Chap. 2, section 2.12.

Dirichlet B.C.: $u(0)=\alpha$, $u(1)=\beta$.

Neumann boundary cond.: $\begin{cases} u'(0)=\sigma & (N) \\ u(1)=\beta & (D) \end{cases}$

U_j, $j=0,\dots,N+1$

$U_{N+1}=\beta$

U_0 is an unknown.

Impose e.g. $\dfrac{U_1-U_0}{h}=\sigma$ => add a row

$$\underbrace{\frac{1}{h^2}\begin{bmatrix} -h & h & 0 & \cdots & 0 \\ -2 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \cdots & 0 \\ & \ddots & \ddots & \ddots & \\ & & & & 1 \\ 0 & & & 1 & -2 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} U_0 \\ U_1 \\ \vdots \\ \\ U_N \end{bmatrix}}_{U} = \underbrace{\begin{bmatrix} \sigma \\ f(x_1) \\ \vdots \\ f(x_{N-1}) \\ f(x_N)-\frac{\beta}{h^2} \end{bmatrix}}_{F}$$

Only 1st order accurate: LTE for the 1st row

$$\tau_0 = \frac{1}{h}\left(u(x_1)-u(x_0)\right)-\sigma$$

$$= u'(x_0)+\frac{1}{2}hu''(x_0)+O(h^2)-\sigma$$

$$= \frac{1}{2}hu''(x_0)+O(h^2)$$

=> $E_j \sim h$ as well.

-> $\begin{cases} \text{More accurate one-sided FD.} \\ \text{Use } U_{-1}\text{, impose eq. at } U_0\text{, centered diff.} \end{cases}$

Chap. 4 Iterative methods.

- Jacobi method
- Multigrid
- Krylov subspace methods.

Consider

$$A\,U = F \quad , \text{ with } A \in \mathbb{R}^{N \times N}$$

- large
- sparse (only a few nonzeros per row and column)
- usually fills in when subjected to Gaussian elimination.
- "ill-conditioned": to be defined later.

Applications:

- elliptic problems such as $\Delta u = f$
- Helmholtz equation: $(\Delta + \omega^2) u = f$.
- Implicit time-stepping for parabolic/hyperbolic eq.

(- Many optimization problems
- Integral equations, etc.)

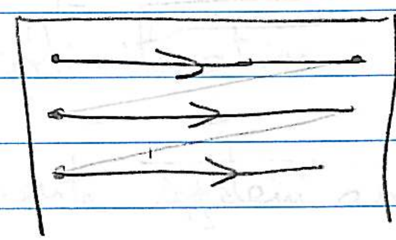
Ex. $u'' = f \Rightarrow$

$$A = \frac{1}{h^2}\begin{bmatrix} 2 & -1 & & 0 \\ -1 & 2 & -1 & \\ & \ddots & \ddots & \ddots \\ 0 & & -1 & 2 \end{bmatrix}$$

Ex. $\Delta u = f$, $x \in [0,1]^2$. , $\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$

5-point Laplacian: $\frac{u_{i-1,j} + u_{i,j-1} + u_{i+1,j} + u_{i,j+1} - 4u_{ij}}{h^2}$

Order the $N = m^2$ unknowns in rowwise / raster scan ordering



$$U = \begin{bmatrix} u_{11} \\ \vdots \\ u_{1m} \\ u_{21} \\ \vdots \\ u_{2m} \\ \vdots \end{bmatrix}$$

Then

$$A = \begin{bmatrix} T & I & & 0 \\ I & T & \ddots & \\ & \ddots & \ddots & I \\ 0 & & I & T \end{bmatrix} \in \mathbb{R}^{m^2 \times m^2}$$

with I is the $m \times m$ identity

$$T = \begin{bmatrix} -4 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & -4 \end{bmatrix} \in \mathbb{R}^{m \times m}$$

Band size: m (bandwidth).

Fill-in under Gaussian elimination:

- becomes full matrix within a band of width m
- $O(m^4)$ complexity!
- Smart about ordering: $O(m^3)$ (see section 3.7 in LeVeque) → lowest complexity for GE.

Iterative methods:
- do not build A or A^{-1} explicitly
- start from a right-hand side, iterate, and converge toward the solution.

Ex. Jacobi iteration for $\Delta u = f$

Rewrite system as

$$u_{ij} = \frac{1}{4}\left[u_{i-1,j} + u_{i,j-1} + u_{i+1,j} + u_{i,j+1}\right] - \frac{h^2}{4} f_{ij}$$

(If $f=0$, a harmonic function at a point equal to its average along a closed curve containing the point)

$\Rightarrow$ iterative method from $u_{ij}^{[k]}$ to $u_{ij}^{[k+1]}$:

$$u_{ij}^{[k+1]} = \frac{1}{4}\left[u_{i-1,j}^{[k]} + u_{i,j-1}^{[k]} + u_{i+1,j}^{[k]} + u_{i,j+1}^{[k]}\right] - \frac{h^2}{4} f_{ij}$$

Ex. Gauss-Seidel: use $u_{i-1,j}^{[k+1]}$ and $u_{i,j-1}^{[k+1]}$ instead.

