Uncertainty estimates for fitting Zernike polynomials to discrete data

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Overview

- The Big Picture: Vector Spaces of Functions & Their Properties
- Family of Orthogonal Polynomials
- Example Orthographic Projection
- Least Squares Approximation & Uncertainty Estimates
- Conclusions & Wrap-up

Vector Spaces

<u>Collections of mathematical objects</u>

- Meet properties listed in table
- Vectors:
  - $\mathbb{R}^2$, $\mathbb{R}^3$, $\mathbb{R}^N$
- Functions (some examples):
  - Polynomials of degree N & less
  - Fourier Series (both real & complex)

<u>Example vector spaces of functions</u> (n = 0,1,2,…,N):

$$f_n(x) = x^n, \qquad -1 \le x \le 1$$

$$f_n(x) = \sin(n\theta), \qquad 0 \le \theta \le 2\pi$$

$$f_n(x) = \ e^{in} \ , \qquad -\infty \le \theta \le \infty$$

Properties of a Vector Space, $\mathbb{V}$

		Vector addition		**Scalar Multiplication**
<u>Must be closed</u>	**1.**	$\boldsymbol{f}(x) + \boldsymbol{g}(x) \in \mathbb{V}$	6.	$a\boldsymbol{f}(x) \in \mathbb{V}$
	2.	$\boldsymbol{f} + \boldsymbol{g} = \boldsymbol{g} + \boldsymbol{f}$	7.	$a(b\boldsymbol{f}) = (ab)\boldsymbol{f}$
	3.	$(\boldsymbol{f} + \boldsymbol{g}) + \boldsymbol{h} = \boldsymbol{f} + (\boldsymbol{g} + \boldsymbol{h})$	8.	$(a + b)\boldsymbol{f} = a\boldsymbol{f} + b\boldsymbol{f}$
<u>Needs to include the zero “vector”</u>	**4**	$\bar{\boldsymbol{0}} + \boldsymbol{f} = \boldsymbol{f}$	9.	$a(\boldsymbol{f} + \boldsymbol{g}) = a\boldsymbol{f} + a\boldsymbol{g}$
	5	$\boldsymbol{f} + (-\boldsymbol{f}) = \bar{\boldsymbol{0}}$	10.	$1\boldsymbol{f} = \boldsymbol{f}$

Inner Product

- Operation that measures length, distance, and orientation
- Vectors (dot product):

$$\mathbf{u} \cdot \mathbf{v} = u_1 v_1 + u_2 v_2 + \cdots + u_n v_n$$

- Functions (inner product):

$$\langle f, g \rangle = \int_a^b w(x) f(x) \underbrace{g^*(x)}_{\text{complex conjugate}} dx$$

Choice of weight, w(x) along with a vector space makes an inner product space

Length = RMS when,

$$w(x) = \frac{1}{b-a}$$

Measure	Formula
length	$\sqrt{\langle \boldsymbol{f}, \boldsymbol{f} \rangle}$
Distance	$\sqrt{\langle \boldsymbol{f} - \boldsymbol{g}, \boldsymbol{f} - \boldsymbol{g} \rangle}$
Orientation	$\langle \boldsymbol{f}, \boldsymbol{g} \rangle$

	Properties that define an Inner Product
1.	$\langle \boldsymbol{f} + \boldsymbol{g}, \boldsymbol{h} \rangle = \langle \boldsymbol{f}, \boldsymbol{g} \rangle + \langle \boldsymbol{f}, \boldsymbol{h} \rangle$
2.	$\langle a\boldsymbol{f}, \boldsymbol{g} \rangle = a \langle \boldsymbol{f}, \boldsymbol{g} \rangle$
3.	$\langle \boldsymbol{f}, \boldsymbol{g} \rangle = \langle \boldsymbol{g}, \boldsymbol{f} \rangle^*$
4.	$\langle \boldsymbol{f}, \boldsymbol{f} \rangle > 0, \boldsymbol{f} \neq 0$

