# Uncertainty Quantification for Complex Systems

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# Outline

## Discussion Points

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## Discussion Points

# Uncertainty

## Two Types

- Aleatory - True Randomness
  - Quantum effects
  - Particle-Material interactions (gold foil)
  - Brownian Motion

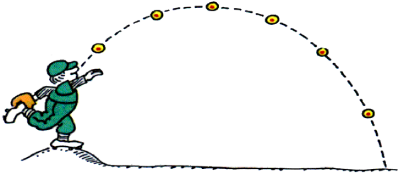
- Epistemic - Unmeasured Uncertainty
  - Tool Accuracy
  - Complicated Dependencies (arrow, double pendulum)
  - Documentation

# Example Stochastic Problem

## Projectile Motion

$$y_f = y_i + v\sin(\theta)t - \frac{1}{2}gt^2,$$

$$x_f = v\cos(\theta)t.$$



Solution: $x_f = \frac{v\cos\theta}{g}\left(v\sin\theta + \sqrt{v^2\sin^2\theta + 2gy_i}\right)$

# Example Stochastic Problem

## Solved!

$$x_f = \frac{v \cos\theta}{g}\left(v\sin\theta + \sqrt{v^2\sin^2\theta + 2gy_i}\right)$$

- initial height $y_i = 2$ m
- initial velocity $v = 35$ m/s
- initial trajectory $\theta = 35^o$
- accel. gravity $g = -9.81$ m/s/s

Solution: $x_f \approx 120$ m

# Example Stochastic Problem

## Uncertainty

$$x_f = \frac{v\cos\theta}{g}\left(v\sin\theta + \sqrt{v^2\sin^2\theta + 2gy_i}\right)$$

- initial height $y_i = 1 \pm 1$ m
- initial velocity $v = 35.5 \pm 2.5$ m/s
- initial trajectory $\theta = 45 \pm 10^o$
- accel. gravity $g = 9.7988 \pm 0.0349$ m/s/s

Solution: $x_f$=?

# Uncertainty Quantification

## Methods

Some way to quantify uncertainty:

# Uncertainty Quantification

## Methods

Some way to quantify uncertainty:

- Min-Max
  - Good for monotonic problems

# Uncertainty Quantification

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Some way to quantify uncertainty:

- Min-Max
  - Good for monotonic problems
- Analytic Uncertainty
  - Good for analytic solutions

# Uncertainty Quantification

## Methods

Some way to quantify uncertainty:

- Min-Max
  - Good for monotonic problems
- Analytic Uncertainty
  - Good for analytic solutions
- Perturbation
  - Valid for small uncertainty

# Uncertainty Quantification

$$x_f = \frac{v\cos\theta}{g}\left(v\sin\theta + \sqrt{v^2\sin^2\theta + 2gy_i}\right)$$

## Min-Max

$$x_{f,\text{min}} = \frac{(33)(0.5736)}{9.8337}\left((33)(0.8192) + \sqrt{(33)^2(0.8192)^2 + 2(9.8337)(0)}\right) = 105.46 \text{ m}$$

$$x_{f,\text{max}} = \frac{(55)(0.8192)}{9.7369}\left((55)(0.5736) + \sqrt{(55)^2(0.5736)^2 + 2(9.8337)(2)}\right) = 142.17 \text{ m}$$

Result: $x_f \approx 124 \pm 18.3$ m

# Uncertainty Quantification

$$x_f = \frac{v\cos\theta}{g}\left(v\sin\theta + \sqrt{v^2\sin^2\theta + 2gy_i}\right)$$

## Min-Max

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Result: $x_f \approx 124 \pm 18.3$ m

## Flawed Reasoning

- $\theta$ not monotonic!
- Does increasing $\theta$ make a longer or shorter range?

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# Uncertainty Quantification

Analytic Uncertainty

$$\sigma_{x_f} = \sqrt{\left(\frac{\partial x_f}{\partial y_i}\right)^2 \sigma_{y_i}^2 + \left(\frac{\partial x_f}{\partial v}\right)^2 \sigma_v^2 + \left(\frac{\partial x_f}{\partial g}\right)^2 \sigma_g^2 + \left(\frac{\partial x_f}{\partial \theta}\right)^2 \sigma_\theta^2}$$

Works well for simple functions

- Simple derivatives
- Analytic solution
- Assumes mean is reference value

# Uncertainty Quantification

$$x_f = \frac{v\cos\theta}{g}\left(v\sin\theta + \sqrt{v^2\sin^2\theta + 2gy_i}\right)$$

