SOR

Extrapolated Gauss-Seidel
(SOR(ω) - Successive over-relaxation)

ω - relaxation parameter
(usually $\omega \in (0,2)$)

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

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

(Gauss-Seidel)

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

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

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 always converge

② if we have equality

ie. $|a_{ii}| \geq \sum_{i \neq j} |a_{ij}|$

we need irreducability

③ For SOR $\omega \in (0,2)$ positive definite is sufficient

④ If adjacency graph $G(A)$ is bipartite $\Rightarrow$ we can compare convergence rates & compute optimal ω

Thm: If A is SDD

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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 $\quad |a_{ii}| \left\{ \underbrace{\begin{matrix} > \\ \geq \end{matrix}}_{\text{strict or not ineq.}} \right\} \sum_{j \neq i} |a_{ij}|$

<u>Thm</u>: 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 $j \neq i$

<u>Claim</u>: 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

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

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

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

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

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

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

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

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

Conjugate Gradient

Let A be positive definite

$$f(x) = \frac{1}{2} x^T A x - b^T x$$

minimized at

$$\nabla f(x) = Ax - b = 0$$

→ use gradient descent

→ every direction is conjugate to previous direction

→ conjugate vectors iff $x^T A y = 0$

$$\langle x, y \rangle_A = x^T A y$$

!

orthogonal for this weighted scalar product

Idea

1. pick x_0
2. direction: $b - Ax_0$
3. Choose conjugate direction
4. line search for next approximation
5. Repeat

Algorithm

① $r = b - Ax$

$p_0 = r_0$

② Repeat until $\|r_k\|^2 < \varepsilon$ ← small

- $\alpha_k = \dfrac{r_k^T r_k}{p_k^T A p_k}$

- $x_{k+1} = x_k - \alpha_k p_k$ (next approx)

- $r_{k+1} = r_k - \alpha_k A p_k$ (gradient of remainder)

- $\beta_k = \dfrac{r_{k+1}^T r_{k+1}}{r_k^T r_k}$ $\quad p_{k+1} = r_{k+1} + \beta_k p_k$ (conjugated gradient)

Properties

- Converges if A is pos. def & symmetric
- w/ infinite precision - converges in n-steps.
- often faster than n
- only multiplication is needed
- No fill in - space needed constant

Overdetermined systems

- SVD
- Moore-Penrose inverse
- QR

<u>Def</u>: Overdetermined systems

$Ax = b \qquad A = \mathbb{R}^{n \times m} \qquad$ if $n > m$

(more often $n >> m$)

Generically, no solution exists

$\Rightarrow$ why $\Rightarrow$ each row is a constraint
(lose a dimension)

So find x such that error is minimized

$$\min_x \|Ax - b\|$$

$\Rightarrow$ usually choose $\|\cdot\|_2$

- examples : curve fitting
  statistical modeling

<u>Other norms</u> : $\|\cdot\|_\infty$ - no very large error
(in any one dim)

$\|\cdot\|_1$ - sparse errors (most should be very small)

Polynomial Approximation

- Find coefficients for cubic equation

$$p(x) = a_3 x^3 + a_2 x^2 + a_1 x + a_0$$

Minimize $\displaystyle\sum_{i=1}^{n} (a_3 x_i^3 + a_2 x_i^2 + a_1 x_i + a_0 - y_i)^2$

$$\begin{pmatrix} 1 & x_1 & x_1^2 & x_1^3 \\ 1 & x_2 & x_2^2 & x_2^3 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 & x_n^3 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} \Rightarrow LS$$

SVD

Thm: $A \in \mathbb{R}^{n \times m}$ then there exists

- orthogonal matrices $U \in \mathbb{R}^{n \times n}$ $V \in \mathbb{R}^{m \times m}$

  $(UU^T = I_n)$ $(V^T V = I_m)$

- a diagonal matrix $\Sigma = \mathrm{diag}(\sigma_1, \ldots, \sigma_{\min(m,n)})$

  w/ $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_{\min(m,n)} \geq 0$

& $\boxed{A = U \Sigma V^T}$

U: left singular vectors $\leadsto$ $AA^T u = \lambda u$

V: right singular vectors $\leadsto$ $A^T A v = \lambda v$

Def: $\lambda(A^T A) = \sigma_i^2$

$A^T A v_i = \sigma_i^2 v_i$

Claim: $\|A\|_2 = \sigma_1$

$u_i = \dfrac{A v_i}{\sigma_i} \Rightarrow A v_i = \sigma_i u_i$

Moore-Penrose inverse

If $A \in \mathbb{R}^{n \times m}$, the MP inverse is $A^+ \in \mathbb{R}^{m \times n}$ & satisfies 4 conditions:

