Simulation Based Inference (Part I)

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Outline

Motivation

Monte Carlo

Important Sampling

Conclusion

▶ In statistics, direct calculation of the moments of a random variable is usually not feasible.

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- ▶ Applied widely in finance and financial econometrics.
- Sometimes are time consuming. C/C++, MATLAB call C, or R call C have to be used.

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Sometimes we can but most of times we can't get this done analytically.

If we can decompose f(x) = h(x)p(x), where p(x) is a simple probability density function (pdf), then we have

$$\int_a^b f(x)dx = \int_a^b h(x)p(x)dx = \mathbf{E}_{p(x)}[h(x)]$$

Why MC Works? Law of Large Numbers (LLN)

► Given an independent and identically distributed (iid) sequence of randome variables $Y_1, Y_2, ..., Y_n$ with $\bar{Y}_n = n^{-1} \sum_{i=1}^n Y_i$ and $E(Y_i) = \mu$, then for any $\epsilon > 0$ we have

$$P(|\bar{Y}_n - \mu| > \epsilon) \to 0$$

as $n \to \infty$.

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▶ According to LLN, as $n \to \infty$, \bar{Y}_n will close to μ , and the approximation will be more accurate.

MC for integral

▶ If we can generate a random sample $\{x_1, ..., x_n\}$ from p(x), then

$$\int_{a}^{b} f(x)dx = \int_{a}^{b} h(x)p(x)dx = E_{p(x)}[h(x)] \approx \frac{1}{n} \sum_{i=1}^{n} h(x_{i})$$

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A simple case. Integrating a function of f(x) over [a, b] is nothing else than computing the mean of f(x) assuming that $x \sim U[0, 1]$, then

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► If we can simulate a random variable *X* over many times from its distribution, we will know almost everything about *X*.

► In Bayesian inference, MC integration can be used to approximate posterior distribution

$$I(y) = \int_a^b f(y|x)p(x)dx \approx \hat{I}(y) = \frac{1}{n} \sum_{i=1}^n f(y|x_i)$$

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► The estimated MC standard error is given by

$$SE^{2}[\hat{I}(y)] = \frac{1}{n} \left(\frac{1}{n-1} \sum_{i=1}^{n} \left(f(y|x_{i}) - \hat{I}(y) \right)^{2} \right)$$

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- ► This is often used to fit latent state time series models where the augmented parameters are highly correlated.
- ► This is also widely applied in particle filter methods in terms of one-step and multi-step ahead forecasting.

Example 1 – with a Normal distribution

► Suppose we want to calculate the expectation of $g(x) = x^d$, $d \in R$, where $x \sim N(0, \sigma^2)$ with pdf $p(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$ truncated in [a, b].

$$E[g(x)] = \int_{a}^{b} g(x)p(x)dx$$
$$= \int_{a}^{b} x^{d} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^{2}}{2\sigma^{2}}\right) dx$$

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We can simulate either the normal distribution or a uniform distribution over [a, b].

$$E[g(x)] = \int_a^b \frac{b-a}{\sqrt{2\pi}\sigma} x^d \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \frac{1}{b-a} dx$$

Example 1 – with a Normal distribution (Cont'd)

Table: Estimate the expectation of g(X) = X with $X \sim N(0, 1)$

	N(0, 1)		U[-5, 5]	
n	Average	SD	Average	SD
5000	0.009268	1.00122	0.014602	1.176178
10,000	0.006634	0.99461	-0.002638	1.180575
15,000	-0.004639	0.99906	0.013984	1.197937
20,000	0.003777	0.99015	0.010644	1.182507

Example 1 – with a Normal distribution (Cont'd)

Table: Estimate the expectation of $g(X) = X^2$ with $X \sim N(0, 1)$

	N(0, 1)		U[-7, 7]		
n	Average	SD	Average	SD	
5000	1.00234	1.4116	0.9809	1.3898	
10,000	0.98920	1.4030	0.9879	1.3928	
15,000	0.99809	1.3942	1.0172	1.4101	
20,000	0.98037	1.3954	0.9916	1.3963	

Example 2 – with a Gamma distribution

▶ Suppose we want to calculate the expectation of $g(x) = x^d$, where $x \sim Gamma(\alpha, \beta)$ with pdf $p(x) = \frac{1}{\Gamma(\alpha)\beta^{\alpha}}x^{\alpha-1}\exp\left(-\frac{x}{\beta}\right)$ truncated in [a,b].

$$E[g(x)] = \int_{a}^{b} g(x)f(x)dx$$
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$$E[g(x)] = \int_{a}^{b} \frac{b-a}{\Gamma(\alpha)\beta^{\alpha}} x^{d+\alpha-1} \exp\left(-\frac{x}{\beta}\right) \frac{1}{b-a} dx$$

