UQ for high dimensional problems

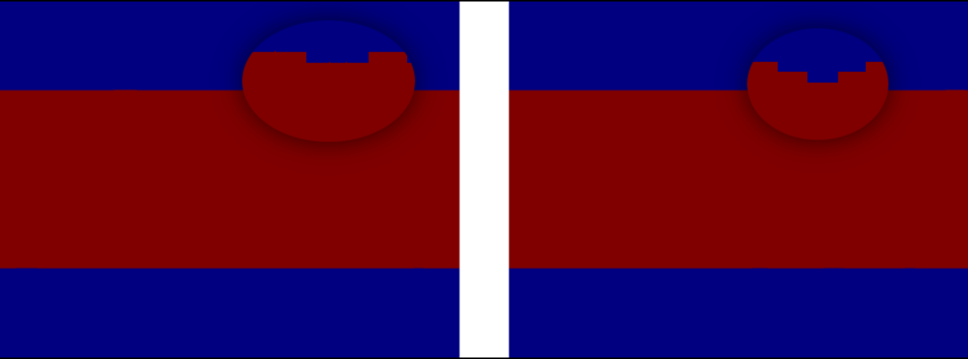
with a view towards hyperbolic conservation laws

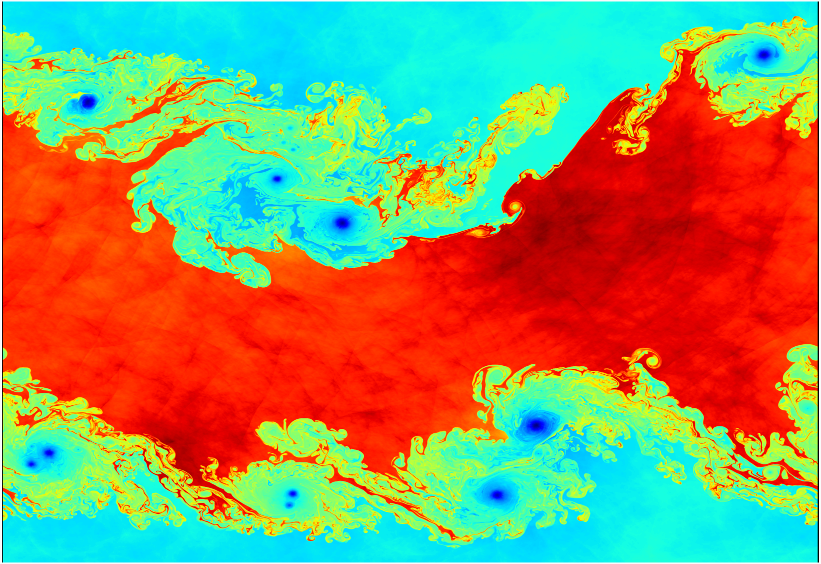
Kjetil Olsen Lye

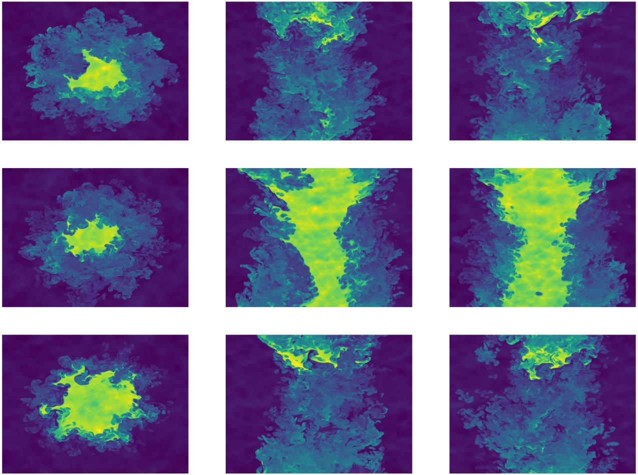
ETH Zurich

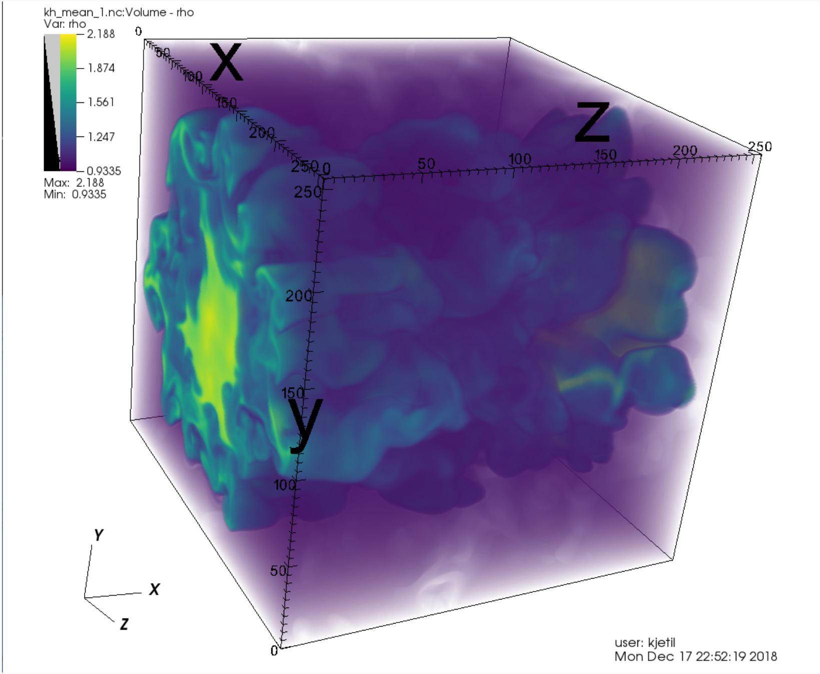
About me

- PhD student at ETH Zürich
- Research interests:
    - Non-linear hyperbolic equations
    - Uncertainty quantifications
    - (Machine learning)





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50
100
150
200
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Y
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user: kjetil
