Introduction to Monte Carlo Methods & Random Variable Generation

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- Review of the Bayesian inference framework, Introducing the Monte Carlo simulation, reviewing the central Limit Theorem and Law of Large Numbers, indicator functions, error approximations
- Examples showing convergence of the MC simulator, Generalization of the MC Estimator in High Dimensions
- Sample Representation of the Monte Carlo Estimator
- Deterministic vc MC integration, Using MC for Computing integrals, expectations and Bayes factors
- Need for sampling methods, Sampling from a discrete distribution, Reverse sampling for continuous distributions, Transformation Methods, Box-Muller Algorithm, sample from the Gaussian

Following closely:

- C. Robert, G. Casella, Monte Carlo Statistical Methods (Ch.. 1, 2, 3.1, & 3.2) (google books, slides, video)
- J. S. Liu, MC Strategies in Scientific Computing (Chapters 1 & 2)
- J-M Marin and C. P. Robert, Bayesian Core (Chapter 2)
- Statistical Computing & Monte Carlo Methods, A. Doucet (course notes, 2007)

The Bayesian Model

- Let us revisit our Bayesian model

$$\pi(\theta \mid x) = \frac{\pi(\theta) f(x \mid \theta)}{\int_{\Theta} \pi(\theta) f(x \mid \theta) d\theta}$$

- In most problems of interest there are no analytical closed forms for the posterior (using conjugate priors is one exception).

- Also note that the denominator in the Bayes' equation above implies the calculation of the following high-dimensional integral:

$$\int_{\Theta} \pi(\theta) f(x \mid \theta) d\theta$$

The Bayesian Model

- Consider the posterior model

$$\pi(\theta \mid x) = \frac{\pi(\theta) f(x \mid \theta)}{\int_{\Theta} \pi(\theta) f(x \mid \theta) d\theta}$$

- Typical point estimates based on the posterior include the following:

$$\mathbb{E}\left[\theta \mid x\right] = \int_{\Theta} \theta \pi(\theta \mid x) d\theta$$

$$Var\left[\theta \mid x\right] = \int_{\Theta} \theta^2 \pi(\theta \mid x) d\theta - \left(\mathbb{E}\left[\theta \mid x\right]\right)^2$$

- We are often interested in the mode of the posterior $\pi(\theta \mid x)$

$$\theta^{MAP} = \arg\max_{\theta} \pi(\theta \mid x)$$

- If $\theta = (\theta_1, \theta_2)$ and θ_2 is a nuisance parameter, marginal distributions are also often needed:

$$\pi(\theta_1 \mid x) = \int \pi(\theta_1, \theta_2 \mid x) d\theta_2$$

The Bayesian Model

- Consider the posterior model

$$\pi(\theta \mid x) = \frac{\pi(\theta) f(x \mid \theta)}{\int_{\Theta} \pi(\theta) f(x \mid \theta) d\theta}$$

- The predictive distribution of Y, $Y \sim g(y|x)$, and its mean $\mathbb{E}[Y \mid x]$, are:

$$g(y \mid x) = \int f(y \mid \theta) \pi(\theta \mid x) d\theta$$

$$\mathbb{E}[Y \mid x] = \iint y f(y \mid \theta) \pi(\theta \mid x) d\theta dy$$

- Similarly, for model selection, we have seen that the posterior takes the form:

$$\pi(k, \theta_k \mid x) = \frac{\pi(k) \pi_k(\theta_k) f_k(x \mid k, \theta_k)}{\sum_{k=1}^{\infty} \pi(k) \int_{\Theta_k} \pi_k(\theta_k) f_k(x \mid k, \theta_k) d\theta_k}$$

Monte Carlo Simulation

- All of the calculations reviewed earlier require computing high-dimensional integrals.

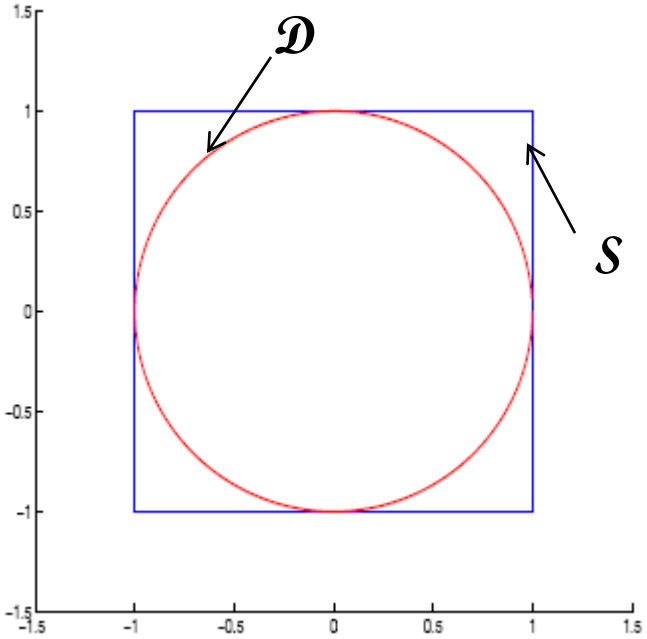
- Monte Carlo simulation provides the means for effective calculation of these integrals and for resolving many more issues.

Some historical (early) references on Monte Carlo Methods:

- N. Metropolis and S. Ulam, The Monte Carlo Method, J Amer. Statist. Ass., Vol. 44, pp. 335-341 (1949)
- N. Metropolis, The Beginning of the Monte Carlo Method, Los Alamos Science Special Issue (1987)

Introducing Monte Carlo Simulation

- Consider a 2×2 square $\mathcal{S} \subset \mathbb{R}^2$ as shown in the Figure below.



- Let an inscribed circle $\mathcal{D}$ of radius 1 in the square $\mathcal{S}$.

Introducing Monte Carlo Simulation

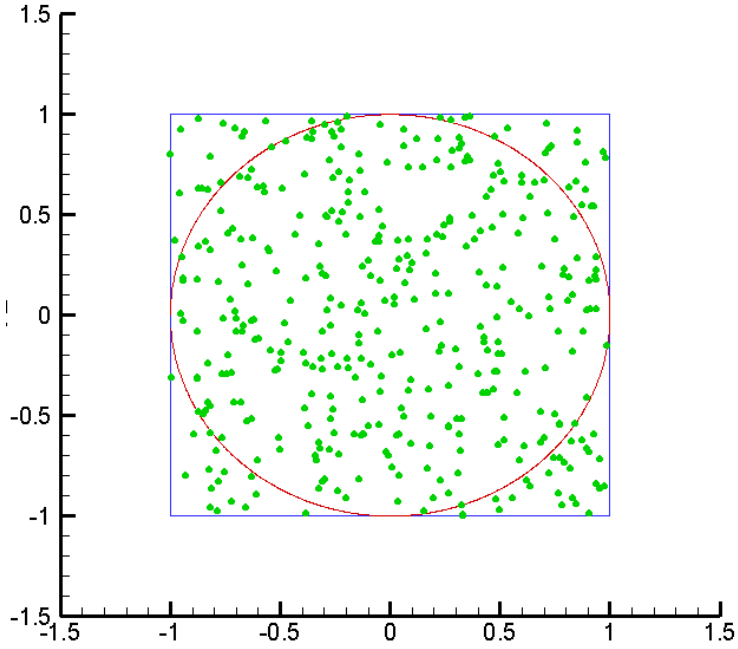
- Let us consider dropping darts uniformly on the square $\mathcal{S}$. This means that the probability of the dart falling in a subdomain A of $\mathcal{S}$ is proportional to the area of A.

- Let $D = (x, y)$ define a random variable on $\Theta = \mathcal{S}$ that represents the location of the drop of the dart. We have:

$$P(D \in A) = \frac{\int_A dxdy}{\int_{\mathcal{S}} dxdy}$$

- Assume N independent drops of the dart on the square $\mathcal{S}$, i.e.

$$\{D_1, D_2, ..., D_N\}$$



Introducing Monte Carlo Simulation

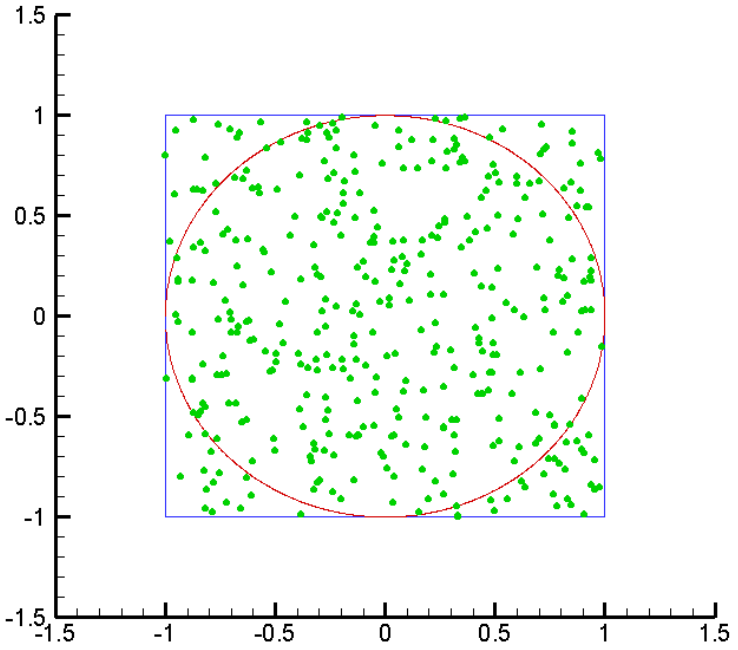
$$P(D \in A) = \frac{\int_A dxdy}{\int_S dxdy}$$

- A common sense estimation of the above probability would be

$$P(D \in A) \simeq \frac{Times\ the\ dart\ fell\ in\ A}{N}$$

where N is the total number of dart falls.

- Can we give a statistical justification of this result?



Indicator Functions

- Let us introduce the indicator function for the event A, i.e. let

$$\mathbb{I}_A(x,y) = \begin{cases} 1 \ if \ drop \ point \ of \ dart \ d = (x,y) \in A, \\ 0, otherwise \end{cases}$$

- Let us compute the probability for $D \in A$.

$$P(D \in A) = \frac{\int_S \mathbb{I}_A(x,y)dxdy}{\int_S dxdy} = \frac{\int_S \mathbb{I}_A(x,y)dxdy}{4} = \int_S \mathbb{I}_A(x,y)\frac{1}{4}dxdy$$

- The above results come immediately noticing that

$$\int_S \mathbb{I}_A(x,y)dxdy = \int_A \mathbb{I}_A(x,y)dxdy + \int_{S\setminus A} \mathbb{I}_A(x,y)dxdy = \int_A 1dxdy + \int_{S\setminus A} 0dxdy = \int_A 1dxdy$$

Indicator Functions

$$P(D \in A) = \frac{\int_S \mathbb{I}_A(x,y)dxdy}{\int_S dxdy} = \frac{\int_S \mathbb{I}_A(x,y)dxdy}{4} = \int_S \mathbb{I}_A(x,y)\frac{1}{4}dxdy$$

- The probability density associated to P is ¼ - this is the density of the uniform distribution on S denoted as $\mathcal{U}_S$
- Let us introduce the random variable $V(D) := \mathbb{I}_A(D) := \mathbb{I}_A(X,Y),$ where X, Y are the random variables representing the Cartesian coordinates of a uniformly distributed point $d = (x,y)$ on S, $D \sim \mathcal{U}_S$, where a dart falls.
- With this notation

$$P(d \in A) = \int_S \mathbb{I}_A(x,y)\frac{1}{4}dxdy = \mathbb{E}_{\mathcal{U}_S}(V)$$

Strong Law of Large Numbers

- Let X_i for $i = 1, 2, \ldots, N$ be independent and identically distritbuted random variables (i.i.d.) with mean $\mathbb{E}(X_i) = \mu$ and variance $V(X_i) = \sigma^2 < \infty$, the strong LLN states for the sample mean $\overline{X}_N$ the following:

$$\lim_{N \to \infty} \overline{X}_N = \mu \ almost \ surely$$

Weak Law of Large Numbers

- Let X_i for $i = 1, 2, \ldots, N$ be independent and identically distritbuted random variables (i.i.d.) with mean $\mathbb{E}(X_i) = \mu$ and variance $V(X_i) = \sigma^2 < \infty$, the weak LLN states that the sample mean $\overline{X}_N$ is a random variable that converges to the true mean as $N \to \infty$, i.e.

$$\overline{X}_N = \frac{\sum_{i=1}^{N} X_i}{N} \to \mu \ as \ N \to \infty$$

- More formally:

$$\lim_{N \to \infty} \Pr\left[\left|\overline{X}_N - \mu\right| \geq \varepsilon\right] = 0 \quad \forall \varepsilon > 0$$

- Note that

$$\mathbb{E}[\overline{X}_N] = \frac{\sum_{i=1}^{N} \mathbb{E}[X_i]}{n} = \frac{\sum_{i=1}^{N} \mu}{n} = \mu \ and \ \text{var}[\overline{X}_N] = \frac{\sum_{i=1}^{N} \text{var}[X_i]}{N^2} = \frac{\sum_{i=1}^{N} \sigma^2}{N^2} = \frac{\sigma^2}{N}$$

The Central Limit Theorem

- Let X_i *for* $i = 1, 2, \ldots, N$ be independent and identically distributed (i.i.d) random variables each with expectation μ and variances σ^2. Then:

$$\mathbb{E}\left[\overline{X}_N\right] = \mathbb{E}\left[\frac{\sum_{i=1}^{N} X_i}{N}\right] = \frac{1}{N}\sum_{i=1}^{N}\mathbb{E}(X_i) = \frac{1}{N}\sum_{i=1}^{N}\mu_i = \frac{1}{N}N\mu = \mu$$

$$Var\left[\overline{X}_N\right] = Var\left[\frac{\sum_{i=1}^{N} X_i}{N}\right] = \frac{1}{N^2}\sum_{i=1}^{N}Var(X_i) = \frac{1}{N^2}\sum_{i=1}^{N}\sigma^2 = \frac{1}{N}N\sigma^2 = \frac{\sigma^2}{N}$$

- Under some weak conditions (such as finite variance), the sample mean $\overline{X}_N = \frac{\sum_{i=1}^{N} X_i}{N}$ has a limiting normal distribution:

$$\lim_{N\to\infty} \frac{\bar{X}_N - \mu}{\sqrt{\frac{\sigma^2}{N}}} \sim \mathcal{N}(0,1)$$

$$or\ as\ N \to \infty\ \bar{X}_N \sim \mathcal{N}(\mu, \frac{\sigma^2}{N})$$

Back to Indicator Functions

- Let X_i for $i = 1, 2, \ldots, N$ be an indicator function for an event F, i.e. let

$$X_i = \begin{cases} 1 \ if \ the \ outcome \ of \ the \ experiment \ i \ is \ F, \\ 0, \ otherwise \end{cases}$$

Then as a result of the law of large numbers,

$$\overline{X}_N = \sum_{i=1}^{N} \frac{X_i}{N} \Rightarrow \Pr(F) \ as \ N \to \infty$$

- Note that herein we used that

$$\mathbb{E}\left[X_i\right] = 1 \times \Pr(F) + 0 \times \Pr(\overline{F}) = \Pr(F)$$

Returning to Our Dart Drop Experiment

- Let us introduce the random variables $\{V_i := V(D_i) := \mathbb{I}_A(D_i), i = 1, 2., , N\}$ associated to the drops $\{D_i, i = 1, 2, ..., N\}$ and consider the sum

$$S_N = \underbrace{\frac{\sum_{i=1}^{N} V_i}{N}}_{\substack{Empirical\ average \\ of\ i.i.d.\{V_i := V(D_i), i=1,2.,,N\}}} = \frac{number\ of\ drops\ that\ fell\ in\ A}{N}$$

- Assuming ($N \to \infty$), then the law of large numbers (since $\mathbb{E}_{\mathcal{U}_S}(|V|) < +\infty$) yields

$$\lim_{N \to \infty} S_N = \mathbb{E}_{\mathcal{U}_S}(V)\ (almost\ surely)$$

where we already proved that $\Pr(D \in A) = \mathbb{E}_{\mathcal{U}_S}(V)$

- When $N \to \infty$, this justifies our intuitive result introduced earlier.