Example 2 – with a Gamma distribution (Cont'd)

Table: Estimate the expectation of g(X) = X with $X \sim Gamma(1, 0.5)$

Gamma(1, 0.5)		U[0, 5]		
n	Average	SD	Average	SD
5000	0.50094	0.50042	0.49119	0.60671
10,000	0.49756	0.49354	0.49277	0.60859
15,000	0.50293	0.50395	0.49519	0.61078
20,000	0.50148	0.50725	0.49931	0.61285

Example 3 – Value at risk (VaR)

Suppose we want to estimate $F_Y(y) = P(Y \ge y) = \mathbb{E}[I_{[y,+\infty)}(Y)]$, where $Y \sim N(0,1)$.

$$E[I_{[y,+\infty)}(Y)] = \int_{y}^{+\infty} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right) dx$$
$$= \int_{-\infty}^{+\infty} h(x) \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right) dx$$

where h(x) = 0 if x < y and h(x) = 1 if $x \ge y$.

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where h(x) = 0 if x < y and h(x) = 1 if $x \ge y$.

▶ Draw an iid sample $\{Y_1, ..., Y_n\}$ from N(0, 1), then the estimator is

$$E[I_{(y,+\infty)}(Y)] = \frac{1}{n} \sum_{i=1}^{n} h(Y_i) = \frac{\text{\# of draws } \ge y}{n}$$

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- ▶ Define h(x, y) = 1 if $x^2 + y^2 \le 1$ and h(x, y) = 0 otherwise.

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- ▶ Define h(x, y) = 1 if $x^2 + y^2 \le 1$ and h(x, y) = 0 otherwise.
- ▶ Draw an iid sample $\{(x_1, y_1), ..., (x_n, y_n)\}$ from $X \sim U(-1, 1)$ and $Y \sim U(-1, 1)$, then the estimator is

$$\pi = \mathrm{E}[h(x,y)] \approx \frac{4}{n} \sum_{i=1}^{n} h(x_i,y_i) = \frac{4*(\# \text{ of draws satisfying } x_i^2 + y_i^2 \le 1)}{n}$$

Example 4 – how to calculate π ? (Cont'd)

Table: Estimate π

n	MC	SD
5000	3.056	0.0034
1000	3.224	0.0016
1500	3.211	0.0011
2000	3.136	0.0008
50000000	3.133	8.240823e-05

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- Suppose the density p(x) roughly approximates the density (of interest) q(x), then

$$\int_{a}^{b} f(x)q(x)dx = \int_{a}^{b} f(x) \left(\frac{q(x)}{p(x)}\right) p(x)dx = \mathbf{E}_{p(x)} \left[f(x) \left(\frac{q(x)}{p(x)}\right) \right]$$

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▶ Give a sample $\{x_i, i = 1, ..., n\}$ drawn from p(x), the IS estimator is

$$\int_{a}^{b} f(x)q(x)dx \approx \frac{1}{n} \sum_{i=1}^{n} f(x_i) \left(\frac{q(x_i)}{p(x_i)}\right)$$

Why Important Sampling (IS)?

▶ In Bayesian statistics, we have,

$$J(y) = \int_{a}^{b} f(y|x)q(x)dx,$$

which can be approximated by

$$J(y) \approx \frac{1}{n} \sum_{i=1}^{n} f(y|x_i) \left(\frac{q(x_i)}{p(x_i)} \right).$$

An alternative

► An alternative formulation of IS is

$$\int_{a}^{b} f(x)q(x)dx \approx \hat{I}(x) = \frac{1}{n} \sum_{i=1}^{n} \omega_{i} f(x_{i}) / \sum_{i=1}^{n} \omega_{i}, \text{ where } \omega_{i} = \frac{q(x_{i})}{p(x_{i})},$$

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$$\int_a^b f(x)q(x)dx \approx \hat{I}(x) = \frac{1}{n} \sum_{i=1}^n \omega_i f(x_i) \Big/ \sum_{i=1}^n \omega_i, \text{ where } \omega_i = \frac{q(x_i)}{p(x_i)},$$

which is called weighted average.

▶ The associated MC variance is

$$\operatorname{Var}(\hat{I}) = \frac{1}{n} \sum_{i=1}^{n} \omega_i (f(x_i) - \hat{I}(x))^2 / \sum_{i=1}^{n} \omega_i$$

Example 3 – Value at risk (VaR) (Cont'd)

▶ Suppose we want to estimate $P(Y \ge 3)$, where $Y \sim N(0, 1)$.

$$P(Y \ge 3) = \int_{3}^{+\infty} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^{2}}{2}\right) dx = \int_{-\infty}^{+\infty} h(x) \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^{2}}{2}\right) dx,$$

where h(x) = 0 if x < 3 and h(x) = 1 if $x \ge 3$.

