Monte Carlo Methods

MATH 565

Git website and repository

Canvas

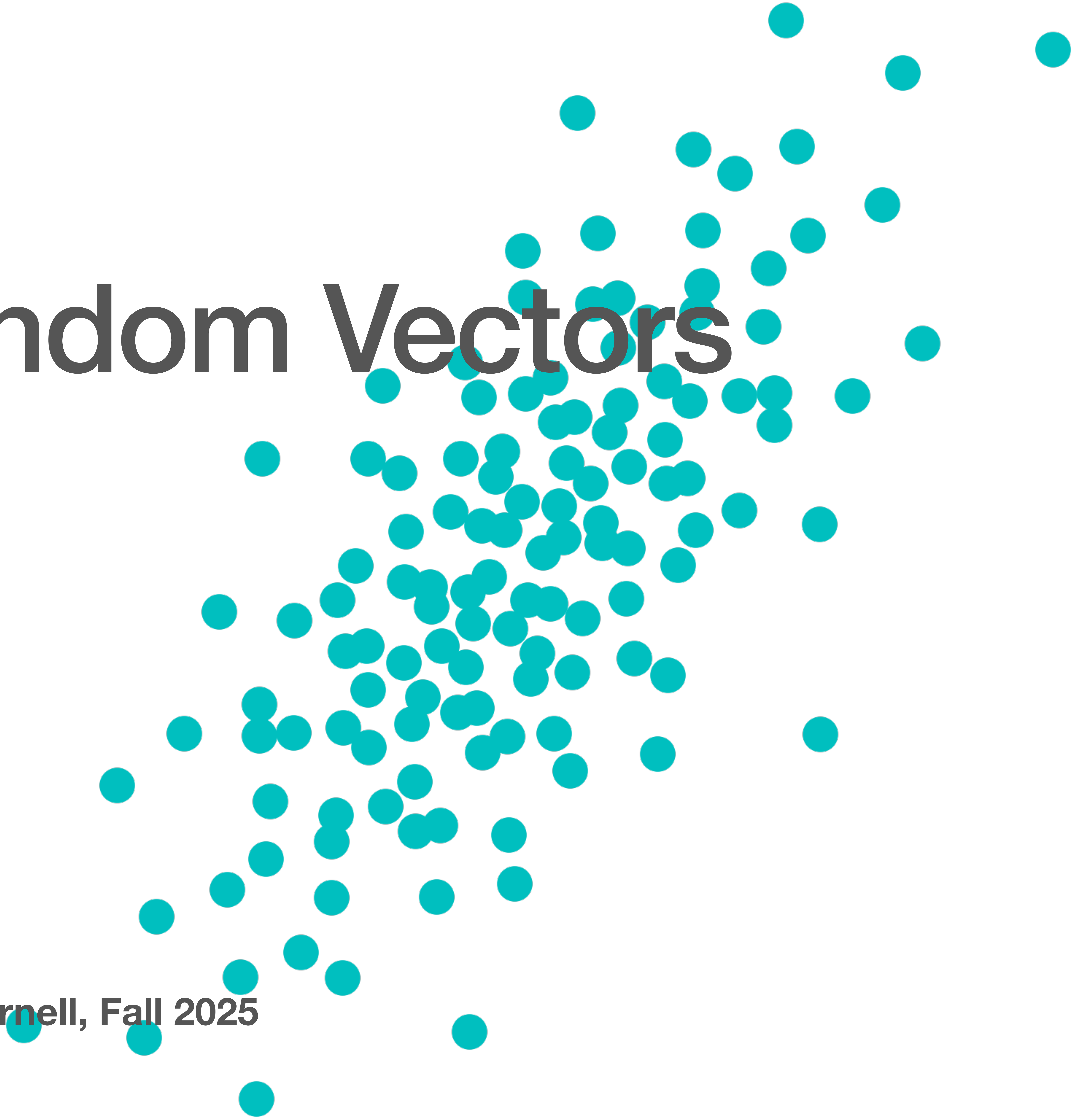
Fred Hickernell, Fall 2025

Updated 2025 August 25

Generating Random Vectors

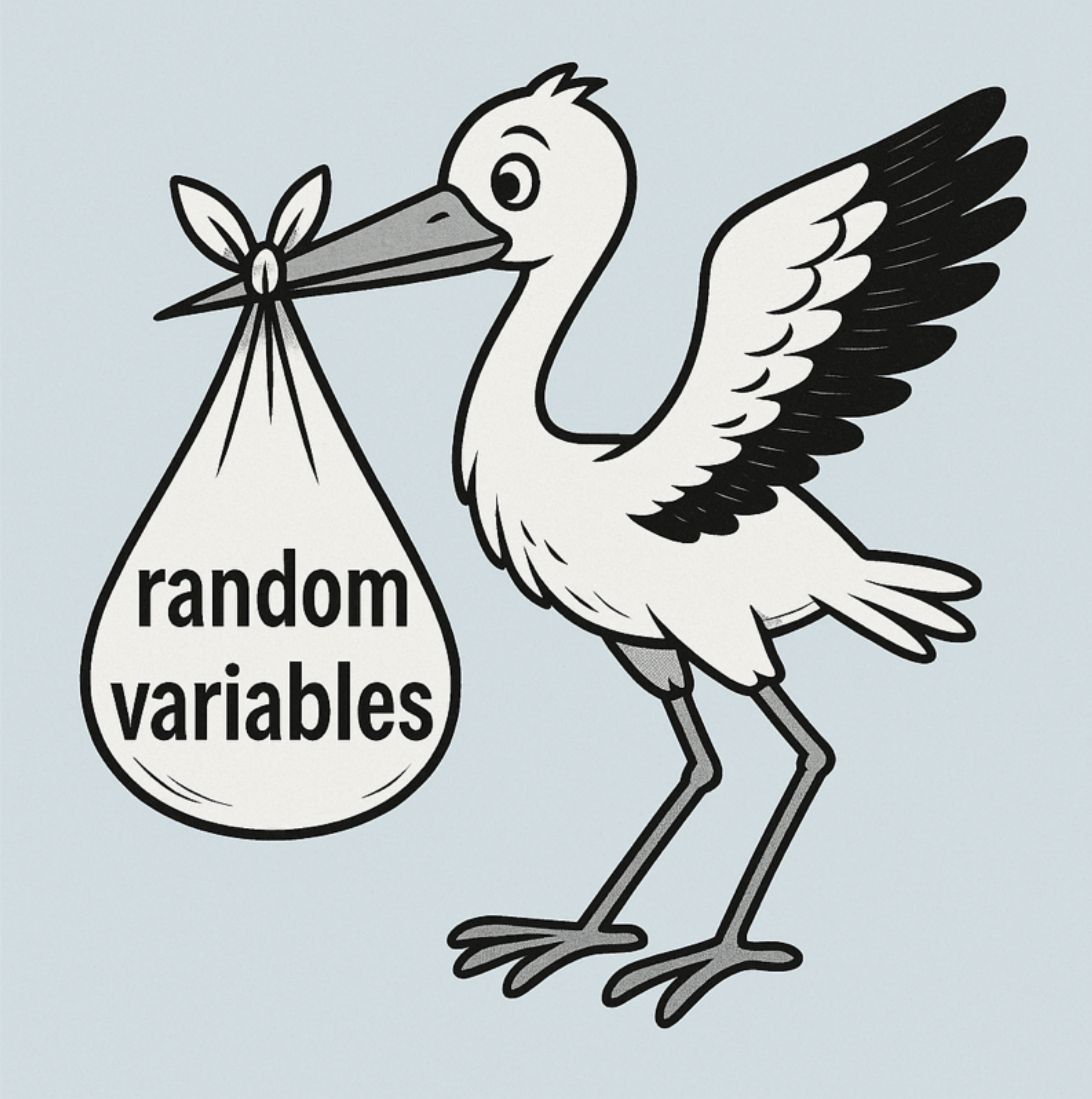
Owen, Chapters 3 & 4

Assignment ?



MATH 565 Monte Carlo Methods, Fred Hickernell, Fall 2025

Where do random variables come from?



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- Pseudo-random number generators are tested to ensure that their output looks IID random in every way possible
- Care must be taken when working on multiple processors
- For a drastic failure see RANDU
- Physical random number generators may be random, but cannot be guaranteed to be IID random of the desired distribution

Quantile function gives non-uniform random numbers

- Most random number generators output $U_1, U_2, \ldots$ that mimic IID $\mathcal{U}[0,1]$.
- To get $X_1, X_2, \ldots$ IID with cumulative distribution function F, we use the quantile function, Q, where $Q(u) := \inf\{x \in \mathcal{X} : F(x) \geq u\}$. Note that

$$Q(u) \leq x \iff u \leq F(x)$$

- Letting $X := Q(U)$, it follows that

$$\mathbb{P}(X \leq x) = \mathbb{P}(Q(U) \leq x) = \mathbb{P}(U \leq F(x)) = F(x)$$

and so $X \sim F$, and

$$X_1 := Q(U_1), X_2 := Q(U_2), \ldots \overset{\text{IID}}{\sim} F$$

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$x \in$	$[0,1)$	$[1,2)$	$[2,3)$	$[3,\infty)$
$\varrho(x)$	0.4^3	$2(0.6)(0.4^2)$	$2(0.6^2)(0.4)$	0.6^3
$\varrho(x)$	0.064	0.288	0.432	0.216
$F(x)$	0.064	0.352	0.784	1
$u \in$	$(0,0.064]$	$(0.064,0.352]$	$(0.352,0.784]$	$(0.784,1]$
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Note that F is right-continuous and Q is left-continuous