Mean Square Error

- Since $P(d \in \mathcal{D}) = \int_{\mathcal{D}} \frac{1}{4} dxdy = \frac{\pi}{4}$, S_N is an unbiased estimator of $\frac{\pi}{4}$.

$$S_N \text{ is a random variable} : S_N = \frac{\pi}{4} + \underbrace{E_N}_{\text{Error term}}$$

- To characterize the precision of the estimator, we can use the following:

$$Var(E_N) = Var(S_N) = \frac{1}{N^2} \sum_{i=1}^{N} Var(V_i) = \frac{1}{N} Var(V_1) \quad (\text{recall the } V_i\text{'s are i.i.d.})$$

- This means that

$$\sqrt{Var(S_N)} = \sqrt{\mathbb{E}\left[\left(S_N - \mathbb{E}(S_N)\right)^2\right]} = \sqrt{\mathbb{E}\left[\left(S_N - \Pr(D \in \mathcal{D})\right)^2\right]} = \frac{1}{\sqrt{N}} \sqrt{Var(V_1)}$$

Thus the mean square error between S_N and $\Pr(D \in \mathcal{D})$ decreases as $\frac{1}{\sqrt{N}}$

- For our problem $Var(V_1) = P(D \in \mathcal{D}) - \left(P(D \in \mathcal{D})\right)^2 = \frac{\pi}{4} - \left(\frac{\pi}{4}\right)^2 = 0.1685.$

Properties of the Estimator

- Applying the central limit theorem (since $Var(V) < +\infty$) :

$$S_N \xrightarrow[d]{} \mathcal{N}\left(\frac{\pi}{4}, \frac{Var(V)}{N}\right)$$

- The probability of the error being larger than $\varepsilon = 2\sqrt{\frac{\text{var}(V)}{N}}$ is given as:

$$\Pr\left[\left|S_N - \frac{\pi}{4}\right| \geq 2\sqrt{\frac{\text{var}(V)}{N}}\right] = 2\left\{1 - \Phi\left(\frac{2\sqrt{\frac{\text{var}(V)}{N}}}{\sqrt{\frac{\text{var}(V)}{N}}}\right)\right\} = 2\left(1 - \Phi(2)\right) = 0.0456$$

where $\Phi(x)$ *the CDF of* $\mathcal{N}(0,1)$.

- One can similarly prove that for any integer $N \geq 1$ *and* $\varepsilon > 0$,

$$\Pr\left[\left| S_N - \frac{\pi}{4} \right| \geq \varepsilon\right] = 2\left\{1 - \Phi\left(\frac{\varepsilon}{\sqrt{\frac{\text{var}(V)}{N}}}\right)\right\} = erfc\,\frac{\varepsilon}{\sqrt{2\frac{\text{var}(V)}{N}}} < Ce^{-\varepsilon^2 \frac{N}{2\,\text{var}(V)}}\sqrt{\frac{\text{var}(V)}{N\varepsilon^2}}$$

where $\Phi(x) = \frac{1}{2}\left(1 + erf\left(\frac{x}{\sqrt{2}}\right)\right)$ and *for large* x : $erfc(x) \approx \frac{e^{-x^2}}{x\sqrt{\pi}}$ (see here).

Coefficient of Variation

- The coefficient of variation for our Monte Carlo estimator is given as:

$$Coeff.\ of\ Var. \equiv COV\left(S_N\right) = \frac{\sqrt{\text{var}\left(S_N\right)}}{\mathbb{E}(S_N)} = \frac{\sqrt{\pi/4\,(1-\pi/4)}}{\pi/4\sqrt{N}} = \sqrt{\frac{4(1-\pi/4)}{N\pi}} = \frac{0.5233}{\sqrt{N}}$$

- For different COVs, the number of samples needed is given as:

$$COV = 10\% \Rightarrow N = 28$$
$$COV = 5\% \Rightarrow N = 110$$
$$COV = 1\% \Rightarrow N = 2739$$

- With all of the above error estimates, we conclude that the approximation error varies as $O\left(\frac{1}{\sqrt{N}}\right)$.

Properties of the Estimator

- An alternative non-asymptotic error estimate[a] using a Bernstein type inequality is:

$$\forall N \geq 1 \; and \; \varepsilon > 0, \; P\left(\left| S_N - \frac{\pi}{4} \right| > \varepsilon \right) \leq 2e^{-2N\varepsilon^2}$$

- Using this result, we can show that:

$$\forall \alpha \in (0,1], \; P\left(\left| S_N - \frac{\pi}{4} \right| > \varepsilon \right) < \alpha \; for \; N \geq \frac{\log(2/\alpha)}{2\varepsilon^2}$$

- Alternatively, for any $N \geq 1$, using the Eq. above we can write:

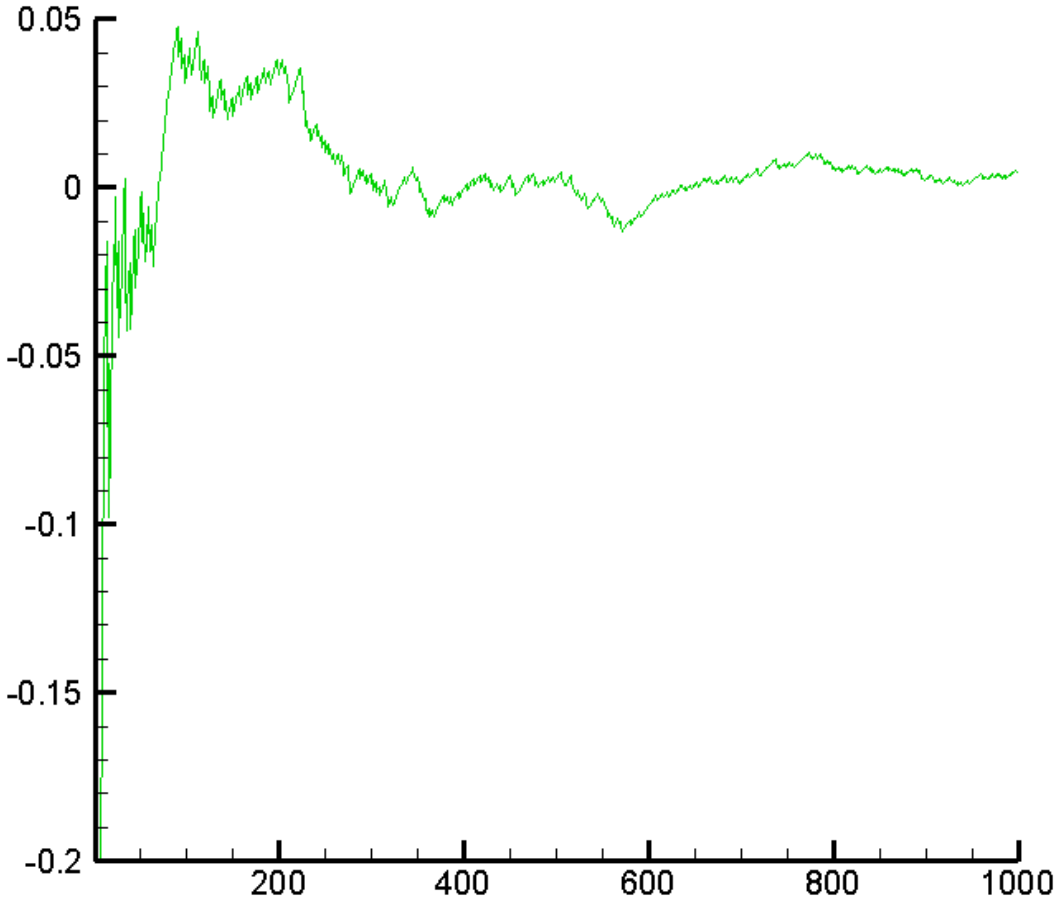
$$\Pr\left[\left| S_N - \frac{\pi}{4} \right| > \sqrt{\frac{\log(40)}{2N}} \right] \leq 0.05$$

- These expressions for the approximation error show that it is inversely proportional to $\sqrt{N}$.

[a]From **Statistical Computing & Monte Carlo Methods**, A. Doucet.

Convergence of the Simulator

- Convergence of $S_N - \frac{\pi}{4}$ as a function of N (one realization)

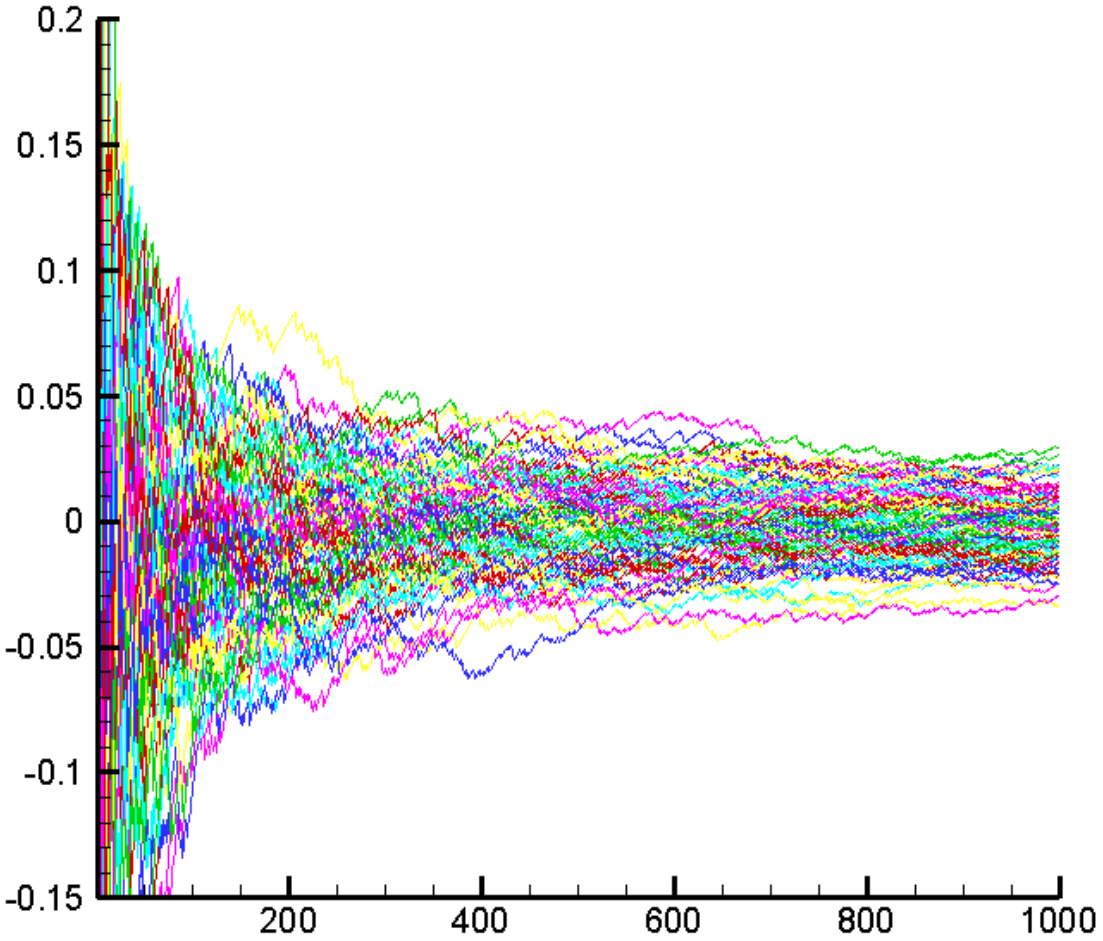


See here for a C++ implementation (Meanerror_plt)

Convergence of the Simulator

- Convergence of $S_N - \frac{\pi}{4}$ as a function of N (one hundred realizations)

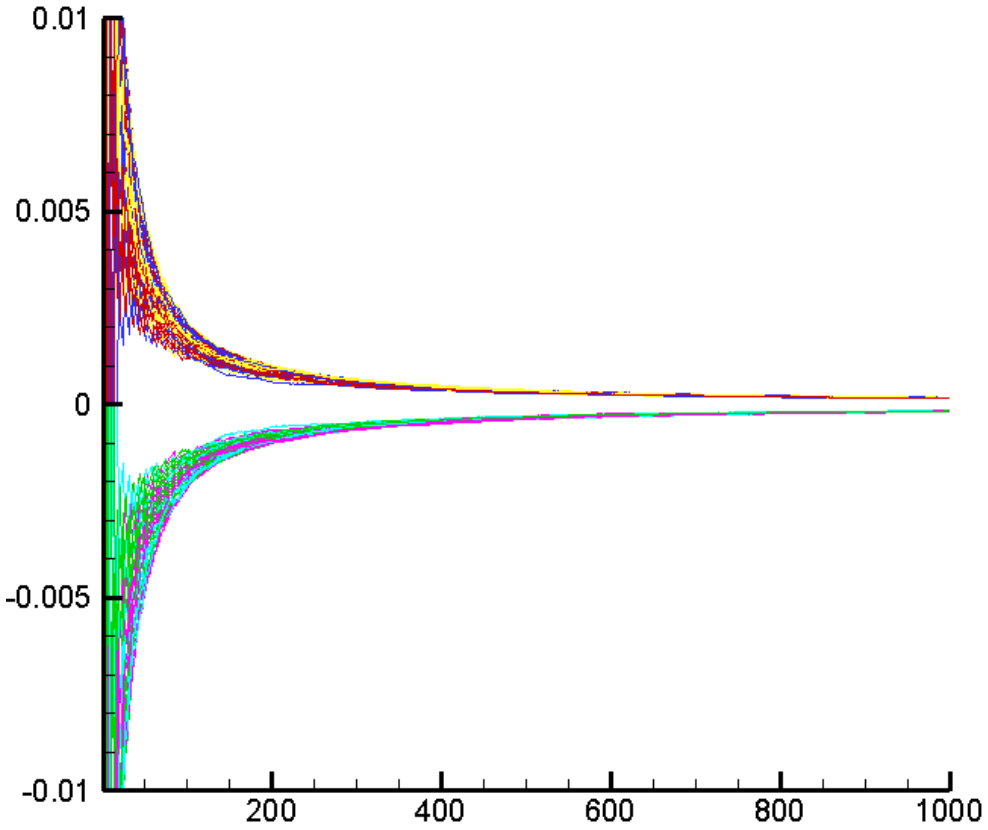
See here for a C++ implementation (Meanerror.plt)



Convergence of the Simulator

- Square root empirical mean square error $S_N - \frac{\pi}{4}$ across 100 realizations as a function of N and $\pm\sqrt{\frac{Var(V)}{N}}$ (dotted)

See here for a C++ implementation (Var_error.plt)

