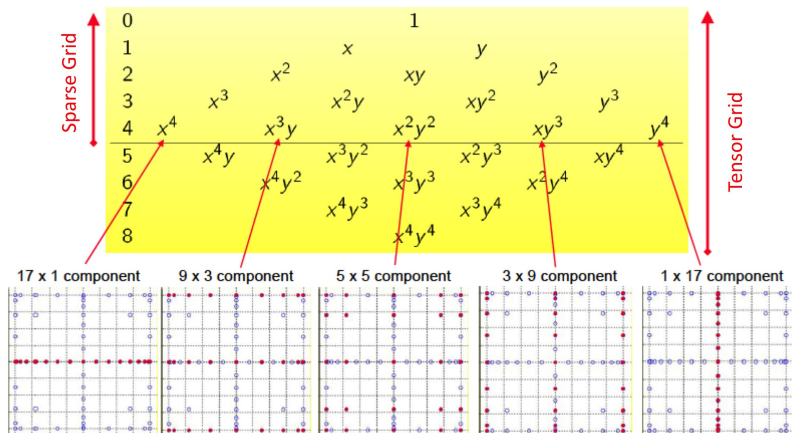
Figure: From Tensor grid to Sparse grid in 2D

The method is based on a linear combination of tensor products to build the actual sparse grid

# Sparse Grids

## Rationale

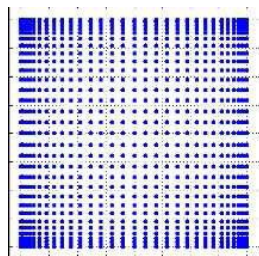
The key is to *reinterpret* the concept of "polynomial exactness"



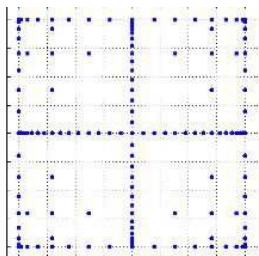
Modified from Eldred 2009

# Sparse Grids

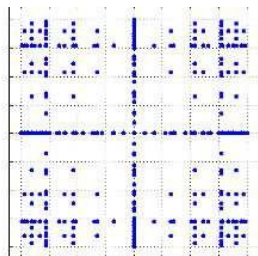
## Stochastic Collocation



Isotropic FT



Smolyak C-C



Smolyak Gauss

Table: Abscissas for  $N = 5$  in each dimension

	$d = 2$	$d = 3$	$d = 4$	$d = 5$	$d = 6$	$d = 7$
Tensor Gauss	25	125	625	3125	15625	78125
Smolyak Gauss	17	31	49	71	97	127
Smolyak CC	13	25	41	61	85	113

# Sparse Grids

## Summary

- ▶ A fundamental advance in the development of stochastic collocation approaches in multiD
- ▶ Becoming more and more popular



# Sparse Grids

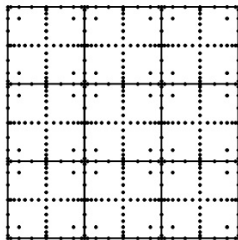
## Summary

- ▶ A fundamental advance in the development of stochastic collocation approaches in multiD
- ▶ Becoming more and more popular
- ▶ **Not perfect**
  - ▶ Not straightforward to construct (implementation errors)
  - ▶ Does not *solve* the curse of dimensionality, although it is better than tensor grids
  - ▶ Not very flexible. Increasing the accuracy requires a large increase in number of solutions...

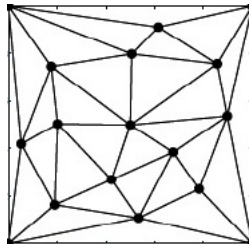
# From Global to Local Basis

## Multi-Element Methods

- ▶ The classical construction of the stochastic collocation method relies on polynomial basis defined over the entire domain spanned by the input uncertainties
- ▶ In many cases it is useful to compute the integrals over subdomains
  - ▶ Capture local features (including discontinuities)
  - ▶ Allow more control on the number of simulations to perform
  - ▶ ...



Multi-Element SC



Simplex SC

# Basis Selection

## Adaptivity & Anisotropy

- ▶ In multi-dimensional problem it is *unlikely* that all the input uncertainty have the same importance with respect to the quantity of interest
- ▶ How can we **selectively** increase the accuracy of the integration?

