LDL decomposition for symmetric matrices

Claim: if $A = A^T$

$A = LU$, $U = \underset{\substack{\downarrow \\ \text{diagonal matrix}}}{\tilde{D}}L^T \Rightarrow \boxed{A = LDL^T}$

Proof: $LU = A = A^T = (LU)^T = U^T L^T$

Multiply on the left w/ (L^{-1})

$L^{-1}LU = L^{-1}(U^T L^T)$

Multiply on the right w/ $(L^T)^{-1}$

$U(L^T)^{-1} = L^{-1}U^T L^T \cdot (L^T)^{-1}$

$\underbrace{U(L^T)^{-1}}_{\text{2 upper triangular}} = \underbrace{L^{-1} \cdot U^T}_{\text{2 lower triangular}} = D$ only matrix which is upper & lower triangular $\Rightarrow$ diagonal

$U(L^T)^{-1} = D \Rightarrow U = DL^T$

$$\boxed{A = LU = LDL^T}$$

Cholesky Decomposition

For positive definite matrices

* A is symmetric positive def. iff

$$A^T = A \quad \& \quad x^T A x > 0 \text{ for all } x \neq 0$$

Then there exists a lower triangular matrix V such that

$$\boxed{A = VV^T}$$

where $V = LD^{1/2}$

<u>Proof</u>: $A = LDL^T$

<u>Claim</u>: all diagonal entries of D are strictly positive so $D^{1/2}$ is well-defined

$\rightarrow x^T A x > 0$

$\underbrace{x^T L}_{y} D \underbrace{L^T x}_{y} > 0 \quad \Rightarrow \quad y^T D y > 0$

can pick x so $y = e_i$

$\Rightarrow A = LDL^T$

$= LD^{1/2} \cdot D^{1/2} L^T = LD^{1/2} (D^{1/2})^T L^T$

transpose of diagonal matrix is the same

$= LD^{1/2} (LD^{1/2})^T$

$= VV^T$

Algorithm

for $k = 1 \ldots n$

$$v_{kk} = \left(a_{kk} - \sum_{i=1}^{k-1} v_{ki}^2 \right)^{1/2}$$

for $j = k+1 \ldots n$

for $i = 1, \ldots, k-1$

$$a_{jk} \leftarrow a_{jk} - v_{ji} v_{ki}$$

$$v_{jk} = a_{jk} / v_{kk}$$

Cost: $\frac{n^3}{3} + O(n^2)$

↑ cheapest computationally

Solving $Ax = b$

① Compute $A = VV^T$ $\left(\frac{n^3}{3} + O(n^2) \right)$

② Solve $Vy = b$ (n^2)

③ Solve $V^T x = y$ (n^2)

Numerically stable

Geometric Interpretation

V is lower triangular $\rightarrow$

first axes $\Leftrightarrow$ first dimension

second axis $\Leftrightarrow$ in the first 2 dimensions

Blockwise derivation

$$A = \begin{pmatrix} A_{11} & A_{21}^T \\ A_{21} & A_{22} \end{pmatrix}$$

LDL decomposition

$$A = \begin{pmatrix} I & 0 \\ L_{21} & I \end{pmatrix} \begin{pmatrix} D_{11} & 0 \\ 0 & S \end{pmatrix} \begin{pmatrix} I & L_{21}^T \\ 0 & I \end{pmatrix}$$

where

$$D_{11} = A_{11} \qquad L_{21} = A_{22} A_{12}^{-1} \qquad S = \underbrace{A_{22} - A_{21} A_{11}^{-1} A_{21}^T}_{\text{Schur complement}}$$

(we will see this soon)

Make
$$\begin{pmatrix} D_{11} & 0 \\ 0 & S \end{pmatrix} = \underbrace{\begin{pmatrix} G_{11} & 0 \\ 0 & G_{22} \end{pmatrix}}_{\text{square root}} \underbrace{\begin{pmatrix} G_{11}^T & 0 \\ 0 & G_{22}^T \end{pmatrix}}$$

So

$$A = \left(\begin{pmatrix} I & 0 \\ L_{21} & I \end{pmatrix} \begin{pmatrix} G_{11} & 0 \\ 0 & G_{22} \end{pmatrix} \right) \left(\begin{pmatrix} I & 0 \\ L_{21} & I \end{pmatrix} \begin{pmatrix} G_{11} & 0 \\ 0 & G_{22} \end{pmatrix} \right)^T$$

Hence,

$$V = \begin{pmatrix} I & 0 \\ L_{21} & I \end{pmatrix} \begin{pmatrix} G_{11} & 0 \\ 0 & G_{22} \end{pmatrix} = \begin{pmatrix} G_{11} & 0 \\ L_{21}G_{11} & G_{22} \end{pmatrix}$$

