Why Iterative Methods?

Solving large problems using Gaussian elimination can be very expensive. Many large problems (e.g. simulations of fluid flow in the environment or industry) result in systems of hundreds or thousands or millions of equations:

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

However, the coefficient matrix $\mathbf{A}$ is often **sparse** (has many zeros and very few non-zero elements). In these cases, iterative methods can sometimes be much faster than direct methods (i.e. Gaussian elimination).

Idea: As in fixed point iteration, set up iteration:

$$\mathbf{x}^{(k+1)} = \mathbf{T}\mathbf{x}^{(k)} + \mathbf{c}$$

where the fixed point $\mathbf{p}$ (defined by $\mathbf{p} = \mathbf{T}\mathbf{p} + \mathbf{c}$) corresponds to the solution of the system $\mathbf{A}\mathbf{x} = \mathbf{b}$.

Jacobi Iteration

Consider the 3×3 system:

$$\begin{array}{rcrcrcr} 4x & - & y & + & z & = & 7 \\ 4x & - & 8y & + & z & = & -21 \\ -2x & + & y & + & 5z & = & 15 \end{array}$$

Rewrite the system as follows and then use the old values of x, y and z to compute the new values.

$$\begin{array}{lrcl} \text{Row 1:} & x & = & \frac{1}{4}(7+y-z) \\ \text{Row 2:} & y & = & \frac{1}{8}(21+4x+z) \\ \text{Row 3:} & z & = & \frac{1}{5}(15+2x-y) \end{array} \quad \longrightarrow \quad \begin{array}{rcl} x^{(k+1)} & = & \frac{1}{4}\left(7+y^{(k)}-z^{(k)}\right) \\ y^{(k+1)} & = & \frac{1}{8}\left(21+4x^{(k)}+z^{(k)}\right) \\ z^{(k+1)} & = & \frac{1}{5}\left(15+2x^{(k)}-y^{(k)}\right) \end{array}$$

Take an initial guess $(x^{(0)}, y^{(0)}, z^{(0)})$ and iterate to find a solution. Let the kth iteration be $\mathbf{x}^{(k)} = (x^{(k)}, y^{(k)}, z^{(k)})$, then we have converged when $\|\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}\| < TOL$.

With an initial guess of $\mathbf{x}^{(0)} = \mathbf{0}$, Jacobi converges to within a tolerance of 10^{-6} in 15 iterations. The solution is $(x, y, z) = (2, 4, 3)$.

That worked very well the first time through. Let's look at another case. Try the same equations in a different order:

$$\begin{array}{rcrcrcr} -2x & + & y & + & 5z & = & 15 \\ 4x & - & 8y & + & z & = & -21 \\ 4x & - & y & + & z & = & 7 \end{array}$$

This system has the same solution as before. Set up iteration:

$$\begin{array}{lrcl} \text{Row 1:} & x & = & \frac{1}{2}(-15+y+5z) \\ \text{Row 2:} & y & = & \frac{1}{8}(21+4x+z) \\ \text{Row 3:} & z & = & 7-4x+y \end{array} \quad \longrightarrow \quad \begin{array}{rcl} x^{(k+1)} & = & \frac{1}{2}\left(-15+y^{(k)}+5z^{(k)}\right) \\ y^{(k+1)} & = & \frac{1}{8}\left(21+4x^{(k)}+z^{(k)}\right) \\ z^{(k+1)} & = & 7-4x^{(k)}+y^{(k)} \end{array}$$

What happens? The iterations diverge. In 100 iterations, the error has reached 10^{18} and is still going. $\longrightarrow$ We need some way to predict when the iteration will converge.

Definition A matrix is *strictly diagonal dominant* if $|a_{ii}| > \sum_{\substack{j=1 \\ j \neq i}}^{N} |a_{ij}|$.

Theorem If a matrix $\mathbf{A}$ is strictly diagonal dominant, then $\mathbf{Ax} = \mathbf{b}$ has a unique solution $\mathbf{x} = \mathbf{p}$. Then, Jacobi (and Gauss-Seidel) iteration produce a sequence $\{\mathbf{p}^{(k)}\}$ that converges to $\mathbf{p}$ for any $\mathbf{p}^{(0)}$.

Let's look at our two examples in this light:

$$\text{Case 1:}\quad \begin{array}{rcrcrcr} 4x & - & y & + & z & = & 7 \\ 4x & - & 8y & + & z & = & -21 \\ -2x & + & y & + & 5z & = & 15 \end{array} \qquad \mathbf{A} = \begin{pmatrix} 4 & -1 & 1 \\ 4 & -8 & 1 \\ -2 & 1 & 5 \end{pmatrix}$$

$$\begin{array}{lrclcl} \text{Row 1:} & |4| & > & |-1|+|1| & = & 2 \\ \text{Row 2:} & |-8| & > & |4|+|1| & = & 5 \\ \text{Row 3:} & |5| & > & |-2|+|1| & = & 3 \end{array} \longrightarrow \begin{array}{l} \text{strictly} \\ \text{diagonal} \\ \text{dominant} \end{array}$$

$$\text{Case 2:}\quad \begin{array}{rcrcrcr} -2x & + & y & + & 5z & = & 15 \\ 4x & - & 8y & + & z & = & -21 \\ 4x & - & y & + & z & = & 7 \end{array} \qquad \mathbf{A} = \begin{pmatrix} -2 & 1 & 5 \\ 4 & -8 & 1 \\ 4 & -1 & 1 \end{pmatrix}$$

$$\begin{array}{lrclcl} \text{Row 1:} & |2| & < & |1|+|5| & = & 6 \\ \text{Row 2:} & |-8| & > & |4|+|1| & = & 5 \\ \text{Row 3:} & |1| & < & |4|+|-1| & = & 5 \end{array} \longrightarrow \begin{array}{l} \text{not strictly} \\ \text{diagonal} \\ \text{dominant} \end{array}$$

Note that convergence is not guaranteed for the second case. It might converge for some initial guesses, but it is not guaranteed to converge for any. Best to look to see if equations can be swapped to make the system diagonally dominant and guarantee convergence.

