Computational Statistics

Instructor: Ming Lin

Computational Statistics

- **Time and Location:**
  - 16:40-18:20, Tuesday; Room 208, Nanqiang Building
  - 14:30-16:10, Thursday; Room 208, Nanqiang Building
- **Course Instructor:** Ming Lin
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  - Office Hour: 13:00-16:00, Tuesday
- **Teaching Assistant:** Shuhui Ai
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- **QQ Group:** 745075488

Computational Statistics

- **Prerequisties:** Calculus, Linear Algebra, Probability Theory, Mathematical Statistics

- **References:**
  - Computational Statistics , Geof H. Givens and Jennifer A. Hoeting, John Wiley & Sons, Inc., 2nd edition, 2013.
  - Numerical Optimization, Jorge Nocedal and Stephen J. Wright, Springer, 2nd edition, 2006.
  - Simulation, Sheldon M. Ross, Elsevier, 5th edition, 2013.
  - Monte Carlo Statistical Methods, Christian P. Robert and George Casella, Springer, New York, 2nd edition, 2004.

- **Homework:**
  - Homework assignments are due on Tuesday, **before the class.**
  - You need use Python to do programming.
- **Grade Policy:**
  - Homework 35%,
  - Midterm Exam 30%,
  - Final Exam 35%.

- **Course Outline:**

  1. Optimization and Solving Nonlinear Equations
  2. EM Optimization Methods
  3. Numerical Integration
  4. Simulation and Monte Carlo Integration
  5. Markov Chain Monte Carlo
  6. Nonparametric Density Estimation
  7. Bootstrapping
  8. Combinational Optimization

1. Optimization and Solving Nonlinear Equations

- **Optimization Problem:** We want to find a point $\theta^* \in \Theta$ (for example, $\Theta = \mathbb{R}^p$) to maximize (or minimize) an *objective function* $g(\theta)$, denoted by

$$\theta^* = \arg\max_{\theta \in \Theta} g(\theta).$$

Under certain conditions, it is equivalent to solving equation $\nabla g(\theta) = 0$.

- **Maximum Likelihood Estimate (MLE):** Let $X_1, X_2, \cdots, X_n$ be a random sample following a distribution with probability density function (PDF) $f(x_1, \cdots, x_n; \theta)$, where θ is a $p \times 1$ vector.
  - For each given $x_1, \cdots, x_n$, $f(x_1, \cdots, x_n; \theta)$ considered as a function of the parameter θ is called the *likelihood function* and denoted by $l(\theta)$.
  - The MLE of θ is

$$\hat{\theta}_{MLE} = \arg\max_{\theta \in \Theta} l(\theta) = \arg\max_{\theta \in \Theta} \log l(\theta).$$

