Statistical Computation

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Contents

1 Review

1.1 Complex Number

Definition 1.1. A complex number z consists of two component, real and imaginary:

$$z = x + \iota y$$

where $\iota = \sqrt{-1}$.

Property 1.1. If $z_1 = x_1 + \iota y_1, z_2 = x_2 + \iota y_2$ then

$$\begin{aligned} z_1 + z_2 &= (x_1 + x_2) + \iota(y_1 + y_2) \\ z_1 z_2 &= (x_1 x_2 - y_1 y_2) + \iota(x_1 y_2 + x_2 y_1) \end{aligned}$$

Property 1.2. $\exp(\iota\theta) = \cos(\theta) + \iota \sin(\theta)$.

Property 1.3. $z = x + \iota y = r\exp(\iota\theta)$ where $r = |z| = \sqrt{x^2 + y^2}, x = r\cos(\theta), y = r\sin(\theta)$.

Property 1.4. $\exp(\iota(\theta_1 + \theta_2)) = \cos(\theta_1 + \theta_2) + \iota \sin(\theta_1 + \theta_2)$.

1.2 Markov Chain

Definition 1.2 (Transition Density)**.** Transition density $q(\mathbf{x}, \mathbf{y})$ is the conditional density of $\mathbf{X}_i$ given $\mathbf{X}_{i-1} = \mathbf{x}$, i.e.,

$$q(\mathbf{x}, \mathbf{y}) = q(\mathbf{x} \to \mathbf{y}) = q(\mathbf{y}|\mathbf{x})$$

Definition 1.3 (Stationary)**.** The Markov chain is stationary with stationary (invariant) density $f(\mathbf{x})$ if

$$f(\mathbf{y}) = \int \cdots \int q(\mathbf{x}, \mathbf{y}) f(\mathbf{x}) \mathrm{d}\mathbf{x}$$

Definition 1.4 (Reversibility)**.** A transition density $q(\mathbf{x}, \mathbf{y})$ will have $f(\mathbf{x})$ as its stationary density if we have

$$f(\mathbf{x})q(\mathbf{x}, \mathbf{y}) = f(\mathbf{y})q(\mathbf{y}, \mathbf{x}) \text{ (Reversibility condition)}$$

1.3 Linear Algebra

Definition 1.5 (Lower Triangular Matrix)**.** We define lower triangular matrix to be

$$L = \begin{pmatrix} a_{11} & 0 & 0 & \cdots & 0 \\ a_{21} & a_{22} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} \end{pmatrix}$$

where $a_{ij} = 0$ for $i < j$.

Definition 1.6 (Upper Triangular Matrix)**.** We define upper triangular matrix to be

$$U = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ 0 & a_{22} & a_{23} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ 0 & 0 & 0 & \cdots & a_{nn} \end{pmatrix}$$

where $a_{ij} = 0$ for $i > j$.

Note. For upper and lower triangular matrices, A^{-1} exists iff $a_{11}, \cdots, a_{nn}$ are all non-zero.

Example 1.1. Suppose we solve $A\mathbf{x} = \mathbf{b}$ for lower triangular matrix A, where $\mathbf{b} = (b_1 \quad \cdots \quad b_n)^T$ and $\mathbf{x} = (x_1 \quad \cdots \quad x_n)^T$ Then

$$\begin{aligned}
x_1 &= \frac{b_1}{a_{11}} \\
x_2 &= \frac{b_2 - a_{21}x_1}{a_{22}} \\
x_3 &= \frac{b_3 - a_{31}x_1 - a_{32}x_2}{a_{33}} \\
&\vdots \\
x_n &= \frac{b_n - a_{n1}x_1 - a_{n2}x_2 - \cdots - a_{n,n-1}x_{n-1}}{a_{nn}}
\end{aligned}$$

Note 1. The algorithm for upper triangular matrix is similar.
Note 2. In R, we use `backsolve` and `forwardsolve`.

Definition 1.7 (Norm)**.** Suppose $\mathbf{x} = (x_1 \quad \cdots \quad x_n)^T$ is a vector. A norm $\|\mathbf{x}\|$ satisfies the following conditions:

1. $\|\mathbf{x} + \mathbf{y}\| \leqslant \|\mathbf{x}\| + \|\mathbf{y}\|$.
2. $\|a\mathbf{x}\| = |a|\|\mathbf{x}\|$.
3. $\|\mathbf{x}\| = 0$ implies $\mathbf{x} = \mathbf{0}$.

Note. $\|\mathbf{x}\|$ gives a measure of the size or length of $\mathbf{x}$.

Example 1.2 (General L_p Norm)**.**

$$\|\mathbf{x}\|_p = \left(\sum_{i=1}^{n} |x_i|^p\right)^{1/p}, p \geqslant 1$$

Example 1.3 (Euclidean Norm)**.**

$$\|\mathbf{x}\|_2 = \left(\sum_{i=1}^{n} x_i^2\right)^{1/2}$$

Example 1.4 (Manhattan Distance)**.**

$$\|\mathbf{x}\|_1 = \sum_{i=1}^{n} |x_i|$$

Example 1.5 (L_∞ Norm)**.**

$$\|\mathbf{x}\|_\infty = \max_{1 \leqslant i \leqslant n} |x_i|$$

Definition 1.8 (Frobenius Norm)**.** The Frobenius norm of an $m \times n$ matrix is

$$\|A\|_F = \left(\sum_{i=1}^{m}\sum_{j=1}^{n} a_{ij}^2\right)^{1/2}$$

Definition 1.9 (L_p Norm for Matrix)**.** Suppose A is an $m \times n$ matrix. We define the L_p norm of A as

$$\|A\|_p = \sup_{\mathbf{x}} \frac{\|A\mathbf{x}\|_p}{\|\mathbf{x}\|_p} = \sup_{\mathbf{x}:\|\mathbf{x}\|_p = 1} \|A\mathbf{x}\|_p$$

Property 1.5.

1. $\|AB\|_p \leqslant \|A\|_p \|B\|_p$.
2. $\|A^k\|_p \leqslant \|A\|_p^k$.
3. $\|I\|_p = \|AA^{-1}\|_p = 1 \Rightarrow \|A^{-1}\|_p \geqslant \dfrac{1}{\|A\|_p}$.
4. For any vector $\mathbf{x}$, $\|A\mathbf{x}\|_p \leqslant \|A\|_p \|\mathbf{x}\|_p$.
5. When $p = 2$,
$$\|A\|_2 = \sqrt{\text{Maximum eigenvalue of } A^T A}$$

Note. If A is symmetric then $\|A\|_2$ is the maximum absolute eigenvalue of A.

Example 1.6 (L_∞ Norm for Matrix)**.** Consider vectors $\mathbf{x}$ whose elements are all ± 1, i.e., $\|\mathbf{x}\|_\infty = 1$. We maximize $\|A\mathbf{x}\|_\infty$ by taking $\mathbf{x}$ so that $\sum_{j=1}^{n} a_{ij} x_j$ is maximized and

$$\|A\|_\infty = \max_{1 \leqslant i \leqslant m} \sum_{j=1}^{n} |a_{ij}|$$

Example 1.7 (L_1 Norm for Matrix)**.** Consider vectors $\mathbf{x}$ whose elements are one 1 and $(n-1)$ 0s, i.e., $\|\mathbf{x}\|_1 = 1$. $A\mathbf{x}$ picks out one column of A and

$$\|A\|_1 = \max_{1 \leqslant j \leqslant n} \sum_{i=1}^{m} |a_{ij}|$$

Theorem 1.1. Suppose A is an $n \times n$ matrix with real-valued eigenvalues $\lambda_1, \cdots, \lambda_n$. Then

$$\max_{1 \leqslant k \leqslant n} |\lambda_k| \leqslant \|A\|_p, p \geqslant 1$$

Proof. Suppose that $A\mathbf{v} = \lambda_k \mathbf{v}$ where $\|\mathbf{v}\|_p = 1$. Then for all $k = 1, \cdots, n$,

$$|\lambda_k| = \|A\mathbf{v}\|_p \leqslant \|A\|_p$$

$\square$

Note. The result holds if there are complex-valued eigenvalues where $|\lambda_k|$ is the modulus if λ_k is complex-valued.

Definition 1.10 (Diagonally Dominant Matrix)**.** An $n \times n$ matrix A is (row) diagonally dominant if

$$|a_{ii}| \geqslant \sum_{j \neq i} |a_{ij}|, i = 1, \cdots, n$$

If $\geqslant$ is replaced by $>$ then A is strictly diagonally dominant.

Property 1.6. A strictly diagonally dominant matrix is invertible.

Theorem 1.2 (Gershgorin Circle Theorem)**.** Suppose A is an $n \times n$ matrix with elements $\{a_{ij}\}$. Define $r_i = \sum_{j \neq i} |a_{ij}|$ and

$$C_i = \{z \in \mathbb{C} : |z - a_{ii} \leqslant r_i|\}$$

which is a circle on the complex plane centered at a_{ii} with radius r_i. If λ is an eigenvalue of A, then $\lambda \in C_i$ for some i.

Theorem 1.3. Suppose A and B are matrices s.t. both AB and BA are well-defined, then

$$\text{trace}(BA) = \text{trace}(AB)$$

Example 1.8. If $\mathbf{u}$ and $\mathbf{v}$ are vectors then

$$\mathbf{u}^T A\mathbf{v} = \text{trace}(A\mathbf{v}\mathbf{u}^T) = \text{trace}(\mathbf{v}\mathbf{u}^T A)$$

Definition 1.11 (Determinant)**.** Suppose A is $n \times n$ matrix with eigenvalues $\lambda_1, \cdots, \lambda_n$, the determinant of A is

$$\det(A) = \prod_{i=1}^{n} \lambda_i$$

Theorem 1.4. Suppose A is symmetric positive definite, then $\lambda_1, \cdots, \lambda_n$ are strictly positive. We have

$$\det(A) = \exp(\text{trace}[\ln(A)])$$

1.3.1 Application: Condition Numbers

Theorem 1.5. If $\|B\|_p < 1$ for some p then

$$(I - B)^{-1} = I + B + B^2 + \cdots = \sum_{k=0}^{\infty} B^k$$

We use $(A+E)^{-1} - A^{-1}$ to check the sensitivity of A^{-1} to round-off error, where E is small relative to A.

We have

$$\begin{aligned} (A+E)^{-1} &= A^{-1}(I + EA^{-1})^{-1} \\ &= A^{-1}[I - EA^{-1} + (EA^{-1})^2 + \cdots] \\ &\approx A^{-1} - A^{-1}EA^{-1} \end{aligned}$$

and thus

$$(A+E)^{-1} - A^{-1} \approx -A^{-1}EA^{-1}$$

Then

$$\|(A+E)^{-1} - A^{-1}\|_p \approx \|A^{-1}EA^{-1}\|_p \leqslant \|A^{-1}\|_p^2 \|E\|_p$$

and

$$\frac{\|(A+E)^{-1} - A^{-1}\|_p}{\|A^{-1}\|_p} \leqslant \|A^{-1}\|_p \|E\|_p = \kappa_p(A)\frac{\|E\|_p}{\|A\|_p}$$

where $\kappa_p(A) = \|A\|_p \|A^{-1}\|_p \geqslant 1$ is called the condition number of A. If the condition number of A is large then the numerical solution of $A\mathbf{x} = \mathbf{b}$ may be unstable.

Example 1.9. Let

$$A = \begin{pmatrix} 1 & 1-\varepsilon \\ 1+\varepsilon & 1 \end{pmatrix}$$

then

$$A^{-1} = \begin{pmatrix} \varepsilon^{-2} & \varepsilon^{-1} - \varepsilon^{-2} \\ -\varepsilon^{-1} - \varepsilon^{-2} & \varepsilon^{-2} \end{pmatrix}$$

for $\varepsilon > 0$ and small. We have $\|A\|_1 = \|A\|_\infty = 2 + \varepsilon$ and $\|A^{-1}\|_1 = \|A^{-1}\|_\infty = 2\varepsilon^{-2} + \varepsilon^{-1}$. Thus

$$\kappa(A) = 4\varepsilon^{-2} + 4\varepsilon^{-1} + 1 \approx 4\varepsilon^{-2}$$

for small ε.

1.3.2 Gram-Schmidt Orthogonalization

Given vectors $\mathbf{v}_1, \cdots, \mathbf{v}_r$, suppose we want to find orthonormal vectors $\mathbf{q}_1, \cdots, \mathbf{q}_r$ with the same span, i.e., if $\mathbf{x} = \sum_{i=1}^{r} a_i \mathbf{v}_i$, then

$$\mathbf{x} = \sum_{i=1}^{r} b_i \mathbf{q}_i$$

for some $b_1, \cdots, b_r$.

The Gram-Schmidt algorithm is:

1. Define $\mathbf{u}_1 = \mathbf{v}_1$.
2. For $i = 2, \cdots, r$, define

$$\mathbf{u}_i = \mathbf{v}_i - \sum_{j=1}^{i-1} \frac{\mathbf{v}_i^T \mathbf{u}_j}{\mathbf{u}_j^T \mathbf{u}_j} \mathbf{u}_j$$

3. Set $\mathbf{q}_i = \dfrac{\mathbf{u}_i}{\|\mathbf{u}_i\|}$ for $i = 1, \cdots, r$.

2 Basics

2.1 Floating Point

2.1.1 Floating Point Representation

Definition 2.1. A ***floating point number*** is represented by three components: (S, F, E) where S is the sign of the number (± 1), F is a fraction (lying between 0 and 1), E is an exponent. S, F, E are all represented as binary digits (bits). The ***floating point representation*** of x, $\mathrm{fl}(x)$ is

$$\mathrm{fl}(x) = S \times F \times 2^E$$

Note. x and $\mathrm{fl}(x)$ need not be the same, since $\mathrm{fl}(x)$ is a binary approximation to x, and there are only a finite number of floating point numbers.

2.1.2 Round-Off Error

Mathematical operations introduce further approximation errors

$$f(\mathrm{fl}(x)) = f(x + \varepsilon) \approx f(x) + \varepsilon f'(x)$$

and the goal is to make the round-off error $|f(x) - \mathrm{fl}(f(\mathrm{fl}(x)))|$ as small as possible.

2.1.3 Machine Epsilon and Other Constants

For a given real number x, we have

$$|\mathrm{fl}(x) - x| \leqslant U|x| \text{ or } \mathrm{fl}(x) = x(1 + u), |u| \leqslant U$$

where U is ***machine epsilon*** or ***machine unit***. U is machine dependent but very small. In R, $U = 2^{-52} = 2.220 \times 10^{-16}$.

Other machine dependent constants include:

1. The minimum and maximum positive floating point numbers: $x_{\min} = 2^{-1022} = 2.225 \times 10^{-308}$ and $x_{\max} = 2^{1024} - 1 = 1.798 \times 10^{308}$.
2. The maximum integer: $2147383647 = 2^{31} - 1$.

2.1.4 Overflow and Underflow Error

Definition 2.2. If the result of a floating point operation exceeds $x_{\max}$, then the value returned is `Inf`.

Note. `Inf` indicates an ***overflow error***.

Definition 2.3. If the result of a floating point operation is undefined then `NaN` is returned.

Definition 2.4 (Underflow Error)**.** An underflow error occurs when the result of a floating point calculation is smaller (in absolute value) than $x_{\min}$.

Note. There are two possible outcomes: an error is reported or an exact 0 is returned. The latter outcome may cause problems in subsequent computations (e.g., division by 0).

Note. There are some ways to avoid overflow and underflow errors:

1. Use logarithmic scale: Changes multiplication/division into addition/subtraction, e.g., `lgamma`, `lfactorial`, `lchoose`.
2. Use series expansions (e.g., Taylor series).

Example 2.1. For x close to 0, $\frac{\exp(x)-1}{x} \approx 1$. Naive computation of $\frac{\exp(x)-1}{x}$ is problematic for x close to 0 due to possible round-off and underflow errors:

$$\frac{\text{fl}(\exp(x)-1)}{\text{fl}(x)} \neq \frac{\exp(x)-1}{x}$$

We solve the problem by using a series approximation, for $|x| \leqslant \varepsilon$,

$$\frac{\exp(x)-1}{x} = \frac{x + x^2/2 + x^3/6 + \cdots}{x} = 1 + \frac{x}{2} + \frac{x^2}{6} + \cdots$$

2.1.5 Catastrophic Cancellation

Suppose $z_1 = g_1(x_1, \cdots, x_n)$ and $z_2 = g_2(x_1, \cdots, x_n)$. We want to compute $y = z_1 - z_2$. What we actually compute is

$$y^* = \text{fl}(\text{fl}(z_1) - \text{fl}(z_2))$$

where $\text{fl}(z_1) = z_1(1+u_1)$ and $\text{fl}(z_2) = z_2(1+u_2)$. We have

$$\text{fl}(z_1) - \text{fl}(z_2) = \underbrace{z_1 - z_2}_{y} + \underbrace{z_1 u_1 - z_2 u_2}_{\text{error}}$$

If z_1 and z_2 are large but $y = z_1 - z_2$ is small then the magnitude of the error may be larger than the magnitude of y - ***catastrophic cancellation***.

2.2 Sparse Matrices

Definition 2.5 (Sparse Matrix). We say an $n \times n$ matrix is sparse if it has $k \times n$ non-zero elements where $k \ll n$.

Note 1. An $n \times n$ matrix needs at least n non-zero elements to be invertible.

Note 2. Sparse matrices are useful because we need only store non-zero elements and their row and column indices; multiplication by and addition to 0 are free operations.

2.3 Application: Computation of Probability Distributions

Question: Suppose X_i are independent discrete r.v.s. taking values $0, \cdots, l$ with

$$P(X_i = x) = p(x), x = 0, \cdots, l$$

Define $S = X_1 + \cdots + X_n$ and find the probability distribution of S.

2.3.1 Brute Force Approach

Start with $n = 2$ and proceed inductively:

$$p_2(x) := P(X_1 + X_2 = x) = \sum_{y=0}^{x} P(X_1 = y, X_2 = x - y)$$

$$p_3(x) := P(X_1 + X_2 + X_3 = x) = \sum_{y=0}^{x} P(X_1 + X_2 = y, X_3 = x - y)$$

$$\vdots$$

$p_k(x)$ requires $x+1$ multiplications and to evaluate $p_k(x)$ for $x = 0, \cdots, kl$, we need

$$N(k) = \sum_{x=0}^{kl}(x+1) \approx \frac{(kl)^2}{2} \text{ multiplications}$$

Thus the total number of multiplications is

$$\sum_{k=2}^{n} N(k) \approx \frac{n^3 l^2}{6} = O(n^3 l^2)$$

2.3.2 Probability Generating Function

Definition 2.6 (Probability Generating Function)**.** If X is a discrete r.v. taking values $0, 1, \cdots$, then its probability generating function is

$$\phi(t) = \mathbb{E}[t^X] = \sum_{x=0}^{\infty} P(X = x)t^x$$

Note. If X takes values $0, \cdots, l$, then $P(X = x)$ can be recovered from evaluating $\phi(t)$ at $l+1$ distinct (non-zero) points $t_0, \cdots, t_l$.