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Introduction

Uncertainty quantifications

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- PDF, CDF, ...

Focus of talk

Compute

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

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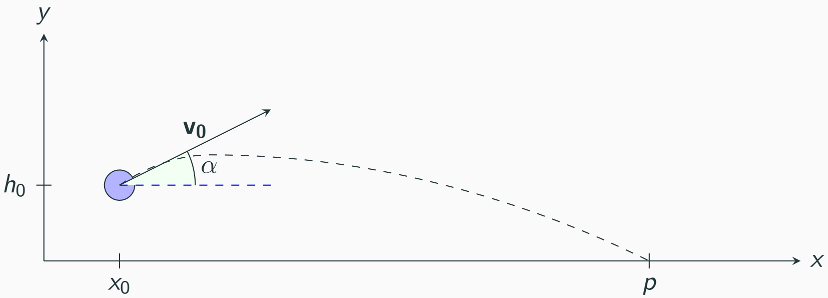
- d is large
- f could be ill-behaved (eg. discontinuous)

Example



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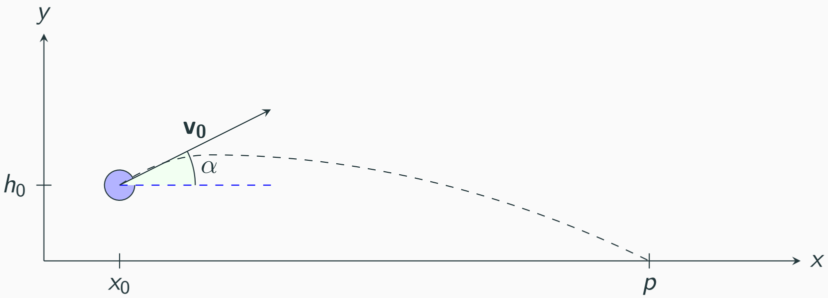

$$p(h_0) = v_0 \cos(\alpha) \frac{v_0 \sin(\alpha) + \sqrt{(v_0 \sin(\alpha))^2 + 2gh_0}}{g} + x_0$$

