A primer on uncertainty quantifications

Kjetil Olsen Lye

Uncertainty quantification

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- How do these uncertainties affect the model predictions?

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- How do these uncertainties affect the model predictions?
- **Goal:** How can we effectively compute statistics of quantities of interest given uncertainties in input data?

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$$\text{Quantity of interest } Q = Q(\underbrace{\text{Model input}}_{\text{uncertain}}) = Q(\mathbf{y})$$

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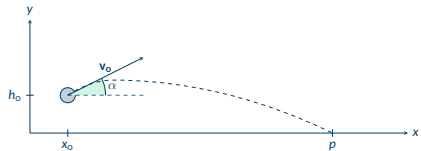

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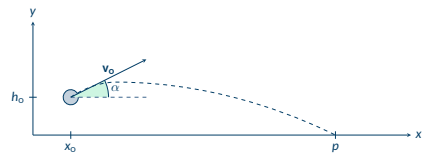

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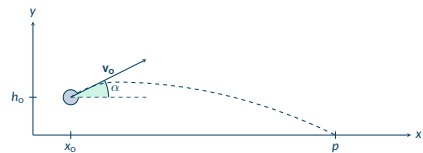

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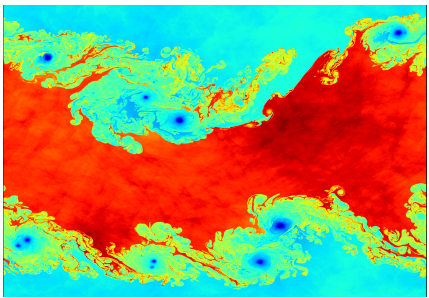

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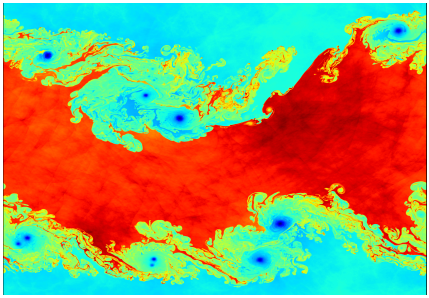

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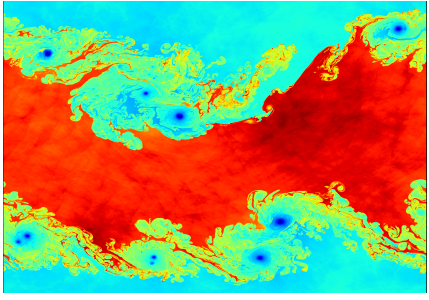

Next three lectures summarized in one slide

- $\mathbf{y} \in D \subset \mathbb{R}^d$ uncertain parameters

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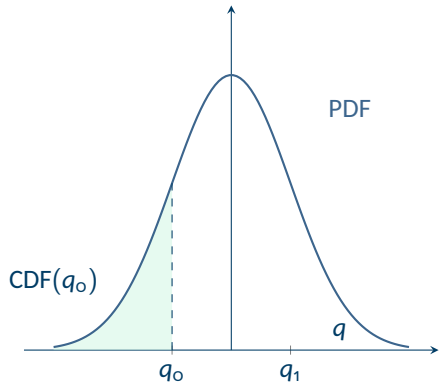
- PDF, CDF, ...



Focus of talk

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$$\int_{[0,1]^d} Q(\mathbf{y})\, d\mathbf{y}$$

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- Q is expensive to compute
- d is large
- Q could be ill-behaved (eg. discontinuous)
- Q could be vector-valued (or even function-valued)

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Random variables

- A random variable X is a measurable function $X : \Omega \to \mathbb{R}^d$

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- The **law** (or distribution) of X is the pushforward measure

$$\mu_X(A) = \mathbb{P}(X^{-1}(A)) \text{ for } A \subset \mathbb{R}^d \text{ Borel}$$

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- If μ_X is absolutely continuous w.r.t. Lebesgue measure: $\mu_X = \rho \cdot dx$
- Then ρ is the probability density function (PDF)

Common distributions

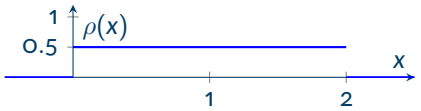
Uniform distribution $X \sim \mathcal{U}[a, b]$

- PDF: $\rho(x) = \frac{1}{b-a}\mathbf{1}_{[a,b]}(x)$
- $\mu_X = \frac{1}{b-a}dx$ on $[a, b]$

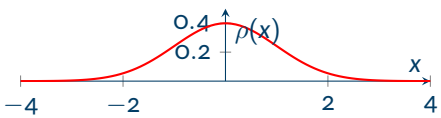
Normal distribution $X \sim \mathcal{N}(\mu, \sigma^2)$

- PDF: $\rho(x) = \frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{(x-\mu)^2}{2\sigma^2}}$
- $\mu_X = \rho(x)dx$ on $\mathbb{R}$

Uniform $\mathcal{U}[0, 2]$

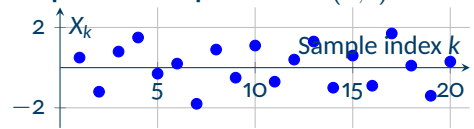


Normal $\mathcal{N}(0, 1)$



Visual interpretation: i.i.d. samples

Independent samples from $\mathcal{N}(0, 1)$



- Each X_k is drawn from same distribution
- Knowing X_1 tells us nothing about X_2

How computers generate random numbers

- Computers are deterministic machines

In Julia:

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using Random
Random.seed!(1234)
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- Same seed $\Rightarrow$ same sequence (reproducibility!)

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Computers: from uniform to other distributions

- Start with $U \sim \mathcal{U}[0, 1]$

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using Random, Distributions
X = rand(Exponential(lambda))
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  - Sample: $X = -\frac{1}{\lambda} \ln(1 - U)$
- Other methods: Box-Muller transform for normal distribution, rejection sampling, etc.

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  - Organize into M vectors of dimension d

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- For M independent samples $\mathbf{Y}_1, \ldots, \mathbf{Y}_M$:
  - Generate $M \times d$ independent uniform random numbers
  - Organize into M vectors of dimension d
- **Example in Julia:**
  - `Y = rand(M, d)  # M samples in R^d`

Monte Carlo algorithm

Goal: Approximate $\mathbb{E}(Q(\mathbf{Y}))$ where $\mathbf{Y} \sim \mathcal{U}([0,1]^d)$

Algorithm:

1. Draw M independent samples $\mathbf{Y}_1, \ldots, \mathbf{Y}_M \sim \mathcal{U}([0,1]^d)$
2. Compute $Q(\mathbf{Y}_k)$ for each $k = 1, \ldots, M$
3. Approximate:

$$\mathbb{E}(Q(\mathbf{Y})) \approx \frac{1}{M} \sum_{k=1}^{M} Q(\mathbf{Y}_k)$$

Error bound:

$$\mathbb{E}\left(\left| \frac{1}{M} \sum_{k=1}^{M} Q(\mathbf{Y}_k) - \mathbb{E}(Q(\mathbf{Y})) \right|^2 \right)^{1/2} = \frac{\mathrm{Var}(Q(\mathbf{Y}))^{1/2}}{\sqrt{M}}$$

Key property: Error decreases as $\mathcal{O}(M^{-1/2})$, *independent of dimension d*.

Monte Carlo algorithm

Goal: Approximate $\mathbb{E}(Q(\mathbf{Y}))$ where $\mathbf{Y} \sim \mathcal{U}([0,1]^d)$

Algorithm:

1. Draw M independent samples $\mathbf{Y}_1, \ldots, \mathbf{Y}_M \sim \mathcal{U}([0,1]^d)$
2. Compute $Q(\mathbf{Y}_k)$ for each $k = 1, \ldots, M$
3. Approximate:

$$\mathbb{E}(Q(\mathbf{Y})) \approx \frac{1}{M} \sum_{k=1}^{M} Q(\mathbf{Y}_k)$$

Error bound:

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Monte Carlo for general integrals

- Can approximate *any* integral of the form:

$$\int_D f(\mathbf{y})\, d\mathbf{y}$$

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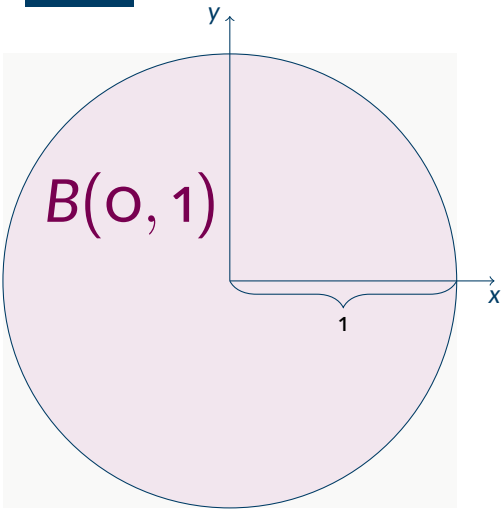
- For $D = [0,1]^d$: simply $\frac{1}{M} \sum_{k=1}^{M} f(\mathbf{Y}_k)$

