Lecture 3: Classical Simulation

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The Road Ahead

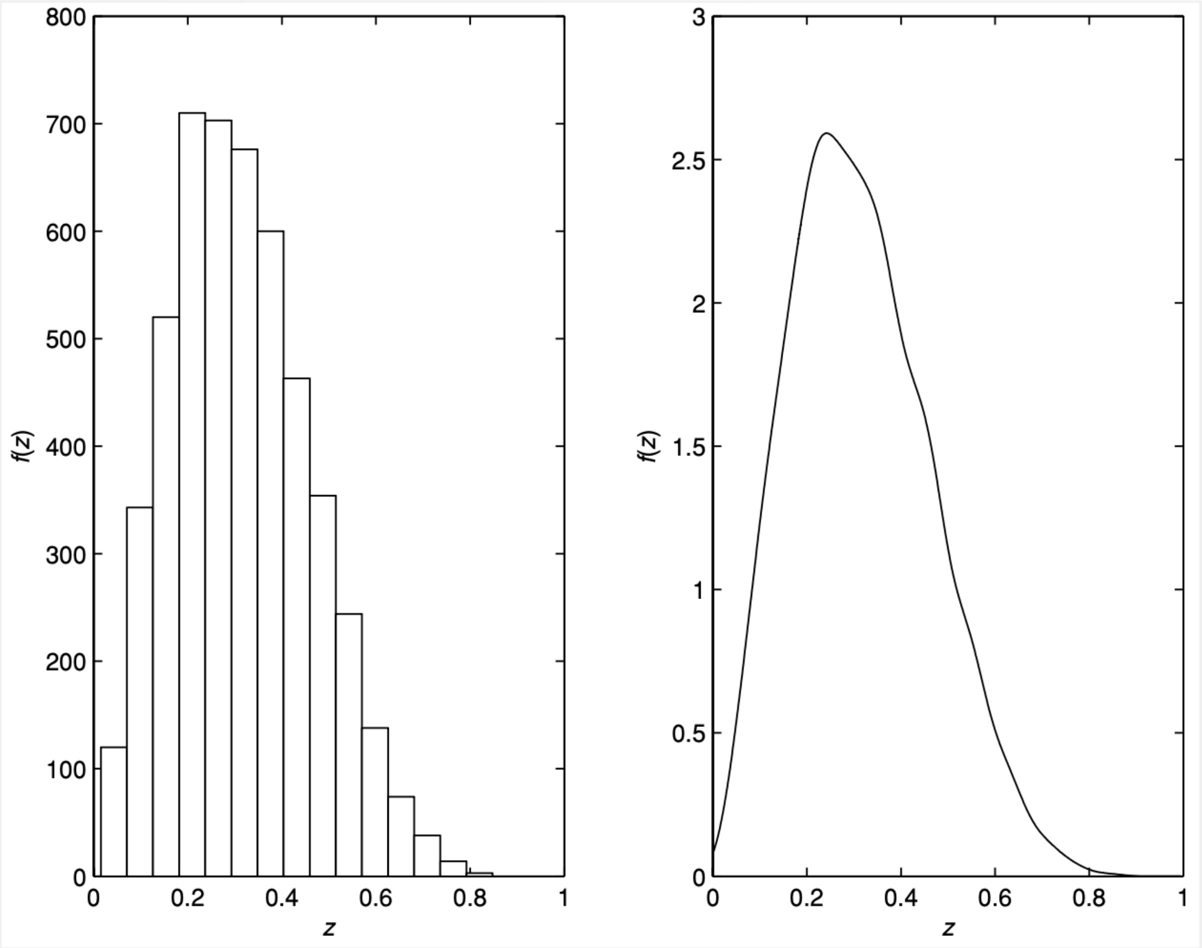
Using Simulated Output

- Use $\{y^{(g)}\}_{g=1}^{G} \sim f(y)$ to investigate properties of $f(y)$, e.g.
  - approximate distribution of $X = h(Y)$, e.g. moments; numerical standard error (n.s.e.) = $\sqrt{\mathbb{V}(X)/G}$
  - 90% credible set: $0.05G$-th & $0.95G$-th ordered $y^{(g)}$
  - marginal (column) vs. joint (row) distribution

$$\{\theta^{(g)}\}_{g=1}^{G} = \begin{bmatrix} \theta_1^{(1)} & \theta_2^{(1)} & \cdots & \theta_d^{(1)} \\ \theta_1^{(2)} & \theta_2^{(2)} & \cdots & \theta_d^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ \theta_1^{(G)} & \theta_2^{(G)} & \cdots & \theta_d^{(G)} \end{bmatrix}$$

- Example: learn distribution $f(z)$ of $Z = XY$, $X \sim \mathcal{B}(3,3)$ and $Y \sim \mathcal{B}(5,3)$ are independent. Sample $\{x^{(g)}\}_{g=1}^{G}$, $\{y^{(g)}\}_{g=1}^{G}$, then $z^{(g)} = x^{(g)} y^{(g)} \sim f(z)$

Using Simulated Output (Cont'd)



