Can you solve this?

$\sqrt{2}\, x_1 + \sqrt{2}\, x_2 = 1$? $\begin{cases} x_2 = 0 \\ x_1 = 1/\sqrt{2} \end{cases}$

$x_1 = x_2 = \frac{1}{2\sqrt{2}}$. $\begin{cases} x_1 = 0 \\ x_2 = 1/\sqrt{2} \end{cases}$

$A = \begin{bmatrix} \sqrt{2} & \sqrt{2} \end{bmatrix}$ $m < n$.

under-determined!

$Ax = b$, $A \in \mathbb{R}^{m \times n}$, $m < n$

classical soln. exists if $\mathrm{rank}(A) = \mathrm{rank}([A\ b])$

$\leq$ least squares.

Let $S = \{ x \in \mathbb{R}^n,\ x$ is the minimizer of $\|Ax - b\|_2 \}$

The SVD solution is

$$x^* = \min_{x \in S} \|x\|_2$$

If $m = n$, $\mathrm{rank}(A) = n$, then

$x^* = A^{-1} b$, otherwise the soln is $x = A^+ b$

1. minimizer of $\|b - Ax\|_2$
2. has the least 2-norm.

any m and $r = \mathrm{rank}(A)$

$A \in \mathbb{C}^{m\times n}$, $\exists\ U \in \mathbb{C}^{m\times m}$, $V \in \mathbb{C}^{n\times n}$

such that $A = U \Sigma V^H$

$$\Sigma_1 = \begin{bmatrix} \sigma_1 & & 0 \\ & \sigma_2 & \\ 0 & & \ddots \ \sigma_p \end{bmatrix}, \quad = U \begin{bmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{bmatrix}_{m\times n} V^H$$

$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p$, $\mathrm{rank}(A) = p$

$$A^+ = V \begin{bmatrix} \frac{1}{\sigma_1} & & 0 & \\ 0 & \ddots & \frac{1}{\sigma_p} & 0 \\ & 0 & & 0 \end{bmatrix}_{n\times m} U^H$$

$\mathrm{Cond}_2(A) = \sigma_1 / \sigma_p$

In matlab $x = \mathrm{pinv}(A) * b;$

$$A = \begin{bmatrix} \sqrt{2} \\ \sqrt{2} \end{bmatrix}$$

$$A^+ = [\sqrt{2} \quad \sqrt{2}]$$

$$A = \underbrace{\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}}_{U} \underbrace{\begin{bmatrix} 2 \\ 0 \end{bmatrix}}_{\Sigma} \underbrace{[1]}_{V^H}$$

$$A^T = [1]\,[2 \quad 0] \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} = \bar{U} \bar{\Sigma} \bar{V}^H$$

$$(A^T)^+ = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \frac{1}{2} \\ 0 \end{bmatrix} [1]$$

Classical soln with minimized two norm.

Soln.

$$x = (A^T)^+ b = \begin{bmatrix} \frac{1}{2\sqrt{2}} \\ \frac{1}{2\sqrt{2}} \end{bmatrix},$$

as expected.

Ex 3 $A = \begin{bmatrix} 2 & 1 & 2 \\ 1 & 0 & 1 \end{bmatrix}$, $b = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$.

$[U \quad D \quad V] = \text{svd}(A)$

$U = \begin{bmatrix} 0.9106 & 0.4132 \\ 0.4132 & -0.9106 \end{bmatrix}$

format short e

$\Sigma = \begin{bmatrix} 3.2886 & 0 & 0 \\ 0 & 0.43 & 0 \end{bmatrix}$

$V = \begin{bmatrix} \quad \end{bmatrix}$

$x^* = \begin{bmatrix} \frac{1}{2} \\ -1 \\ \frac{1}{2} \end{bmatrix}$.

Pseudo-inverse.

$$A = U \Sigma V^H \qquad \Sigma = \begin{bmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{bmatrix}$$

$$A^+ = V \begin{bmatrix} \Sigma_1^{-1} & 0 \\ 0 & 0^+ \end{bmatrix} U^H$$

$\Sigma_1 = \mathrm{diag}(\sigma_1, \sigma_2, \dots \sigma_p)$
$\sigma_i > 0$
$i = 1, 2, \dots p.$

Prop 1

$$AA^+ \overset{X}{=} I$$

properties:

$$\begin{cases} AA^+A = A \\ A^+AA^+ = A^+ \\ A^+A = (A^+A)^H \\ AA^+ = (AA^+)^H \end{cases}$$

Another definition of pseudo-inverse.