Obligatory example: Computing π



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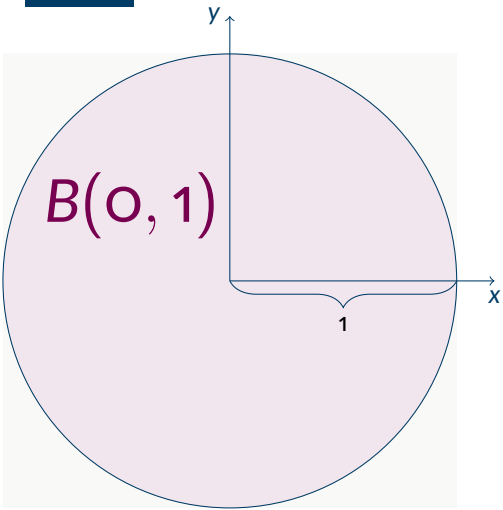

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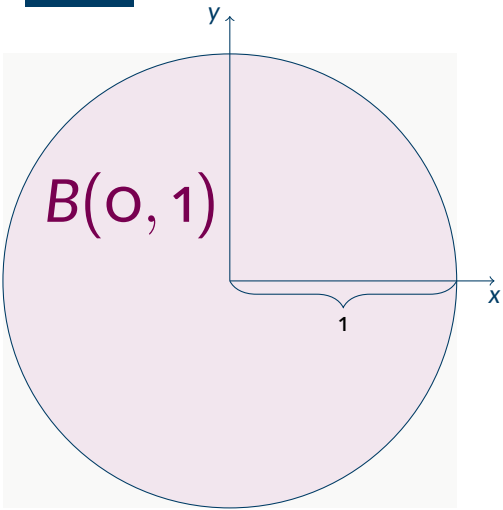

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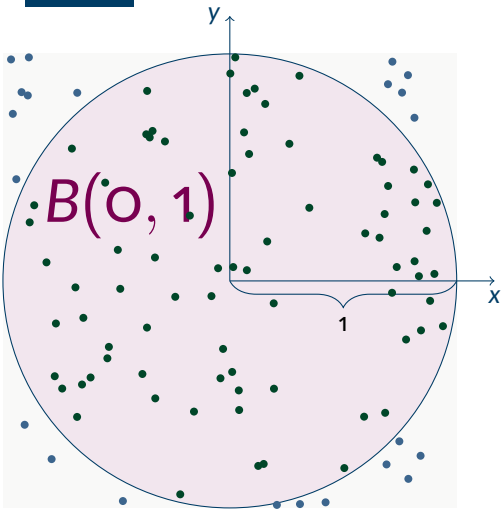

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$$\approx 4 \cdot \frac{1}{M}\sum_{k=1}^{M} \mathbf{1}_{B(o,1)}(X_k, Y_k)$$

$X_k \sim \mathcal{U}[-1,1], Y_k \sim \mathcal{U}[-1,1]$
independent random variables

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Summary in Julia

```
## Drawing random samples:
using Random
using Distributions
X = rand(Uniform(a, b), M)  # M samples from U[a,b]
Y = rand(Normal(mu, sigma), M)   # M samples from N(mu,sigma^2)
```