Interesting quantities

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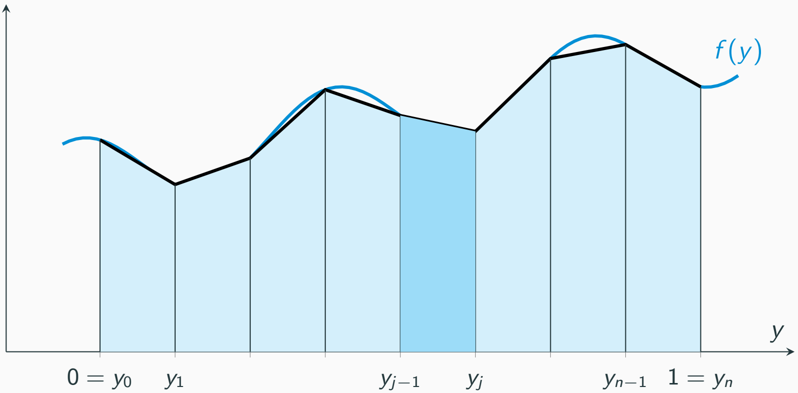
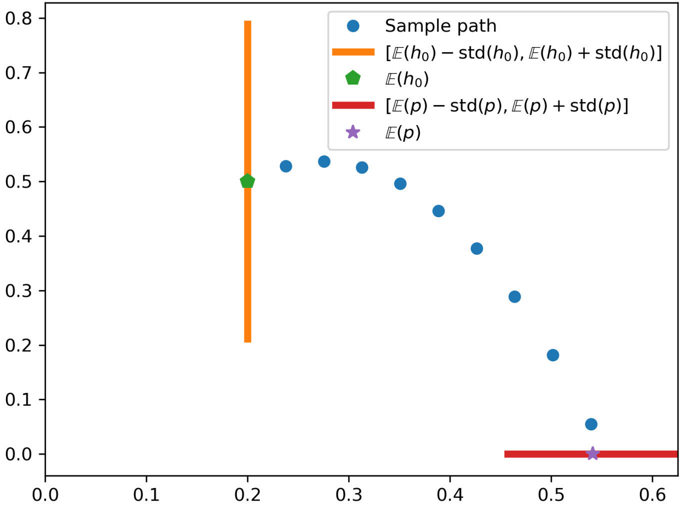
Both quantities involving the integral!

Approximate by Trapezoidal rule

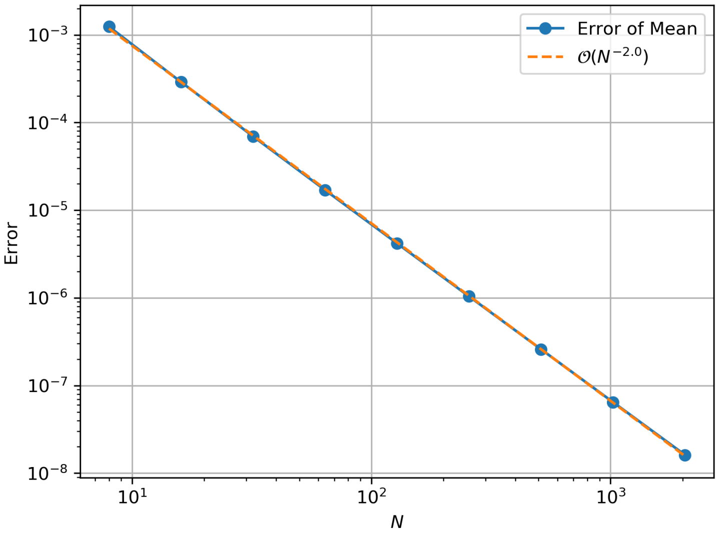
$$\int_0^1 f(y)\,dy \approx \frac{\Delta y}{2}\left(f(y_0) + 2\sum_{i=1}^{N-1} f(y_{i-1}) \cdot + f(y_N)\right)$$



Results varying initial height



Error versus number of evaluations



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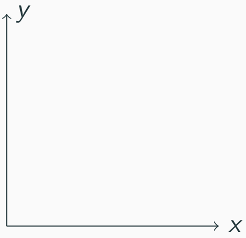
- Integration in 2D?

Trapezoidal rule for two dimensions

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



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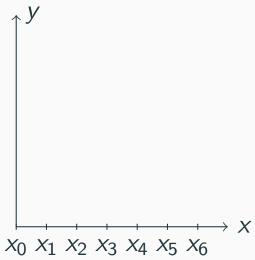

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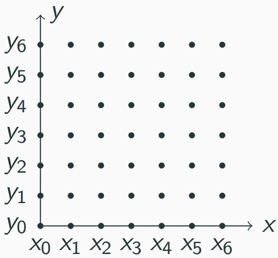
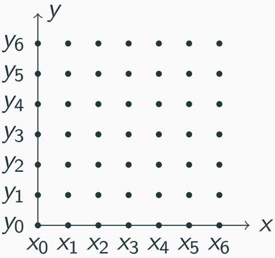
$$\approx \Big(f(0,0) + f(1,0) + f(0,1) + f(1,1) + 4\sum_{i=1}^{N-1}\sum_{i=1}^{N-1} f(x_i,y_i)$$

