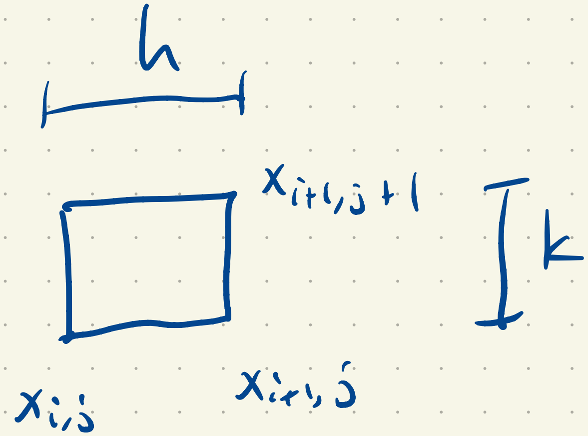
Numerical Strategy:

Centered Differences.



$0 \le i \le N, \quad 0 \le j \le M$

$$-\Delta u \approx \frac{-u_{i+1,j}+2u_{i,j}-u_{i-1,j}}{h^2} + \frac{-u_{i,j+1}+2u_{i,j}-u_{i,j-1}}{k^2}$$

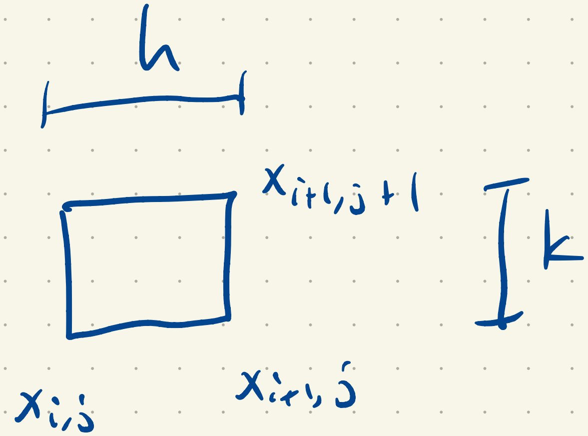
$$-\Delta u = -\partial_x^2 u - \partial_y^2 u = -u_{xx} - u_{yy}$$

$-\Delta u = f$

$f(x_{ij})$

Numerical Strategy:

Centered Differences.



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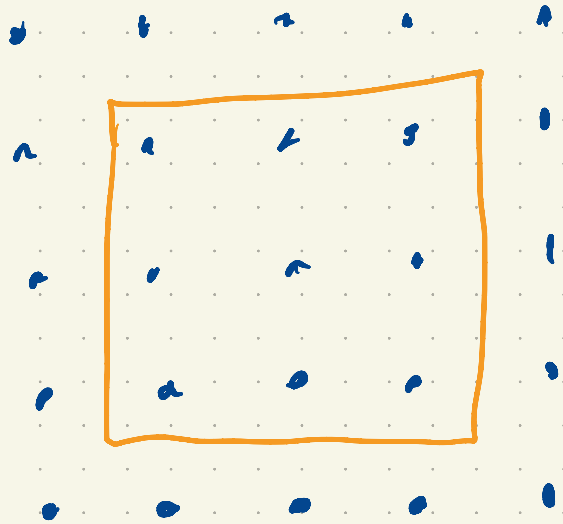
$$-\Delta u \approx \frac{-u_{i+1,j}+2u_{i,j}-u_{i-1,j}}{h^2} + \frac{-u_{i,j+1}+2u_{i,j}-u_{i,j-1}}{k^2}$$

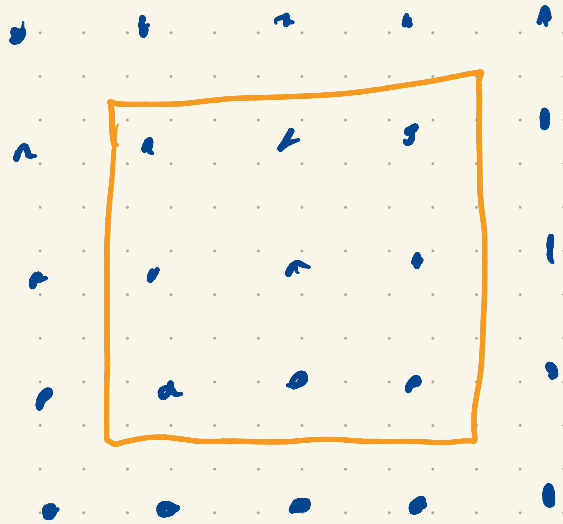
$$= \frac{1}{k^2}\Big[-\lambda^2\left(u_{i+1,j}+u_{i-1,j}\right)+2\left(1+\lambda^2\right)u_{i,j} - \left(u_{i,j-1}+u_{i,j+1}\right)\Big]$$

$$\lambda = \frac{k}{h} \qquad \left(\beta = 2\left(1+\lambda^2\right)\right)$$



$$\begin{matrix} x_{13} & x_{23} & x_{33} \\ x_{12} & x_{22} & x_{32} \\ x_{11} & x_{21} & x_{31} \end{matrix}$$