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## Monte Carlo integration:
function monte_carlo_integral(f, M, d)
  sum = 0.0
  for k in 1:M
    y = rand(d)  # Sample in [0,1]^d
    sum += f(y)
  end
  return sum / M  # Approximate integral
end
```

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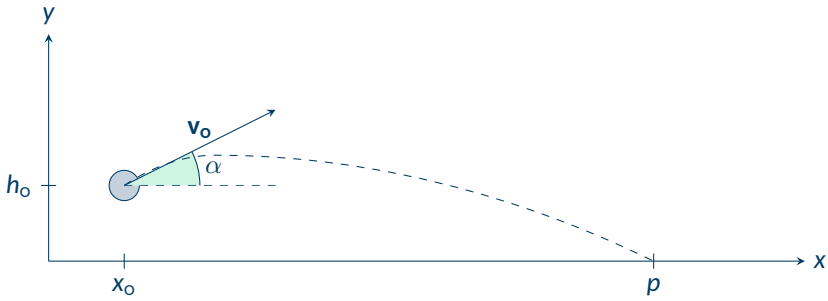
- **Balance errors:** Choose $M \sim \Delta^{-2\gamma}$ to get total error $\mathcal{O}(\Delta^\gamma)$

Example



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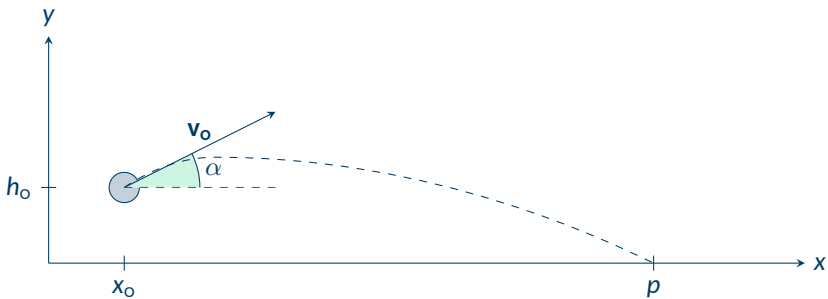

$$p(h_o) = v_o \cos(\alpha) \frac{v_o \sin(\alpha) + \sqrt{(v_o \sin(\alpha))^2 + 2gh_o}}{g} + x_o$$

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Interesting quantities

Assume $h_0 \sim \mathcal{U}[0, 1]$

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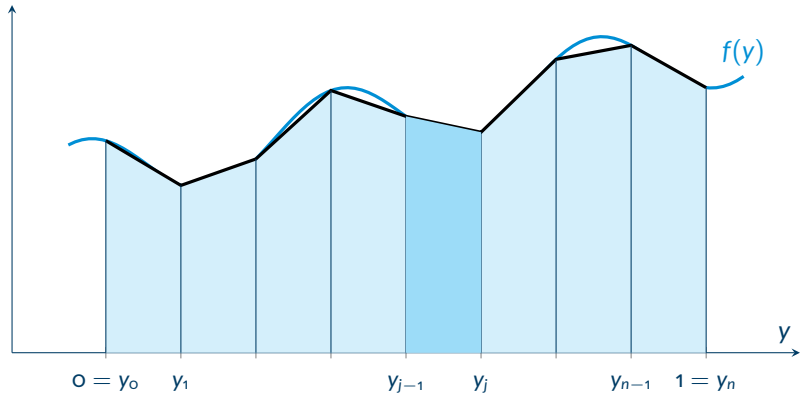
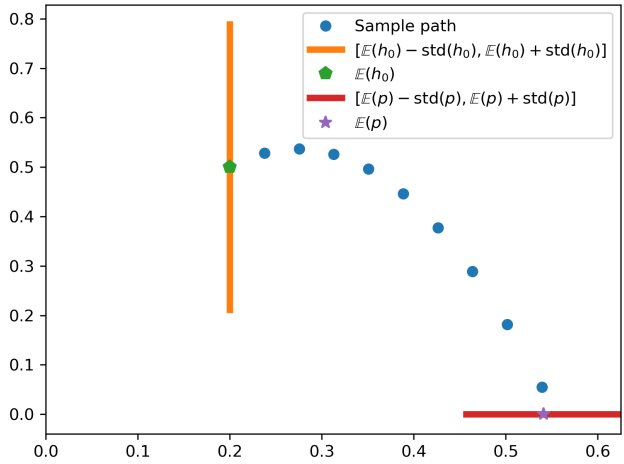
All quantities involving the integral!

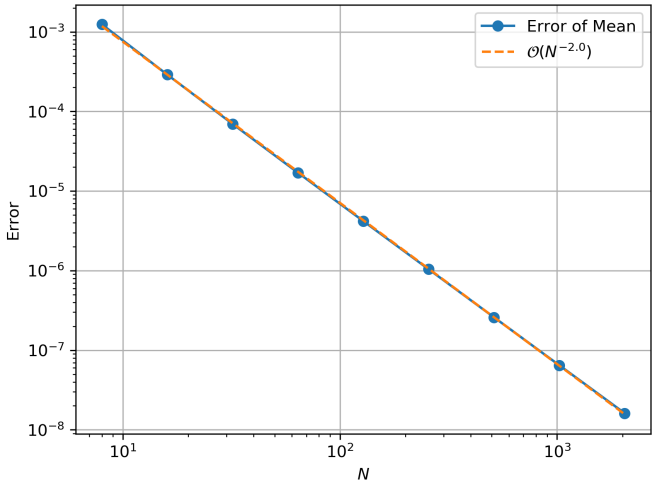
Approximate by Trapezoidal rule



Results varying initial height



Error versus number of evaluations



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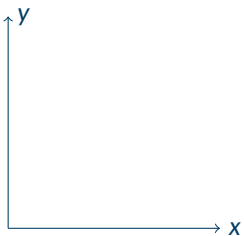
- Integration in 2D?

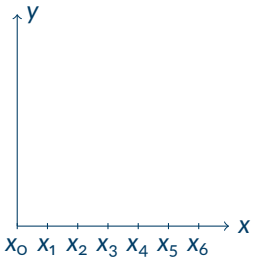
Trapezoidal rule for two dimensions

$$\int_0^1 \int_0^1 f(x, y)\, dx\, dy$$



Trapezoidal rule for two dimensions

$$\int_0^1 \int_0^1 f(x,y)\,dx\,dy \approx \int_0^1 \left(f(x_0,y) + 2\sum_{i=1}^{N-1} f(x_i,y) + f(x_N,y) \right) \Delta x\,dy$$



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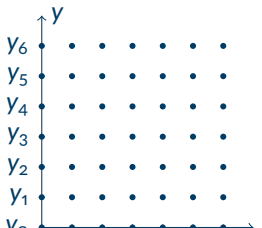
$$\approx \Big(f(0,0) + f(1,0) + f(0,1) + f(1,1) + 4\sum_{i=1}^{N-1}\sum_{i=1}^{N-1} f(x_i,y_i)$$

$$+ 2\sum_{i=1}^{N-1} f(x_i,0) + 2\sum_{i=1}^{N-1} f(x_i,1) + 2\sum_{i=1}^{N-1} f(1,y_i) + 2\sum_{i=1}^{N-1} f(0,y_i) \Big)$$



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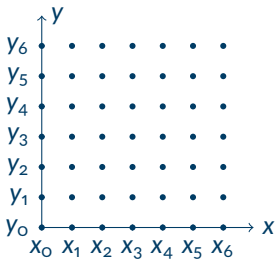

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Even more complications

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- **Seven** parameters

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Landing position depends on 7 parameters

$$p(h_o, \alpha, v_o, C_D, r, \rho, m) = \ldots$$

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$$p(h_0, \alpha, v_0, C_D, r, \rho, m) \frac{dm\ dr\ dC_D\ dv_0\ d\alpha\ dh_0}{20 \cdot 5\pi/12 \cdot 0.2 \cdot 0.015 \cdot 0.3 \cdot 0.07}$$

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How many evaluations of p do we need?

- We have 7 parameters ($d = 7$)
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Require Error $< 1/25 \approx 4\%$

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- $\Rightarrow N^d = N^7 = 5^7 = 78125$ evaluations

Finding p

Governing ODE

$$\begin{cases} \dfrac{d^2}{dt^2}\mathbf{x}(t) = -\mathbf{F}_D(C_D, r, \rho, \dfrac{d}{dt}\mathbf{x}(t))/m - g\mathbf{e}_2 \\ \mathbf{x}(0) = \begin{pmatrix} x_0 \\ y_0 \end{pmatrix} \\ \mathbf{x}'(0) = \begin{pmatrix} v_0 \cos(\alpha) \\ v_0 \sin(\alpha) \end{pmatrix} \end{cases}$$

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Finding p

$\mathbf{x}(t)$ depends on the parameters

$$\begin{cases} \dfrac{d^2}{dt^2}\mathbf{x}(h_o, \alpha, v_o, C_D, r, \rho, m; t) = -\mathbf{F}_D(C_D, r, \rho, \dfrac{d}{dt}\mathbf{x}(\ldots; t))/m - g\mathbf{e}_2 \\ \mathbf{x}(h_o, \alpha, v_o, C_D, r, \rho, m; 0) = \begin{pmatrix} 0 \\ y_o \end{pmatrix} \\ \dfrac{d}{dt}\mathbf{x}(h_o, \alpha, v_o, C_D, r, \rho, m; 0) = \begin{pmatrix} v_o \cos(\alpha) \\ v_o \sin(\alpha) \end{pmatrix} \end{cases}$$

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Assuming underlying probability space Ω

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for $\omega \in \Omega$.

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for $\omega \in \Omega$. Solve using eg. Forward-Euler:

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Set $p^{\Delta t}(\omega) = y^{N,\Delta t}(\omega)$.

Algorithm: Compute expected position using Trapezoidal rule

Input: $\Delta t, \Delta h_o, \Delta\alpha, \Delta v_o \ \ldots$

1. Initialize mean $E = 0$
2. For each integration point $h_o^i,\ \alpha^j,\ v_o^k, \ldots$:
   - 2.1 Use forward Euler to compute
   $$p^{\Delta t}(h_o^i, \alpha^j, v_o^k, \ldots)$$
   - 2.2 Update mean
   $$E = E + w_{i,j,k,\ldots} \cdot p^{\Delta t}(h_o^i, \alpha^j, v_o^k, \ldots)$$

Each evaluation is expensive when done 100 000 times!

Runtime to obtain an error ϵ:

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$$\overbrace{\mathcal{O}(\epsilon^{-1})}^{\text{Forward Euler}} \cdot \underbrace{\mathcal{O}(\epsilon^{-7/2})}_{\text{Trapezoidal}} = \mathcal{O}(\epsilon^{-4.5}).$$

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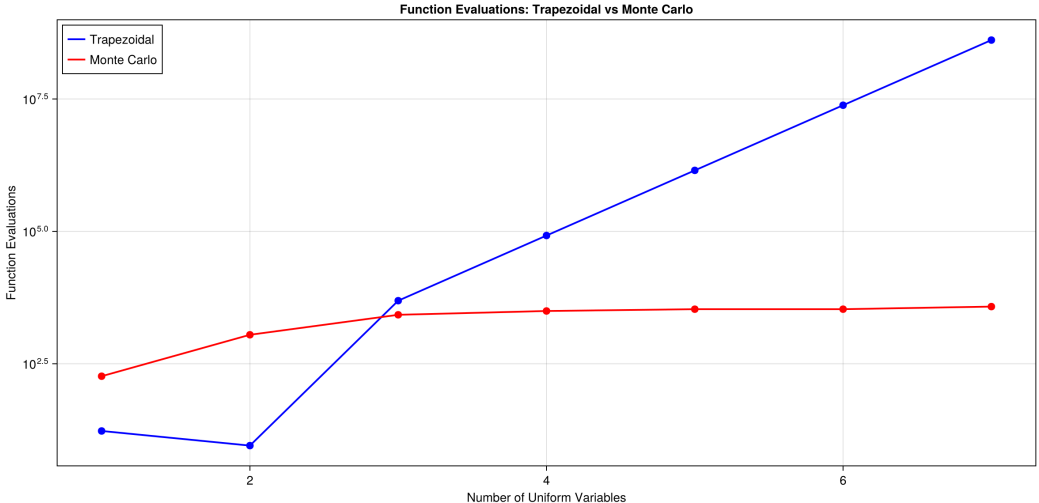
Then

$$E \approx \mathbb{E}(u(\cdot, T))$$

Function evaluations comparison: Trapezoidal vs Monte Carlo



Various smaller remarks

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Computing variance and means online

- Problem: Computing variance requires two passes over data. Alternatively:

$$\mathrm{Var}(X) = \mathbb{E}(X^2) - \mathbb{E}(X)^2$$ Sensitive to cancellation

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Welford's online algorithm:

$$M_k = M_{k-1} + \frac{X_k - M_{k-1}}{k} \qquad \text{(running mean)}$$

$$S_k = S_{k-1} + (X_k - M_{k-1})(X_k - M_k) \qquad \text{(running sum of squares)}$$

Then: $\mathbb{E}(X) \approx M_k$, $\mathrm{Var}(X) \approx S_k/(k-1)$

Storage: Only need to keep M_k and S_k (constant memory!)

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Programming tips: Use an explicit random generator

- `seed!`, —randn()—, `rand()`, etc modify global state

Prefer to use an explicit random number generator (available in Julia, Python, C++, ...):

```
using Random
using Distributions
rng = MersenneTwister(1234)
U = rand(rng)
X = rand(rng, Exponential(lambda))
Y = rand(rng, Normal(mu, sigma))
Z = rand(rng, Uniform(a, b), (10, 10))
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- What happens if other parts of the code also use random numbers?
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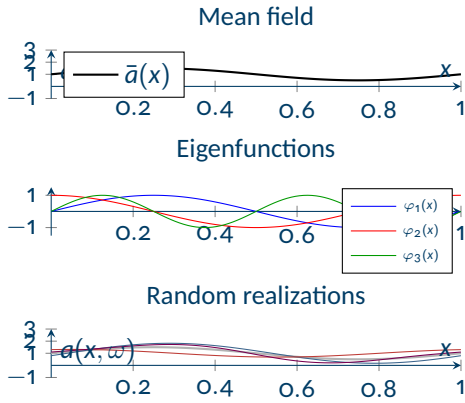
Uncertain functions: Karhunen-Loève expansion

- Sometimes uncertainty is in a *function*, not just parameters



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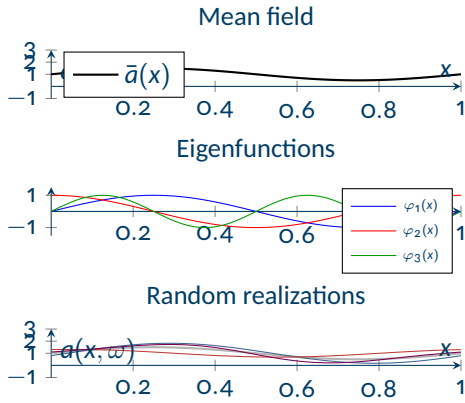

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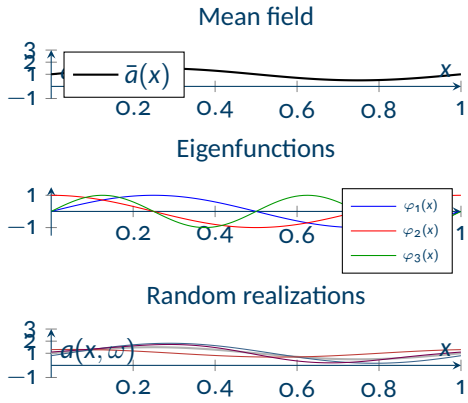