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- ▶ Define a sensor based on
  - ▶ sensitivity
  - ▶ variance decomposition
  - ▶ error estimate
- ▶ Tailor the interpolation basis
  - ▶ Increase the polynomial order selectively (anisotropy)
  - ▶ Choose special basis (enrichment)
  - ▶ Increase the resolution locally (subdomain decomposition)

# Discontinuous Surface Responses - Approaches

This is not a new problem....

- ▶ Multi-element approaches (Wan & Karniadakis, ...)
- ▶ Wavelet-based polynomial chaos (LeMaitre et al.)
- ▶ Basis-enrichment (Ghosh & Ghanem, ...)
- ▶ Polynomial Annihilation (Jakeman & Xiu)
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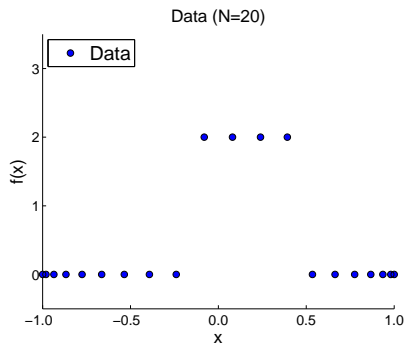
- ▶ Prefer a global approach
- ▶ No prior knowledge of the location of discontinuity
- ▶ Avoid adaptivity
- ▶ **Reuse/extend stochastic collocation framework**



# Padé-Legendre (PL) Method

- ▶ Consider  $f(x) = \text{sign}(x + 0.2) - \text{sign}(x - 0.5)$ .

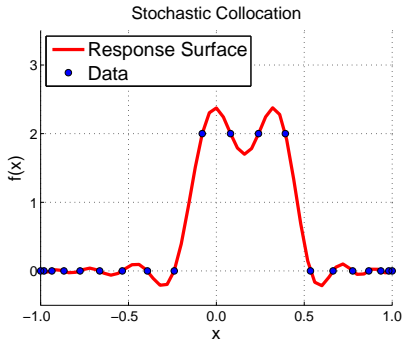
Data: Number of data points:  $N = 20$



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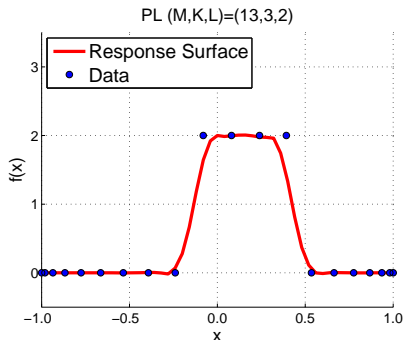
## Stochastic Collocation solution



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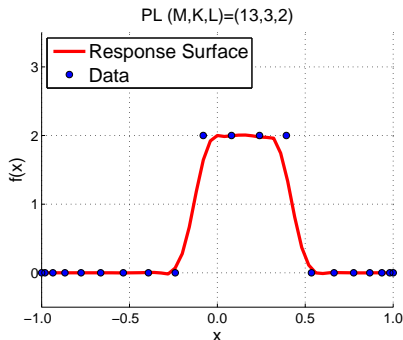
PL with "tuned" parameters (e.g. polynomial orders)



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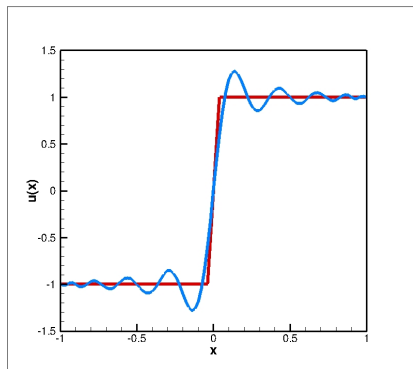
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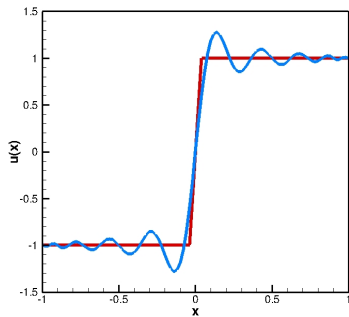
How to **construct** the PL approximant?  
How to **choose** the tuning parameters?