If $\phi(t) = \mathbb{E}[t^{X_i}]$, then the probability generating function of S is

$$\mathbb{E}[t^S] = \mathbb{E}[t^{X_1+\cdots+X_n}] = [\phi(t)]^n$$

Thus we can recover $P(S = x)$ for $x = 0, \cdots, nl$ by evaluating $[\phi(t)]^n$ at $t_0, \cdots, t_{nl}$. We have $nl+1$ linear equations in $nl+1$ unknowns, and solving typically requires $O(n^3 l^3)$ operations, which is slower than the brute force approach.

2.3.3 Discrete Fourier Transform (DFT)

A choice for $t_0, \cdots, t_{nl}$ are complex exponentials

$$t_j = \exp\left(-2\pi\iota \frac{j}{nl+1}\right), j = 0, \cdots, nl$$

where $\iota = \sqrt{-1}$. Since $p(x) = 0$ for $x = l+1, \cdots, nl$, we have

$$\phi(t_j) = \sum_{x=0}^{l} p(x) \exp\left(-2\pi\iota \frac{jx}{nl+1}\right) = \sum_{x=0}^{nl} p(x) \exp\left(-2\pi\iota \frac{jx}{nl+1}\right)$$

$\phi(t_0), \cdots, \phi(t_{nl})$ is the ***discrete Fourier transform*** (DFT) of $p(0), \cdots, p(nl)$, and thus, the DFT of $P(S = 0), \cdots, P(S = nl)$ is $[\phi(t_0)]^n, \cdots, [\phi(t_{nl})]^n$. Hence, given $\phi(t_0), \cdots, \phi(t_{nl})$, we can compute the probability distribution of S using the inverse DFT:

$$P(S = x) = \frac{1}{nl+1} \sum_{j=0}^{nl} [\phi(t_j)]^n \exp\left(2\pi\iota \frac{jx}{nl+1}\right), x = 0, \cdots, nl$$

Naive computation of $P(S = x)$ using DFT requires $O(n^3 l^2)$ multiplications; but with divide-and-conquer algorithm, we can reduce the number of multiplications by a factor of n.

In R, if `x` is a vector of length n we can compute its DFT with `fft(x)` and the inverse DFT with `fft(tx, inv=T) / length(x)`:

```
probs = # The vector for P(X=x)
dft = fft(probs)
dft.s = dtf^n # S=X1+...+Xn
idft.s = fft(dft.s, inv=T) / length(probs)
Re(idft.s) # Real component of idft.s, or P(S=x)
```

Note. `fft` is the fast Fourier transform, which is an efficient algorithm for computing the DFT when the length of the sequence is a product of small primes.

2.4 Application: Image Processing

Question: We observe an image denoted by $x(i,j).i = 1,\cdots,m, j = 1,\cdots,n$, where (i,j) denotes a pixel location. We want:

1. Denoising: Think of $\{x(i,j)\}$ as a image corrupted by noise

$$x(i,j) = \underbrace{s(i,j)}_{\text{True}} + \underbrace{\varepsilon(i,j)}_{\text{Noise}}$$

2. Compression: Approximate $x(i,j)$ by $x^*(i,j)$ where

$$x^*(i,j) = \sum_{k=1}^{p} \beta_k \phi_k(i,j)$$

where $p \ll m \times n$ and $\phi_1,\cdots,\phi_p$ are known functions.

2.4.1 Transformation

Define X to be the $m \times n$ matrix whose elements are $x(i,j)$. Define orthogonal matrices H_1 $(m \times m)$ and H_2 $(n \times n)$ and define $\widehat{X} = H_1 X H_2$, which has the same dimensions as X. Since for orthogonal matrix H, $H^{-1} = H^T$ and so $X = H_1^T \widehat{X} H_2^T$. Assume the noisy image model $X = S + E$, if H_1 and H_2 are chosen appropriately,

$$\widehat{X} = \underbrace{H_1 S H_2}_{\text{Sparse}} + \underbrace{H_1 E H_2}_{\approx 0}$$

Therefore,

1. Denoising: Given $\widehat{X}$, find a transformation $\widehat{X} \mapsto T(\widehat{X})$ and define the denoised image

$$X_{\text{dn}} = H_1^T T(\widehat{X}) H_2^T$$

where we assume the smallest elements of $\widehat{X}$ are due to noise and set these equal to 0

$$T(\widehat{X})(i,j) = 0, |\widehat{X}(i,j)| \leqslant \text{Threshold}$$

2. Compression: The same idea is used for compression: for some T,

$$X_{\text{c}} = H_1^T T(\widehat{X}) H_2^T$$

Note. T is usually defined more deterministically. The form of T depends on the amount of compression and the type of image.

2.4.2 Hadamard Matrices and Walsh-Hadamard Transform

Definition 2.7 (Hadamard Matrix)**.** A Hadamard matrix is an $n \times n$ matrix whose elements are all ± 1 with orthogonal rows s.t. $HH^T = nI$.

Note 1. $H^{-1} = \dfrac{H^T}{n}$.

Note 2. Hadamard matrices only exist if $n = 1, n = 2$, or n is a multiple of 4.

Note 3. We focus on the case where $n = 2^k$ since it is simple to construct and we can write the Hadamard matrix as a product of sparse matrices. We start with the trivial 1×1 Hadamard matrix $H_1 = 1$, and then define $H_2, H_4, H_8, \cdots$ recursively:

$$H_2 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$H_{2^k} = \begin{pmatrix} H_{2^{k-1}} & H_{2^{k-1}} \\ H_{2^{k-1}} & -H_{2^{k-1}} \end{pmatrix}$$

for $k = 2, 3, \cdots$.

Note 4. H_2 is symmetric and so H_{2^k} is symmetric and thus $H_{2^k}^{-1} = \dfrac{H_{2^k}}{2^k}$.

Definition 2.8 (Kronecker Product)**.** Given arbitrary matrices A and B, the Kronecker product $A \otimes B$ is

$$A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B & \cdots & a_{1n}B \\ a_{21}B & a_{22}B & \cdots & a_{2n}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}B & a_{m2}B & \cdots & a_{mn}B \end{pmatrix}$$

for an $m \times n$ matrix A.

Property 2.1. Assume below that any matrix sums, products or inverses are well-defined.

1. $A \otimes (B + C) = (A \otimes B) + (A \otimes C)$.
2. $(B + C) \otimes A = (B \otimes A) + (C \otimes A)$.
3. $A \otimes (B \otimes C) = (A \otimes B) \otimes C$.
4. $(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$.
5. $(A \otimes B)^T = A^T \otimes B^T$.
6. $(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$.

Note. For Hadamard matrices, $H_{2^k} = H_2 \otimes H_{2^{k-1}}$. We rewrite it as $H_{2^k} = (H_2 I_2) \otimes (I_{2^{k-1}} H_{2^{k-1}})$ and using the property, we have

$$H_{2^k} = (H_2 \otimes I_{2^{k-1}})(I_2 \otimes H_{2^{k-1}})$$

Repeating the process with $H_{2^{k-1}}, H_{2^{k-2}}, \cdots$, we get

$$H_{2^k} = \underbrace{(H_2 \otimes I_{2^{k-1}})(I_2 \otimes H_2 \otimes I_{2^{k-2}})(I_4 \otimes H_2 \otimes I_{2^{k-3}}) \cdots (I_{2^{k-1}} \otimes H_2)}_{k = \log_2(n) \text{ terms}}$$

Definition 2.9 (Walsh-Hadamard Transform)**.** Given an $n \times n$ Hadamard matrix H and a vector $\mathbf{x}$ of length n, we define its Walsh-Hadamard transform by $\widehat{\mathbf{x}} = H\mathbf{x}$.

Note 1. Given the W-H transform, we can recover $\mathbf{x}$

$$\mathbf{x} = \frac{1}{n} H^T \widehat{\mathbf{x}}$$

Note 2. If $n = 2^k$, since $H = H^T$, then

$$\mathbf{x} = \frac{1}{n} H \widehat{\mathbf{x}}$$

2.5 Application: Denoising

Question: Suppose we observe $\mathbf{x} = (x_1, \cdots, x_n)^T$ where we assume that

$$\mathbf{x} = \mathbf{s} + \mathbf{e} = \text{Signal} + \text{Noise}$$

We want to recover or estimate the signal $\mathbf{s}$.

2.5.1 Assumption

Assume $\mathbf{s}$ is structured so that its W-H transform $\widehat{\mathbf{s}} = H\mathbf{s}$ contains mostly 0s

$$\widehat{\mathbf{x}} = H\mathbf{x} = \underbrace{H\mathbf{s}}_{\text{Sparse}} + \underbrace{H\mathbf{e}}_{\text{Relatively small}}$$

2.5.2 Thresholding

We shrink smaller components of $\widehat{\mathbf{x}}$ towards 0, and then estimate $\mathbf{s}$ by the inverse W-H transform of the thresholded $\widehat{\mathbf{x}}$. Thresholded W-H transform $\widehat{\mathbf{x}}_s$ is an estimate of the W-H transform of $\mathbf{s}$, and thus we can estimate $\mathbf{s}$ by the inverse W-H transform

$$\widetilde{\mathbf{s}} = \frac{1}{n} H^T \widehat{\mathbf{x}}_s$$

Define thresholds $\lambda_1, \cdots, \lambda_n \geqslant 0$. The ***hard thresholding*** is to modify $\widehat{\mathbf{x}}$ as follows:

$$\widehat{\mathbf{x}}_s = \begin{pmatrix} \widehat{x}_1 I(|\widehat{x}_1| \geqslant \lambda_1) \\ \vdots \\ \widehat{x}_n I(|\widehat{x}_n| \geqslant \lambda_n) \end{pmatrix}$$

The ***soft thresholding*** is to modify $\widehat{\mathbf{x}}$ as follows:

$$\widehat{\mathbf{x}}_s = \begin{pmatrix} \operatorname{sgn}(\widehat{x}_1)(|\widehat{x}_1| - \lambda_1)_+ \\ \vdots \\ \operatorname{sgn}(\widehat{x}_n)(|\widehat{x}_n| - \lambda_n)_+ \end{pmatrix}$$

where $\operatorname{sgn}(y)$ is the sign of y, and y_+ equals y if $y > 0$ and 0 if $y \leqslant 0$.

Typically we set $\lambda_1 = 0$, and use knowledge of the problem to decide $\lambda_2, \cdots, \lambda_n$; or take $\lambda_2 = \cdots = \lambda_n$ and choose the common value based on tools such as half normal plots.

2.5.3 The Fast W-H Transform

A Hadamard matrix H consists of ± 1 so computation of $H\mathbf{x}$ involves only additions and subtractions, but naive computation involves $n(n-1) = O(n^2)$ additions and subtractions, which is less than ideal if n is very large. We can write H as a product of sparse matrices to reduce complexity.

Example 2.2 ($n = 2^3 = 8$)**.** The 8×8 Hadamard matrix is

$$H_8 = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \end{pmatrix}$$

Naive computation of $H_8\mathbf{x}$ needs 56 additions and subtractions. But if $H_8 = A^3$ where

$$A = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 \end{pmatrix}$$

Computation of $AAA\mathbf{x}$ needs $3 \times 8 = 24$ additions and subtractions.

2.5.4 R code for FWHT

The function `fwht` below computes the W-H transform of data in a vector `x`.

```
fwht = function(x) {
  h=1
  len = length(x)
  while (h < len) {
    for (i in seq(1, len, by=h*2)) {
      for (j in seq(i, i+h-1)) {
        a = x[j]
        b = x[j+h]
        x[j] = a + b
        x[j+h] = a - b
      }
    }
  h = 2 * h
  }
  x
}
```

We can compute the inverse W-H transform using `fwht` by dividing the output by the length of the vector.

2.6 Fast Fourier Transform (FFT)

Definition 2.10 (Discrete Fourier Transform)**.** Suppose we have data $x_0, \cdots, x_{n-1}$, and define $\widehat{x}_0, \cdots, \widehat{x}_{n-1}$ by

$$\widehat{x}_j = \sum_{t=0}^{n-1} \exp\left(-2\pi\iota\frac{j}{n}t\right) x_t$$

where $\iota = \sqrt{-1}$.

Property 2.2 (Inverse DFT)**.** Given DFT, recover the original sequence by

$$x_t = \frac{1}{n}\sum_{j=0}^{n-1} \exp\left(2\pi\iota\frac{j}{n}t\right) \widehat{x}_j$$

Proof. For complex numbers z,

$$\sum_{j=0}^{n-1} z^j = \begin{cases} n, & z = 1 \\ \dfrac{1-z^n}{1-z}, & \text{otherwise} \end{cases}$$

Thus if $z = \exp\left(\dfrac{2\pi\iota t}{n}\right)$ for an integer t. we have

$$\sum_{j=0}^{n-1} z^j = \sum_{j=0}^{n-1} \exp\left(2\pi\iota \frac{t}{n} j\right) = \frac{1-\exp(2\pi\iota t)}{1-\exp(2\pi\iota t/n)} = 0$$

since $\exp(2\pi\iota t) = \cos(2\pi t) + \iota\sin(2\pi t) = 1$. Hence,

$$\begin{aligned} \frac{1}{n}\sum_{j=0}^{n-1} \exp\left(2\pi\iota \frac{j}{n} t\right) \widehat{x}_j &= \frac{1}{n}\sum_{j=0}^{n-1}\sum_{s=0}^{n-1} \exp\left(2\pi\iota \frac{t-s}{n} j\right) x_s \\ &= \frac{1}{n}\sum_{s=0}^{n-1} x_s \sum_{j=0}^{n-1} \exp\left(2\pi\iota \frac{t-s}{n} j\right) \\ &= x_t \end{aligned}$$

since

$$\sum_{j=0}^{n-1} \exp\left(2\pi\iota \frac{t-s}{n} j\right) = \begin{cases} n, & s = t \\ 0, & s \neq t \end{cases}$$

□

Definition 2.11 (Matrix Formulation of DFT)**.** Define $\mathbf{x} = (x_0, \cdots, x_{n-1})^T$ and $\widehat{\mathbf{x}} = (\widehat{x}_0, \cdots, \widehat{x}_{n-1})^T$. Then

$$\widehat{\mathbf{x}} = F\mathbf{x}$$

where F is an $n \times n$ matrix whose jth row and kth column is

$$f_{jk} = \exp\left(-2\pi\iota \frac{(j-1)(k-1)}{n}\right)$$

The elements of F^{-1} are

$$\overline{f}_{jk} = \frac{1}{n}\exp\left(2\pi\iota \frac{(j-1)(k-1)}{n}\right)$$

Note 1. Using the matrix form directly, we need $O(n^2)$ additions and multiplications to compute the DFT (and its inverse).

Note 2. We can write F as a product of sparse matrices, but unlike the W-H transform, factorization of the DFT matrix is more complicated.

2.6.1 FFT Derivation

Assume n is a product of prime numbers $n_1, \cdots, n_k : n = n_1 \times \cdots \times n_k$.

2.6.1.1 Case I: Even Number and Product of Small Prime Numbers

Assume n is even, then

$$\begin{aligned}\widehat{x}_j &= \sum_{t=0}^{n/2-1} \exp\left(-2\pi\iota\frac{j}{n}2t\right)x_{2t} + \sum_{t=0}^{n/2-1} \exp\left(-2\pi\iota\frac{j}{n}(2t+1)\right)x_{2t+1} \\ &= \underbrace{\sum_{t=0}^{n/2-1} \exp\left(-2\pi\iota\frac{j}{n/2}t\right)x_{2t}}_{\text{DFT of } x_0, x_2, \cdots} + \exp\left(-2\pi\iota\frac{j}{n}\right) \underbrace{\sum_{t=0}^{n/2-1} \exp\left(-2\pi\iota\frac{j}{n/2}t\right)x_{2t+1}}_{\text{DFT of } x_1, x_3, \cdots}\end{aligned}$$

Hence, the DFT of $x_0, \cdots, x_{n-1}$ is a linear combination of the DFT of the even and odd indices. Our rearrangement into DFT of odd and even indices can be written in matrix form as

$$\widehat{\mathbf{x}} = \underbrace{\begin{pmatrix} I & \Omega \\ I & -\Omega \end{pmatrix}}_{\text{Sparse}} \underbrace{\begin{pmatrix} F_{n/2} & 0 \\ 0 & F_{n/2} \end{pmatrix}}_{\text{Sparser}} P\mathbf{x}$$

where Ω is a diagonal matrix (sparse) and P is a permutation matrix (sparse), i.e., if n is even, we can write F as a product of two sparse matrices and a matrix that is sparser than F ($n^2/2$ 0s).

If $n/2$ is divisible by a prime number n', we can perform a similar decomposition of $F_{n/2}$ and F is now the product of sparser matrices. When $n_1, \cdots, n_k$ are small then we need $O(n\ln(n))$ additions and multiplications.

2.6.1.2 Case II: Prime Number with Zero-Padding

Definition 2.12 (Zero Padding)**.** Add 0s to the end of the sequence so that the length of the ***zero padded*** sequence is a product of small prime numbers:

$$x_0, \cdots, x_{n-1}, \underbrace{0, \cdots, 0}_{m}$$

with $n + m = n_1 \times \cdots \times n_k$ where $n_1, \cdots, n_k$ are small primes.

Note 1. The function `nextn` is useful for zero-padding.

Note 2. Adding 0s to a sequence changes the nature of the sequence - creating a large discontinuity, which is reflected in the DFT.

2.6.2 Analysis of DFT Approach

For the application in computation of probability distributions with DFT approach, we take $m \geqslant nl = 1$ where m is a product of small prime numbers, and follow the steps:

1. Define $\widehat{p}_i(0), \cdots, \widehat{p}_i(m-1)$ to be the DFT of $p_i(0), \cdots, p_i(m-1)$ for $i = 1, \cdots, n$.
2. Define
$$\widehat{p}_s(k) = \prod_{i=1}^{n} \widehat{p}_i(k), k = 0, \cdots, m-1$$
3. Inverse DFT: $P(S = 0), \cdots, P(S = m-1)$ is the inverse DFT of $\widehat{p}_s(0), \cdots, \widehat{p}_s(m-1)$.

The number of multiplications at each step is:

1. DFT: $n \times O(m\ln(m)) = O(nm\ln(m))$.
2. Product of DFTs: $O(nm)$.

3. Inverse DFT: $O(m \ln(m))$.

The total number of multiplications is $O(nm \ln(m))$ and thus if $m \approx nl$, the number of multiplications is $O(n^2 l \ln(nl))$ versus $O(n^3 l^2)$ for the brute force algorithm.