Basis Functions

- Basis Vectors (**i**, **j**, **k**)

$$\mathbf{v} = v_x\mathbf{i} + v_y\mathbf{j} + v_z\mathbf{k}$$

- Basis Functions ($e_k(x)$)

$$f(x) = \beta_0 e_0(x) + \beta_1 e_1(x) + \cdots + \beta_n e_n(x)$$

- If orthogonal, the inner product finds the coefficients

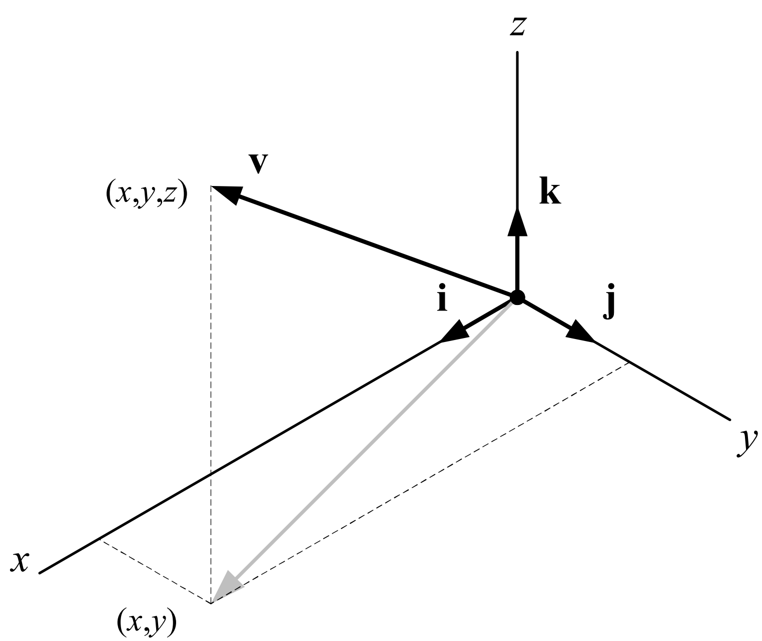
$$\langle e_n, e_m \rangle = \alpha \underbrace{\delta_{n,m}}_{\text{Kronecker delta function}} \Rightarrow \beta_k = \frac{1}{\alpha}\langle f, e_k \rangle$$

- If orthonormal $\langle e_k, e_k \rangle = 1$

$$\beta_k = \langle f, e_k \rangle$$

Example orthonormal bases:

$$\left\langle e^{im\theta}, e^{in\theta} \right\rangle = \frac{1}{2\pi}\int_0^{2\pi} e^{i(m-n)\theta}\, d\theta = \delta_{m,n}$$



Family of Orthogonal Polynomials

Jacobi Polynomials (most general)

$$P_\ell^{(\alpha,\beta)}(x) = \frac{(-1)^\ell}{2^\ell \ell!(1-x)^\alpha (1+x)^\beta} \frac{d^\ell}{dx^\ell}\left[(1-x)^{\alpha+\ell}(1+x)^{\beta+\ell}\right]; \quad -1 \le x \le 1$$

$\alpha,\beta = -½$

Chebyshev Polynomials

$\alpha,\beta = 0$

Legendre Polynomials

$\beta = 0$, $n = 2\ell + m$, $x = 2\rho^2 - 1$

Zernike Radial Polynomials

$$R_n^m(\rho) = \rho^m P_{(n-m)/2}^{(0,m)}\left(2\rho^2 - 1\right); \quad 0 \le \rho \le 1$$

Multiply by $e^{im\theta}$

Zernike Circle Polynomials (complex function)

$$V_n^m(\rho,\theta) = \sqrt{n+1} R_n^m(\rho) e^{im\theta}; \quad 0 \le \theta \le 2\pi$$

Real component

$$Z_n^m(\rho,\theta) = \begin{cases} N_n^m R_n^{|m|} \cos(m\theta); & m \ge 0 \\ -N_n^m R_n^{|m|} \sin(m\theta); & m < 0 \end{cases}$$