Sensitivity issue.

$$\Sigma = \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_p \end{bmatrix}$$

$\sigma_1 = O(1)$

$\vdots$

$\sigma_s = O(1)$

$\sigma_i = O(10^{-4})$

$\sigma_i = O(10^{-12})$

$\sigma_i = O(10^{-15})$

real singular values or round-off errors,

$\|A^+\|$ would be very large.

Cut-off criterion. $tol = 10^{-10}$

if $\sigma_i \leq tol$, $\sigma_i = 0$.

Example of singular value decomposition

Ex 1. $A = \begin{bmatrix} \sqrt{2} \\ \sqrt{2} \end{bmatrix}$ $\qquad A^TA = [\sqrt{2}\ \sqrt{2}] \begin{bmatrix} \sqrt{2} \\ \sqrt{2} \end{bmatrix} = 4$

$\sigma_1 = 2 \qquad x_1 = [1] \qquad V = [1]$

$$y_1 = \frac{A x_1}{\sigma_1} = \frac{1}{2} \begin{bmatrix} \sqrt{2} \\ \sqrt{2} \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix},$$

$$y_2 = \begin{bmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}, \qquad U = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix},$$

$U \qquad \Sigma \quad V^T$

$$U^TAV = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \sqrt{2} \\ \sqrt{2} \end{bmatrix} [1] = \begin{bmatrix} 2 \\ 0 \end{bmatrix}$$

Ex 2. $A = \begin{bmatrix} 1 & 1 \\ \sqrt{2} & 0 \\ 0 & \sqrt{2} \end{bmatrix}$, $\qquad A^TA = \begin{bmatrix} 1 & \sqrt{2} & 0 \\ 1 & 0 & \sqrt{2} \end{bmatrix} \begin{bmatrix} 1 & 1 \\ \sqrt{2} & 0 \\ 0 & \sqrt{2} \end{bmatrix}$

$$= \begin{bmatrix} 3 & 1 \\ 1 & 3 \end{bmatrix}$$

$(\lambda - 3)^2 = 1$

$\lambda_1 = 4, \quad \lambda_2 = 2, \qquad \sigma_1 = 2, \quad \sigma_2 = \sqrt{2}$

Choose σ_2 first (σ_1 is a little more complicated for U)

$(2I - A^TA)\, x_1 = 0 \qquad \begin{bmatrix} -1 & -1 \\ -1 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = 0, \quad x_1 = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix}$

$$V_1 = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}$$

$$y_1 = \frac{1}{\sqrt{2}} A x_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ \sqrt{2} & 0 \\ 0 & \sqrt{2} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix}$$

$$y_2 = \begin{bmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}, \qquad y_3 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

$$U_1 = \begin{bmatrix} 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{bmatrix}$$

$$U_1^T A V_1 = \begin{bmatrix} \sqrt{2} & 0 \\ 0 & \sqrt{2} \\ 0 & \sqrt{2} \end{bmatrix}$$

$$V_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \qquad U_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}$$

$$U_2^T U_1^T A V_1 V_2 = \begin{bmatrix} \sqrt{2} & 0 \\ 0 & 2 \\ 0 & 0 \end{bmatrix}$$

$$(P_{12}^T)_{3\times 3} U_2^T U_1^T A V_1 V_2 (P_{12})_{2\times 2} = \begin{bmatrix} 2 & 0 \\ 0 & \sqrt{2} \\ 0 & 0 \end{bmatrix}$$

$$A = \begin{bmatrix} 2 & 1 & 2 \\ 1 & 0 & 1 \end{bmatrix}, \qquad b = \begin{bmatrix} 1 \\ 1 \end{bmatrix}. \qquad \text{solve } Ax = b.$$

$$[U \ D \ V] = svd(A) \qquad A = UDV'$$

$$U = \begin{bmatrix} 0.9106 & 0.4132 \\ 0.4132 & -0.9106 \end{bmatrix}$$

$$D = \begin{bmatrix} 3.2886 & 0 & 0 \\ 0 & 0.4300 & 0 \end{bmatrix}$$

$$V = \begin{bmatrix} 0.6795 & -0.1958 & -0.7071 \\ 0.2769 & 0.9609 & 0 \\ 0.6795 & -0.1958 & 0.7071 \end{bmatrix}$$

$$x^* = \begin{bmatrix} \frac{1}{2} \\ -1 \\ 1/2 \end{bmatrix} = pinv(A) * b.$$

$$A^+ = V \begin{bmatrix} 0.3041 & 0 \\ 0 & 2.3254 \\ 0 & 0 \end{bmatrix} U'$$

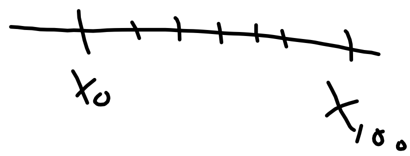
$$x^* = V \begin{bmatrix} 0.3041 & 0 \\ 0 & 2.3254 \\ 0 & 0 \end{bmatrix} U' \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \\ -1 \\ \frac{1}{2} \end{bmatrix}$$

$$Ax^* - b = 0. \qquad \|x^*\|_2 = \sqrt{\frac{1}{4} + 1 + \frac{1}{4}} = \frac{\sqrt{6}}{2}.$$

Krylov subspace iterative methods for solving $Ax=b$.