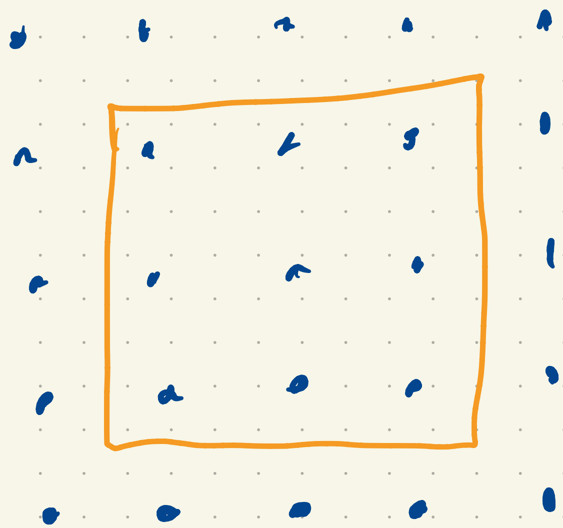
$$Au = f \qquad -\Delta u = f$$



$$\begin{array}{ccc} x_{13} & x_{23} & x_{33} \\ x_{12} & x_{22} & x_{32} \\ x_{11} & x_{21} & x_{31} \end{array}$$

$$\downarrow$$

$$\begin{array}{ccc} v_7 & v_8 & v_9 \\ v_4 & v_5 & v_6 \\ v_1 & v_2 & v_3 \end{array}$$



$$\begin{array}{ccc} x_{13} & x_{23} & x_{33} \\ x_{12} & x_{22} & x_{32} \\ x_{11} & x_{21} & x_{31} \end{array}$$

$$\downarrow$$

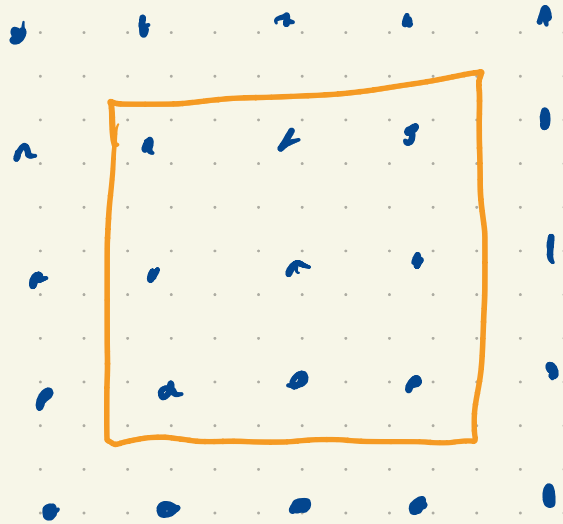
$$\begin{array}{ccc} v_7 & v_8 & v_9 \\ v_4 & v_5 & v_6 \\ v_1 & v_2 & v_3 \end{array}$$

A

First row (0 boundary conditions)

$$B \quad -\lambda^2 \quad 0 \quad -1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0$$

$$\begin{bmatrix} u_{11} \\ u_{21} \\ u_{31} \\ u_{12} \\ u_{22} \\ \vdots \end{bmatrix}$$