Matrix expression of Jacobi:

$$A = \underset{\substack{\text{diag,}\\ -\frac{4}{h^2} I}}{M} - \underset{\substack{\text{nondiag}\\ \frac{1}{h^2} \text{ on shifted diags}}}{N}$$ with M easily invertible

$$AU = F \Rightarrow MU - NU = F$$

$$U = \underbrace{M^{-1}N}_{G}U + \underbrace{M^{-1}F}_{c}$$

Iteration:

$$U^{[k+1]} = GU^{[k]} + c$$

U is a fixed point / equilibrium of the iteration. Is it stable?

Let $e^{[k]} = U^{[k]} - U$ (exact)

$$\Rightarrow e^{[k+1]} = Ge^{[k]}$$

$$\Rightarrow e^{[k]} = G^k e^{[0]}$$

Stable fixed point means that G is contractive, i.e. $\lim_{k\to\infty} G^k = 0$

Since $\|e^{[k+1]}\| \le \|G\| \, \|e^{[k]}\|$,

$$\|e^{[k]}\| \le \|G\|^k \|e^{[0]}\|,$$

suffices to show

$$\boxed{\|G\| < 1}$$

in some norm.

e.g. $\|G\|_2 = \max_j |\lambda_j(G)|$ if $G = G^T$.
(spectral radius)

(see LeVeque for the case $G \neq G^T$)

$\rightarrow$ check $|\lambda|_{max}$ of $G = M^{-1}N$.

<u>Ex</u>. $u'' = f$, centered diff.

$$A = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & -2 \end{bmatrix} \qquad M = -\frac{2}{h^2} I$$

$$= M - N \qquad N = \frac{1}{h^2}\begin{bmatrix} 0 & -1 & & \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 0 \end{bmatrix} = M - A$$

$$M^{-1} = -\frac{h^2}{2} I, \quad M^{-1}N = M^{-1}(M - A)$$

$$= I - M^{-1}A$$

$$= I + \frac{h^2}{2} A$$

So $G = I + \frac{h^2}{2} A$

Eigenvectors: same as A

Eigenvalues: $\lambda_m(G) = 1 + \frac{h^2}{2}\lambda_m(A)$

We know $\lambda_m(A) = \frac{-4}{h^2}\sin^2\left(\frac{m\pi h}{2}\right)$

$$\Rightarrow \lambda_m(G) = \cos(m\pi h) \qquad m = 1, \ldots, N \quad h = 1/_{N+1}$$

$$\lambda_{max}(G) = \cos(\pi h) \quad (m = 1)$$

$$\|G\|_2 = \lambda_{max}(G) = \cos(\pi h)$$
$$= 1 - \frac{\pi^2 h^2}{2} + O(h^4) \simeq 0.999$$

Convergence $\|G\|_2 < 1$? YES. ✓
Fast ? NO because $\|G\|_2$ very close to 1.
How many iterations?

$$\|e^{[k]}\| \leq \underbrace{\|G\|^k}_{=\varepsilon} \|e^{[0]}\|$$

Want error reduction factor ε.

$$\Rightarrow \|G\|^k = \varepsilon$$
$$k \log \|G\| = \log \varepsilon$$
$$k = \log \varepsilon / \log \|G\|$$

with $\log \|G\|_2 = \log\left(1 - \frac{\pi^2 h^2}{2}\right)$ $(\log = \ln)$

$$\simeq -\frac{\pi^2 h^2}{2}$$

$$k \simeq (\log \varepsilon) \cdot \frac{-2}{\pi^2 h^2}$$
$$= \left(\frac{2}{\pi^2}\right)(N+1)^2 \log\left(\frac{1}{\varepsilon}\right) = O(N^2)$$

$\rightarrow O(N^2)$ iterations to reach a fixed error level!
Each iteration: $O(N)$ complexity
$\rightarrow O(N^3)$ total complexity $\rightarrow$ unacceptable.

02/23/10

Slowness of Jacobi, and multigrid.

$$u'' = f \quad \rightarrow \quad AU = F$$

$$A = M - N$$

$\llcorner$ diag.

$$U = \underbrace{M^{-1}N}_{G}\, U + M^{-1}F$$

$$U^{[k+1]} = G U^{[k]} + M^{-1}F.$$

$$e^{[k]} = U^{[k]} - U$$

$$\boxed{e^{[k+1]} = G e^{[k]}}$$

Need $\|G\|_2 < 1$

$G = G^T$,

$\|G\|_2 = |\lambda|_{max}(G)$

N in code → look → $M = N+1$

Eigen-analysis of A.
(Fourier sine)

