Monte Carlo and Empirical Methods for Stochastic Inference (MASM11/FMS091)

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Lecture 3
Importance sampling
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Last time: MC output analysis

- We used the CLT

$$\sqrt{N}\,(\tau_N - \tau) \xrightarrow{\text{d.}} \mathcal{N}(0, \sigma^2(\phi))$$

to target τ by the approximate two-sided confidence interval

$$\left(\tau_N - \lambda_{\alpha/2}\frac{\sigma(\phi)}{\sqrt{N}}, \tau_N + \lambda_{\alpha/2}\frac{\sigma(\phi)}{\sqrt{N}}\right).$$

- In addition, we discussed how to estimate $\varphi(\tau)$ for some function $\varphi : \mathbb{R} \to \mathbb{R}$ having at hand an estimator τ_N of τ. If $\varphi \in \mathcal{C}^1$ one may prove the CLT

$$\sqrt{N}\,(\varphi(\tau_N) - \varphi(\tau)) \xrightarrow{\text{d.}} \mathcal{N}(0, \varphi'(\tau)^2\sigma^2(\phi)).$$

Consequently, the natural estimator $\varphi(\tau_N)$ works fine, at least asymptotically (but suffers in general from bias for finite N's).

Example: Buffon's needle

Consider a a wooden floor with parallel boards of width d on which we randomly drop a needle of length ℓ, with $\ell \leq d$. Let

$$\begin{cases} X = \text{distance from the lower needlepoint to the upper board edge line,} \\ \theta = \text{angle between the needle and the board edge normal.} \end{cases}$$

Then

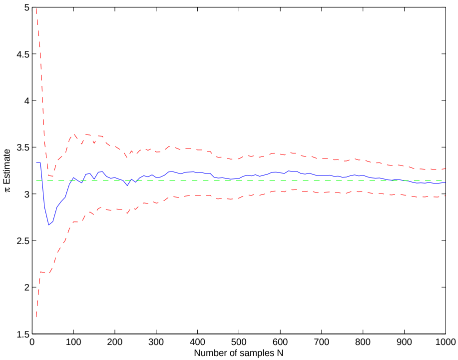
$$\tau = \mathbb{P}\,(\text{needle intersects board edge}) = \mathbb{P}(X \leq \ell \cos\theta) = \ldots = \frac{2\ell}{\pi d}.$$

or, equivalently,

$$\pi = \frac{2\ell}{\tau d}.$$

Example: Buffon's needle (cont.)

Since $\tau = \mathbb{P}(\text{needle intersects board edge}) = \mathbb{E}(\mathbb{1}_{\{X \leq \ell \cos\theta\}})$ can be easily estimated by means of MC, an approximation of $\pi = \varphi(\tau) = 2\ell/(\tau d)$ can be obtained via the delta method:



Last time: pseudo-random number generation

- We discussed (briefly) how to generate pseudo-random, uniformly distributed numbers (U_n) using the linear congruential generator

$$U_n = (a \cdot U_{n-1} + c) \mod m.$$

- Having at hand such $\mathcal{U}(0,1)$-distributed numbers U, we also looked at how to generate random numbers X from an arbitrary distribution F by means of the inversion method, i.e., by letting

$$X = F^{\leftarrow}(U) = \inf\{x \in \mathbb{R} : F(x) \geq U\}.$$

Conditional methods

Let f be a multivariate density on $\mathbb{R}^d$. By decomposing f into conditional densities according to

$$f(x_1, \ldots, x_d) = f(x_1) \prod_{\ell=2}^{d} f(x_\ell | x_1, \ldots, x_{\ell-1}),$$

the problem of sampling from a multivariate density can be reduced to that of sampling from several univariate densities:

draw $X_1 \sim f(x_1)$
for $\ell = 2 \to d$ **do**
  draw $X_\ell \sim f(x_\ell | X_1, \ldots, X_{\ell-1})$
end for
return $X = (X_1, \ldots, X_d)$

Trivially, the resulting draw X has the correct distribution f. This method presumes that the conditional densities are easily obtained, which is not always the case.