$A \in \mathbb{R}^{n \times n}$, $\operatorname{rank}(A)=n$. A is large and sparse.

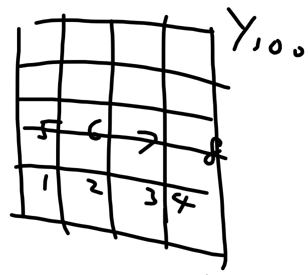
$u_{xx} = f$



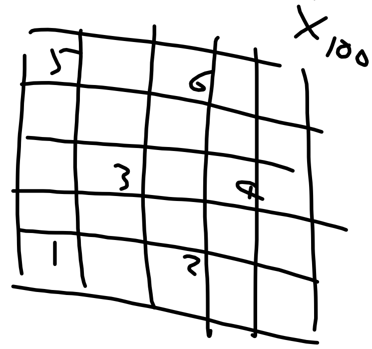
$$\frac{U_{i-1} - 2U_i + U_{i+1}}{h^2} = f(x_i)$$

$AU = F \qquad A \in \mathbb{R}^{100,100}$

In 2D $A \in \mathbb{R}^{100^2, 100^2}$



Natural ordering



Red/Black ordering

$A_{nat} \sim A_{r/b}$

switch rows and columns.

$P^T A_{nat} P = A_{r/b}$.

Iterative method.

Simple (stationary) $\underline{x^{k+1} = R x^k + c}$

R : Jacobi — Solve for the diagonal

G-S, — $R_J = D^{-1}(L+U)$

SOR(ω) — $c = D^{-1} b$

$R_{GS} = (D-L)^{-1} U$

$c = (D-L)^{-1} b$

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

No. of iterations

for Poisson Eqn — J, GS — $O(n^2)$

elliptic PDEs

Optimal ω,

only for Poisson Eqn. — $\underline{\underline{O(n)}}$

Better methods. Criteria.

1. Errors keep decreasing.
2. Error is orthogonal to some spaces.

Given vector r.

$\varphi_1, \varphi_2, \ldots \varphi_n$ are a set of basis in R^n,

$r^T \varphi_j = 0, \quad j = 1, 2 \ldots n,$

$r = 0$ residual

Conjugate Gradient (CG)

method and analysis.

$Ax=b$. A is an SPD, $A=A^T$. GMRES

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

$$\nabla\varphi = 0 \Rightarrow Ax-b.$$

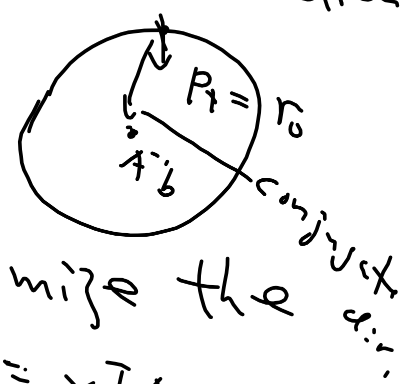
Given $x_0 \in R^n$, $r_0 = b - Ax_0$.

If $r_0=0$, done! $A^{-1}b - x_0$, not computable; computable

$x_1 = x_0 - \alpha_1 p_1$, $p_1 = r_0$, search direction

$b - Ax_1 = b - Ax_0 + \alpha_1 A p_1$

$r_1 = r_0 + \alpha_1 A p_0$



($x_1 - x^* = x_0 - x^* - \alpha_1 p_1$; error in some norm) minimize the

$$\|x\|_{A^{\frac{1}{2}}} = x^T A x$$

$$\begin{cases} x_1 = x_0 - \alpha_1 p_1, & p_1 = r_0 \\ p_2 = r_1 + \beta_2 p_1, & \text{New search direction} \end{cases}$$

$r_1 = r_0 + \alpha_1 A p_1$, $p_1 = r_0$, $Ax_1 = Ax_0 - \alpha_1 A p_1$

(I) Choose α_1 such that $r_0^T r_1 = 0$

$r_0^T r_1 = r_0^T r_0 + \alpha_1 p_1^T A p_1$ $\quad \alpha_1 = -\dfrac{r_0^T r_0}{p_1^T A p_1}$