Analytic Uncertainty

$$\sigma_{x_f} = \sqrt{\left(\frac{\partial x_f}{\partial y_i}\right)^2 \sigma_{y_i}^2 + \left(\frac{\partial x_f}{\partial v}\right)^2 \sigma_v^2 + \left(\frac{\partial x_f}{\partial g}\right)^2 \sigma_g^2 + \left(\frac{\partial x_f}{\partial \theta}\right)^2 \sigma_\theta^2}$$

Result: $x_f = 120 \pm 62.44$ m

# A More Difficult Problem
## Air Resistance

With Air Resistance:

$$y_f = \frac{v_T}{g}(v\sin\theta + v_T)\left(1 - e^{-gt/v_T}\right) - v_T t,$$

$$x_f = \frac{v v_T \cos\theta}{g}\left(1 - e^{-gt/v_T}\right).$$

$$v_T = \frac{mg}{D}, \qquad D = \frac{\rho C A}{2}, \qquad A = \pi r^2$$

Solve numerically to get $x_f$ (Forward Euler).

# A More Difficult Problem

## Aside: Forward Euler

Take small $\Delta_t$ time steps `while` $y^t > 0$: $\quad t = t + \Delta_t$,

$$a_x^{(t+\Delta_t)} = \frac{-D}{m} v^{(t)}\ v_x^{(t)}, \qquad a_y^{(t+\Delta_t)} = -g - \frac{D}{m} v^{(t)}\ v_x^{(t)},$$

$$v_x^{(t+\Delta_t)} = v_x^{(t)} + a_x^{(t+\Delta_t)}\Delta_t, \qquad v_y^{(t+\Delta_t)} = v_y^{(t)} + a_y^{(t+\Delta_t)}\Delta_t,$$

$$x^{(t+\Delta_t)} = x^{(t)} + v_x^{(t+\Delta_t)}\Delta_t + \frac{1}{2}a_x^{(t+\Delta_t)}\Delta_t^2,$$
$$y^{(t+\Delta_t)} = y^{(t)} + v_y^{(t+\Delta_t)}\Delta_t + \frac{1}{2}a_y^{(t+\Delta_t)}\Delta_t^2.$$

(video)

# A More Difficult Problem

## Uncertainty Summary

$$
\begin{aligned}
y_i &= 1 \pm 1 \text{ m},\\
v &= 35.5 \pm 2.5 \text{ m/s},\\
\theta &= 45 \pm 10^o,\\
g &= 9.7988 \pm 0.0349,\\
m &= 0.145 \pm 0.0725 \text{ kg},\\
r &= 0.0336 \pm 0.00336 \text{ m},\\
C &= 0.5 \pm 0.5,\\
\rho_{\text{air}} &= 1.2 \pm 0.1 \text{ kg/m}^3.
\end{aligned}
$$

Sensitivity Study

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# A More Difficult Problem

## Equation Summary

$$y_f = \frac{v_T}{g}(v \sin\theta + v_T)\left(1 - e^{-gt/v_T}\right) - v_T t,$$

$$x_f = \frac{v v_T \cos\theta}{g}\left(1 - e^{-gt/v_T}\right).$$

$$v_T = \frac{mg}{D}, \qquad D = \frac{\rho C A}{2}, \qquad A = \pi r^2$$

# Uncertainty Quantification

## Complicated Problems

How do we quantify uncertainty for problems without simple analytic solutions?

- Monte Carlo sampling
- Stochastic Collocation
- High Density Model Reduction (low-order)

# Uncertainty Quantification

## Monte Carlo

- Let $u(Y)$ be any system, like $x_f(y_i, v, \theta, g, m, r, C, \rho)$
- Randomly sample input parameters, record outputs
- Repeat $M$ times
- Calculate moments (mean, variance, skew, kurtosis)

$$\text{Mean: } \bar{u} \approx \frac{1}{M} \sum u\left(Y^{(m)}\right)$$

(video)

# Uncertainty Quantification

## Stochastic Collocation

- Let $u(Y)$ be any system, like $x_f(y_i, v, \theta, g, m, r, C, \rho)$
- Represent original model with polynomials
- Calculate moments (mean, variance, skew, kurtosis)

$$u(Y) \approx \sum_{k \in \Lambda} c_k \Phi_k(Y),$$

$$\Phi_k(Y) = \phi_{k_1}(Y_1) \cdot \phi_{k_2}(Y_2) \cdot \ldots \cdot \phi_{k_N}(Y_N)$$

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# Uncertainty Quantification