3 Generation of Random Variates

3.1 Generation of Random Numbers

Example 3.1 (Importance Sampling)**.** Suppose we want to estimate

$$I = \int \cdots \int g(\mathbf{x}) \mathrm{d}\mathbf{x}$$

for some integrand $g : \mathbb{R}^p \to \mathbb{R}$. If f is a probability density function on $\mathbb{R}^p$, then

$$I = \int \cdots \int g(\mathbf{x}) \mathrm{d}\mathbf{x} = \int \cdots \int \frac{g(\mathbf{x})}{f(\mathbf{x})} f(\mathbf{x}) \mathrm{d}\mathbf{x} = \mathbb{E}_f \left[\frac{g(\mathbf{X})}{f(\mathbf{X})} \right]$$

where $\mathbf{X}$ has a density f. We can use the law of large numbers to estimate the expected value provided $\mathrm{Var}_f \left[\frac{g(\mathbf{X})}{f(\mathbf{X})} \right] < \infty$. Take $\mathbf{X}_1, \cdots, \mathbf{X}_n$ independent from f, LLN gives

$$\widehat{I} = \frac{1}{n} \sum_{i=1}^{n} \frac{g(\mathbf{X}_i)}{f(\mathbf{X}_i)} \approx \int \cdots \int g(\mathbf{x}) \mathrm{d}\mathbf{x}$$

Note. We choose f satisfying precision and expediency:

1. Precision: Minimize the variance of $\widehat{I}$.
2. Expediency: Be able to sample from f.

Example 3.2 (Monte Carlo Estimation of π)**.** If X and Y are independent Unif$(-1, 1)$ r.v.s., then

$$P(X^2 + Y^2 \leqslant 1) = \frac{\pi}{4}$$

We generate independent pairs and have

$$\widehat{\pi} = \frac{4}{n} \sum_{i=1}^{n} I(X_i^2 + Y_i^2 \leqslant 1)$$

3.2 Generation of Unif$(0, 1)$

To generate pseudo-random $U_1, U_2, \cdots$, we generate integers $V_1, V_2, \cdots$ from a uniform distribution on $\{1, \cdots, N\}$ and define $U_i = \frac{V_i}{N+1}$ for $i = 1, 2, \cdots$. Note that $U_1, U_2, \cdots$ are uniform on the set $\{1/(N+1), \cdots, N/(N+1)\}$. If N is large enough, $U_1, U_2, \cdots$ are independent Unif$(0, 1)$ r.v.s.:

$$\sup_{0 \leqslant x \leqslant 1} |P(U_i \leqslant x) - x| \leqslant \frac{1}{N}$$

3.2.1 Linear Congruential RNG

Define $V_1, V_2, \cdots$ via the recursion:

$$V_{k+1} = (aV_k + b) \mod m$$

for some integers a, b, and m.

Note 1. The initial value V_0 is the ***seed*** of the RNG.

Note 2. $V_1, V_2, \cdots$ take values in the set $\{0, \cdots, m-1\}$.

Note 3. If $b = 0$ then we have a ***multiplicative congruential*** RNG.

Note 4. We have $V_{k+p} = V_k$ for some $p \leqslant m$, and p is the ***period*** of the RNG.

Property 3.1. If $b = 0$, then the maximum possible period is $m - 1$. Furthermore, if m is prime, and

$$a^{(m-1)/q} \mod m \neq 1$$

for every prime factor q of $m - 1$ then the RNG has period $m - 1$.

Example 3.3. Take $m = 5$ and $m - 1 = 4$ has a single prime factor 2. We need $a^2 \mod 5 \neq 1$ so we can take $a = 3$ (for example).

Example 3.4. Let m to be the largest possible prime number $m = 2^{31} - 1$. We can take $a = 16807$ or 48271, or 397204094.

3.2.2 Combining Unif$(0, 1)$ RNGs

Combination increases the period of the RNG.

Example 3.5 (Wichmann-Hill RNG)**.** Combine three multiplicative congruential RNGs:

$$\begin{aligned} V_{k+1}^{(1)} &= 171V_k^{(1)} \mod 30269 \\ V_{k+1}^{(2)} &= 172V_k^{(2)} \mod 30307 \\ V_{k+1}^{(3)} &= 170V_k^{(3)} \mod 30323 \end{aligned}$$

where the periods are short ($\approx 3 \times 10^4$). Then

$$U_k = \left(\frac{V_k^{(1)}}{30269} + \frac{V_k^{(2)}}{30307} + \frac{V_k^{(3)}}{30323} \right) \mod 1$$

where the period is

$$p = \frac{30268 \times 30306 \times 30322}{4} = 6.9536 \times 10^{12}$$

3.2.3 Shift Register Method

We use the binary representation of Unif$(0, 1)$. Suppose $Z_1, Z_2, \cdots$ are independent binary r.v.s. with

$$P(Z_k = 0) = P(Z_k = 1) = \frac{1}{2}$$

then

$$U = \sum_{k=1}^{\infty} \frac{Z_k}{2^k} \sim \text{Unif}(0, 1)$$

In practice, we define U as a finite sum

$$U = \sum_{k=1}^{r} \frac{Z_k}{2^k}$$

where r is the number of bits.

We generate $\{Z_k\}$ via ***exclusive-or*** operations for binary variables x and y. We construct $\{Z_k\}$ as follows:

$$Z_k = Z_{k-p} \oplus Z_{k-p+q}, 1 < q < p$$

and

$$U_n = \sum_{k=1}^{r} \frac{Z_{n-s(k)}}{2^k}$$

for some shifts $\{s(k)\}$.

Recall. If Z_1 and Z_2 are independent, and $Z_3 = Z_1 \oplus Z_2$, then Z_3 is independent of Z_1 and Z_2.

Note 1. For the shifts, we need $s(k) - s(k-1) \gg p$.

Note 2. Initialization of shift register RNGs is much complicated since Z_k is a function of Z_{k-p} and Z_{k-p+q} and U_n depends on r values of $\{Z_k\}$.

Note 3. We need a $p \times r$ matrix of binary seeds.

Example 3.6 (Lewis-Payne RNG)**.** $p = 98, q = 27$, and $s(k) = 100p(k-1)$ s.t. $s(k)-s(k-1) = 100p$. The period is $2^{98} - 1$.

Example 3.7 (Mersenne Twister)**.** The period is $2^{19937} - 1$.

3.3 Testing Unif$(0, 1)$ RNGs

We need to check:

1. Uniformity on $[0, 1]$: For $0 \leqslant a < b \leqslant 1$,

$$\frac{1}{n}\sum_{i=1}^{n} I(a \leqslant U_i \leqslant b) \approx b - a$$

2. Uniformity of k-tuples on $[0, 1]^k$: For $A \subset [0, 1]^k$,

$$\binom{n}{k}^{-1} \sum_{(i_1,\cdots,i_k)} I[(U_{i_1}, \cdots, U_{i_k}) \in A] \approx \text{Volume}(A)$$

3. Independence: U_i independent of $U_{i+1}, U_{i+2}, \cdots$.

3.4 RNGs in R

The function `RNGkind` that allows a user to specify the RNG used to generate Unif$(0, 1)$ r.v.s. and the method used to generate normal r.v.s..

3.5 Methods for Continuous Distribution

3.5.1 Inverse Method

Suppose F is a univariate distribution and we want to generate $X \sim F$.

Definition 3.1. For a general univariate distribution function F, we define

$$F^{-1}(t) = \inf\{x : F(x) \geqslant t\}, 0 < t < 1$$

Property 3.2. If F is a univariate distribution function with inverse F^{-1} and $U \sim$ Unif$(0, 1)$, then

$$X = F^{-1}(U) \sim F$$

Proof. We need to show $P(F^{-1}(U) \leqslant x) = F(x)$ or equivalently $[F^{-1}(U) \leqslant x] = [U \leqslant F(x)]$. By definition of F^{-1}, $[U \leqslant F(x)]$ implies $[F^{-1}(U) \leqslant x]$. If $F^{-1}(U) \leqslant x$ then $F(x + \varepsilon) \geqslant U, \forall \varepsilon > 0$. F is right continuous so $[F^{-1}(U) \leqslant x]$ implies $[U \leqslant f(x)]$. □

Example 3.8 (Exponential Distribution). $F(x) = 1 - \exp(-\lambda x)$ for $x \geqslant 0, \lambda > 0$. Solving $F(F^{-1}(t)) = t$ for $F^{-1}(t)$, we have

$$F^{-1}(t) = -\frac{\ln(1-t)}{\lambda}$$

Thus $X = -\dfrac{\ln(1-U)}{\lambda}$ has an exponential distribution. Since $1 - U \sim \text{Unif}(0,1)$ so we define $X = -\dfrac{-\ln(U)}{\lambda}$.

Example 3.9 (Logistic Distribution). $F(x) = \dfrac{\exp(x)}{1+\exp(x)}$. Solving $F(F^{-1}(t)) = t$, we have

$$F^{-1}(t) = \ln\left(\frac{t}{1-t}\right)$$

which is called logit function. Thus $X = \ln\left(\dfrac{U}{1-U}\right)$ has a Logistic distribution.

Example 3.10 (Approximation of Euler's Constant). The Euler's constant is

$$\begin{aligned}\gamma &= \lim_{m\to\infty}\left[\sum_{k=1}^{m}\frac{1}{k} - \ln(m)\right] \\ &= \int_1^\infty \left(\frac{1}{\lfloor x\rfloor} - \frac{1}{x}\right)\mathrm{d}x \\ &= \int_1^\infty x^2\left(\frac{1}{\lfloor x\rfloor} - \frac{1}{x}\right)x^{-2}\mathrm{d}x\end{aligned}$$

where $f(x) = x^{-2}$ is a density function on $[1,\infty)$. If we can sample $X_1, \cdots, X_n$ from $f(x)$, we can estimate γ by

$$\widehat{\gamma} = \frac{1}{n}\sum_{i=1}^{n} X_i^2\left(\frac{1}{\lfloor X_i\rfloor} - \frac{1}{X_i}\right)$$

The distribution function is $F(x) = 1 - x^{-1}$ whose inverse is $F^{-1}(t) = (1-t)^{-1}$. We can use inverse method to sample from $f(x)$.

```
n = 1000000
u = runif(n)
x = 1 / (1 - u)
gammahat = mean(x^2 * (1 / floor(x) - 1 / x))
```

3.5.2 Rejection Sampling

Assume F is continuous with density function f and $F^{-1}(t)$ is not easily computable. Suppose we want to sample X from a density f. We define a proposal density g s.t. $f(x) \leqslant Mg(x)$ for all x and some $M < \infty$. We sample Y from g and $U \sim \text{Unif}(0,1)$ where Y and U are independent, and define $T = \dfrac{f(Y)}{Mg(Y)}$. If $U \leqslant T$, then set $X = Y$; if $U > T$, then reject and repeat until acceptance. The algorithm works: Given independent $Y \sim g$ and $U \sim \text{Unif}(0,1)$,

$$\begin{aligned}P(X \leqslant x) &= P\left(Y \leqslant x \middle| U \leqslant \frac{f(Y)}{Mg(Y)}\right) \\ &= \frac{P(Y \leqslant x, U \leqslant f(Y)M^{-1}g^{-1}(Y))}{P(U \leqslant f(Y)M^{-1}g^{-1}(Y))}\end{aligned}$$

Since $Y \perp U$, the joint density of (Y,U) is

$$h(y,u) = \begin{cases} g(y), & 0 \leqslant u \leqslant 1 \\ 0, & \text{otherwise} \end{cases}$$

Therefore,

$$\begin{aligned} P(\text{Accept})P\left(U \leqslant \frac{f(Y)}{Mg(Y)}\right) &= \int_{-\infty}^{\infty}\int_{0}^{f(y)M^{-1}g^{-1}(y)} g(y)\mathrm{d}u\mathrm{d}y \\ &= \frac{1}{M}\int_{-\infty}^{\infty} f(y)\mathrm{d}y \\ &= \frac{1}{M} \end{aligned}$$

and

$$\begin{aligned} P\left(Y \leqslant x, U \leqslant \frac{f(Y)}{Mg(Y)}\right) &= \int_{-\infty}^{x}\int_{0}^{f(y)M^{-1}g^{-1}(y)} g(y)\mathrm{d}u\mathrm{d}y \\ &= \frac{1}{M}\int_{-\infty}^{x} f(y)\mathrm{d}y \\ &= \frac{P(X \leqslant x)}{M} \end{aligned}$$

Note 1. The probability of acceptance of a given proposal is $\frac{1}{M}$.
Note 2. If f and g are close then M will be close to 1.
Note 3. We can evaluate M by maximizing $\frac{f(x)}{g(x)}$ but we do not need to find the smallest possible M with $f(x) \leqslant Mg(x)$ since rejection sampling will work with a sub-optimal M with a lower probability of acceptance.
Note 4. f and g can be joint density functions or probability mass functions.

Example 3.11 (Half-Normal Distribution with Exponential Proposal)**.** Suppose we want to sample X from a half-normal distribution whose density is

$$f(x) = \frac{2}{\sqrt{2\pi}}\exp\left(-\frac{x^2}{2}\right), x \geqslant 0$$

i.e., if $X \sim \mathcal{N}(0,1)$, then $|X| \sim f$. Since X takes values on $[0,\infty)$, a natural proposal distribution is exponential

$$g(y) = \exp(-y), y \geqslant 0$$

since the tails of the exponential are heavier than those of the normal distribution so M should be finite.

To fine M, we need to maximize $\frac{f(x)}{g(x)}$ over $x \geqslant 0$, i.e.,

$$\max \ln[f(x)] - \ln[g(x)]$$

After calculation, we find $\frac{f(x)}{g(x)}$ is maximized at $x = 1$ and

$$M = \frac{f(1)}{g(1)} = 1.315489$$

and the probability of acceptance of a given proposal is

$$\frac{1}{M} = 0.76$$

The code to generate half-normal r.v.s. is:

```
x = NULL
count = 0
total = 0 # Number of proposals generated
while (count < 100) {
  reject = T
  while (reject) {
    y = rexp(1)
    u = runif(1)
    total = total + 1
    if (u <= 2*dnorm(y)/(1.315489*dexp(y))) {
      x = c(x, y)
      count = count + 1
      reject = F
    }
  }
}
```

Example 3.12 (Cauchy Distribution)**.** Suppose we want to sample X from a Cauchy distribution whose density is

$$f(x) = \frac{1}{\pi(1+x^2)}$$

The distribution function is

$$F(x) = \frac{1}{2} + \frac{1}{\pi}\tan^{-1}(x)$$

and

$$F^{-1}(t) = \tan\left[\pi\left(t - \frac{1}{2}\right)\right], 0 < t < 1$$

We can generate r.v.s. from a Cauchy distribution using the inverse method bug floating point evaluation of $\tan(x)$ is not always straightforward.

We can write $f(x)$ as a mixture of two densities

$$f(x) = \frac{1}{2}f_1(x) + \frac{1}{2}f_2(x)$$

where

$$f_1(x) = \frac{2}{\pi(1+x^2)}, |x| \leqslant 1$$
$$f_2(x) = \frac{2}{\pi(1+x^2)}, |x| > 1$$

We know that if $X \sim f_1$, then $X^{-1} \sim f_2$. Therefore, we generate Z from f_1 and $U \sim \text{Unif}(0,1)$ with $Z \perp U$. If $U > \frac{1}{2}, X = Z$; if $U < \frac{1}{2}, X = \frac{1}{Z}$. Hence, we can use rejection sampling to sample from

f_1. Taking g to be a uniform distribution on $[-1.1]$ is a reasonable choice, and $\dfrac{f_1(x)}{g(x)}$ is maximized at $x = 0$. Thus

$$M = \frac{f_1(0)}{g(0)} = \frac{4}{\pi} = 1.273$$

and

$$P(\text{Accept}) = \frac{\pi}{4} = 0.785$$

3.6 Sampling from Mixture Densities

Suppose we want to sample from a density $f(x)$ which can be written as a mixture of k components:

$$f(x) = \lambda_1 f_1(x) + \cdots + \lambda_k f_k(x)$$

where $f_1(x), \cdots, f_k(x)$ are densities, $\lambda_1 + \cdots + \lambda_k = 1$. We sample a discrete r.v. J from a discrete distribution with $P(J = j) = \lambda_j$ (and we can do with a single Unif$(0,1)$ r.v.). Given $J = j$, sample X from $f_j(x)$. The algorithm works best if k is small or if $\lambda_1 = \cdots = \lambda_k = \dfrac{1}{k}$: $J = \lceil kU \rceil$.

3.6.1 Application: Walker's Alias Method

Suppose we want to sample X from a discrete distribution

$$f(x_j) = P(X = x_j) = p_j, j = 1, \cdots, k$$

where $p_1 + \cdots + p_k = 1$. We can write f as a mixture of k components each with weight k^{-1} :

$$f(x) = P(X = x) = \frac{1}{k} f_1(x) + \cdots + \frac{1}{k} f_k(x), x = x_1, \cdots, x_k$$

$f_1, \cdots, f_k$ are discrete distribution putting mass at two points:

$$f_j(x) = \begin{cases} \tau_j, & x = x_j \\ 1 - \tau_j, & x = a_j \end{cases}$$

where $a_j \in \{x_1, \cdots, x_k\}$ is called an alias.

Given $\tau_1, \cdots, \tau_k$ and $a_1, \cdots, a_k$, we sample X from f as follows: Generate $U_1 \sim$ Unif$(0,1)$ and set $J = \lceil kU_1 \rceil$; generate $U_2 \sim$ Unif$(0,1)$ and define $X = x_J$ if $U_2 \leqslant \tau_J$ and $X = a_J$ if $U_2 > t_J$.

Note 1. We require a separate algorithm to construct $\tau_1, \cdots, \tau_k$ and $a_1, \cdots, a_k$.

Note 2. Walker's alias method is used by the R function `sample` when the option `replace=T` is given.

Example 3.13 (Binomial Distribution)**.** Take $X \sim$ Binom$(3, 0.4)$:

$$f(x) = P(X = x) = \binom{3}{x} 0.4^x 0.6^{3-x}, x = 0, 1, 2, 3$$

where $f(0) = 0.216, f(1) = 0.432, f(2) = 0.288, f(3) = 0.064$. We need to write

$$f(x) = \frac{1}{4} \sum_{i=0}^{3} f_i(x)$$

with $f_i(x) = \tau_i$ is $x = i$ and $f_i(x) = 1 - \tau_i$ if $x = a_i$ where $a_i \in \{0, 1, 2, 3\}$. We let

$$\begin{aligned} \tau_0 &= 0.272 \quad a_0 = 1 \\ \tau_1 &= 1 \quad \text{No alias} \\ \tau_2 &= 0.408 \quad a_2 = 0 \\ \tau_3 &= 0.256 \quad a_3 = 2 \end{aligned}$$

3.7 Generation of Normal Random Variables

3.7.1 Inverse Method

Define the $\mathcal{N}(0, 1)$ distribution function

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} \exp\left(-\frac{t^2}{2}\right) \mathrm{d}t$$

$\Phi(x)$ is strictly increasing so we can define its inverse by $\Phi(\Phi^{-1}(t)) = t$ for $0 \leqslant t \leqslant 1$. Thus given $U \sim \text{Unif}(0, 1), X = \Phi^{-1}(U) \sim \mathcal{N}(0, 1)$.