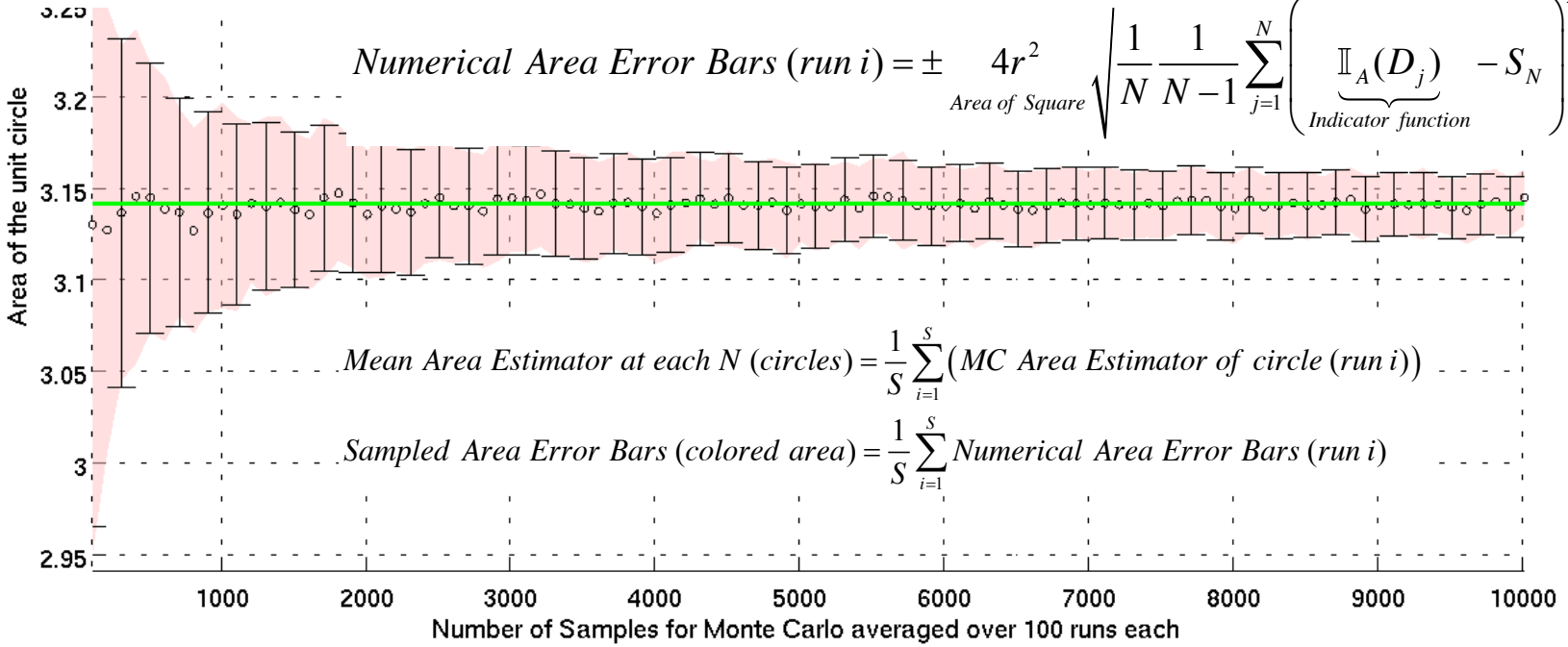


Convergence of the Estimator

$$MC\ Estimator\ of\ the\ area\ A\ of\ circle\ (run\ i) = \underbrace{Area\ of\ square}_{4r^2} \times \underbrace{Number\ of\ counts\ of\ samples\ falling\ in\ circle\ /\ N}_{our\ S_N\ MC\ estimator}$$

$$Theoretical\ Area\ Error\ Bars\ (solid\ lines) = \pm \underbrace{4r^2}_{Area\ of\ Square} \underbrace{\sqrt{\frac{\pi}{4} - \left(\frac{\pi}{4}\right)^2} \Big/ \sqrt{N}}_{exact\ std\ of\ our\ S_N\ MC\ estimator}$$

$$Numerical\ Area\ Error\ Bars\ (run\ i) = \pm \underbrace{4r^2}_{Area\ of\ Square} \sqrt{\frac{1}{N}\frac{1}{N-1}\sum_{j=1}^{N}\left(\underbrace{\mathbb{I}_A(D_j)}_{Indicator\ function} - S_N\right)^2}$$



$$Mean\ Area\ Estimator\ at\ each\ N\ (circles) = \frac{1}{S}\sum_{i=1}^{S}\left(MC\ Area\ Estimator\ of\ circle\ (run\ i)\right)$$

$$Sampled\ Area\ Error\ Bars\ (colored\ area) = \frac{1}{S}\sum_{i=1}^{S} Numerical\ Area\ Error\ Bars\ (run\ i)$$

- Monte Carlo estimator of the area of a unit circle: (a) Circles: MC mean averaged over the S=100 runs; (b) Theoretical error bars using the estimator discussed earlier; (c) Average of the MC numerical error bars (from the S=100 MC runs for each N). MatLab implementation is given here.

Generalization of the Dart Drop Experiment

- Consider now the case where $\Theta = \mathbb{R}^{n_\theta}$, $n_\theta >> 1$. We assume a hypercube $\mathcal{S}^{n_\theta}$ and the inscribed hyperball $\mathcal{D}^{n_\theta}$ in Θ.

- We can build the same estimator as in $2D$. Our indicator function now becomes $\mathbb{I}_{\mathcal{D}^{n_\theta}}(D)$.

- All of our earlier derivations are still applicable. The rate of convergence of the estimator in the mean square sense is independent of n_θ and equal to $1/\sqrt{N}$.

- This is not the case using a deterministic method on a grid of regularly spaced points where the convergence rate is typically of the form $1/N^{r/n_\theta}$ where r is related to the smoothness of the contours of $\mathcal{D}^{n_\theta}$.

- Monte Carlo methods are thus attractive when n_θ is large.

Generalization of the Dart Drop Experiment

- Assume you are interested in computing the volume of the hypersphere of radius $R = 1$ in n_θ–dimensions:

$$vol\left(\mathcal{S}_{n_\theta}\right) = \frac{\pi^{\frac{n_\theta}{2}}}{\Gamma\left(\frac{n_\theta}{2}+1\right)} \to 0 \; as \; n_\theta \to \infty$$

- We want to do so using samples from the hypercube $\left[-1,1\right]^{n_\theta}$ of volume 2^{n_θ}.

- Using N samples, the variance of our MC estimator is

$$\frac{Var\left(X\right)}{N} = \frac{p_{n_\theta}\left(1-p_{n_\theta}\right)}{N} \approx \frac{p_{n_\theta}}{N} \; as \; n_\theta \to \infty$$

$$where: X \sim Bernoulli(p_{n_\theta}) \; with \; p_{n_\theta} = \frac{vol\left(\mathcal{S}_{n_\theta}\right)}{2^{n_\theta}}.$$

Monte Carlo and the Curse of Dimensionality

- The coefficient of variation is then:

$$COV = \frac{\sqrt{\frac{Var(X)}{N}}}{\mathbb{E}(X)} \approx \frac{\sqrt{\frac{p_{n_\theta}}{N}}}{p_{n_\theta}} = \frac{1}{\sqrt{N p_{n_\theta}}} \; as \; n_\theta \to \infty$$

- To obtain a reasonable relative error, we would need $N \approx 100\, p_{n_\theta}^{-1}$.
- For this choice: $COV \approx 0.1$
- For

$$n_\theta = 20,\; N \approx 100\, p_{n_\theta}^{-1} = 100 \times 2^{20} \frac{\Gamma(11)}{\pi^{10}} = 100 \times 2^{20} \frac{10!}{\pi^{10}} \approx 4.06 \times 10^9$$

- Clearly a plain Monte Carlo approach is not as helpful in 20 and higher dimensions! You are trying in a huge volume of the hypercube to hit the infinitesimal hypersphere!

Generalization of the Dart Drop Experiment

$$Consider: \mathbb{E}(X) = 1, \; and \; Var(X) = C\alpha^{n_\theta}, \; with \; \alpha > 1.$$

$$Then: For \; \frac{Var(X)}{N} \leq \varepsilon \Rightarrow N \geq \frac{C\alpha^{n_\theta}}{\varepsilon}.$$

- To obtain a fixed precision ε in the variance, a number of samples that is exponential in the dimension is needed!
- So using a plain Monte Carlo method still suffers from the curse of dimensionality
  - ✓ MC not appropriate for rare events modeling.

Generalization

- Assume $N >> 1$ i.i.d. samples $\theta^{(i)} \sim \pi \ (i = 1, 2, ..., N)$

- Now consider any set $A \subset \Theta$ and assume that we are interested in $\pi(A) = P(\theta \in A)$, $for\ \theta \sim \pi$. We naturally choose the following estimator:

$$\pi(A) \simeq \frac{number\ of\ samples\ in\ A}{total\ number\ of\ samples}$$

which by the law of large numbers is a consistent estimator of $\pi(A)$ since

$$\lim_{N \to +\infty} \frac{1}{N} \sum_{i=1}^{N} \mathbb{I}_A(\theta^{(i)}) = \mathbb{E}_\pi(\mathbb{I}_A(\theta)) = \pi(A)$$

Generalization

- Now we generalize the idea to tackle the generic problem of estimating

$$\mathbb{E}_{\pi}(f(\theta)) = \int_{\Theta} f(\theta)\pi(\theta)d\theta$$

where $f : \Theta \to \mathbb{R}^{n_f}$ and π is a probability distribution on $\Theta \subset \mathbb{R}^{n_x}$.

- We assume that $\mathbb{E}_{\pi}(|f(\theta)|) < +\infty$ and that $\mathbb{E}_{\pi}(f(\theta))$ cannot be calculated analytically.

Generalization

- To evaluate $\mathbb{E}_\pi(f(\theta))$, we consider the unbiased estimator

$$S_N(f) = \frac{1}{N}\sum_{i=1}^{N} f(\theta^{(i)})$$

- From the law of large numbers $S_N(f)$ will converge and

$$\lim_{N\to+\infty} \frac{1}{N}\sum_{i=1}^{N} f(\theta^{(i)}) = \mathbb{E}_\pi(f(\theta))\ (a.s.)$$

- A good measure of the approximation is the variance of $S_N(f)$,

$$Var_\pi\left[S_N(f)\right] = Var_\pi\left[\frac{1}{N}\sum_{i=1}^{N} f(\theta^{(i)})\right] = \frac{Var_\pi\left[f(\theta)\right]}{N}$$

- From the central limit (if $\text{var}_\pi\left[f(\theta)\right] < +\infty$), we have:

$$\sqrt{N}\left(S_N(f) - \mathbb{E}_\pi\left(f(\theta)\right)\right) \underset{d}{\overset{N\to+\infty}{\to}} \mathcal{N}\left(0, Var_\pi\left[f(\theta)\right]\right) \text{ or}$$

$$S_N(f) \underset{d}{\overset{N\to+\infty}{\to}} \mathcal{N}\left(\mathbb{E}_\pi\left(f(\theta)\right), \frac{Var_\pi\left[f(\theta)\right]}{N}\right)$$

Generalization

- The rate of convergence is independent of the dimension of Θ
- Integration in complex domains is now not a problem.
- The method is easy to implement and rather general. You will need
  - to be able to evaluate $f(\theta)\ \forall \theta \in \Theta$
  - to be able to produce samples distributed according to π

Some historical references on Monte Carlo Methods:

- N. Metropolis and S. Ulam, The Monte Carlo Method, J Amer. Statist. Ass., Vol. 44, pp. 335-341 (1949)
- N. Metropolis, The Beginning of the Monte Carlo Method, Los Alamos Science Special Issue (1987)

Sample Representation of the MC Estimator

- Let us introduce the Dirac-Delta function $\delta_{\theta_0}(\theta)$ for $\theta_0 \in \Theta$ defined for any $f : \Theta \leftarrow \mathbb{R}^{n_f}$ as follows:

$$\int_{\Theta} f(\theta)\delta_{\theta_0}(\theta)d\theta = f(\theta_0)$$

- Note that this implies in particular that for $A \subset \Theta$

$$\int_{\Theta} \mathbb{I}_A(\theta)\delta_{\theta_0}(\theta)d\theta = \int_{A} \delta_{\theta_0}(\theta)d\theta = \mathbb{I}_A(\theta_0)$$

- For $\theta^{(i)} \sim \pi, i = 1,...,N$, we can introduce the following mixture of Delta-Dirac functions:

$$\hat{\pi}_N(\theta) := \frac{1}{N}\sum_{i=1}^{N} \delta_{\theta^{(i)}}(\theta)$$

which is the empirical measure, and consider for any $A \subset \Theta$

$$\hat{\pi}_N(A) \triangleq \int_A \hat{\pi}_N(\theta)d\theta = \sum_{i=1}^{N} \int_A \frac{1}{N}\delta_{\theta^{(i)}}(\theta)\, d\theta = \frac{1}{N}\sum_{i=1}^{N} \mathbb{I}_A(\theta^{(i)}) = S_N(A)\ (\#\ of\ samples\ in\ A)$$

Sample Representation of π

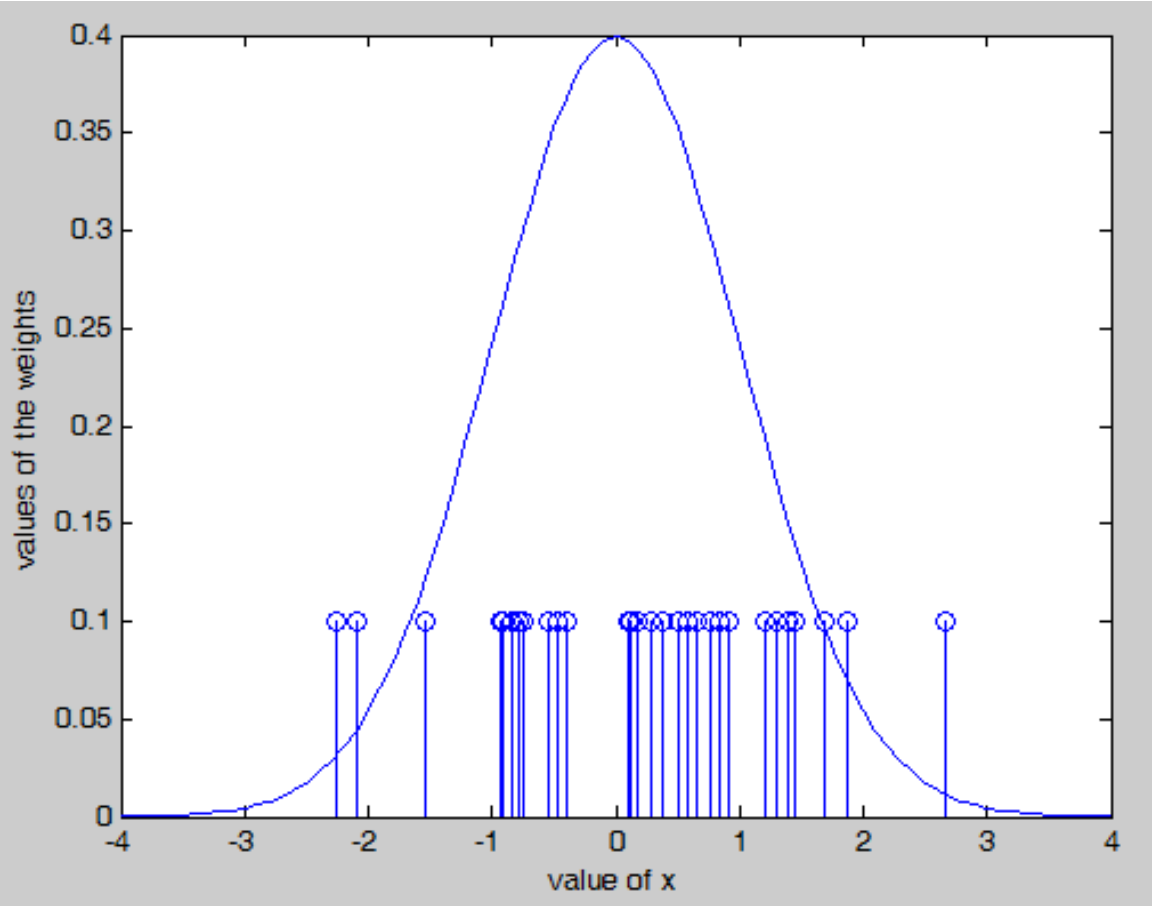
- The concentration of points in a given region of the space represents π

- This is contrast with parametric statistics where one starts with samples and then introduces a distribution with an algebraic representation of the underlying population.