## Stochastic Collocation

For example:

$$x_f(y_i, v, \theta, g, m, r, C, \rho) \approx \sum_{k \in \Lambda} c_k \Phi_k(y_i, v, \theta, g, m, r, C, \rho),$$

$$\Phi_k(y_i, v, \theta, g, m, r, C, \rho) = \phi_{y_i}(y_i) \cdot \phi_v(v) \cdot \ldots \cdot \phi_\rho(\rho).$$

For $k = (1, 1, 2, 2, 3, 3, 4, 4)$ and
$\phi$ as monomials $(1, x^2, x^3, x^4, \ldots)$,

$$\Phi_k(y_i, v, \theta, g, m, r, C, \rho) = y_i \cdot v \cdot \theta^2 \cdot g^2 \cdot m^3 \cdot r^3 \cdot C^4 \cdot \rho^4.$$

# Uncertainty Quantification

## Stochastic Collocation

Comparison

| Monte Carlo | Stochastic Collocation |
|---|---|
| Dimension-independent | Calculations grow with dimension* |
| Slow converging | Very fast convergence* |
| | Can replace original model |

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# Uncertainty Quantification

## Results: pdf

TODO

# Uncertainty Quantification

## Results: Expected Value, Values

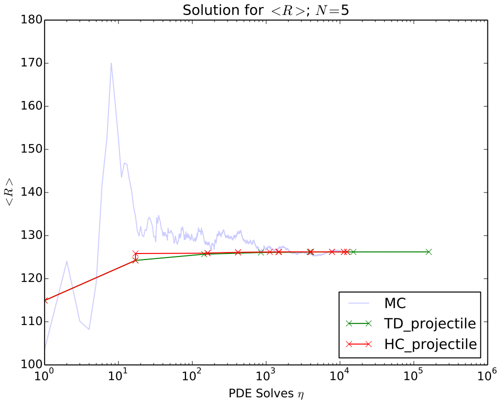


Figure : $\mathbb{E}[x_f]$

# Uncertainty Quantification

## Results: Expected Value, Errors

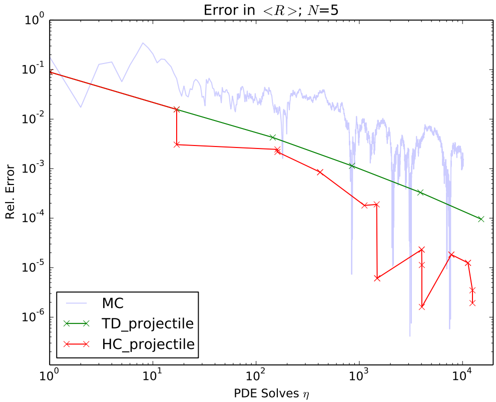


Figure : Error in $\mathbb{E}[x_f]$

# Sensitivity Analysis

## Polynomial Expansion Revisited

Recall: $u(Y) \approx \sum_{k\in\Lambda} c_k\Phi_k(Y)$, so for $x_f(y_i, v, \theta, g, m, r, C, \rho)$:

$$
\begin{aligned}
x_f \approx\ & c_{(0,0,0,0,0,0,0,0)} \\
& + c_{(1,0,0,0,0,0,0,0,0)} y_i + c_{(0,1,0,0,0,0,0,0,0)} v + c_{(0,0,1,0,0,0,0,0,0)} \theta + \ldots \\
& + c_{(2,0,0,0,0,0,0,0,0)} y_i^2 + c_{(1,1,0,0,0,0,0,0,0)} y_i \cdot v + c_{(1,0,1,0,0,0,0,0,0)} y_i \cdot \theta + \ldots \\
& + c_{(3,0,0,0,0,0,0,0,0)} y_i^3 + c_{(1,1,0,0,0,0,0,0,0)} y_i \cdot v \cdot \theta + \ldots \\
& \ldots
\end{aligned}
$$

# Sensitivity Analysis

## Polynomial Expansion Revisited

Rearrange:

$$
\begin{aligned}
x_f \approx\ & c_{(0,0,0,0,0,0,0,0)} \\
& + c_{(1,0,0,0,0,0,0,0,0)} y_i + c_{(2,0,0,0,0,0,0,0,0)} y_i^2 + c_{(3,0,0,0,0,0,0,0,0)} y_i^3 + \dots \\
& + c_{(0,1,0,0,0,0,0,0,0)} v + c_{(0,2,0,0,0,0,0,0,0)} v^2 + c_{(0,3,0,0,0,0,0,0,0)} v^3 + \dots \\
& \dots \\
& + c_{(1,1,0,0,0,0,0,0,0)} y_i \cdot v + c_{(1,2,0,0,0,0,0,0,0)} y_i \cdot v^2 + \dots \\
& \dots
\end{aligned}
$$

