Residual + Stopping criteria

$$r = b - Ax \qquad e_k = x_k - x$$
$$r_k = b - Ax_k$$

$\|r_k\|$ small

When is that good enough?

We actually want $\|e_k\|$ small

$$\begin{aligned}\|r_k\| &= \|b - Ax_k\| \\ &= \|Ax - Ax_k\| \\ &= \|A(x - x_k)\| \\ &= \|Ae_k\| \le \|A\|\,\|e_k\|\end{aligned}$$

$$r_k = -Ae_k$$

$$\Rightarrow e_k = -A^{-1} r_k$$

$$\|e_k\| = \|A^{-1} r_k\| \le \|A^{-1}\|\,\|r_k\|$$

divide both sides by $\|x_k\|$

$$\frac{\|e_k\|}{\|x_k\|} \le \frac{\|A^{-1}\|\,\|r_k\|}{\|x_k\|}$$

multiply numerator + denominator on rhs by $\|A\|$

$$\frac{\|e_k\|}{\|x_k\|} \le \frac{\|A^{-1}\|\,\|A\|\,\|r_k\|}{\|x_k\|\,\|A\|} = \mathrm{cond}_2(A)\,\frac{\|r_k\|}{\|A\|\,\|x_k\|}$$

small relative residual and well-conditioned $A \Rightarrow$ $\boxed{\text{small relative error!}}$

Q What if relative residual is large?

Let E be s.t. $(A+E)x_k = b$

i.e., x_k is the exact soln to $(A+E)x = b$

$$\|r_k\| = \|b - Ax_k\| = \|Ex_k\| \le \|E\|\,\|x_k\|$$

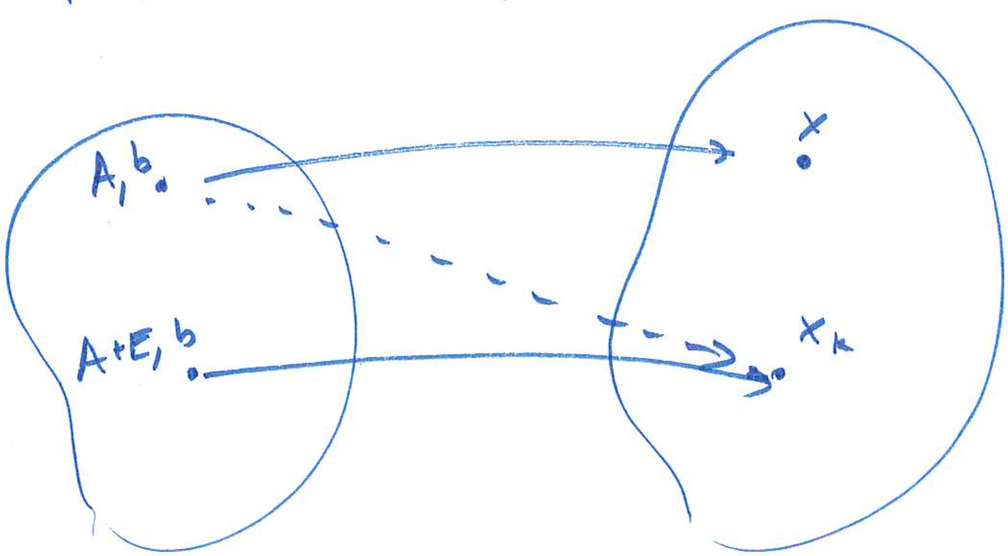
Divide both sides by $\|A\|\,\|x_k\|$:

$$\frac{\|r_k\|}{\|A\|\,\|x_k\|} \le \frac{\|E\|}{\|A\|}\,\frac{\cancel{\|x_k\|}}{\cancel{\|x_k\|}}$$

result:

$$\boxed{\frac{\|r_k\|}{\|A\|\,\|x_k\|} \le \frac{\|E\|}{\|A\|}}$$

large relative residual $\Rightarrow$ large backward error



Linear Systems by Arnoldi & GMRES

Solve $Ax = b$

GMRES = generalized minimal residuals

$$\mathcal{K}_r = \text{span}\{b, Ab, \dots, A^{r-1}b\}$$

Krylov subspace

main idea of GMRES:

at step k, choose $x_k \in \mathcal{K}_k$ that minimizes the norm of the residual $r_k = b - Ax_k$.

$$\underset{x \in \mathcal{K}_k}{\arg\min} \|b - Ax\|_2 = x_k$$

Arnoldi gives us an orthonormal basis for $\mathcal{K}_k$.

