Quantifying Uncertainty in Engineering Analysis

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Motivation

Engineering analysis assumes perfect knowledge of the geometry and mathematical model.

Engineering design assumes we can manufacture exactly what is designed.

In reality, there is much uncertainty:

- manufacturing tolerances
- uncertain modelling parameters

Next big trend in engineering analysis is to quantify the consequences of these.

Approaches

At one extreme, there are stochastic PDEs, able to cope with extremely large uncertainties (e.g. variation in rock porosity in oil reservoir modelling), but very complex and computationally demanding.

We're interested in the other extreme:

- limited to very small uncertainties
- relatively simple and computationally inexpensive
- usually only concerned with one or two output functionals (e.g. lift, drag)
- often interested only in first order (variance) and second order (mean perturbation) effects
- sometimes, also interested in confidence limits

Explicit Uncertainty Propagation

- Monte Carlo simulations;
- Moment method with first, second and third order Taylor expansions;
- Moment method with adjoint error correction.

Taylor Expansion

$$
\begin{aligned}
y = f(x) \quad &= \quad f(\mu_x) + f'(\mu_x)(x - \mu_x) + \frac{f''(\mu_x)}{2!}(x - \mu_x)^2 \\
&\quad + \frac{f'''(\mu_x)}{3!}(x - \mu_x)^3 + O((x - \mu_x)^4)
\end{aligned}
$$

where the primes denote derivative with respect to x, and μ_x is mean of x.

First Order Taylor series approximation:

$$
\begin{aligned}
\mu_y \quad &= \quad f(\mu_x) \\
\sigma_y^2 \quad &= \quad \big(f'(\mu_x)\big)^2 \; \sigma_x^2
\end{aligned}
$$