Note 1. It is the default method in R.

Note 2. Though $\Phi^{-1}(t)$ is not a nice function, it is very well approximated.

3.7.2 Box-Muller Method

If X_1 and X_2 are independent $\mathcal{N}(0, 1)$, then their joint density is

$$f(x_1, x_2) = \frac{1}{2\pi} \exp\left(-\frac{x_1^2 + x_2^2}{2}\right)$$

Convert to polar coordinates: $X_1 = R\cos(\Theta)$ and $X_2 = R\sin(\Theta)$, and (R, Θ) has joint density

$$g(r, \theta) = \frac{1}{2\pi} \exp\left(-\frac{r^2}{2}\right) r, r > 0, 0 \leqslant \theta < 2\pi$$

where $g(r, \theta) = g_1(r)g_2(\theta)$ and so $R \perp \Theta$. $\Theta \sim \text{Unif}(0, 2\pi)$ and $R = \sqrt{V}$ where V is exponential with mean 2. We generate R from $g_1(r)$ and Θ from $g_2(\theta)$, and

$$X_1 = R\cos(\Theta), X_2 = R\sin(\Theta)$$

If U_1 and U_2 are independent Unif$(0, 1)$, then we can define

$$\Theta = 2\pi U_1, R = \sqrt{-2\ln(U_2)}$$

3.7.3 Kinderman-Ramage Method

Consider half-normal distribution

$$f(x) = \frac{2}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right)$$

and we write $f(x)$ as a mixture of two distributions

$$\begin{aligned} f(x) &= \lambda_1 f_1(x) + \lambda_2 f_2(x) \\ &= 0.884 \times \underbrace{\text{Triangular density}}_{0.90-0.41x} + 0.116 f_2(x) \end{aligned}$$

Note 1. It is easy to generate from the triangular density $f_1(x)$: U_1 and U_2 are independent Unif$(-1, 1)$, then $V = \dfrac{2.216|U_1 + U_2|}{2}$ has density $f_1(x)$.

Note 2. It is not easy to generate from $f_2(x)$.

3.7.4 Monty Python Method

We generate independent r.v.s. U_1 and U_2 s.t. (U_1, U_2) have a uniform distribution on

$$\mathcal{B} = [0, \sqrt{2\pi}] \times \left[0, \frac{1}{\sqrt{2\pi}}\right]$$

and divide $\mathcal{B}$ into 4 regions - depending on which region (U_1, U_2), we can define a r.v. X with a half-normal distribution.

Define

$$f(x) = \frac{2}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right)$$

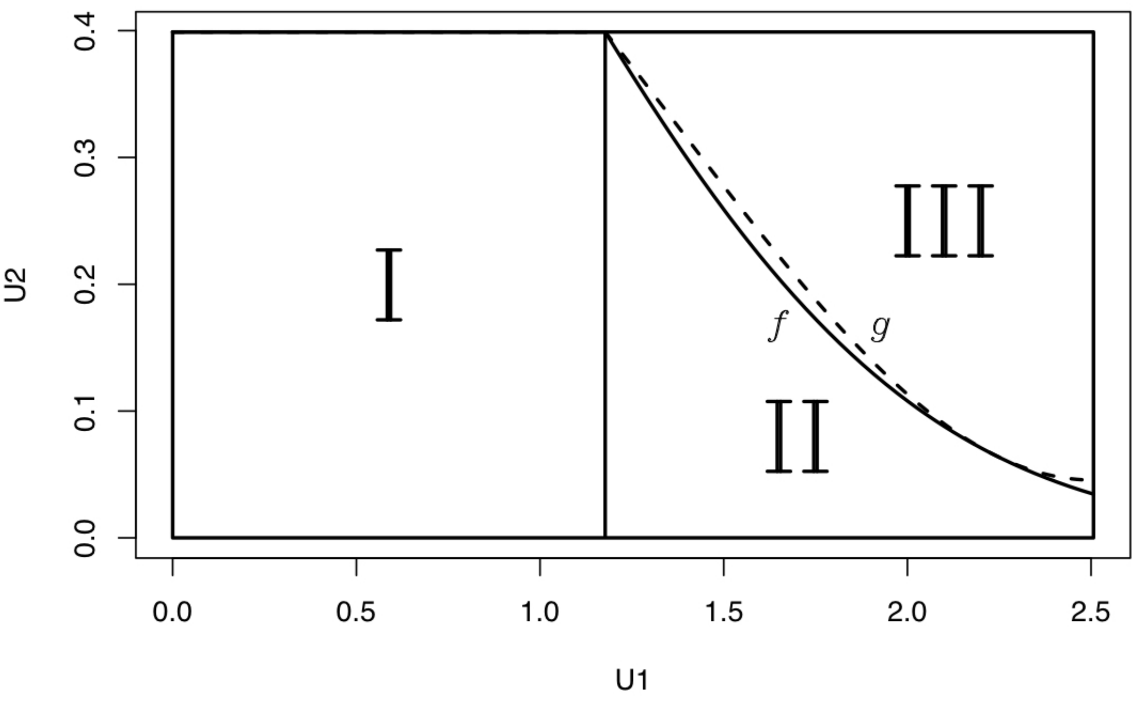
Define $g(x)$ to be $f(x)$ rotated and rescaled into $\mathcal{B}$ for x s.t.

$$f(x) > \frac{1}{\sqrt{2\pi}} = \frac{1}{b} \text{ or } x < \sqrt{\ln(4)} = a$$

i.e.,

$$g(x) = \frac{1}{b} - \frac{a}{b-a}\left[f\left(\frac{a(b-x)}{b-a}\right) - \frac{1}{b}\right]$$

for $\sqrt{\ln(4)} = a \leqslant x \leqslant b = \sqrt{2\pi}$. We can refine regions I, II, and III in terms of $f(x)$ and $g(x)$.



We generate (U_1, U_2) on $\mathcal{B}$: $U_1 \sim \text{Unif}(0, \sqrt{2\pi})$ and $U_2 \sim \text{Unif}(0, 1/\sqrt{2\pi})$. If $(U_1, U_2) \in \text{I}$, then $X = U_1$; if $(U_1, U_2) \in \text{II}$, then $X = U_1$; if $(U_1, U_2) \in \text{III}$, then $X = \frac{a(b-U_1)}{b-a}$; otherwise, we need to generate X from the tail ($x > \sqrt{2\pi}$) of the half-normal distribution (by rejection sampling with a shifted exponential proposal).

3.7.5 Sum of Uniforms

We sum k independent Unif$(0,1)$ r.v.s. $U_1, \cdots, U_k$ and define

$$X = \frac{U_1 + \cdots + U_k - k/2}{\sqrt{k/12}}$$

where the normalization guarantees $\mathbb{E}[X] = 0$ and $\mathrm{Var}[X] = 1$.

Note. $k = 12$ works well.

3.8 Markov Chain Monte Carlo

3.8.1 Construction of Reversible Markov Chain

We first assume that $f(\mathbf{x})q(\mathbf{x},\mathbf{y}) > f(\mathbf{y})q(\mathbf{y},\mathbf{x})$. Define $q^*(\mathbf{x},\mathbf{y}) = \alpha(\mathbf{x},\mathbf{y})q(\mathbf{x},\mathbf{y})$ s.t.

$$f(\mathbf{x})q^*(\mathbf{x},\mathbf{y}) = f(\mathbf{y})q^*(\mathbf{y},\mathbf{x})$$

The solution is

$$\begin{aligned} \alpha(\mathbf{x},\mathbf{y}) &= \frac{f(\mathbf{y})q(\mathbf{y},\mathbf{x})}{f(\mathbf{x})q(\mathbf{x},\mathbf{y})} \\ \alpha(\mathbf{y},\mathbf{x}) &= 1 \end{aligned}$$

We can do the similar thing if $f(\mathbf{x})q(\mathbf{x},\mathbf{y}) < f(\mathbf{y})q(\mathbf{y},\mathbf{x})$. In general,

$$\alpha(\mathbf{x},\mathbf{y}) = \min\left\{\frac{f(\mathbf{y})q(\mathbf{y},\mathbf{x})}{f(\mathbf{x})q(\mathbf{x},\mathbf{y})}, 1\right\}$$

Note. $q^*(\mathbf{x},\mathbf{y})$ may not be a transition density (unless $\alpha(\mathbf{x},\mathbf{y}) = 1$ for all $\mathbf{x},\mathbf{y}$). Given $\mathbf{X}_{i-1} = \mathbf{x}$, we can fix by allowing $\mathbf{X}_i = \mathbf{x}$ w.p.

$$\alpha(\mathbf{x},\mathbf{x}) = 1 - \int \cdots \int q^*(\mathbf{x},\mathbf{y})\mathrm{d}\mathbf{y}$$

which ideally should be small.

3.8.2 Metropolis-Hastings Algorithm

Suppose we want to generate $\mathbf{X}_i$ from $f(\mathbf{x})$ and we have a proposal transition density $q(\mathbf{x},\mathbf{y})$. Given $\mathbf{X}_{i-1} = \mathbf{x}$, we generate $\mathbf{Y}$ from $q(\mathbf{x},\mathbf{y})$ (density in $\mathbf{y}$ for each $\mathbf{x}$) and $U \sim$ Unif$(0,1)$ independent of $\mathbf{Y}$. If $U \leqslant \alpha(\mathbf{X}_{i-1},\mathbf{Y})$, then $\mathbf{X}_i = \mathbf{Y}$; if $U > \alpha(\mathbf{X}_{i-1},\mathbf{Y})$, then $\mathbf{X}_i = \mathbf{X}_{i-1}$.

We want to sample $\mathbf{X}_i$ s.t.

$$\frac{1}{n}\sum_{i=1}^{n} h(\mathbf{X}_i) \text{ converges to } \int \cdots \int h(\mathbf{x})f(\mathbf{x})\mathrm{d}\mathbf{x}$$

as fast as possible for any function h, and the convergence speed is determined largely by

$$\mathrm{Var}\left[\frac{1}{n}\sum_{i=1}^{n} h(\mathbf{X}_i)\right] \approx \frac{1}{n}\left\{\mathrm{Var}[h(\mathbf{X}_i)] + 2\sum_{s=1}^{\infty}\mathrm{Cov}[h(\mathbf{X}_i), h(\mathbf{X}_{i+s})]\right\}$$

The choice of $q(\mathbf{x},\mathbf{y})$ is important – it determines $\alpha(\mathbf{x},\mathbf{y})$, i.e., how often $\mathbf{X}_{i-1} = \mathbf{X}_i$, and how quickly $\mathbf{X}_i$ move around the space – we want to make the autocovariance terms small.

Example 3.14. Suppose we want to generate X_i from

$$P(X_i = x) = \binom{2}{x} 0.3^2 0.7^{2-x}, x = 0, 1, 2$$

Using simple transition matrix

$$Q = \begin{pmatrix} 1/3 & 1/3 & 1/3 \\ 1/3 & 1/3 & 1/3 \\ 1/3 & 1/3 & 1/3 \end{pmatrix}$$

s.t. $q(x, y) = \dfrac{1}{3}$ for $x, y = 0, 1, 2$. Our acceptance probability is

$$\alpha(x, y) = \min\left\{\frac{f(y)q(y, x)}{f(x)q(x, y)}, 1\right\} = \min\left\{\frac{\binom{2}{y}}{\binom{2}{x}} 0.3^{y-x} 0.7^{x-y}, 1\right\}$$

3.8.2.1 Application to Bayesian Inference

$\alpha(\mathbf{x}, \mathbf{y})$ depends on f only via the ratio $\dfrac{f(\mathbf{y})}{f(\mathbf{x})}$ and we only need to know $f(\mathbf{x})$ up to a multiplicative constant. Hence, we do not need to know the constant to sample from the posterior density.

3.8.2.2 Random Walk (Metropolis) Sampler

$q(\mathbf{x}, \mathbf{y}) = g(\mathbf{y} - \mathbf{x})$ for some density g :

$$\alpha(\mathbf{x}, \mathbf{y}) = \min\left\{\frac{f(\mathbf{y})g(\mathbf{x} - \mathbf{y})}{f(\mathbf{x})g(\mathbf{y} - \mathbf{x})}, 1\right\}$$

Given $\mathbf{X}_{i-1} = \mathbf{x}$, we would generate the proposal $\mathbf{Y}$ by

$$\mathbf{Y} = \mathbf{x} + \mathbf{Z}$$

where the density of $\mathbf{Z}$ is g.

Note. If g is symmetric around 0, then

$$\alpha(\mathbf{x}, \mathbf{y}) = \min\left\{\frac{f(\mathbf{y})}{f(\mathbf{x})}, 1\right\}$$

3.8.2.3 Independence (Hastings) Sampler

$q(\mathbf{x}, \mathbf{y}) = g(\mathbf{y})$: For each i, the distribution of the proposal $\mathbf{Y}$ is independent of $\mathbf{X}_{i-1}$

$$\alpha(\mathbf{x}, \mathbf{y}) = \min\left\{\frac{f(\mathbf{y})g(\mathbf{x})}{f(\mathbf{x})g(\mathbf{y})}, 1\right\}$$

Note. The independence sampler somewhat resembles rejection sampling (but without the rejection).

Example 3.15 (Poisson Distribution)**.** Suppose we want to sample X_i from a Poisson distribution with mean $\lambda > 0$. We use independence sampler with a geometric proposal

$$g(x) = (1 - \theta)\theta^x, x = 0, 1, \cdots$$

whose expected value is $\dfrac{\theta}{1-\theta}$. We choose θ s.t. $\dfrac{\theta}{1-\theta} = \lambda$, i.e., $\theta = \dfrac{\lambda}{1+\lambda}$. We can sample from a geometric distribution by $\lfloor V \rfloor$ where V as an exponential distribution with mean $-\dfrac{1}{\ln(\theta)}$.

The code for $\lambda = 5$ is:

```
lambda = 5
x = 5
samp = NULL
theta = lambda / (1 + lambda)
for (i in 1:10000) {
  v = -rexp(1) / log(theta)
  y = floor(v)
  u = runif(1)
  if (u <= dpois(y, lambda) * theta^(x-y) / dpois(x, lambda)) x = y
  samp = c(samp, x)
}
eprob = NULL
for (i in 0: 10) eprob = c(eprob, sum(samp==i) / 10000)
```

3.8.3 Practical Issues of MCMC

MCMC is often very sensitive to initial conditions. We can discard the first m iterations of the MCMC algorithm.

Note. This is important when sampling high dimensional random vectors.

It is useful to treat the output of an MCMC algorithm as a time series, and we can look at time series plots to see when the output has achieved stationarity, and autocorrelation $\widehat{\rho}(1), \cdots$.

The effective sample size is

$$n_{\text{eff}} = \left[1 + 2\sum_{s=1}^{\infty} \rho(s)\right]^{-1} n$$

4 Numerical Linear Algebra

4.1 Solving Linear Equations

Theorem 4.1 (Sherman-Morrison-Woodbury Formula/Woodbury Matrix Identity)**.**

$$(A + UCV)^{-1} = A^{-1} - A^{-1}U(C^{-1} + VA^{-1}U)^{-1}VA^{-1}$$

Note. If A and C are diagonal matrices, then computation of $(A + UCV)^{-1}$ is easy.

Example 4.1. Let $\mathbf{u}$ and $\mathbf{v}$ be vectors of length n and so $\mathbf{u}\mathbf{v}^T$ has rank 1. We can now use the Woodbury matrix identity setting $A = I, C = 1, U = \mathbf{u}, V = \mathbf{v}^T$

$$\begin{aligned}(I + \mathbf{u}\mathbf{v}^T)^{-1} &= I - I\mathbf{u}(1 + \mathbf{v}^T I\mathbf{u})^{-1}\mathbf{v}^T I \\ &= I - \frac{1}{1 + \mathbf{v}^T\mathbf{u}}\mathbf{u}\mathbf{v}^T\end{aligned}$$

and thus

$$A^{-1}\mathbf{b} = \mathbf{b} - \frac{\mathbf{v}^T\mathbf{b}}{1 + \mathbf{v}^T\mathbf{u}}\mathbf{u}$$

Example 4.2. Define

$$A = \begin{pmatrix} 1 & 1-\varepsilon \\ 1+\varepsilon & 1 \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & -\varepsilon \\ \varepsilon & 0 \end{pmatrix}}_{B_\varepsilon} + \underbrace{\begin{pmatrix} 1 \\ 1 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix}^T}_{\mathbf{v}\mathbf{v}^T}$$

where $B_\varepsilon^{-1} = B_{1\varepsilon}$ (both off-diagonal matrices). We can apply the Woodbury identity to evaluate $A^{-1}\mathbf{b}$:

$$\begin{aligned}A^{-1}\mathbf{b} &= B_\varepsilon^{-1}\mathbf{b} - \frac{1}{1 + \mathbf{v}^T B_\varepsilon^{-1}\mathbf{v}} B_\varepsilon^{-1}\mathbf{v}\mathbf{v}^T B_\varepsilon^{-1}\mathbf{b} \\ &= B_\varepsilon^{-1}\mathbf{b} - \frac{\mathbf{v}^T B_\varepsilon^{-1}\mathbf{b}}{1 + \mathbf{v}^T B_\varepsilon^{-1}\mathbf{v}} B_\varepsilon^{-1}\mathbf{v}\end{aligned}$$

The R code is:

```
eps = 1.e-7
B = matrix(c(0, -eps, eps, 0), ncol=2, byrow=T)
b = c(1, 1)
v = c(1, 1)
solve(B, b) - sum(v*solve(B, b)) * solve(B, v) / (1 + sum(v*solve(B, v)))
```

Definition 4.1 (Pivoting)**.** Pivoting means exchanging rows. Let P be a permutation matrix where each row and column has exactly one 1 and $n - 1$ 0s, then $P\mathbf{b}$ rearranges elements of $\mathbf{b}$ while PA rearranges rows of A.

Gaussian elimination with partial pivoting is essentially the approach used by R function `solve`. For some permutation matrix P, we find lower and upper triangular matrices L and U s.t.

$$PA = LU$$

Then

$$\begin{aligned}PA\mathbf{x} &= P\mathbf{b} \\ L\underbrace{U\mathbf{x}}_{\mathbf{y}} &= P\mathbf{b}\end{aligned}$$

We solve $L\mathbf{y} = P\mathbf{b}$ for $\mathbf{y}$ and then solve $U\mathbf{x} = \mathbf{y}$ for $\mathbf{x}$.

4.2 Matrix Factorizations

4.2.1 Cholesky Factorization

If A is a symmetric ($A = A^T$) and positive definite ($\mathbf{x}^T A\mathbf{x} > 0$ for $\mathbf{x} \neq \mathbf{0}$) $n \times n$ matrix, then we can write

$$A = LL^T$$

where L is lower triangular.