# Padé-Legendre (PL) Method

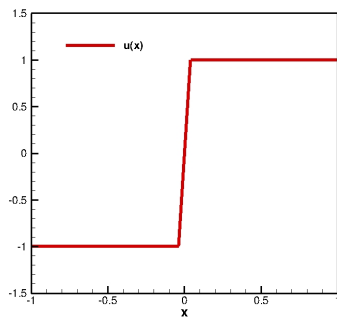


Gibbs phenomena. Polynomial interpolation

# Padé-Legendre (PL) Method

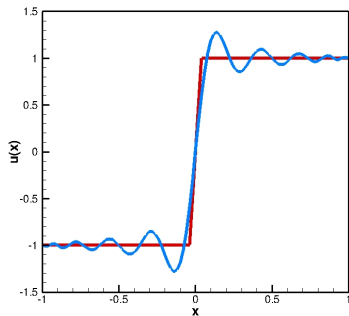


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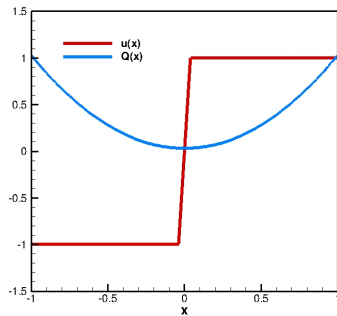


Data

# Padé-Legendre (PL) Method

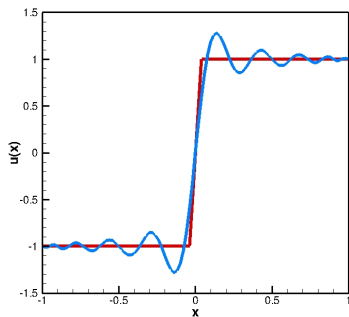


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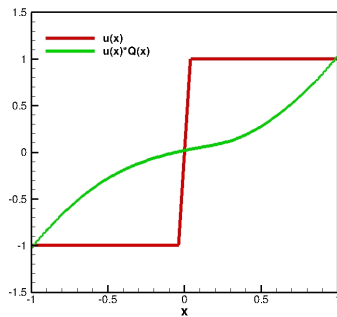


Auxiliary function  $Q(x)$

# Padé-Legendre (PL) Method



Gibbs phenomena. Polynomial interpolation



Preconditioned function  $Q(x)u(x)$



## PL Formulation (1-D)

- ▶ Given data  $u(x_k)$ ,  $k = 0, 1, \dots, N$
- ▶ Find the approximation  $R(x) \approx u(x)$  in the form of

$$R(x) = \frac{P(x)}{Q(x)} = \frac{\sum_{j=0}^M \hat{p}_j \Psi_j(x)}{\sum_{j=0}^L \hat{q}_j \Psi_j(x)}, \quad (\text{A1})$$

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such that

$$\langle P - Qu, \phi \rangle_N = 0, \quad \forall \phi \in \mathbb{P}_N, \quad (\text{A2})$$

where where  $\Psi_j$ 's are the Legendre polynomial basis and  $\langle \cdot, \cdot \rangle_N$  is the discrete inner product.

\* J. Hesthaven, et al, Padé–Legendre interpolants for Gibbs reconstruction, J. Sci. Comput. 28 (2006) 337-359.

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Solve the following linear system for coefficients of  $Q$ :

$$\begin{bmatrix} \langle u\psi_0, \psi_{M+1} \rangle_N & \cdots & \langle u\psi_L, \psi_{M+1} \rangle_N \\ \vdots & \ddots & \vdots \\ \langle u\psi_0, \psi_{M+L} \rangle_N & \cdots & \langle u\psi_L, \psi_{M+L} \rangle_N \end{bmatrix} \begin{bmatrix} \hat{q}_0 \\ \vdots \\ \hat{q}_L \end{bmatrix} = \underline{0}.$$

Matrix size:  $L \times (L + 1)$ . Solve for nonzero  $Q$ .

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- ▶  $R = P/Q \approx u$ .

# 1-D to $n$ -D

## One-dimensional PL

- ▶ There are  $N + 1$  equations, one for each  $\Psi_n$ .
- ▶ We split the equations into  $M$  and  $L$  ( $M + L = N + 1$ ).
- ▶ The last  $L$  equations are used to calculate  $Q$ .
- ▶ The first  $M$  equations are then used to calculate  $P$ .