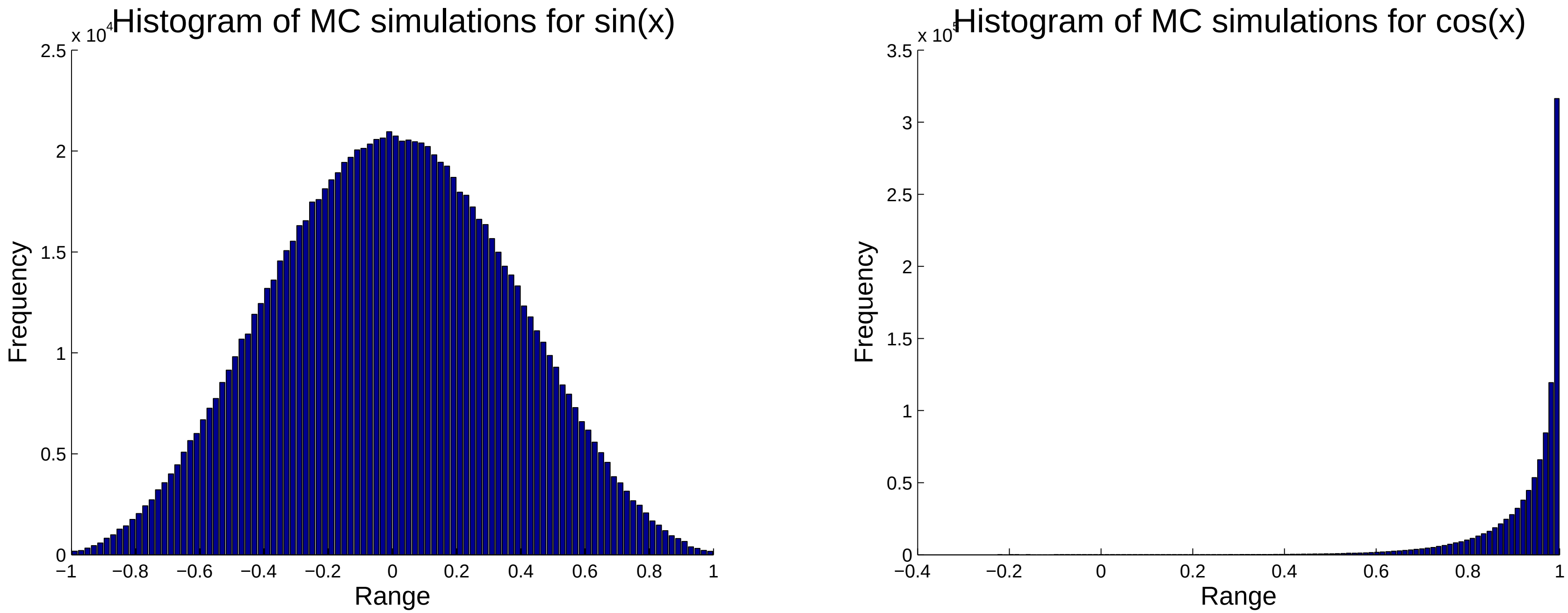
Taylor Expansion

Second Order Taylor series approximation:

$$
\begin{aligned}
\mu_y &= f(\mu_x) + \frac{f''(\mu_x)}{2!}\,\sigma_x^2 \\
\sigma_y^2 &= f''(\mu_x)^2\,\sigma_x^2 + f'(\mu_x)\,f''(\mu_x)\,S(x)\,\sigma_x^3 \\
&\quad + \frac{f''(\mu_x)}{2!}^2 (K(x)-1)\,\sigma_x^4
\end{aligned}
$$

- Similarly third order Taylor series approximation can be derived involving skewness and Kurtosis terms.

MC for Test Functions



Frequency distribution for sin(x) and cos(x) for normally distributed x with $\mu_x = 0$, $\sigma_x = \frac{\pi}{4}$ – sample size = 10^6.