4.2.1.1 Computation of L

Define A_k to be the upper left $k \times k$ sub-matrix of A where $A_1 = a_{1,1}$ and $A_n = A$. A_k is symmetric positive definite so $A_k = L_k L_k^T$ where L_k is lower triangular and L_k is a sub-matrix of L_{k+1}.

Define $\mathbf{v}_{k-1} = (l_{k,1}, \cdots, l_{k,k-1})^T$ and $\mathbf{a}_{k-1} = (a_{1,k}, \cdots, a_{k-1,k})^T$, then

$$\begin{aligned} A_k &= \begin{pmatrix} A_{k-1} & \mathbf{a}_{k-1} \\ \mathbf{a}_{k-1}^T & a_{k,k} \end{pmatrix} \\ &= \begin{pmatrix} A_{k-1} & L_{k-1}\mathbf{v}_{k-1} \\ \mathbf{v}_{k-1}^T L_{k-1}^T & l_{k,1}^2 + \cdots + l_{k,k}^2 \end{pmatrix} \end{aligned}$$

Thus we have

$$L_{k-1}\mathbf{v}_{k-1} = \mathbf{a}_{k-1} \text{ (Lower triangular system)}$$

and

$$l_{k,k} = \sqrt{a_{k,k} - (l_{k,1}^2 + \cdots + l_{k,k-1}^2)}$$

Then we can successively compute $L_1 = \sqrt{a_{1,1}}, L_2, \cdots, L_n = L$:

$$L_k = \begin{pmatrix} & L_{k-1} & & 0 \\ l_{k,1} & \cdots & l_{k,k-1} & l_{k,k} \end{pmatrix}$$

Example 4.3. Let

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$$

Then

$$L_1 = l_{1,1} = \sqrt{a_{1,1}} = \sqrt{2}$$

and

$$L_2 = L = \begin{pmatrix} \sqrt{2} & 0 \\ l_{2,1} & l_{2,2} \end{pmatrix}$$

We have

$$\sqrt{2}l_{2,1} = a_{1,2} = 1 \Rightarrow l_{2,1} = \frac{1}{\sqrt{2}}$$

and

$$l_{2,2} = \sqrt{a_{2,2} - l_{2,1}^2} = \sqrt{\frac{3}{2}}$$

Thus

$$L = \begin{pmatrix} \sqrt{2} & 0 \\ \sqrt{1/2} & \sqrt{3/2} \end{pmatrix}$$

4.2.1.2 Application: Generating Multivariate Normal Random Vectors

Suppose we want to generate a random vector $\mathbf{X}$ from a p-variate normal distribution with mean vector $\mathbf{0}$ and $p \times p$ covariance matrix C where we assume C is positive definite.

We generate $Y_1, \cdots Y_p$ independent $\mathcal{N}(0,1)$ r.v.s. and define $\mathbf{Y} = (Y_1, \cdots, Y_p)^T$, and compute L in the Cholesky factorization of C. We define $\mathbf{X} = L\mathbf{Y}$ and $\mathbf{X} \sim \mathcal{N}_p(\mathbf{0}, LL^T = C)$.

Note. In R, we use function `chol` that returns L^T.

4.3 Iterative Matrix Method

Suppose we solve $A\mathbf{x} = \mathbf{b}$ for $\mathbf{x}$ where A is an $n \times n$ matrix with n very large. If A is not too complicated then we can solve iteratively, i.e., find a sequence $\{\mathbf{x}_k\}$ s.t. $\mathbf{x}_k$ converges to the solution. We write $A = A_1 + A_2$ where A_1 is nice (e.g., diagonal, lower or upper triangular) and define $\mathbf{x}_1, \mathbf{x}_2, \cdots$ s.t.

$$A_1\mathbf{x}_{k+1} = \mathbf{b} - A_2\mathbf{x}_k \text{ or } \mathbf{x}_{k+1} = A_1^{-1}\mathbf{b} - A_1^{-1}A_2\mathbf{x}_k$$

4.3.1 Jacobi and Gauss-Seidel Algorithm

Suppose we want to solve

$$\begin{pmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ \vdots \\ b_n \end{pmatrix}$$

For each $i = 1, \cdots, n$, we have

$$b_i = \sum_{j=1}^{n} a_{ij}x_j = a_{ii}x_i + \sum_{j \neq i} a_{ij}x_j$$

so that

$$x_i = \frac{1}{a_{ii}} \left(b_i - \sum_{j \neq i} a_{ij}x_j \right)$$

Then,

1. Jacobi algorithm:

$$x_i^{(k+1)} = \frac{1}{a_{ii}} \left(b_i - \sum_{j \neq i} a_{ij}x_j^{(k)} \right)$$

2. Gauss-Seidel algorithm:

$$x_i^{(k+1)} = \frac{1}{a_{ii}} \left(b_i - \sum_{j<i} a_{ij}x_j^{(k+1)} - \sum_{j>i} a_{ij}x_j^{(k)} \right)$$

Note. The Gauss-Seidel algorithm computes $\mathbf{x}_{k+1}$ in place, which is more efficient for memory; while for the Jacobi algorithm, we need to store both $\mathbf{x}_{k+1}$ and $\mathbf{x}_k$.

Let $A = L + D + U$:

$$A = \begin{pmatrix} 0 & 0 & \cdots & 0 & 0 \\ a_{21} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{n,n-1} & 0 \end{pmatrix} + \begin{pmatrix} a_{11} & 0 & \cdots & 0 \\ 0 & a_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{pmatrix} + \begin{pmatrix} 0 & a_{12} & \cdots & a_{1,n-1} & a_{nn} \\ \vdots & \cdots & \ddots & \cdots & \vdots \\ 0 & 0 & \cdots & a_{n-1,n-1} & a_{n-1,n} \\ 0 & 0 & \cdots & 0 & 0 \end{pmatrix}$$

We can write both the Gauss-Seidel and Jacobi iterations in terms of L, D and U :

1. Jacobi: $\mathbf{x}_{k+1} = D^{-1}[\mathbf{b} - (L+U)\mathbf{x}_k]$.
2. Gauss-Seidel: $(L+D)\mathbf{x}_{k+1} = \mathbf{b} - U\mathbf{x}_k$ or $\mathbf{x}_{k+1} = (L+D)^{-1}(\mathbf{b} - U\mathbf{x}_k)$.

4.3.1.1 Convergence of Gauss-Seidel and Jacobi Algorithm

Suppose $\mathbf{x}_k \to \mathbf{x}^*$ as $k \to \infty$, then

1. Jacobi: $\mathbf{x}^* = D^{-1}[\mathbf{b} - (L+U)\mathbf{x}^*]$ or $(L+D+U)\mathbf{x}^* = \mathbf{b}$.
2. Gauss-Seidel: $\mathbf{x}^* = (L+D)^{-1}(\mathbf{b} - U\mathbf{x}^*)$ or $(L+D+U)\mathbf{x}^* = \mathbf{b}$.

4.3.1.2 Comment

1. When n is large and A is relatively sparse, then iterative method can be much more efficient than direct method.
2. Iterative method is easy to program.
3. We can extend the basic idea behind the Gauss-Seidel algorithm to other problems, such as back-fitting, coordinate descent, etc.
4. We can improve the algorithm with successive over-relaxation (S0OR) method.

4.3.1.3 Application: Quadratic Minimization

Suppose we want to minimize the quadratic function

$$g(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T A\mathbf{x} - \mathbf{x}^T\mathbf{b} + c$$

where A is symmetric positive definite, i.e., $A^T = A$ and $\mathbf{x}^T A\mathbf{x} > 0$ for all $\mathbf{x} \neq \mathbf{0}$.

We can write out $g(\mathbf{x})$ explicitly:

$$g(\mathbf{x}) = g(x_1, \cdots, x_n) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}x_i x_j - \sum_{i=1}^{n} x_i b_i + c$$

Now fix $\{x_i : i \neq k\}$ and minimize $g(\mathbf{x})$ w.r.t. x_k :

$$\frac{\partial}{\partial x_k} g(\mathbf{x}) = \sum_{i=1}^{n} a_{ik}x_i - b_k = a_{kk}x_k + \sum_{i\neq k} a_{ik}x_i - b_k$$

Setting the partial derivative to 0, we have

$$x_k = \frac{1}{a_{kk}}\left(b_k - \sum_{i\neq k} a_{ik}x_i\right)$$

which is simply a Gauss-Seidel iteration.

4.4 Solving Least Squares Problems

4.4.1 Additive Regression Models

Definition 4.2 (Additive Regression Model). Given data $\{(x_{i1}, \cdots, x_{ip}, y) : i = 1, \cdots, n\}$, we assume that

$$y_i = \beta_0 + f_1(x_{i1}) + \cdots + f_p(x_{ip}) + \varepsilon_i, i = 1, \cdots, n$$

where $\{x_{ij} : i = 1, \cdots, n; j = 1, \cdots, p\}$ are predictor variables, $f_1, \cdots, f_p$ are unknown smooth functions, and $\{\varepsilon_i\}$ are r.v.s. with mean 0 and finite variance.

Note 1. For identifiability reasons, we assume that

$$\sum_{i=1}^{n} f_j(x_{ij}) = 0, j = 1, \cdots, p$$

Note 2. Suppose we have a single predictor, we observe $(x_1, y_1), \cdots, (x_n, y_n)$ and the model is $y_i = g(x_i) + \varepsilon_i, i = 1, \cdots, n$ where g is smooth function. We estimate $g(x)$ by a weighted average of $\{y_i : |x_i - x| \leqslant h\}$ where h is a tuning parameter (bandwidth) that controls the smoothness of the estimate $\widehat{g}(x)$ (***non-parametric estimation***).

Note 3. Vector from:

$$\mathbf{y} = \beta_0 \mathbf{1} + \mathbf{f}_1 + \cdots + \mathbf{f}_p + \varepsilon$$

Definition 4.3 (Smoothing Matrix)**.** Define vectors

$$\widehat{\mathbf{g}} = \begin{pmatrix} \widehat{g}(x_i) \\ \vdots \\ \widehat{g}(x_n) \end{pmatrix} \text{ and } \mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

We have

$$\widehat{\mathbf{g}} = S\mathbf{y}$$

where the $n \times n$ matrix S is a smoothing matrix.

Note 1. For simplicity, we assume S is symmetric.

Note 2. S typically depends on some tuning parameters (e.g., a bandwidth parameter).

Note 3. The eigenvalues $\lambda_1, \cdots, \lambda_n$ of a smoothing matrix S satisfy:

1. $-1 < \lambda_1, \cdots, \lambda_n \leqslant 1$.
2. At least one eigenvalue is 1.
3. Special case: Projection matrix (eigenvalues 0 and 1).

Note 4. The space spanned by eigenvectors of S with eigenvalue 1 typically includes simple functions (e..g, linear functions and possibly low order polynomials) $S(a\mathbf{1} + b\mathbf{x}) = a\mathbf{1} + b\mathbf{x}$.

Definition 4.4. For a given smoothing matrix S, we define the equivalent degrees of freedom or equivalent number of parameters of S as

$$\text{eqdf}(S) = \text{trace}(S) = \text{Measure of model complexity}$$

Example 4.4 (Penalized Least Squares)**.** Define $\widehat{\mathbf{g}}$ to minimize

$$\underbrace{\sum_{i=1}^{n}(y_i - g(x_i))^2}_{\|\mathbf{y}-\mathbf{g}\|^2 = (\mathbf{y}-\mathbf{g})^T(\mathbf{y}-\mathbf{g})} + \lambda \mathbf{g}^T A \mathbf{g}$$

where A is non-negative definite. Then

$$\widehat{\mathbf{g}} = \underbrace{(I + \lambda A)^{-1}}_{S} \mathbf{y}$$

4.4.2 The Backfitting Algorithm

Define smoothing matrices $S_0, \cdots, S_k$ where

$$S_0 = \begin{pmatrix} 1/n & \cdots & 1/n \\ \vdots & \ddots & \vdots \\ 1/n & \cdots & 1/n \end{pmatrix}$$

and $S_k\mathbf{1} = \mathbf{0}$ for $k = 1, \cdots, p$. Given current estimates $\widehat{\beta}_0, \widehat{\mathbf{f}}_1, \cdots, \widehat{\mathbf{f}}_p$, we update $\widehat{\mathbf{f}}_k$ as

$$\widehat{\mathbf{f}}_k \leftarrow S_k \left(\mathbf{y} - \widehat{\beta}_0 \mathbf{1} - \sum_{j \neq k} \widehat{\mathbf{f}}_j \right)$$

Then $\widehat{\beta}_0$ is updated as

$$\widehat{\beta}_0 \mathbf{1} \leftarrow S_0 \left(\mathbf{y} - \sum_{j=1}^{p} \widehat{\mathbf{f}}_j \right)$$

Suppose the backfitting estimate converges, then at convergence, we would have

$$\widehat{\mathbf{f}}_k = S_k \left(\mathbf{y} - \widehat{\beta}_0 \mathbf{1} - \sum_{j \neq k} \widehat{\mathbf{f}}_j \right), k = 1, \cdots, p$$

and

$$\widehat{\beta}_0 \mathbf{1} = S_0 \left(\mathbf{y} - \sum_{j=1}^{p} \widehat{\mathbf{f}}_j \right)$$

We can write in matrix form:

$$\begin{pmatrix} I & S_1 & S_1 & \cdots & S_1 & S_1 \\ S_2 & I & S_2 & \cdots & S_2 & S_2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ S_p & S_p & S_p & \cdots & I & S_p \\ S_0 & S_0 & S_0 & \cdots & S_0 & I \end{pmatrix} \begin{pmatrix} \widehat{\mathbf{f}}_1 \\ \widehat{\mathbf{f}}_2 \\ \vdots \\ \widehat{\mathbf{f}}_p \\ \widehat{\beta}_0 \mathbf{1} \end{pmatrix} = \begin{pmatrix} S_1\mathbf{y} \\ S_2\mathbf{y} \\ \vdots \\ S_p\mathbf{y} \\ S_0\mathbf{y} \end{pmatrix}$$

4.4.3 Application: Measure of Dependence

Suppose X and Y are r.v.s. with some joint distribution. The measure of linear dependence or association is

$$\rho = \frac{\mathrm{Cov}(X, Y)}{\sqrt{\mathrm{Var}[X]\mathrm{Var}[Y]}}$$

Given bivariate data $\{(x_i, y_i) : i = 1, \cdots, n\}$ from distribution and we can estimate ρ by

$$\widehat{\rho} = \frac{\sum_{i=1}^{n} (x_i - \overline{x})(y_i - \overline{y})}{\sqrt{\sum_{i=1}^{n} (x_i - \overline{x})^2} \sqrt{\sum_{i=1}^{n} (y_i - \overline{y})^2}}$$

Recall. $\rho = 0$ does not imply $X \perp Y$, and two r.v.s. can be highly dependent and have $\rho = 0$.

Definition 4.5 (Maximal Correlation)**.** Functions ψ and ϕ to maximize the correlation between $\psi(X)$ and $\phi(Y)$.

Note. The computation for ψ and ϕ are difficult. Assume X and Y have joint PDF $f(x,y)$ with respective marginal density functions $f_X(x)$ and $f_Y(y)$. To compute the maximal correlation, we need to maximize $\mathbb{E}[\psi(X)\phi(Y)]$ over all functions ψ and ϕ satisfying $\mathbb{E}[\psi(X)] = \mathbb{E}[\phi(Y)] = 0$ and $\mathbb{E}[\psi^2(X)] = \mathbb{E}[\phi^2(Y)] = 1$, then ψ and ϕ must satisfy the conditions

$$\mathbb{E}[\psi(X)|Y=y] = \int_{-\infty}^{\infty} \psi(x)\frac{f(x,y)}{f_Y(y)}\mathrm{d}x = \lambda\phi(y)$$

and

$$\mathbb{E}[\phi(Y)|X=x] = \int_{-\infty}^{\infty} \phi(y)\frac{f(x,y)}{f_X(x)}\mathrm{d}y = \lambda\psi(x)$$

where $\lambda \in [0,1]$ is the maximal correlation.

Example 4.5. Suppose $X \sim \text{Unif}(-1,1)$ and $Y = X^2$, then $\text{Cov}(X,Y) = \mathbb{E}[XY] = \mathbb{E}[X^3] = 0$. If we take $\psi(X) = X^2$ and $\phi(Y) = Y = X^2$, then the correlation between $\psi(X)$ and $\phi(Y)$ is 1.

4.4.3.1 Computing λ : The Alternating Conditional Expectation (ACE) Algorithm

Given data $(x_1,y_1),\cdots,(x_n,y_n)$ we can estimate ψ and ϕ by iterative smoothing:

1. Estimate $\psi(x)$ by smoothing $\{\widehat{\phi}(y_i)\}$ as a function of $\{x_i\}$.
2. Estimate $\phi(y)$ by smoothing $\{\widehat{\psi}(x_i)\}$ as a function of $\{y_i\}$.
3. Iterate the process until convergence.

The R function for the ACE algorithm is:

```
ace = function(x, y, niter=5, span=0.75) {
  x1 = scale(x)
  y1 = scale(y)
  for (i in 1:niter) {
    r = loess(y1~x, span=span)
    x1 = scale(r$fitted)
    r = loess(x1~y, span=span)
    y1= scale(r$fitted)
    }
  corr =cor(x1, y1)
  r = list(x=x, y=y, xhat=x1, yhat=y1, cor=corr)
  }
```

Note 1. `loess` is the locally weighted quadratic smoother.

Note 2. `span=0.75` parameter in `loess` means we use approximately 75% of the data.

Note 3. The estimates of ψ and ϕ are contained in the components `$xhat` and `$yhat`, respectively. The maximal correlation is in `$cor`.

4.4.4 Least Squares

The general least squares problem is to minimize

$$\|\mathbf{y} - X\beta\|^2$$

where X is an $n \times r$ matrix with $n > r$ and $\|\cdot\|$ is the L_2 norm. The problem is called and overdetermined system of equations.

4.4.4.1 Linear Regression Model

Suppose the linear regression model is

$$y_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \varepsilon_i = \mathbf{x}_i^T \beta + \varepsilon_i, i = 1, \cdots, n.$$

We can write the model in matrix form

$$\mathbf{y} = X\beta + \varepsilon$$

where

$$\mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}, X = \begin{pmatrix} \mathbf{x}_1^T \\ \vdots \\ \mathbf{x}_n^T \end{pmatrix} \text{ and } \varepsilon = \begin{pmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{pmatrix}$$

The least squares problem is to find $\widehat{\beta}$ to minimize

$$\sum_{i=1}^{n} (y_i - \mathbf{x}_i^T \beta)^2 = \|\mathbf{y} - X\beta\|^2.$$

If $\{\varepsilon_i\}$ are independent $\mathcal{N}(0, \sigma^2)$ then $\widehat{\beta}$ is the MLE of β. If we differentiable the objective function w.r.t. β and set the partial derivatives to 0, we get the ***normal equations*** for $\widehat{\beta}$

$$(X^T X)\widehat{\beta} = X^T \mathbf{y}$$

If $X^T X$ is invertible then

$$\widehat{\beta} = (X^T X)^{-1} X^T \mathbf{y}$$

where $X^T X$ is invertible if $\text{rank}(X) = p + 1$.