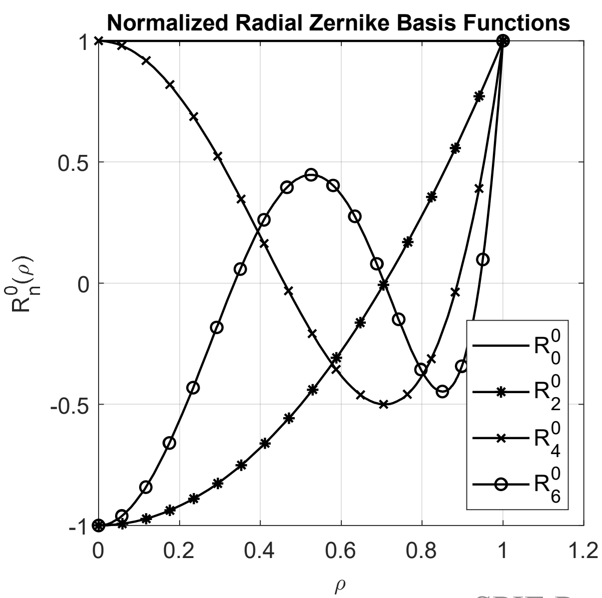
Orthographic Projection of a Hemisphere

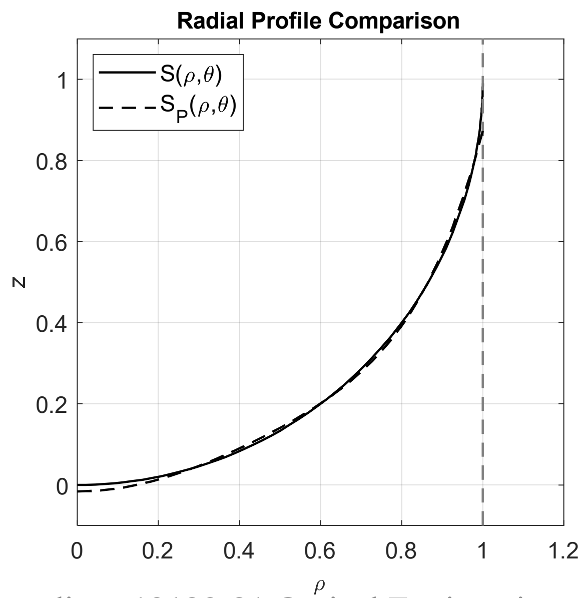
Project sag equation onto basis:

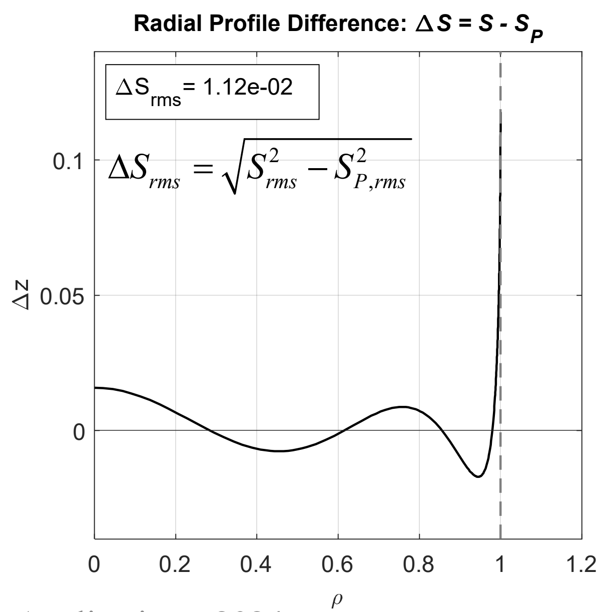
$$S = 1 - \sqrt{1-\rho^2}, \quad 0 \le \rho \le 1$$

$$S_P = \sum_n \beta_{n,0} N_n^0 R_n^0, \quad n = 0, 2, 4, 6$$

Index		Normalization	Basis polynomials	Projected coefficient	Aberration
n	**m**	$N_n^0 = \sqrt{n+1}$	$R_n^0(\rho)$	$\beta_{n,0}$	
0	0	1	1	0.3333	**Piston**
2	0	$\sqrt{3}$	$-1 + 2\rho^2$	0.2309	**Defocus**
4	0	$\sqrt{5}$	$1 - 6\rho^2 + 6\rho^4$	4.259e-2	**1st-Spherical**
6	0	$\sqrt{7}$	$-1 + 12\rho^2 - 30\rho^4 + 20\rho^6$	1.680e-2	**2nd-Spherical**