Mean: Moment Methods

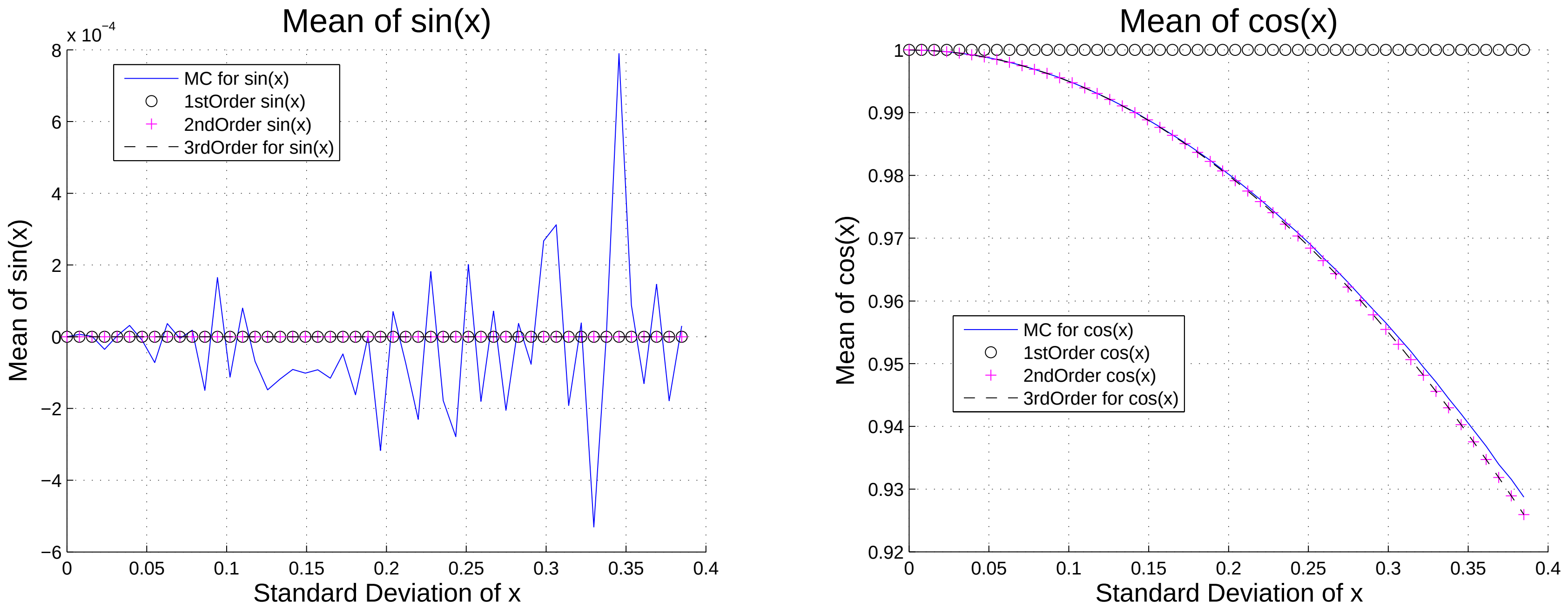
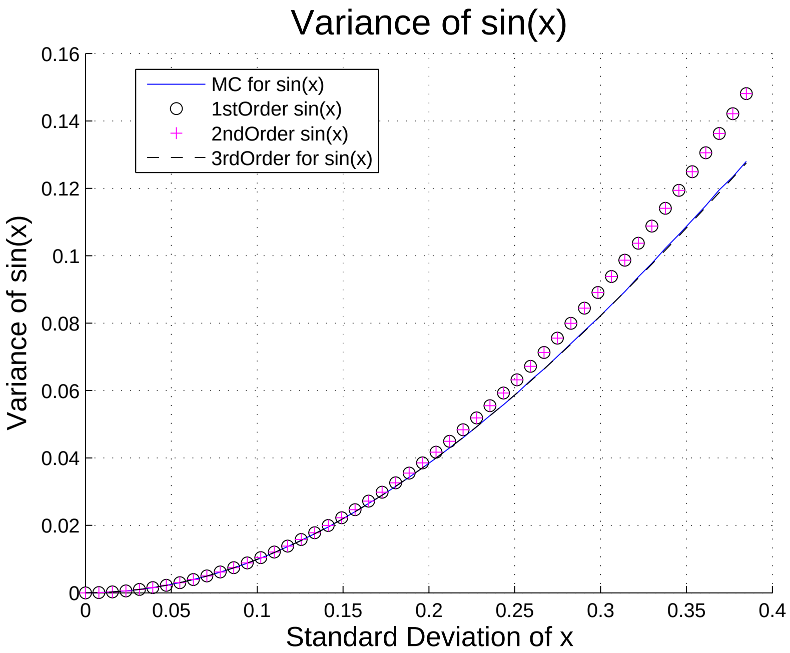