Note 1. One simple algorithm (Cholesky): If $X^T X$ is positive definite and $\text{rank}(X) = p+1$, then Cholesky factorization gives $X^X = LL^T$ where L is lower triangular, and we can solve $LL^T \widehat{\beta} = X^T \mathbf{y}$.

Note 2. The Cholesky algorithm relies on being able to compute $X^T X$ and $X^T \mathbf{y}$ with minimal round-off error. Computation of $X^T X$ and $X^T \mathbf{y}$ is moderately expensive: $O(np^2)$ floating point operations for $X^T X$ and $O(np)$ floating point operations for $X^T \mathbf{y}$. If the columns of X are collinear, the condition number of $X^T X$ is large, then round-off error in computation of $X^T X$ is magnified and the Cholesky factorization does not work.

4.4.4.2 Least Square Estimation with the QR Decomposition

Suppose the columns of X are orthogonal vectors $\mathbf{q}_0, \cdots, \mathbf{q}_p$:

$$\mathbf{q}_j^T \mathbf{q}_k = 0, j \neq k$$

then $X^T X = D$, a diagonal matrix with diagonal elements $\mathbf{q}_0^T \mathbf{q}_0, \cdots, \mathbf{q}_p^T \mathbf{q}_p$ and

$$\widehat{\beta} = D^{-1} X^T \mathbf{y}$$

We write $X = QR$ where the columns of Q are orthonormal vectors (norm is 1) and R is upper triangular. We want to minimize

$$\|\mathbf{y} - X\beta\|^2 = \|\mathbf{y} - QR\beta\|^2$$

Define $\alpha = R\beta$ and minimize

$$\|\mathbf{y} - Q\alpha\|^2$$

w.r.t. α. The normal equations for $\widehat{\alpha}$ are

$$\widehat{\alpha} = (Q^TQ)^{-1}Q^T\mathbf{y} = Q^T\mathbf{y}$$

since Q has orthonormal columns. We can then compute $\widehat{\beta}$ by solving the upper triangular system

$$R\widehat{\beta} = \widehat{\alpha}$$

Write

$$X = \begin{pmatrix} 1 & x_{11} & \cdots & x_{1p} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & \cdots & x_{np} \end{pmatrix} = \begin{pmatrix} \mathbf{v}_0 & \cdots & \mathbf{v}_p \end{pmatrix}$$

We can use the Gram-Schmidt algorithm to orthogonalize the vectors $\mathbf{v}_0, \cdots, \mathbf{v}_p$ to get Q. Note that $\mathbf{v}_0$ depends only on the first column of $Q, \mathbf{q}_0$ and for $j = 1, \cdots, p, \mathbf{v}_j$ depends on $\mathbf{q}_0, \cdots, \mathbf{q}_j$. Thus $X = QR$ where R is upper triangular.

Note 1. The Gram-Schmidt algorithm is numerically unstable: Due to round-off error, $\mathbf{q}_1, \cdots, \mathbf{q}_r$ are not exactly orthogonal, i.e., $Q^Q \neq I$. The lack of orthogonality is worse if the condition number of X^TX is large (collinear columns).

Note 2. Alternative algorithms for computing Q and R that are more numerically stable:

1. Modified Gram-Schmidt (adjusts the vectors to improve orthogonality).
2. Householder reflections (best method for achieving orthogonality).

Example 4.6 (Leverage Score)**.** In regression, the fitted values $\widehat{\mathbf{y}} = X\widehat{\beta}$ can be written as

$$\widehat{\mathbf{y}} = X(X^TX)^{-1}X^T\mathbf{y} = H\mathbf{y}$$

where matrix H is the hat matrix. The diagonal element h_{ii} of H is the leverage score that measure the potential influence of observation i. Using the QR decomposition $X = QR$, we have

$$\begin{aligned} H &= QR(R^TQ^TQR)^{-1}R^TQ^T \\ &= QR(R^TR)^{-1}R^TQ^T \text{ (Since } Q^TQ = I) \\ &= QRR^{-1}(R^T)^{-1}R^TQ^T \\ &= QQ^T \end{aligned}$$

If $\mathbf{v}_1, \cdots, \mathbf{v}_n^T$ are the rows of Q then $h_{ii} = \mathbf{v}_i^T\mathbf{v}_i$.

4.5 Randomized Numerical Linear Algebra

If we want to infer the properties of a matrix A using random sampling, we can sample random vectors $\mathbf{V}_1, \cdots, \mathbf{V}_m$ from some distribution, evaluate $\mathbf{X}_1 = A\mathbf{V}_1, \cdots, \mathbf{X}_m = A\mathbf{V}_m$, and use the empirical distribution of $\mathbf{X}_1, \cdots, \mathbf{X}_m$ to infer properties of A. The random vectors $\mathbf{V}_1, \cdots, \mathbf{V}_m$ are probing vectors.

4.5.1 Hutchinson's Method

Theorem 4.2. Suppose that $\mathbf{V}$ is a random vector with $\mathbb{E}[\mathbf{V}\mathbf{V}^T] = I$, then

$$\mathbb{E}[\mathbf{V}^TA\mathbf{V}] = \text{trace}(A)$$

Proof. Define $Z = \mathbf{V}\mathbf{V}^T$ whose elements are r.v.s. $\{Z_{ij}\}$ with $\mathbb{E}[Z_{ij}] = 1$ if $i = j$, and 0 otherwise. Then

$$\begin{aligned}\mathbb{E}[\mathbf{V}^T A\mathbf{V}] = \mathbb{E}[\text{trace}(AZ)] = \mathbb{E}\left[\sum_{i=1}^n\sum_{j=1}^n a_{ij}Z_{ji}\right] \\ = \sum_{i=1}^n\sum_{j=1}^n a_{ij}\mathbb{E}[Z_{ji}] \\ = \sum_{i=1}^n a_{ii} = \text{trace}(A)\end{aligned}$$

□

Note 1. We can now use the law of large numbers to approximate $\mathbb{E}[\mathbf{V}^T A\mathbf{V}] = \text{trace}(A)$. If $\mathbf{V}_1, \cdots, \mathbf{V}_m$ are independent random vectors with $\mathbb{E}[\mathbf{V}_i\mathbf{V}_i^T] = I$, then

$$\widehat{\text{trace}}(A) = \frac{1}{m}\sum_{i=1}^m \mathbf{V}_i^T A\mathbf{V}_i \approx \text{trace}(A)$$

for large m.

Note 2. The variance of $\widehat{\text{trace}}(A)$ is

$$\text{Var}[\widehat{\text{trace}}(A)] = \frac{1}{n}\text{Var}[\mathbf{V}^T A\mathbf{V}]$$

and we can find the distribution of $\mathbf{V}$ to minimize $\text{Var}[\mathbf{V}^T A\mathbf{V}]$ over distributions where $\mathbb{E}[\mathbf{V}\mathbf{V}^T] = I$.

Theorem 4.3. For any $A, \text{Var}[\mathbf{V}^T A\mathbf{V}]$ is minimized for $\mathbf{V} = (V_1, \cdots, V_n)^T$ where $V_1, \cdots, V_n$ are independent with

$$P(V_i = 1) = P(V_i = -1) = \frac{1}{2}$$

which is the Rademacher distribution.

4.5.1.1 Application: Equivalent Degrees of Freedom for Loess

Suppose the model

$$\mathbf{y} = \mathbf{g} + \varepsilon$$

We estimate $\mathbf{g}$ by $\widehat{\mathbf{g}} = S\mathbf{y}$ for some smoothing matrix S that is not explicitly defined. Recall that eqdf$(S) = \text{trace}(S)$. Using Hutchinson's method, we have

$$\widehat{\text{eqdf}}(S) = \frac{1}{M}\sum_{i=1}^m \mathbf{V}_i^T S\mathbf{V}_i$$

The code computing Hutchinson estimate in R is:

```
tracedf = function(x, span=0.7, m=100) {
  traces = NULL
  n = length(x)
  for (i in 1:m) {
    v = ifelse(runif(n)>0.5, 1, -1)
    r = loess(v~x, span=span)
    traces = c(traces, sum(v*r$fitted))
    }
enp = mean(traces)
std.err = sd(traces) / sqrt(m)
r = list(enp=enp, std.err=std.err)
return(r)
}
```

4.5.1.2 Function of Symmetric Matrix and Trace

Suppose that A is symmetric ($A^T = A$), then

$$A = \Gamma\Lambda\Gamma^T$$

where Γ is a diagonal matrix whose elements are the eigenvalues $\lambda_1, \cdots, \lambda_n$ of A and Λ is an orthogonal matrix whose columns are the eigenvectors of A.

If $f(x)$ is a function with $f(\lambda_1), \cdots, f(\lambda_n)$ well-defined, then we can define

$$f(A) = \Gamma f(\Lambda)\Gamma^T$$

where $f(\Lambda)$ is a diagonal matrix matrix with diagonal elements $f(\lambda_1), \cdots, f(\lambda_n)$.

Note. $\text{trace}[f(A)] = \sum_{i=1}^{n} f(\lambda_i)$.

If f is a polynomial

$$f(A) = \alpha_0 I + \alpha_1 A + \cdots + \alpha_p A^p$$

then approximating trace$[f(A)]$ using Hutchinson's method is straightforward

$$\widehat{\text{trace}}[f(A)] = \frac{1}{m}\sum_{i=1}^{m}\sum_{k=0}^{p} \mathbf{V}_i^T A^k \mathbf{V}_i$$

where $A^k\mathbf{V}_i = A(A^{k-1}\mathbf{V}_i)$.

If f is not a polynomial, then we may be able to approximate it by a polynomial, such as Taylor series, i.e., for some A_0 we have

$$f(A) = f(A_0) + f'(A_0)(A - A_0) + \frac{1}{2}f''(A_0)(A - A_0)^2 + \cdots$$

4.5.1.3 Estimating $\det(A)$

Suppose that $A = I - B$ where the eigenvalues of B lie in $(-1, 1)$, then eigenvalues of A lie in $(0, 2)$. We have

$$\begin{aligned}
\ln(\det(A)) &= \sum_{i=1}^{n} \ln(1 - \lambda_i) \\
&= -\sum_{i=1}^{n}\sum_{k=1}^{\infty} \frac{\lambda_i^k}{k} \\
&= -\sum_{k=1}^{\infty}\left(\frac{1}{k}\sum_{i=1}^{n}\lambda_i^k\right) \\
&= -\sum_{k=1}^{\infty}\frac{\text{trace}(B^k)}{k}
\end{aligned}$$

To apply Hutchinson's method, we need to find r s.t.

$$\sum_{k=r+1}^{\infty} \frac{\operatorname{trace}(B^k)}{k} \approx 0$$

Then we can estimate $\det(A)$ by

$$\widehat{\det}(A) = \exp\left(- \sum_{k=1}^{r} \sum_{i=1}^{m} \frac{\mathbf{V}_i^T B^k \mathbf{V}_i}{km} \right)$$

for probing vectors $\mathbf{V}_1, \cdots, \mathbf{V}_m$ with $\mathbb{E}[\mathbf{V}_i \mathbf{V}_i^T] = I$.

We can extend the method to a general symmetric positive definite matrix A :

1. Write $A = D(I - B)$ where D is diagonal and eigenvalues of B lie in $(-1, 1)$. We have $B = I - D^{-1}A$.
2. We have $\det(A) = \det(D)\det(I - B)$. Note that we need to know the eigenvalues of A to define D.

5 Optimization

We want to minimize or maximize some objective function $g(\mathbf{x})$ for $\mathbf{x} \in \mathcal{C}$. If $\mathcal{C}$ is an open set, i.e., every point in $\mathcal{C}$ is an interior point, we use unconstrained optimization. If $\mathcal{C}$ is not an open set, i.e., some points in $\mathcal{C}$ lie on the boundary of $\mathcal{C}$, we use constrained optimization.

5.1 Unconstrained Optimization

Consider minimizing $g(\mathbf{x})$ over an open set $\mathcal{O}$, or equivalently maximizing $-g(\mathbf{x})$ over $\mathcal{O}$. If g is differentiable over $\mathcal{O}$, then $\mathbf{x}^*$ minimizing g must satisfy

$$\nabla g(\mathbf{x}^*) = \begin{pmatrix} \frac{\partial}{\partial x_1} g(\mathbf{x}^*) \\ \vdots \\ \frac{\partial}{\partial x_p} g(\mathbf{x}^*) \end{pmatrix} = \mathbf{0}$$

Note. We may have multiple solutions and we check the second partial derivatives to determine if we have a local maximum or local minimum.

5.2 Convex Function

Convex minimization is ubiquitous in statistics and machine learning.

Definition 5.1 (Convex)**.** A function $g(\mathbf{x})$ is convex if

$$g(\lambda\mathbf{x} + (1-\lambda)\mathbf{y}) \leqslant \lambda g(\mathbf{x}) + (1-\lambda)g(\mathbf{y})$$

for any $\lambda \in [0,1]$. If the inequality holds strictly for $\lambda \in (0,1)$, then g is strictly convex.

Note 1. If $p = 1$ and $g''(x) \geqslant 0$ for all x, then g is convex. For $p > 1$, if the $p \times p$ matrix of second partial derivatives is non-negative definite for all $\mathbf{x}$, then g is convex.

Note 2. Convex functions are not necessarily differentiable at all $\mathbf{x}$. E.g., $g(x) = |x|$.

Note 3. If $g(\mathbf{x})$ is a strictly convex and differentiable function, then $\mathbf{x}^*$ satisfying $\nabla g(\mathbf{x}^*) = \mathbf{0}$ is the unique minimizing value of g, which follows from the fact that for strictly convex function,

$$g(\mathbf{x}_0) + [\nabla g(\mathbf{x}_0)]^T(\mathbf{x} - \mathbf{x}_0) < g(\mathbf{x})$$

for all $\mathbf{x} \neq \mathbf{x}_0$.

5.2.1 Sub-Gradient

Definition 5.2 (Sub-Gradient)**.** Suppose $g(\mathbf{x})$ is a convex function, the sub-gradient $\partial g(\mathbf{x})$ is

$$\partial g(\mathbf{x}) = \{\mathbf{v} : g(\mathbf{y}) \geqslant g(\mathbf{x}) + \mathbf{v}^T(\mathbf{y} - \mathbf{x}) \text{ for all } \mathbf{y}\}$$

Note 1. In general, $\partial g(\mathbf{x})$ is set-valued (a closed convex set).

Note 2. If g is defined on the real line, then

$$\partial g(x) = \{v : g(y) \geqslant g(x) + v(y - x) \text{ for all } y\}$$

i.e., $\phi_x(y) = g(x) + v(y-x)$ is a line with slope v s.t. $\phi_x(x) = g(x)$ and $\phi_x(y) \leqslant g(y)$ for all y.

Example 5.1. $g(x) = x^2$. We have $g'(1) = \partial g(1) = 2$.

Example 5.2. $g(x) = x^2 + 2|x-1|$. We have $\partial g(1) = [0,4]$.

Example 5.3. $g(x) = |x|$. We have

$$\partial g(x) = \begin{cases} -1, & x < 0 \\ 1, & x > 0 \\ [-1,1], & x = 0 \end{cases}$$

Example 5.4. $g(x) = g_0(x) + |x|$ where g_0 is differentiable. We have

$$\partial g(x) = \begin{cases} g_0'(x) - 1, & x < 0 \\ g_0'(x) + 1, & x > 0 \\ [g_0'(0) - 1, g_0'(0) + 1], & x = 0 \end{cases}$$

Example 5.5. $g(x) = \max\{0, 1-x\}$ is not differentiable at $x = 1$ with $\partial g(1) = [-1, 0]$.

5.2.2 Sub-Gradient and Convex Optimization

If $g(\mathbf{x})$ is a convex function with sub-gradient $\partial g(\mathbf{x})$, then $\mathbf{x}^*$ minimizes g iff

$$\mathbf{0} \in \partial g(\mathbf{x}^*)$$

If g is strictly convex, then $\mathbf{x}^*$ satisfying $\mathbf{0} \in \partial g(\mathbf{x}^*)$ is unique.

5.3 Constrained Optimization

We want to find $\mathbf{x}^*$ to minimize $g(\mathbf{x})$ for $\mathbf{x} \in \mathcal{C}$ subject to some conditions. One general approach to solve constrained optimization problems is to make the problem an unconstrained minimization problem.

Two basic approaches:

1. Introduce Lagrange multipliers and slack variables: Minimize

$$g(\mathbf{x}) + \sum_{j=1}^{k} \lambda_j (g_j(\mathbf{x}) - z_j^2)$$

w.r.t. $\mathbf{x}$, Lagrange multipliers $\lambda_1, \cdots, \lambda_k$, and slack variables $z_1, \cdots, z_k$.

2. Approximate the constrained problem by a sequence of unconstrained problems: Find $\mathbf{x}_\lambda^*$ to minimize

$$g(\mathbf{x}) + \text{Penalty}_\lambda(\mathbf{x})$$

so that $\mathbf{x}_\lambda^* \to \mathbf{x}^*$ as $\lambda \to 0$.

5.4 Fixed Point Algorithm

Start with a single variable $h : \mathbb{R} \to \mathbb{R}$ and we want to find x^* s.t. $h(x^*) = 0$. We consider iterative methods of the form

$$x_k = \phi(x_{k-1}), k = 1, 2, \cdots$$

for some function ϕ. If the algorithm converges ($x_k \to x^*$) then $x^* = \phi(x^*)$, where x^* is called a ***fixed point*** of ϕ.

We re-express $h(x^*) = 0$: If $a(x) \neq 0$ for all x, then

$$h(x^*) = 0 \Rightarrow \frac{h(x^*)}{a(x^*)} = 0 \Rightarrow \frac{h(x^*)}{a(x^*)} + x^* = x^*$$

which suggests that we can define $\phi(x) = x + \dfrac{h(x)}{a(x)}$ and so

$$x_k = x_{k-1} + \frac{h(x_{k-1})}{a(x_{k-1})}$$

5.4.1 Analysis of Fixed Point Algorithm

Suppose $x_k = \phi(x_{k-1})$ and $x_k \to x^*$ where x^* is a fixed point of ϕ. Assume $|x_{k-1} - x^*| = \delta$. The Taylor series expansion of $|x_k - x^*|$ is

$$\begin{aligned} |\phi(x_{k-1}) - \phi(x^*)| &= |\phi'(\xi)(x_{k-1} - x^*)| \\ &= |\phi'(\xi)||x_{k-1} - x^*| \end{aligned}$$

and so $|x_k - x^*| < \delta$ if $|\phi'(\xi)| < 1$, which suggests that the convergence of the fixed point iteration depends on $|\phi'(x)|$ for $x \in [a, b]$.