1. Optimization and Solving Nonlinear Equations

- We often use an iterative updating step

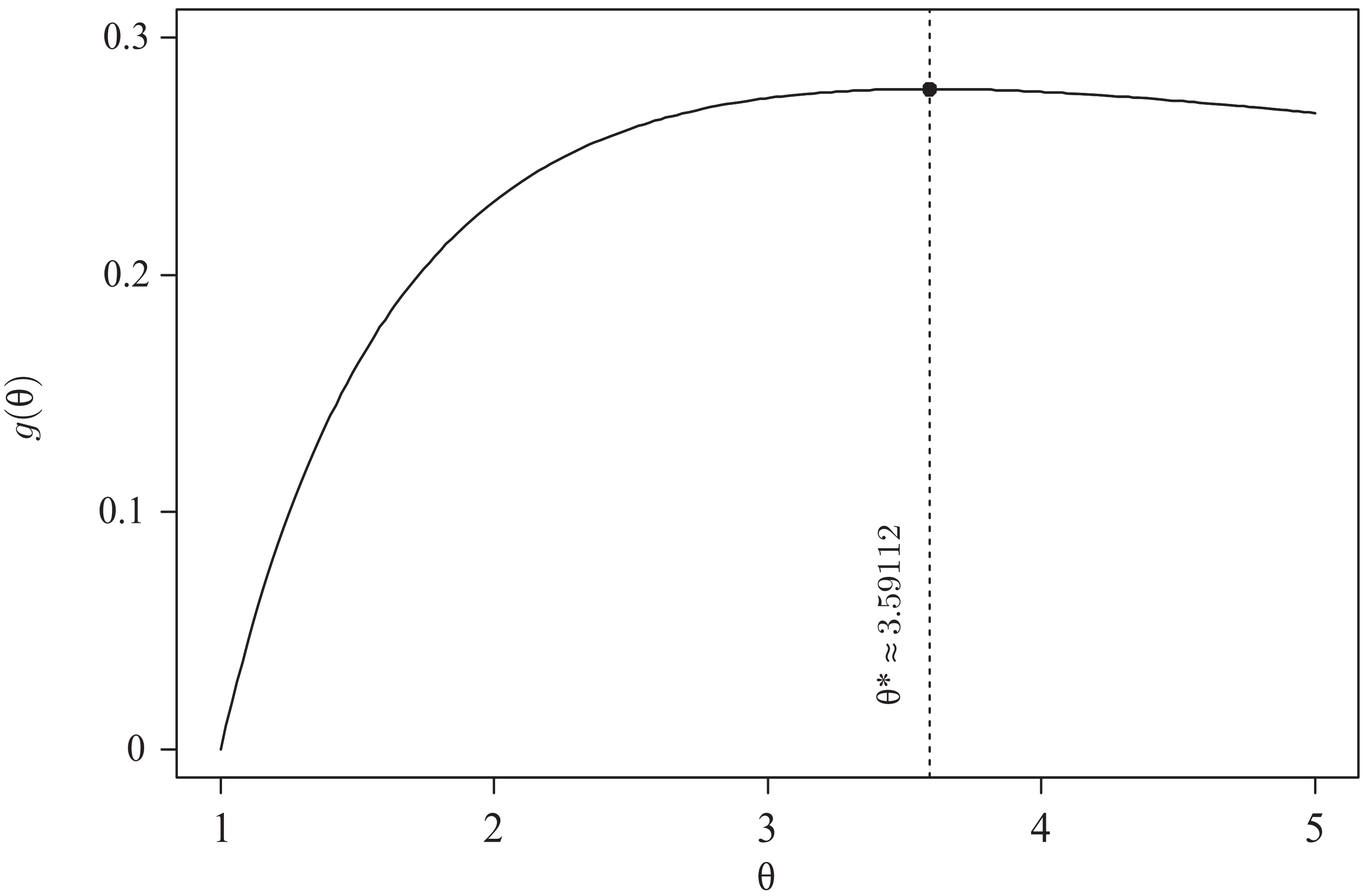
$$\theta^{(t+1)} = \theta^{(t)} + \alpha_t u^{(t)}$$

to search for θ^*, where $u^{(t)}$ is a $p \times 1$ direction vector and $\alpha_t > 0$ is the *step size*. Consider Taylor series expansion, we have

$$g(\theta^{(t+1)}) = g(\theta^{(t)} + \alpha_t u^{(t)}) \approx g(\theta^{(t)}) + \alpha_t \nabla g(\theta^{(t)})^T u^{(t)}.$$

When $\nabla g(\theta^{(t)})^T u^{(t)} > 0$ and α_t is not too large, we can have $g(\theta^{(t+1)}) > g(\theta^{(t)})$.

  - How to choose $u^{(t)}$?
  - How to decide α_t?