Rejection sampling

- In many cases we do not know the inverse of F or not even the normalizing constant of the density f. However, if g is another density such that $f(x) \leq Kg(x)$ for all $x \in \mathbb{R}^d$ and some constant $1 \leq K < \infty$, we may use rejection sampling:

  repeat

  draw $X^* \sim g$

  draw $U \sim \mathcal{U}(0, 1)$

  until $U \leq \frac{f(X^*)}{Kg(X^*)}$

  $X \leftarrow X^*$

  return X

Rejection sampling (cont)

Theorem (Rejection sampling)

The output X of the rejection sampling algorithm is a random variable with density function f. Moreover, the expected number of trials needed before acceptance is K.

Example

We wish to simulate $f(x) = \exp(\cos^2(x))/c$, $x \in (-\pi/2, \pi/2)$, where $c = \int_{-\pi/2}^{\pi/2} \exp(\cos^2(z))\,\mathrm{d}z = \pi e^{1/2} I_o(1/2)$ is the normalizing constant.

However, since for all $x \in (-\pi/2, \pi/2)$,

$$f(x) = \frac{\exp(\cos^2(x))}{c} \leq \frac{e}{c} = \underbrace{\frac{e\pi}{c}}_{K} \times \underbrace{\frac{1}{\pi}}_{g},$$

where g is the density of $\mathcal{U}(-\pi/2, \pi/2)$, we may use rejection sampling where a candidate $X^* \sim \mathcal{U}(-\pi/2, \pi/2)$ is accepted if

$$U \leq \frac{f(X^*)}{Kg(X^*)} = \frac{\exp(\cos^2(X^*))/c}{e/c} = \exp(\cos^2(X^*) - 1).$$

```
prob = @(x) exp((cos(x))^2 - 1);
trial = 1;
accepted = false;
while ~accepted,
    Xcand = - pi/2 + pi*rand;
    if rand < prob(Xcand),
        accepted = true;
        X = Xcand;
    else
    trial = trial + 1;
    end
end
```

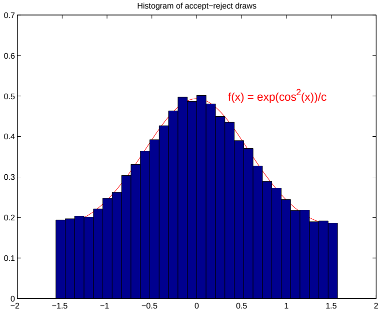


Figure: Plot of a histogram of $20{,}000$ accept-reject draws together with the true density. The average number of trials was $1.5555 (\approx K = e^{1/2}/I_0(1/2) \approx 1.5503)$.

Plan of today's lecture

1. Importance sampling (IS)
2. Self-normalized IS
3. Home assignment 1 (HA1)

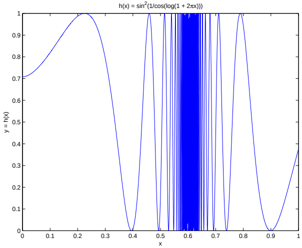
We are here $\longrightarrow \bullet$

1. Importance sampling (IS)
2. Self-normalized IS
3. Home assignment 1 (HA1)

Advantages of the MC method

The MC method

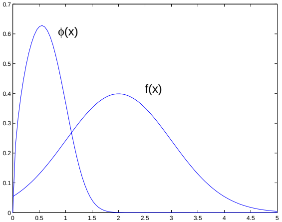
- is more efficient than deterministic methods in high dimensions,
- does in general not require knowledge of the normalizing constant of a density for computing expectations, and
- handles efficiently “strange” integrands that may cause problems for deterministic methods.