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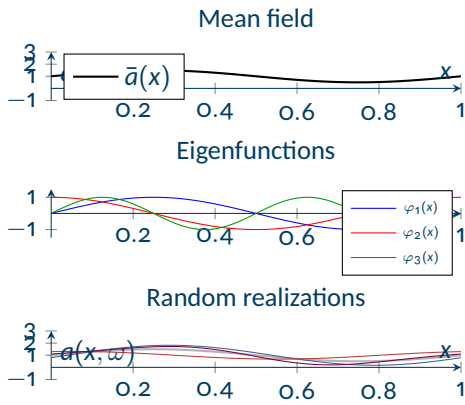

Uncertain functions: Karhunen-Loève expansion

- Sometimes uncertainty is in a *function*, not just parameters
- Example: Random field $a(x, \omega)$ for $x \in D$, $\omega \in \Omega$
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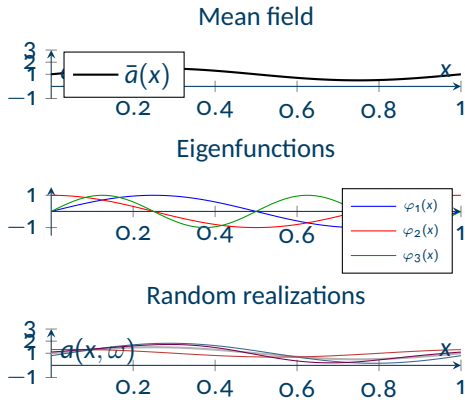

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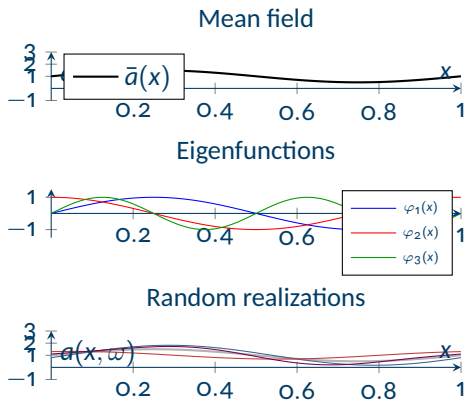

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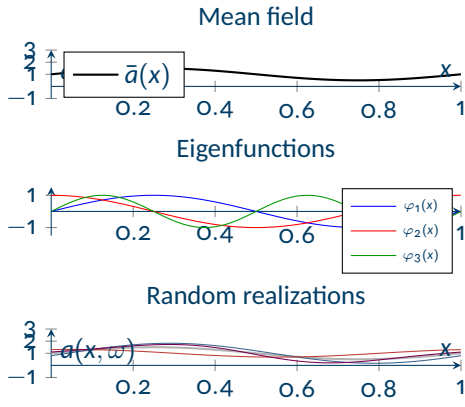

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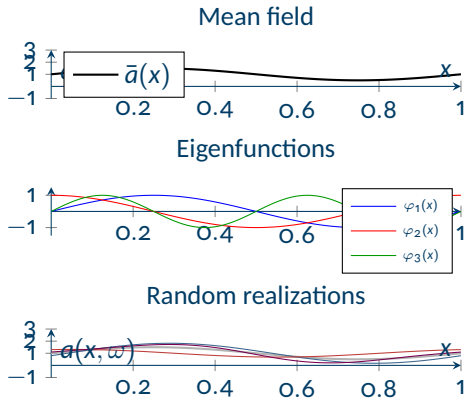

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Programming tips: Make sure you use a suitable random number generator

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- Some generators have limits on how many random numbers can be drawn
- However: Mersenne Twister has period of $2^{19937} - 1 \approx 4.3 \times 10^{6000}$

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Conclusion

- Monte Carlo

$$\mathbb{E}(Q(\mathbf{Y})) = \int_{[0,1]^d} Q(\mathbf{y})\, d\mathbf{y} \approx \frac{1}{M} \sum_{k=1}^{M} Q(\mathbf{Y}_k)$$

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- Error of Monte Carlo

$$\mathbb{E}\left(\left(\frac{1}{M} \sum_{k=1}^{M} Q(\mathbf{Y}_k) - \mathbb{E}(Q(\mathbf{Y}))\right)^2\right)^{1/2} = \frac{\mathrm{Var}(Q(\mathbf{Y}))^{1/2}}{M^{1/2}}$$

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- Motivation for the coming part: Monte Carlo is *slow*
- …but sometimes the best we have

Recap

Convergence of Monte Carlo

$$\left(\mathbb{E}\left[\mathbb{E}(X) - \frac{1}{M} \sum_{k=1}^{M} X_k \right]^2 \right)^{1/2} = \frac{\mathrm{Var}(X)^{1/2}}{M^{1/2}}$$

New notation:

$$\|f\|_{L^2(\Omega)} := \left(\mathbb{E}(f^2)\right)^{1/2}, \quad f \in L^2(\Omega)$$

Thus,

$$\left\| \mathbb{E}(X) - \frac{1}{M} \sum_{k=1}^{M} X_k \right\|_{L^2(\Omega)} = \frac{\mathrm{Var}(X)^{1/2}}{M^{1/2}}$$

Model Problem

$$\begin{cases} \dfrac{d}{dt}u(\omega;t) = F(u(\omega;t)), \\ u(\omega;0) = u_0(\omega), \end{cases}$$

Let $u_0^1, \ldots, u_0^M$ be i.i.d. samples of u_0.
Let

$$u^k_{\Delta t,T}(\omega) = F_{\Delta t,T}(\omega; u_0^k),$$

where $F_{\Delta t,T}(\omega;\cdot)$ is a numerical scheme.

Approximate:

$$\mathbb{E}(u(\cdot;T)) \approx \frac{1}{M}\sum_{k=1}^{M} u^k_{\Delta t,T}(\omega)$$

Error Estimation

Triangle inequality:

$$\left\| \mathbb{E}(u(\cdot;T)) - \frac{1}{M}\sum_{k=1}^{M} u^k_{\Delta t,T} \right\|_{L^2(\Omega)} \leq \varepsilon_1 + \varepsilon_2$$

where

$$\varepsilon_1 = \left\| \mathbb{E}(u(\cdot;T)) - \mathbb{E}(u^k_{\Delta t,T}) \right\|_{L^2(\Omega)}$$

$$\varepsilon_2 = \left\| \mathbb{E}(u^k_{\Delta t,T}) - \frac{1}{M}\sum_{k=1}^{M} u^k_{\Delta t,T} \right\|_{L^2(\Omega)}$$

Bounding the Errors

Assume

$$|u(\omega; T) - u^k_{\Delta t, T}(\omega)| \leq C\Delta t^s \quad \forall \omega \in \Omega$$

Then

$$\varepsilon_1 \leq C\Delta t^s$$

And by Monte Carlo convergence,

$$\varepsilon_2 \leq \frac{\mathrm{Var}(u_{\Delta t, T})^{1/2}}{M^{1/2}}$$

Hence,

$$\left\| \mathbb{E}(u(\cdot; T)) - \frac{1}{M} \sum_{k=1}^{M} u^k_{\Delta t, T} \right\|_{L^2(\Omega)} \leq C\Delta t^s + \frac{\mathrm{Var}(u_{\Delta t, T})^{1/2}}{M^{1/2}}$$

Equilibrating the Error

Choose

$$C\Delta t^s \approx \frac{\mathrm{Var}(u_{\Delta t,T})^{1/2}}{M^{1/2}}$$

This gives

$$M = \mathcal{O}(\Delta t^{-2s})$$

Total cost:

$$\text{Cost} = M \cdot \text{Cost per sample} = \mathcal{O}(\Delta t^{-2s}) \cdot \mathcal{O}(\Delta t^{-1}) = \mathcal{O}(\Delta t^{-(2s+1)})$$

So if we want to go from an error tolerance of ϵ to $\epsilon/2$, we need to increase the computational cost by a factor of

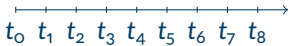
$$\left(\frac{\epsilon}{\epsilon/2}\right)^{2+\frac{1}{s}} = 2^{2+\frac{1}{s}}$$

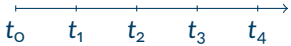
Multilevel Monte Carlo

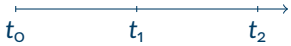
Multilevel telescoping sum

Numerical approximation u^{Δ}

Multilevel telescoping sum

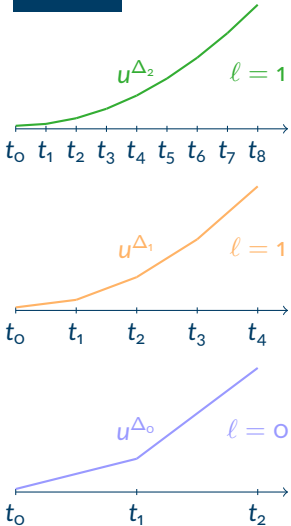






Numerical approximation u^{Δ}

Multilevel telescoping sum



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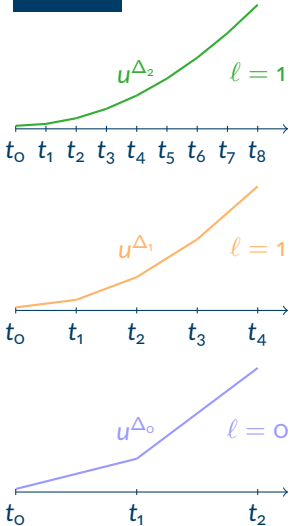