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where h(x) = 0 if x < 3 and h(x) = 1 if $x \ge 3$.

▶ Draw an iid sample $\{y_1, ..., y_n\}$ from $N(\mu, 1)$, then the estimator is

$$E[I_{[3,+\infty)}(Y)] \approx \frac{1}{n} \sum_{i=1}^{n} \frac{h(y_i)f(y_i)}{g(y_i)},$$

where f(y) is the density of N(0, 1) and g(y) is the density of $N(\mu, 1)$.

Example 3 – Value at risk (VaR) (Cont'd)

Table: Estimate p(Y > 3) = 0.001349898

	$\mu = 0$	$\mu = 3$	$\mu = 4$
n	Average	Average	Average
5000	0.001	0.001352	0.001352
10,000	0.0016	0.001296	0.001295
15,000	0.0007	0.001394	0.001372
20,000	0.0013	0.001389	0.001389

Example 4

▶ Suppose we want to calculate the expectation of $g(X) = \exp\left(-\frac{1}{2\exp(X)}\right)$, where $X \sim N(\mu, \sigma^2)$ with pdf f(X).

$$E[g(X)] = \int_{-\infty}^{+\infty} g(x)f(x)dx$$

$$= \int_{-\infty}^{+\infty} \exp\left(-\frac{1}{2\exp(x)}\right) \frac{1}{\sqrt{2\pi}\sigma^2} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) dx$$

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$$= \int_{-\infty}^{+\infty} \exp\left(-\frac{1}{2\exp(x)}\right) \frac{1}{\sqrt{2\pi}\sigma^2} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) dx$$

Notice that $\exp(-x)$ is a convex function which is bounded above by a linear function of μ . By taking Taylor expansion for $\exp(-x)$ at μ we get

$$\log(g(x)) = -\frac{1}{2}e^{-x} \le -\frac{1}{2}\left[\exp(-\mu)(1+\mu) - x\exp(-\mu)\right]$$

▶ Then we get

$$\begin{split} g(x)*f(x) & \leq \exp\bigg(-\frac{1}{2}\big[\exp(-\mu)(1+\mu) - x\exp(-\mu)\big]\bigg) \\ & \times \frac{1}{\sqrt{2\pi}\sigma^2}\exp\bigg(-\frac{(x-\mu)^2}{2\sigma^2}\bigg) \end{split}$$

▶ Then we get

$$g(x) * f(x) \le \exp\left(-\frac{1}{2}\left[\exp(-\mu)(1+\mu) - x\exp(-\mu)\right]\right)$$
$$\times \frac{1}{\sqrt{2\pi}\sigma^2} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

▶ After eliminating some constant terms, we get

$$g(x) * f(x) \le k \cdot f_N \left(\mu + \frac{\sigma^2}{2} \exp(\mu), \sigma^2 \right) \stackrel{\text{def}}{=} k \cdot f^*$$

▶ The expectation of g(X) is

$$E[g(X)] = \int_{\infty}^{\infty} g(x) \left(\frac{f(x)}{f^*(x)} \right) f^*(x) dx = E_{f^*(x)} \left[g(x) \left(\frac{f(x)}{f^*(x)} \right) \right]$$
$$\approx \frac{1}{n} \sum_{i=1}^{n} \frac{g(x_i) f(x_i)}{f^*(x_i)}$$

Table: Estimate
$$g(X) = \exp\left(-\frac{1}{2\exp(X)}\right)$$
 with $X \sim N(3, 1)$

	IS	MC
n	Average	Average
5000	0.96089	0.96113
10,000	0.96125	0.96140
15,000	0.96088	0.96078
20,000	0.96146	0.96154

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- Monte Carlo methods are useful for obtaining integrals, especially for truncated distributions.
- Important sampling is even useful for integrals with complicated functions.
- ▶ MC and IS are widely used in financial engineering.

Motivation Monte Carlo Important Sampling Conclusion

Thank you!

References

- [1] McLeish, D. L. Monte Carlo Simulation and Finance. Wiley, New York (2005) (full text).
- [2] McLeish, D. L. and Z. Men. 2015. Extreme Value Importance Sampling for Rare Event Risk Measurement. K. Glau et al. (eds.), Innovations in Quantitative Risk Management. Springer Proceedings in Mathematics & Statistics. Volume 99, 2015, pp 317-335. (full text).
- [3] Paul Glasserman. 2013. Monte Carlo Methods in Financial Engineering (Stochastic Modelling and Applied Probability) . (Springer).