5.4.2 Fixed Point Theorem

Theorem 5.1 (Fixed Point Theorem)**.** Suppose $\phi(x)$ has a fixed point $x^* \in [a, b]$, i.e., $\phi(x^*) = x^*$ and $|\phi'(x)| \leqslant \lambda < 1$ for $x \in [a, b]$. If $x_0 \in (a, b)$ and $x_k = \phi(x_{k-1})$ for $k \geqslant 1$, then $x_k \to x^*$ as $k \to \infty$.

Proof. From the mean value theorem

$$x_1 - x^* = \phi(x_0) - \phi(x^*) = \phi'(\xi)(x_0 - x^*)$$

where ξ lies between x_0 and x^*. Thus $\xi \in [a, b]$ and so $|\phi'(\xi)| \leqslant \lambda < 1$. Iterating the process, we have

$$|x_k - x^*| \leqslant \lambda^k \underbrace{|x_0 - x^*|}_{\leqslant b-a} \to 0$$

□

Definition 5.3 (Linear Convergence Rate)**.** A fixed point algorithm satisfying the conditions of fixed point theorem has

$$|x_k - x^*| \leqslant \lambda |x_{k-1} - x^*|, \lambda < 1$$

which is called a linear convergence rate.

Note. We have a faster convergence rate if $|\phi'(x)|$ is closer to 0.

5.4.3 Multivariate Fixed Point Theorem

Suppose we want to solve $\mathbf{h}(\mathbf{x}^*) = \mathbf{0}$ for some function $\mathbf{h} : \mathbb{R}^p \to \mathbb{R}^p$. Consider iterative algorithms of the form

$$\mathbf{x}_k = \mathbf{x}_{k-1} + A^{-1}(\mathbf{x}_{k-1})\mathbf{h}(\mathbf{x}_{k-1}) = \phi(\mathbf{x}_{k-1})$$

where the matrix $A(\mathbf{x})$ is invertible for all $\mathbf{x}$.

We can replace $\phi'(x)$ by the Jacobian matrix of ϕ

$$J(\mathbf{x}) = \begin{pmatrix} [\nabla\phi_1(\mathbf{x})]^T \\ \vdots \\ [\nabla\phi_p(\mathbf{x})]^T \end{pmatrix}$$

where $J(\mathbf{x})$ is a $p \times p$ matrix. We would like to have

$$\|\mathbf{x}_k - \mathbf{x}^*\| < \|\mathbf{x}_{k-1} - \mathbf{x}^*\|$$

for some norm. From the definition of matrix norms, we have

$$\|\mathbf{x}_k - \mathbf{x}^*\| \leqslant \|J(\xi)\|\|\mathbf{x}_{k-1} - \mathbf{x}^*\|$$

Thus if $\|J(\mathbf{x})\| < 1$ for $\mathbf{x}$ in some large enough set, then we will have

$$\|\mathbf{x}_k - \mathbf{x}^*\| < \|\mathbf{x}_{k-1} - \mathbf{x}^*\|$$

and $\mathbf{x}_k \to \mathbf{x}^*$.

Note 1. Iterative algorithms require a leap of faith in their implementation.

Note 2. When p is large, we prefer simple algorithms (such as gradient descent).

5.5 Newton-Raphson Algorithm

Suppose we solve $h(x^*) = 0$ where $h(x)$ is differentiable, and we take $a(x) = -h'(x)$ so that

$$x_k = x_{k-1} - \frac{h(x_{k-1})}{h'(x_{k-1})}$$

We have

$$\phi'(x) = 1 - \frac{[h'(x)]^2 - h(x)h''(x)}{[h'(x)]^2} = \frac{h(x)h''(x)}{[h'(x)]^2}$$

If $h'(x) \neq 0$ for x close to x^*, we have $\phi'(x^*) = 0$ and $|\phi'(x)| \leqslant \varepsilon < 1$ for $|x - x^*| < \delta$. Thus, if x_{k-1} is close to x^*, we have a ***quadratic convergence rate***

$$|x_k - x^*| \leqslant C|x_{k-1} - x^*|^2$$

Note 1. N-R applies only when x_k is close to x^*.

Note 2. δ could be small and the radius of convergence of N-R could be very narrow.

Note 3. We may lose the quadratic convergence rate if $h'(x^*) = 0$.

Example 5.6 (Logistic Location MLE)**.** Suppose data $x_1, \cdots, x_n$ is from a Logistic distribution with unknown location (center) θ :

$$f(x;\theta) = \frac{\exp(x-\theta)}{[1+\exp(x-\theta)]^2}$$

The log-likelihood function is

$$\ln(\mathcal{L}(\theta)) = \sum_{i=1}^{n}[x_i - \theta - 2\ln(1+\exp(x_i-\theta))]$$

Differentiating w.r.t. θ, the MLE $\widehat{\theta}$ satisfies

$$S(\widehat{\theta}) = \sum_{i=1}^{n} \left[\frac{2\exp(x_i - \widehat{\theta})}{1 + \exp(x_i - \widehat{\theta})} - 1 \right] = 0$$

where $S(\widehat{\theta})$ is called the ***score function***. Using N-R:

$$\widehat{\theta}_k = \widehat{\theta}_{k-1} + \frac{S(\widehat{\theta}_{k-1})}{H(\widehat{\theta}_{k-1})}$$

where

$$H(\theta) = 2\sum_{i=1}^{n} \frac{\exp(x_i - \theta)}{[1 + \exp(x_i - \theta)]^2}$$

Note 1. The Logistic distribution is symmetric around 0, and thus a natural choice of initial estimate $\widehat{\theta}_0$ is a measure of the center (sample mean or sample median) of the distribution.

Note 2. If we assume that $x_1, \cdots, x_n$ come from a Logistic distribution, then we can use $H(\widehat{\theta})$, the ***observed Fisher information*** to estimate the standard error of $\widehat{\theta}$

$$\widehat{\text{SE}}(\widehat{\theta}) = [H(\widehat{\theta})]^{-1/2}$$

5.5.1 Variations on Newton-Raphson

5.5.1.1 Partial N-R Steps

For some $\alpha > 0$,

$$x_k = x_{k-1} - \alpha \frac{h(x_{k-1})}{h'(x_{k-1})} = \phi_\alpha(x_{k-1})$$

with

$$\phi'_\alpha(x) = 1 - \alpha + \alpha\phi'_1(x)$$

Note 1. By adjusting α, we may be able to increase the radius of convergence.

Note 2. Typically, $\alpha(0, 1)$, but $\alpha > 1$ is possible.

5.5.1.2 Secant Method

Replace $h'(x_{k-1})$ in N-R by the secant approximation

$$\widetilde{h}'(x_{k-1}) = \frac{h(x_{k-1}) - h(x_{k-2})}{x_{k-1} - x_{k-2}}$$

which has a slightly slower convergence rate

$$|x_k - x^*| \leqslant C|x_{k-1} - x^*|^{1.618}$$

5.5.2 Newton-Raphson and Reweighted Least Squares

We have

$$S(\theta) = \sum_{i=1}^{n} S_i(\theta) = \sum_{i=1}^{n} \frac{\partial}{\partial\theta} \ln(f(x_i; \theta))$$

and

$$H(\theta) = \sum_{i=1}^{n} H_i(\theta) = -\sum_{i=1}^{n} \frac{\partial^2}{\partial\theta^2} \ln(f(x_i; \theta))$$

The N-R iterations are

$$\widehat{\theta}_k = \widehat{\theta}_{k-1} + \frac{S(\widehat{\theta}_{k-1})}{H(\widehat{\theta}_{k-1})}$$

We have

$$\widehat{\theta}_k = \sum_{i=1}^{n} w_i(\widehat{\theta}_{k-1}) \left(\widehat{\theta}_{k-1} + \frac{S_i(\widehat{\theta}_{k-1})}{H_i(\widehat{\theta}_{k-1})} \right)$$

where

$$w_i(\theta) = \frac{H_i(\theta)}{H_1(\theta) + \cdots + H_n(\theta)}$$

Note that $w_1(\theta) + \cdots + w_n(\theta) = 1$ for all θ. We can think of N-R update at step k as a weighted average of pseudo-data

$$\widehat{\theta}_{k-1} + \frac{S_1(\widehat{\theta}_{k-1})}{J_1(\widehat{\theta}_{k-1})}, \cdots, \widehat{\theta}_{k-1} + \frac{S_n(\widehat{\theta}_{k-1})}{H_n(\widehat{\theta}_{k-1})}$$

Thus at convergence, $\widehat{\theta}$ is the weighted average of

$$\widehat{\theta} + \frac{S_1(\widehat{\theta})}{H_1(\widehat{\theta})}, \cdots, \widehat{\theta} + \frac{S_n(\widehat{\theta})}{H_n(\widehat{\theta})}$$

which can be used to obtain an estimate of the standard error of $\widehat{\theta}$ (***sandwich estimate***):

$$\widehat{\text{SE}}(\widehat{\theta}) = \left[\frac{S_1^2(\widehat{\theta}) + \cdots + S_n^2(\widehat{\theta})}{[H_1(\widehat{\theta}) + \cdots + H_n(\widehat{\theta})]^2} \right]^{1/2}$$

5.5.3 Multivariate N-R Algorithm

We take

$$A(\mathbf{x}) = -\begin{pmatrix} [\nabla h_1(\mathbf{x})]^T \\ \vdots \\ [\nabla h_p(\mathbf{x})]^T \end{pmatrix}$$

5.5.4 Application: Maximum Likelihood Estimation

Suppose data $x_1, \cdots, x_n$ with log-likelihood function $\ln(\mathcal{L}(\theta)) = \ln(f(x_1, \cdots, x_n; \theta))$ defined for $\theta \in \Theta$ (parameter space). Assume that the MLE $\widehat{\theta}$ satisfies

$$\nabla \ln(\mathcal{L}(\widehat{\theta})) = \mathbf{S}(\widehat{\theta}) = \mathbf{0}$$

$H(\theta)$ is the matrix of negative second derivatives:

$$h_{ij}(\theta) = -\frac{\partial^2}{\partial\theta_i \partial\theta_j} \ln(\mathcal{L}(\theta))$$

The N-R iteration is

$$\widehat{\theta}_k = \widehat{\theta}_{k-1} + [H(\widehat{\theta}_{k-1})]^{-1}\mathbf{S}(\widehat{\theta}_{k-1})$$

We can estimate the variance-covariance matrix of $\widehat{\theta}$ by $[H(\widehat{\theta})]^{-1}$.

Example 5.7 (Weibull Distribution)**.** Suppose $x_1, \cdots, x_n$ are independent observations from a Weibull distribution (which is often used to model lifetime data or failure data). The density function is

$$f(x;\alpha,\sigma) = \left(\frac{\alpha}{\sigma}\right)\left(\frac{x}{\sigma}\right)^{\alpha-1}\exp\left[-\left(\frac{x}{\sigma}\right)^{\alpha}\right], x > 0$$

where $\alpha > 0$ and $\sigma > 0$ are unknown parameters: α is a shape parameter and σ is a scale parameter. Note that

$$\mathbb{E}[X] = \int_0^\infty x f(x;\alpha,\sigma)\mathrm{d}x = \sigma\Gamma\left(1+\frac{1}{\alpha}\right)$$

The ***hazard function*** is given by

$$h(x) = \frac{f(x;\alpha,\sigma)}{1-F(x;\alpha,\sigma)} = \frac{\alpha}{\sigma^\alpha}x^{\alpha-1}$$

The MLEs of α and σ satisfy the likelihood equations

$$\sum_{i=1}^n \left[\frac{1}{\widehat{\alpha}} + \ln\left(\frac{x_i}{\widehat{\sigma}}\right) - \ln\left(\frac{x_i}{\widehat{\sigma}}\right)\left(\frac{x_i}{\widehat{\sigma}}\right)^{\widehat{\alpha}}\right] = 0$$

and

$$\sum_{i=1}^n \left[\frac{\widehat{\alpha}}{\widehat{\sigma}}\left(\frac{x_i}{\widehat{\sigma}}\right)^{\widehat{\alpha}} - \frac{\widehat{\alpha}}{\widehat{\sigma}}\right] = 0$$

To compute the MLEs, we can use the N-R algorithm to solve the likelihood equations.

We need to choose proper initial values for α and σ in the N-R algorithm since it can be critical in guaranteeing that the N-R algorithm converges. We consider two basic criteria:

1. $\widehat{\alpha}_0$ and $\widehat{\sigma}_0$ should be easy to compute.
2. $\widehat{\alpha}_0$ and $\widehat{\sigma}_0$ should be good estimates of α and σ.

Criterion 2 is much more important, and we can use method of moments estimates: We find functions g_1 and g_2 s.t.

$$\mathbb{E}[g_1(X)] = \psi_1(\alpha,\sigma)$$
$$\mathbb{E}[g_2(X)] = \psi_2(\alpha,\sigma)$$

We estimate $\mathbb{E}[g_1(X)]$ and $\mathbb{E}[g_2(X)]$ by sample means and define $\widehat{\alpha}_0$ and $\widehat{\sigma}_0$ as follows:

$$\frac{1}{n}\sum_{i=1}^n g_1(x_i) = \psi_1(\widehat{\alpha}_0,\widehat{\sigma}_0)$$
$$\frac{1}{n}\sum_{i=1}^n g_2(x_i) = \psi_2(\widehat{\alpha}_0,\widehat{\sigma}_0)$$

If $\mathrm{Var}[g_1(X)]$ and $\mathrm{Var}[g_2(X)]$ are both finite, then $\widehat{\alpha}_0$ and $\widehat{\sigma}_0$ are good estimates. Note that if we can estimate α by $\widehat{\alpha}_0$, then we can define

$$\widehat{\sigma}_0 = \frac{\overline{x}}{\Gamma(1+1/\widehat{\alpha}_0)}$$

We can use a Weibull plot to define $\widehat{\alpha}_0$: Note that

$$1-F(x;\alpha,\sigma) = \exp\left[-\left(\frac{x}{\sigma}\right)^{\alpha}\right]$$

and so

$$\ln(-\ln(1-F(x))) = \alpha\ln(x) - \alpha\ln(\sigma) \Rightarrow \ln(x) = \frac{1}{\alpha}\ln(-\ln(1-F(x))) + \ln(\sigma)$$

i.e., $\ln(x)$ is linear function of $\ln(-\ln(1-F(x)))$. The Weibull plot is constructed as follows:

1. Order the data from smallest to largest: $x_{(1)} \leqslant \cdots \leqslant x_{(n)}$.
2. Plot $\ln(x_{(i)})$ versus $t_i = \ln\left(-\ln\left(1-\frac{i}{n+1}\right)\right)$ for $i = 1, \cdots, n$.

For Weibull data, the points should lie close to a straight line with slope $\frac{1}{\alpha}$ and intercept $\ln(\sigma)$. We can use the Weibull plot to obtain $\widehat{\alpha}_0$ and possibly $\widehat{\sigma}_0$ using least squares to estimate the slope and intercept. The R code for Weibull plot is:

```
weibullplot = function(x, line=T){
  x = sort(x)
  n = length(x)
  s = 1 - c(1:n)/(n+1)
  plot(log(-log(s)), log(x), pch=20)
  r = lm(log(x)~log(-log(s)))
  alpha = 1/r$coef[2]
  sigma = exp(r$coef[1])
  if (line){
    abline(r, col="red", lwd=3)
    title(main=paste("alpha = ", round(alpha, 2), "sigma = ", round(sigma, 2)),
       cex=0.5)
    }
  else{
    a = list(alpha=alpha, sigma=sigma)
    a
    }
  }
```

5.6 Fisher Scoring

We replace the matrix $H(\theta)$ in the N-R algorithm by its expected value $\mathcal{H}(\theta) = \mathbb{E}_\theta[H(\theta)]$:

$$\widehat{\theta}_k = \widehat{\theta}_{k-1} + [\mathcal{H}(\widehat{\theta}_{k-1})]^{-1}\mathbf{S}(\widehat{\theta}_{k-1})$$

Fisher scoring tends to converge slower than N-R and may be more sensitive to initial values. In exponential family models where the joint density has the general form

$$f(\mathbf{x};\theta) = \exp[\theta^T\mathbf{T}(\mathbf{x}) - c(\theta) + d(\mathbf{x}))]$$

Fisher scoring and N-R are essentially the same.

Example 5.8 (Weibull Distribution)**.** The form of $H(\alpha,\sigma)$ is rather complicated: It depends on $y_i = \frac{x_i}{\sigma}$ for $i = 1, \cdots, n$ via the following sums:

$$\sum_{i=1}^n \ln(y_i)y_i^\alpha, \sum_{i=1}^n y_i^\alpha, \sum_{i=1}^n [\ln(y_i)]^2 y_i^\alpha$$

We can compute $\mathcal{H}(\alpha,\sigma)$ by taking expected values:

$$\mathcal{H}(\alpha,\sigma) = n \begin{pmatrix} \dfrac{6+\pi^2-12\gamma+6\gamma^2}{6\alpha^2} & \dfrac{\gamma-1}{\sigma} \\ \dfrac{\gamma-1}{\sigma} & \dfrac{\alpha^2}{\sigma^2} \end{pmatrix}$$

where $\gamma = 0.5772\cdots$ is Euler's constant.

5.6.1 Quasi-Likelihood Estimation

Suppose the data is $\{(\mathbf{x}_i, y_i) : i = 1,\cdots,n\}$. For a generalized linear model, we specify the variance function $V(\mu_i)$ and the link function $\phi(\mu_i) = \mathbf{x}_i^T\beta$. If the variance function corresponds to a particular distribution, then we can estimate β by maximum likelihood estimation; otherwise, we define a ***quasi-likelihood*** function and maximize it.