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# Sensitivity Analysis

## ANOVA

ANOVA: [AN]alysis [O]f [VA]riance

- How much does each input contribute to the variance?

| Input | Variance | % Variance | Weight |
|---|---|---|---|
| $C$ | 0.523 | 0.6657 | 1 |
| $\theta$ | 0.236 | 0.3006 | 1/2 |
| $r$ | 0.00868 | 0.0111 | 1/5 |
| $m$ | 0.00862 | 0.0110 | 1/5 |
| $y_i$ | 0.00671 | 0.0085 | 1/5 |
| $\rho$ | 0.00209 | 0.0027 | 1/6 |
| $v$ | 0.000348 | 0.0004 | 1/7 |
| $g$ | $2.83\times10^{-6}$ | $3.601\times10^{-6}$ | 1/12 |

Uncertainty Ranges

# Sensitivity Analysis

## Results: Expected Value, Values

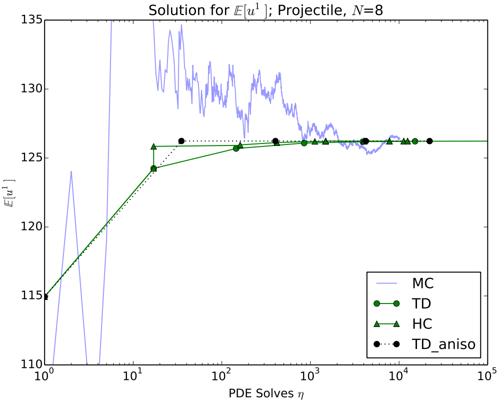


Figure : $\mathbb{E}[x_f]$

# Uncertainty Quantification

## Results: Expected Value, Errors

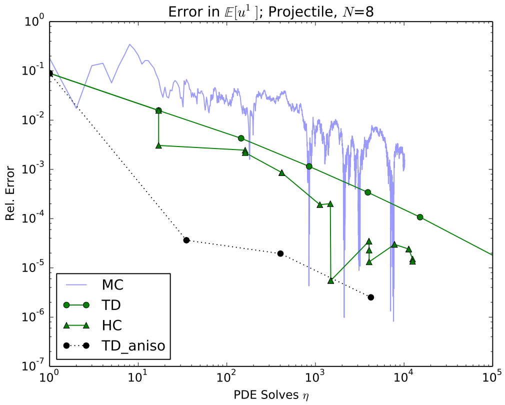


Figure : Error in $\mathbb{E}[x_f]$

# Uncertainty Quantification

## Results: Second Moment, Values

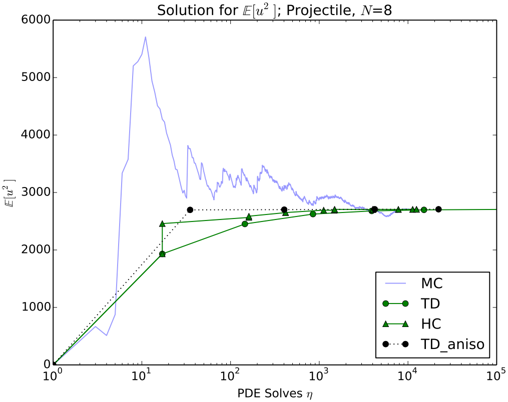


Figure : $\mathbb{E}[x_f^2]$

# Uncertainty Quantification

## Results: Second Moment, Errors

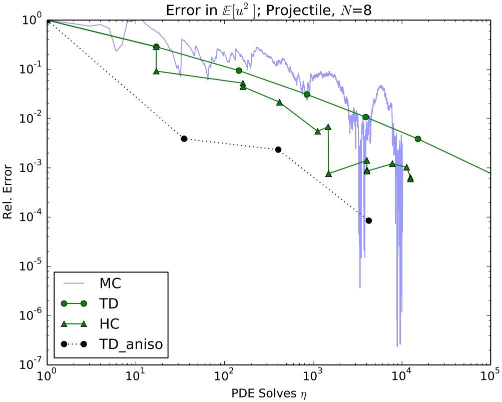


Figure : Error in $\mathbb{E}[x_f^2]$

# Conclusions

- Uncertainty Quantification methods
  - Analytic methods: good, but possible deceiving
  - Numerical methods: expensive, but robust
- Sensitivity Analysis
  - Reveals importance of parameters
  - Tighten uncertainty in experiment/model
- Areas of study
  - Adaptive sampling
  - Sparse quadrature integration
  - Improved Monte Carlo methods
  - Efficient statistics algorithms