Numerical approximation u^{Δ}

$$u^{\Delta_1} = (u^{\Delta_1} - u^{\Delta_0}) + u^{\Delta_0}$$

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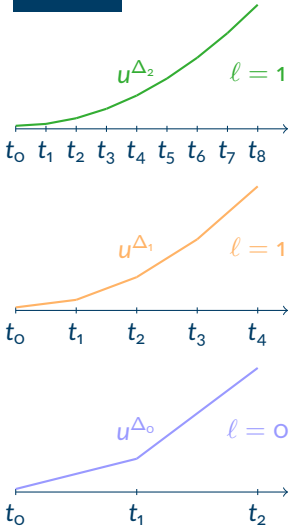

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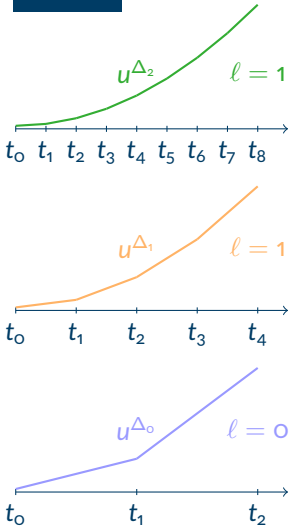

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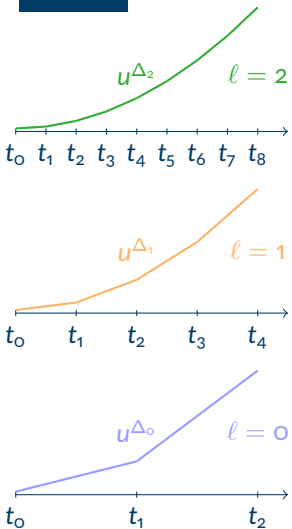

Random variable $u^{\Delta}(\omega)$

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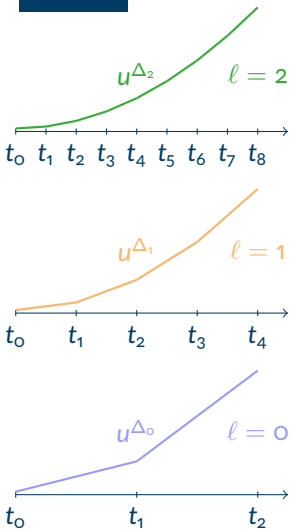

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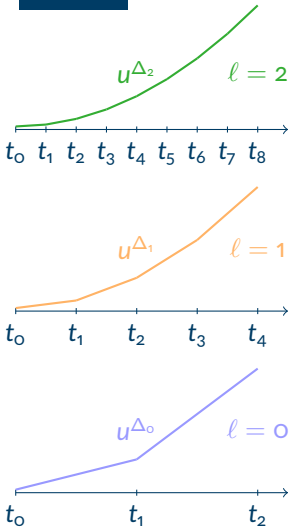

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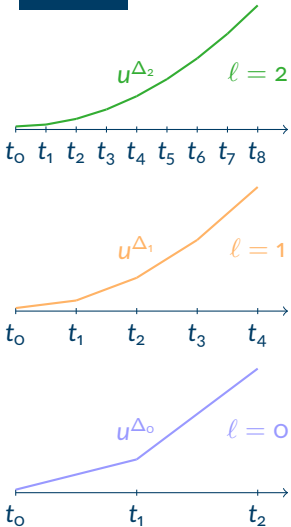

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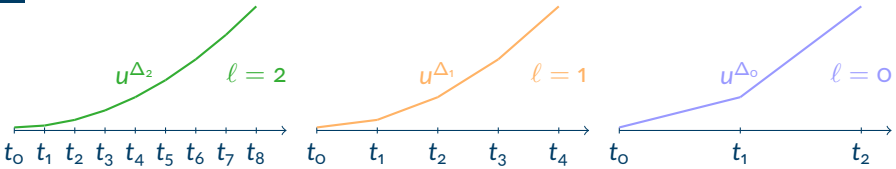
Multilevel Monte Carlo Estimator



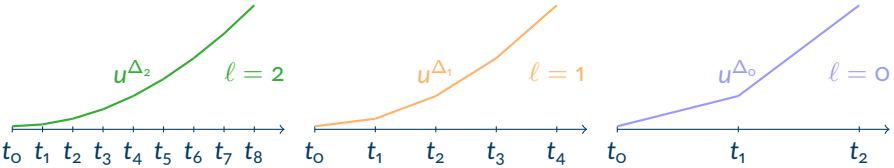
$$E_L(u) = \sum_{\ell=1}^{L} \overbrace{\frac{1}{M_\ell} \sum_{k=1}^{M_\ell} \left(u^{k,\Delta_\ell,+} - u^{k,\Delta_{\ell-1},-}\right)}^{\text{Monte Carlo estimate of } \mathbb{E}(u^{\Delta_\ell} - u^{\Delta_{\ell-1}})} + \underbrace{\frac{1}{M_0} \sum_{k=1}^{M_0} u^{k,\Delta_0}}_{\text{Monte Carlo estimate of } \mathbb{E}(u^{\Delta_0})}$$

Key idea: Use different sample sizes M_ℓ on different levels

Estimator properties:

- Unbiased: $\mathbb{E}(E_L(u)) = \mathbb{E}(u^{\Delta_L})$
- Key idea: $\mathrm{Var}(u^{\Delta_\ell} - u^{\Delta_{\ell-1}})$ decreases with ℓ
- $\Rightarrow$ can use smaller M_ℓ on finer levels

Multilevel Monte Carlo: Drawing samples



Monte Carlo estimate of $\mathbb{E}(u^{\Delta_\ell} - u^{\Delta_{\ell-1}})$

$$E_L(u) = \sum_{\ell=1}^{L} \frac{1}{M_\ell} \sum_{k=1}^{M_\ell} \left(u^{k,\Delta_\ell,+} - u^{k,\Delta_{\ell-1},-}\right) + \frac{1}{M_0} \sum_{k=1}^{M_0} u^{k,\Delta_0}$$

Monte Carlo estimate of $\mathbb{E}(u^{\Delta_0})$

$u^{k,\Delta_\ell,+}$ and $u^{k,\Delta_{\ell-1},-}$ must be computed using the **same** random input.

```
u_delta_l_plus = solve_model(random_input_k, delta_l);
u_delta_lminus = solve_model(random_input_k, delta_lminus);
```

MLMC:General observable

$$E_L(g(u)) = \sum_{\ell=1}^{L} \overbrace{\frac{1}{M_\ell} \sum_{k=1}^{M_\ell} \left(g(u^{k,\Delta_\ell,+}) - g(u^{k,\Delta_{\ell-1},-}) \right)}^{\text{Monte Carlo estimate of } \mathbb{E}(g(u^{\Delta_\ell}) - g(u^{\Delta_{\ell-1}}))} + \underbrace{\frac{1}{M_o} \sum_{k=1}^{M_o} g(u^{k,\Delta_o})}_{\text{Monte Carlo estimate of } \mathbb{E}(g(u^{\Delta_o}))}$$

Picking the numbers of samples

Error Decomposition

Error satisfies

$$\|\mathbb{E}(u) - E_L(u)\|_{L^2(\Omega)} \leq \underbrace{\|\mathbb{E}(u) - \mathbb{E}(u_{\Delta_L})\|_{L^2(\Omega)}}_{\text{Discretization error}} + \underbrace{\|E_L(u) - \mathbb{E}(u_{\Delta_L})\|_{L^2(\Omega)}}_{\text{Stochastic error}}$$

Stochastic error satisfies

$$\|E_L(u) - \mathbb{E}(u_{\Delta_L})\|_{L^2(\Omega)} \leq \sum_{\ell=1}^{L} \frac{\mathrm{Var}(u_{\Delta_\ell} - u_{\Delta_{\ell-1}})^{1/2}}{M_\ell^{1/2}} + \frac{\mathrm{Var}(u_{\Delta_0})^{1/2}}{M_0^{1/2}}$$

Picking the numbers of samples

Assume we have a target tolerance $\tau > 0$ for the stochastic error:

$$\|\mathbb{E}(u_L) - E_L(u)\|_{L^2(\Omega)} \leq \tau$$

We let V_l denote the variance at level ℓ:

$$V_l = \mathrm{Var}(u_{\Delta_\ell} - u_{\Delta_{\ell-1}}), \quad V_0 = \mathrm{Var}(u_{\Delta_0})$$

and the C_l denote the cost per sample at level ℓ:

$$C_l = \text{Cost per sample at level } \ell$$

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Then we want to solve the **optimization problem**

$$\begin{cases} \min\limits_{M_0,\ldots,M_L} \sum\limits_{\ell=0}^{L} M_\ell \cdot C_\ell \\ \text{subject to} \quad \sum\limits_{\ell=0}^{L} \dfrac{V_\ell}{M_\ell} \leq \tau^2 \end{cases}$$