- Note that each sample $\theta^{(i)}$ has a weight of $1/N$, but that it is also possible to consider weighted sample representations of π .

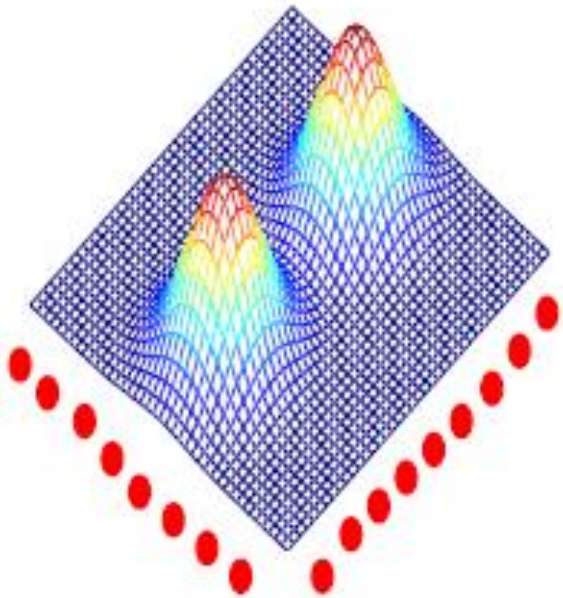
Sample Representation of π

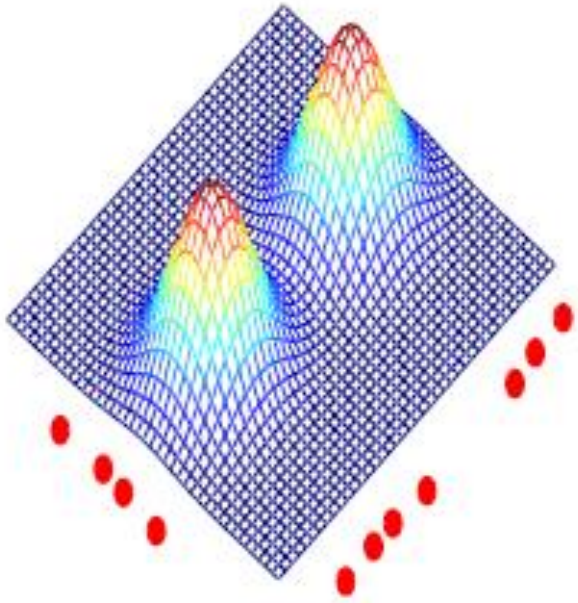
- Sample representation of a Gaussian distribution is shown below.



See here for a MatLab Implementation

Deterministic Vs. Monte Carlo Integration





Sample Representation of the MC Estimator

- Now consider the problem of estimating $\mathbb{E}_\pi(f)$. We simply replace π with its sample representation $\hat{\pi}_N(\theta)$ and obtain:

$$\mathbb{E}_\pi(f) \simeq \int_\Theta f(\theta) \sum_{i=1}^{N} \int_A \frac{1}{N} \delta_{\theta^{(i)}}(\theta)\, d\theta = \sum_{i=1}^{N} \int_\Theta \frac{1}{N} f(\theta) \delta_{\theta^{(i)}}(\theta)\, d\theta = \frac{1}{N} \sum_{i=1}^{N} f\left(\theta^{(i)}\right)$$

- This is precisely $S_N(f)$, the Monte Carlo estimator suggested earlier.
- Clearly based on $\hat{\pi}_N(\theta)$, we can easily estimate $\mathbb{E}_\pi(f)$ for any f.
- For example, the variance of f is approximated as:

$$Var_\pi(f) = \mathbb{E}_\pi(f^2) - \mathbb{E}_\pi^2(f) \simeq \frac{1}{N} \sum_{i=1}^{N} f^2\left(\theta^{(i)}\right) - \left(\frac{1}{N} \sum_{i=1}^{N} f\left(\theta^{(i)}\right) \right)^2$$

From the Algebraic to the Sample Representation

- Similarly, if we have:

$$\hat{\pi}_N(\theta_1, \theta_2) = \frac{1}{N}\sum_{i=1}^{N} \delta_{\theta_1^{(i)}\theta_2^{(i)}}(\theta_1\ , \theta_2\ )$$

- The marginal distribution is given as:

$$\hat{\pi}_N(\theta_1) = \frac{1}{N}\sum_{i=1}^{N} \delta_{\theta_1^{(i)}}(\theta_1\ )$$

- If we want to estimate $\arg\max_{\theta} \pi(\theta)$ and $\pi(\theta)$ is only known up to a normalizing constant, then a reasonable estimate is the following:

$$\arg\max_{\{\theta^{(i)}\}} \pi(\theta^{(i)})$$

Sampling from an Arbitrary Distribution

- We can now see that if we can sample easily from an arbitrary distribution, then we could easily compute any quantities of interest.

- But how do we sample from an arbitrary distribution?

  - We will discuss about MCMC and other methods in follow up lectures

Monte Carlo Integration

- We can use the same estimation for performing integration. Consider computing the following:

$$I = \int_D f(x)dx$$

- We can write this integration as $I = \int_D f(x)dx = \mathbb{E}_{1_D}\left[f(x)\right]$ where the mean is wrt the uniform distribution in D:

$$\pi(x) = \begin{cases} 1 \;\; if \;\; x \in D \\ 0, otherwise \end{cases}$$

- To compute the integral I, we thus need to draw samples from this distribution. Our estimator will then be as follows:

$$\hat{I} = \frac{1}{n}\sum_{i=1}^{n} f(x_i)$$

- The estimator converges as $O(\frac{1}{\sqrt{N}})$.

Monte Carlo Integration

- We can extend this to high (d) dimensions:

$$I = \int_D f(\boldsymbol{x}) d\boldsymbol{x}$$

- The estimator converges as $\mathcal{O}(\frac{1}{\sqrt{N}})$ regardless of the dimensionality d.

- For a Riemann integration of this, the rate of convergence is better $\mathcal{O}(\frac{1}{N})$ where a grid of equally spaced points is used (e.g. for $D = [0,1], \Delta x = 1/N$).

- However, in let us say ten dimensions, $D = [0,1]^{10}$, you will need $\mathcal{O}(N^{10})$ grid points to achieve $\mathcal{O}(\frac{1}{N})$ the same rate of convergence as in 1D!

- Generally, the rate of convergence of the Riemann approximation of the above integral is $\mathcal{O}(1/N^{r/d})$ where N is the total number of grid points and r depends on the smoothness of the domain D.

J. S. Liu, MC Strategies in Scientific Computing (Chapter 2, Introduction)

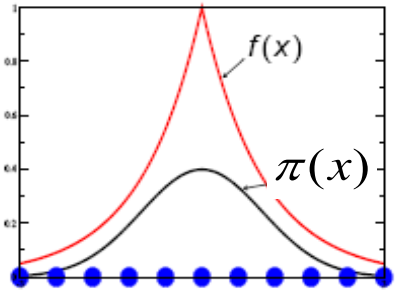
Monte Carlo for Integration

- In computing $I = \int_{D=[0,1]} f(x)dx$ with Riemann integration, one e.g.

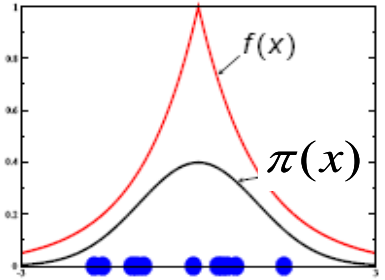
  constructs a grid with $\Delta x = 1/N$, computes $f(x_i) = f(i\Delta x)$ and with approximation error $\mathcal{O}(\Delta x) \propto \mathcal{O}\left(1/N\right)$ evaluates:

$$\hat{I}_N \approx \sum_{i=1}^{N} f(x_i)\Delta x = \frac{1}{N}\sum_{i=1}^{N} f(x_i)$$

- In d −dimensions, we need N^d evaluations $f(x_i)$ to keep an error $\mathcal{O}\left(1/N\right)$
- Clearly the MC estimator is slower in convergence $\mathcal{O}(\frac{1}{\sqrt{N}})$ but it converges independently of the dimension d. It requires no grid of points. But you need to be able to sample from $p(x)$.



Riemann integration



MC integration

Monte Carlo Integration

- Consider calculating for any function $f(x)$, the following integral

$$\mu(f) = \int_0^1 f(x)dx$$

- We can write this integral as:

$$\mu(f) = \int_{-\infty}^{+\infty} f(x)\mathbb{I}_{[0,1]}(x)dx = \mathbb{E}[f(X)]$$

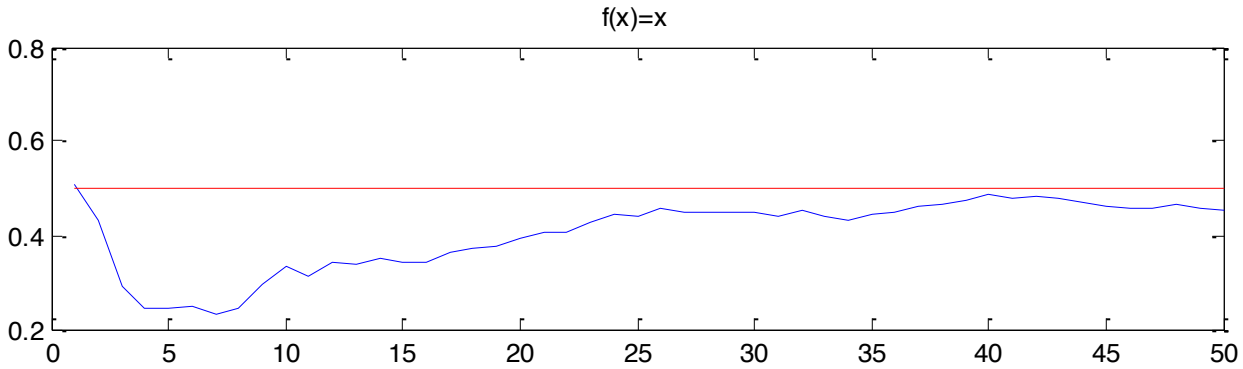
- Here

$$X \sim \mathcal{U}_{[0,1]}$$

- The Monte Carlo estimator of the integral is now:

$$\hat{\mu}_N(f) = \frac{1}{N}\sum_{i=1}^{N} f(X_i)\,,\; X_i \overset{i.i.d}{\sim} U_{[0,1]}$$

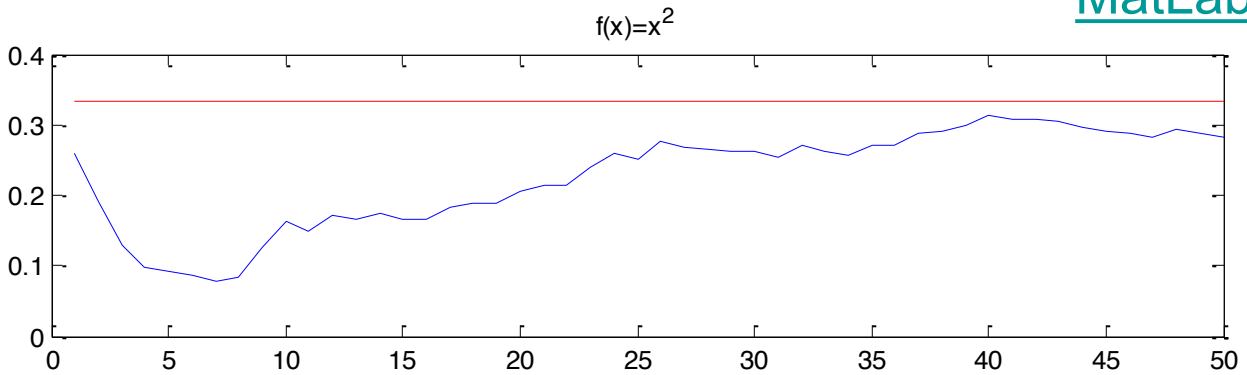
Monte Carlo Integration



$$f(x) = x$$

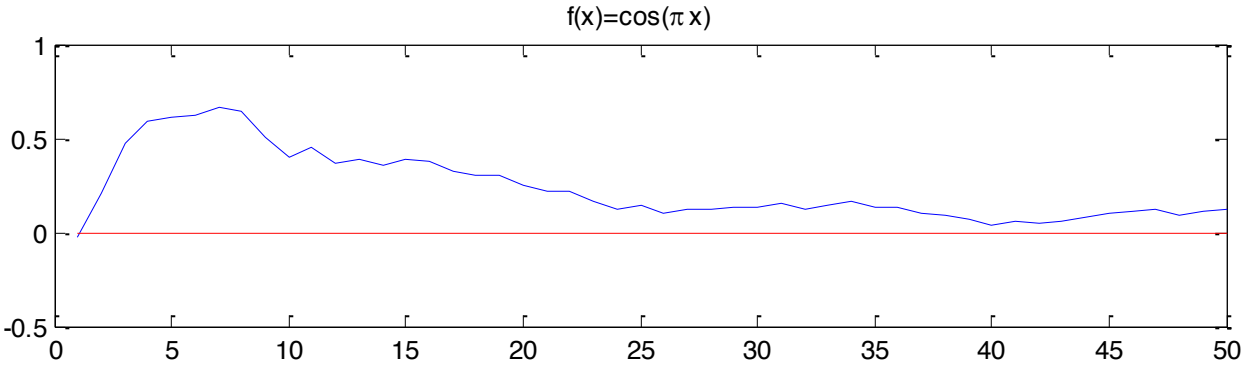
$$\mu = 0.5$$

MatLab Implementation



$$f(x) = x^2$$

$$\mu = 0.333$$



$$f(x) = \cos(\pi x)$$

$$\mu = 0$$

Monte Carlo Integration: Variance

- From the earlier discussed properties of the MC estimator:

$$\mathbb{E}[\hat{\mu}_N] = \mu$$

$$Var[\hat{\mu}_N] = \frac{1}{N} Var[f(X)] = \frac{1}{N}\sigma^2(f), X \sim \mathcal{U}_{[0,1]}$$

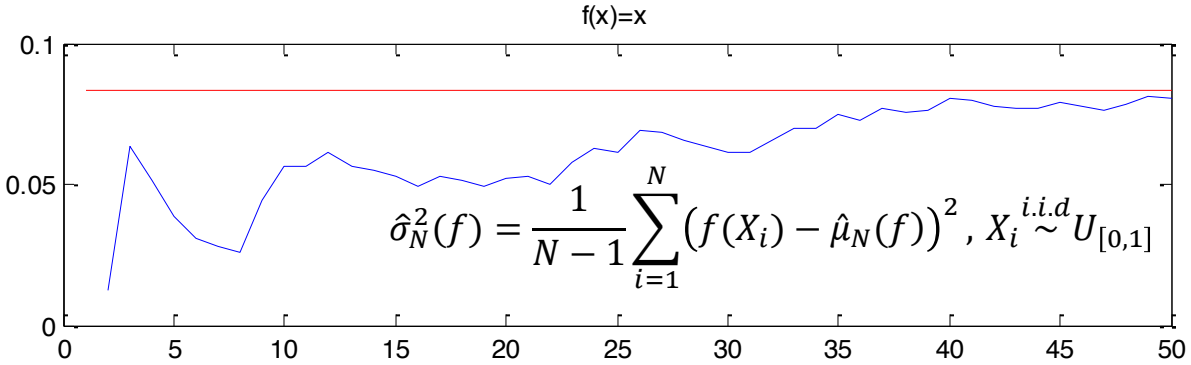
where:

$$\sigma^2(f) \equiv Var\left[f(X)\right] = \int_{-\infty}^{+\infty} \left(f(x) - \mu\right)^2 \mathbb{I}_{[0,1]}(x) dx$$