$m = 1, .., N-1$

$h = 1/N$

$$\lambda_m(A) = \frac{-4}{h^2}\sin^2\left(\frac{m\pi h}{2}\right)$$

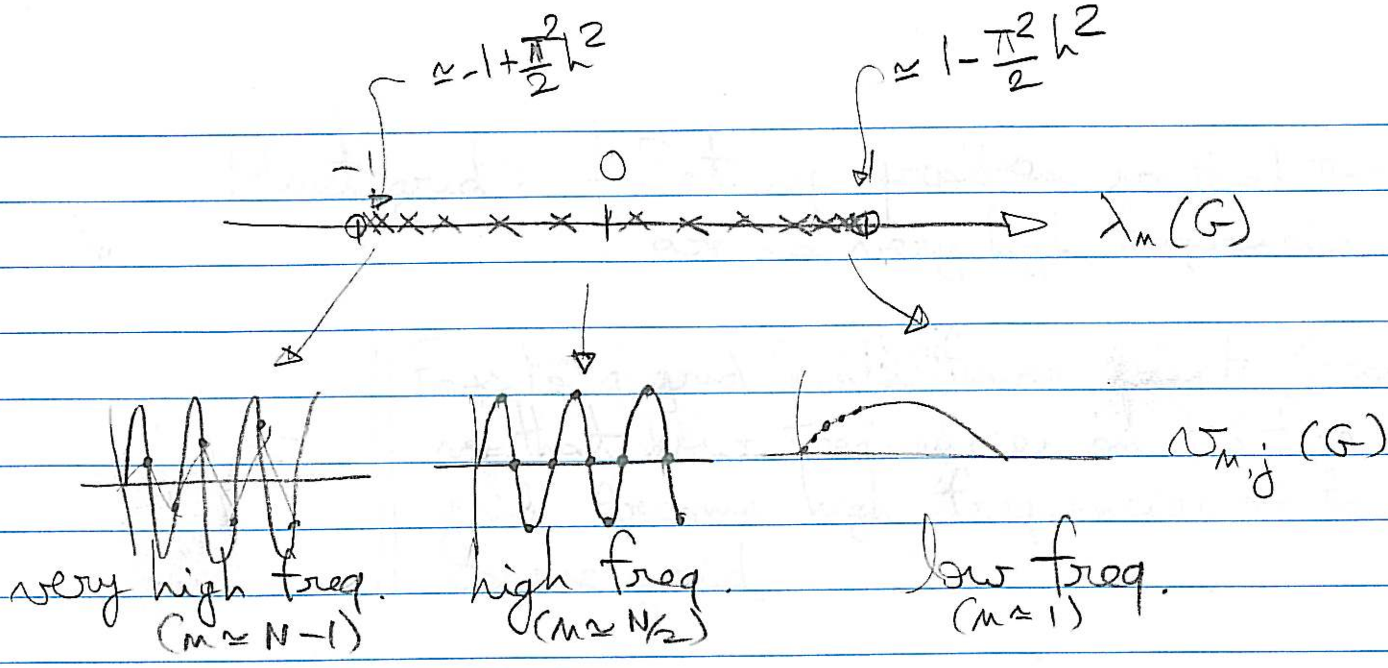
$$v_{m,j}(A) = \sin(m\pi jh)$$

$(x_j = jh)$

$j = 1, .., N-1$

Eigen-analysis of G: $\quad G = I + \frac{h^2}{2}A$

$$\begin{cases} \lambda_m(G) = \cos(m\pi h) \\ v_{m,j}(G) = \sin(m\pi jh) \end{cases}$$



Decompose $\quad e_j^{[0]} = \sum_{m=1}^{N-1} c_m v_{m,j} \quad$ for some c_m.

(Fourier sine expansion)

$$G\, e_j^{[0]} = \sum_{m=1}^{N-1} c_m \lambda_m(G) v_{m,j}$$

$$\Rightarrow e_j^{[k]} = \sum_{m=1}^{N-1} c_m \boxed{\lambda_m^k(G)}\, v_{m,j}$$

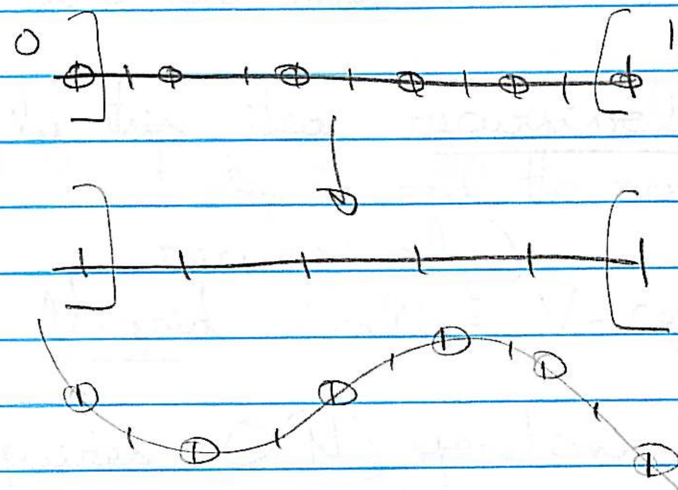
m-th eigencomponent decays like $\lambda_m^k(G)$ as k increases:

- slow when $m \simeq 1$ or $m \simeq N-1$
- fast otherwise (very fast)

e.g. $(0.9)^5 = 0.59\ldots$
$(0.4)^5 = 0.01\ldots$

Multigrid: – Set up problem so that there are no very high frequencies.

Pass to a grid with fewer points (= coarse) so that low frequencies on the fine grid become high frequencies on the coarse grid.



$j = 1, \dots, N-1$

$j = 1, \dots, \frac{N}{2} - 1$

Do not solve the original problem, get an estimate of the error:

- get $u^{[k]}$ from a few iterations of Jacobi

$$\left[\begin{array}{ll} \text{want } e^{[k]} = u^{[k]} - u & \\ \text{have } r^{[k]} = f - Au^{[k]} & \text{(residual error)} \\ \Rightarrow Ae^{[k]} = Au^{[k]} - f = -r^{[k]} & \end{array}\right]$$

- solve $Ae^{[k]} = -r^{[k]}$ at the <u>coarser</u> scale.