## Multi-dimensional PL

- ▶ Let  $d$  be the dimension.
- ▶ There are  $c(N, d) = \frac{(N+d)!}{N!d!}$  equations.
- ▶ There are  $c(L, d) = \frac{(L+d)!}{L!d!}$  coefficients in  $Q$
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and  $\langle P - Qu, \phi \rangle_N$  is minimized for  $\phi \in \mathbb{P}_{M+K}$ .

## PL Construction ( $n$ -D)

- ▶ Similar to 1-D, choose the Legendre basis:  $\phi = \Psi$ .
- ▶ Calculate  $Q$  *approximately* by using  $\phi = \Psi \in \mathbb{P}_{M+K} \setminus \mathbb{P}_M$
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We have to specify  $L$ ,  $M$  and  $K$  ( $N$  is usually given).

# Automatic Parameter Selection

- ▶ Every triplet  $(L, M, K)$  gives a different response surface.
- ▶ We designed a strategy (called APS) to choose the “best” response surfaces among all the possible choices of  $(L, M, K)$

Question: What do we mean by “best?”

Answer: According to 2 error measures.

## Two Error Measures

- ▶  $L_2$ -error (measure of accuracy w.r.t. data)

$$e_{L_2} = \frac{\|\tilde{u} - u\|_{L_2}}{\|u\|_{L_2}} = \left( \frac{\sum_{j=1}^{N_q} w_j (u(x_j) - \tilde{u}(x_j))^2}{\sum_{j=1}^{N_q} w_j u^2(x_j)} \right)^{\frac{1}{2}},$$

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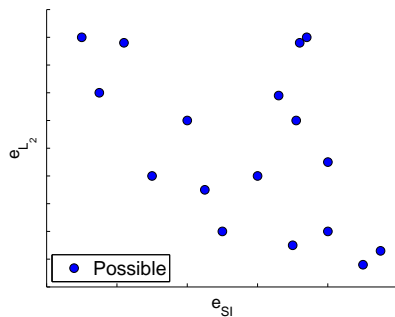
- ▶ Smoothness Indicator (measure of lack of spurious oscillations between data points)

$$e_{SI} = \frac{|\text{SI}(\tilde{u}, G_F) - \text{SI}(u, G_D)|}{\text{SI}(u, G_D)},$$

where  $SI(\cdot)$  is Total Variation,  $G_D$  is a grid consisting of the available data, and  $G_F$  is an additional highly refined grid.

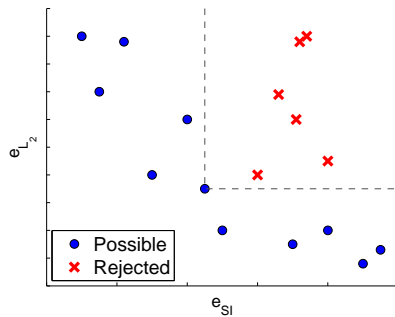
# Pareto Front

Plot all response surfaces according to  $e_{L_2}$  and  $e_{SI}$



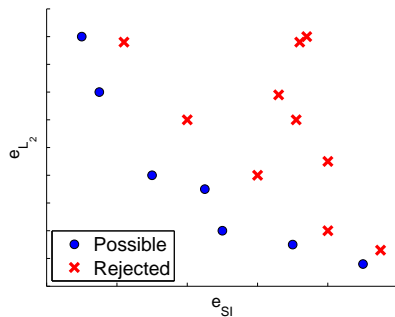
# Pareto Front

Reject all the ones that cannot be best



# Pareto Front

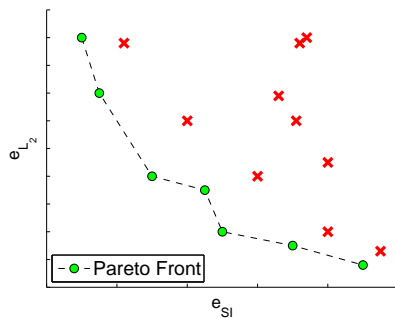
Keep rejecting until we can no longer reject anymore





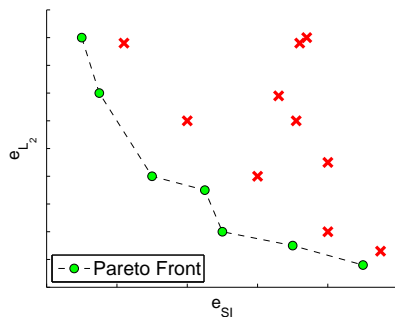
# Pareto Front

The remaining PL surfaces constitute the Pareto front



# Pareto Front

The remaining PL surfaces constitute the Pareto front



- ▶ Bottom-right: most data-accurate, but least smooth
- ▶ Top-left: most smooth, but least data-accurate

# APS

- ▶ Any response surface in the Pareto front is logically acceptable.