0.3
0.2
0.1
0
$g(\theta)$
$\theta^* \approx 3.59112$
1
2
3
4
5
θ

2. EM Optimization Methods

- Suppose we want to estimate parameter θ in model $f_{XY}(x, y; \theta)$, but we can not observe x.
  - In this case, the MLE of θ is

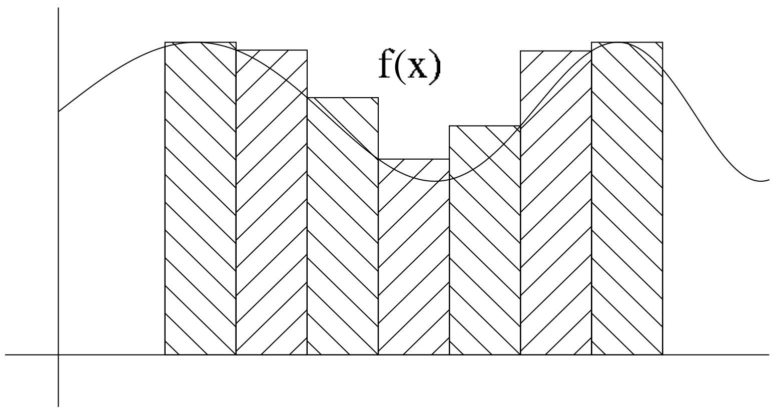
$$\begin{aligned} \theta_{MLE} &= \arg\max_{\theta} l(\theta) \\ &= \arg\max_{\theta} f_Y(y; \theta) = \arg\max_{\theta} \int f_{XY}(x, y; \theta)\, dx. \end{aligned}$$

  - The integration $\int f_{XY}(x, y; \theta)\, dx$ may be difficult to calculate.
  - The expectation-maximization (EM) algorithm provides a strategy to find the MLE in this case.

3. Numerical Integration

- Suppose we want to calculate integration $\int g(x)\,dx$ for some function $g(\cdot)$.
  - For example, when $g(x) = f_{XY}(x,y)$ for a given y, then $\int g(x)\,dx = \int f_{XY}(x,y)\,dx = f_Y(y)$.
  - **Numerical Integration:** Let $a = t_0 < t_1 < \cdots < t_{m-1} < t_m = b$ be a partition of interval $[a,b]$ and ξ_j is any point between t_{j-1} and t_j. Then

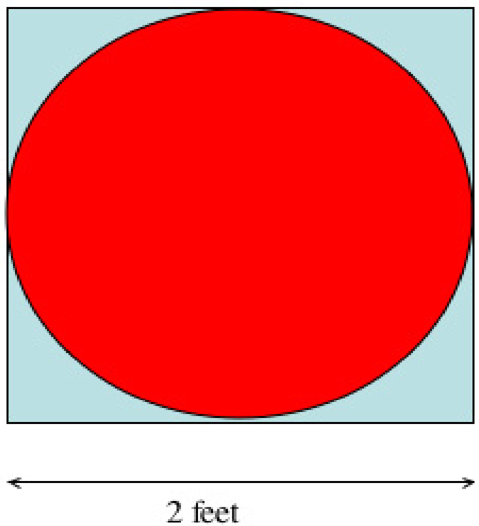
$$\widetilde{\Pi} \triangleq \sum_{j=1}^{m} g(\xi_j)(t_j - t_{j-1}) \to \int_a^b g(x)\,dx.$$



4. Simulation and Monte Carlo Integration

- **Example: Calculating π.** A circle of radius 1 will have area equal to π, and a square drawn around that circle will have area 4. If we draw samples (x_j, y_j), $j = 1, \cdots, m$, uniformly distributed within the square, then

$$\frac{1}{m}\sum_{j=1}^{m} I(x_j^2 + y_j^2 < 1) \approx \pi/4.$$



4. Simulation and Monte Carlo Integration

- Calculate π using simulation:
  - Generate random samples (x_j, y_j), $j = 1, \cdots, m$, where $x_j \sim U(-1, 1)$ and $y_j \sim U(-1, 1)$.
  - Estimate π by

$$\widehat{\pi} = 4 \cdot \frac{1}{m} \sum_{j=1}^{m} I(x_j^2 + y_j^2 < 1),$$

where $I(\cdot)$ is the indicator function.