1. restrict / downsample $r^{[k]}$ to a coarser grid
2. solve $A e^{[k]} = -r^{[k]}$ approximately (Jacobi)
3. interpolate / upsample / (prolong) $e^{[k]}$ to a finer grid $\rightarrow e^*$

- update $u^* = u^{[k]} - e^*$
- do a few more iterations of Jacobi

$\rightarrow$ Apply this idea <u>recursively</u>.
(at step 2, call the routine recursively)

$\rightarrow$ <u>Multigrid</u>. (called V-cycle)

Requires $O(N)$ operations for a V-cycle.
Requires $O(\log N)$ cycles to get error ε
$\Rightarrow$ $O(N \log N)$ complexity
Some variants (full multigrid) require $O(N)$ op.

02/25

Iterative methods for linear systems $Ax = b$.

Black box algorithms:

$$x \to \boxed{} \to Ax. \qquad x \in \mathbb{R}^N,$$

- $O(N^2)$ operations in general.
- can be $O(N)$ if A is sparse or has structure.

(1) Steepest
Gradient descent

(2) Conjugate gradient

Today: Assume $A = A^T$

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

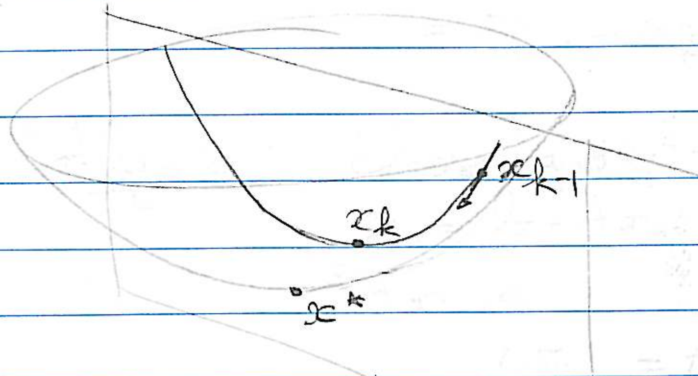
$$\nabla\varphi(x) = Ax - b$$
$$= 0 \text{ when } Ax = b.$$

$\Rightarrow$ solution x^* of $Ax = b$ is a stationary point of $\nabla\varphi(x)$

Def. A is positive definite when $x^T A x \geq 0$ for all x and $x^T A x = 0 \Rightarrow x = 0$.

When A is pos. def.,
$\nabla\varphi(x^*) = 0 \iff x^*$ is the minimum of φ

Rmk. A pos. def. $\Leftrightarrow$ all $\lambda_j(A) > 0$



1 Go downhill.

$$x_k = x_{k-1} - \alpha_{k-1} \nabla\varphi(x_{k-1})$$
$$= x_{k-1} - \alpha_{k-1} [\underbrace{Ax_{k-1} - b}_{-r_{k-1}\text{, residual}}]$$
$$= x_{k-1} + \alpha_{k-1} r_{k-1}$$

$$\alpha_{k-1} : \min_{\alpha} \varphi(x_{k-1} + \alpha_{k-1} r_{k-1})$$

$$\Rightarrow (\ldots) \quad \alpha_{k-1} = \frac{r_{k-1}^T r_{k-1}}{r_{k-1}^T A r_{k-1}}$$

Algo 1 choose guess x_0
for $k = 1, 2, \ldots$
$r_{k-1} = b - Ax_{k-1}$
if $\|r_{k-1}\| < tol$, stop.
$\alpha_{k-1} = \dfrac{r_{k-1}^T r_{k-1}}{r_{k-1}^T A r_{k-1}}$
$x_k = x_{k-1} + \alpha_{k-1} r_{k-1}$
end

notice $r_k = b - Ax_k$

$= b - A(x_{k-1} + \alpha_{k-1} r_{k-1})$

$= r_{k-1} - \alpha_{k-1} \underbrace{A r_{k-1}}_{w_{k-1}}$

<u>Algo 2</u> choose guess x_0

$r_0 = b - Ax_0$

for k

$w_{k-1} = A r_{k-1}$

$$\alpha_{k-1} = \frac{r_{k-1}^T r_{k-1}}{r_{k-1}^T w_{k-1}}$$

$x_k = x_{k-1} + \alpha_{k-1} r_{k-1}$

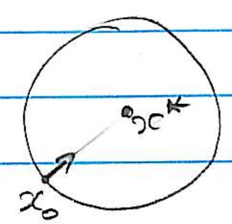
$r_k = r_{k-1} - \alpha_{k-1} w_{k-1}$

if $\|r_k\| <$ tol, stop.

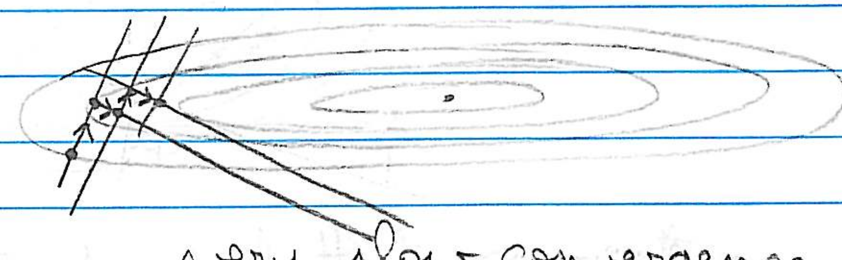
end

$\varphi(x) = \|x\|^2$

$\varphi(x) = \frac{x_1^2}{100} + x_2^2$



1 step



very slow convergence.