We can write the L.S. problem above as

$$y_k = \underset{y}{\arg\min} \|b - AQ_k y\|_2, \quad \text{where } x_k = Q_k y_k$$

Recall from Arnoldi,

$$AQ_k = Q_{k+1} H_{k+1,k}.$$

orthogonal: $Q = \left(Q_{k+1} \,\middle|\, \tilde{Q}_{k+1} \right)$

$$\Rightarrow \|b - AQ_k y\| = \|b - Q_{k+1} H_{k+1,k}\, y\|$$

$$= \|Q_{k+1}^T b - H_{k+1,k}\, y\| + \|\tilde{Q}_{k+1}^T b - \cancelto{0}{\tilde{Q}_{k+1}^T Q_{k+1} H_{k+1,k}\, y}\|$$

$$\| Q_{k+1}^T b - H_{k+1,k} y \|$$

Note $q_1 = \dfrac{b}{\|b\|}$ in Arnoldi. Then

$$Q_{k+1}^T b = \|b\| \vec{e}_1$$

So the least squares problem solved by GMRES is

$$\min_y \| \, \|b\| e_1 - H_{k+1,k} y \|_2$$

At each step k, solve for y. Set $x_k = Q_k y$.

<u>GMRES Algorithm</u> (high level)

$q_1 = b / \|b\|$

for $k = 1, 2, \ldots$

  do step k of Arnoldi

  $\rightsquigarrow \; A Q_k = Q_{k+1} H_{k+1,k}$

  find y that minimizes $\| \, \|b\| e_1 - H_{k+1,k} y \|_2$

  $x_k = Q_k y$

end

Linear Systems by Arnoldi and GMRES

Arnoldi gives an orthonormal basis for each Krylov subspace $\mathcal{K}_1, \mathcal{K}_2, \dots, \mathcal{K}_r$

GMRES: find a vector x_k in $\mathcal{K}_k$ that minimizes $\| b - Ax_k \|$

GMRES = Generalized Minimum RESidual

I.e. $\quad x_k = Q_k y_k$

$$
\begin{aligned}
\min \; & \| b - Ax_k \|_2^2 \\
&= \| b - AQ_k y_k \|_2^2 \\
&= \| Q_{k+1}^T b - Q_{k+1}^T A Q_k y_k \|_2^2 + \| \overset{0}{\cancel{\tilde{Q}_{k+1}^T b}} - \tilde{Q}_{k+1}^T A Q_k y_k \|_2^2 \\
&= \underbrace{\| \, \|b\| \vec{e}_1 - H_{k+1,k} y_k \|_2^2}_{\text{least squares problem}} + \| \overset{0}{\cancel{\underset{(n-k)\times n}{\tilde{Q}_{k+1}^T} \underset{n\times k+1}{Q_{k+1}}}} \underset{k+1\times k}{H_{k+1,k}} y_k \|_2^2
\end{aligned}
$$

The zeros below the first subdiagonal in $H_{k+1,k}$ make this fast.

<u>GMRES</u>:
- calculate q_{k+1} with Arnoldi
- find y_k which minimized $\| r_k \|_2$
- compute $x_k = Q_k y_k$
- stop if residual is small enough.

The L.S. problem can be solved by QR. It is only necessary to update the QR factorization in each iteration by 1 Given rotation (orthogonal matrix)

Conjugate Gradients (CG)

A $n \times n$

A symmetric positive definite

Since A is spd, it gives a norm

$\|\vec{x}\|_A = (\vec{x}^T A \vec{x})^{1/2}$ "A-norm"

CG has the following property:
In each iteration k, it finds $x_k \in \mathcal{K}_k$
that minimizes the A-norm of the
error e_k. I.e., $\|e_k\|_A = \min_{x_k \in \mathcal{K}_k}$

Solution x^* $\quad Ax^* = b$

$$\min_{x_k \in \mathcal{K}_k} (x^* - x_k)^T A (x^* - x_k)$$

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

$$\delta\phi = \frac{1}{2} \delta x^T A x + \frac{1}{2} x^T A \delta x - b^T \delta x$$

$$\nabla\phi = Ax - b$$

$$\begin{aligned}
\phi((x - x^*) + x^*) &= \frac{1}{2}(x - x^*)^T A (x - x^*) \\
&\quad + \frac{1}{2} x^{*T} A x^* + (x - x^*)^T A x^* \\
&\quad - b^T (x - x^*) - b^T x^* + c
\end{aligned}$$

$$\langle Ax^* = b \rangle \quad = \frac{1}{2} e^T A e + \frac{1}{2} b^T x^* + \cancel{e^T b} - \cancel{b^T e} - b^T x^* + c$$

$$\phi(x^* + e) = \frac{1}{2} e^T A e - \frac{1}{2} b^T x^* + c$$

$$= \frac{1}{2} e^T A e + \text{constant}$$

x_0 , $r_0 = b - Ax_0$, $s_0 = r_0$

for $k = 0, 1, 2, \ldots$

$\alpha_k = ?$

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

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

$s_{k+1} = ?$

end

C.G.