4. Simulation and Monte Carlo Integration

- **Monte Carlo Methods:**
  - Wikipedia: Monte Carlo methods are a broad class of computational algorithms that rely on repeated **random sampling** to obtain numerical results.
  - It was named, by Stanislaw Ulam and Nicholas Metropolis, after the Monte Carlo Casino.

4. Simulation and Monte Carlo Integration

- **Monte Carlo Integration:** Suppose we want to calculate $\int g(x)\,dx$.
  - Generate random samples $x^{(1)}, \cdots, x^{(m)}$ from a *trial distribution* (or *sampling distribution*) with PDF $q(x)$.
  - Calculate

$$\begin{aligned} \widehat{\Pi} &= \frac{1}{m}\sum_{j=1}^{m}\frac{g(x^{(j)})}{q(x^{(j)})} \\ &\to E\left(\frac{g(x^{(j)})}{q(x^{(j)})}\right) = \int \frac{g(x)}{q(x)}\,q(x)dx = \int g(x)\,dx. \end{aligned}$$

- **Example: Calculating π.** We want to calculate integration

$$\pi = \int_{x^2+y^2<1} 1\, dxdy = \int I(x^2+y^2<1)\, dxdy.$$

  – Generate random samples (x_j, y_j), $j = 1, \cdots, m$, where $x_j \sim U(-1,1)$ and $y_j \sim U(-1,1)$. The PDF of the trial distribution is

$$q(x,y) = 1/4 \quad \text{for } -1 < x, y < 1.$$

  – Estimate π by

$$\begin{aligned} \widehat{\pi} &= \frac{1}{m}\sum_{j=1}^{m} \frac{I(x_j^2+y_j^2<1)}{q(x_j,y_j)} \\ &= 4 \cdot \frac{1}{m}\sum_{j=1}^{m} I(x_j^2+y_j^2<1). \end{aligned}$$

4. Simulation and Monte Carlo Integration

- The convergence rate of Monte Carlo integration is

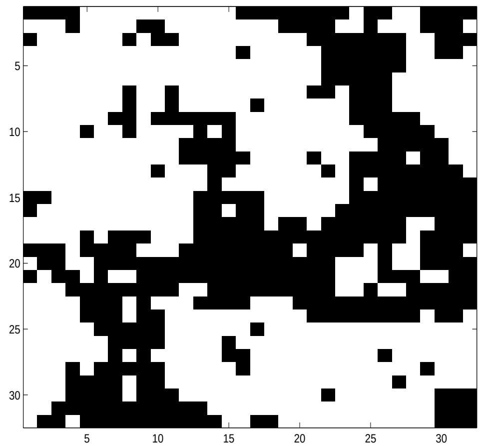
$$\sqrt{\mathrm{Var}(\widehat{\Pi})} = \sqrt{\frac{1}{m}\mathrm{Var}\left(\frac{g(x^{(j)})}{q(x^{(j)})}\right)} = \frac{c}{\sqrt{m}}.$$

- In one-dimensional cases, the convergence rate of numerical integration is $1/m$.

- However, the convergence rate of numerical integration will decrease as the dimension of x increases.

- **Markov Chain Monte Carlo (MCMC):** We want to compute $E_f[g(X)] = \int g(x)f(x)\,dx$, where the dimension of x is large. The MCMC algorithm generates a sequence of random variables $x^{(1)}, \cdots, x^{(m)}$ (a Markov chain), so that $\frac{1}{m}\sum_{i=1}^{m} g(x^{(i)}) \xrightarrow{a.s.} E_f[g(x)]$.

- **Ising Model:** In a magnet field, the atomic spins on a $N \times N$ lattice space, $\mathcal{L} = \{(i,j) : i,j = 1, \cdots, N\}$, can be represented by a random matrix $\boldsymbol{X} = \{X_{i,j}\}_{N \times N}$. Each $X_{i,j}$ is either 1 or -1.



