3.36pt

Advanced Simulation - Lecture 1

George Deligiannidis

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Lecture 1

- First half of course: GD, second half: Lawrence Murray
- Website: www.stats.ox.ac.uk/~deligian/sc5.html
- Email: deligian@stats.ox.ac.uk
- Lectures: Mondays 10-11 & Wednesdays 14-15, weeks 1-8, LG01.
- Classes:

Undergraduate: Thursdays 10-11 LG04, weeks 3-8; MSc: Thursdays 11-11 LG03, weeks 4, 5, 7, 8.

- Class tutors:
 - G. Deligiannidis first half, Lawrence Murray second half.
- Hand in solutions by Tuesday, 1pm at the Adv. Simulation tray.

- Solutions of many scientific problems involve intractable high-dimensional integrals.
- Standard deterministic numerical integration deteriorates rapidly with dimension.
- Monte Carlo methods are stochastic numerical methods to approximate high-dimensional integrals.
- Main application in this course: Bayesian statistics.
- Other applications: statistical/quantum physics, econometrics, ecology, epidemiology, finance, signal processing, weather forecasting...
- More than 2,000,000 results for "Monte Carlo" in Google Scholar.

• For
$$f : \mathbb{X} \to \mathbb{R}$$
, let
$$I = \int_{\mathbb{X}} f(x) \, dx.$$

• When X = [0, 1], then we can simply approximate *I* through

$$\widehat{I}_n = \frac{1}{n} \sum_{i=0}^{n-1} f\left(\frac{i+1/2}{n}\right).$$

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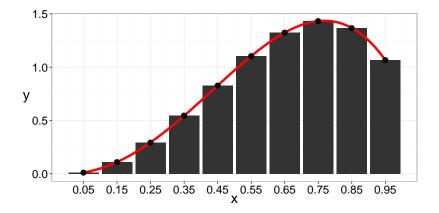


Figure: Riemann sum approximation (black rectangles) of the integral of *f* (red curve).

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Error of naive numerical integration in 1D

■ Naively, for a small interval $[a, a + \varepsilon]$ approximate

•

$$\int_{a}^{a+\varepsilon} f(x) \mathrm{d}x \approx \varepsilon \times f(a).$$

Error bounded above by

$$\left| \int_{a}^{a+\varepsilon} f(x) dx - \varepsilon \times f(a) \right| = \left| \int_{a}^{a+\varepsilon} [f(x) - f(a)] dx \right|$$

$$\leq \int_{a}^{a+\varepsilon} \int_{y=a}^{x} |f'(y)| dy \, dx \leq \sup_{x \in [0,1]} |f'(x)| \frac{\varepsilon^{2}}{2}.$$

■ If sup_{*x*∈[0,1]} |*f*′(*x*)| < *M*, the uniform grid with *n* points gives approximation error at most

$$Mn \times \frac{1}{n^2} = \mathcal{O}(1/n).$$

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Computing High-Dimensional Integrals

• For
$$\mathbb{X} = [0,1] \times [0,1]$$
 using $n = m^2$ evaluations
 $\widehat{I}_n = \frac{1}{m^2} \sum_{i=0}^{m-1} \sum_{j=0}^{m-1} f\left(\frac{i+1/2}{m}, \frac{j+1/2}{m}\right)$

the same calculation shows that the approximation error is

$$Mm^2 \times \frac{1}{m^3} = \mathcal{O}(1/m) = \mathcal{O}\left(n^{-1/2}\right).$$

• Generally for $\mathbb{X} = [0, 1]^d$ we have an approximation error in

$$\mathcal{O}\left(n^{-1/d}\right).$$

- So-called "curse of dimensionality".
- Other integration rules(e.g. Simpson's) also degrade as d increases.

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Monte Carlo Integration

• For $f : \mathbb{X} \to \mathbb{R}$, write

$$I = \int_{\mathbb{X}} f(x) \, dx = \int_{\mathbb{X}} \varphi(x) \pi(x) dx.$$

where π is a probability density function on X and

$$\varphi: x \mapsto f(x) / \pi(x).$$

- Monte Carlo method: sample $X_1, \ldots, X_n \stackrel{\text{i.i.d.}}{\sim} \pi$,
 - compute

$$\widehat{I}_n = \frac{1}{n} \sum_{i=1}^n \varphi(X_i).$$

- Strong law of large numbers: $\widehat{I}_n \to I$ almost surely;
- Central limit theorem: the random approximation error is

$$\mathcal{O}(n^{-1/2})$$

whatever the dimension of the state space X.

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Monte Carlo Integration

Monte Carlo Integration

In many cases the integral of interest is in the form

$$I = \int_{\mathbb{X}} \varphi(x) \pi(x) dx = \mathbb{E}_{\pi} \left[\varphi(X) \right],$$

for a specific function φ and distribution π .