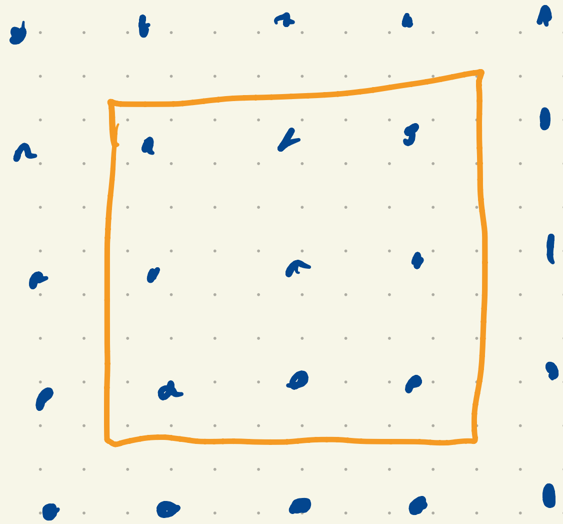


$V_7 \quad V_8 \quad V_9$

$V_4 \quad V_5 \quad V_6$

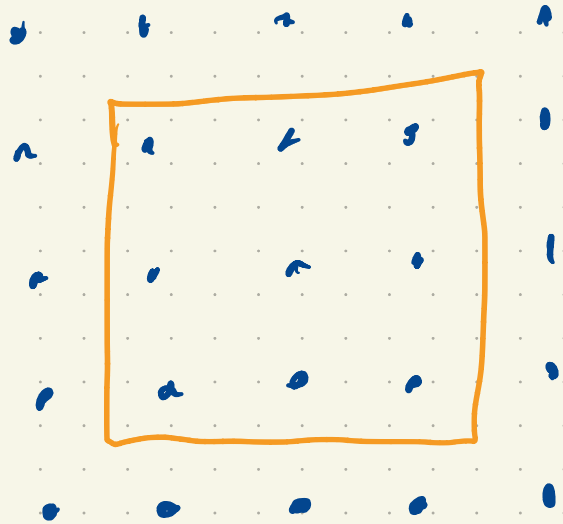
$V_1 \quad V_2 \quad V_3$

$\beta = \lambda^2 \quad 0 \quad -1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0$



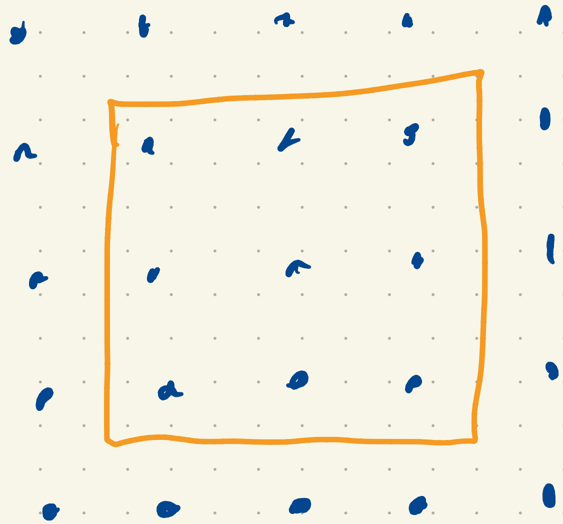
$$\begin{array}{ccc} V_7 & V_8 & V_9 \\ V_4 & V_5 & V_6 \\ V_1 & V_2 & V_3 \end{array}$$

$$\begin{array}{cccccccc} \beta-\lambda^2 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ -\lambda^2 & \beta-\lambda^2 & 0 & -1 & 0 & 0 & 0 & 0 \end{array}$$



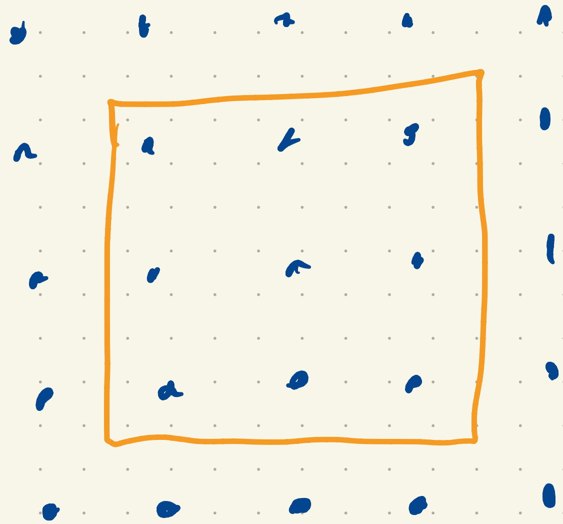
$$\begin{array}{ccc} V_7 & V_8 & V_9 \\ V_4 & V_5 & V_6 \\ V_1 & V_2 & V_3 \end{array}$$

$$\begin{matrix} \beta & -\lambda^2 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ -\lambda^2 & \beta & -\lambda^2 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & -\lambda^2 & \beta & 0 & 0 & -1 & 0 & 0 & 0 \end{matrix}$$