- When the variance $\sigma^2(f) \equiv Var\left[f(X)\right]$ is unknown, we can use its MC estimator instead:

$$\hat{\sigma}_N^2(f) = \frac{1}{N-1}\sum_{i=1}^{N}\left(f(X_i) - \hat{\mu}_N(f)\right)^2, \hat{\mu}_N(f) = \frac{1}{N}\sum_{j=1}^{N} f(X_j), X_i \overset{i.i.d}{\sim} \mathcal{U}_{[0,1]}$$

Monte Carlo Integration: Empirical Variance

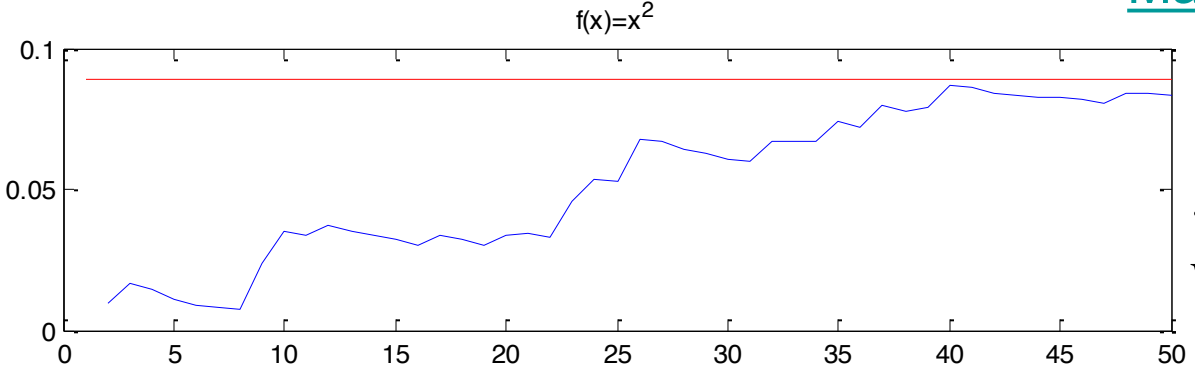


$$\hat{\sigma}_N^2(f) = \frac{1}{N-1}\sum_{i=1}^{N}\left(f(X_i) - \hat{\mu}_N(f)\right)^2, \; X_i \overset{i.i.d}{\sim} U_{[0,1]}$$

$$f(x) = x$$

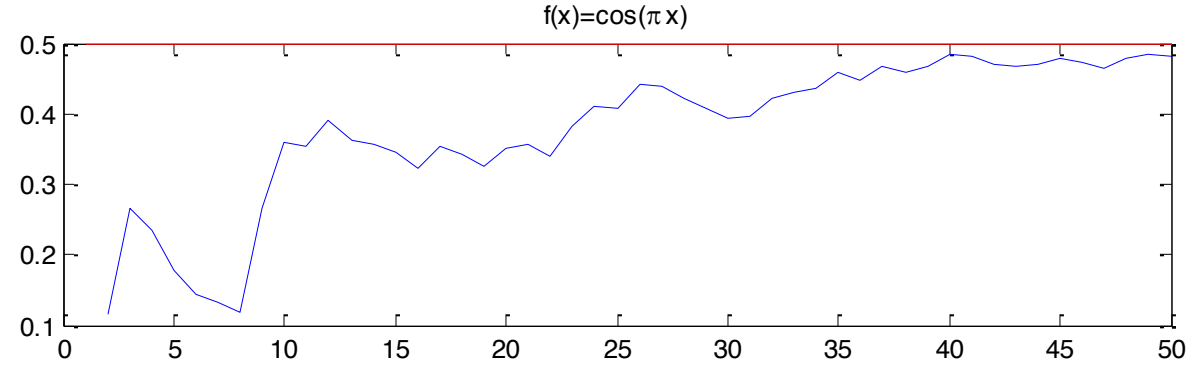
$$Var\left[f(X)\right] = 1/12$$

MatLab Implementation



$$f(x) = x^2$$

$$Var\left[f(X)\right] = 4/45$$



$$f(x) = \cos(\pi x)$$

$$Var\left[f(X)\right] = 1/2$$

Optimal Number of MC Samples

- We can compute the optimal number of MC samples for a desired accuracy of the estimator:

$$\Pr(|\hat{\mu}_N(f) - \mu(f)| \leq \varepsilon) = 1 - \alpha \Rightarrow \Pr\left(\frac{|\hat{\mu}_N(f) - \mu(f)|}{\sigma/\sqrt{N}} \leq \frac{\varepsilon\sqrt{N}}{\sigma}\right) = 1 - \alpha$$

- From the asymptotic properties $\sqrt{N}(\hat{\mu}_N - \mu) \underset{N\to\infty}{\overset{D}{\to}} \mathcal{N}(0, \sigma^2(f))$ we can estimate:

$$X_\alpha = \varepsilon\sqrt{\frac{N}{\sigma^2(f)}} \Rightarrow N = \left(\frac{X_\alpha}{\varepsilon}\right)^2 \sigma^2(f)$$

where:

$$X_\alpha = \Phi^{-1}\left(1 - \frac{\alpha}{2}\right), \Phi^{-1} \text{ inverse cdf of } \mathcal{N}[0,1]$$

- Approximating the variance $\sigma^2(f)$, the number of needed N should satisfy:

$$\hat{\sigma}_N^2(f) \leq \frac{N\varepsilon^2}{X_\alpha^2}$$

Optimal Number of MC Samples

- The condition $\hat{\sigma}_N^2(f) \leq \frac{N\varepsilon^2}{X_\alpha^2}$ can be satisfied iteratively
  - 1. Start with n_1 MC samples from $X_1,\ldots,X_{n_1} \sim \mathcal{U}[0,1]$
  - 2. If $\hat{\sigma}_{n_1}^2(f) \leq \frac{n_1\varepsilon^2}{X_\alpha^2}$ then stop; otherwise
  - 3. Evaluate $k_1 = \left\lfloor \frac{X_\alpha^2 \hat{\sigma}_{n_1}^2(f)}{\varepsilon^2} - n_1 \right\rfloor$ and generate k_1 samples $X_{n_1+1},\ldots,X_{n_1+k} \sim \mathcal{U}[0,1]$ where here $\lfloor x \rfloor$ indicates the integer part of x.

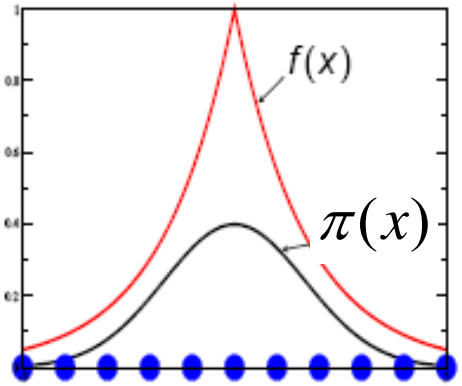
Computing Expectations

- Expectations with respect to any distribution also involve high-dimensional integration:

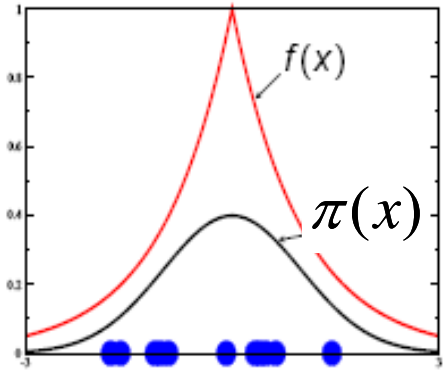
$$I = \int_D f(\boldsymbol{x})\pi(\boldsymbol{x})d\boldsymbol{x}$$

If we can draw samples from $\pi(\boldsymbol{x})$, then we can use the estimator

$$\hat{I} = \frac{1}{N}\sum_{i=1}^{N} f(x_i), \; with\, Coeff.\, of\, Variat.\, (\hat{I}) = \frac{\sqrt{Var\big(f(x)\big)}}{\sqrt{N}\mathbb{E}_{\pi(x)}[f(x)]}$$



Riemann integration



MC integration

Bayes Factor Approximation

- For the CMBdata, consider 2 subsamples $(x_1,...,x_n)$ and $(y_1,...,y_n)$.
- We consider that both come from distributions $x_1,\ldots,x_n \sim \mathcal{N}(\mu_x,\sigma^2)$ and $y_1,\ldots,y_n \sim \mathcal{N}(\mu_y,\sigma^2)$.
- We want to decide if both means are the same, i.e. test $H_0:\mu_x=\mu_y$.
- We assume that the variance (error) σ^2 is the same for both models and use a prior

$$\pi_\sigma(\sigma^2)=1/\sigma^2$$

- The Bayes factor B_{10}^{π} can then be computed as follows:

$$B_{10}^{\pi}=\frac{\int \ell(\mu_x,\mu_y,\sigma^2\mid\mathcal{D}_n)\pi(\mu_x,\mu_y)\pi_\sigma(\sigma^2)d\sigma^2 d\mu_x d\mu_y}{\int \ell(\mu,\sigma^2\mid\mathcal{D}_n)\pi_\mu(\mu)\pi_\sigma(\sigma^2)d\sigma^2 d\mu}$$

- Note that the Bayes factor does not depend on the normalizing constant of $\pi_\sigma(\sigma^2)$ and thus the use of an improper prior $\pi_\sigma(\sigma^2)=1/\sigma^2$ is fine.

J-M Marin and C. P. Robert, Bayesian Core, Chapter 2

Bayes Factor Approximation

- We introduce a new parametrization by writing:

$$\mu_x = \mu - \xi,\ \mu_y = \mu + \xi$$

with the prior

$$\pi(\mu, \xi) = \pi_\mu(\mu)\pi_\xi(\xi)$$

This allows the same prior $\pi_\mu(\mu)$ to be used in both H_0 and the alternative H_1: $\mu_x \neq \mu_y$.

- We choose the improper prior $\pi_\mu(\mu) = 1$ and $\xi \sim \mathcal{N}(0,1)$.

- The Bayes' factor can now be re-written as:

$$B_{10}^{\pi} = \frac{\int \ell\left(\mu_x, \mu_y, \sigma^2 \mid \mathcal{D}_n\right)\pi\left(\mu_x, \mu_y\right)\pi_\sigma\left(\sigma^2\right)d\sigma^2 d\mu_x d\mu_y}{\int \ell\left(\mu, \sigma^2 \mid \mathcal{D}_n\right)\pi_\mu(\mu)\pi_\sigma\left(\sigma^2\right)d\sigma^2 d\mu} =$$

$$= \frac{\int \left(\sigma^2\right)^{-n/2} \exp\left\{-\left(n\left(\mu - \xi - \bar{x}\right)^2 + s_x^2\right)\Big/2\sigma^2\right\}\left(\sigma^2\right)^{-n/2} \exp\left\{-\left(n\left(\mu + \xi - \bar{y}\right)^2 + s_y^2\right)\Big/2\sigma^2\right\}\frac{1}{\sqrt{2\pi}} e^{-\frac{\xi^2}{2}}\left(\sigma^2\right)^{-1} d\sigma^2 d\mu d\xi}{\int \left(\sigma^2\right)^{-n/2} \exp\left\{-\left(n\left(\mu - \bar{x}\right)^2 + s_x^2\right)\Big/2\sigma^2\right\}\left(\sigma^2\right)^{-n/2} \exp\left\{-\left(n\left(\mu - \bar{y}\right)^2 + s_y^2\right)\Big/2\sigma^2\right\}\left(\sigma^2\right)^{-1} d\sigma^2 d\mu}$$

Bayes Factor Approximation

- To simplify the Bayes factor, let us define:

$$S^2 = \frac{s_x^2}{n} + \frac{s_y^2}{n} = \frac{\sum_{i=1}^{n}\left(x_i - \bar{x}\right)^2}{n} + \frac{\sum_{i=1}^{n}\left(y_i - \bar{y}\right)^2}{n}$$

- We can then write:

$$B_{10}^{\pi} = \frac{\int \left(\sigma^2\right)^{-n-1} e^{-\frac{n}{2\sigma^2}\left(\left(\mu-\xi-\bar{x}\right)^2+\left(\mu+\xi-\bar{y}\right)^2+S^2\right)} \frac{1}{\sqrt{2\pi}} e^{-\frac{\xi^2}{2}} d\sigma^2 d\mu d\xi}{\int \left(\sigma^2\right)^{-n-1} e^{-\frac{n}{2\sigma^2}\left(\left(\mu-\bar{x}\right)^2+\left(\mu-\bar{y}\right)^2+S^2\right)} d\sigma^2 d\mu}$$

- Performing the integrals in σ^2:

$$B_{10}^{\pi} = \frac{\int \left[\left(\mu-\xi-\bar{x}\right)^2+\left(\mu+\xi-\bar{y}\right)^2+S^2\right]^{-n} \frac{1}{\sqrt{2\pi}} e^{-\frac{\xi^2}{2}} d\mu d\xi}{\int \left[\left(\mu-\bar{x}\right)^2+\left(\mu-\bar{y}\right)^2+S^2\right]^{-n} d\mu}$$

- Lets now integrate in μ. Start with the denominator. Note that:

$$\left(\mu-\bar{x}\right)^2+\left(\mu-\bar{y}\right)^2 = 2\left(\mu-\frac{\bar{x}+\bar{y}}{2}\right)^2 + \frac{\left(\bar{x}-\bar{y}\right)^2}{2}$$

Student-t

Bayes Factor Approximation

$$B_{10}^{\pi} = \frac{\int \left[\left(\mu - \xi - \bar{x}\right)^2 + \left(\mu + \xi - \bar{y}\right)^2 + S^2 \right]^{-n} \frac{1}{\sqrt{2\pi}} e^{-\frac{\xi^2}{2}} d\mu d\xi}{\int \left[\left(\mu - \bar{x}\right)^2 + \left(\mu - \bar{y}\right)^2 + S^2 \right]^{-n} d\mu}$$

- So the denominator takes the form:

$$\int \left[\left(\mu - \bar{x}\right)^2 + \left(\mu - \bar{y}\right)^2 + S^2 \right]^{-n} d\mu = 2^{-n} \int \left[\left(\mu - \frac{\bar{x} + \bar{y}}{2} \right)^2 + \frac{\left(\bar{x} - \bar{y}\right)^2}{4} + \frac{S^2}{2} \right]^{-n} d\mu$$

