Numerical Methods

assume A is SPD (symmetric positive definite)

Recall: we've been studying non-stationary methods for $A\underline{x} = \underline{b}$, of the form

$$\underline{x}^{k+1} = \underline{x}^k + \alpha_k \underline{p}^k, \quad k = 0, 1, \ldots$$

next guess; current guess; increment direction; (relative) step length

(then residual updates by $\underline{r}^{k+1} = \underline{r}^k - \alpha_k A \underline{p}^k$)

In the gradient method, $\underline{p}^k = \underline{r}^k \quad (= \underline{b} - A\underline{x}^k)$

Choosing α_k appropriately gave $\|\underline{e}^k\|_A \leq \left(\dfrac{K_2(A)-1}{K_2(A)+1}\right)^k \|\underline{e}^0\|_A$ $\quad K_2(A) = \dfrac{\lambda_{max}}{\lambda_{min}}$

Q: Can we improve on this using a different choice of $\underline{p}^k$?

In the gradient method, $\underline{p}^k$ and $\underline{p}^{k-1}$ are orthogonal w.r.t. Euclidean inner product:

$$\begin{aligned}
(\underline{p}^k, \underline{p}^{k-1}) = (\underline{r}^k, \underline{r}^{k-1}) &= (\underline{r}^{k-1} - \alpha_{k-1} A \underline{r}^{k-1}, \underline{r}^{k-1}) \\
&= (\underline{r}^{k-1}, \underline{r}^{k-1}) - \alpha_{k-1}(\underline{r}^{k-1}, A\underline{r}^{k-1}) \\
&= \|\underline{r}^{k-1}\|_2^2 - \alpha_{k-1}\|\underline{r}^{k-1}\|_A^2 \\
&= 0 \text{ by def'n of } \alpha_{k-1} = \frac{\|\underline{r}^{k-1}\|_2^2}{\|\underline{r}^{k-1}\|_A^2}.
\end{aligned}$$

In the conjugate gradient method we choose $\underline{p}^k$ to be orthogonal w.r.t. $(\cdot,\cdot)_A$. ("A-orthogonal" or "conjugate orthogonal")

in fact, $(\underline{p}^k, \underline{p}^j)_A = 0$ for all $j \in \{0, 1, \ldots, k-1\}$.

(recall: $(\underline{v}, \underline{w})_A = (\underline{v}, A\underline{w}) = \underline{v}^T A \underline{w}$)

We'll see this leads to faster convergence.

Conjugate gradient algorithm: (CG)

Given $\underline{x}^0$, set $\underline{r}^0 = \underline{b} - A\underline{x}^0$, and $\underline{p}^0 = \underline{r}^0$.

Then iterate until convergence (stopping criterion):

update current guess

- $\alpha_k = \dfrac{(\underline{r}^k, \underline{p}^k)}{\|\underline{p}^k\|_A^2}$ ← comes from minimising $\|\underline{e}^{k+1}\|_A$ as a function of α_k.
- $\underline{x}^{k+1} = \underline{x}^k + \alpha_k \underline{p}^k$

update residual

- $\underline{r}^{k+1} = \underline{r}^k - \alpha_k A \underline{p}^k$

update search direction

- $\beta_k = \dfrac{(\underline{r}^{k+1}, \underline{p}^k)_A}{\|\underline{p}^k\|_A^2}$ ← this A is missing in eqn (4.48) in notes. cf. Gram-Schmidt orthogonalisation
- $\underline{p}^{k+1} = \underline{r}^{k+1} - \beta_k \underline{p}^k$ projection of $\underline{r}^{k+1}$ onto $\underline{p}^k$ w.r.t. $(\cdot,\cdot)_A$

Properties:

- $(\underline{p}^k, \underline{p}^j)_A = 0, \quad 0 \leq j < k$
- $(\underline{r}^k, \underline{r}^j) = 0, \quad 0 \leq j < k$.

Theorem (proof not supplied – see e.g. Quarteroni (4.47))

Let A be SPD. Then the error $\underline{e}^k = \underline{x} - \underline{x}^k$ after k steps of CG satisfies

$$\|\underline{e}^k\|_A \leq 2\left(\frac{\sqrt{K_2(A)} - 1}{\sqrt{K_2(A)} + 1}\right)^k \|\underline{e}^0\|_A, \quad k = 0, 1, \ldots$$

Comparing this to the gradient method, for which $\|\underline{e}^k\|_A \leq \left(\frac{K_2(A) - 1}{K_2(A) + 1}\right)^k \|\underline{e}^0\|_A$, we see that CG beats gradient once k is sufficiently large, ← to deal with the factor of 2.

since $\dfrac{\sqrt{t} - 1}{\sqrt{t} + 1} = 1 - \dfrac{2}{\sqrt{t} + 1} < 1 - \dfrac{2}{t+1} = \dfrac{t-1}{t+1}$ for $t > 1$.

(recall: $K_2(A) \geq 1$)

Interestingly, the orthogonality property means that CG reaches the exact solution $\underline{x}$ after at most n iterations!

(But when n is large we rarely see this happen since we want to stop well before $k \simeq n$.)

Stopping criteria

When to stop iteration? Ideally, when $\dfrac{\|\underline{x}^k - \underline{x}\|}{\|\underline{x}\|} \leq tol$

problem is we can't compute this!

user-specified tolerance.

As for nonlinear eqns, we have different options:

- Use an a priori bound, if we can estimate $K_2(A)$, $\|\underline{e}^0\|_A$ etc.
- Use a residual-based criterion, stopping when

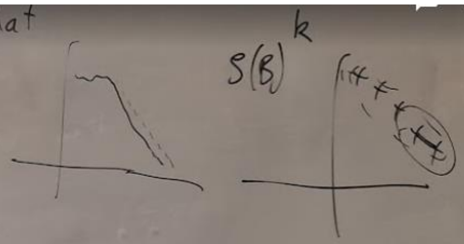
$$\frac{\|\underline{r}^k\|}{\|\underline{b}\|} = \frac{\|\underline{b} - A\underline{x}^k\|}{\|\underline{b}\|} \leq \widetilde{tol}$$

- Use an increment-based criterion, stopping when

$$\|\underline{x}^{k+1} - \underline{x}^k\| \leq \widetilde{\widetilde{tol}}.$$

Recall from section on condition numbers that

$$\underbrace{\frac{1}{K(A)} \frac{\|\underline{r}^k\|}{\|\underline{b}\|}}_{\text{rel. residual}} \leq \underbrace{\frac{\|\underline{x}^k - \underline{x}\|}{\|\underline{x}\|}}_{\text{rel. error}} \leq K(A) \underbrace{\frac{\|\underline{r}^k\|}{\|\underline{b}\|}}_{\text{rel. residual}}$$



So if $K(A) \approx 1$ a residual-based criterion works well.

But not if $K(A) \gg 1$.

Similar observations can be made about increment-based criteria - see notes.

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix}, \quad \underline{b} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \underline{x} = \begin{pmatrix} 3/5 \\ -1/5 \end{pmatrix}$$

$\underline{x}^{k+1} = B\underline{x}^k + \underline{c}$, convergence iff $\rho(B) < 1$.

$P\underline{x}^{k+1} = \ldots$

A\b produces the solution of $A\underline{x} = b$ via a direct method (LU factorisation?)

$Ax = b$ $x = A\backslash b$ "norm(x)" calculates $\|x\|_2$ by default.