- The distribution π is often called the "target distribution".
- Monte Carlo approach relies on independent copies of

 $X \sim \pi$.

Hence the following relationship between integrals and sampling:

Monte Carlo method to approximate $\mathbb{E}_{\pi} [\varphi(X)]$ \Leftrightarrow simulation method to sample π

Thus Monte Carlo sometimes refer to simulation methods.

Monte Carlo Integration

Ising Model

- Consider a simple 2D-Ising model on a finite lattice
 G = {1,2,...,m} × {1,2,...,m} where each site σ = (i, j) hosts a particle with a +1 or -1 spin modeled as a r.v. X_σ.
- The distribution of $X = \{X_{\sigma}\}_{\sigma \in \mathcal{G}}$ on $\{-1, 1\}^{m^2}$ is given by

$$\pi_{\beta}(x) = \frac{\exp\left(-\beta U\left(x\right)\right)}{Z_{\beta}}$$

where $\beta > 0$ is called the inverse temperature and the potential energy is

$$U(x) = J \sum_{\sigma \sim \sigma'} x_{\sigma} x_{\sigma'}.$$

- Physicists are interested in computing $\mathbb{E}_{\pi_{\beta}}[U(X)]$ and Z_{β} .
- The dimension is m^2 , where *m* can easily be 10^3 .

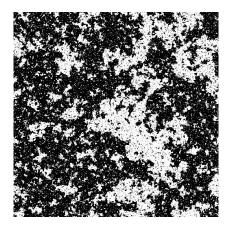


Figure: One draw from the Ising model on a 500 \times 500 lattice.

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- Let S(t) denote the price of a stock at time t.
- European option: grants the holder the right to buy the stock at a fixed price *K* at a fixed time *T* in the future; the current time being *t* = 0.
- At time *T* the holder achieves a payoff of

$$\max\{S_T-K,0\}.$$

• With interest rate r, the expected discounted value at t = 0 is

$$\exp\left(-rT\right)\mathbb{E}\left[\max\left(0,S\left(T\right)-K\right)\right].$$

- If we knew explicitly the distribution of S(T) then $\mathbb{E}[\max(0, S(T) K)]$ is a low-dimensional integral.
- **Problem**: We only have access to a complex stochastic model for $\{S(t)\}_{t \in \mathbb{N}}$

$$S(t+1) = g(S(t), W(t+1))$$

= g(g(S(t-1), W(t)), W(t+1))
=: g^{t+1}(S(0), W(1), ..., W(t+1))

where $\{W(t)\}_{t \in \mathbb{N}}$ is a sequence of random variables and *g* is a known function.

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The price of the option involves an integral over the *T* latent variables

 $\left\{W\left(t\right)\right\}_{t=1}^{T}.$

- Assume these are independent with probability density function *p*_W.
- We can write

$$\mathbb{E}\left[\max\left(0, S\left(T\right) - K\right)\right]$$

= $\int \max\left[0, g^{T}\left(s\left(0\right), w\left(1\right), ..., w\left(T\right)\right) - K\right]$
 $\times \left\{\prod_{t=1}^{T} p_{W}\left(w\left(t\right)\right)\right\} dw\left(1\right) \cdots dw\left(T\right),$

a high-dimensional integral.

- Given $\theta \in \Theta$, we assume that *Y* follows a probability density function $p_Y(y; \theta)$.
- Having observed Y = y, we want to perform inference about θ .
- In the frequentist approach θ is unknown but fixed; inference in this context can be performed based on

 $\ell(\theta) = \log p_{Y}(y;\theta).$

 In the Bayesian approach, the unknown parameter is regarded as a random variable θ and assigned a prior p_θ (θ).

- Probabilities refer to limiting relative frequencies. They are (supposed to be) objective properties of the real world.
- Parameters are fixed unknown constants. Because they are not random, we cannot make any probability statements about parameters.
- Statistical procedures should have well-defined long-run properties. For example, a 95% confidence interval should include the true value of the parameter with limiting frequency at least 95%.

- Probability describes degrees of subjective belief, not limiting frequency.
- We can make probability statements about parameters, e.g.

 $\mathbb{P}\left(\theta \in \left[-1,1\right] \mid Y = y\right)$

- Observations produce a new probability distribution for the parameter, the posterior.
- Point estimates and interval estimates may then be extracted from this distribution.

Bayesian inference relies on the *posterior*

$$p_{\vartheta|Y}(\theta|y) = \frac{p_{Y}(y;\theta) p_{\vartheta}(\theta)}{p_{Y}(y)}$$

where

$$p_{Y}(y) = \int_{\Theta} p_{Y}(y;\theta) p_{\vartheta}(\theta) d\theta$$

is the so-called *marginal likelihood* or *evidence*.