Since $L_{21} = A_{21} A_{11}^{-1}$

• $(X^{-1})^T = (X^T)^{-1}$

$L_{21} G_{11} = A_{21} A_{11}^{-1} G_{11}$; $A_{11} = G_{11} G_{11}^T$

$\Rightarrow A_{11}^{-1} = (G_{11}^{-1})^T G_{11}^{-1}$

$A_{11}^{-1} G_{11} = (G_{11}^{-1})^T$

↓

$L_{21} G_{11} = A_{21} (G_{11}^{-1})^T$

So $G = \begin{pmatrix} G_{11} & 0 \\ A_{22}(G_{21}^{-1})^T & G_{22} \end{pmatrix}$

w/ $G_{22} G_{22}^T = A_{22} - A_{21} A_{11}^{-1} A_{21}^T$

Start w/ G_{11} as a scalar.

Derivation 2

$A = VV^T$ $\qquad$ $V \sim$ lower triangular

So

$$a_{jk} = \sum_{i=1}^{\min(j,k)} v_{jk} v_{ki}$$

Take $j = k$

$$a_{kk} = \sum_{i=1}^{k} v_{ki}^2$$

$$a_{kk} = \sum_{i=1}^{k-1} v_{ki}^2 + v_{kk} \Rightarrow v_{kk} = \sqrt{a_{kk} - \sum_{i=1}^{k-1} v_{ki}^2}$$

square root ok since $v_{kk} > 0$

Now for off-diagonal

Take $j > k$

$$a_{jk} = \sum_{i=1}^{k} v_{ji} v_{ki}$$

$$= \sum_{i=1}^{k-1} v_{ji} v_{ki} + v_{jk} v_{kk}$$

$$\Rightarrow v_{jk} = \frac{1}{v_{kk}} \left(a_{jk} - \sum_{i=1}^{k-1} v_{ji} v_{ki} \right) \quad \text{for } j > k$$

Iterative Methods

- Jacobi iteration
- Gauss-Seidel iteration
- SOR iteration

- Others: Chebyshev, SSOR, Krylov methods, Conjugate gradient, FFT, Multigrid methods

Still solving $Ax = b$

→ Now looking for approximate solution $\hat{x}$

$$\|\hat{x} - x^*\| \leq \varepsilon$$

for some ε, where x^* is the exact solution

__Advantages__: - Sparse matrices ⇒ much faster
- Can stop when we are "close" enough

__Basic idea__

$$Ax = b \Rightarrow x = Rx + c \quad \text{(so solution is a fixed point)}$$

Approximate

$$x_{n+1} = Rx_n + c$$

if $x_{m+1} = Rx_m + c$ converges $\Rightarrow x_\infty = x^*$

How to choose R & c so x_i converges?

Derivation (Basic)

$A = M - K$ w/ M non-singular

$Ax = Mx - Kx = b \Rightarrow x = \underbrace{M^{-1}K}_{R}x + \underbrace{M^{-1}b}_{c}$

$\Rightarrow x_{m+1} = Rx_m + c$

When does this converge?

Thm: Let $\|\cdot\|$ denote a matrix norm so that $\|R\| \leq 1$, then
$x_{m+1} = Rx_m + c \xrightarrow{m\to\infty} x_\infty \to x^*$ where $Ax^* = b$
for all x_0.

Proof: $Ax^* = b \iff x^* = Rx^* + c$

$\|x_{m+1} - x^*\| = \|R(x_m - x^*)\|$

$\leq \|R\|\,\|x_m - x^*\| \leq \|R^2\|\|x_{m-1} - x^*\|$

$\leq \cdots \leq \|R\|^m \|x_0 - x^*\|$

Since $\|R\| < 1 \Rightarrow \|R\|^m \to 0$ so $\|x_{m+1} - x^*\| \leq 0$

.

Spectral Radius

The spectral radius of $R \in \mathbb{R}^{n\times n}$ is defined as

$$\rho(R) = \max_j |\lambda_j(R)|$$

where λ_j is the j-th eigenvector of R

Note: in standard form this is often written as $\lambda_1(R)$,
since $|\lambda_1| \geq |\lambda_2| \geq \dots \geq |\lambda_n|$

Thm:

① For every choice of matrix norm $\|\cdot\|$, $\rho(R) \le \|R\|$

② For every $\varepsilon > 0$ there exists a matrix norm $\|\cdot\|_*$ such that $\|R\|_* \le \rho(R) + \varepsilon$