Figure 1: Prediction of μ_y with increasing σ_x

Variance: Moment Methods



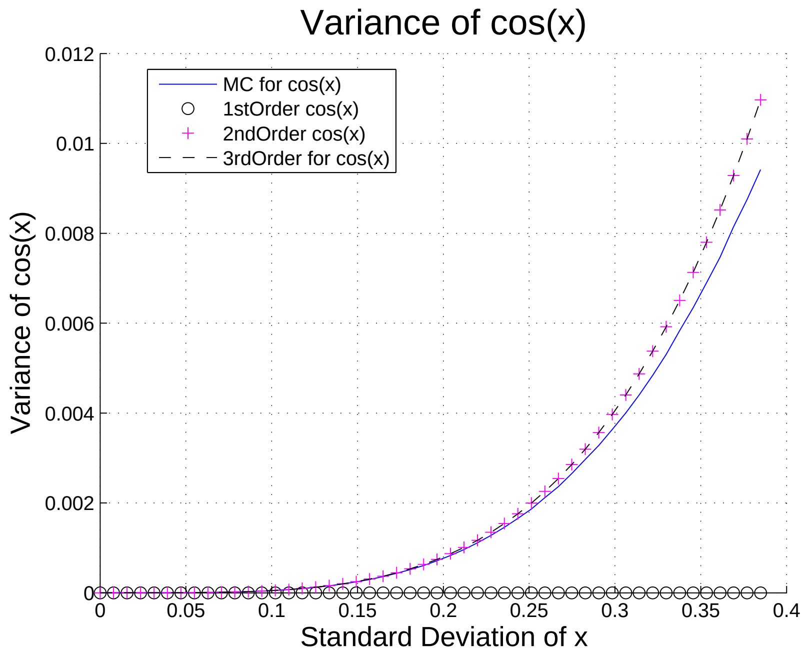


Figure 2: Prediction of σ_y^2 with increasing σ_x

Implicit Uncertainty Propagation

Let u be the solution of a set of non-linear algebraic equations

$$f(u(x), x) = 0,$$

and an output functional of interest, $J(u(x), x)$.

The adjoint equation corresponding to this functional is

$$\left(\frac{\partial f}{\partial u}\right)^T \overline{f} + \left(\frac{\partial J}{\partial u}\right)^T = 0.$$

Given approximate solutions u^* and $\overline{f}^*$,

$$J(u(x), x) \approx J(u^*, x) + (\overline{f}^*)^T f(u^*, x).$$

MC using Adjoint Error Correction

To avoid the cost of computing exact u, Monte-Carlo simulations are performed using adjoint error correction.

The following options are available:

- $u^* = u_{\mu_x}, \quad \overline{f}^* = \overline{f}_{\mu_x}$
- $u^* = u_{\mu_x} + \dfrac{du}{dx}(x-\mu_x), \quad \overline{f}^* = \overline{f}_{\mu_x}$
- $u^* = u_{\mu_x} + \dfrac{du}{dx}(x-\mu_x), \quad \overline{f}^* = \overline{f}_{\mu_x} + \dfrac{d\overline{f}}{dx}(x-\mu_x)$