Solution via Lagrange multipliers

$$\begin{cases} \min\limits_{M_0,\ldots,M_L} \sum\limits_{\ell=0}^{L} M_\ell \cdot C_\ell \\ \text{subject to} \quad \sum\limits_{\ell=0}^{L} \dfrac{V_\ell}{M_\ell} \leq \tau^2 \end{cases}$$

One can show that the solution to the optimization problem is

$$M_\ell = \left\lceil \frac{1}{\tau^2} \sqrt{\frac{V_\ell}{C_\ell}} \sum_{k=0}^{L} \sqrt{V_k C_k} \right\rceil, \quad \ell = 0, \ldots, L \tag{3.1}$$

SINTEF

Convergence rates and MLMC complexity [Giles, 2015]

Theorem

Assume

$$V_\ell \leq c_2 2^{-\beta \ell},$$

$$C_\ell \leq c_3 2^{\gamma \ell},$$

the computational cost of MLMC to achieve a root mean square error (RMSE) of τ is bounded by

$$\begin{cases} c_4 \tau^{-2}, & \beta > \gamma, \\ c_4 \tau^{-2} (\log \tau)^2, & \beta = \gamma, \\ c_4 \tau^{-2-(\gamma-\beta)/\alpha}, & \beta < \gamma. \end{cases}$$

MLMC for the projectile motion

$$C_\ell = C\Delta t_\ell^{-1} = \mathcal{O}(\text{Number of timesteps}) \qquad V_\ell = \text{Var}(u_{\Delta_\ell} - u_{\Delta_{\ell-1}}) = \mathcal{O}(\Delta t_\ell^2)$$

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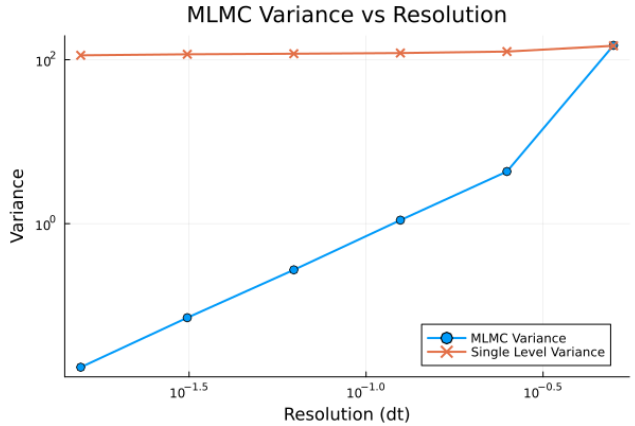
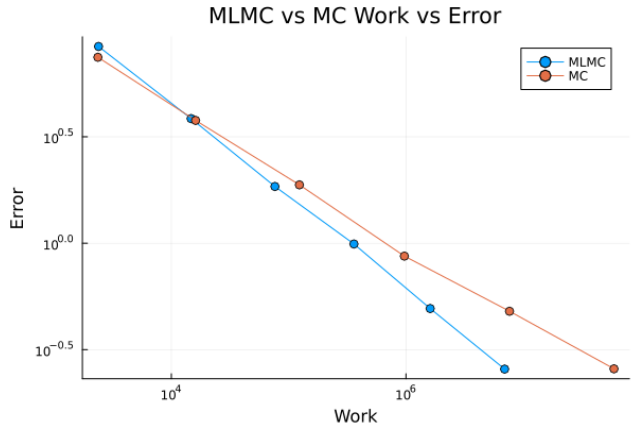


MLMC for the projectile motion: Work comparison



Pesudo-sketch for MLMC

```
function simulate_mlmc_samples(resolutions, required_samples)
    samples = []
    for (level, M) in enumerate(required_samples)
        push!(samples, [])
        for _ in 1:M
            parameters = rand(base_parameters)
            fine_solution = model(parameters; dt = timestepsizes[level])
            if level == 1
                push!(samples[level], fine_solution)
            else
                coarse_solution = model(parameters;
                    dt = timestepsizes[level-1])
                push!(samples[level], (fine_solution, coarse_solution))
            end
        end
    end
    return samples
end
```

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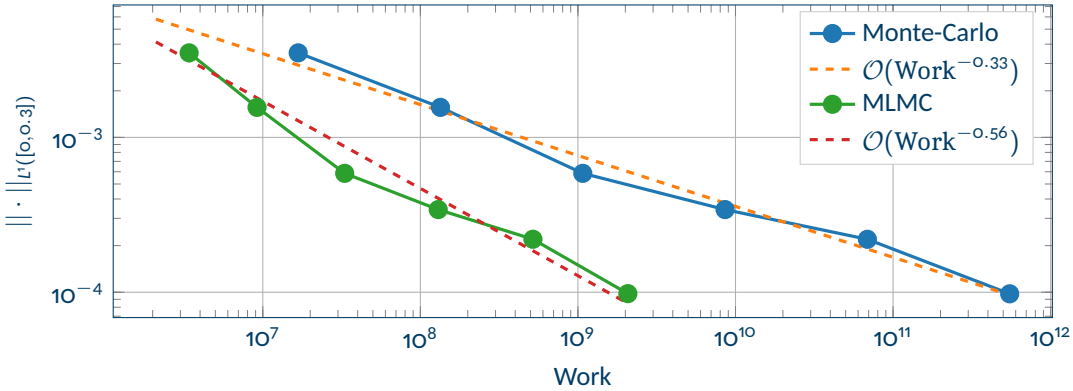
Pesudo-sketch for MLMC: Computing mean of a quantity of interest

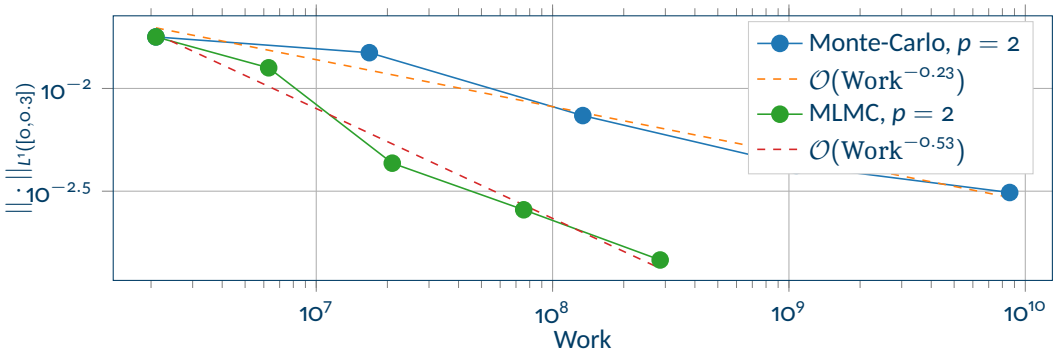
```
function mlmc_estimate(mlmc_samples, g = x -> x)
    mean_estimate = zero(typeof(g(mlmc_samples[1][1])))

    for level in 1:length(mlmc_samples)
        if level == 1
            mean_estimate += mean(g.(mlmc_samples[level]))
        else
            # last element is coarse, first is fine (only two elements per sample)
            mean_estimate += mean(g.(first.(mlmc_samples[level])) \
                                  .- g.(last.(mlmc_samples[level])))
        end
    end
    return mean_estimate
end
```

Academic examples

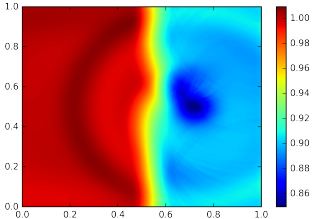
Burgers': Uncertain shock location: MLMC



