Numerical Linear Algebra: iterative methods

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Two different approaches

Solve $Ax = b$

Direct methods:

- Deterministic
- Exact up to machine precision
- Expensive (in time and space)

Iterative methods:

- Only approximate
- Cheaper in space and (possibly) time
- Convergence not guaranteed

Iterative methods

Choose any x_0 and repeat

$$x^{k+1} = Bx^k + c$$

until $\|x^{k+1} - x^k\|_2 < \epsilon$ or until $\frac{\|x^{k+1}-x^k\|_2}{\|x^k\|} < \epsilon$

Example of iterative solution

Example system

$$\begin{pmatrix} 10 & 0 & 1 \\ 1/2 & 7 & 1 \\ 1 & 0 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 21 \\ 9 \\ 8 \end{pmatrix}$$

with solution $(2, 1, 1)$.

Suppose you know (physics) that solution components are roughly the same size, and observe the dominant size of the diagonal, then

$$\begin{pmatrix} 10 & & \\ & 7 & \\ & & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 21 \\ 9 \\ 8 \end{pmatrix}$$

might be a good approximation: solution $(2.1, 9/7, 8/6)$.

Iterative example′

Example system

$$\begin{pmatrix} 10 & 0 & 1 \\ 1/2 & 7 & 1 \\ 1 & 0 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 21 \\ 9 \\ 8 \end{pmatrix}$$

with solution $(2, 1, 1)$.

Also easy to solve:

$$\begin{pmatrix} 10 & & \\ 1/2 & 7 & \\ 1 & 0 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 21 \\ 9 \\ 8 \end{pmatrix}$$

with solution $(2.1, 7.95/7, 5.9/6)$.

Iterative example''

Instead of solving $Ax = b$ we solved $L\tilde{x} = b$. Look for the missing part: $\tilde{x} = x + \Delta x$, then $A\Delta x = A\tilde{x} - b \equiv r$. Solve again $L\widetilde{\Delta x} = r$ and update $\tilde{\tilde{x}} = \tilde{x} - \widetilde{\Delta x}$.

iteration	1	2	3
x_1	2.1000	2.0017	2.000028
x_2	1.1357	1.0023	1.000038
x_3	0.9833	0.9997	0.999995

Two decimals per iteration. *This is not typical*

Exact system solving: $O(n^3)$ cost; iteration: $O(n^2)$ per iteration. Potentially cheaper if the number of iterations is low.

Abstract presentation

- To solve $Ax = b$; too expensive; suppose $K \approx A$ and solving $Kx = b$ is possible
- Define $Kx_0 = b$, then error correction $x_0 = x + e_0$, and $A(x_0 - e_0) = b$
- so $Ae_0 = Ax_0 - b = r_0$; this is again unsolvable, so
- $K\tilde{e}_0$ and $x_1 = x_0 - \tilde{e}_0$.
- now iterate: $e_1 = x_1 - x$, $Ae_1 = Ax_1 - b = r_1$ et cetera

Error analysis

- One step

$$\begin{aligned} r_1 &= Ax_1 - b = A(x_0 - \tilde{e}_0) - b && (1) \\ &= r_0 - AK^{-1}r_0 && (2) \\ &= (I - AK^{-1})r_0 && (3) \end{aligned}$$

- Inductively: $r_n = (I - AK^{-1})^n r_0$ so $r_n \downarrow 0$ if $|\lambda(I - AK^{-1})| < 1$
  Geometric reduction (or amplification!)
- This is 'stationary iteration': every iteration step the same.
  Simple analysis, limited applicability.

Computationally

If

$$A = K - N$$

then

$$Ax = b \Rightarrow Kx = Nx + b \Rightarrow Kx_{i+1} = Nx_i + b$$

Equivalent to the above, and you don't actually need to form the residual.