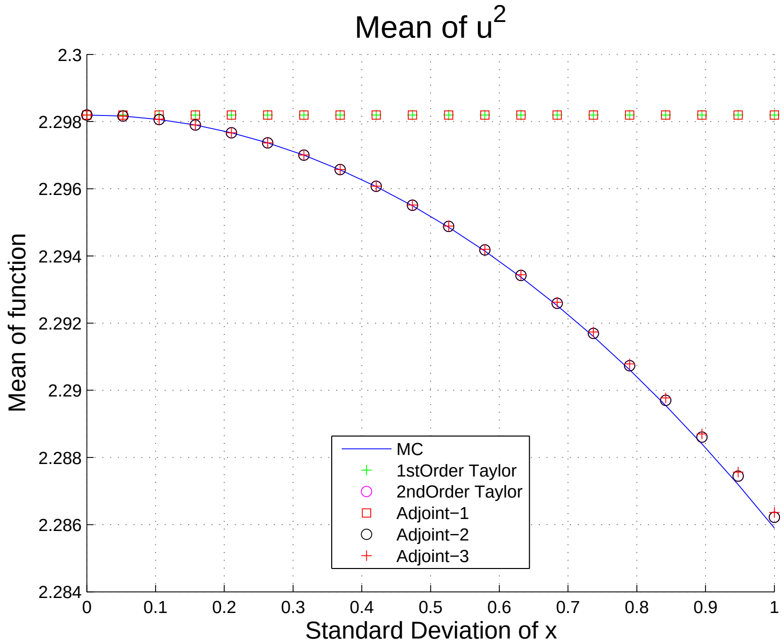
Test Case

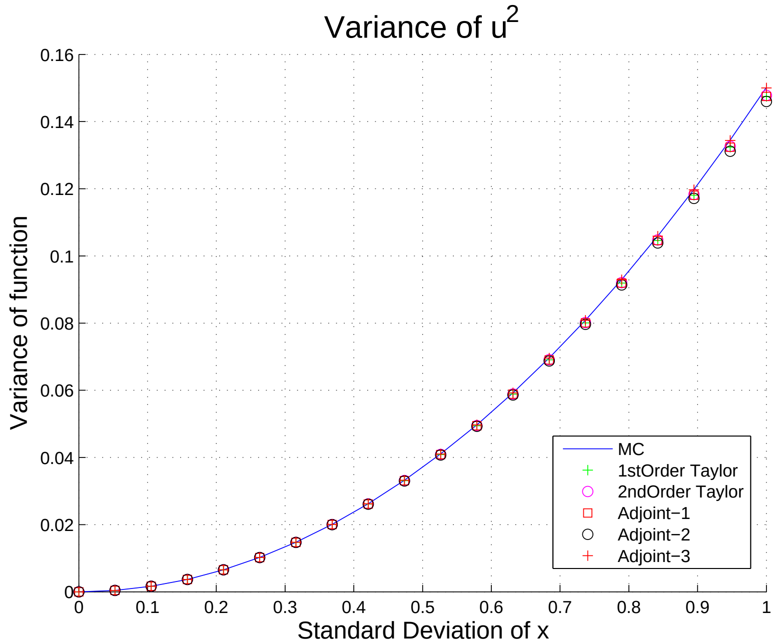
$$N(u(x),x) = u + u^3 - x = 0, \qquad J(u(x),x) = u^2.$$

- nonlinear equation solved by Newton iteration;
- adjoints are calculated analytically;
- $\dfrac{du}{dx}$ and $\dfrac{d\overline{f}}{dx}$ are calculated analytically.