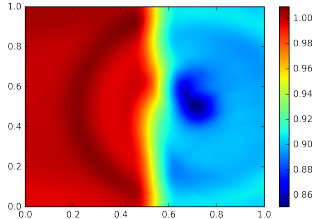
Burgers': Brownian initial data: MLMC



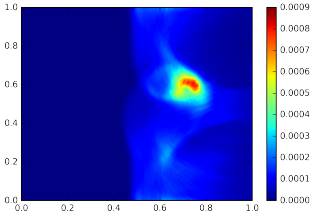
MLMC test: Shock-Vortex



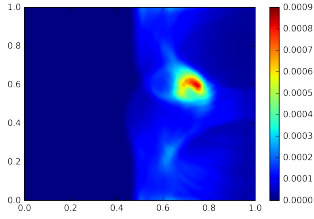
Mean, MLMC



Mean, MC



Variance, MLMC



Variance, MC

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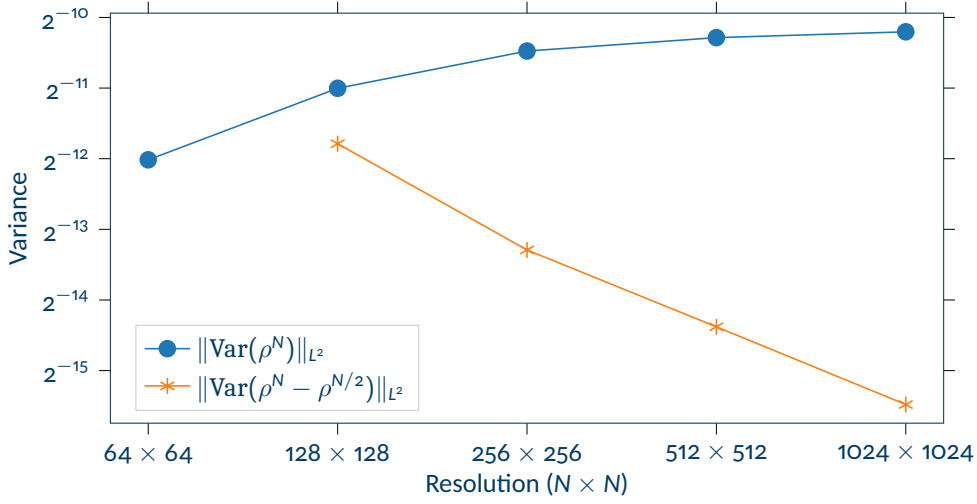
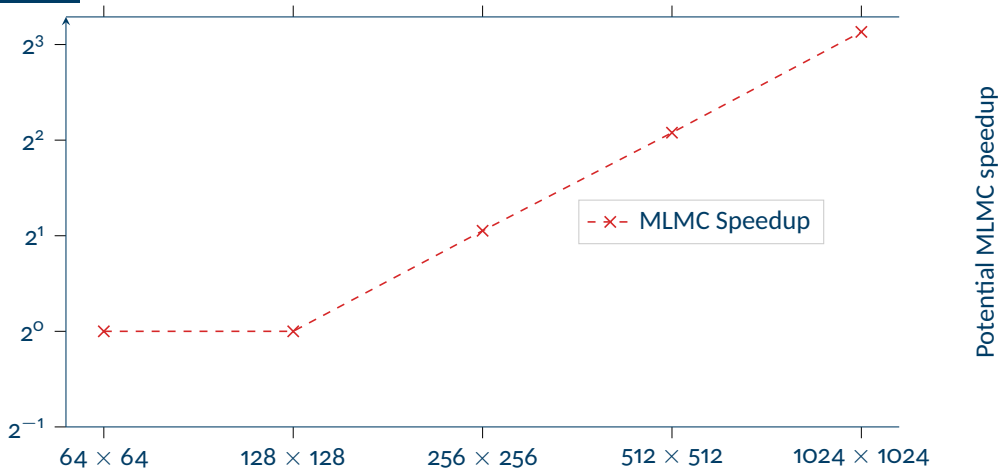
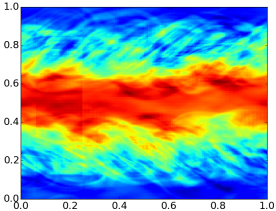
Shock-Vortex: Variance decay



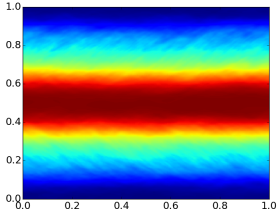
Shock-Vortex: Speedup



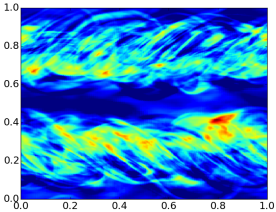
Kelvin–Helmholtz + MLMC

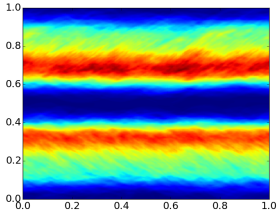


Mean, MLMC



Mean, MC





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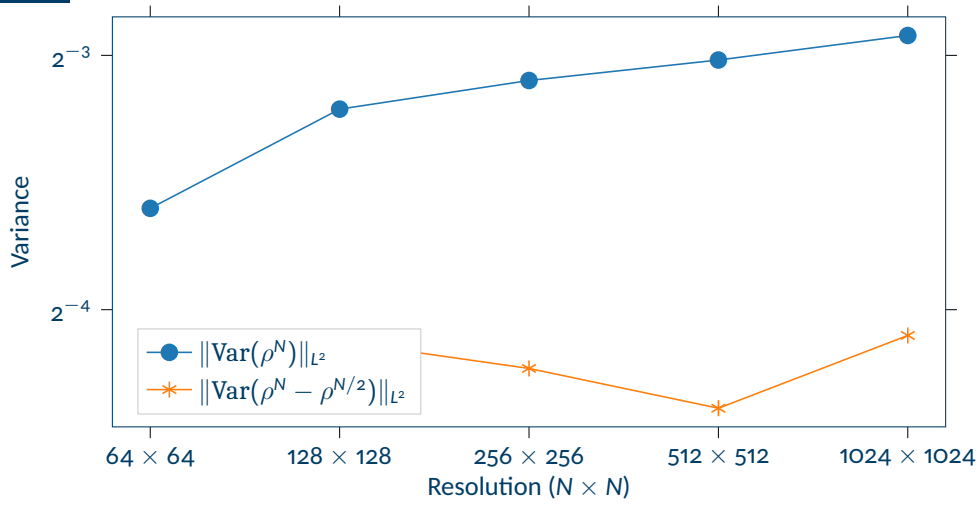
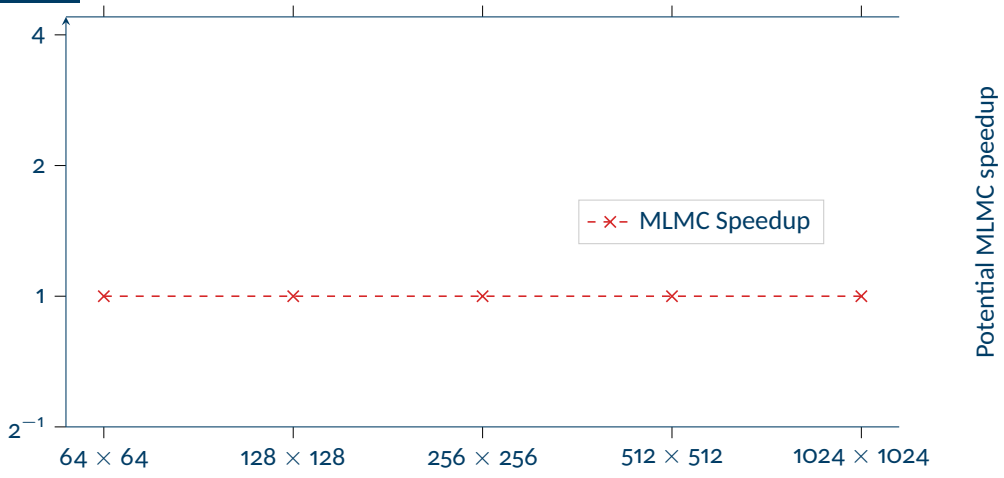
Kelvin–Helmholtz: Variance decay



Kelvin–Helmholtz: Speedup



Industrial examples

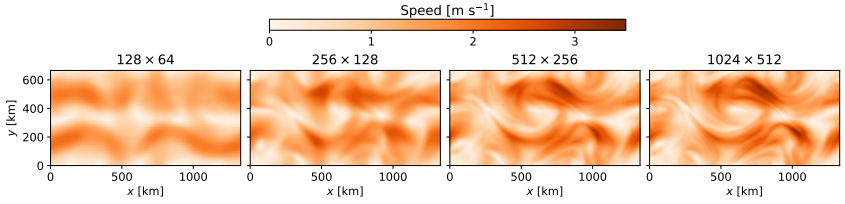
Multilevel EnKF for Shallow Water Equations (Beiser, Holm, Lye, Eidsvik, 2024)

Assimilate (synthetic) momentum observations in a 2D shallow water model:

$$\frac{\partial \eta}{\partial t} + \frac{\partial (hu)}{\partial x} + \frac{\partial (hv)}{\partial y} = 0$$

$$\frac{\partial (hu)}{\partial t} + \frac{\partial}{\partial x}\left(\frac{(hu)^2}{H+\eta} + \frac{1}{2}g(H+\eta)^2\right) + \frac{\partial}{\partial y}\left(\frac{(hu)(hv)}{H+\eta}\right) = -g(H+\eta)\frac{\partial B}{\partial x}$$

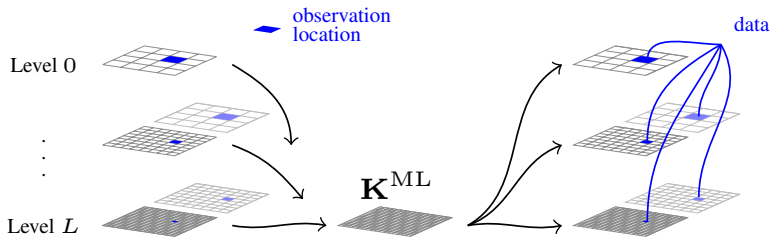
$$\frac{\partial (hv)}{\partial t} + \frac{\partial}{\partial x}\left(\frac{(hu)(hv)}{H+\eta}\right) + \frac{\partial}{\partial y}\left(\frac{(hv)^2}{H+\eta} + \frac{1}{2}g(H+\eta)^2\right) = -g(H+\eta)\frac{\partial B}{\partial y}$$



Multilevel EnKF for Shallow Water Equations (Beiser, Holm, Lye, Eidsvik, 2024)