We define the function $\mathcal{Q}(y;\mu)$ by the differential equation

$$\frac{\partial}{\partial\mu}\mathcal{Q}(y;\mu) = \frac{y-\mu}{V(\mu)}$$

Given $\{(\mathbf{x}_i, y_i)\}$ with functions ϕ and V, we maximize

$$\sum_{i=1}^{n} \mathcal{Q}(y_i;\mu_i) = \sum_{i=1}^{n} \mathcal{Q}(y_i;\phi^{-1}(\mathbf{x}_i^T\beta))$$

w.r.t. β. Note that the gradient of $\mathcal{Q}(y_i;\mu_i)$ w.r.t. β is

$$\nabla\mathcal{Q}(y_i;\phi^{-1}(\mathbf{x}_i^T\beta)) = \underbrace{\left[\frac{\partial}{\partial\mu_i}\mathcal{Q}(y_i;\mu_i)\right]}_{(y_i-\mu_i)/V(\mu_i)} \underbrace{[\nabla\phi^{-1}(\mathbf{x}_i^T\beta)]}_{[\phi'(\phi^{-1}(\mathbf{x}_i^T\beta))]^{-1}\mathbf{x}_i}$$

The maximum quasi-likelihood estimate $\widehat{\beta}$ satisfies

$$\mathbf{S}(\widehat{\beta}) = \sum_{i=1}^{n}\left[\frac{y_i-\mu_i(\widehat{\beta})}{V(\mu_i(\widehat{\beta}))\phi'(\mu_i(\widehat{\beta}))}\right]\mathbf{x}_i = \mathbf{0}$$

where $\mu_i(\beta) = \phi^{-1}(\mathbf{x}_i^T\beta)$. We can solve these equations using N-R or Fisher scoring, and the Fisher scoring algorithm is simple:

$$\widehat{\beta}_k = \widehat{\beta}_{k-1} + [\mathcal{H}(\widehat{\beta}_{k-1})]^{-1}\mathbf{S}(\widehat{\beta}_{k-1})$$

where

$$\mathcal{H}(\beta) = \sum_{i=1}^{n}\frac{\mathbf{x}_i\mathbf{x}_i^T}{[\phi'(\mu_i(\beta))]^2 V(\mu_i(\beta))}$$

5.6.2 Fisher Scoring and Iteratively Reweighted Least Squares

We want to find a stable implementation of the Fisher scoring algorithm. Define

$$X = \begin{pmatrix} \mathbf{x}_1^T \\ \vdots \\ \mathbf{x}_n^T \end{pmatrix}$$

and $W(\beta)$ to be a diagonal matrix with diagonal elements

$$w_i(\beta) = \frac{1}{[\phi'(\mu_i(\beta))]^2 V(\mu_i(\beta))}$$

for $i = 1, \cdots, n$. Then

$$\mathcal{H}(\beta) = X^T W(\beta) X$$

We can define $\widehat{\beta}_k$ as a weighted least squares estimate minimizing

$$\sum_{i=1}^{n} w_i(\widehat{\beta}_{k-1})(z_i(\widehat{\beta}_{k-1}) - \mathbf{x}_i^T \beta)^2$$

w.r.t. β Note that

$$\begin{aligned}
\widehat{\beta}_k &= \widehat{\beta}_{k-1} + [\mathcal{H}(\widehat{\beta}_{k-1})]^{-1}\mathbf{S}(\widehat{\beta}_{k-1}) \\
&= (X^T W(\widehat{\beta}_{k-1})X)^{-1}[X^T W(\widehat{\beta}_{k-1})X\widehat{\beta}_{k-1} + \mathbf{S}(\widehat{\beta}_{k-1})] \\
&= (X^T W(\widehat{\beta}_{k-1})X)^{-1} X^T W(\widehat{\beta}_{k-1})\mathbf{z}(\widehat{\beta}_{k-1})
\end{aligned}$$

where

$$z_i(\beta) = \mathbf{x}_i^T \beta + \phi'(\mu_i(\beta))(y_i - \mu_i(\beta))$$

We call $\{z_i(\beta)\}$ as the ***adjusted dependent variable***.

Example 5.9 (Logistic Regression)**.** Suppose the model is $\{Y_i\}$ binary with $\mathbb{E}[Y_i|\mathbf{x}_i] = \mu_i$, $\mathrm{Var}[Y_i|\mathbf{x}_i] = \mu_i(1-\mu_i) = V(\mu_i)$, and logit link

$$\ln\left(\frac{\mu_i}{1-\mu_i}\right) = \mathbf{x}_i^T \beta$$

so that

$$\mu_i(\beta) = \frac{\exp(\mathbf{x}_i^T \beta)}{1 + \exp(\mathbf{x}_i^T \beta)}$$

We have

$$w_i(\beta) = \mu_i(\beta)(1 - \mu_i(\beta))$$

and

$$z_i(\beta) = \mathbf{x}_i^T \beta + \frac{y_i - \mu_i(\beta)}{\mu_i(\beta)(1-\mu_i(\beta))}$$

5.6.2.1 Application: Poisson Regression

Suppose the model is $Y_i \sim$ Poisson with mean μ_i, with $V(\mu) = \mu$ and log link $\phi(\mu_i) = \ln(\mu_i) = \mathbf{x}_i^T \beta$ Then $\mu_i = \mu_i(\beta) = \exp(\mathbf{x}_i^T \beta)$. For IRLS algorithm, we define

$$w_i(\beta) = \frac{1}{[\phi'(\mu_i)]^2 V(\mu_i)} = \mu_i(\beta)$$

and

$$z_i(\beta) = \mathbf{x}_i^T \beta + \frac{y_i - \mu_i(\beta)}{\mu_i(\beta)}$$

5.7 Application: M-Estimation

Least squares estimation is very sensitive to outliers, and the M-estimation is to minimize

$$\sum_{i=1}^{n} \rho(y_i - \mathbf{x}_i^T \beta)$$

where $\dfrac{\rho(x)}{x^2} \to 0$ as $|x| \to \infty$. E.g., $\rho(x) = |x|^r$ for $1 \leqslant r < 2$.

Suppose we define $\widehat{\beta}$ to minimize the objective function of M-estimation, where $\rho(t)$ is a twice differentiable function s.t. $\rho(0) = 0$ and $\rho(t)$ increases as $|t|$ increases. We define $\psi(t) = \rho'(t)$ and $\psi'(t) = \rho''(t)$. M-estimates are often defined in terms of $\psi(t)$. $\widehat{\beta}$ satisfies the condition

$$\sum_{i=1}^{n} \psi(y_i - \mathbf{x}_i^T \beta)\mathbf{x}_i = \mathbf{0}$$

Example 5.10 (Huber Estimate)**.** Define $\rho(t)$ so that $\rho(t) = Ct^2$ for $|t|$ close to 0 and $\rho(t) \approx C|t|$ for larger $|t|$. Define $\psi(t) = \psi_c(t)$ as follows:

$$\psi_c(t) = \begin{cases} -c, & t < -c \\ t, & |t| \leqslant c \\ c, & t > c \end{cases}$$

where c is a tuning parameter. Note that $\psi_c'(t)$ is not defined at $t = \pm c$. The corresponding $\rho_c(t)$ is defined as follows:

$$\rho_c(t) = \begin{cases} \dfrac{t^2}{2}, & |t| < c \\ c|t| - \dfrac{c^2}{2}, & |t| > c \end{cases}$$

5.7.1 N-R for M-Estimation

The M-estimate $\widehat{\beta}$ satisfies the equation

$$\mathbf{S}(\widehat{\beta}) = \sum_{i=1}^{n} \psi(y_i - \mathbf{x}_i^T \beta)\mathbf{x}_i = \mathbf{0}$$

Since we assume that ψ' exists, we can use the N-R algorithm to compute $\widehat{\beta}$:

$$\widehat{\beta}_k = \widehat{\beta}_{k-1} + [H(\widehat{\beta}_{k-1})]^{-1}\mathbf{S}(\widehat{\beta}_{k-1})$$

where

$$H(\beta) = \sum_{i=1}^{n} \psi'(y_i - \mathbf{x}_i^T \beta)\mathbf{x}_i\mathbf{x}_i^T$$

5.7.2 IRLS for M-Estimation

We write

$$H(\beta) = X^T W(\beta) X$$

where $W(\beta)$ is a diagonal matrix with diagonals

$$w_i(\beta) = \psi'(y_i - \mathbf{x}_i^T \beta)$$

for $i = 1, \cdots, n$. Then we have

$$\widehat{\beta}_k = (X^T W(\widehat{\beta}_{k-1}) X)^{-1} X^T W(\widehat{\beta}_{k-1}) \mathbf{z}(\widehat{\beta}_k)$$

where

$$z_i(\beta) = \mathbf{x}_i^T \beta + \frac{\psi(y_i - \mathbf{x}_i^T \beta)}{\psi'(y_i - \mathbf{x}_i^T \beta)}$$

for $i = 1, \cdots, n$.

5.7.3 Fisher Scoring Modification

We can replace the matrix $W(\beta)$ and the vector $\mathbf{z}(\beta)$ by $W(\beta) = \tau(\beta) I$ where

$$\tau(\beta) = \frac{1}{n} \sum_{i=1}^{n} \psi'(y_i - \mathbf{x}_i^T \beta)$$

and

$$\mathbf{z}(\beta) = \mathbf{x}_i^T \beta + \frac{\psi(y_i - \mathbf{x}_i^T \beta)}{\tau(\beta)}$$

Example 5.11 (Huber Estimate)**.** $\widehat{\beta}$ satisfies

$$\sum_{i=1}^{n} \psi_c(y_i - \mathbf{x}_i^T \beta) \mathbf{x}_i = \mathbf{0}$$

where

$$\psi_c(t) = \begin{cases} -c, & t < -c \\ t, & |t| \leqslant c \\ c, & t > c \end{cases}$$

Then $\psi_c'(t) = 1$ for $|t| < c$ and $\psi_c'(t) = 0$ for $|t| > c$. For IRLS, we have $w_i(\beta) = 0$ if $|y_i - \mathbf{x}_i^T \beta| > c$, and $w_i(\beta) = 1$ and $z_i(\beta) = y_i$ if $|y_i - \mathbf{x}_i^T \beta| \leqslant c$. The R code is:

```
huber = function(x, y, c, niter=10){
   # Ues LS as initial estimate
   r = lm(y~x)
   if (missing(c)) c = median(abs(r$resid)) * 1.35
   for (i in 1:niter){
      resid = r$resid
      fitted = r$fitted
      wt = ifelse(abs(resid)>c, 0, 1)
      z = y
      r = lm(y~x, weights=wt)
      }
   beta = r$coef
   beta
   }
```

5.8 L_∞ Estimation and Lawson's Algorithm

The L_∞ estimation is to minimize

$$\max_{1\leqslant i\leqslant n} |y_i - \mathbf{x}_i^T\beta| = \|\mathbf{y} - X\beta\|_\infty$$

w.r.t. β. L_∞ estimation is useful if we know $y_i \approx \mathbf{x}_i^T\beta$ for some β and the approximation error is very small and bounded. For example, minimize median$|y_i - \mathbf{x}_i^T\beta|$, which is the least median of squares (LMS) estimate, is an L_∞ estimate on a subset of the data.

The L_∞ is essentially determined by $p+1$ points where p is the length of the vector β. If these points are $(\mathbf{x}_{i_1}, y_{i_1}), \cdots, (\mathbf{x}_{i_{p+1}}, y_{i_{p+1}})$ then

$$\max_{1\leqslant i\leqslant n} |y_i - \mathbf{x}_i^T\widehat{\beta}| = |y_{i_j} - \mathbf{x}_{i_j}^T\widehat{\beta}|$$

for $j = 1,\cdots,p+1$. We successively downweight observations with small absolute residuals until only $p+1$ points have positive weights. The Lawson's algorithm is:

1. Define $\widehat{\beta}_0$ to be the LS estimate and weights $w_1^{(0)} = \cdots = w_n^{(0)} = \dfrac{1}{n}$.
2. For $k = 1, 2, \cdots$:

   (1) Define weights $\{w_i^{(k)}\}$ to be

$$w_i^{(k)} = \frac{w_i^{(k-1)}|y_i - \mathbf{x}_i^T\widehat{\beta}_{k-1}|}{\sum_{j=1}^n w_j^{(k-1)}|y_j - \mathbf{x}_j^T\widehat{\beta}_{k-1}|}$$

for $i = 1,\cdots,n$.

   (2) Define $\widehat{\beta}_k$ to minimize

$$\sum_{i=1}^n w_i^{(k)}(y_i - \mathbf{x}_i^T\beta)^2$$

We need to exclude points where $w_i^{(k)} = 0$ for some k, and at convergence we will have

$$w_i^* = \frac{w_i^*|y_i - \mathbf{x}_i^T\widehat{\beta}|}{\sum_{j=1}^n w_j^*|y_j - \mathbf{x}_i^T\widehat{\beta}|}$$

for some non-negative weights $w_q^*, \cdots, w_n^*$.

5.9 Gradient Descent Algorithm

Suppose we want to minimize $g(\mathbf{x})$ over some open set $\mathcal{O}$ and $\mathbf{x}^*$ satisfies

$$\nabla g(\mathbf{x}^*) = \mathbf{0}$$

For small $\varepsilon > 0$, we have

$$g(\mathbf{x} + \varepsilon\mathbf{u}) \approx g(\mathbf{x}) + \varepsilon\mathbf{u}^T\nabla g(\mathbf{x})$$

where the right hand side above decreases most rapidly over unit vectors $\mathbf{u}$ taking

$$\mathbf{u} = -\frac{\nabla g(\mathbf{x})}{\|\nabla g(\mathbf{x})\|}$$

which suggests the gradient descent algorithm

$$\mathbf{x}_k = \mathbf{x}_{k-1} - \varepsilon\nabla g(\mathbf{x}_{k-1}) = \phi(\mathbf{x}_{k-1})$$

where the parameter $\varepsilon > 0$ is called the ***learning rate*** in machine learning, and ε may depend on k, i.e., $\varepsilon = \varepsilon_k$.

5.9.1 Convergence of Gradient Descent

We would have convergence of $\mathbf{x}_k$ to $\mathbf{x}^*$ if the Jacobian matrix of ϕ, $J_\phi(\mathbf{x})$, has all eigenvalues with modulus less than 1 for $\mathbf{x}$ in some region. Note that

$$J_\phi(\mathbf{x}) = I - \varepsilon J_{(\nabla g)}(\mathbf{x})$$

Because of minimization, $J_{(\nabla g)}(\mathbf{x})$ should be symmetric positive definite for $\mathbf{x}$ in some region and will have positive eigenvalues in this region. Thus the eigenvalues of $J_\phi(\mathbf{x})$ will be less than 1 in absolute value for ε small enough, which implies convergence.

Example 5.12. Suppose $g(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T A\mathbf{x} - \mathbf{x}^T\mathbf{b}$ where A is symmetric positive definite. Then $\nabla g(\mathbf{x}) = A\mathbf{x} - \mathbf{b}$, $\mathbf{x}^*$ minimizing g satisfies $A\mathbf{x}^* = \mathbf{b}$, and $J_{(\nabla g)}(\mathbf{x}) = A$. Therefore, $J_\phi(\mathbf{x}) = I - \varepsilon A$. If $\lambda_1 \geqslant \cdots \geqslant \lambda_p > 0$ are the eigenvalues of A, then $1 - \varepsilon\lambda_1, \cdots, 1 - \varepsilon\lambda_p$ are the eigenvalues of $J_\phi(\mathbf{x})$. We need to take $0 < \varepsilon < \frac{2}{\lambda_1}$ for convergence.

5.10 Robbins-Monro Procedure

5.10.1 Stochastic Approximation

Suppose we want to solve $\mathbf{h}(\mathbf{x}^*) = \mathbf{0}$ for $\mathbf{x}^*$. We can write

$$\mathbf{h}(\mathbf{x}) = \sum_{i=1}^{n} \mathbf{h}_i(\mathbf{x})$$

5.10.2 Robbins-Monro Procedure

Suppose we want to solve

$$\mathbb{E}_F[\mathbf{h}(X;\theta)] = \mathbf{0}$$

for θ. Assume that for each x, $\mathbf{h}(x;\theta)$ is the gradient (w.r.t. θ) of a convex function. The algorithm is

$$\theta_k = \theta_{k-1} - a_k\mathbf{h}(X_k;\theta_{k-1})$$

for some $\{a_k\}$ of positive numbers, and $X_1, \cdots$ are independent r.v.s. with distribution F. The conditions on $\{a_k\}$ are needed for convergence: $a_k \to 0$ as $k \to \infty$ but not too quickly or too slowly, i.e.,

1. $\sum_{k=1}^{\infty} a_k = \infty$.
2. $\sum_{k=1}^{\infty} a_k^2 < \infty$.

5.10.3 Application: Convex Minimization

Suppose we want to minimize $g(\mathbf{x})$ where $g(\mathbf{x}) = \sum_{i=1}^{n} g_i(\mathbf{x})$ and each g_i is convex and differentiable. If $\mathbf{x}^*$ minimizes $g(\mathbf{x})$, then

$$\nabla g(\mathbf{x}^*) = \sum_{i=1}^{n} \nabla g_i(\mathbf{x}^*) = \mathbf{0}$$

We can uas a stochastic approximation approach to approximate $\mathbf{x}^*$. We write the condition for $\mathbf{x}^*$ as an expected value:

$$\mathbf{0} = \frac{1}{n}\sum_{i=1}^{n} \nabla g_i(\mathbf{x}^*) = \mathbb{E}[\nabla g_{\mathcal{I}}(\mathbf{x}^*)]$$

where $P(\mathcal{I} = i) = \dfrac{1}{n}$ for $i = 1, \cdots, n$.

5.11 Stochastic Gradient Descent Algorithm

Suppose we want to minimize convex function g where

$$\nabla g(\mathbf{x}) = \sum_{i=1}^{n} \nabla g_i(\mathbf{x})$$

The algorithm is:

$$\mathbf{x}_k = \mathbf{x}_{k-1} - a_k \nabla g_{\mathcal{I}_k}(\mathbf{x}_{k-1})$$

where $\mathcal{I}_1, \cdots$ are independent r.v.s. with $P(\mathcal{I}_j = i) = \dfrac{1}{n}$ for $i = 1, \cdots, n$, $\sum_{k=1}^{\infty} a_k = \infty$, and $\sum_{k=1}^{\infty} a_k^2 < \infty$.

Suppose $a_k = \dfrac{\alpha}{k}$ for some $\alpha > 0$:

1. α too small: Take small steps and convergence may be too slow - significant bias if m is too small, i.e., low variance and high bias.
2. α too large: Take large steps and possibly inflate the variance of the estimates, i.e., low bias and high variance.

Example 5.13 (Huber Estimate in Regression)**.** $\widehat{\beta}$ satisfies

$$\sum_{i=1}^{n} \psi_c(y_i - \mathbf{x}_i^T \beta)\mathbf{x}_i = \mathbf{0}$$

where

$$\psi_c(t) = \begin{cases} -c, & t < -c \\ t, & |t| \leqslant c \\ c, & t > c \end{cases}$$

The stochastic gradient descent iteration is:

$$\widehat{\beta}_k = \widehat{\beta}_{k-1} + a_k \psi(y_{\mathcal{I}_k} - \mathbf{x}_{\mathcal{I}_k}^T \widehat{\beta}_{k-1})$$

where $P(\mathcal{I}_k = i) = \dfrac{1}{n}$ for $i = 1, \cdots, n$. The R code for stochastic gradient descent is:

```
stochapprox = function(x, y, c, alpha=1, nrep=10000){
  x = cbind(1, x)
  p = ncol(x)
  beta = rep(0, p)
  betas = NULL
  n = length(y)
  for (k in 1:nrep){
    i = sample(c(1:n), size=1)
    resi = y[i] - sum(beta*x[i, ])
    psi = ifelse(abs(resi)<c, resi, c*sign(resi))
    beta = beta + alpha * psi * x[i, ] / k
    betas = rbind(betas, beta)
    }
  betas
  }
```

Bias decreases as k increases, and bias persists for $\alpha = 1$ even for large k. Variance decreases as k increases, and is larger for larger values of α.