Pf: ① Let v be the eigenvector for λ

$$|\lambda| \le \frac{\|Rv\|}{\|v\|} \le \|R\| \quad \Rightarrow \quad \rho(R) \le \|R\|$$

↑ definition of eigenvalue/vector

② Let $J = \bigoplus_{i=1}^{k} J_{n_i}(\lambda_i)$ be the Jordan block decomp. of A. There exists an invertible matrix S such that

$$S^{-1} A S = J$$

We can show that for $D_\varepsilon = \operatorname{diag}(1, \varepsilon, \dots \varepsilon^{n-1})$

$$D_\varepsilon^{-1} J D_\varepsilon = \bigoplus_{i=1}^{k} J_{n_i}(\lambda_i, \varepsilon)$$

where $J_{n_i}(\lambda_i, \varepsilon) = \lambda_i I_{n-i} + \varepsilon E_{n_i}$

$E_{n_i} := \mathbb{R}^{n_i \times n_i}$ w/ 1 on the first upper diagonal & 0 elsewhere

e.g $\begin{pmatrix} 0 & 1 & & 0 \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ 0 & & & 0 \end{pmatrix}$

So for $D_\varepsilon^{-1} J D_\varepsilon$ all Jordan blocks

$$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & \varepsilon \\ 0 & 1 \end{pmatrix}$$

So $\|D_\varepsilon^{-1} J D_\varepsilon\|_\infty \le \rho(R) + \varepsilon$

Define $\|x\|_* = \|(SD_\varepsilon)^{-1} x\|_\infty$

$$\Rightarrow \|R\|_* \le \|D_\varepsilon^{-1} J D_\varepsilon\|_\infty \quad \blacksquare$$

Consequence of Theorem

For $x_{m+1} = Rx_m + c$ $\quad x_m \to x^*$ iff $\rho(R) < 1$

Rate of convergence is given by

$$r(R) := -\log_{10} \rho(R)$$

describes # of steps required to get an error of ε (in decimal notation)

Goals in for finding $A = M - K$

① $Rx = M^{-1}Kx$ & $M^{-1}b$ should be easy to compute

② $\rho(R)$ should be as small as possible

① & ② are opposing goals,

eg. set $M = I \Rightarrow \rho(R)$ can be large

set $M = A \Rightarrow$ "hard" to compute

Lets write $\boxed{A = D - \tilde{L} - \tilde{U}}$

(D: diag., $\tilde{L}$: lower triang, $\tilde{U}$: upper triang.)

Jacobi iteration

Set $M = D$

$K = \tilde{L} + \tilde{U}$

$\Rightarrow R_J := D^{-1}(\tilde{L} + \tilde{U})$

$c_J := D^{-1} b$

If $x^{(j)} = \begin{pmatrix} x_1^{(j)} \\ \vdots \\ x_n^{(j)} \end{pmatrix} \Rightarrow x_i^{(k)} = \frac{1}{a_{ii}} \left(b_i - \sum_{\substack{j=1 \\ j \neq i}}^{n} a_{ij} x_j^{(k-1)} \right)$

Computational Cost

if each column has at most m non-zero entries $\rightarrow$ each iteration $O(mn)$

Gauss-Seidel

$M = D - \tilde{L}$ $\quad R_{GS} = (D-\tilde{L})^{-1}\tilde{U}$

$K = \hat{U}$ $\quad C_{GS} = (D-\tilde{L})^{-1} b$

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

Computation Cost: Same as Jacobi iteration

$O(mn)$ (w/ m non-zero entries / row or col)

Advantage: Don't need to store $x^{(k-1)}$

(can overwrite the vector since the calculation is split $i<j$ & $j<i$)

SOR

(Successive over relaxation)

Extrapolated Gauss-Seidel (SOR(ω))

where $\omega \in \mathbb{R}$ is the relaxation parameter.
(usually $\omega \in (0,2)$)

$$x_i^{(k)} = (1-\omega)x^{(k-1)} + \omega x_i^{(k)}$$

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

(Gauss-Seidel)

$$\Rightarrow \quad R_{SOR(\omega)} = (D - \omega\tilde{L})^{-1}((1-\omega)D + \omega\tilde{U})$$

$$c_{SOR(\omega)} = \omega(D - \omega\tilde{L})^{-1}b$$

Convergence Criteria

A matrix is strongly (row) diagonally dominant if for all i
(SDD)

$$|a_{ii}| > \sum_{\substack{j=i \\ i\neq j}}^{n} |a_{ij}|$$

① Jacobi & Gauss-Seidel for SDD matrices always converge (GS converges faster)

② Incase of equality → need irreducability (cannot be permuted to upper triangular)