Multi-Level Monte Carlo (MLMC) for Covariance

$$\mathbf{\Sigma}^{\mathrm{ML}}[\mathbf{x}^L, \mathbf{x}^L] = \frac{1}{N^{\mathrm{o}} - 1} \sum_{e=1}^{N^{\mathrm{o}}} \tilde{\mathbf{x}}_e^{\mathrm{o}} (\tilde{\mathbf{x}}_e^{\mathrm{o}})^\top + \sum_{l=1}^{L} \frac{1}{N^l - 1} \sum_{e=1}^{N^l} \left(\tilde{\mathbf{x}}_e^{l+} (\tilde{\mathbf{x}}_e^{l+})^\top - \tilde{\mathbf{x}}_e^{l-} (\tilde{\mathbf{x}}_e^{l-})^\top \right),$$



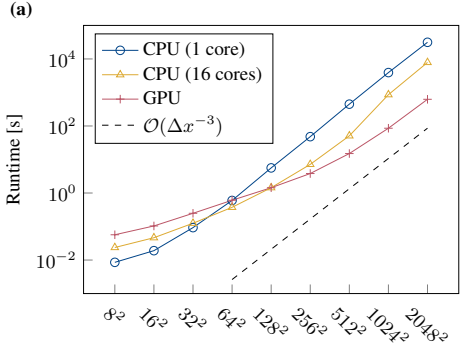
Speedup from MLMC for EnKF (SWE Model)

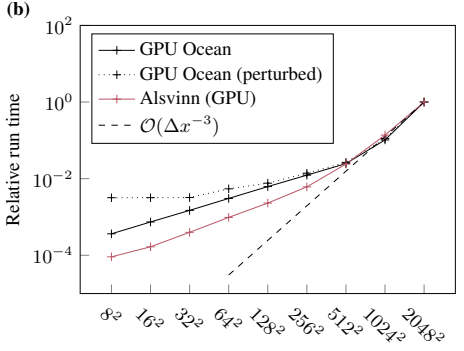
Theoretical speedup: 2.3, **practical speedup**: 1.7.

Speedup from MLMC for EnKF (SWE Model)

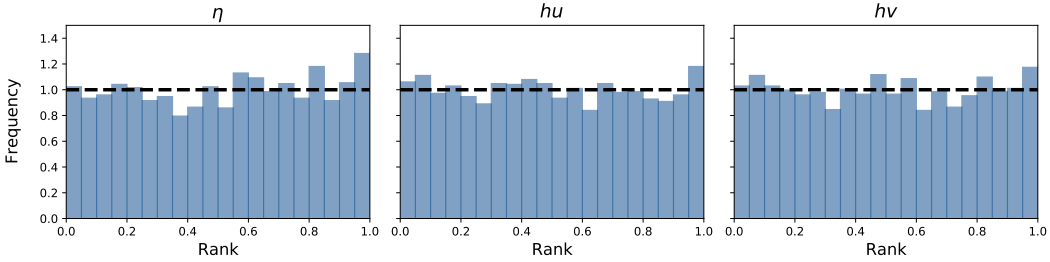
Theoretical speedup: 2.3, **practical speedup**: 1.7.

Numerical code does not always scale perfectly!





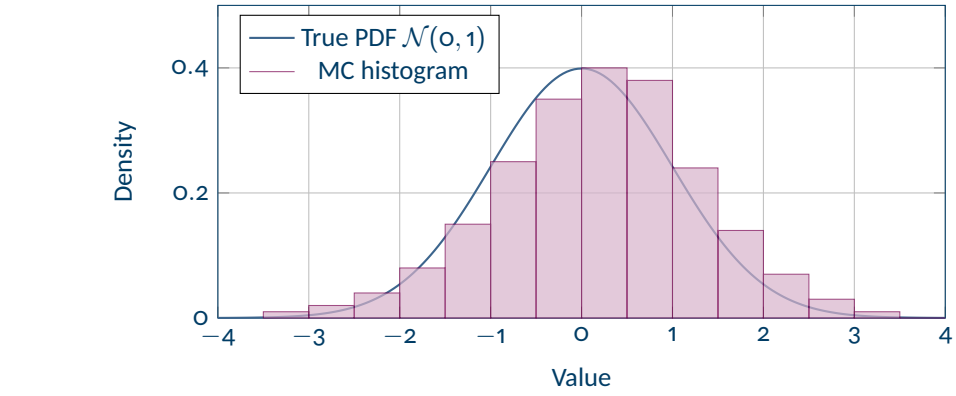
Rank Histograms (SWE Model)



Estimating probability density functions with MLMC

Probability density function and MLMC

With singlelevel Monte Carlo, the histogram approximates the PDF well:



However, with MLMC, the histogram is not easily available.

SINTEF

Orthogonal series density estimation: Estimating the PDF with MLMC

Recall:

$$E_L(g(u)) \approx \mathbb{E}(g(u)) = \int g(u) f_U(u) du$$

where $f_U(u)$ is the PDF of u.

Orthogonal series density estimation: Estimating the PDF with MLMC

Recall:

$$E_L(g(u)) \approx \mathbb{E}(g(u)) = \int g(u) f_U(u) du$$

where $f_U(u)$ is the PDF of u. Let $(\varphi_i)_{i=1}^N$ be a set of orthonormal basis functions (e.g., polynomials, wavelets, etc.). We can write

$$f_U(u) \approx \sum_{i=1}^{N} \alpha_i \varphi_i(u)$$

with coefficients

$$\alpha_i = \int \varphi_i(u) f_U(u) du = \mathbb{E}(\varphi_i(u)) \approx E_L(\varphi_i(u))$$

We can thus estimate the PDF by estimating the coefficients α_i using MLMC.

Estimating the PDF with MLMC using maximum entropy*

Let $(\varphi_i)_{i=0}^{N}$ be a set of orthonormal basis functions. Let

$$\tilde{\alpha}_i = E_L(\varphi_i(u)), \quad i = 0, \ldots, N.$$

The maximum entropy method finds the PDF $\tilde{f}_U(u)$ that maximizes the entropy by finding λ_i such that

$$\begin{cases} \tilde{f}_U(u) := \exp\left(\sum_{k=0}^{N} \tilde{\lambda}_k \varphi_k(u)\right), & \tilde{\lambda}_k \in \mathbb{R}, \\ \tilde{\alpha}_k = \int_I \varphi_k(u)\, \tilde{f}_U(u)\, du, & 0 \leq k \leq N. \end{cases}$$

then

$$\tilde{f}_U(u) = \exp\left(\sum_{k=0}^{N} \tilde{\lambda}_k \varphi_k(u)\right) \approx f_U(u)$$

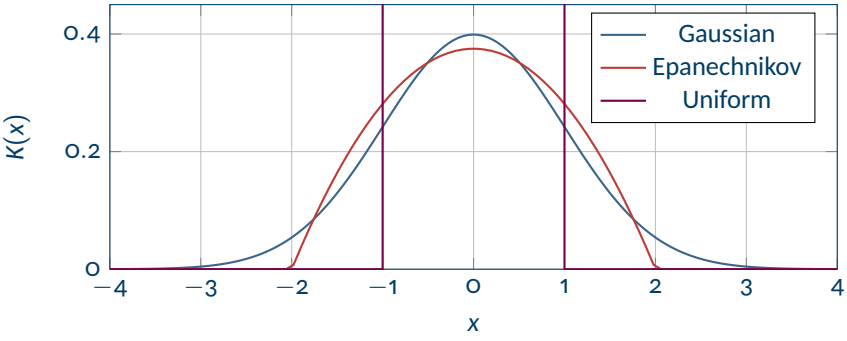
* Bierig and Chernov, 2016

Estimating the PDF with Kernel Density Estimation (KDE)

Idea: Let K_ϵ be a kernel with bandwidth $\epsilon > 0$.

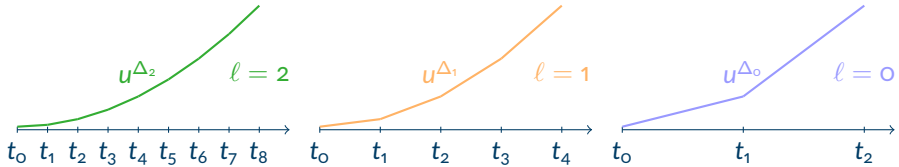
$$f_U(u) \approx \int K_\epsilon(u - v) f_U(v)\, dv = \mathbb{E}\left(K_\epsilon(u - U)\right) \approx E_L\left(K_\epsilon(u - U)\right)$$

Common kernel functions



Conclusions

- Monte Carlo is a simple and robust method for uncertainty quantification
- Monte Carlo converges slowly: error $\sim M^{-1/2}$
- Multilevel Monte Carlo can significantly reduce the computational cost
- Main motivation for Multilevel Monte Carlo: Get the same spatial accuracy at lower cost



Monte Carlo estimate of $\mathbb{E}(u^{\Delta_\ell} - u^{\Delta_{\ell-1}})$

$$E_L(u) = \sum_{\ell=1}^{L} \frac{1}{M_\ell} \sum_{k=1}^{M_\ell} \left(u^{k,\Delta_\ell,+} - u^{k,\Delta_{\ell-1},-} \right) + \underbrace{\frac{1}{M_0} \sum_{k=1}^{M_0} u^{k,\Delta_0}}_{\text{Monte Carlo estimate of } \mathbb{E}(u^{\Delta_0})}$$