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# Polynomial Index Sets

## Choosing what polynomial degrees to use

- Tensor Product:

$$\Lambda_{\text{TP}}(L) = \left\{ \bar{p} = [p_1, ..., p_N] : \max_{1 \leq n \leq N} p_n \leq L \right\}, \eta = (L+1)^N$$

- Total Degree:

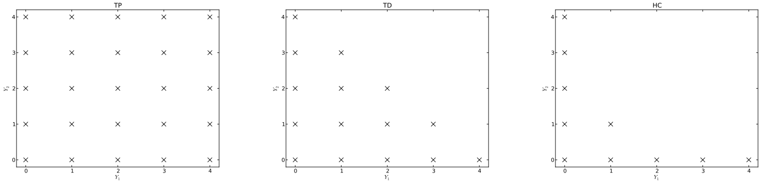
$$\Lambda_{\text{TD}}(L) = \left\{ \bar{p} = [p_1, ..., p_N] : \sum_{n=1}^{N} p_n \leq L \right\}, \eta = \binom{L+N}{N}$$

- Hyperbolic Cross:

$$\Lambda_{\text{HC}}(L) = \left\{ \bar{p} = [p_1, ..., p_N] : \prod_{n=1}^{N} p_n + 1 \leq L + 1 \right\}, \eta \leq (L+1)(1+\log(L+1))^{N-1}$$

# Polynomial Index Sets

## 2D Example




(a) Tensor Product (b) Total Degree (c) Hyperbolic Cross

Figure : Index Set Examples: $N = 2, L = 4$

# Calculating $c_k$

Where the algorithmic rubber hits the mathematical road.

$$u(Y) \approx \mathcal{S}_{N,\Lambda(L)}[u](Y) = \sum_{\boldsymbol{i}\in\Lambda(L)} c(\boldsymbol{i}) \bigotimes_{n=1}^{N} \mathcal{U}_{n,p(i_n)}[u](Y),$$

$$c(\boldsymbol{i}) = \sum_{\substack{\boldsymbol{j}=\{0,1\}^N,\\ \boldsymbol{i}+\boldsymbol{j}\in\Lambda(L)}} (-1)^{|\boldsymbol{j}|_1},$$

$$\bigotimes_{n=1}^{N} \mathcal{U}_{n,p(i_n)}[u](Y) \equiv \sum_{k_1=0}^{p(i_1)} \cdots \sum_{k_N=0}^{p(i_N)} u_h\left(Y^{(k_1)}, \cdots, Y^{(k_N)}\right) \prod_{n=1}^{N} \mathcal{L}_{k_n}(Y_n),$$

$$= \sum_{k}^{p(\vec{i})} u_h\left(Y^{(k)}\right) \mathcal{L}_k(Y),$$

# Calculating $c_k$

## 2D Examples

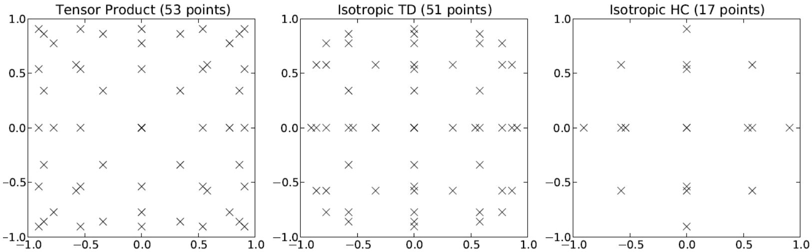



Figure : Sparse Grids, $N = 2, L = 4, p(i) = i$, Legendre points

# Calculating $c_k$

## Some Numbers

| | | TP | TD | | HC | |
|---|---|---|---|---|---|---|
| $N$ | $L$ | $\lvert\Lambda(L)\rvert$ | $\lvert\Lambda(L)\rvert$ | $\eta$ | $\lvert\Lambda(L)\rvert$ | $\eta$ |
| 3 | 4 | 125 | 35 | 165 | 16 | 31 |
| | 8 | 729 | 165 | 2,097 | 44 | 153 |
| | 16 | 4,913 | 969 | 41,857 | 113 | 513 |
| | 32 | 35,737 | 6,545 | 1,089,713 | 309 | 2,181 |
| 5 | 2 | 293 | 21 | 61 | 11 | 11 |
| | 4 | 3,125 | 126 | 781 | 31 | 71 |
| | 8 | 59,049 | 1,287 | 28,553 | 111 | 481 |

Table : Index Set and Collocation Size Comparison