Assume $AV = V\Lambda$ with $A = A^T$

$V^T = V^{-1}$
(orthogonal eigenvec.)

$\Rightarrow A = V \Lambda V^T$

$x^T A x = \underbrace{x^T V}_{y^T} \Lambda \underbrace{V^T x}_{y}$

$= y^T \Lambda y = \sum \lambda_j y_j^2$

$$\Rightarrow \varphi(x) = \sum_{j=1}^{N} \left(\frac{y_j}{1/\sqrt{\lambda_j}}\right)^2 + \text{linear}$$

Lengths of semi-axes: $1/\sqrt{\lambda_j}$

Eccentricity $= \sqrt{\dfrac{\lambda_{max}}{\lambda_{min}}} = \sqrt{\kappa(A)}$

where $\kappa(A) = \dfrac{\lambda_{max}}{\lambda_{min}}$ is the

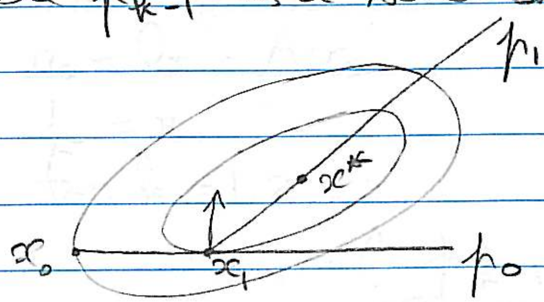
<u>condition number</u> (when $A = A^T$)

(2) Conjugate gradients. (Hestenes, Stiefel '52)

A needs to be symm. pos. def.

$x_k = x_{k-1} + \alpha_{k-1} p_{k-1}$

where p_{k-1} is a well chosen <u>direction</u>



$x \in \mathbb{R}^2$: choose p_1 such that $x_2 = x^*$

$\Rightarrow p_1 = x^* - x_1$

$-\nabla\varphi(x_1) = r_1 = b - Ax_1$

$p_0 \perp \nabla\varphi(x_1) \Rightarrow \quad p_0^T(b - Ax_1) = 0$

$p_0^T(Ax^* - Ax_1)$

$p_0^T A(x^* - x_1)$

$\boxed{p_0^T A p_1 = 0}$

$\Rightarrow p_0$ and p_1 are A-conjugate

Choose directions as follows:

$p_0 = r_0 \quad \rightarrow \quad x_1$ min of φ over $x_0 + \langle p_0 \rangle$

p_1 conj. $p_0 \quad \rightarrow \quad x_2$ min of φ over $x_0 + \langle p_0, p_1 \rangle$

p_2 conj. $p_0, p_1 \quad \rightarrow \quad x_3$ ——— $x_0 + \langle p_0, p_1, p_2 \rangle$

etc.

Rmk Terminates after N steps where $A \in \mathbb{R}^{N \times N}$, because $\langle p_0, \dots, p_{N-1} \rangle = \mathbb{R}^N$.

Algo (CG)

choose guess x_0

$r_0 = b - Ax_0$

$p_0 = r_0$

for $k = 1, 2, \dots$

$w_{k-1} = A p_{k-1}$ (temp.)

$\alpha_{k-1} = \dfrac{(r_{k-1}^T r_{k-1})}{p_{k-1}^T w_{k-1}}$ (line search)

$x_k = x_{k-1} + \alpha_{k-1} p_{k-1}$ (new)

$r_k = r_{k-1} - \alpha_{k-1} w_{k-1}$ (as before)

if $\|r_k\| < tol$, stop

$\beta_{k-1} = \dfrac{(r_k^T r_k)}{r_{k-1}^T r_{k-1}}$ (new)

$p_k = r_k + \beta_{k-1} p_{k-1}$

end.

Rmk $x_0 = 0 \Rightarrow p_0 = r_0 = b, \quad \langle p_0 \rangle = \langle b \rangle$

$$p_1 = r_1 + \beta_0 p_0$$
$$= b - Ax_1 - \beta_0 b$$
$$\quad \llcorner\, x_1 = x_0 + \alpha_0 p_0$$
$$\qquad = \alpha_0 b$$
$$= (1-\beta_0)\boxed{b} - \alpha_0 \boxed{Ab}$$

$$\Rightarrow \quad \langle p_0, p_1 \rangle = \langle b, Ab \rangle$$

etc.

$$\langle p_0, \ldots, p_{k-1} \rangle = \langle b, \ldots, A^{k-1} b \rangle$$
$$= K_k$$

called a Krylov space
- of dimension k
- associated with b

$\Rightarrow$ CG minimizes $\varphi(x)$ over K_k at step k
(If $x_0 \neq 0$, min. $\varphi(x)$ over $x_0 + K_k$.)