ΔS is orthogonal to all the basis functions

Least Squares Approximation with Discrete Points

Matrix representation of the surface:

$$\mathbf{S} = \mathbf{Z}\boldsymbol{\beta} + \Delta\mathbf{S}$$

$$\begin{bmatrix} S(\rho_1,\theta_1) \\ \vdots \\ S(\rho_N,\theta_N) \end{bmatrix} = \begin{bmatrix} 1 & Z_2(\rho_1,\theta_1) & \cdots & Z_J(\rho_1,\theta_1) \\ \vdots & \vdots & & \vdots \\ 1 & Z_2(\rho_N,\theta_N) & \cdots & Z_J(\rho_N,\theta_N) \end{bmatrix} \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_J \end{bmatrix} + \begin{bmatrix} \Delta S(\rho_1,\theta_1) \\ \vdots \\ \Delta S(\rho_N,\theta_N) \end{bmatrix}$$

Estimate of the coefficients:

$$\hat{\boldsymbol{\beta}} = \underbrace{\left(\mathbf{Z}^{\mathrm{T}}\mathbf{Z}\right)^{-1}\mathbf{Z}^{\mathrm{T}}}_{\text{Moore-Penrose pseudoinverse matrix}}\mathbf{S}$$

Estimate of the difference:

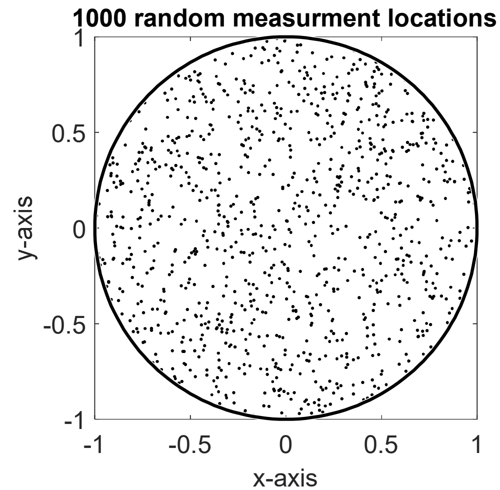
$$\Delta\hat{\mathbf{S}} = \mathbf{S} - \mathbf{Z}\hat{\boldsymbol{\beta}}$$

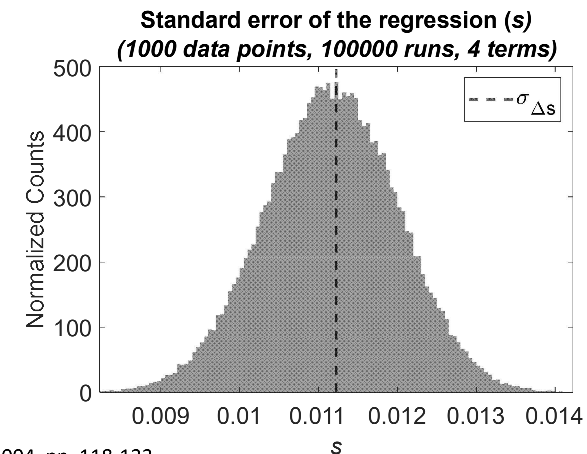
Estimate the standard error of the regression:

$$s^2 = \frac{\Delta\hat{\mathbf{S}}^{\mathrm{T}}\Delta\hat{\mathbf{S}}}{N-J}$$

Variance of the coefficients (with non-stochastic **Z**):

$$\mathrm{var}\left(\hat{\boldsymbol{\beta}}\right) \approx \frac{1}{N}s^2$$





C. Heij, "Least squares in matrix form," in Econometric methods with applications in business and economics, USA, Oxford University Press, 2004, pp. 118-133.