Choice of K

- The closer K is to A, the faster convergence.
- Diagonal and lower triangular choice mentioned above: let

$$A = D_A + L_A + U_A$$

  be a splitting into diagonal, lower triangular, upper triangular part, then
- Jacobi method: $K = D_A$ (diagonal part),
- Gauss-Seidel method: $K = D_A + L_A$ (lower triangle, including diagonal)
- SOR method: $K = \omega D_A + L_A$

Jacobi

$$K = D_A$$

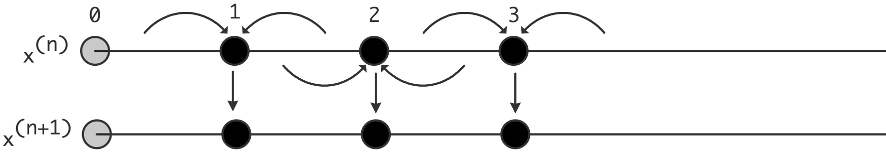
Algorithm:

$$\begin{array}{l} \textit{for } k = 1, \ldots \textit{ until convergence, do:} \\ \quad \textit{for } i = 1 \ldots n\textit{:} \\ \qquad // a_{ii} x_i^{(k+1)} = \sum_{j \neq i} a_{ij} x_j^{(k)} + b_i \Rightarrow \\ \qquad x_i^{(k+1)} = a_{ii}^{-1} (\sum_{j \neq i} a_{ij} x_j^{(k)} + b_i) \end{array}$$

Implementation:

$$\begin{array}{l} \textit{for } k = 1, \ldots \textit{ until convergence, do:} \\ \quad \textit{for } i = 1 \ldots n\textit{:} \\ \qquad t_i = a_{ii}^{-1} (-\sum_{j \neq i} a_{ij} x_j + b_i) \\ \quad \textit{copy } x \leftarrow t \end{array}$$

Jacobi in pictures:



Gauss-Seidel

$$K = D_A + L_A$$

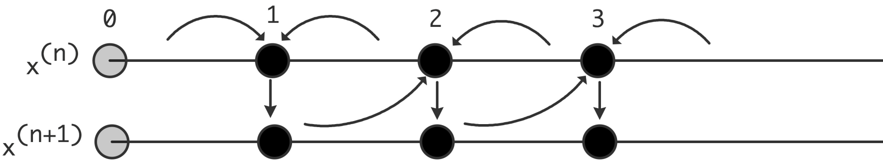
Algorithm:

$$\begin{array}{l} \textit{for } k = 1, \ldots \textit{ until convergence, do:} \\ \quad \textit{for } i = 1 \ldots n\textit{:} \\ \qquad // a_{ii} x_i^{(k+1)} + \sum_{j<i} a_{ij} x_j^{(k+1)}) = \sum_{j>i} a_{ij} x_j^{(k)} + b_i \Rightarrow \\ \qquad x_i^{(k+1)} = a_{ii}^{-1}(-\sum_{j<i} a_{ij} x_j^{(k+1)}) - \sum_{j>i} a_{ij} x_j^{(k)} + b_i) \end{array}$$

Implementation:

$$\begin{array}{l} \textit{for } k = 1, \ldots \textit{ until convergence, do:} \\ \quad \textit{for } i = 1 \ldots n\textit{:} \\ \qquad x_i = a_{ii}^{-1}(-\sum_{j \neq i} a_{ij} x_j + b_i) \end{array}$$

GS in pictures:



Choice of K through incomplete LU

- Inspiration from direct methods: let $K = LU \approx A$

Gauss elimination:

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for k,i,j:
   a[i,j] = a[i,j] - a[i,k] * a[k,j] / a[k,k]
```

Incomplete variant:

```
for k,i,j:
  if a[i,j] not zero:
    a[i,j] = a[i,j] - a[i,k] * a[k,j] / a[k,k]
```

$\Rightarrow$ sparsity of $L + U$ the same as of A

Stopping tests

When to stop converging? Can size of the error be guaranteed?

- Direct tests on error $e_n = x - x_n$ impossible; two choices
- Relative change in the computed solution small:

$$\|x_{n+1} - x_n\| / \|x_n\| < \epsilon$$

- Residual small enough:

$$\|r_n\| = \|Ax_n - b\| < \epsilon$$

Without proof: both imply that the error is less than some other ϵ'.

General form of iterative methods 1.

System $Ax = b$ has the same solution as $K^{-1}Ax = K^{-1}b$.

Let $\tilde{x}$ be a guess and

$$\tilde{r} = K^{-1}A\tilde{x} - K^{-1}b.$$

then

$$x = A^{-1}b = \tilde{x} - A^{-1}K\tilde{r} = \tilde{x} - (K^{-1}A)^{-1}\tilde{r}.$$

A little linear algebra

Cayley-Hamilton theorem:

$$A \text{ nonsingular} \Rightarrow \exists_\phi\colon \phi(A) = 0.$$

Write

$$\phi(x) = 1 + x\pi(x),$$

Apply this to $K^{-1}A$:

$$0 = \phi(K^{-1}A) = I + K^{-1}A\pi(K^{-1}A) \Rightarrow (K^{-1}A)^{-1} = -\pi(K^{-1}A)$$

General form of iterative methods 2.

Recall

$$x = \tilde{x} - (K^{-1}A)^{-1}\tilde{r}.$$

Define iterates x_i and residuals $r_i = Ax_i - b$, then $\tilde{r} = K^{-1}r_0$.

Use Cayley-Hamilton:

$$x = x_0 - \pi(K^{-1}A)K^{-1}r_0 = x_0 - K^{-1}\pi(AK^{-1})r_0.$$

so that $x = \tilde{x} + \pi(K^{-1}A)\tilde{r}$. Now, if we let $x_0 = \tilde{x}$, then $\tilde{r} = K^{-1}r_0$, giving the equation

$$x = x_0 + \pi(K^{-1}A)K^{-1}r_0 = x_0 + K^{-1}\pi(AK^{-1})r_0.$$

Iterative scheme:

$$x_{i+1} = x_0 + K^{-1}\pi^{(i)}(AK^{-1})r_0 \qquad (4)$$

Residuals

$$x_{i+1} = x_0 + K^{-1}\pi^{(i)}(AK^{-1})r_0$$

Multiply by A and subtract b:

$$r_{i+1} = r_0 + \tilde{\pi}^{(i)}(AK^{-1})r_0$$

So:

$$r_i = \hat{\pi}^{(i)}(AK^{-1})r_0$$

where $\hat{\pi}^{(i)}$ is a polynomial of degree i with $\hat{\pi}^{(i)}(0) = 1$.

$\Rightarrow$ convergence theory

Juggling polynomials

For $i = 1$:

$$r_1 = (\alpha_1 AK^{-1} + \alpha_2 I)r_0 \Rightarrow AK^{-1}r_0 = \beta_1 r_1 + \beta_0 r_0$$

for some values α_i, β_i.

For $i = 2$

$$r_2 = (\alpha_2 (AK^{-1})^2 + \alpha_1 AK^{-1} + \alpha_0)r_0$$

for different values α_i.

Together:

$$(AK^{-1})^2 r_0 \in [\![r_2, r_1, r_0]\!],$$

and inductively

$$(AK^{-1})^i r_0 \in [\![r_i, \ldots, r_0]\!]. \tag{5}$$

General form of iterative methods 3.

$$x_{i+1} = x_0 + \sum_{j\leq i} K^{-1} r_j \alpha_{ji}.$$

or equivalently:

$$x_{i+1} = x_i + \sum_{j\leq i} K^{-1} r_j \alpha_{ji}.$$

More residual identities

$$x_{i+1} = x_i + \sum_{j\leq i} K^{-1} r_j \alpha_{ji}.$$

gives

$$r_{i+1} = r_i + \sum_{j\leq i} AK^{-1} r_j \alpha_{ji}.$$

Specifically

$$r_1 = r_0 + AK^{-1} r_0 \alpha_{00}.$$

so $AK^{-1}r_0 = \alpha_{00}^{-1}(r_1 - r_0)$.

Next:

$$\begin{aligned} r_2 &= r_1 + AK^{-1}r_1\alpha_{11} + AK^{-1}r_0\alpha_{01} \\ &= r_1 + AK^{-1}r_1\alpha_{11} + \alpha_{00}^{-1}\alpha_{01}(r_1 - r_0) \\ \Rightarrow AK^{-1}r_1 &= \alpha_{11}^{-1}(r_2 - (1 + \alpha_{00}^{-1}\alpha_{01})r_1 + \alpha_{00}^{-1}\alpha_{01}r_0) \end{aligned}$$

so $AK^{-1}r_1 = r_2\beta_2 + r_1\beta_1 + r_0\beta_0$, and that $\sum_i \beta_i = 0$.

Inductively:

$$
\begin{array}{rll}
r_{i+1} & = r_i + AK^{-1} r_i \delta_i + \sum_{j\leq i+1} r_j \alpha_{ji} & \\
r_{i+1}(1-\alpha_{i+1,i}) & = AK^{-1} r_i \delta_i + r_i(1+\alpha_{ii}) + \sum_{j<i} r_j \alpha_{ji} & \\
r_{i+1}\alpha_{i+1,i} & = AK^{-1} r_i \delta_i + \sum_{j\leq i} r_j \alpha_{ji} & \text{substituting } \begin{array}{l}\alpha_{ii} := 1+\alpha_{ii} \\ \alpha_{i+1,i} := 1-\alpha_{i+}\end{array} \\
& & \text{note that } \alpha_{i+1,i} = \sum_{j\leq i} \alpha_{ji} \\
r_{i+1}\alpha_{i+1,i}\delta_i^{-1} & = AK^{-1} r_i + \sum_{j\leq i} r_j \alpha_{ji} \delta_i^{-1} & \\
r_{i+1}\alpha_{i+1,i}\delta_i^{-1} & = AK^{-1} r_i + \sum_{j\leq i} r_j \alpha_{ji} \delta_i^{-1} & \\
r_{i+1}\gamma_{i+1,i} & AK^{-1} r_i + \sum_{j\leq i} r_j \gamma_{ji} & \text{substituting } \gamma_{ij} = \alpha_{ij}\delta_j^{-1}
\end{array}
$$

and we have that $\gamma_{i+1,i} = \sum_{j\leq i} \gamma_{ji}$.

General form of iterative methods 4.

$$r_{i+1}\gamma_{i+1,i} = AK^{-1}r_i + \sum_{j\leq i} r_j\gamma_{ji}$$

and $\gamma_{i+1,i} = \sum_{j\leq i}\gamma_{ji}$.

Write this as $AK^{-1}R = RH$ where

$$H = \begin{pmatrix} -\gamma_{11} & -\gamma_{12} & \ldots \\ \gamma_{21} & -\gamma_{22} & -\gamma_{23} & \ldots \\ 0 & \gamma_{32} & -\gamma_{33} & -\gamma_{34} \\ \emptyset & \ddots & \ddots & \ddots & \ddots \end{pmatrix}$$

H is a Hessenberg matrix, and note zero column sums.

Divide A out:

$$x_{i+1}\gamma_{i+1,i} = K^{-1}r_i + \sum_{j\leq i} x_j\gamma_{ji}$$

General form of iterative methods 5.

$$\begin{cases} r_i = Ax_i - b \\ x_{i+1}\gamma_{i+1,i} = K^{-1}r_i + \sum_{j\leq i} x_j\gamma_{ji} \\ r_{i+1}\gamma_{i+1,i} = AK^{-1}r_i + \sum_{j\leq i} r_j\gamma_{ji} \end{cases}$$

where $\gamma_{i+1,i} = \sum_{j\leq i} \gamma_{ji}$.

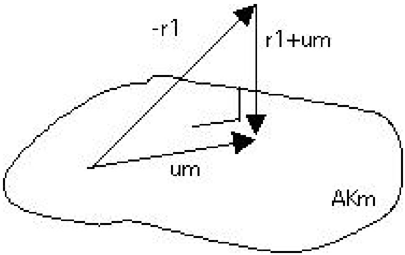
Orthogonality

Idea one:

> *If you can make all your residuals orthogonal to each other, and the matrix is of dimension n, then after n iterations you have to have converged: it is not possible to have an $n + 1$-st residuals that is orthogonal and nonzero.*

Idea two:

> *The sequence of residuals spans a series of subspaces of increasing dimension, and by orthogonalizing the initial residual is projected on these spaces. This means that the errors will have decreasing sizes.*


-r1
r1+um
um
AKm

Full Orthogonalization Method

Let r_0 *be given*
For $i \geq 0$*:*
  let $s \leftarrow K^{-1}r_i$
  let $t \leftarrow AK^{-1}r_i$