- With the definitions $\sigma^2 = \dfrac{\dfrac{\left(\bar{x} - \bar{y}\right)^2}{4} + \dfrac{S^2}{2}}{2n-1}$ and $\nu = 2n-1$, we can simplify as:

$$\int \left[\left(\mu - \bar{x}\right)^2 + \left(\mu - \bar{y}\right)^2 + S^2 \right]^{-n} d\mu = \left(2\sigma^2\nu\right)^{-n} \int \left[1 + \left(\mu - \frac{\bar{x} + \bar{y}}{2} \right)^2 \Big/ \sigma^2\nu \right]^{-(\nu+1)/2}$$

$$d\mu = \left(2\sigma^2\nu\right)^{-n} \sigma \frac{\sqrt{\nu\pi}\,\Gamma\left(\frac{\nu}{2}\right)}{\Gamma\left(\frac{\nu+1}{2}\right)} =$$

$$\frac{\sqrt{\nu\pi}}{(2\nu)^n \sigma^{2n-1}} \Gamma\left(\frac{\nu+1}{2}\right) \Big/ \Gamma\left(\frac{\nu}{2}\right) = \underbrace{\frac{\sqrt{\pi}}{2^n} \Gamma\left(\frac{\nu+1}{2}\right) \Big/ \Gamma\left(\frac{\nu}{2}\right)}_{\text{Common Factor in the demomin. and numer.of } B_{10}^{\pi}} \frac{1}{\left(\left(\frac{\bar{x} - \bar{y}}{2}\right)^2 + \frac{S^2}{2} \right)^{n-1/2}}$$

Here we use the normalizing constant of the t-distribution

$$p(\theta) = \frac{\Gamma((\nu+1)/2)}{\Gamma(\nu/2)\sqrt{\nu\pi}\sigma} \left(1 + \frac{1}{\nu}\left(\frac{\theta-\mu}{\sigma}\right)^2\right)^{-(\nu+1)/2}$$

Bayes Factor Approximation

- Thus for the normal case with

$$x_1, \ldots, x_n \sim \mathcal{N}(\mu + \xi, \sigma^2)$$
$$y_1, \ldots, y_n \sim \mathcal{N}(\mu - \xi, \sigma^2) \quad \text{and} \quad H_0 : \xi = 0$$

under prior $\pi(\mu, \sigma^2) = 1/\sigma^2$ and $\xi \sim \mathcal{N}(0,1)$

$$B_{01}^{\pi} = \frac{1}{B_{10}^{\pi}} = \frac{\left[\left(\bar{x} - \bar{y}\right)^2 + 2S^2\right]^{-n+1/2}}{\int \left[\left(2\xi + \bar{x} - \bar{y}\right)^2 + 2S^2\right]^{-n+1/2} e^{-\xi^2/2} d\xi \Big/ \sqrt{2\pi}}$$

For CMBdata, we simulate $\xi_1, \ldots, \xi_{1000} \sim \mathcal{N}(0,1)$ and approximate B_{01}^{π} with (for one simulation that we run)

$$\widehat{B_{01}^{\pi}} = \frac{[(\bar{x} - \bar{y})^2 + 2S^2]^{-n+1/2}}{\sum_{i=1}^{1000} [(2\xi_i + \bar{x} - \bar{y})^2 + 2S^2]^{-n+1/2} / 1000} = 43.3309$$

when $\bar{x} = 0.0888, \bar{y} = 0.1078, S^2 = 0.00875, n = 100$. Thus H_0 is much more likely with the data available.

Precision Evaluation in Bayes Factor

- For an estimator, $I = \int h(\boldsymbol{x})\pi(\boldsymbol{x})d\boldsymbol{x}$ with $x_i \sim \pi(\boldsymbol{x})$, the variance can be computed (in terms of the empirical mean) as

$$v_N = \frac{1}{N}\frac{1}{N-1}\sum_{j=1}^{N}\left[h(x_j) - \overline{h_N}\right]^2$$

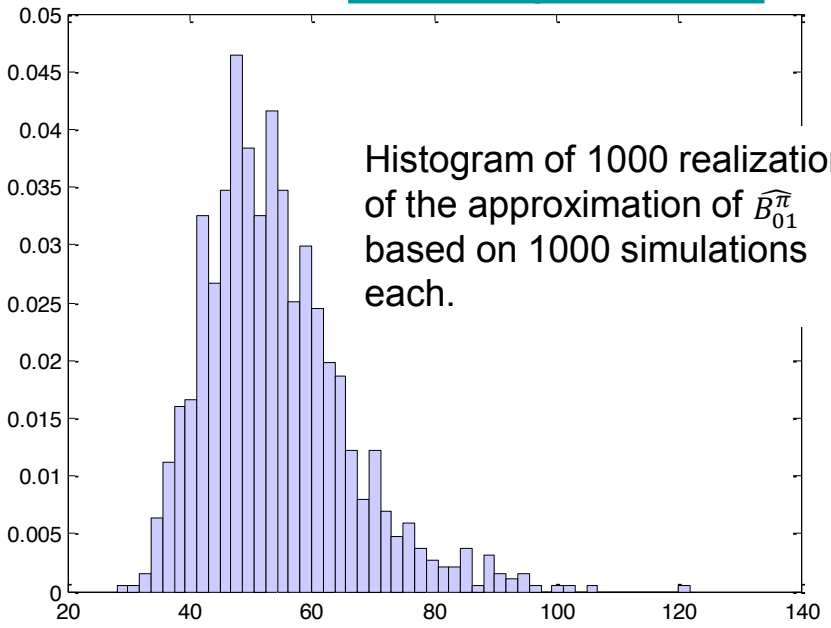
and for N large,

$$\left\{\overline{h_N} - \mathbb{E}_f[h(X)]\right\}/\sqrt{v_N} \sim \mathcal{N}(0,1)$$

We can thus find the variability in the Bayes factor estimation.

We construct a convergence test and of confidence bounds on the approximation of $\widehat{B_{01}^{\pi}}$

MatLab Implementation



Histogram of 1000 realizations of the approximation of $\widehat{B_{01}^{\pi}}$ based on 1000 simulations each.

Example (Cauchy-Normal)

- For estimating a normal mean, a robust prior is a Cauchy prior

$$x \sim \mathcal{N}(\theta,1), \qquad \theta \sim \mathcal{C}(0,1)$$

Under squared error loss, the posterior mean is given as:

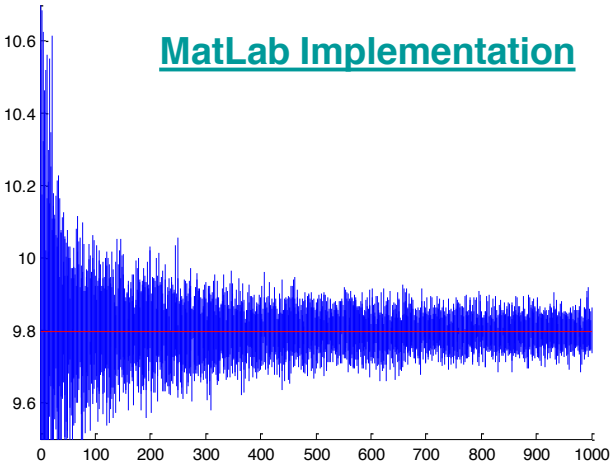
$$\delta^{\pi}(x) = \frac{\int_{-\infty}^{+\infty} \frac{\theta}{1+\theta^2} e^{-(x-\theta)^2/2} d\theta}{\int_{-\infty}^{+\infty} \frac{1}{1+\theta^2} e^{-(x-\theta)^2/2} d\theta}$$

Form of δ^{π} suggests simulating i.i.d. variables $\theta_1, \cdots, \theta_m \sim \mathcal{N}(x,1)$ and calculate

$$\widehat{\delta_m^{\pi}}(x) = \frac{\sum_{i=1}^{m} \frac{\theta_i}{1+\theta_i^2}}{\sum_{i=1}^{m} \frac{1}{1+\theta_i^2}}$$

LLN implies $\widehat{\delta_m^{\pi}}(x) \to \delta^{\pi}(x) \;\; as \;\; m \to \infty$

MatLab Implementation



Random Variable Generation

The Problem of Interest

- $\boldsymbol{x} \equiv$ vector of k –random variables.
- $\pi(\boldsymbol{x}) \equiv$ distribution function. In the context of Bayesian analysis, this will be the posterior distribution.
- Goal is to evaluate $\mathbb{E}_{\pi}\{f(\boldsymbol{x})\}$

$$\mathbb{E}_{\pi}\{f(\boldsymbol{x})\} \equiv \frac{\int f(\boldsymbol{x})\pi(\boldsymbol{x})d\boldsymbol{x}}{\int \pi(\boldsymbol{x})d\boldsymbol{x}}$$

- $\int \pi(\boldsymbol{x})d\boldsymbol{x}$ is the normalizing constant.
- In most algorithms to be discussed in this and the following lectures, we do not need to know this normalization constant.

Monte Carlo Integration: Review

- Monte Carlo integration evaluates $\mathbb{E}_\pi\{f(\mathbf{x})\}$ by drawing samples $\{\boldsymbol{x}_t; t = 1,\dots N\}$ from $\pi(\boldsymbol{x})$ and then approximating

$$\mathbb{E}_\pi\left(f(\mathbf{x})\right) \equiv \frac{1}{N}\sum_{t=1}^{N} f(\mathbf{x}_t),\ \mathbf{x}_t\ i.i.d.$$

- That is, the population mean of $f(X)$ is estimated by a sample mean.
- When $\boldsymbol{x}_t$ are i.i.d., LLN ensures that the approximation can be accurate as desired by increasing N.
- N is the number of samples we use to approximate $\mathbb{E}_\pi\left(f(\mathbf{x})\right)$
- As we have seen, the convergence rate is $\frac{1}{\sqrt{N}}$.

Sampling From an Arbitrary Distribution

- Let us assume that we need to estimate

$$\mathbb{E}_{\pi}\left(f(\mathbf{x})\right) = \int f(\mathbf{x})\pi(\mathbf{x})d\mathbf{x}, \mathbf{x} \in \mathcal{X}$$

- The basic steps in MC are the following:
  - Generate i.i.d samples

$$\mathbf{x}_i \sim \pi(\mathbf{x})$$

But how do we sample from an arbitrary distribution?

  - Evaluate

$$\hat{f} = \frac{1}{N}\sum_{i=1}^{N} f(\mathbf{x}_i)$$

- We have shown that this estimator is unbiased:

$$\mathbb{E}(\hat{f}) = \mathbb{E}_{\pi}(f(\mathbf{x}))$$

- The variance of the estimator is:

$$Var(\hat{f}) = \frac{Var(f(\mathbf{x}))}{N}$$

Sampling From an Arbitrary Distribution

- Consider an arbitrary probability density $\pi(\mathbf{x})$

- Monte Carlo approximation is given by

$$\hat{\pi}_N(\mathbf{x}) = \frac{1}{N}\sum_{i=1}^{N} \delta_{X^{(i)}}(\mathbf{x}) \text{ , } where\ X^{(i)} \overset{i.i.d.}{\sim} \pi$$

- For any function $f : \mathcal{X} \to \mathbb{R}$

$$\mathbb{E}_{\hat{\pi}_N}(f) = \frac{1}{N}\sum_{i=1}^{N} f(X^{(i)}) \cong \mathbb{E}_{\pi}(f)$$

But how do we sample from an arbitrary distribution?

or more precisely:

$$\mathbb{E}_X\left[\mathbb{E}_{\hat{\pi}_N}(f)\right] = \mathbb{E}_{\pi}(f) \ and \ Var_X\left(\mathbb{E}_{\hat{\pi}_N}(f)\right) = \frac{Var_{\pi}\ (f)}{N}$$

Sampling Uniform Random Variables

- Most sampling algorithms rely on generating uniform random variables in $[0, 1]$.
- We only have algorithms for generating pseudo-random numbers which look like they are i.i.d. $\mathcal{U}$ [0, 1].
- There are several standard uniform random number generators available.

Sampling From a Discrete Distribution

- Consider $\mathcal{X} = \{1, 2, 3\}$ and

$$\pi(X = 1) = 1/6,\ \pi(X = 2) = 2/6,\ \pi(X = 3) = 1/2$$

- Define the cdf of X for $x \in [0, 3]$ as

$$F_X(x) = \sum_{i=1}^{3} \pi(X = i)\mathbb{I}(i \leq x)$$

and its inverse for $u \in [0, 1]$

$$F_X^{-1}(u) = \inf\{x \in \mathcal{X}; F_X(x) \geq u\}$$

Sampling from a Discrete Distribution

- Consider the distribution of a discrete random variable
- To sample from this discrete distribution, sample $u \sim \mathcal{U}[0,1]$
- Define the following:

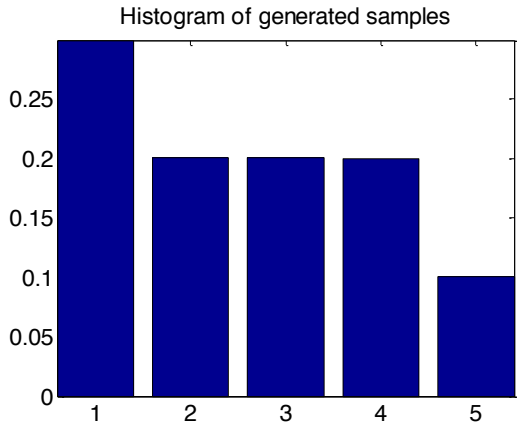
$$P_k = \sum_{j=1}^{k} p_j \in [0,1],\ P_0 = 0,\ P_1 = p_1,\ P_\infty = 1$$

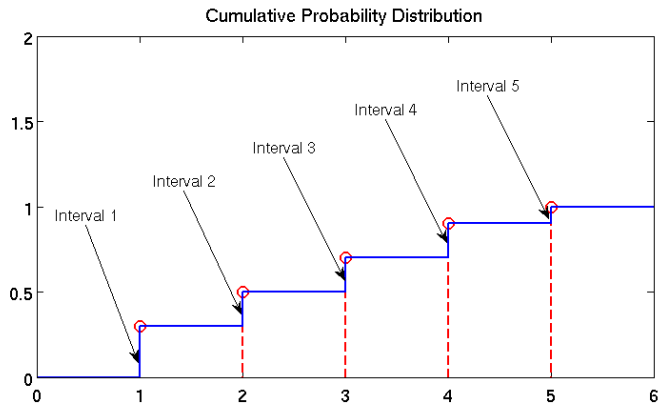
- Obviously

$$P_k = \Pr[X \le k]$$

- Set $x = k$, where

$$k = \min\{k \in \{1,2,3,\ldots,+\infty\} \ \ such\ that \ \ u \le P_k\}$$





MatLab Implementation

Sampling from a Discrete Distribution

- Consider a discrete random variable X taking values $\{1,2,3,\ldots,\infty\}$ with probability $\Pr[X=k]=p_k, with \sum_{i=1}^{\infty} p_i = 1$
- We want by sampling $u \sim \mathcal{U}[0,1]$ to generate samples $x \sim p(X)$
- Let $P_k \in [0,1], s.t.\ P_k = \Pr[X \le k] = \sum_{j=1}^{k} p_j$
- Draw $u \sim \mathcal{U}[0,1]$.
- Then set $x = k$, where $k = \min\{k \in \{1,2,3,\ldots,+\infty\} \ such\ that \ u \le P_k\}$

$$Note: \Pr[x=k] = \Pr[P_{k-1} < u \le P_k] = \int_{P_{k-1}}^{P_k} 1 du$$

$$= P_k - P_{k-1} = \sum_{j=1}^{k} p_j - \sum_{j=1}^{k-1} p_j = p_k, i.e. \quad the\ desired\ distribution$$

Sampling from a Continuous Distribution

- Assume the distribution has a density, then the CDF takes the form:

$$Note: F_X(x) = Pr(X \le x) = \int_{-\infty}^{+\infty} \pi(u)\mathbb{I}(u \le x)du = \int_{-\infty}^{x} \pi(u)du$$

- Algorithm: $u \sim U[0,1]$ and then set $X = F_X^{-1}(u)$. Do we have $X \sim \pi$?

$$Proof: Pr(X \le x) = \Pr\left(u \le F_X(x)\right) \text{ since } F_X \text{ is non-decreasing}$$

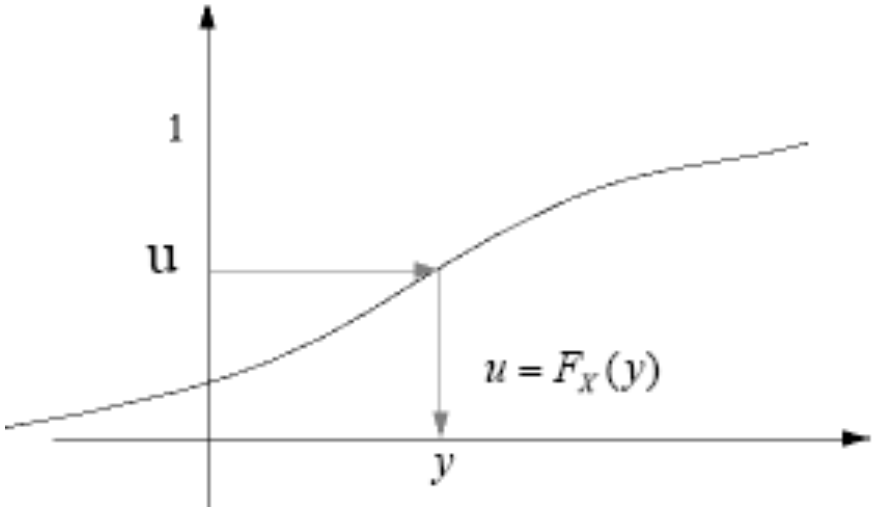
$$= \int_0^1 \mathbb{I}(u \le F_X(x))du \text{ since } u \sim \mathcal{U}[0,1]$$

$$= F_X(x) \text{ which is precisely the CDF of } \pi$$

Reverse Sampling for Continuous Distributions

- Simplest method
- Used frequently for non-uniform random number generation
- Sample a random number u from $\mathcal{U}[0,1)$
- Set $x = y$, where $u = F_X(y)$ (i.e. $x = F_X^{-1}(u)$)
- Simple, but you need the functional form of F.