Point estimates, e.g. posterior mean of ϑ

$$\mathbb{E}\left(\vartheta|y\right) = \int_{\Theta} \theta \, p_{\vartheta|Y}\left(\theta|y\right) \mathrm{d}\theta$$

can be computed.

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• Credible intervals: an interval *C* such that

 $\mathbb{P}\left(\vartheta\in C|\,y\right)=1-\alpha.$

Assume the observations are independent given θ = θ then the predictive density of a new observation Y_{new} having observed Y = y is

$$p_{Y_{new}|Y}(y_{new}|y) = \int_{\Theta} p_{Y}(y_{new};\theta) p_{\vartheta|Y}(\theta|y) d\theta$$

 Above predictive density takes into account the *uncertainty about the parameter* θ.

Compare to simple plug-in rule $p_Y(y_{new}; \hat{\theta})$ where $\hat{\theta}$ is a point estimate of θ (e.g. the MLE).

Bayesian Inference: Gaussian Data

- Let $Y = (Y_1, ..., Y_n)$ be i.i.d. random variables with $Y_i \sim \mathcal{N}(\theta, \sigma^2)$ with σ^2 known and θ unknown.
- Assign a prior distribution on the parameter: $\vartheta \sim \mathcal{N}(\mu, \kappa^2)$, then one can check that

$$p(\theta|y) = \mathcal{N}(\theta; \nu, \omega^2)$$

where

$$\omega^2 = \frac{\kappa^2 \sigma^2}{n\kappa^2 + \sigma^2}, \ \nu = \frac{\sigma^2}{n\kappa^2 + \sigma^2} \mu + \frac{n\kappa^2}{n\kappa^2 + \sigma^2} \overline{y}.$$

• Thus $\mathbb{E}(\vartheta|y) = \nu$ and $\mathbb{V}(\vartheta|y) = \omega^2$.

If
$$C := (\nu - \Phi^{-1} (1 - \alpha/2) \omega, \nu + \Phi^{-1} (1 - \alpha/2) \omega)$$
, then
 $\mathbb{P} (\vartheta \in C | y) = 1 - \alpha.$

• If $Y_{n+1} \sim \mathcal{N}(\theta, \sigma^2)$ then

$$p(y_{n+1}|y) = \int_{\Theta} p(y_{n+1}|\theta) p(\theta|y) d\theta = \mathcal{N}(y_{n+1};\nu,\omega^2 + \sigma^2).$$

 No need to do Monte Carlo approximations: the prior is conjugate for the model.

Bayesian Inference: Logistic Regression

• Let $(x_i, Y_i) \in \mathbb{R}^d \times \{0, 1\}$ where $x_i \in \mathbb{R}^d$ is a covariate and

$$\mathbb{P}\left(\left.Y_{i}=1\right|\theta\right)=\frac{1}{1+e^{-\theta^{T}x_{i}}}$$

Assign a prior $p(\theta)$ on ϑ . Then Bayesian inference relies on

$$p\left(\theta | y_{1},...,y_{n}\right) = \frac{p\left(\theta\right)\prod_{i=1}^{n} \mathbb{P}\left(Y_{i} = y_{i} | \theta\right)}{\mathbb{P}\left(y_{1},...,y_{n}\right)}$$

■ If the prior is Gaussian, the posterior is not a standard distribution: $\mathbb{P}(y_1, ..., y_n)$ cannot be computed.

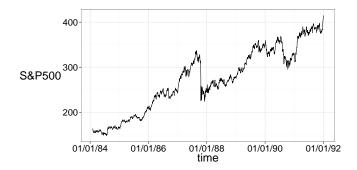


Figure: S&P 500 daily price index (p_t) between 1984 and 1991.

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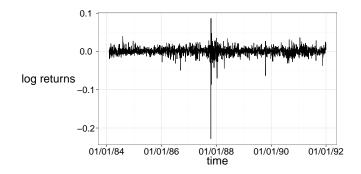


Figure: Daily returns $y_t = \log(p_t/p_{t-1})$ between 1984 and 1991.

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Bayesian Inference: Stochastic Volatility Model

• Latent stochastic volatility $(X_t)_{t \ge 1}$ of an asset is modeled through

$$X_{t} = \varphi X_{t-1} + \sigma V_{t}, \ Y_{t} = \beta \exp\left(X_{t}\right) W_{t}$$

where $V_t, W_t \sim \mathcal{N}(0, 1)$.

- Intuitively, log-returns are modeled as centered Gaussians with dependent variances.
- Popular alternative to ARCH and GARCH models (Engle, 2003 Nobel Prize).
- Estimate the parameters (φ, σ, β) given the observations.
- Estimate X_t given $Y_1, ..., Y_t$ on-line based on $p(x_t | y_1, ..., y_t)$.
- No analytical solution available!