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



Trapezoidal rule for two dimensions

$$\int_0^1 \int_0^1 f(x,y)\,dx\,dy \approx \sum_{i=0}^{N} \sum_{j=0}^{N} w_{i,j} f(x_i, y_j)$$



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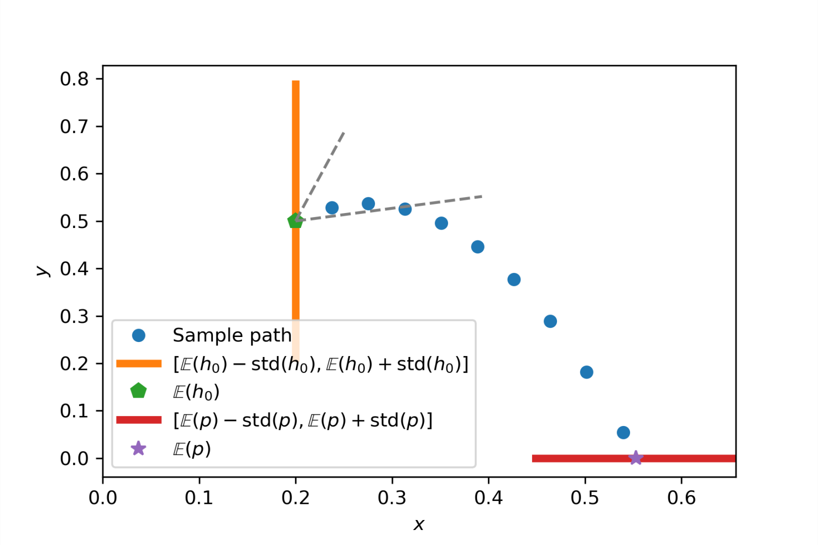

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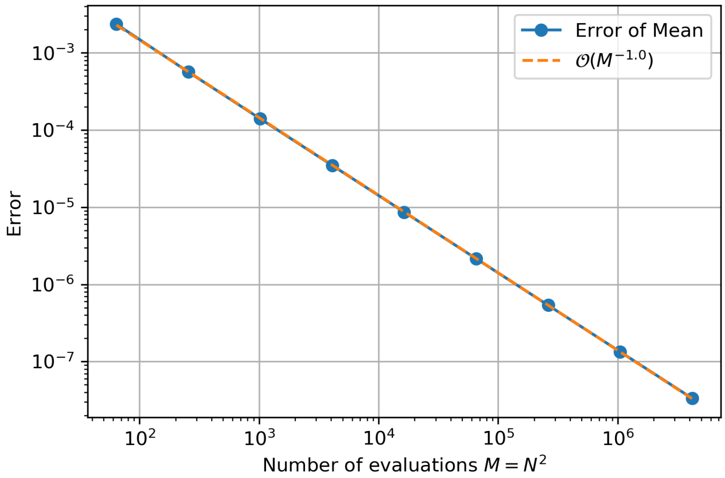

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- **Seven** parameters

Landing position depends on 7 parameters

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

How many evaluations of p do we need?

- We have 7 parameters ($d = 7$)
- Trapezoidal rule error

$$\text{Error} \leqslant Ch^2$$

Require Error $< 1/25 \approx 4\%$

- $\Rightarrow h \leqslant \sqrt{1/25} = 1/5$

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

Finding p

Governing ODE

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

Finding p

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

$$\begin{cases} \dfrac{d^2}{dt^2}\mathbf{x}(h_0, \alpha, v_0, C_D, r, \rho, m; t) = -\mathbf{F}_D(C_D, r, \rho, \dfrac{d}{dt}\mathbf{x}(\ldots; t))/m - g\mathbf{e}_2 \\ \mathbf{x}(h_0, \alpha, v_0, C_D, r, \rho, m; 0) = \begin{pmatrix} 0 \\ y_0 \end{pmatrix} \\ \dfrac{d}{dt}\mathbf{x}(h_0, \alpha, v_0, C_D, r, \rho, m; 0) = \begin{pmatrix} v_0 \cos(\alpha) \\ v_0 \sin(\alpha) \end{pmatrix} \end{cases}$$

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for $\omega \in \Omega$.

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

$$\mathbf{x}^{n,\Delta t}(\omega) = \mathbf{x}^{n-1,\Delta t}(\omega) + \Delta t \mathbf{v}^{n-1,\Delta t}(\omega)$$
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Set $p^{\Delta t}(\omega) = y^{N,\Delta t}(\omega)$.