$$\begin{array}{ccc} V_7 & V_8 & V_9 \\ V_4 & V_5 & V_6 \\ V_1 & V_2 & V_3 \end{array}$$

$$\begin{array}{ccccccccc}
\beta & -\lambda^2 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
-\lambda^2 & \beta & -\lambda^2 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & -\lambda^2 & \beta & 0 & 0 & -1 & 0 & 0 & 0 \\
-1 & 0 & 0 & \beta & -\lambda^2 & 0 & -1 & 0 & 0
\end{array}$$



$$
\begin{array}{ccc}
V_7 & V_8 & V_9 \\
V_4 & V_5 & V_6 \\
V_1 & V_2 & V_3
\end{array}
$$

$$
A = \left(\begin{array}{ccc|ccc|ccc}
\beta & -\lambda^2 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
-\lambda^2 & \beta & -\lambda^2 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & -\lambda^2 & \beta & 0 & 0 & -1 & 0 & 0 & 0 \\
\hline
-1 & 0 & 0 & \beta & -\lambda^2 & 0 & -1 & 0 & 0 \\
0 & -1 & 0 & -\lambda^2 & \beta & \lambda^2 & 0 & -1 & 0 \\
0 & 0 & -1 & 0 & -\lambda^2 & \beta & 0 & 0 & -1 \\
\hline
 & * & & & * & & & * &
\end{array}\right)
$$

What about nonzero boundary values?

$$\underbrace{-\lambda^2 u_{01}} - \lambda^2 u_{21} + \beta u_{11} \underbrace{- u_{10}} - u_{12}$$

$\rightarrow$ These are known, become part of r.h.s

$$\beta \quad -\lambda^2 \quad 0 \quad -1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0$$

as before.

Discrete problem

$$A\vec{u} = k^2 \vec{f}$$

$$\begin{array}{cc} & NM \\ NM & \begin{bmatrix} T & -I & \ddots & 0 \\ -I & T & \ddots & \\ & \ddots & \ddots & -I \\ 0 & \ddots & -I & T \end{bmatrix} \end{array}$$

T, tridiagonal

[sparse, symmetric]

$(NM) \times (NM)$ matrix

($1000 \times 1000 \Rightarrow$ $\underline{1\,000\,000} \times \underline{1\,000\,000}$ matrix)

7.3 TB

Features of continuous system

1) $-\Delta$ has eigenvalues $\pi^2\left(\left(\frac{k}{a}\right)^2+\left(\frac{\ell}{b}\right)^2\right)>0$

$-\nabla u \cdot n\, v$

$\left(\geq \pi^2\left(\frac{1}{a^2}+\frac{1}{b^2}\right)\right)$

They are positive, $\nearrow \infty$.

2) Symmetry: $\displaystyle\int_\Omega (-\Delta u)v = \int_\Omega \nabla u \cdot \nabla v = \int_\Omega u(-\Delta v)$

$(u, v = 0 \text{ on } \partial\Omega)$

$(Au)\cdot v = u \cdot (Av)$

These manifest themselves in A:

1) A is symmetric: $A^T = A$

2) A has eigenvalues

$$\lambda^{p,q} = \frac{4}{h^2} \sin^2\left(\frac{ph\pi}{2a}\right) + \frac{4}{k^2} \sin^2\left(\frac{qh\pi}{2b}\right) \geq 0$$

$$1 \leq p \leq N \qquad 1 \leq q \leq M$$

$$\lambda^{1,1} \to \pi^2 \left(\frac{1}{a^2} + \frac{1}{b^2}\right) \qquad \left(\|A^{-1}\|_2 \leq 1/\lambda^{1,1}\right)$$

How to solve?

$$Ax = b \qquad A \ \overbrace{\text{pos def}}^{\text{all } \lambda > 0}, \ \text{symmetric.}$$

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

How to solve?

$$Ax = b \qquad A \text{ pos def, symmetric.}$$

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

Job: minimize J

$$\left.\frac{d}{dt}\right|_{t=0} J(x+ty) = 0$$

How to solve?

$$Ax = b \qquad A \text{ pos def, symmetric.}$$

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

Job: minimize J

$$\left.\frac{d}{dt}\right|_{t=0} J(x+ty) = 0$$

At a minimum: $\frac{1}{2} y^T A x + \frac{1}{2} x^T A y - y^T b = 0$

$$y^T [Ax - b] = 0 \ \forall y.$$

This comes from a continuous property too:

To solve $-\Delta u = f$

$$u|_{\partial\Omega} = 0$$

minimize

$$J(u) = \int_{\Omega} \frac{1}{2}|\nabla u|^2 - uf$$

Optimization

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

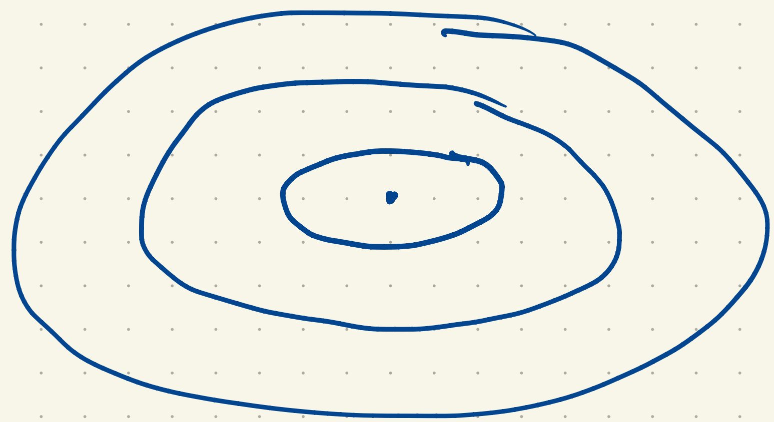
Optimization

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

$$x^2 + 2y^2$$

$$A = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}$$

$$b = 0$$



level sets

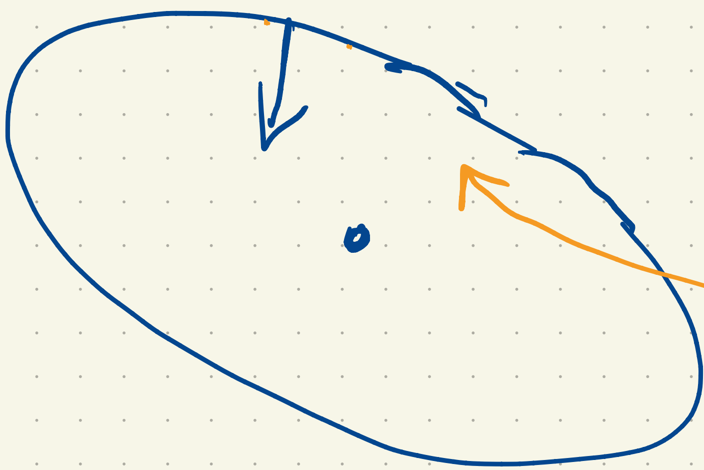
Descent Methods

$$J = \frac{1}{2} x^T A x - x^T b$$

$$\nabla J = \underbrace{(Ax-b)}_{-r}{}^T \quad \text{, residual}$$

$$Ax = b$$

$$r = 0$$



$$r = -\nabla J$$

Descent Methods:

Start at a guess x_0

$$x_1 = x_0 + \alpha_0 d_0$$

search direction, e.g. $-\nabla J = r_0$

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α_0 determined by $\dfrac{d}{d\alpha} J(x_0 + \alpha d_0) = 0$

Descent Methods:

Start at a guess x_0

$$x_1 = x_0 + \alpha_0 d_0$$

search direction, e.g. $-\nabla J = r_0$

α_1 determined by $\dfrac{d}{d\alpha} J(x_0 + \alpha d_0) = 0$

$$d_0^T A(x_0 + \alpha_0 d_0) - d_0^T b = 0$$

$$d_0^T \underbrace{[A x_0 - b]}_{-r_0} + \alpha_0 d_0^T A d_0 = 0$$

$$\alpha_0 = \frac{d_0^T r_0}{d_0^T A d_0}$$

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Now repeat: (Given a search direction d_k)

$$r_k = A x_k - b$$

$$\alpha_k = \frac{d_k^T r_k}{d_k^T A d_k}$$

$$x_{k+1} = x_k + \alpha_k d_k$$

Note: residual is orthogonal to d_k

new

$$d_k^T \left[A(x_k + \alpha_k d_k) - b_k \right] = 0$$

$$d_{k+1}^T r_k = 0$$

is exactly the equation that determines α_k

Steepest Descent:

At each stage, pick $d_k = r_k$.