Problems with MC integration

OK, MC integration looks promising. We may however run into problems if

- it is hard to sample from f or
- if the integrand ϕ and the density f are dissimilar; in this case we will end up with a lot of draws where the integrand is small, and consequently only a few draws will contribute to the estimate. This gives a large variance.



These problems can often be solved using importance sampling.

Importance sampling (IS, Ch. 6.4.1)

The basis of importance sampling is to take an instrumental density g on X such that $g(x) = 0 \Rightarrow f(x) = 0$ and rewrite the integral as

$$\begin{aligned}\tau = \mathbb{E}_f\left(\phi(X)\right) &= \int_{\mathsf{X}} \phi(x) f(x)\,\mathrm{d}x = \int_{f(x)>0} \phi(x) f(x)\,\mathrm{d}x \\ &= \int_{g(x)>0} \phi(x) \frac{f(x)}{g(x)} g(x)\,\mathrm{d}x = \mathbb{E}_g\left(\phi(X)\frac{f(X)}{g(X)}\right) = \mathbb{E}_g\left(\phi(X)\omega(X)\right),\end{aligned}$$

where

$$\omega : \{x \in \mathsf{X} : g(x) > 0\} \ni x \mapsto \frac{f(x)}{g(x)}$$

is the so-called importance weight function.

Importance sampling (IS, Ch. 6.4.1) (Generalization)

The basis of importance sampling is to take an instrumental density g on X such that $g(x) = 0 \Rightarrow \phi(x) f(x) = 0$ and rewrite the integral as

$$\tau = \mathbb{E}_f\left(\phi(X)\right) = \int_{\mathsf{X}} \phi(x) f(x)\,\mathrm{d}x = \int_{|\phi(x)|f(x)>0} \phi(x) f(x)\,\mathrm{d}x$$
$$= \int_{g(x)>0} \phi(x) \frac{f(x)}{g(x)} g(x)\,\mathrm{d}x = \mathbb{E}_g\left(\phi(X)\frac{f(X)}{g(X)}\right) = \mathbb{E}_g\left(\phi(X)\omega(X)\right),$$

where

$$\omega : \{x \in \mathsf{X} : g(x) > 0\} \ni x \mapsto \frac{f(x)}{g(x)}$$

is the so-called importance weight function.

Importance sampling (cont.)

We may now estimate $\tau = \mathbb{E}_g(\phi(X)\omega(X))$ using standard MC:

for $i = 1 \to N$ **do**
  draw $X_i \sim g$
end for
set $\tau_N \leftarrow \sum_{i=1}^{N} \phi(X_i)\omega(X_i)/N$
return τ_N

Here, trivially,

$$\mathbb{V}(\tau_N) = \frac{1}{N}\mathbb{V}_g(\phi(X)\omega(X))$$

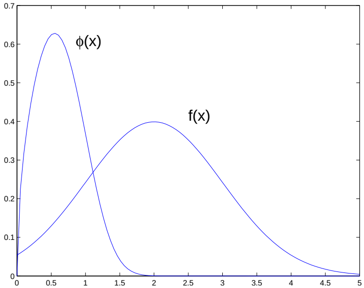
and we should thus aim at choosing g so that the function $x \mapsto \phi(x)\omega(x)$ is close to constant in the support of g. This gives a minimal variance.

Example: A tricky normal expectation

Let X have $\mathcal{N}(2,1)$ distribution and try to compute

$$\tau = \mathbb{E}\left(\mathbb{1}_{X\geq 0}\sqrt{X}\exp(-X^3)\right) = \int \underbrace{\mathbb{1}_{x\geq 0}\sqrt{x}\exp(-x^3)}_{=\phi(x)}\underbrace{\mathcal{N}(x;2,1)}_{=f(x)}\,\mathrm{d}x,$$