Estimating Variance with Discrete Random Points

<u>When (ρ,θ) is stochastic and uniformly distributed:</u>

- Define new function $\Lambda_j(\rho,\theta)$

$$\Lambda_j(\rho,\theta) = Z_j(\rho,\theta)\Delta S(\rho,\theta)$$

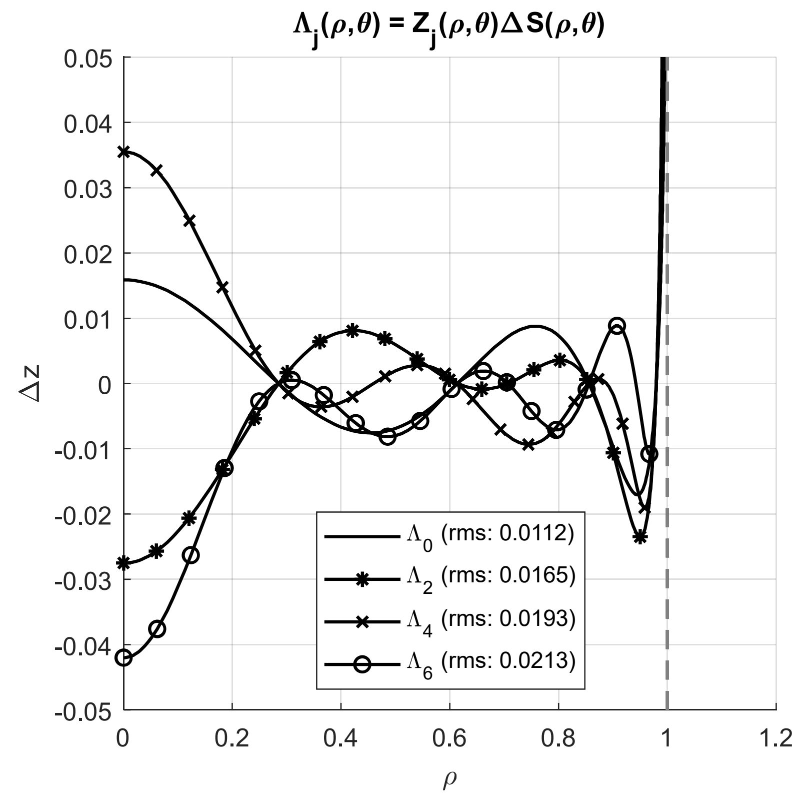
- Covariance Matrix of Λ

$$\boldsymbol{\Sigma}_\Lambda = \begin{bmatrix} \mathrm{var}(\Lambda_1) & \cdots & \mathrm{cov}(\Lambda_1,\Lambda_J) \\ \vdots & & \vdots \\ \mathrm{cov}(\Lambda_J,\Lambda_1) & \cdots & \mathrm{var}(\Lambda_J) \end{bmatrix}$$

- The variance of the estimated coefficients is

$$\mathrm{var}(\hat{\boldsymbol{\beta}}) = \frac{1}{N}\boldsymbol{\Sigma}_\Lambda \xrightarrow{\text{Swap } \Delta\hat{S} \text{ for } \Delta S} \widehat{\mathrm{var}}(\hat{\boldsymbol{\beta}}) = \frac{1}{N}\hat{\boldsymbol{\Sigma}}_\Lambda$$