Rmk. CG also minimizes the following function of x over K_k:
$$\|e\|_A = \sqrt{e^T A e}, \quad \text{where } e = x - x^*$$

Indeed, $\|e\|_A^2 = (x - x^*)^T A (x - x^*)$
$$= x^T A x - 2 x^T \underbrace{A x^*}_{= b}$$
$$+ (x^*)^T A x^*$$
$$= \varphi(x) + \underbrace{(x^*)^T A x^*}_{\text{constant}}$$

Also, $x_k = x_0 + \alpha_0 p_0 + \dots + \alpha_{k-1} p_{k-1}$

$\Rightarrow e_k = e_0 + \alpha_0 p_0 + \dots + \alpha_{k-1} p_{k-1}$

Since $x_k \in x_0 + K_k$,

$\alpha_0 p_0 + \dots + \alpha_{k-1} p_{k-1} \in K_k$

$\Rightarrow e_k - e_0 \in K_k$

$\Rightarrow e_k = P_k(A) e_0$

$\hookrightarrow$ polynomial of degree k in the matrix A:

$$P_k(A) = I + c_1 A + c_2 A^2 + \dots + c_k A^k$$

$\Rightarrow$ CG implicitly constructs P such that

$$\min_{\deg P = k} \| P(A) e_0 \|_A .$$

$$\left(\begin{aligned} A = V \Lambda V^{-1} \quad &\Rightarrow \quad A^k = V \Lambda^k V^{-1} \\ &\Rightarrow \quad P_k(A) = V P_k(\Lambda) V^{-1} \\ \text{where } P_k(\Lambda) = &\begin{pmatrix} P_k(\lambda_1) & & 0 \\ & \ddots & \\ 0 & & P_k(\lambda_n) \end{pmatrix} \end{aligned} \right)$$

Claim: $\| P(A) e_0 \|_A \le \max_j |P(\lambda_j)| \, \|e_0\|_A$

$$\Rightarrow \boxed{\frac{\|e_k\|_A}{\|e_0\|_A} \le \min_{\deg P = k} \max_j |P(\lambda_j)|}$$

How large can a deg-k polynomial be on the spectrum of A? $\to$ det. convergence

Claim: There exists a pol. of deg k such that

$$\frac{\|P(A)e_0\|_2}{\|e_0\|_2} \leq 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^k$$

$$\simeq 2\left(1-\frac{2}{\sqrt{\kappa}}\right)^k$$

$$\simeq 2e^{-2k/\sqrt{\kappa}}$$

where $\kappa = \lambda_{max}(A)/\lambda_{min}(A)$ is the condition number of A.

Ex. $A = \frac{1}{h^2}\begin{pmatrix} -2 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & -2 \end{pmatrix}$, consider $-A$

$$\Rightarrow \lambda_{max}(-A) \simeq 4/h^2$$

$$\lambda_{min}(-A) \simeq \pi^2$$

$$\kappa(-A) \simeq \frac{4}{\pi^2 h^2} = O(N^2)$$

$\Rightarrow$ CG requires $O(\sqrt{\kappa}) = O(N)$ steps to converge

Not very good in 1D but OK in nD, $n \geq 2$, where N is the number of points per dimension.

03/02 CG; heat eqn.

One in a family of Krylov subspace methods

	$Ax=b$	$Av=\lambda v$
$A=A^*$	CG	LANCZOS
$A\neq A^*$	GMRES	ARNOLDI $\to$ Matlab's eigs

Krylov subspace:

$$\mathcal{K}_k = \{ b, Ab, \ldots, A^{k-1} b \}$$ (big round k)

CG: • minimizes $\phi(x) = x^T A x - x^T b$
for $x \in \mathcal{K}_k$ at step k.
• also min $\|e\|_A = \sqrt{e^T A e}$,
$e = x - x^*$. $Ax^* = b$
for $x \in \mathcal{K}_k$ at step k.

(\$) $$e_k = e_0 + \underbrace{c_1 A e_0 + c_2 A^2 e_0 + \ldots + c_k A^k e_0}_{\in \mathcal{K}_k \text{ because } Ae_0 = -b}$$

$$= P(A) e_0 \quad \text{with } P(A) = I + c_1 A + \ldots + c_k A^k$$
$$P(0) = I$$

$\to$ CG solves $$\min_{\substack{\deg P = k \\ P(0) = I}} \| P(A) e_0 \|_A / \| e_0 \|_A$$

$$A = V \Lambda V^{-1} \qquad P(A) = V\, P(\Lambda)\, V^{-1}$$

with $P\left(\begin{matrix} \lambda_1 & \\ & \ddots \\ & & \lambda_n \end{matrix}\right) = \left(\begin{matrix} P(\lambda_1) & \\ & \ddots \\ & & P(\lambda_n) \end{matrix}\right)$

$$\| P(A) e_0 \|_A^2 = e_0^T P(A)^T A\, P(A)\, e_0$$
$$= e_0^T V^{-T} P(\Lambda) V^T \underbrace{V \Lambda V^T}_{A} V P(\Lambda) V^{-1}$$