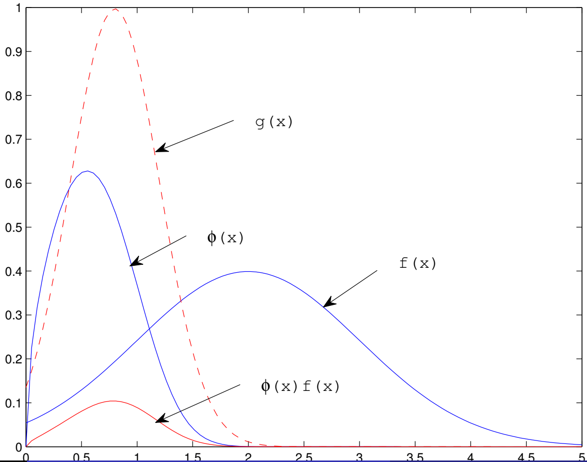
where $\mathcal{N}(x;\mu,\sigma^2)$ denotes the density of the normal distribution.



Here the support of f is significantly larger than that of ϕ.

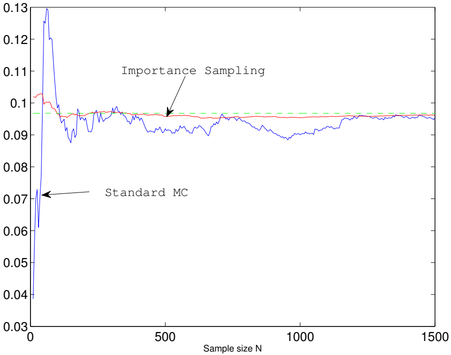
Example: A tricky normal expectation (cont.)

Thus, standard MC will lead to a waste of computational power. Better is to use IS with g being a scale-location-transformed normal-distribution:



Example: A tricky normal expectation (cont.)

```
phi = @(x) (x >= 0).*sqrt(x).*exp(- x.^3);
mu = 0.8;
sigma = 0.4;
omega = @(x) normpdf(x,2,1)./normpdf(x,mu,sigma);
X = sigma*randn(1,N)+mu;
tau = mean(phi(X).*omega(X));
```



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Self-normalized IS (Ch. 6.4.1)

Often $f(x)$ is known only up to a normalizing constant $c > 0$, i.e. $f(x) = z(x)/c$, where we can evaluate $z(x) = cf(x)$ but not $f(x)$. Then, as before,

$$\tau = \mathbb{E}_f(\phi(X)) = \int_{\mathsf{X}} \phi(x) f(x)\,\mathrm{d}x = \frac{c\int_{f(x)>0} \phi(x) f(x)\,\mathrm{d}x}{c\int_{f(x)>0} f(x)\,\mathrm{d}x}$$

$$= \frac{\int_{g(x)>0} \phi(x) \frac{cf(x)}{g(x)} g(x)\,\mathrm{d}x}{\int_{g(x)>0} \frac{cf(x)}{g(x)} g(x)\,\mathrm{d}x} = \frac{\int_{g(x)>0} \phi(x) \frac{z(x)}{g(x)} g(x)\,\mathrm{d}x}{\int_{g(x)>0} \frac{z(x)}{g(x)} g(x)\,\mathrm{d}x}$$

$$= \frac{\int_{g(x)>0} \phi(x)\omega(x) g(x)\,\mathrm{d}x}{\int_{g(x)>0} \omega(x) g(x)\,\mathrm{d}x} = \frac{\mathbb{E}_g(\phi(X)\omega(X))}{\mathbb{E}_g(\omega(X))},$$

where we are able to evaluate

$$\omega : \{x \in \mathsf{X} : g(x) > 0\} \ni x \mapsto \frac{z(x)}{g(x)}.$$

Self-normalized IS (cont.)