Gauss-Seidel Iteration

Gauss-Seidel is a modification of Jacobi iteration that can converge faster in some cases. **Idea:** Use the most up-to-date information available.

Example:(same as before)

$$\begin{array}{rcrcrcr} 4x & - & y & + & z & = & 7 \\ 4x & - & 8y & + & z & = & -21 \\ -2x & + & y & + & 5z & = & 15 \end{array}$$

As before, we can rewrite the system as follows:

$$\begin{array}{lrcl} \text{Row 1:} & x & = & \frac{1}{4}(7+y-z) \\ \text{Row 2:} & y & = & \frac{1}{8}(21+4x+z) \\ \text{Row 3:} & z & = & \frac{1}{5}(15+2x-y) \end{array} \longrightarrow \begin{array}{rcl} x^{(k+1)} & = & \frac{1}{4}\left(7+y^{(k)}-z^{(k)}\right) \\ y^{(k+1)} & = & \frac{1}{8}\left(21+4x^{(k+1)}+z^{(k)}\right) \\ z^{(k+1)} & = & \frac{1}{5}\left(15+2x^{(k+1)}-y^{(k+1)}\right) \end{array}$$

Now at each step, we use the most up-to-date value of each variable available. After solving for $x^{(k+1)}$, we immediately use this new value to solve for $y^{(k+1)}$.

Strength: Can speed convergence.

Weaknesses: Doesn't always converge when Jacobi does, doesn't parallelize well.

How does it work on this example? Converges to a tolerance of 10^{-6} in 9 iterations. (Almost twice as fast as Jacobi.)

Relaxation Methods

Commonly used in conjunction with Gauss-Seidel to speed or slow convergence by taking larger or smaller steps at each iteration.

For our standard problem from today:

$$
\begin{aligned}
x^{(k+1)} &= (1-\omega)x^{(k)} + \frac{\omega}{4}\left(7 + y^{(k)} - z^{(k)}\right) \\
y^{(k+1)} &= (1-\omega)y^{(k)} + \frac{\omega}{8}\left(21 + 4x^{(k+1)} + z^{(k)}\right) \\
z^{(k+1)} &= (1-\omega)z^{(k)} + \frac{\omega}{5}\left(15 + 2x^{(k+1)} - y^{(k+1)}\right)
\end{aligned}
$$

- In standard Gauss-Seidel, $\omega = 1$.
- Setting $0 < \omega < 1$ (under-relaxation) slows convergence but can obtain convergence in some systems that do not converge with Gauss-Seidel.
- Setting $1 < \omega < 2$ (over-relaxation) can speed convergence in some problems that converge with Gauss-Seidel. Referred to as **SOR** or successive over-relaxation.

How to measure error?

If you know the exact solution to a linear system $\mathbf{Ax} = \mathbf{b}$, then the absolute error is the norm of the difference between your approximation $\mathbf{x}^{(k)}$ and the solution $\mathbf{x}$:

$$E^{(k)} = \|\mathbf{x} - \mathbf{x}^{(k)}\|$$

If you don't know the solution beforehand, the *residual* tells you how close you have come to solving the linear system:

$$\mathbf{r}^{(k)} = \mathbf{b} - \mathbf{Ax}^{(k)}$$

To draw an analogy with root finding:

$$\begin{aligned} \|\mathbf{r}^{(k)}\| \quad &\longleftrightarrow \quad |f(x_k)| \\ \|\mathbf{x}^{(k)} - \mathbf{x}^{(k-1)}\| \quad &\longleftrightarrow \quad |x_k - x_{k-1}| \end{aligned}$$

Iterative Schemes at Work

Consider the linear system:

$$\begin{array}{rcrcr} 3x_1 & + & x_2 & = & 7 \\ x_1 & - & 4x_2 & = & -2 \end{array}$$

Rearrange and form iterative schemes:

Jacobi

$$\begin{aligned} x_1^{(k)} &= \tfrac{1}{3}\left(7 - x_2^{(k-1)}\right) \\ x_2^{(k)} &= \tfrac{1}{4}\left(2 + x_1^{(k-1)}\right) \end{aligned}$$

Gauss-Seidel

$$\begin{aligned} x_1^{(k)} &= \tfrac{1}{3}\left(7 - x_2^{(k-1)}\right) \\ x_2^{(k)} &= \tfrac{1}{4}\left(2 + x_1^{(k)}\right) \end{aligned}$$

SOR

$$\begin{aligned} x_1^{(k)} &= (1-\omega)x_1^{(k-1)} + \tfrac{\omega}{3}\left(7 - x_2^{(k-1)}\right) \\ x_2^{(k)} &= (1-\omega)x_2^{(k-1)} + \tfrac{\omega}{4}\left(2 + x_1^{(k)}\right) \end{aligned}$$