CS205 – Class 10

Covered in class: All
Reading: Shewchuk Paper on course web page

1. Let’s go back to linear systems of equations Ax=b.
   a. Assume that A is square, symmetric, positive definite
   b. If A is dense we might use a direct solver, but for a sparse A, iterative solvers are better as they only deal with nonzero entries
   c. Quadratic Form  \( f(x) = \frac{1}{2} x^T A x - b^T x + c \)
   d. If A is symmetric positive definite then f(x) is minimized by the solution x to Ax=b!
      i.  \( \nabla f(x) = A x + \frac{1}{2} A^T x - b = A x - b \) since A is symmetric
      ii. \( \nabla f(x) = 0 \) is equivalent to Ax=b
          1. this makes sense considering the scalar equivalent
             \( f(x) = \frac{1}{2} ax^2 - bx + c \) where the line of symmetry is \( x = b/a \)
               which is the solution of ax=b and the location of the maximum or minimum
      iii. The Hessian is H=A, and since A is symmetric positive definite so is H, and a solution to \( \nabla f(x) = 0 \), or Ax=b is a minimum
          1. note that symmetric negative definite A lead to maxima
          2. in the scalar case \( f(x) = 1/2 ax^2 - bx + c \), H=[a] and when a>0 the parabola is concave up and \( x = b/a \) represents a minima
          3. Even if A is not symmetric, the Hessian \( H = \frac{1}{2}(A + A^T) \) is symmetric itself, as expected since the quadratic function we considered has continuous second derivatives
   iv. Moreover, since H=A is constant, f(x) has a bowl shape everywhere –

\[
\begin{align*}
\text{Consider this in 1D. We have} & \\
f(x) &= \frac{1}{2} ax^2 - bx + c = \frac{1}{2} ax^2 - bx + c \\
f'(x) &= ax - b
\end{align*}
\]

minimum is \( x = b/a \). Then the second derivative sign is analogous to
the positive or negative definiteness of the general matrix case. Here

vi. \( f(x) = \frac{1}{2} \cdot 2 \cdot x^2 + 3x - 10 \) minimum is at \( b/a = 3/2 \).

2. Steepest Descent – for \( Ax = b \)
   a. We look in the direction \(-\nabla f = b - Ax = r\). As we have shown, the residual direction is the steepest descent direction!
   b. Another way to think about the residual is \( r = b - Ax = \)
      \( = Ax_{\text{exact}} - Ax = A(x_{\text{exact}} - x) = -Ae \) where \( e = x - x_{\text{exact}} \) is the error. Thus, the residual is the error transformed by \( A \) into the space where \( b \) resides.
   c. \(-\nabla f = r = -Ae\) so the search direction is predicted by \( r \), not by \( e \), whereas \( e \) is the correct search direction. Note that in 1d the directions of \( e \) and \( r \) are coincident, but in multi-d this problem manifests itself. The residual may or may not be a good measure of error. Consider a 1D example with \( r = ae \). Suppose \( r = 10^{-8} \). Then \( e \) could be arbitrarily large as we make \( a \) smaller (where \( a \) is the concavity).
   d. Recall that we choose \( \alpha \) using a 1D minimization problem
      i. The solution occurs where the new \( \nabla f(x) \) is orthogonal to the search line,
         1. i.e. go in the direction until you reach a spot where direction is tangent to level curves
         2. i.e. \( \perp \) to \( \nabla f(x) \)
         3. i.e. \( \nabla f(x) \perp s_k \) where \( s_k \) is search direction at iteration \( k \)
         4. i.e. \( \nabla f(x) \cdot s_k = 0 \)
         5. i.e. \( \nabla f(x_{k+1}) \cdot r_k = 0 \)
         6. i.e. \( r_{k+1} \cdot r_k = 0 \).
      ii. If we knew the absolute error \( e_k \), we could use it to write:
          \( x_{k+1} = x_k + s_k \alpha = x_k - e_k \alpha = x_k - (x_k - x_{\text{exact}}) \alpha \) gives \( x_{k+1} = x_{\text{exact}} \) for \( \alpha = 1 \).
      iii. However, using \( r_{k+1} \cdot r_k = 0 \) implies \( (b - Ax_{k+1}) \cdot r_k = 0 \) or
          \( (b - A(x_k + r_k \alpha)) \cdot r_k = 0 \) or \( (b - Ax_k) \cdot r_k - (Ar_k \alpha) \cdot r_k = 0 \) or
          \( r_k \cdot r_k - \alpha r_k \cdot Ar_k = 0 \) so that \( \alpha = \frac{r_k \cdot r_k}{r_k \cdot Ar_k} = \frac{r_k^T r_k}{r_k^T Ar_k} \).
      e. So, the steepest descent method applied to the quadratic form is \( r_k = b - Ax_k \),
         \( \alpha = \frac{r_k^T r_k}{r_k^T Ar_k} \), \( x_{k+1} = x_k + r_k \alpha \); this can also be seen as solving \( Ax = b \).
f. Sometimes people iterate on the residual directly using
\[ r_{k+1} = b - Ax_{k+1} = b - A(x_k + r_k \alpha) = r_k - \alpha Ar_k \]
to find the \( r_k \), while still updating along the way (although \( x \) no longer feeds back into the algorithm)

i. The advantage of this is that we no longer need the extra multiplication by \( A \) in \( r_k = b - Ax_k \). Both the computation of \( \alpha = \frac{r_k^T r_k}{r_k^T Ar_k} \) and
\[ r_{k+1} = r_k - \alpha Ar_k \]
use the same \( Ar_k \)

3. Steepest Descent for Ax=b (continued)
   a. Suppose that our initial guess is such that the error term, \( e = x - x_{\text{exact}} \), is an eigenvector of the matrix \( A \)
      i. Then \( r = -Ae = -\lambda e \)
      ii. \[ x_{k+1} = x_k + \left( \frac{r_k \cdot r_k}{r_k \cdot Ar_k} \right) e = x_k + \left( \frac{r_k \cdot r_k}{r_k \cdot Ar_k} \right) (-\lambda e) = x_k + \left( \frac{r_k \cdot r_k}{r_k \cdot Ar_k} \right) e \]
      Then \( x_{k+1} = x_k + \left( \frac{r_k \cdot r_k}{r_k \cdot Ar_k} \right) e = x_k + \left( \frac{r_k \cdot r_k}{r_k \cdot (-\lambda e)} \right) e = x_k - e = x_{\text{exact}} \) and we’re done!
   iii. In this case, we lie exactly on one of the coordinate axis of the ellipsoid and \( \nabla f \) and \( e \) point in the same direction:
\[ -\nabla f = r = -Ae = -\lambda e \]
   b. When all the eigenvalues are equal, we have circles instead of ellipses. Then \( \nabla f \) and \( e \) always point in the same direction, and the steepest descent method converges in one iteration
   c. In general, the error is a linear combination of the eigenvectors
      i. I.e., we do not lie on the principle axis of the ellipse
      ii. I.e. \( \nabla f \) and \( e \) point in different directions.