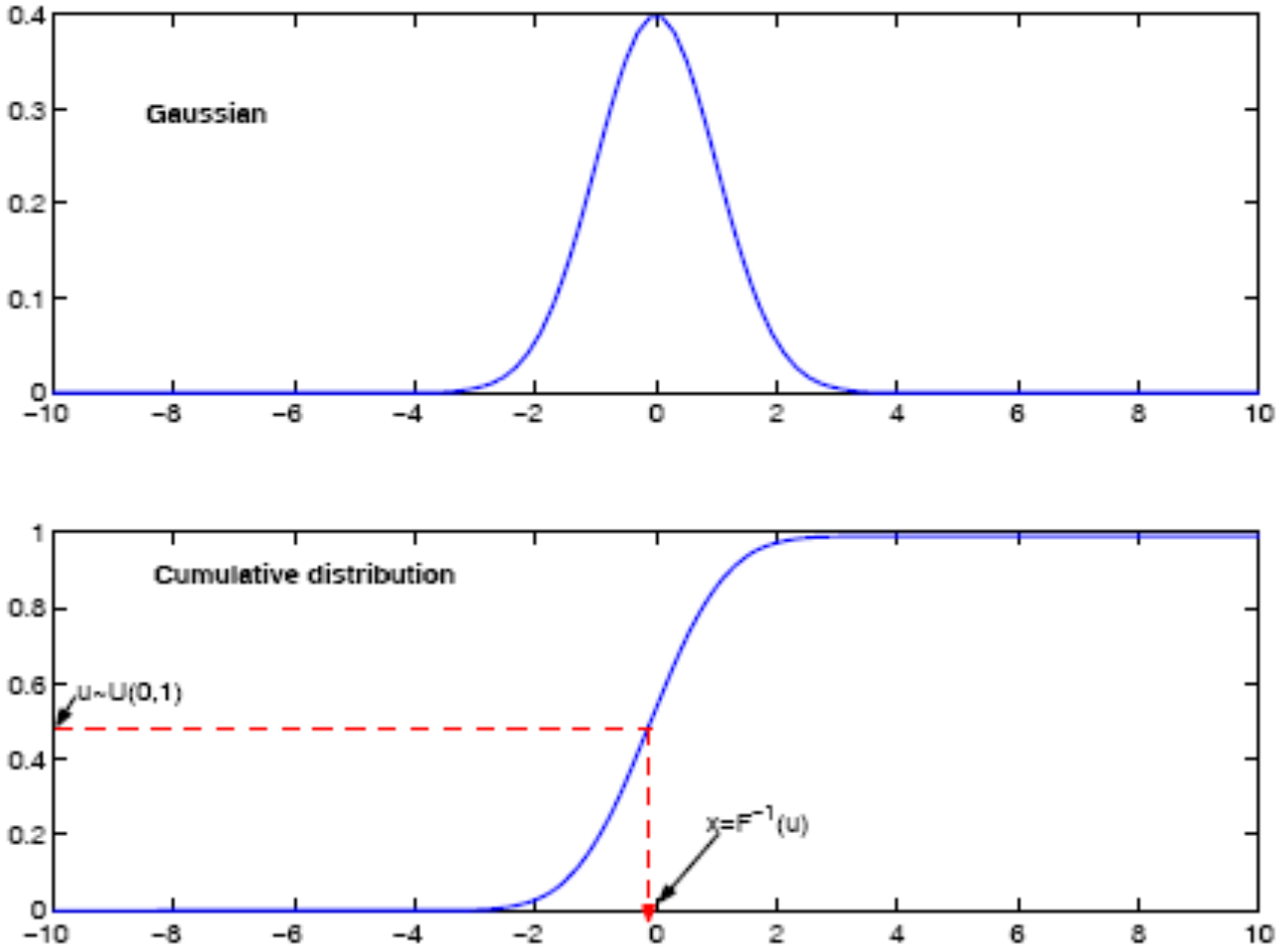
$$Indeed: \Pr[x \le y] = \Pr[u \le F_X(y)]$$
$$= \int_0^{F_X(y)} 1 du = F_X(y)$$



Sampling using the inverse of the CDF

Sampling from a Continuous Distribution

- The distribution and the CDF of a normal distribution



Inverse Method: Exponential Distribution

- Consider the exponential distribution with parameter λ:

$$\pi(x) = \lambda e^{-\lambda x} \mathbb{I}_{[0,+\infty)}$$

- The CDF of X is:

$$F_X(x) = \int_{-\infty}^{x} \pi(z)dz = \begin{cases} 0 \; if \;\; x \le 0 \\ 1 - e^{-\lambda x} \;\; if \;\; x > 0 \end{cases}$$

- Thus the inverse CDF is:

$$1 - e^{-\lambda x} = u \Leftrightarrow x = -\frac{1}{\lambda}\log(1-u) = F_X^{-1}(u)$$

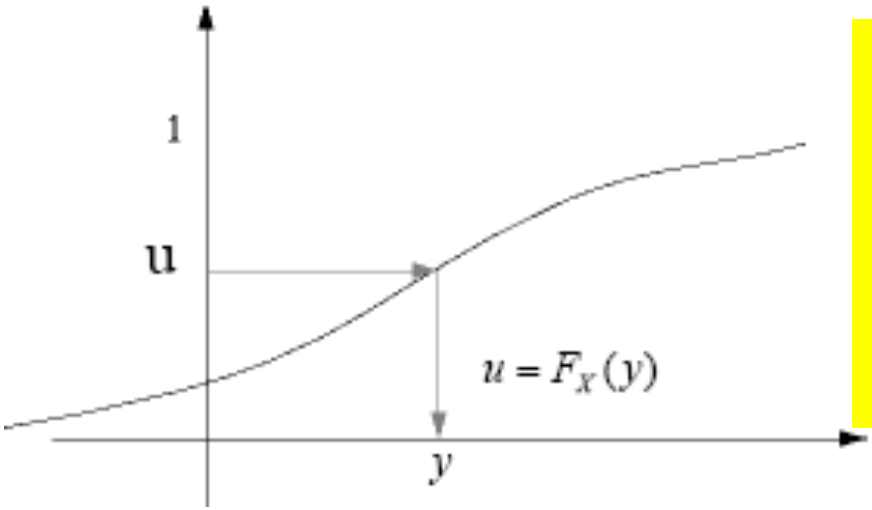
- Inverse method: $u \sim \mathcal{U}[0,1]$, then $X = -\frac{1}{\lambda}\log(1-U) \sim \pi \equiv \mathcal{E}xp(\lambda)$

- Similarly if $u \sim \mathcal{U}[0,1]$, then $X = -\frac{1}{\lambda}\log U \sim \mathcal{E}xp(\lambda)$. Indeed:

$$\Pr(X \le x) = \Pr(-\log U \le \lambda x) = \Pr\left(U \ge e^{-\lambda x}\right) = 1 - e^{-\lambda x} \Rightarrow X \sim \mathcal{E}xp(\lambda)$$

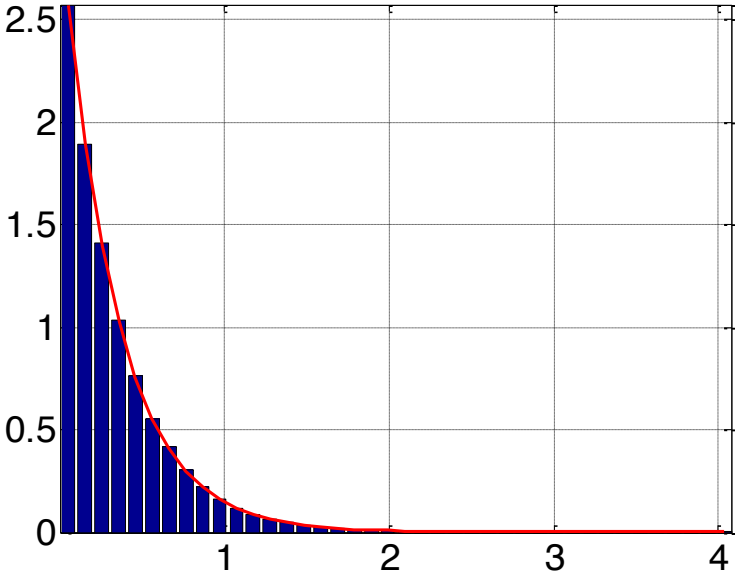
Inverse Method: Exponential Distribution

Exponential(λ): $\pi(x) = \lambda e^{-\lambda x}$, $F_X(y) = 1 - e^{-\lambda y}$, $x = -\ln(1-u)/\lambda$



As $F(y)$ is area under $\pi(y)$, $y = F^{-1}(u)$ prescribes that

- Choose $u = (0, 1]$, then find value y that has that *fraction u of area to the left of y, or $u = F(y)$*
- Return that value of $x = y$.



MatLab Implementation

Inverse Method: Example

- Consider N i.i.d. random variables $X_i \sim f_X$ (with CDF F_X). We are interested to sample from the following distribution:

$$Z = \max\left(X_1, \ldots, X_N\right)$$

- You can use an inverse approach as follows:

$$F_Z(z) = \Pr\left(X_1 \le z, \ldots, X_N \le z\right)$$

$$= \prod_{i=1}^{N} \Pr\left(X_i \le z\right) = \left[F_X(z)\right]^N$$

- Thus for any $U \sim \mathcal{U}[0,1]$, we can sample $Z \sim f_Z$ as follows:

$$Z = F_Z^{-1}(U) = F_X^{-1}(U^{1/N})$$

Inverse Method: Limitations

- Practical and simple method for univariate distributions.
- Limited to cases where the inverse cdf has an analytical form that can be tabulated.
- Its practical use is very limited.

Transformation Methods

- We have seen an example of the transformation method:

$$If\ u \sim \mathcal{U}[0,1] \Rightarrow X = -\frac{1}{\lambda}\log(1-U) \sim \mathcal{E}xp(\lambda)$$

$$If\ u \sim \mathcal{U}[0,1] \Rightarrow X = -\frac{1}{\lambda}\log U \sim \mathcal{E}xp(\lambda)$$

- We use the fact that π is related to other transformations easier to sample from.
- These methods are specific to some distributions, e.g.

$$\text{If } X_i \sim \mathcal{E}xp(1)\ then: Y = 2\sum_{i=1}^{\nu} X_i \sim \chi^2_{2\nu}, \quad Y = \beta\sum_{i=1}^{\alpha} X_i \sim \mathcal{G}amma(\alpha,\beta),$$

$$Y = \frac{\sum_{i=1}^{\alpha} X_i}{\sum_{i=1}^{\alpha+\beta} X_i} \sim \mathcal{B}e(\alpha,\beta)$$

Transformation Methods

- Starting with samples from the uniform distribution, these transformations are very simple to apply:

$$Y = -2\sum_{i=1}^{\nu} \log\left(U_i\right) \sim \chi^2_{2\nu},$$

$$Y = -\beta\sum_{i=1}^{\alpha} \log\left(U_i\right) \sim \mathcal{Gamma}(\alpha, \beta)$$

$$Y = \frac{\sum_{i=1}^{\alpha} \log\left(U_i\right)}{\sum_{i=1}^{\alpha+\beta} \log\left(U_i\right)} \sim \mathcal{Be}(\alpha, \beta)$$

- With this approach, we cannot generate Gamma random variables with a non-integer shape parameter α.

- Cannot generate χ^2_1 which will give us a $\mathcal{N}(0,1)$ variable.

Box Muller Algorithm to Sample Gaussians

- Consider (x, y) coordinates $X_1 \sim \mathcal{N}(0,1)$ *and* $X_2 \sim \mathcal{N}(0,1)$, then the polar coordinates (R, θ) of this point are independent and distributed according to

$$R^2 = X_1^2 + X_2^2 \sim \mathcal{Exp}\left(\frac{1}{2}\right)$$
$$\theta \sim \mathcal{U}[0, 2\pi]$$

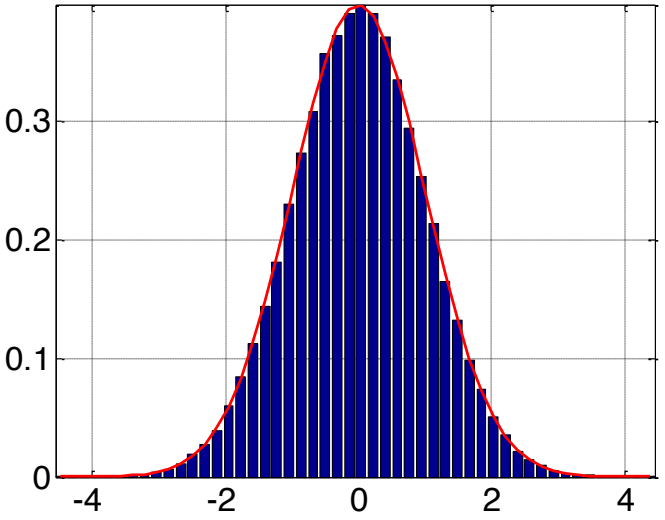
If $X_1 \sim \mathcal{N}(0,1), \ldots, X_n \sim (0,1)$, then $X_1^2 + \ldots + X_n^2 \sim x_n^2$. For n=2, $x_{n=2}^2 \sim \mathcal{E}xp\left(\frac{1}{2}\right)$.