Results

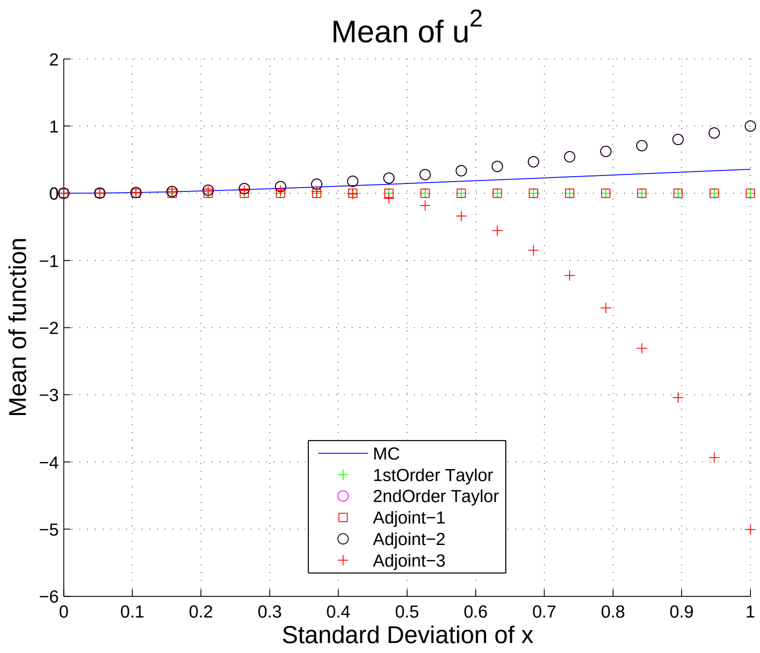
- $\mu_x = 5; \sigma_x^2 = 1$

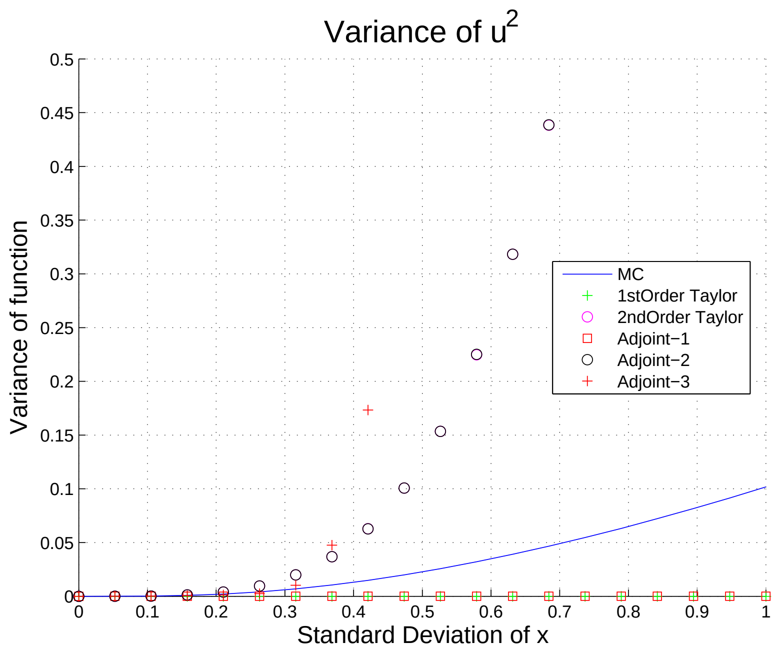




Results

- $\mu_x = 0; \sigma_x^2 = 1$





Computational Cost

- One nonlinear solution
- One adjoint solution
- N linear solutions for $\frac{du}{dx}$ (N = # of uncertain parameters)
- N linear solutions for $\frac{d\overline{f}}{dx}$
- M inexpensive approximate MC evaluations

Cheap Hessian Evaluation

Functional and nonlinear equations:

$$j(x) = J(u,x) \quad \Longrightarrow \quad \frac{\partial j}{\partial x_i} = \frac{\partial J}{\partial u}\,\frac{\partial u}{\partial x_i} + \frac{\partial J}{\partial x_i}.$$

$$f(x,u) = 0 \quad \Longrightarrow \quad \frac{\partial f}{\partial u}\,\frac{\partial u}{\partial x_i} + \frac{\partial f}{\partial x_i} = 0.$$

Adjoint equation and gradient:

$$\left(\frac{\partial f}{\partial u}\right)^T \overline{f} + \left(\frac{\partial J}{\partial u}\right)^T = 0,$$

$$\frac{\partial j}{\partial x_i} \;=\; -\,\frac{\partial J}{\partial u}\left(\frac{\partial f}{\partial u}\right)^{-1}\frac{\partial f}{\partial x_i} + \frac{\partial J}{\partial x_i} \;=\; \overline{f}^T\,\frac{\partial f}{\partial x_i} + \frac{\partial J}{\partial x_i}.$$

Cheap Hessian Evaluation

Second derivative of functional and nonlinear equations:

$$\frac{\partial^2 j}{\partial x_i \partial x_j} = \frac{\partial J}{\partial u}\,\frac{\partial^2 u}{\partial x_i \partial x_j} + D^2_{i,j} J,$$

$$\frac{\partial f}{\partial u}\,\frac{\partial^2 u}{\partial x_i \partial x_j} + D^2_{i,j} f = 0,$$

$$D^2_{i,j} J \equiv \frac{\partial^2 J}{\partial u^2}\,\frac{\partial u}{\partial x_i}\,\frac{\partial u}{\partial x_j} + \frac{\partial^2 J}{\partial u \partial x_i}\,\frac{\partial u}{\partial x_j} + \frac{\partial^2 J}{\partial u \partial x_j}\,\frac{\partial u}{\partial x_i} + \frac{\partial^2 J}{\partial x_i \partial x_j}$$

and $D^2_{i,j} f$ is defined similarly.

$$\Longrightarrow \quad \frac{\partial^2 j}{\partial x_i \partial x_j} = \overline{f}^T D^2_{i,j} f + D^2_{i,j} J.$$

Cheap Hessian Evaluation

Computational cost:

- One nonlinear solution;
- N_o adjoint solutions, one for each output;
- N_i linear solutions, one for each input;
- inexpensive evaluation of $D^2_{i,j}f$, $D^2_{i,j}J$ using forward-on-forward AD.

Not a new idea (Taylor, Green, Newman and Putko, 2003) but worth pursuing?