A good trade-off between smoothness and data-accuracy depends on applications

- ▶ Data-accuracy is always good, but ...
- ▶ How accurate is the given data?
- ▶ Do we want to extract gradient information?
- ▶ Do we want to calculate extrema?

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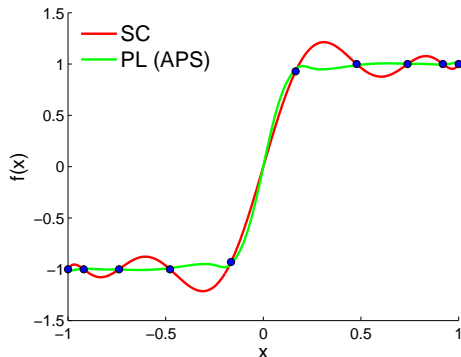
## Example

Underlying function:  $f(x) = \tanh(10x)$ ,  $x \in [-1, 1]$

APS strategy: Most data-accurate.

Stochastic Collocation (SC) vs Padé-Legendre (PL) method

Number of data points:  $N = 10$



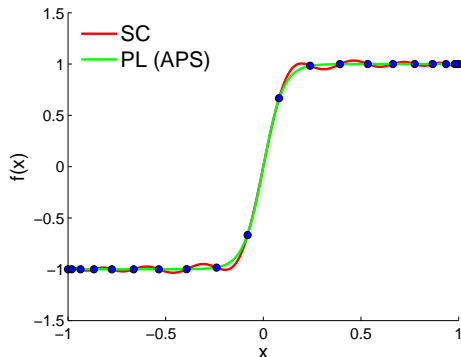
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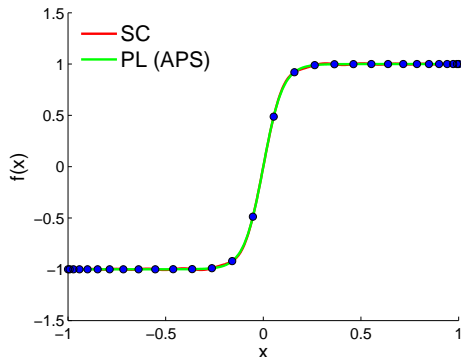
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Number of data points:  $N = 30$



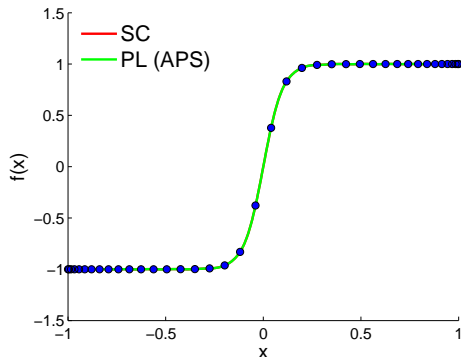
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Number of data points:  $N = 40$





## Convergence to SC for Smooth Underlying Functions

Consider  $f(x) = \tanh(x/\delta)$ . Vary the number of data points,  $N$ .  
Observe  $L$  of the most data-accurate response surfaces.

	$\delta = 0.2$		$\delta = 0.3$		$\delta = 0.4$	
$N$	$e_{SI}[SC]$	$L$	$e_{SI}[SC]$	$L$	$e_{SI}[SC]$	$L$
8	9.744e-1	2	2.852e-1	2	1.045e-1	2
10	5.882e-1	4	1.474e-1	4	2.627e-2	4
12	3.281e-1	4	6.224e-2	4	7.192e-3	4
14	2.141e-1	6	2.508e-2	6	2.414e-3	0
16	1.311e-1	6	8.718e-3	6	6.083e-4	0
18	7.265e-2	8	3.359e-3	0	2.535e-4	0
20	4.124e-2	8	1.069e-3	0	8.143e-5	0
22	2.352e-2	8	3.840e-4	0	2.603e-5	0
24	1.257e-2	9	1.656e-4	0	8.291e-6	0
26	6.967e-3	0	6.731e-5	0	2.596e-6	0
28	3.665e-3	0	2.839e-5	0	1.143e-6	0

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