- It is simple to simulate $R = \sqrt{-2\log(U_1)}$ *and* $\theta \sim 2\pi U_2$, where

$U_1 \sim \mathcal{U}[0,1]$ *and* $U_2 \sim \mathcal{U}[0,1]$. *Then*

$$X_1 = R\cos\theta = \sqrt{-2\log(U_1)}\cos(2\pi U_2)$$
$$X_2 = R\sin\theta = \sqrt{-2\log(U_1)}\sin(2\pi U_2)$$

- By construction X_1 and X_2 are two independent $\mathcal{N}(0,1)$ random variables. A plot of one of them is shown here.



MatLab Implementation

Box Muller Algorithm to Sample Gaussians

- Let us see a simpler approach to sample from a spherical Gaussian. We sample z_1, z_2 uniformly from a unit circle: $p(z_1, z_2) = \frac{1}{\pi}\mathbb{I}(z \; inside \; unit \; circle)$. This can be done by sampling uniformly on the cube $[-1\ 1]^2$ and disregarding the samples outside the circle.

- Consider polar coordinates (r, θ). You can show that $\left|\frac{\partial(z_1,z_2)}{\partial(r,\theta)}\right| = \left|\frac{\partial(rcos\theta, rsin\theta)}{\partial(r,\theta)}\right| = r$.

- Define $y_1 = (-2lnr^2)^{1/2}cos\theta, y_2 = (-2lnr^2)^{1/2}sin\theta$. With simple algebra you can show that $\left|\frac{\partial(y_1,y_2)}{\partial(r,\theta)}\right| = -\frac{2}{r}$.
- The distribution of y_1, y_2 can now be computed as:

$$p(y_1, y_2) = p(z_1, z_2)\left|\frac{\partial(z_1, z_2)}{\partial(r, \theta)}\right|\left|\frac{\partial(y_1, y_2)}{\partial(r, \theta)}\right|^{-1} = \frac{1}{\pi}r\frac{r}{2} = \frac{r^2}{2\pi} = \frac{1}{2\pi}exp\left(-\frac{1}{2}(y_1^2 + y_2^2)\right)$$

- Thus we obtain the desired result:

$$p(y_1, y_2) = \frac{1}{\sqrt{2\pi}}exp\left(-\frac{1}{2}y_1^2\right)\frac{1}{\sqrt{2\pi}}exp\left(-\frac{1}{2}y_2^2\right)$$

Sampling from the Bivariate Normal Density

To sample from the bivariate density,

1) Generate two, uncorrelated, standard normal variates, z_1 *and* z_2.

$$z \sim \mathcal{N}\left(\mu = 0, \sigma^2 = 1\right)$$

2) Compute the correlated X_1 and X_2

$$X_1 = \mu_1 + \sigma_1 z_1$$
$$X_2 = \mu_2 + \sigma_2 \left[z_1 \rho + z_2 \sqrt{1 - \rho^2} \right]$$

3) X_1 *and* X_2 will have means μ_1 and μ_2, standard deviations σ_1 and σ_2, and correlation ρ

Sampling from the Bivariate Normal Density

Example 1. data are sampled from the standard bivariate normal distribution

Example 2. data are sampled from the bivariate normal distribution with

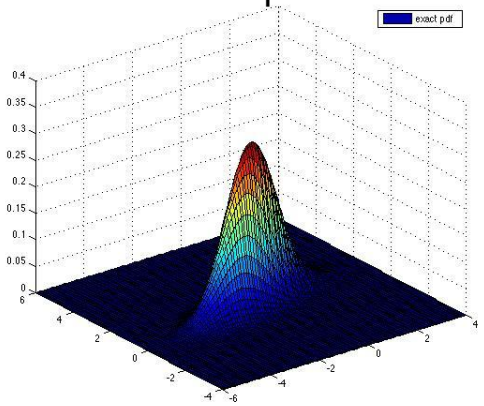
Mean vector $\{\mu_1, \mu_2\} = \{-1, 1\}$

Covariance matrix $\Sigma = \begin{bmatrix} 1.44 & 0.3 \\ 0.3 & 0.25 \end{bmatrix}$

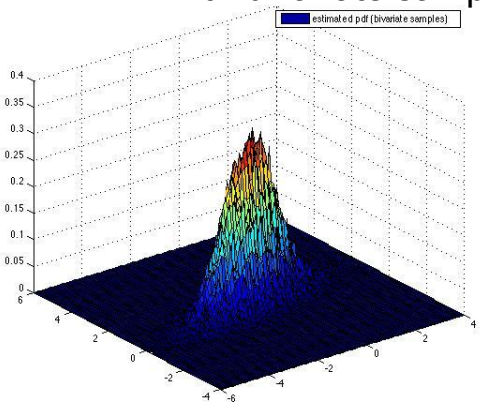
Sampling from the Bivariate Normal Density

Validation of the algorithm

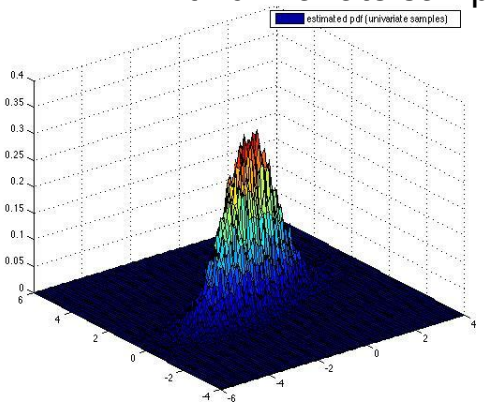
Exact pdf



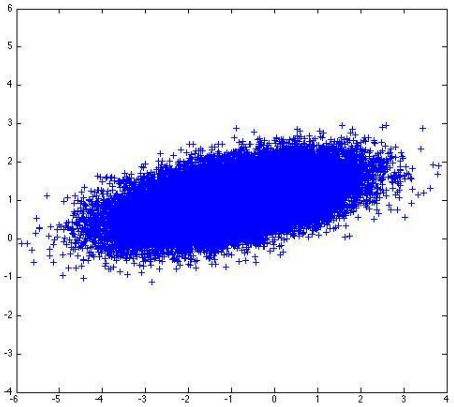
PDF with bivariate samples

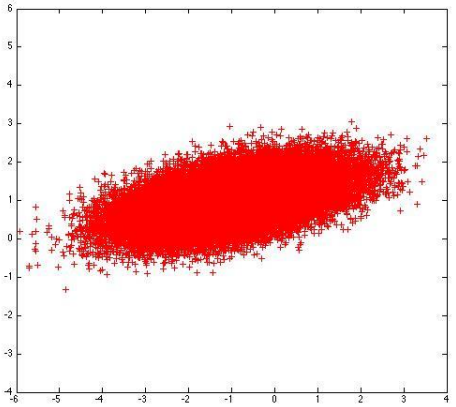


PDF with univariate samples



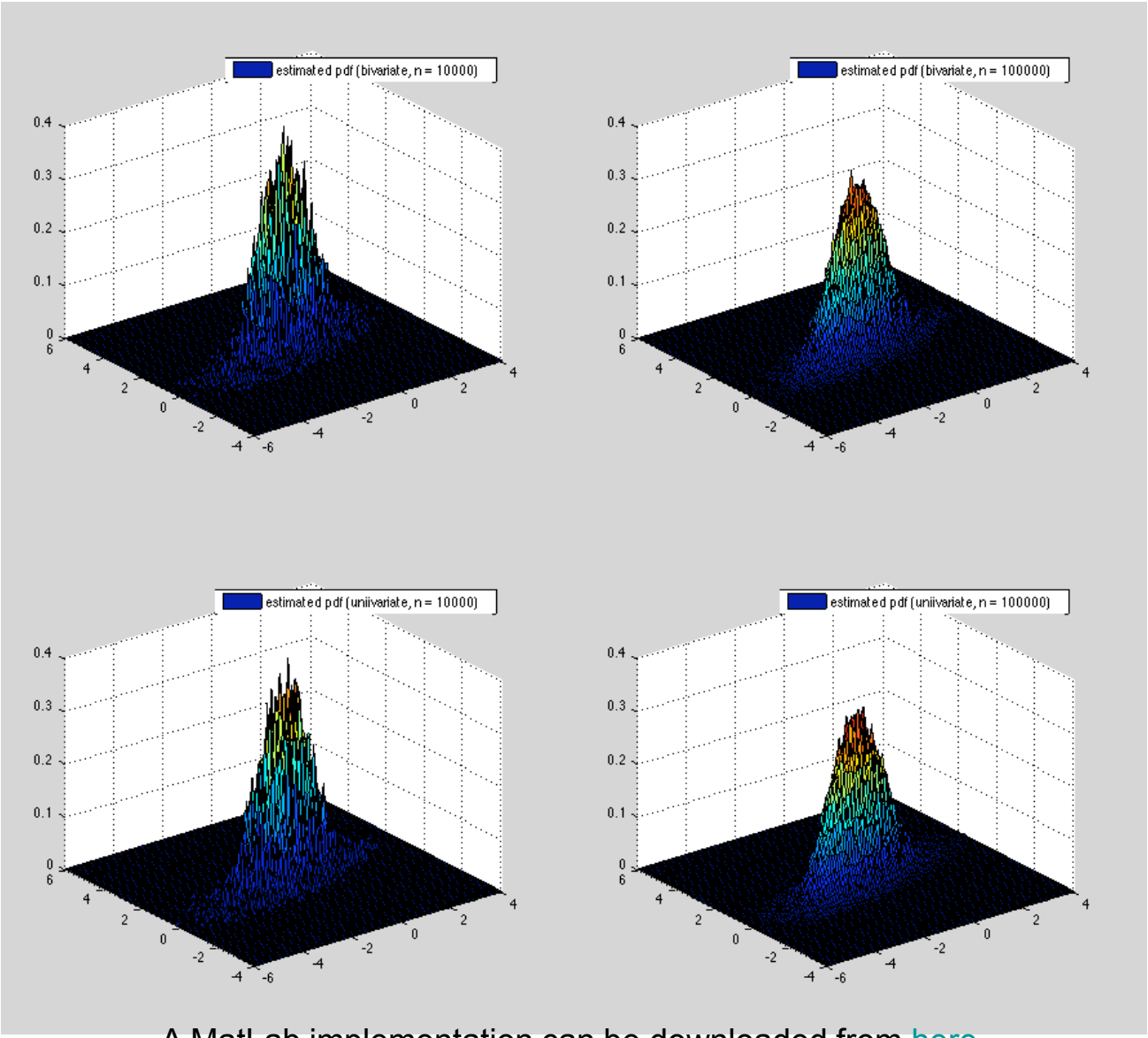
The pdf generated from samples compared with the true standard bivariate Gaussian pdf





A MatLab implementation can be downloaded from here.

Sampling from the Bivariate Normal Density



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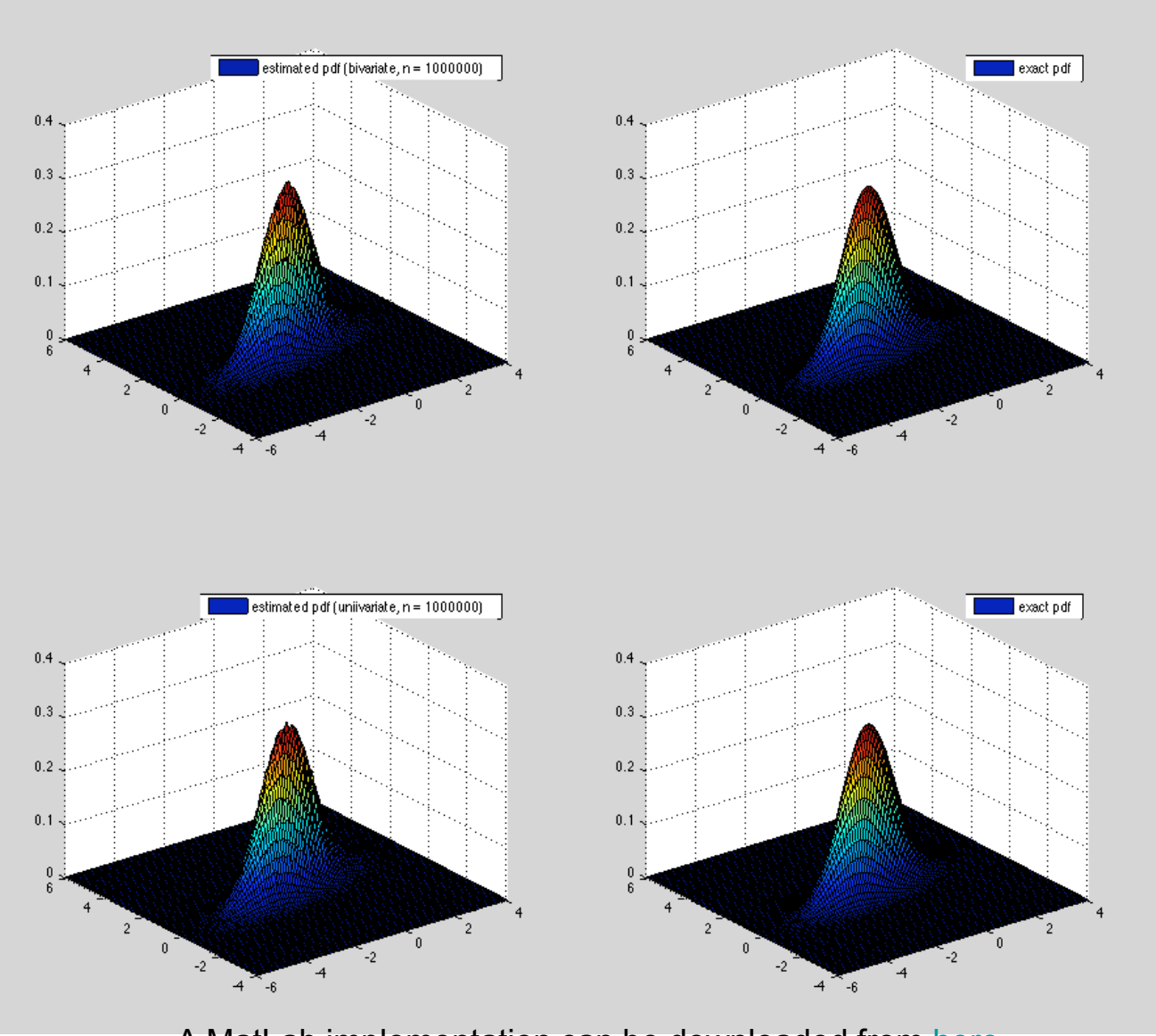
Sampling from the Bivariate Normal Density



A MatLab implementation can be downloaded from here.

Sampling from the Multivariate Gaussian

- In principle, the same approach can work:
  - Sample $\boldsymbol{u} \sim \mathcal{U}[0,1]^d$
  - Set $\boldsymbol{x} = F_X^{-1}(\boldsymbol{u})$
- How about for the multivariate Gaussian: $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$
  - Draw $z_i \sim \mathcal{N}(0,1)$ i.i.d.
  - Introduce the Cholesky decomposition of $\boldsymbol{\Sigma}$: $\boldsymbol{\Sigma} = \boldsymbol{S}\boldsymbol{S}^T$
  - Set

$$\boldsymbol{x} = \boldsymbol{\mu} + \boldsymbol{S}\boldsymbol{z}$$

$$Indeed: \mathbb{E}\left[(\boldsymbol{x} - \boldsymbol{\mu})(\boldsymbol{x} - \boldsymbol{\mu})^T \right] = \mathbb{E}\left[\boldsymbol{S}\boldsymbol{z}\boldsymbol{z}^T \boldsymbol{S}^T \right] =$$

$$= \boldsymbol{S}\mathbb{E}\left[\boldsymbol{z}\boldsymbol{z}^T \right] \boldsymbol{S}^T = \boldsymbol{S}\boldsymbol{S}^T = \boldsymbol{\Sigma}$$