- Histogram (left) vs. kernel-smoothed density (right)

Probability Integral Transform

Algorithm 1

Step 1: draw $u \sim \mathcal{U}(0,1)$
Step 2: return $y = F^{-1}(u)$ as a draw from $f(y)$

- Represent $f(y)$ with $\mathbb{P}(Y \leq y) = F(y)$ by simulating *independent* samples from uniform distribution
  - useful for sampling from truncated $F(y)$: $\frac{F(y)-F(c_1)}{F(c_2)-F(c_1)}$ for $c_1 \leq y \leq c_2$
  - not applicable for multivariate as F is not injective
- Example: $f(y) = \frac{3}{8}y^2$ for $0 \leq y \leq 2$ and 0 otherwise
  - compute $F(y) = \frac{1}{8}y^3$ for $0 \leq y \leq 2$
  - draw $u \sim \mathcal{U}(0,1) \Rightarrow y = 2u^{\frac{1}{3}} \sim f(y)$

Python Code

```python
import numpy as np
import scipy.stats as stats
import matplotlib.pyplot as plt

# Generate random numbers
u = np.random.rand(10000)   # uniform
x = 2 * u**(1/3)   # probability integral transform

# Plot
plt.hist(x, bins=50, density=True, color="red", alpha=0.5)
plt.xlabel("x")
plt.ylabel("Probability Density")
plt.title("Histogram")
plt.show()
```

Composition

Algorithm 2

$$\text{Step 1: draw } y \sim h(y)$$

$$\text{Step 2: draw } x \sim g(x|y) \;\Rightarrow\; x \sim f(x) = \int g(x|y)h(y)dy$$

- Example: sample regression error $u_i|\sigma^2 \sim t_\nu(0, \sigma^2)$

$$f(u_i|\sigma^2) = \int \underbrace{g(u_i|\lambda_i, \sigma^2)}_{\mathcal{N}(u_i|0,\sigma^2/\lambda_i)} \; \underbrace{h(\lambda_i)}_{\mathcal{G}(\lambda_i|\nu/2,\nu/2)} \; d\lambda_i$$

  - conditional heteroskedasticity: $\mathbb{V}(u_i|\lambda_i, \sigma^2) = \lambda_i^{-1}\sigma^2$
  - unconditional homoskedasticity: $\mathbb{V}(u_i|\sigma^2) = \frac{\nu}{\nu-2}\sigma^2$

- Finite mixture distribution

$$f(x) = \sum_{i=1}^{K} p_i f_i(x), \qquad \sum_{i=1}^{K} p_i = 1$$

Python Code

```python
def mix_normal(w, dist, n):
    """
    Try help(mix_normal) at runtime to display docstring
    """
    m = len(w)
    index = np.random.choice(m, size=n, p=w)   # categorical random variable
    sample = np.zeros(n)   # sample each component
    for i in range(m):
        k = np.where(index == i)
        sample[k] = dist[i].rvs(size=len(k[0]))
    return sample

# Sample mixture normal
w = [0.5, 0.5]
dist = [stats.norm(loc=-3, scale=1), stats.norm(loc=3, scale=1)]
sample = mix_normal(w, dist, 10000)
```