Algorithm: Compute expected position using Trapezoidal rule

Input: $\Delta t, \Delta h_0, \Delta\alpha, \Delta v_0 \ldots$

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Then

$$E \approx \mathbb{E}(p)$$

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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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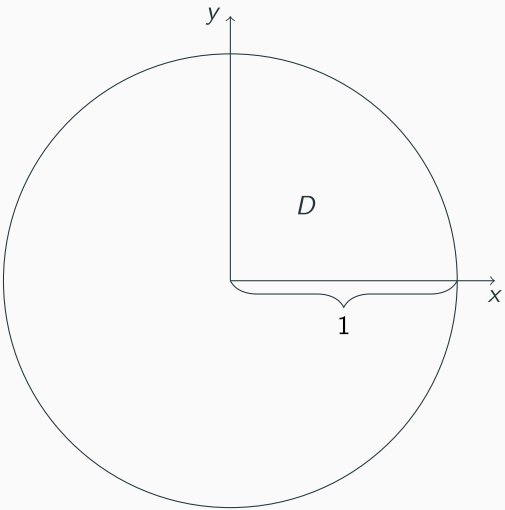
Monte Carlo methods

Obligatory example: Computing π



$$|D| = \frac{\pi}{4}$$

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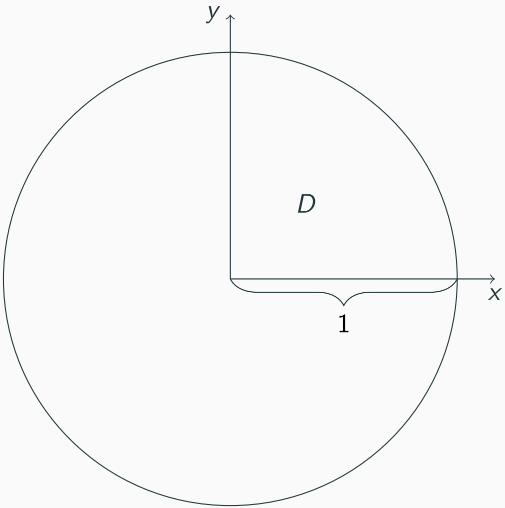

$$|D| = \frac{\pi}{4}$$

$$|D| = \int_0^1 \int_0^1 \mathbf{1}_{B(0,1)}(x, y)\, dx\, dy$$

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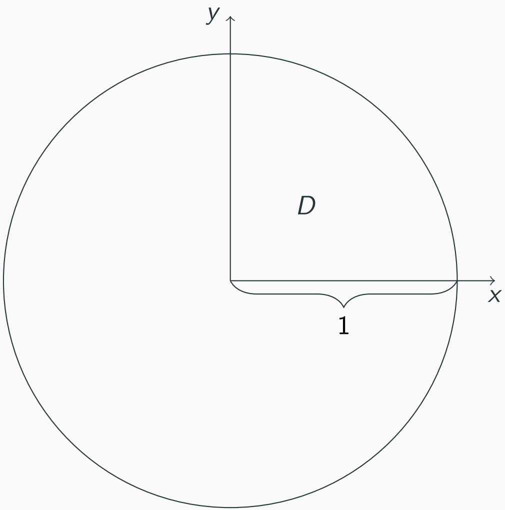

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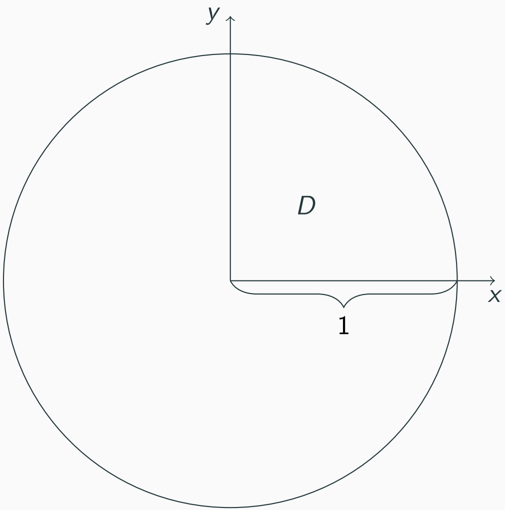