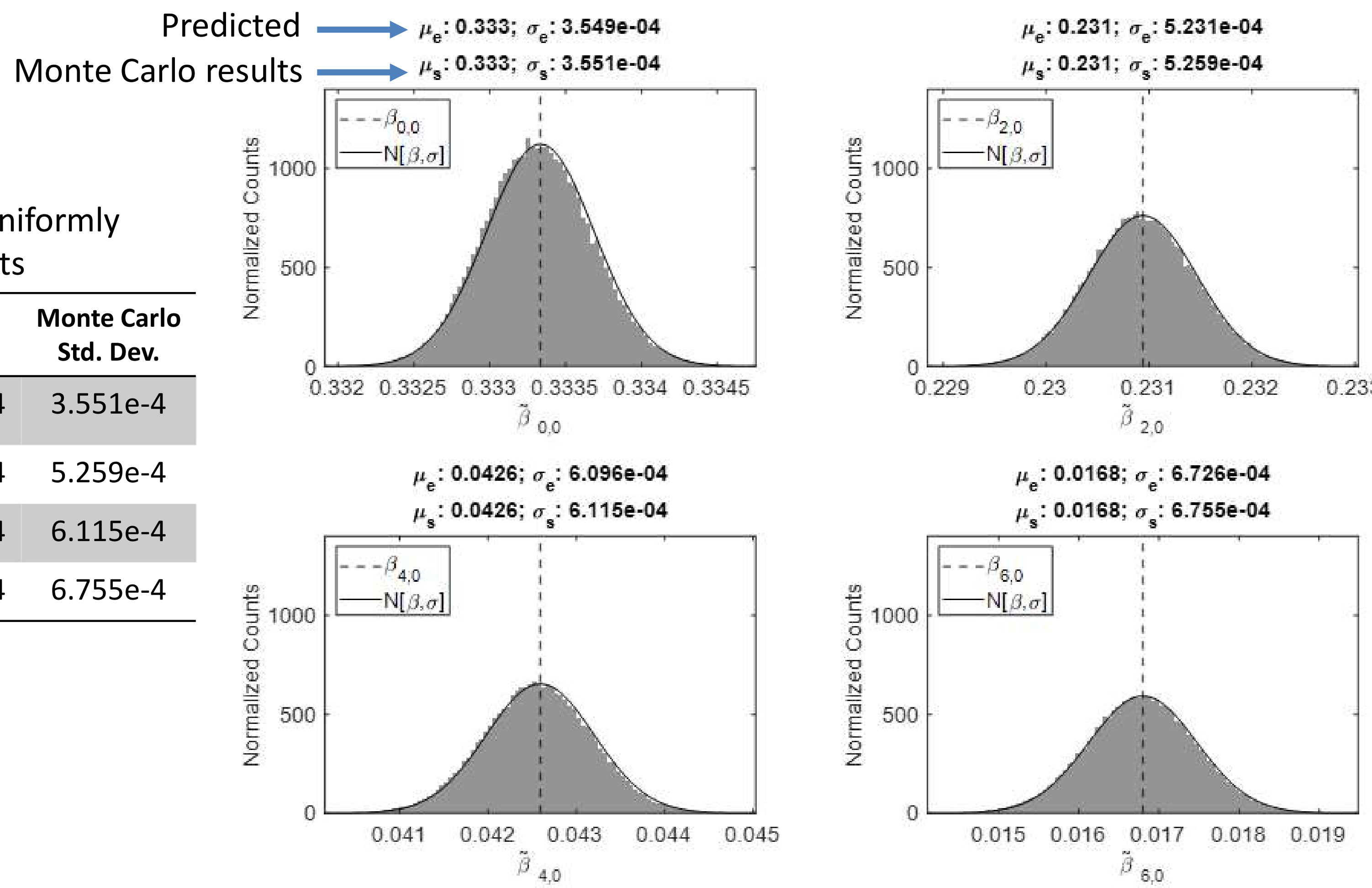
Variance is proportional to the rms of $\Lambda_j(\rho,\theta)$