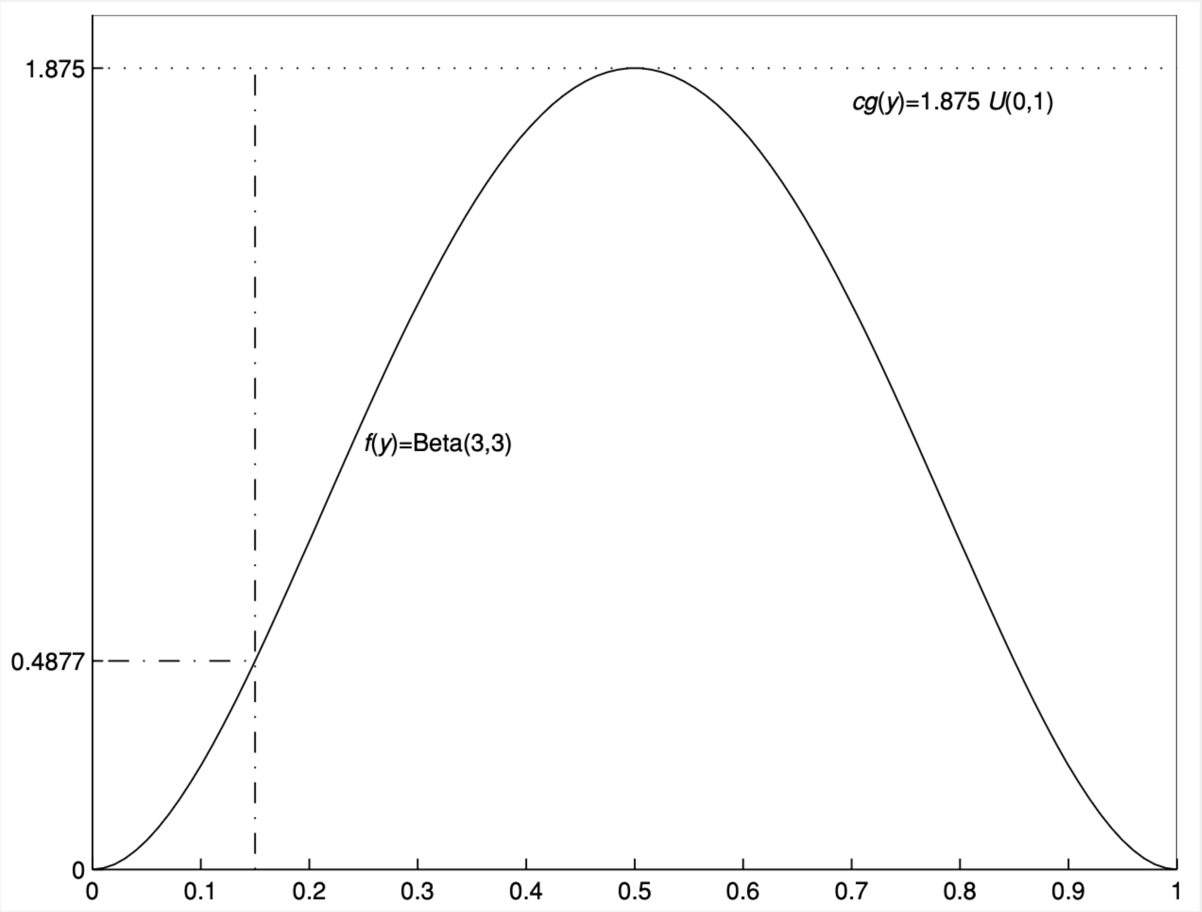
Accept-Reject

Algorithm 3

$$\begin{aligned}&\text{Step 1: draw } y \sim g(y)\\&\text{Step 2: draw } u \sim \mathcal{U}(0,1)\\&\text{Step 3: accept } y \text{ as a draw from } f(y) \text{ if } u \leq \frac{f(y)}{cg(y)};\\&\qquad\qquad \text{otherwise reject and return to step 1}\end{aligned}$$

- Represent target $f(y)$ by simulating *independent* samples from proposal $g(y)$ with $f(y) \leq cg(y)$ for some $c \geq 1$
  - $1/c$ = probability of acceptance $\Rightarrow$ choose small c
  - difficult to find proposal in multivariate case
- Example: sample $y \sim \mathcal{B}(3,3)$? Choose proposal $\mathcal{U}(0,1)$ and set $c = f(.5)/g(.5) = 1.875$

Accept-Reject (Cont'd)



- Efficient sampler tailors proposal to mimic target

Python Code

```python
def target(x):
    return stats.beta.pdf(x, a=3, b=3)

def proposal(x):
    return stats.uniform.pdf(x)

def accept_reject(target, proposal, c, n):
    sample = []
    while len(sample) < n:
        x = np.random.uniform(0, 1)
        u = np.random.uniform(0, 1)
        if u <= target(x) / (proposal(x)*c):
            sample.append(x)
    return np.array(sample)

# Sample beta
c = target(0.5) / proposal(0.5)
sample = accept_reject(target, proposal, c, 10000)
```

Importance Sampling

Algorithm 4

$$\mathbb{E}[g(X)] \approx \frac{1}{G}\sum_{g=1}^{G} g(x^{(g)})\underbrace{f(x^{(g)})/h(x^{(g)})}_{\text{importance weight}}, \quad \{x^{(g)}\}_{g=1}^{G} \sim h(x)$$

- Monte Carlo integration: estimate $\mathbb{E}[g(X)] = \int g(x)f(x)dx$ by simulating *independent* samples from proposal $h(x)$
  - efficiency requires tailoring $h(x)$ to $f(x)$
  - why Gaussian is not suitable for $h(x)$? (thin tails)
- Example: $\mathbb{E}[(1+x^2)^{-1}]$, $x \sim \text{Exponential}(1)$ truncated to $[0,1]$
  - step 1: sample $\{x^{(g)}\}_{g=1}^{G} \sim \mathcal{B}(2,3)$
  - step 2: compute $\frac{1}{G}\sum_{g=1}^{G} \frac{1}{1+(x^{(g)})^2} \frac{e^{-x^{(g)}}}{1-e^{-1}} \frac{\mathbb{B}(2,3)}{x^{(g)}(1-(x^{(g)})^2)}$

Python Code

```python
def imp_sampler(target, proposal, sampler, n):
    sample = sampler(n)
    w = target(sample) / proposal(sample)
    return sample, w

# Monte Carlo integration
target = lambda x: stats.expon.pdf(x, scale=1)
proposal = lambda x: stats.beta.pdf(x, a=2, b=3)
sampler = lambda n: stats.beta.rvs(a=2, b=3, size=n)
n = 10000
sample, w = imp_sampler(target, proposal, sampler, n)
estimate = sum(1 / (1+sample**2) * w) / n
```

Readings

- DeGroot & Schervish (2002), "Probability and Statistics," Addison-Wesley
- Robert & Casella (2004), "Monte Carlo Statistical Methods," Springer-Verlag