Explorations in generating random vectors

Generating Random Vectors

Zero-inflated exponential

Suppose that X is a non-negative random variable with probability p_0 of being zero and otherwise an exponential distribution

$$F(x) = \begin{cases} 0 & -\infty < x < 0 \\ p_0 + (1 - p_0)\exp(-\lambda x) & 0 \le x < \infty \end{cases}$$

To generate $X_1, X_2, \ldots \overset{\text{IID}}{\sim} F$ from $U_1, U_2, \ldots \overset{\text{IID}}{\sim} \mathcal{U}[0,1]$, we need the quantile function

Quantile function for zero-inflated exponential

$$F(x) = \begin{cases} 0 & -\infty < x < 0 \\ p_0 + (1 - p_0)\exp(-\lambda x) & 0 \leq x < \infty \end{cases}$$

$$u = F(x) \implies \begin{cases} x = 0, & 0 < u \leq p_0 \\ u = p_0 + (1 - p_0)\exp(-\lambda x), & p_0 \leq u < 1 \end{cases}$$

$$\iff \begin{cases} x = 0, & 0 < u \leq p_0 \\ \dfrac{u - p_0}{1 - p_0} = \exp(-\lambda x), & p_0 \leq u < 1 \end{cases}$$

$$\iff x = Q(u) = \begin{cases} 0, & 0 < u \leq p_0 \\ \lambda \log\left(\dfrac{1 - p_0}{u - p_0}\right), & p_0 \leq u < 1 \end{cases}$$

Random vectors with independent marginals

Suppose that $\boldsymbol{X} = (X_1, \ldots, X_d)$ is a random vector with independent marginals. Then

$$\boldsymbol{X} = \big(Q_1(\boldsymbol{U}_1), \ldots, Q_d(\boldsymbol{U}_d)\big), \quad \boldsymbol{U} \sim \mathcal{U}[0,1]^d$$

has the desired distribution, provided that $Q_1, \ldots, Q_d$ are the corresponding quantile functions.

We express n samples of $\boldsymbol{X}$ as an $n \times d$ matrix or array,

$\mathsf{X} = \begin{pmatrix} X_{11} & X_{12} & \cdots & X_{1d} \\ \vdots & \vdots & & \vdots \\ X_{11} & X_{12} & \cdots & X_{1d} \end{pmatrix}$ where X_{ij} is the j^{th} component of the i^{th} sample

Multivariate normal distribution

If $\boldsymbol{Z} \sim \mathcal{N}(\mathbf{0}_d, \mathrm{I}_d)$, i.e., a d-dimensional standard normal random variable, then $\boldsymbol{X} = \mathrm{A}\boldsymbol{Z} + \boldsymbol{b}$ (thinking of $\boldsymbol{Z}$ as a column vector) has

$$
\begin{aligned}
\boldsymbol{\mu} &= \mathbb{E}(\boldsymbol{X}) = \boldsymbol{b} \\
\Sigma &= \mathrm{cov}(\boldsymbol{X}) = \mathbb{E}[(\boldsymbol{X} - \boldsymbol{\mu})(\boldsymbol{X} - \boldsymbol{\mu})^\top] \\
&= \mathbb{E}[\mathrm{A}\boldsymbol{Z}\boldsymbol{Z}^T\mathrm{A}^T] = \mathrm{A}\mathrm{A}^\top
\end{aligned}
$$

So $\boldsymbol{X} \sim \mathcal{N}(\boldsymbol{b}, \Sigma)$, where Σ is symmetric and positive-definite. So, give a desired $\boldsymbol{\mu}$ and Σ, one needs only to find A with $\Sigma = \mathrm{A}\mathrm{A}^\top$, and then

$$\boldsymbol{X} = \mathrm{A}\boldsymbol{Z} + \boldsymbol{\mu} \sim \mathcal{N}(\boldsymbol{\mu}, \Sigma)$$

Note that there are multiple ways to decompose $\Sigma = \mathrm{A}\mathrm{A}^\top$.

Low discrepancy sampling

Acceptance–rejection sampling

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Bias–variance decomposition