What is NA?

Last week: Solve $A\vec{c} = F$, $A > 0$, symmetric.

$$\Updownarrow$$

$$\min E(\vec{c}) = \frac{1}{2}\vec{c}^T A \vec{c} - F^T \vec{c}$$

Gradient method:
- Start with $\vec{c}_0 \in \mathbb{R}^N$
- Find min of E on line $\{\vec{c}_0 + \alpha \nabla_c E(c_0) : \alpha \in \mathbb{R}\}$
- Choose as $\vec{c}_1$
- Repeat.

Issue: **Thm:** $\|\vec{c}_k - \vec{c}_0\|_A \le \left(\frac{K-1}{K+1}\right)^k \|\vec{c}_0 - \vec{c}\|_A$

, where $K = \dfrac{\lambda_{max}(A)}{\lambda_{min}(A)}$.

So as $K \to \infty$, $\dfrac{K-1}{K+1} \to 1$ $\rightsquigarrow$ Slow convergence.

Key Idea: Choose orthogonal directions for minimisation s.t. a method will converge in N steps.

Conjugate Gradient Method: Given A-orthogonal directions $d_0, \dots, d_{N-1}$ (which form a basis); For exact soln:

$$d_\ell^T A c = d_\ell^T \sum_{k=0}^{N-1} \alpha_k A d_k = \alpha_\ell d_\ell^T A d_\ell \Rightarrow c = \sum \alpha_\ell d_\ell$$

with $\alpha_\ell = \dfrac{d_\ell^T A c}{d_\ell^T A d_\ell} = \dfrac{d_\ell^T F}{d_\ell^T A d_\ell}$.

(Δ) Challenge: Find the orthogonal basis $\{d_0, \dots, d_{N-1}\}$.

Lemma: The sequence $x_{k+1} = x_k + \alpha_k d_k$ with $\alpha_k = -\dfrac{d_k^T (A x_k - F)}{d_k^T A d_k}$ gives the solution x after N steps. (For any $x_0 \in \mathbb{R}^N$.)

$\nwarrow$ $Ax = F$

Proof:

$$c - c_0 = \sum_i \alpha_i d_i \quad \text{where } \alpha_k = \frac{d_k^T A (c - c_0)}{d_k^T A d_k}$$

$$= -\frac{d_k^T (A c_0 - F)}{d_k^T A d_k}$$

Note that $d_k^T A (c_k - c_0) = 0$ as $c_k = \sum_{j=0}^{k-1} \beta_j d_j + c_0$ and d_k is orthogonal to $\{d_0, \dots, d_{k-1}\}$.

Thus, $\alpha_k = -\dfrac{d_k^T (A c_k - F)}{d_k^T A d_k}$. //

Lemma: c_k minimizes $E(c) = \frac{1}{2} c^T A c - F^T c$, not only on the line $\{c_{k-1} + \alpha d_{k-1} : \alpha \in \mathbb{R}\}$, but over the subspace $\{c_0 + \sum_{j=0}^{k-1} \alpha_j d_j : \alpha_j \in \mathbb{R}, \forall j\}$.

In particular $d_i^T (A c_k - F) = 0 \quad \forall i < k$. (*)

Proof of (*): By algorithm:

$$c_{k+1} = c_k + \alpha_k d_k \quad ; \quad \alpha_k = -\frac{d_k^T (Ac_k - F)}{d_k^T A d_k}.$$

With this choice of d_k: $d_k^T (Ac_{k+1} - F) = 0$, $\forall k$.

$\rightsquigarrow$ (*) holds for $k=0$. Induction. $\square$

If we know A-orthogonal directions $\{d_0, \dots, d_{N-1}\}$, then method converges in N steps.

Back to (Δ):

Conj. grad. algo.: • Let $c_0 \in \mathbb{R}^N$. Set $d_0 = F - Ac_0$
$= -g_0$

• For $k = 0, 1, \dots$

• Compute: $\alpha_k = \dfrac{g_k^T g_k}{d_k^T A d_k}$

$$c_{k+1} = c_k + \alpha_k d_k$$

$$g_{k+1} = g_k + \alpha_k A d_k$$

$$\beta_k = \frac{g_{k+1}^T g_{k+1}}{g_k^T g_k}$$

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

Lemma: d_k's are A-orthogonal.

Corrolary: Method terminates after N steps.

Thm: $\|c_k - c\|_A \le \cancel{\frac{\sqrt{\kappa-1}}{\sqrt{\kappa+1}}}\; 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^k \|c_0 - c\|_A$

where $\kappa = \frac{\lambda_{max}}{\lambda_{min}}$.

Related methods

Minimize error in $\|c_k - c\|_{A^\mu}$; $\mu \ge 1$

Eg.:
$$
\begin{aligned}
\|c_k - c\|_{A^2}^2 &= (c_k - c)^T A^2 (c_k - c) \\
&= (A(c_k - c))^T (A(c_k - c)) \\
&= \|Ac_k - F\|_{\mathbb{R}^N}^2 \qquad \text{(least squares)} \\
&= c_k^T A^2 c - 2F^T A c_k + \text{const.}
\end{aligned}
$$

minimises the above energy. MINRES.

Variations of CG also for nonsymmetric A : BICGSTAB.

Outlook:
- Time dependent problems.
- Time stepping methods:
  - convergence
  - (in-) stability.
- Linearized Navier-Stokes (Stokes problem).