Step size α_k

$f(x_k + \alpha_k s_k)$ one-dim. minimization

$\phi(\alpha_k) = f(x_k + \alpha_k s_k)$

$$\frac{d\phi}{d\alpha}(\alpha_k) = \nabla f(x_k + \alpha_k s_k)^T s_k = 0$$

For C.G., $\nabla f(x) = b - Ax = r$

$$\Rightarrow \left(\frac{d\phi}{d\alpha}(\alpha_k) = 0\right) \Rightarrow$$

$$r_{k+1}^T s_k = \left[b - A(x_k + \alpha_k s_k)\right]^T s_k$$

$$= b^T s_k - x_k^T A^T s_k - \alpha_k s_k^T A^T s_k = 0$$

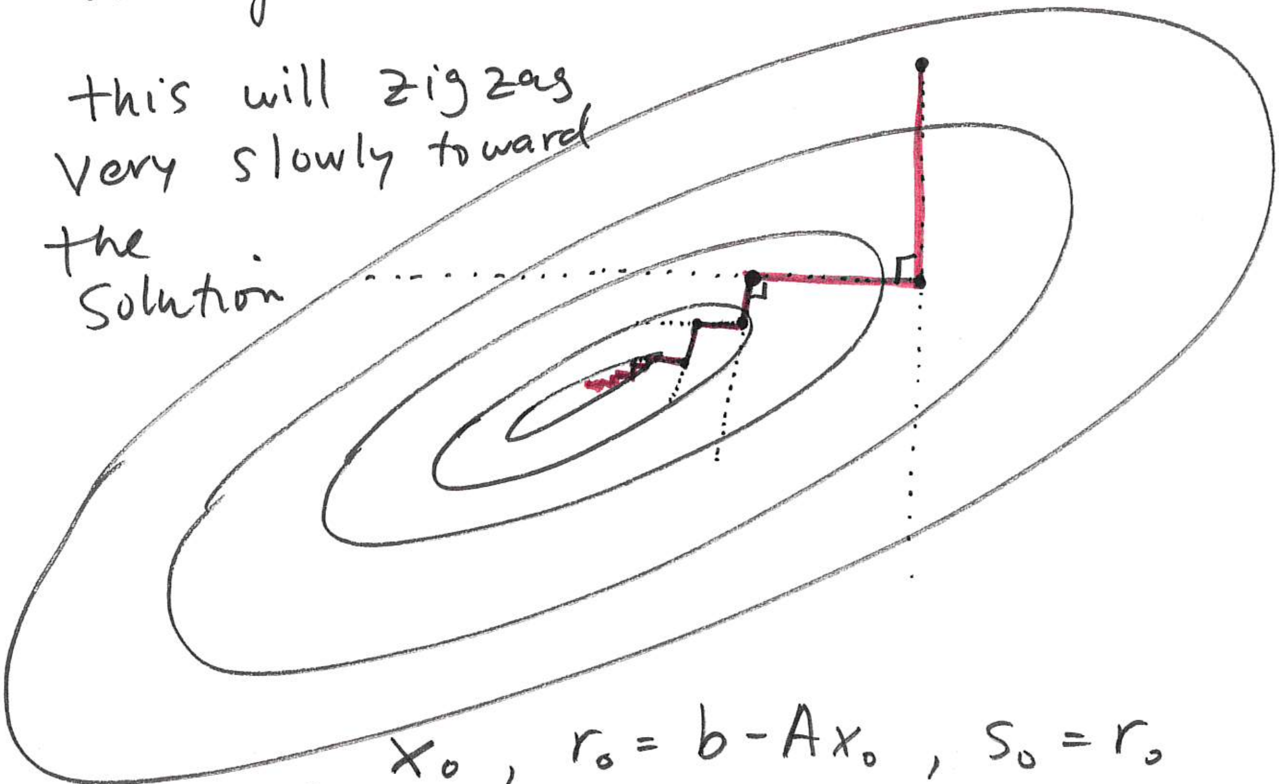
$$= (b - Ax_k)^T s_k - \alpha_k s_k^T A^T s_k = 0$$

$$\Rightarrow \boxed{\alpha_k = \frac{r_k^T s_k}{s_k^T A s_k}}$$

Steepest Descent Method

or gradient descent

this will zigzag very slowly toward the solution



$$x_0, \quad r_0 = b - Ax_0, \quad s_0 = r_0$$

for $k = 0, 1, 2, \ldots$

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

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

$$s_{k+1} = s_k - \alpha_k A s_k$$

end

Progress

$$\frac{\phi(x_k) - \phi(x^*)}{\phi(x_{k-1}) - \phi(x^*)} \le 1 - \frac{1}{\text{Cond } A}$$