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$$\Rightarrow \pi = 4 \int_0^1 \int_0^1 \mathbf{1}_{B(0,1)}(x, y)\, dx\, dy$$

$$\approx 4 \frac{1}{M} \sum_{k=1}^{M} \mathbf{1}_{B(0,1)}(X_k, Y_k)$$

$X_k \sim \mathcal{U}[0, 1]$, $Y_k \sim \mathcal{U}[0, 1]$ independent random variables

Convergence of Monte Carlo

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

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

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

Convergence of Monte Carlo

$$\begin{aligned}
\left(\frac{1}{M}\sum_{k=1}^{M} X_k - \mathbb{E}(X)\right)^2 &= \left(\frac{1}{M}\sum_{k=1}^{M} X_k - \frac{1}{M}\sum_{k=1}^{M}\mathbb{E}(X)\right)^2 \\
&= \frac{1}{M^2}\left(\sum_{k=1}^{M}\left(X_k - \mathbb{E}(X)\right)\right)^2 \\
&= \frac{1}{M^2}\sum_{k=1}^{M}\left(X_k - \mathbb{E}(X)\right)^2 \\
&\quad + \frac{1}{M^2}\sum_{k=1}^{M}\sum_{j\neq k}\left(X_k - \mathbb{E}(X)\right)\left(X_j - \mathbb{E}(X)\right)
\end{aligned}$$

$$\left(\frac{1}{M}\sum_{k=1}^{M} X_k - \mathbb{E}(X)\right)^2 = \frac{1}{M^2}\sum_{k=1}^{M}(X_k - \mathbb{E}(X))^2 + \frac{1}{M^2}\sum_{k=1}^{M}\sum_{j\neq k}(X_k - \mathbb{E}(X))(X_j - \mathbb{E}(X))$$

Now take the expectation

$$\mathbb{E}\left(\left(\frac{1}{M}\sum_{k=1}^{M} X_k - \mathbb{E}(X)\right)^2\right) = \mathbb{E}\left(\frac{1}{M^2}\sum_{k=1}^{M}(X_k - \mathbb{E}(X))^2\right) + \frac{1}{M^2}\sum_{k=1}^{M}\sum_{j\neq k}\underbrace{\mathbb{E}\left((X_k - \mathbb{E}(X))(X_j - \mathbb{E}(X))\right)}_{=0}$$

$$\left(\frac{1}{M}\sum_{k=1}^{M} X_k - \mathbb{E}(X)\right)^2 = \frac{1}{M^2}\sum_{k=1}^{M} (X_k - \mathbb{E}(X))^2 + \frac{1}{M^2}\sum_{k=1}^{M}\sum_{j\neq k} (X_k - \mathbb{E}(X))(X_j - \mathbb{E}(X))$$

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

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&= \mathbb{E}\left(\frac{1}{M^2}\sum_{k=1}^{M}\left(X_k - \mathbb{E}(X)\right)^2\right) \\
&= \frac{1}{M}\mathrm{Var}(X)
\end{aligned}$$

Monte Carlo error

In *expectation* we converge

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

Algorithm: Using Monte Carlo for ODE

$$\begin{cases} u'(\omega; t) = F(u(\omega, t)) \\ u(\omega, 0) = u_0(\omega) \end{cases}$$

Approximate: $\mathbb{E}(u(\cdot; T))$

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    $$E = E + \frac{1}{M} u^k_{\Delta T, N}$$

Then

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

Example

See notebook

Conclusion

- Monte Carlo

$$\int_{\Omega} f(X(\omega))\, d\mathbb{P}(\omega) \approx \frac{1}{M} \sum_{k=1}^{M} f(X_k(\omega))$$

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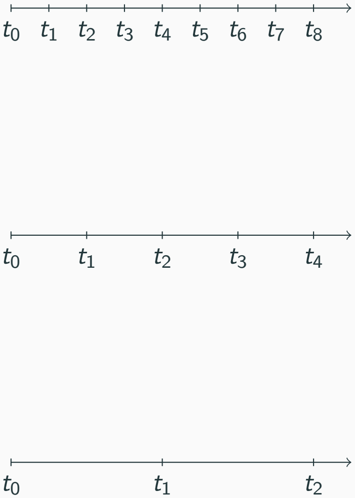
- Motivation for tomorrow: Monte Carlo is *slow*
- ... but sometimes the best we have