with $V^T V = I$ $(A = A^*)$

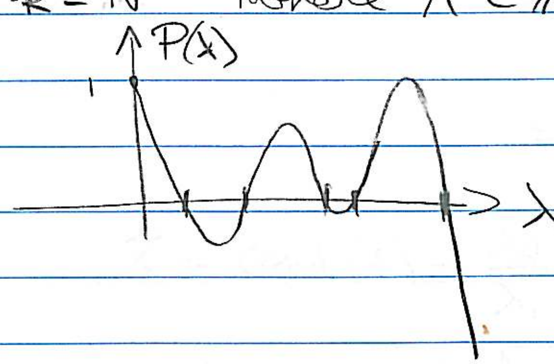
$$= e_0^T V \operatorname{diag}(\lambda_j P(\lambda_j)^2) V^T e_0$$

$$\leq \max_j P(\lambda_j)^2 \underbrace{e_0^T V \Lambda V^T e_0}_{\| e_0 \|_A^2}$$

$$\frac{\| P(A) e_0 \|_A}{\| e_0 \|_A} \leq \max_j P(\lambda_j)$$

then minimize over all P s.t. : $\deg P = k$, $P(0) = 1$.

- ex : $k = N$ where $A \in \mathbb{R}^{N \times N}$.



λ_j , $j = 1, \dots, N$

→ pick

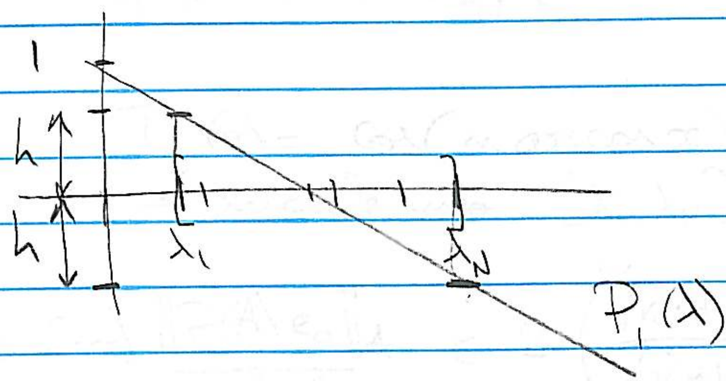
$$P(\lambda) = \frac{\prod_j (\lambda - \lambda_j)}{\prod_j (0 - \lambda_j)}$$

$$\Rightarrow \|e_k\|_A = \min \frac{\|P(A)e_0\|_A}{\|e_0\|_A} \le \max_j |P(\lambda_j)|$$

$$\le 0 \quad \Rightarrow \|e_k\|_A = 0$$

exact!

- ex: $k=1$ $\qquad P(\lambda) = a\lambda + 1$ with $P(0) = 1$



$\rightarrow$ choose a s.t. $P(\lambda_1) = -P(\lambda_N)$

$\rightarrow \quad a\lambda_1 + 1 = -a\lambda_N - 1$

$a(\lambda_1 + \lambda_N) = -2 \quad ; \quad a = \dfrac{-2}{\lambda_1 + \lambda_N}$

$$P_1(\lambda) = 1 - \frac{2}{\lambda_1 + \lambda_N}\lambda$$

$$\max_j |P(\lambda_j)| = P(\lambda_1) = 1 - \frac{2}{\lambda_1 + \lambda_N}\lambda_1$$

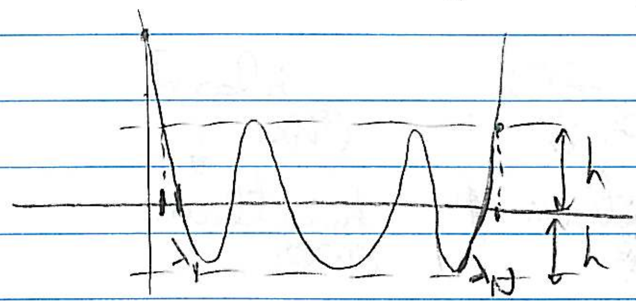
$$= \frac{\lambda_N - \lambda_1}{\lambda_N - \lambda_1} = \frac{\lambda_N/\lambda_1 - 1}{\lambda_N/\lambda_1 + 1}$$

$$= \frac{\kappa - 1}{\kappa + 1},$$

$$\kappa = \mathrm{cond}(A) = \frac{\lambda_N}{\lambda_1}$$ condition number

$\dfrac{\kappa-1}{\kappa+1}$ = bound on the reduction factor of the error after 1 step.

- General case : Chebyshev polynomials



→ equioscillation

$$T_n(x) = \cos(n \arccos x) \qquad x \in [-1,1]$$

→ rescale into $[\lambda_1, \lambda_N]$

$$\Rightarrow (\ldots) \frac{\|P(A) e_0\|_A}{\|e_0\|_A} \leq 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^k$$

$$\simeq 2\left(1 - \frac{2}{\sqrt{\kappa}}\right)^k \qquad (\kappa \text{ large})$$

$$\simeq 2\, e^{-2k/\sqrt{\kappa}}$$

→ $\boxed{\sqrt{\kappa} \text{ governs convergence of the CG algorithm : need } O(\sqrt{\kappa}) \text{ steps to get small error}}$

Ex. $A = \frac{1}{h^2}\begin{pmatrix} -2 & 1 & & \\ 1 & \ddots & & \\ & & & 1 \\ & & 1 & -2 \end{pmatrix} \Rightarrow \kappa(A) = \left|\frac{\lambda_N}{\lambda_1}\right| \simeq \frac{4/h^2}{1/\pi^2} = O(N^2)$

$(h = 1/N)$

$\sqrt{\kappa} = O(N) \quad O(N)$ steps

Jacobi : convergence governed by κ, not $\sqrt{\kappa}$

(N^2 steps)

Redeem CG (and GMRES, etc.) when κ is large:

Jacobi $\xrightarrow{O(N^3)}$ multigrid $O(N)$

CG $\xrightarrow{O(N^2)}$ multigrid $O(N)$

for the matrix $A = \frac{1}{h^2}\begin{pmatrix} -2 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & -2 \end{pmatrix}$

Preconditioning: introduce $M \in \mathbb{R}^{N \times N}$ such that:
- M is easy to invert $\rightarrow M^{-1}$ in a black box.
- M is some approximation to A.