5. Markov Chain Monte Carlo

- The random matrix X follows a distribution with the form

$$\pi(\boldsymbol{x}) = P(\boldsymbol{X} = \boldsymbol{x}) = \frac{1}{S}\, e^{-U(\boldsymbol{x})/kT} \propto e^{-U(\boldsymbol{x})/kT},$$

where $\boldsymbol{x} = \{x_{i,j}\}_{N\times N}$, k is the Boltzmann constant, T is the temperature, $S = \sum_{\boldsymbol{x}} e^{-U(\boldsymbol{x})/kT}$ is the normalizing constant.

  – The potential function is

$$U(\boldsymbol{x}) = -J \sum_{(i,j)\sim(i',j')} x_{i,j}\, x_{i',j'} + \sum_{i,j} h_{i,j}\, x_{i,j},$$

where the symbol $(i,j) \sim (i',j')$ means that the two sites are neighbors, J is called the *interaction strength*, $\{h_{i,j}\}_{N\times N}$ is the magnetic field.

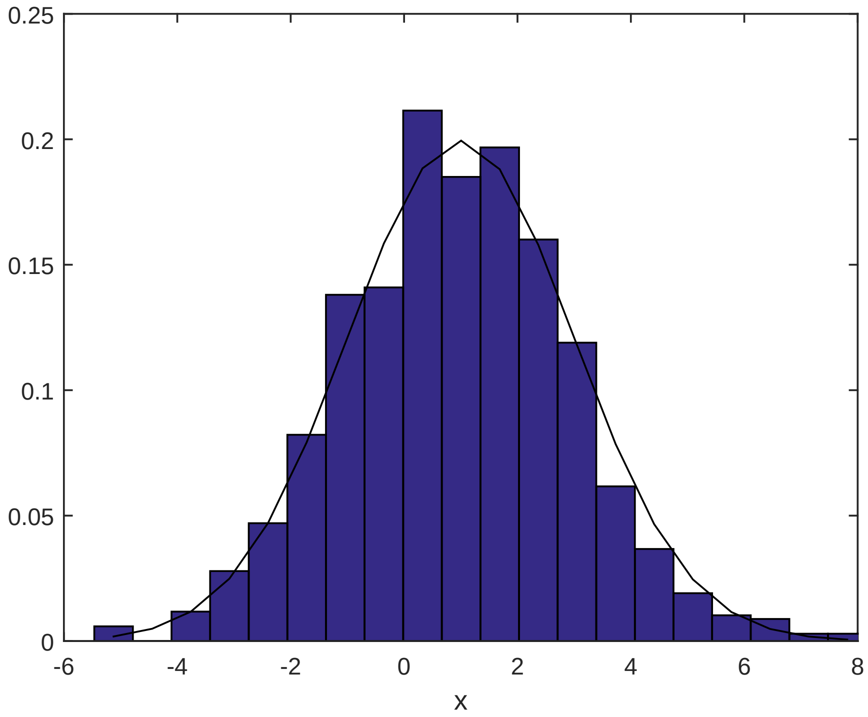
  – We want to calculate the *internal energy*, which is defined as

$$E\big[U(\boldsymbol{X})\big] = \sum_{\boldsymbol{x}} U(\boldsymbol{x})\pi(\boldsymbol{x}) = \frac{\sum_{\boldsymbol{x}} U(\boldsymbol{x}) e^{-U(\boldsymbol{x})/kT}}{\sum_{\boldsymbol{x}} e^{-U(\boldsymbol{x})/kT}}.$$

6. Nonparametric Density Estimation

- Suppose we have i.i.d. samples $X_1, X_2, \cdots, X_n$ from a distribution with unknown density function $f(x)$. How to use the samples to estimate $f(x)$ without assuming its parametric form?