x_0 given

while looping

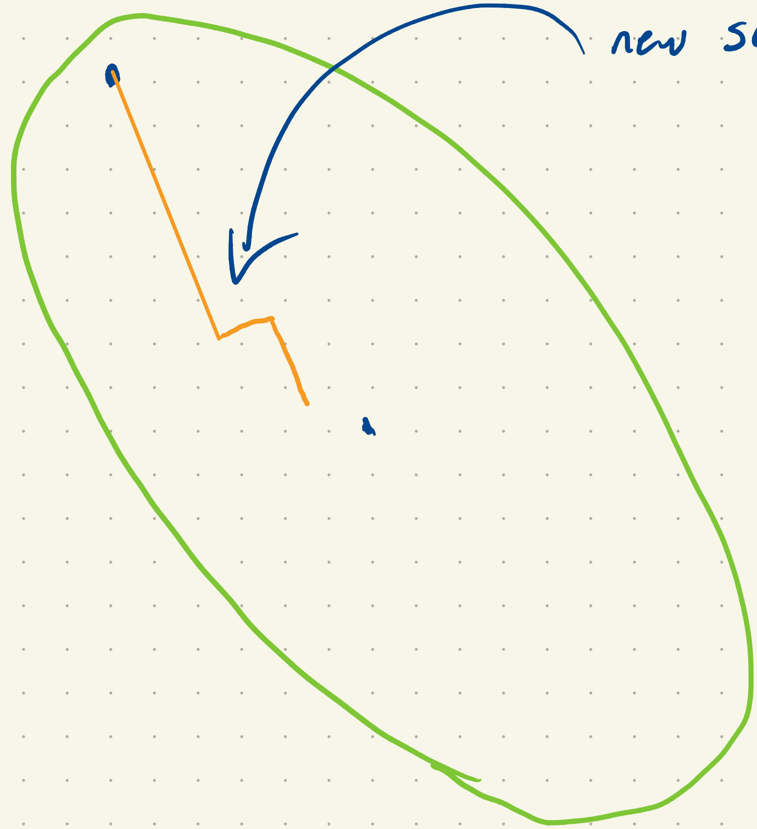
$$r_k = b - A x_k$$

$$d_k = r_k$$

$$\alpha_k = \frac{r_k^T d_k}{d_k A d_k}$$

$$x_{k+1} = x_k + \alpha_k d_k$$

What can go wrong?



new search direction is residual, so is $\perp$ to old search direction.

This is exacerbated if the eigenvalues of A are spread out (large cond #, ours grows like n^2)

Conjugate gradient strategy:

New search direction is A-perp to prior search direction: $\left(d_k^T A d_{k-1} = 0 \right)$

$$d_k = r_k + \beta_k d_{k-1}$$

$$d_{k-1} A \left[r_k + \beta_k d_{k-1} \right] = 0$$

[Magic: Gram Schmidt should have
$d_k = r_k + \sum_{i<k} \beta_{ik} d_k$]

$$-\frac{d_{k-1}^T A r_k}{d_{k-1}^T A d_{k-1}} = \beta_k$$

$$r_k \cdot r_{k-1} = 0$$

$$\Big\downarrow \text{magic}$$

$$\beta_k = \frac{r_k^T r_k}{r_{k-1}^T r_{k-1}}$$

CG Algorithm

x_0 given

$r_0 = b - Ax_0$

$d_0 = r_0$

while looping:

$$\alpha_k = \frac{r_k^T r_k}{d_k^T A d_k}$$

$$x_{k+1} = x_k + \alpha_k d_k$$

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

$$\beta_{k+1} = r_{k+1}^T r_{k+1} / r_k^T r_k$$

$$d_{k+1} = r_{k+1} + \beta_{k+1} d_k$$

CG Algorithm

x_0 given

$r_0 = b - Ax_0$

$d_0 = r_0$

while looping:

$$\alpha_k = \frac{r_k^T r_k}{d_k^T \boxed{A d_k}} \qquad q_k = A d_k$$

$$x_{k+1} = x_k + \alpha_k d_k$$

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

$$\beta_{k+1} = r_{k+1}^T r_{k+1} / r_k^T r_k$$

$$d_{k+1} = r_{k+1} + \beta_{k+1} d_k$$

Fantastic Properties:

- Search directions d_k's are <u>all</u> mutually A-orthogonal.
- Error $(x^* - x_k)$ minimizes A-norm among subspace of search directions
- Residuals r_k are all mutually perpendicular in traditional sense.

Consequence:

If A is $n \times n$,

residual $= 0$ after n

steps in exact arithmetic.

(r_{n+1} is $\perp$ to n mutually orthogonal vectors,

so is 0).