③ For SOR $0<\omega<2$ (neccesary) if A is pos. def. this is sufficient

④ If the adjacency graph of A is bipartite we can compare convergence rates & determine optimal ω in SOR(ω)

Thm: If A is SDD

$$\|R_{GS}\|_\infty \le \|R_J\|_\infty < 1$$

Pf: $\|R_J\|_\infty < 1$

$$\|R_J\|_\infty = \||R_J|\|_\infty = \||R_J|e\|_\infty = \max_i \sum_{j\ne i} \frac{|a_{ij}|}{|a_{ii}|} < 1$$

$\|R_{GS}\| \le \|R_J\|_\infty$

Sufficient to show $|R_{GS}|e \le |R_J|e$ where

$$x \le y \iff x_i \le y_i \quad \forall i$$

$$|R_{GS}|e = |(I-L)^{-1}U|e \overset{\circledast}{\le} |(I-L)^{-1}|\cdot|U|\cdot e$$

$$= \left|\sum_{i=0}^{n-1} L^i\right|\cdot|U|\cdot e \le \sum_{i=0}^{n-1} |L|^i \cdot |U| e$$

$$\overset{\circledast}{=} (I-|L|)^{-1} e$$

$\circledast$ $(I-L)^{-1} = \sum_{i=0}^{\infty} L^i = \sum_{i=0}^{n-1} L^i$ Since $L^n = 0$

$\circledast$ $(I-|L|)^{-1} = \sum_{i=0}^{\infty} |L|^i = \sum_{i=0}^{n-1} |L|^i$ $|L|^n = 0$

So we must show

$$(I-|L|)^{-1}|U||e| \le |R_J|e = |L+U|e$$
$$= (|L|+|U|)e$$

$I-|L|$ is non-negative so

$$|U|e \le (I-|L|)(|L|+|U|)e$$

$$0 \le |L|(I-|L|-|U|)e$$

$$\iff 0 \le (I-|L|-|U|)e \iff \sum_{j\ne i} \frac{|a_{ij}|}{|a_{ii}|} < 1$$

Notes

① The above does not mean GS is always faster than Jacobi (depends on starting condition)

② Because $\|A\|_\infty = \|A^T\|_1$ strongly (column) diagonally dominant also implies convergence

SDD vs DD $\quad |a_{ii}| \left\{ \begin{matrix} > \\ \geq \end{matrix} \right\} \sum_{j \neq i} |a_{ij}|$

strict or not ineq.

Thm: If A is DD & irreducible

$\Rightarrow \rho(R_{GS}) \leq \rho(R_J) < 1$

Irreducibility as a graph property

$G(A)$ for $A \in \mathbb{R}^{n \times n}$ $\quad V = \{1, \dots, n\}$

$E = i \to j$ if $a_{ij} \neq 0$

Directed graph is strongly connected if $\exists$ a path $i \to j$ for all $j \neq i$

Claim: A is irreducible iff $G(A)$ is strongly connected.

Thm:

$\rho(R_{SOR}(\omega)) \geq \omega - 1$ so $\omega \in (0,2)$ is necessary

Pf

$$\det(R_{SOR}(\omega)) = \det\left((D - \omega\tilde{L})^{-1}((1-\omega)D + \omega\tilde{U})\right)$$

$$= \det\left((I - \omega D\tilde{L})^{-1} D^{-1} D\left((1-\omega) + \omega D^{-1}\tilde{U}\right)\right)$$

$$= \det\left((I - \omega D\tilde{L})^{-1} \cdot \det\left((1-\omega) + \omega D^{-1}\tilde{U}\right)\right)$$

$$= 1 \cdot (1-\omega)^n = (1-\omega)^n$$

Thm: Spectral radius $R_{SOR}(\omega)$

If A is positive def. then $\rho(R_{SOR}(\omega)) < 1$ $\forall$ $0 < \omega < 2$

Thm: If $G(A)$ is bipartite

① $\rho(R_{GS}) = \rho(R_J)^2$

② if R_J has real eigenvalues &

$\mu := \rho(R_J) < 1$ then

$$\omega_{opt} = \frac{2}{1 + \sqrt{1 - \mu^2}}$$

$$\rho(R_{SOR}(\omega_{opt})) = \omega_{opt} - 1$$

$$\rho(R_{SOR}(\omega)) = \begin{cases} \omega - 1 & \omega_{opt} \geq \omega < 2 \\ f(\omega, \mu) & 0 < \omega < \omega_{opt} \end{cases}$$

$$f(\omega, \mu) = 1 - \omega + \frac{1}{2}\omega^2\mu^2 + \omega\mu\sqrt{1 - \omega + \frac{1}{4}\omega^2\mu^2}$$