(ii) $p_2 = r_1 + \beta_2 p_1$, Choose β_2 such that $p_2^T A p_1 = 0$. (p_2 and p_1 are A-conjugate)

$A p_2 = A r_1 + \beta_2 A p_1$

$p_1^T A p_2 = p_1^T A r_1 + \beta_2 \, p_1^T A p_1$

$$\beta_2 = -\frac{r_1^T A p_1}{p_1^T A p_1}$$

$p_1^T A r_1$
$= (p_1^T A r_1)^T$
$= r_1^T A p_1$

Summarize $p_0 = r_0$

$$x_k = x_{k-1} - \alpha_k p_k$$

$$(r_k = r_{k-1} + \alpha_k A p_k) \qquad \alpha_k = \frac{-r_{k-1}^T r_{k-1}}{p_k^T A p_k}$$

$$p_{k+1} = r_k + \beta_{k+1} p_k \qquad r_k^T r_{k-1} = 0$$

$$(A p_{k+1} = A r_k + \beta_{k+1} A p_k) \qquad \beta_{k+1} = \frac{-r_k^T A p_k}{p_k^T A p_k}$$

p_k^T

Cost: Only need Ap_k, one matrix-vector multiplication.

Storage x_k, x_{k-1}, p_k, r_k

"Speed"

Pseudo-code CG PCG.

Input x_0, compute $r = b - Ax_0$.

$p = r$

for $k = 1, \ldots,$ until converge

$v = Ap$. $\quad w = v^T p \quad (p^T A p)$

$\alpha = -r^T p / w$

$x = x - \alpha p$

$r = r + \alpha v$

$\beta = -r^T v / w$

$p = r + \beta p$

end

Properties of CG-method

$$\|e_{k+1}\|_{A^{1/2}} < \|e_k\|_{A^{1/2}} = \sqrt{e_k^T \underline{\underline{A e_k}}}$$

$$r_{k+1}^T r_j = 0, \quad j = 1, 2 \ldots, k$$

$$r_{k+1}^T p_j = 0, \quad j = 1, 2, \ldots k.$$

It (CG) converges at most $\min\{n, p_{min}\}$

$p_i^T A p_j = 0$ if $i \neq j$, $\{p_i\}$ is a set of A-conjugate. Math. Induction.

$\{A^{\frac{1}{2}} p_i\}$ is an orthogonal set in R^n space

$$A = Q^T D Q = \underbrace{Q^T D^{\frac{1}{2}} Q}_{A^{\frac{1}{2}}} \underbrace{Q^T D^{\frac{1}{2}} Q}_{A^{\frac{1}{2}}}$$

$$(A^{\frac{1}{2}} p_i)^T (A^{\frac{1}{2}} p_j) = 0$$

$$x_{k+1} = x_k - \alpha_k p_k$$

$$r_{k+1} = r_k + \alpha_k A$$

$$= x_{k-1} - \alpha_{k-1} p_{k-1} \cdots \qquad r_2 = r_1 + \alpha_1 A r_1$$

$$x_{k+1} = x_0 - \sum_{j=1}^{k} \alpha_j p_j$$

$$p_1 = r_0, \qquad p_2 = r_1 - \beta_2 \overset{r_0}{p_1} \in \mathrm{Span}\{r_1, Ar_1\}$$

$$p_3 = r_2 + \beta_3$$

$$p_k \in \mathrm{Span}\{r_0, Ar_0, \ldots A^{k-1} r_0\}.$$

$$x_{k+1} = x_0 - \sum_{j=1}^{k} \alpha_j p_j$$

$$x^* = A^{-1} b$$

$$r_{k+1} = r_0 + \sum_{j=1}^{k} \alpha_j A p_j$$

$$x_{k+1} - x^* = x_0 - x^* - \sum_{j=1}^{k} \alpha_j p_j$$

$$e_{k+1} = e_0 - \sum_{j=1}^{k} \alpha_j A p_j$$

$$\| e_{k+1} \|_{A^{\frac{1}{2}}} = \min_{\alpha_j} \| e_0 - \sum_{j=1}^{k} \alpha_j A p_j \|_{A^{\frac{1}{2}}}$$

$$= \min_{\{\alpha_j\}} \left(e_0 - \sum \alpha_j A p_j \right)^T A \left(\quad \right)$$

$$\alpha_j = \frac{\pm\, r_0^T r_0}{p_j^T A p_j}$$