Model Comparisons with Monte Carlo Simulations

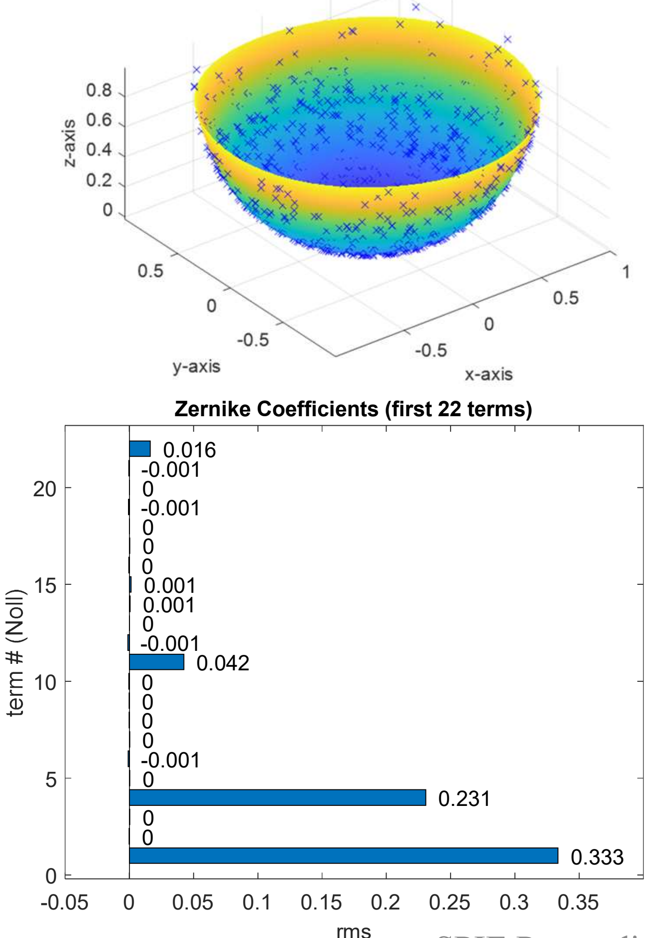
100,000 trials of 1,000 uniformly distributed random points

	$\sqrt{\mathrm{var}(\hat{\boldsymbol{\beta}})}$	**Monte Carlo Std. Dev.**
Piston ($\beta_{0,0}$)	3.549e-4	3.551e-4
Defocus ($\beta_{2,0}$)	5.231e-4	5.259e-4
1st Spherical ($\beta_{4,0}$)	6.096e-4	6.115e-4
2nd Spherical ($\beta_{6,0}$)	6.726e-4	6.755e-4