Thus, having generated a sample $X_1, \ldots, X_N$ from g we may estimate the numerator $\mathbb{E}_g(\phi(X)\omega(X))$ as well as the denominator $\mathbb{E}_g(\omega(X))$ using standard MC:

$$\tau = \frac{\mathbb{E}_g(\phi(X)\omega(X))}{\mathbb{E}_g(\omega(X))}$$

$$\approx \frac{\frac{1}{N}\sum_{i=1}^{N} \phi(X_i)\omega(X_i)}{\frac{1}{N}\sum_{\ell=1}^{N} \omega(X_\ell)} = \sum_{i=1}^{N} \underbrace{\frac{\omega(X_i)}{\sum_{\ell=1}^{N} \omega(X_\ell)}}_{\text{normalized weight}} \phi(X_i).$$

Note that the denominator yields an estimate of the normalizing constant c:

$$c = \mathbb{E}_g(\omega(X)) \approx \frac{1}{N}\sum_{\ell=1}^{N} \omega(X_\ell).$$

Example

We reconsider the density

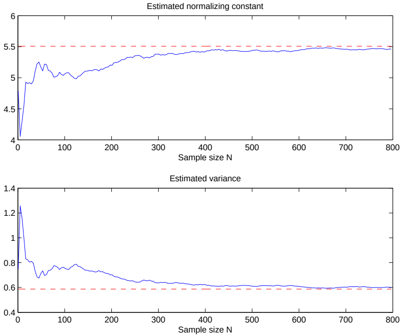
$$f(x) = \exp(\cos^2(x))/c, \quad x \in (-\pi/2, \pi/2),$$

treated last time and estimate its variance as well as the normalizing constant $c > 0$ using self-normalized IS.

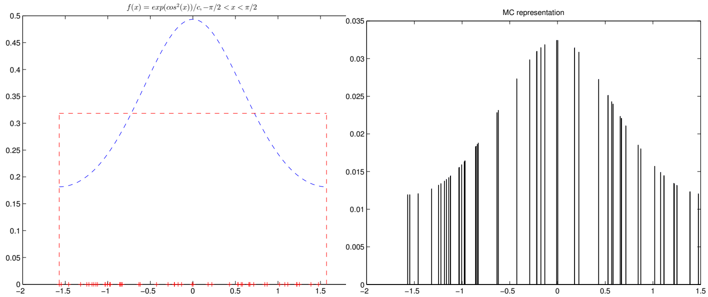
Let the instrumental distribution g be the uniform distribution $\mathcal{U}(-\pi/2, \pi/2)$.

Example (cont.)

```
z = @(x) exp(cos(x).^2);
X = - pi/2 + pi*rand(1,N);
omega = @(x) pi*z(x);
tau = cumsum(X.^2.*omega(X))./cumsum(omega(X));
c = cumsum(omega(X))./(1:N);
subplot(2,1,1);
plot(1:N,c);
subplot(2,1,2);
plot(1:N,tau);
```



The weighted sample $(X_i, \omega(X_i))$ can be viewed as an MC representation of the target distribution f.



$$f(x) \quad \stackrel{\text{IS}}{\Rightarrow} \quad (X_i, \omega(X_i))$$

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HA1: Simulation and Monte Carlo integration

HA1 comprises

- one question on random number generation and
- two larger questions on IS (one- and two-dimensional problems) containing
- two sub questions (2(b) and (d)) on variance reduction (which we will discuss next time).

Submission:

- A written report in PDF format (*No* MS Word-files).
- Upload in CANVAS HA1 before Tuesday 8 Feb, 13:00:00. The uploaded files should include the report file as well as *all* your m-files with a file `proj1.m` that runs your analysis.
- Late submissions do not qualify for marks higher than 3.

Instructions on report writing

- Explain carefully all introduced notation: $X =?$.
- Describe/explain the model.
- The text should be readable without access to the Matlab code; write plain text instead of including Matlab code in the report.
- Include your solutions in the text; do not write "calculations of ? can be found in the matlab code", or similar.
- When referring to the lecture notes or the book, be specific (i.e. refer to Chapter/which lecture).
- Refer to your figures in the text. Explain colors etc. in the figure captions (a figure caption is almost never too long).
- Write clear motivations and discussions when it concerns choice of instrumental distributions etc.