1. $AA^+A = A$
2. $A^+AA^+ = A^+$
3. $(AA^+)^T = AA^+$
4. $(A^+A)^T = A^+A$

Claim: Let $A = U\Sigma V^T$ (be the SVD decomposition) then the Moore-Penrose inverse of A is

$$A^+ = V\Sigma^+ U^T$$

w/ $\Sigma^+ = \mathrm{diag}(\sigma_1^+, \sigma_2^+, \ldots, \sigma_{\min(m,n)}^+)$

$$\sigma_i^+ = \begin{cases} 1/\sigma_i & \text{if } \sigma_i \neq 0 \\ 0 & \text{else} \end{cases}$$

Check

1. $$AA^+A = (U\Sigma V^T)(V\Sigma^+U^T)(U\Sigma V^T)$$
$$= U\Sigma I_m \Sigma^+ I_n \Sigma V^T$$
$$= U\underbrace{(\Sigma\Sigma^+)}_{I_{\min(m,n)}}\Sigma V^T = U\Sigma V^T = A$$

Claim: $A \in \mathbb{R}^{n \times m}$ $n \geq m$ $\mathrm{rank}(A) = m$

LS solution to $Ax = b \Rightarrow x = A^+ b$

Sensitivity

$A \in \mathbb{R}^{n \times m}$ - orthogonal

The condition number of A is defined as

$$\kappa_2(A) = \|A\|_2 \|A^+\|_2$$

Claim: $\kappa_2(A) = \sigma_{max}(A) / \sigma_{min}(A)$

Thm: $A \in \mathbb{R}^{n \times m}$ w/ $\text{rank}(A) = m$ & $n \geq m$

Let - x_0 be the minimizer of $\|Ax - b\|_2^2$

- $r := b - Ax_0$
- x' be the minimizer of

$$\|(b + \Delta b) - (A + \Delta A)x\|_2^2$$

- $\varepsilon := \max\left(\frac{\|\Delta A\|_2}{\|A\|_2}, \frac{\|\Delta b\|_2}{\|b\|_2}\right)$

$$\frac{\|x' - x_0\|}{\|x_0\|} \geq \varepsilon \underbrace{\left(\frac{2\kappa_2(A)}{\cos\theta} + \tan\theta \cdot \kappa_2(A)\right)}_{\kappa_{LS}(A)} + O(\varepsilon^2)$$

↳ condition number for least squares

where $\sin\theta = \frac{\|r\|_2}{\|b\|_2}$

Solution via normal system

$\mathrm{rank}(A)=m$, the solution to $Ax=b$ by least squares is $x \in \mathbb{R}^m$ which solves the normal system/equations

$$A^T A x = A^T b$$

Pf

Let x be the vector which minimizes $\|b-Ax\|_2$ so that $b-Ax$ (error) is orthogonal to A

ie $(b-Ax)^T a_i = 0$ or

$$A^T(b-Ax)=0$$

$$A^T b - A^T A x = 0$$

$$A^T A x = A^T b$$

since $\mathrm{rank}(A)=m \Rightarrow \mathrm{rank}(A^T A)=m$

so system is solvable

Example : Linear Regression

We are looking for the line which best fits

$$(x_1, y_1) \ldots (x_n, y_n)$$

ie. $y = a + bx$

$$\underbrace{\begin{pmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} a \\ b \end{pmatrix}}_{x} = \underbrace{\begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}}_{b}$$

$$x = (A^T A)^{-1} A^T y = \begin{bmatrix} n & \sum x_i \\ \sum x_i & \sum x_i^2 \end{bmatrix}^{-1} \begin{bmatrix} \sum y_i \\ \sum x_i y_i \end{bmatrix}$$

Solving the normal system - Cholesky

$A \in \mathbb{R}^{n \times m}$ $\quad \operatorname{rank}(A) = m \iff A^T A$ is positive definite

So $(A^T A)x = A^T b$ can be solved via Cholesky

① $B = A^T A \quad c = A^T b \quad$ cost: $nm^2 + O(mn)$

compute only top half of $A^T A$ since it is symmetric

② $B = VV^T \quad$ cost $\frac{1}{3} m^3 + O(m^2)$

③ Solve $Vy = c \quad$ cost $O(m^2)$

④ Solve $V^T x = y \quad$ cost $O(m^2)$

<u>Total</u>: $nm^2 + \frac{1}{3} m^3 + O(nm)$

Remember $n \gg m$

QR Decomposition

Let $A \in \mathbb{R}^{n \times m}$ $\exists$ $Q \in \mathbb{R}^{n \times m}$ s.t.