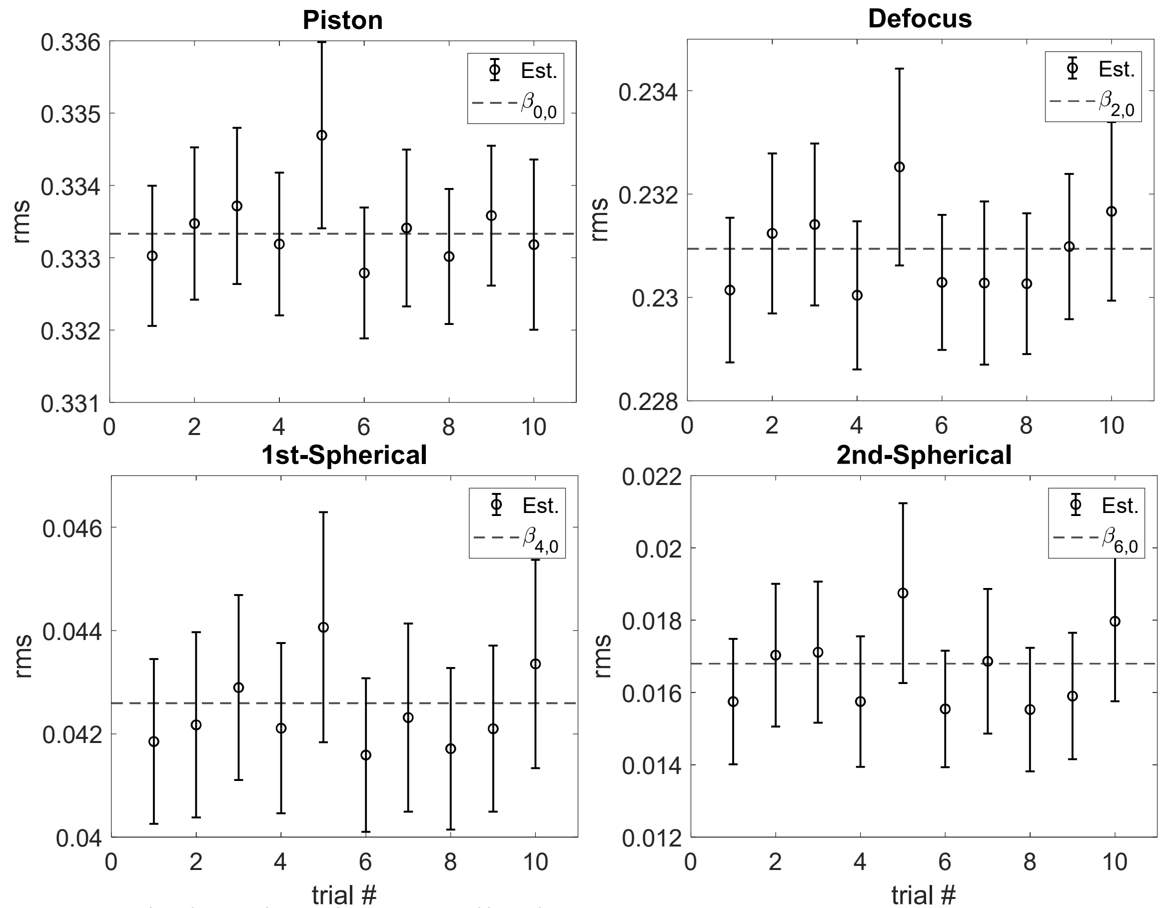


Estimate of Coefficients using $\Delta\hat{S}$

Fitted surface to 1,000 sample points



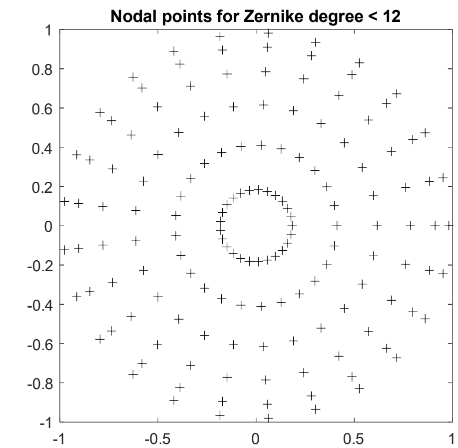
Estimated coefficients for 10 trials of 1,000 randomly sampled surface points along with **3σ** error bars compared to real value

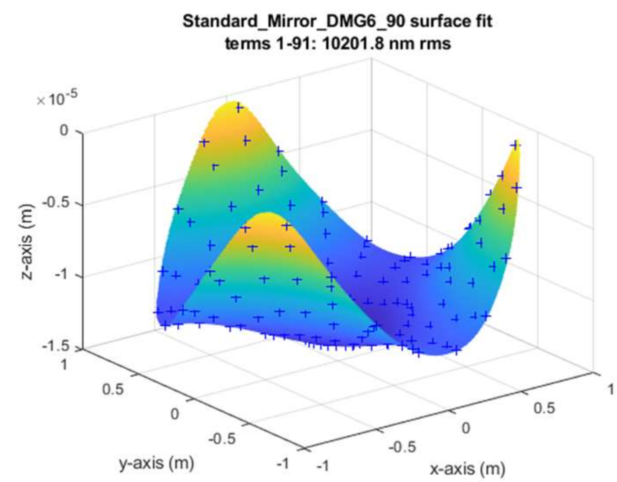


Conclusions

- Estimated coefficient ($\hat{\beta}$) standard deviation agrees with simulations
- Higher order coefficients have increased variance
- Estimates change based on
  - Number of data points
  - Number of Zernike terms (points are not orthogonal)
- Is this the most accurate? – No
  - Instead of random locations, point selection can be intentional
  - Gauss Quadrature to be examined in part II
- <u>Enables informed trade-off between accuracy and speed</u>

<u>Gauss quadrature points</u>





Thank You

Questions?

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