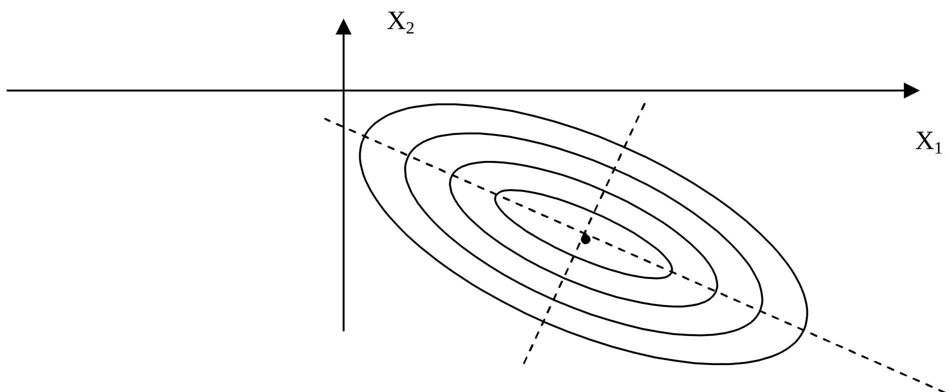
CS205 – Class 10

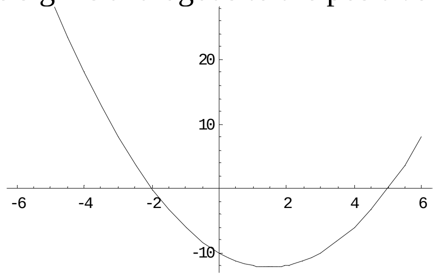
Covered in class: All
Reading: Shewchuk Paper on course web page

1. **Conjugate Gradient Method** – this covers more than just optimization, e.g. we'll use it later as an iterative solver to aid in solving pde's
2. 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 $f(x) = \frac{1}{2} x^T Ax - b^T x + c$
    d. If A is symmetric, positive definite then f(x) is minimized by the solution x to Ax=b!
        i. $\nabla f(x) = \frac{1}{2} Ax + \frac{1}{2} A^T x - b = Ax - b$ 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 $f(x) = 1/2ax^2 - bx + c$, H=[a] and when a>0 the parabola is concave up and $x = b/a$ represents a minima
            3. [Note: Even if A is not symmetric, the Hessian $H = \frac{1}{2}\left(A + A^T\right)$ 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 –



v. Consider this in 1D. We have $f(x) = \frac{1}{2}xax - bx + c = \frac{1}{2}ax^2 - bx + c$, $f'(x) = ax - b$ so 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. $f(x)=1/2 * 2 * x^2-3x-10$ minimum is at $b/a=3/2$.

3. Steepest Decent for $Ax=b$
   a. We look in the direction $-\nabla f = b - Ax = r$. As we have shown, the residual direction is the steepest decent direction!
   b. Another way to think about the residual is $r = b - Ax = \; = Ax_{exact} - Ax = A(x_{exact} - x) = -Ae$ where $e = x - x_{exact}$ 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 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 α 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. $\nabla f(x) to \perp$
         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. 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 $\alpha = \dfrac{r_k \cdot r_k}{r_k \cdot Ar_k} = \dfrac{r_k{}^T r_k}{r_k{}^T Ar_k}$
   e. So, the steepest decent method applied to Ax=b is $r_k = b - Ax_k$, $\alpha = \dfrac{r_k{}^T r_k}{r_k{}^T Ar_k}$, $x_{k+1} = x_k + r_k\,\alpha$
   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 $x_{k+1} = x_k + r_k\,\alpha$ 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 $\alpha = \dfrac{r_k{}^T r_k}{r_k{}^T Ar_k}$ and $r_{k+1} = r_k - \alpha Ar_k$ use the same Ar_k