  for $j \leq i$*:*
    let γ_j *be the coefficient so that* $t - \gamma_j r_j \perp r_j$
  for $j \leq i$*:*
    form $s \leftarrow s - \gamma_j x_j$
    and $t \leftarrow t - \gamma_j r_j$
  let $x_{i+1} = (\sum_j \gamma_j)^{-1}s$, $r_{i+1} = (\sum_j \gamma_j)^{-1}t$.

Modified Gramm-Schmidt

Let r_0 *be given*
For $i \geq 0$*:*
  let $s \leftarrow K^{-1}r_i$
  let $t \leftarrow AK^{-1}r_i$
  for $j \leq i$*:*
    let γ_j *be the coefficient so that* $t - \gamma_j r_j \perp r_j$
    form $s \leftarrow s - \gamma_j x_j$
    and $t \leftarrow t - \gamma_j r_j$
  let $x_{i+1} = (\sum_j \gamma_j)^{-1}s$, $r_{i+1} = (\sum_j \gamma_j)^{-1}t$.

Practical differences

- Modfied GS more stable
- Inner products are global operations: costly

Coupled recurrences form

$$x_{i+1} = x_i - \sum_{j \le i} \alpha_{ji} K^{-1} r_j \tag{6}$$

This equation is often split as

- Update iterate with search direction: direction:

$$x_{i+1} = x_i - \delta_i p_i,$$

- Construct search direction from residuals:

$$p_i = K^{-1} r_i + \sum_{j<i} \beta_{ij} K^{-1} r_j.$$

Inductively:

$$p_i = K^{-1} r_i + \sum_{j<i} \gamma_{ij} p_j,$$

Conjugate Gradients

Basic idea:

$$r_i^t K^{-1} r_j = 0 \quad \text{if } i \neq j.$$

Split recurrences:

$$\begin{cases} x_{i+1} = x_i - \delta_i p_i \\ r_{i+1} = r_i - \delta_i A p_i \\ p_i = K^{-1} r_i + \sum_{j<i} \gamma_{ij} p_j, \end{cases}$$

Symmetric Positive Definite case

Three term recurrence is enough:

$$\begin{cases} x_{i+1} = x_i - \delta_i p_i \\ r_{i+1} = r_i - \delta_i A p_i \\ p_{i+1} = K^{-1} r_{i+1} + \gamma_i p_i \end{cases}$$

Preconditioned Conjugate Gradietns

Compute $r^{(0)} = b - Ax^{(0)}$ for some initial guess $x^{(0)}$
for $i = 1, 2, \ldots$
  solve $Mz^{(i-1)} = r^{(i-1)}$
  $\rho_{i-1} = {r^{(i-1)}}^T z^{(i-1)}$
  if $i = 1$
    $p^{(1)} = z^{(0)}$
  else
    $\beta_{i-1} = \rho_{i-1}/\rho_{i-2}$
    $p^{(i)} = z^{(i-1)} + \beta_{i-1} p^{(i-1)}$
  endif
  $q^{(i)} = Ap^{(i)}$
  $\alpha_i = \rho_{i-1}/{p^{(i)}}^T q^{(i)}$
  $x^{(i)} = x^{(i-1)} + \alpha_i p^{(i)}$
  $r^{(i)} = r^{(i-1)} - \alpha_i q^{(i)}$
  check convergence; continue if necessary
end

Observations on iterative methods

- Conjugate gradients: constant storage and inner products; works only for symmetric systems
- GMRES (like FOM): growing storage and inner products: restarting and numerical cleverness
- BiCGstab and QMR: relax the orthogonality

CG derived from minimization

Special case of SPD:

For which vector x with $\|x\| = 1$ is $f(x) = 1/2x^tAx - b^tx$ minimal? (7)

Taking derivative:

$$f'(x) = Ax - b.$$

Update

$$x_{i+1} = x_i + p_i\delta_i$$

optimal value:

$$\delta_i = \operatorname*{argmin}_\delta \|f(x_i + p_i\delta)\| = \frac{r_i^tp_i}{p_1^tAp_i}$$

Other constants follow from orthogonality.