Iterative Linear Algebra Methods

The following are outlines of the best-known iterative methods for approximately solving $Ax = b$, where $A \in I\!R^{n\times n}$, $x \in I\!R^n$, and $b \in I\!R^n$.

1. The classical iterative methods: Jacobi, Gauss–Seidel, and SOR.

Notation: In describing the matrix-vector forms of the classical iterative methods, we use the decomposition $A = L + D + U$, in which L, D, and U are the strict lower-triangular, diagonal, and strict upper-triangular parts of A, respectively. In describing the componentwise forms, we denote the ith components of x and b and the ijth entry of A by x_i, b_i, and A_{ij}, respectively.

<u>Jacobi Iteration:</u> (matrix-vector form)

Given A, b, and initial x.

Until "stop":

Update $x \leftarrow D^{-1}\big[b - (L + U)x\big]$.

<u>Jacobi Iteration:</u> (componentwise form)

Given A, b, and initial x.

Until "stop":

For $i = 1, \ldots, n$:

Set $x_i^+ = \big(b_i - \sum_{j\neq i} A_{ij}x_j\big)/A_{ii}$.

Update $x \leftarrow x^+$.

Gauss–Seidel Iteration: (matrix-vector form)

Given A, b, and initial x.

Until "stop":

Update $x \leftarrow (L+D)^{-1}(b - Ux)$.

Gauss–Seidel Iteration: (componentwise form)

Given A, b, and initial x.

Until "stop":

For $i = 1, \ldots, n$:

Update $x_i \leftarrow \big(b_i - \sum_{j \neq i} A_{ij} x_j\big)/A_{ii}$.

Successive Overrelaxation (SOR): (matrix-vector form)

Given A, b, initial x, and ω.

Until "stop":

Update $x \leftarrow (\omega L + D)^{-1}\big\{\omega b + \big[(1-\omega)D - \omega U\big]x\big\}$.

Successive Overrelaxation (SOR): (componentwise form)

Given A, b, initial x, and ω.

Until "stop":

For $i = 1, \ldots, n$:

Update $x_i \leftarrow (1-\omega)x_i + \omega\big(b_i - \sum_{j \neq i} A_{ij} x_j\big)/A_{ii}$.

2. Krylov subspace methods: GMRES(m), CG, and PCG.

Notation: In GMRES(m), $e_1 = (1, 0, \ldots, 0)^T \in I\!R^{m+1}$ and w_{k+1} is the $(k+1)$st component of the vector $w \in I\!R^{m+1}$. Generally, subscripted quantities may denote scalars, vectors, or matrices, depending on the context.

$\underline{\text{GMRES}(m)\text{:}}$ (standard Gram–Schmidt implementation)

Given A, b, x, tol, itmax.

INITIALIZE: Set $r \equiv b - Ax$, $v_1 \equiv r/\|r\|_2$, $w \equiv \|r\|_2 e_1 \in I\!R^{m+1}$.

ITERATE: For $k = 1, \ldots, m$, do:

Initialize $v_{k+1} = Av_k$.

For $i = 1, \ldots, k$, do:

Set $h_{ik} = v_i^T v_{k+1}$.

Update $v_{k+1} \leftarrow v_{k+1} - h_{ik} v_i$.

Set $h_{k+1,k} = \|v_{k+1}\|_2$.

If $k > 1$, apply $J_{k-1} \cdots J_1$ to $(h_{1,k}, \ldots, h_{k,k}, h_{k+1,k}, 0, \ldots)^T \in I\!R^{m+1}$.

Determine a Givens rotation J_k such that

$$J_k \cdots J_1 \begin{pmatrix} h_{1,k} \\ \vdots \\ h_{k,k} \\ h_{k+1,k} \\ 0 \\ \vdots \end{pmatrix} \equiv \begin{pmatrix} r_{1,k} \\ \vdots \\ r_{k,k} \\ 0 \\ 0 \\ \vdots \end{pmatrix}.$$

If $k = 1$, form $R_1 \equiv (r_{11})$; else form $R_k \equiv \begin{pmatrix} R_{k-1} & \begin{matrix} r_{1,k} \\ \vdots \end{matrix} \\ 0 \cdots 0 & r_{k,k} \end{pmatrix}$.

Update $w \leftarrow J_k w$. If $|w_{k+1}| \le tol$ or $k = m$, go to SOLVE; else update $v_{k+1} \leftarrow v_{k+1}/h_{k+1,k}$.

SOLVE: Let k be the final iteration number from ITERATE.

Solve $R_k y = \bar{w}$ for y, where $\bar{w} \equiv (w_1, \ldots, w_k)^T$.

Update $x \leftarrow x + (v_1, \ldots, v_k)y$.

If $|w_{k+1}| \le tol$, accept x and stop; otherwise, return to INITIALIZE.

Conjugate Gradient Method (CG):

Given A, b, x, and tol.

Set $r = b - Ax$, $\rho^2 = \|r\|_2^2$, $z = 0$, $\beta = 0$.

Until "stop":

If $\rho \le tol$, update $x \longleftarrow x + z$ and stop.

Update $p \longleftarrow r + \beta p$.

Compute Ap.

Compute $p^T Ap$ and $\alpha = \rho^2 / p^T Ap$.

Update $z \longleftarrow z + \alpha p$ and $r \longleftarrow r - \alpha Ap$.

Update $\beta \longleftarrow \|r\|_2^2 / \rho^2$ and $\rho^2 \longleftarrow \|r\|_2^2$.

Preconditioned Conjugate Gradient Method (PCG):

Given A, b, x, tol, and a symmetric positive-definite preconditioner M.

Set $r = b - Ax$, $r = b - Ax$, $w = M^{-1}r$, $\rho^2 = r^T w$, $z = 0$, $\beta = 0$.

Until "stop":

If $\rho \le tol$, update $x \longleftarrow x + z$ and stop.

Update $p \longleftarrow w + \beta p$.

Compute Ap.

Compute $p^T Ap$ and $\alpha = \rho^2 / p^T Ap$.

Update $z \longleftarrow z + \alpha p$ and $r \longleftarrow r - \alpha Ap$.

Update $w = M^{-1}r$, $\beta = r^T w / \rho^2$, and $\rho^2 = r^T w$.