Multilevel Monte Carlo

Multilevel telescoping sum

Numerical approximation u^{Δ}

Multilevel telescoping sum



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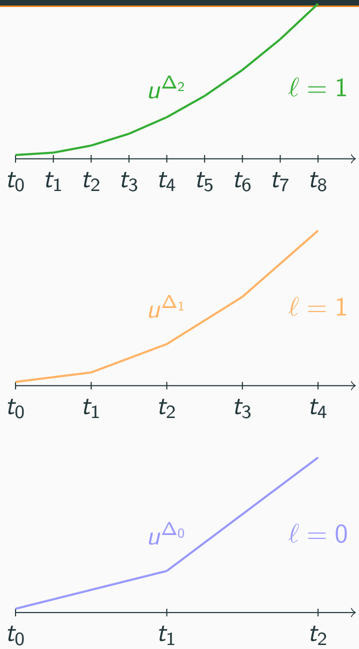

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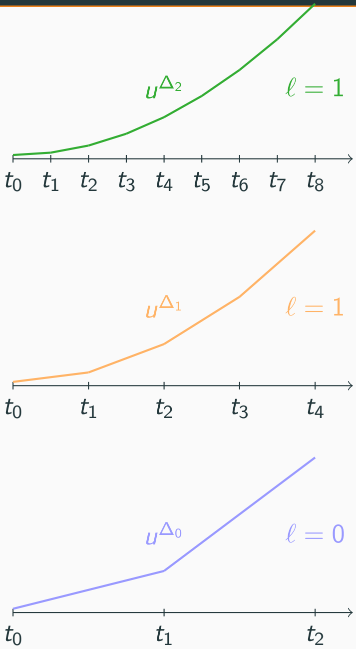
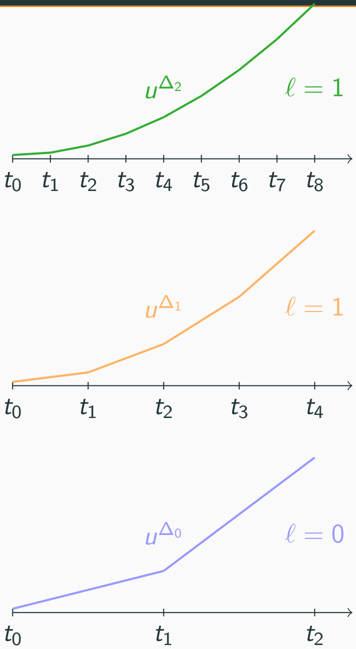


Numerical approximation u^{Δ}

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

Multilevel telescoping sum



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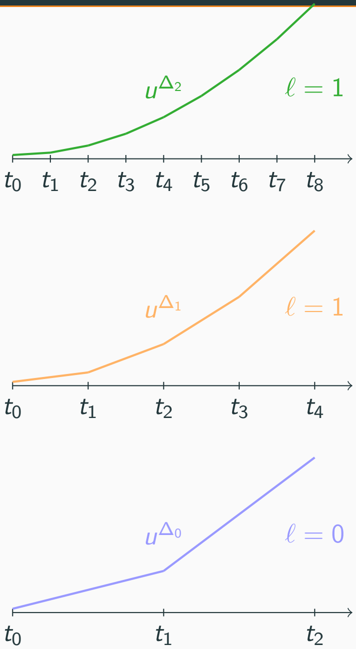

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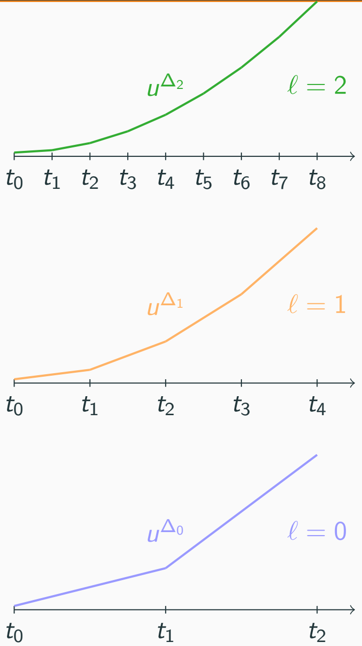
In general,