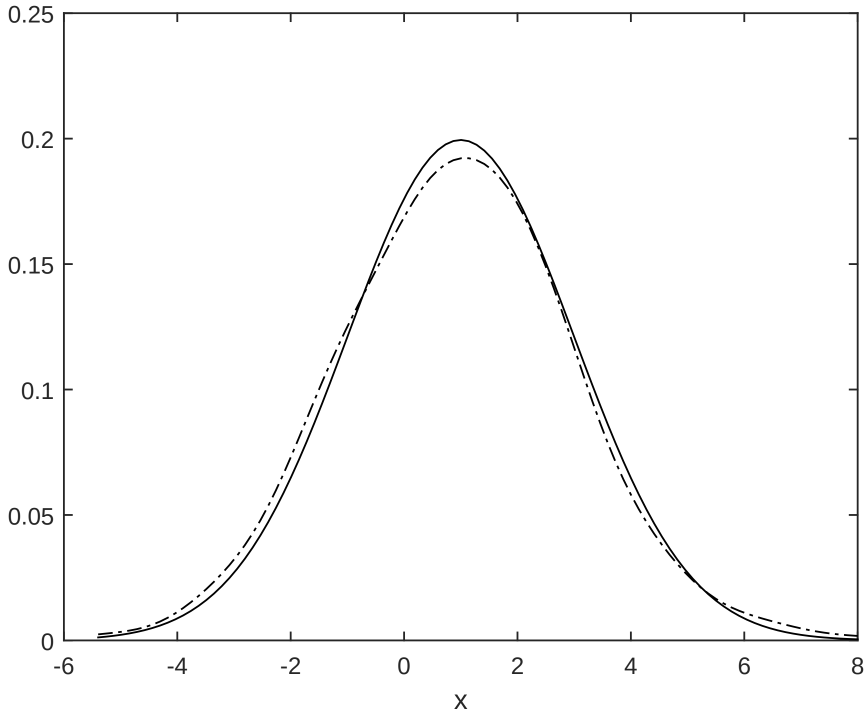
- **Histogram Estimator:** The true distribution is $N(1, 4)$ and $n = 1000$.



- **Kernel Estimator:** Estimate the density function $f(x)$ by

$$f_{K,n}(t) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{h_n} K\left(\frac{t - X_i}{h_n}\right),$$

where $K(t)$ is a kernel function satisfying $K(t) \geq 0$ and $\int K(t)\, dt = 1$.