Left: $\boxed{M^{-1}A}\, x = M^{-1} b$

① compute $M^{-1}b$
② solve with the matrix $M^{-1}A$

Right: $AM^{-1}y = b \quad , \quad x = M^{-1}y$

① solve with $AM^{-1} \rightarrow y$
② compute $M^{-1}y$

Centered: (preserve symmetry and pos. def.)

$$\underbrace{(C^{-T}AC^{-1})}_{\tilde{A}}\ \underbrace{Cx}_{\tilde{x}} = \underbrace{C^{-T}b}_{\tilde{b}}$$

$\rightarrow$ redef. CG (p. 95)

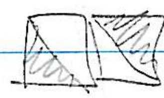
<u>ex</u>. of M^{-1}: 1) solve partially using a cheap multigrid; or multigrid on an easier equation

<u>ex</u>. $\nabla \cdot \alpha(x) \nabla \to \Delta$

<u>ex</u> $\Delta + k^2 I \to \Delta$

2) incomplete Cholesky factorization:

<u>Cholesky</u>: $A = R^T R$ (LU for symm. A)



<u>incomplete</u>: only consider the elements of R at the same locations as those of A; put others to zero.

$\to$ sparse approx. to R, call C

$$A \simeq C^T C = M$$

$\to$ forward and back substitutions with C, C^T.

3) (for GMRES) incomplete LU.

and the list goes on.

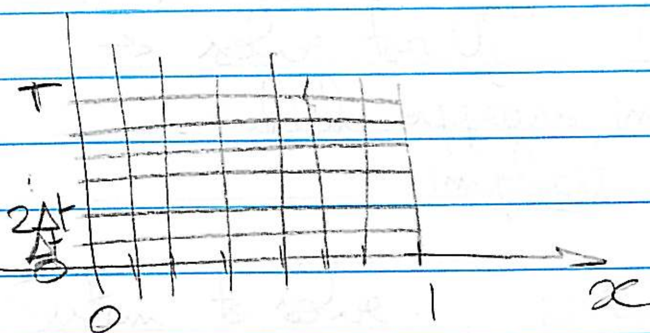
Part II

Initial value problems

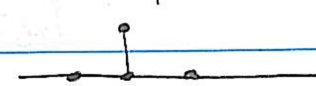
Chap. 9 of LeVeque (2007): diffusion equations

ex (Heat equation)
$$\begin{cases} u_t = \alpha u_{xx} & \alpha = \text{heat conductivity} \\ & x \in [0,1] \\ u(t=0,x) = u_0(x) & \\ u(t,x=0) = g_0(t) & \\ u(t,x=1) = g_1(t) & \end{cases} \Big\} \text{ Dirichlet.}$$

$$x_j = j\underbrace{h}_{\Delta x \text{ (grid spacing)}} \quad ; \quad t_n = n\underbrace{k}_{\Delta t \text{ (time step)}}$$



Stencil for simplest:



$$U_j^n \simeq u(x_j, t_n)$$

$n \to$ time, $j \to$ space

ex. Simplest: $$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \alpha \frac{1}{(\Delta x)^2}\left(U_{j+1}^n - 2U_j^n + U_{j-1}^n\right)$$

$$\Rightarrow U_j^{n+1} = U_j^n + \alpha \frac{\Delta t}{(\Delta x)^2}\left(U_{j+1}^n - 2U_j^n - U_{j-1}^n\right)$$

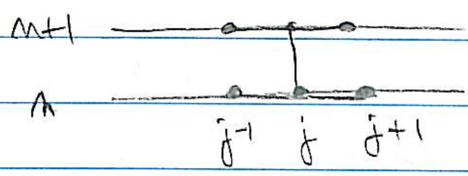
Obtain U_j^{n+1} explicitly from quantities at time t_n

$\rightarrow$ <u>explicit</u> method.

<u>ex.</u> Crank-Nicolson :

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{\alpha}{2}\left[D_{c,2}U_j^{n+1} + D_{c,2}U_j^n\right]$$

$$= \frac{\alpha}{2}\left[\frac{U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}}{(\Delta x)^2} + \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{(\Delta x)^2}\right]$$



$$r = \frac{\alpha \Delta t}{2(\Delta x)^2}$$

$\rightarrow$ solve for U_j^{n+1} (for all j) which appears implicitly

$\rightarrow$ <u>implicit</u> method.

System to solve :

$$\begin{bmatrix} 1+2r & -r & & \\ -r & \ddots & \ddots & \\ & \ddots & \ddots & -r \\ & & -r & 1+2r \end{bmatrix}$$