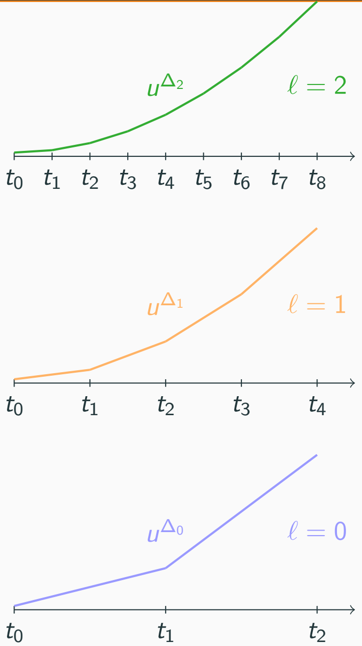
$$u^{\Delta_L} = \sum_{l=1}^{L} (u^{\Delta_\ell} - u^{\Delta_{\ell-1}}) + u^{\Delta_0}$$

Multilevel Monte Carlo [Giles, 2008; Heinrich 2001]



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

Multilevel Monte Carlo [Giles, 2008; Heinrich 2001]



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

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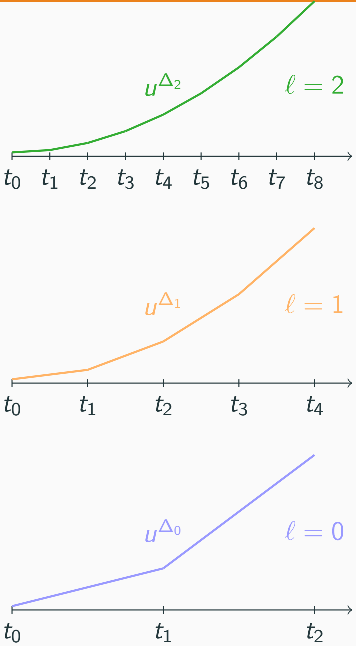

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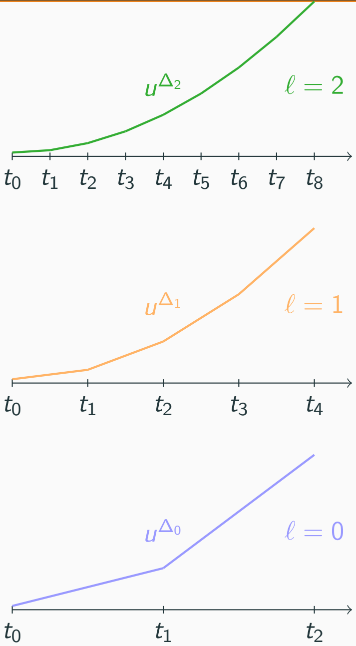

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$$\mathbb{E}(u^{\Delta_1}) = \mathbb{E}(u^{\Delta_1} - u^{\Delta_0}) + \mathbb{E}(u^{\Delta_0})$$

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$$\approx \underbrace{\frac{1}{M_1} \sum_{k=1}^{M_1} \left(u_k^{\Delta_1} - u_k^{\Delta_0} \right)}_{\approx \mathbb{E}(u^{\Delta_1} - u^{\Delta_0})} + \underbrace{\frac{1}{M_0} \sum_{k=1}^{M_0} u_k^{\Delta_0}}_{\approx \mathbb{E}(u^{\Delta_0})}$$

Variance reduction

$$\begin{aligned}
\mathbb{E}(u^{\Delta_1}) &= \mathbb{E}(u^{\Delta_1} - u^{\Delta_0}) + \mathbb{E}(u^{\Delta_0}) \\
&\approx \underbrace{\frac{1}{M_1}\sum_{k=1}^{M_1}\left(u_k^{\Delta_1} - u_k^{\Delta_0}\right)}_{\approx \mathbb{E}(u^{\Delta_1} - u^{\Delta_0})} + \underbrace{\frac{1}{M_0}\sum_{k=1}^{M_0} u_k^{\Delta_0}}_{\approx \mathbb{E}(u^{\Delta_0})} \\
&=: E_{M_0,M_1}(u)
\end{aligned}$$

Error

$$\begin{aligned}
\mathbb{E}\left(\left(E_{M_0,M_1}(u) - \mathbb{E}(u^{\Delta_1})\right)^2\right)^{1/2} &= \mathbb{E}\left(\left(E_{M_0,M_1}(u) - \left(\mathbb{E}(u^{\Delta_1} - u^{\Delta_0}) + \mathbb{E}(u^{\Delta_0})\right)\right)^2\right) \\
&\quad + \mathbb{E}\left(\left(E_{M_0,M_1}(u^{\Delta_0}, u^{\Delta_1}) - \mathbb{E}(u^{\Delta_1})\right)^2\right)^{1/2}
\end{aligned}$$

$$\frac{\mathrm{Var}(X)^{1/2}}{M^{1/2}}$$