$Q^T Q = I_m$ & $R \in \mathbb{R}^{m \times m}$ is upper triang.

with

Q orthonormal

$$\boxed{A = QR}$$

$A = QR$ implies span(A) = span(Q)

column space

columns of Q - orthogonal ($q_i^T q_j = 0$ $i \neq j$ & normalized)

$$\begin{bmatrix} q_1 & q_2 & \cdots & q_m \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1m} \\ & r_{22} & & \vdots \\ 0 & & \ddots & \\ & & & r_{mm} \end{bmatrix} = \begin{bmatrix} a_1 & a_2 & \cdots & a_m \end{bmatrix}$$

$q_1 \cdot r_{11} = a_1 \Rightarrow q_1 = \frac{1}{r_{11}} a_1$

$\|q_1\| = 1 \Rightarrow r_{11} = \|a_1\|$

$a_2 = r_{12} q_1 + r_{22} q_2 \Rightarrow q_2 = \frac{1}{r_{22}} (a_2 - r_{12} q_1)$

need $(a_2 - r_{12} q_1) q_1 = 0 \Rightarrow r_{12}$

& $\|q_2\| = 1 \Rightarrow r_{22}$

$q_m = \frac{1}{r_{mm}} (a_m - r_{1m} q_1 - \cdots - r_{m-1,m} q_{m-1})$

So we can compute the QR decomposition via (modified Gram-Schmidt) orthogonalization

$$r_{11} = \|a_1\|_2$$

$$q_1 = \frac{1}{r_{11}} a_1$$

$$\begin{array}{l}
\text{for } j = 2, \ldots, m \\
\quad q_j = a_j \\
\quad \left.\begin{array}{l}
\text{for } i = 1 \ldots j \\
\quad r_{ij} = q_i^T a_i \quad \color{red}{(r_{ij} = q_i^T q_j)} \\
\quad q_j = q_j - r_{ij} q_i
\end{array}\right\} \ \color{blue}{\text{direction}} \\
\quad \left.\begin{array}{l}
r_{jj} = \|q_j\|_2 \\
q_j = \frac{1}{r_{jj}} q_j
\end{array}\right\} \ \color{purple}{\text{scaling}}
\end{array}$$

So we can compute the QR decomposition via (modified) Gram-Schmidt orthogonalization

$r_{11} = \|a_1\|_2$

$q_1 = \frac{1}{r_{11}} a_1$

for $j = 2 \ldots m$

$\quad q_j = a_j$

$\quad$ for $i = 1 \ldots j$

$\quad\quad r_{ij} = q_i^T a_j \quad (r_{ij} = q_j^T q_j)$

$\quad\quad q_j = q_j - r_{ij} q_i$

direction

$\quad r_{jj} = \|q_j\|_2$

$\quad q_j = \frac{1}{r_{jj}} q_j$

scaling

Using QR for solving $Ax = b$

<u>Lemma</u>: cost of QR $\approx 2nm^2$

<u>Pf</u>: $2n + 2 + \sum_{j=2}^{m} \left(\left(\sum_{i=1}^{j} 4n \right) + 3n \right)$

$\approx 2n + 2 + \sum_{j=2}^{m} (4nj + 3n)$

$\approx 2n + 2 + 4n \sum_{j=2}^{m} (j+1) \approx 2n + 2 + 4n \cdot m^2/2$

$\approx 2nm^2$

Claim: $A \in \mathbb{R}^{n \times m}$ $\text{rank}(A) = m$

Least squares sol. of $Ax = b \iff Rx = Q^T b$

Pf: $A^T A x = (QR)^T (QR) x$

$$= R^T Q^T Q R x$$

$$= R^T R x$$

$$A^T b = R^T Q^T b$$

Obs: R^T is invertible since $\text{rank}(R^T) = m$

$$A^T A x = A^T b$$

$$\Rightarrow R^T R x = R^T Q^T b \quad / \cdot (R^T)^{-1}$$

$$\boxed{Rx = Q^T b}$$