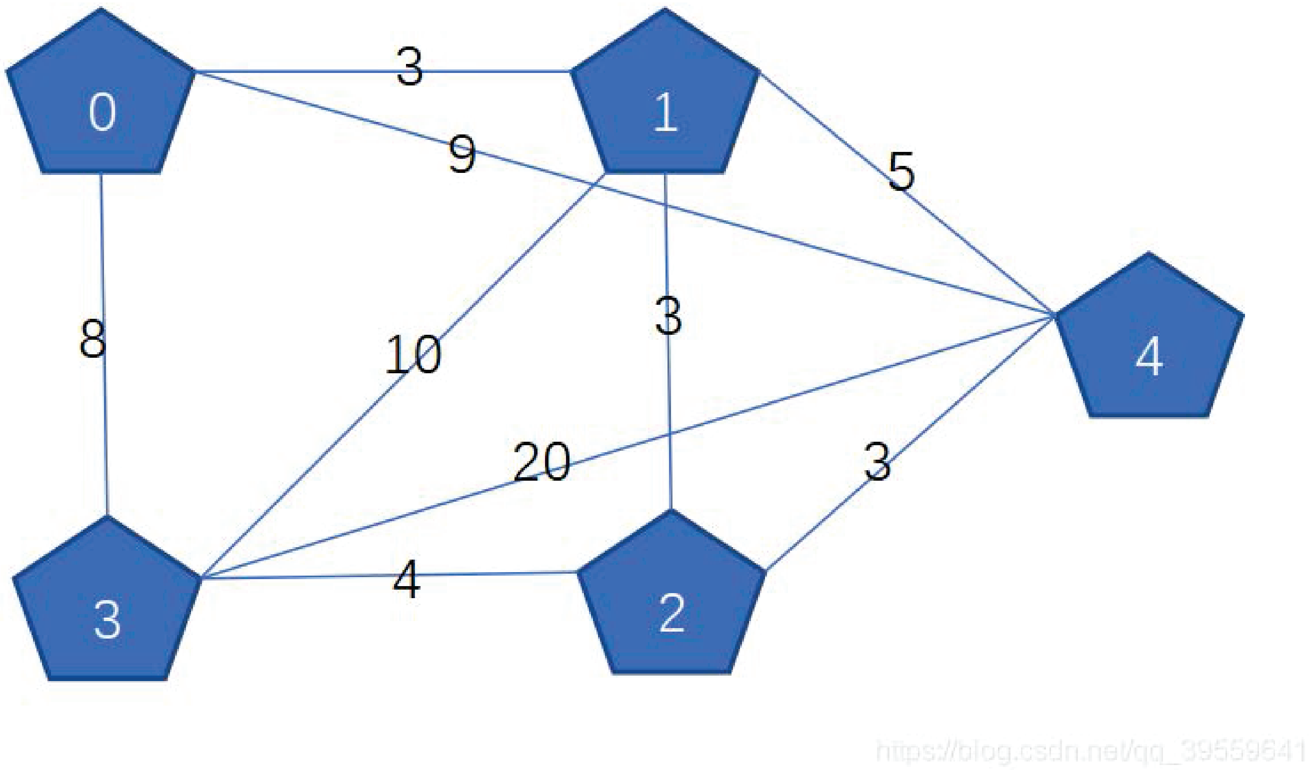
7. Bootstrapping

- Suppose we have one realization $x_1, \cdots, x_n$ of i.i.d. random variables $X_1, \cdots, X_n$. We often want to know the distribution of a statistic $T(X_1, \cdots, X_n)$, especially for testing problems.
  - We only have one observation $T(x_1, \cdots, x_n)$, how to estimate the distribution of $T(X_1, \cdots, X_n)$?
  - **Bootstrap Method:**
    - $\ast$ For $b = 1, \cdots, B$,
      - · Randomly draw samples $\{x_1^{*(b)}, \cdots, x_n^{*(b)}\}$ from $\{x_1, \cdots, x_n\}$ with replacement;
      - · Compute $T^{*(b)} = T(x_1^{*(b)}, \cdots, x_n^{*(b)})$.
    - $\ast$ Under certain conditions, we can use $\{T^{*(1)}, \cdots, T^{*(B)}\}$ to estimate the distribution of $T(X_1, \cdots, X_n)$.

8. Combinational Optimization

- We want to find $\theta^* \in \Theta$ to maximize (or minimize) an objective function $g(\theta)$, where Θ is a discrete set consisting of N elements. Usually N is very large.

- **Travelling Salesman Problem:** There are p cities with pathes connecting any two of them. Starting from one city, the salesman need to visit each of the p cities exactly once and return to his point of origin.
  - There are $(p-1)!/2$ possible routes. How to find the route with the shortest total travel distance?
  - We can not use derivatives to solve this problem.



Travelling Salesman Problem

8. Combinational Optimization

- **Variable Selection in Regression:** Consider a multiple linear regression problem with dependent variable Y and a set of candidate predictors $X_1, \cdots, X_p$.
  - We want to find the best model of the form

    $$Y = \beta_0 + \beta_{j_1} X_{j_1} + \cdots + \beta_{j_s} X_{j_s} + \epsilon,$$

    where $S := \{j_1, \cdots, i_s\}$ is a subset of $\{1, \cdots, p\}$.
  - We can use Akaike information criterion (AIC) to measure the performance of the model, where

    $$AIC(S) = N \log \left\{ \frac{1}{n} \sum_{i=1}^{n} \left(Y_i - \hat{\beta}_0 + \hat{\beta}_{j_1} X_{i,j_1} + \cdots + \hat{\beta}_{j_s} X_{i,j_s} \right)^2 \right\} + 2(s+2),$$

    where n is the sample size and s is the number of predictors in the model.
  - We want to find the model S with the smallest AIC. There are 2^p possible choices of the subset S.