$\boxed{L\#10}$ Sept. 29, 2011 Thursday

Variational Methods

(steepest descent, conjugate gradient, MINRES)

We shall study a new class of methods, called variational method, that are related to minimization of some functional, produced by the original problem $Ax=b$, A nonsingular

The simplest functional is a least-squares

$$J(y) = \frac{1}{2}\|Ay-b\|_2^2 \qquad \|\cdot\|_2 \text{ Euclidean norm}$$

Obviously, minimum of $J(y)$ over $y \in \mathbb{R}^n$ is 0 and achieved for x, solution of the problem $Ax=b$. If we rewrite $J(y)$ using the Euclidean inner product we get

$$J(y) = \frac{1}{2}(Ay-b, Ay-b) \quad \text{if } y=0 \text{ then } J(x)=0$$

Then taking $y = x+u$, x solution of $(*)$ $u \in \mathbb{R}^n$ we get

$$J(x+u) = \frac{1}{2}(Ax+Au-b, Ax+Au-b) = \frac{1}{2}(Au, Au) \geq 0$$

and if $u \neq 0$ $J(x+u) > 0$

The only minimum is at x, solution to $(*)$.

This is not a very good method!

Now we consider the case A an SPD.

<u>Lemma:</u> $Ax = b$ if and only if $J(x) \le J(y)$, $y \in \mathbb{R}^n$

where $J(y) = \frac{1}{2}(Ay, y) - (b, y)$

Indeed $J(y) = \underbrace{\frac{1}{2}(Ay,y) - (Ax,y) + \frac{1}{2}(Ax,x)} - \frac{1}{2}(Ax,x)$

$$= \frac{1}{2}(A(y-x), y-x) + J(x)$$

$$J(x) = \frac{1}{2}(Ax,x) - (Ax,x) = -\frac{1}{2}(Ax,x)$$

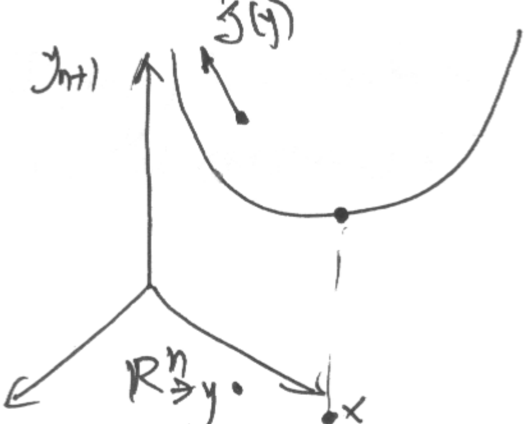
$$J(y) - J(x) = \frac{1}{2}(A(y-x), y-x) > 0$$

& $=$ only if $y = x$

Thus $J(x) = \min_{y \in \mathbb{R}^n} J(y) = \min_{y \in \mathbb{R}^n} \left\{ \frac{1}{2}(Ay,y) - (b,y) \right\}$

Note that $J(y)$ is a quadratic function of the variables $(y_1, y_2, \dots, y_n)$. In $\mathbb{R}^n$ $J(y) = c$ is a surface

$$\boxed{y_{n+1} = J(y)} \quad y \in \mathbb{R}^n$$



Define the gradient of J

$$\nabla J(y) = \left(\frac{\partial J}{\partial y_1}, \frac{\partial J}{\partial y_2}, \dots, \frac{\partial J}{\partial y_n}\right) \in R^n$$

$y \in$ fixed in $\mathbb{R}^n$

∇J is the direction of the greatest increase of J at the point y

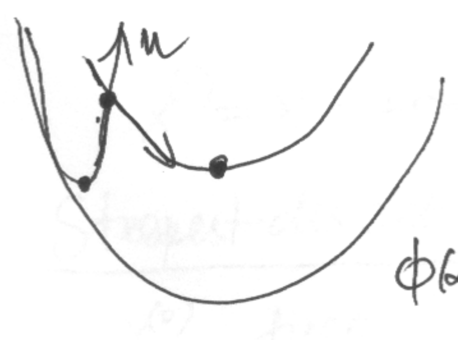
Obviously, $\nabla J(y) = 0$ is equivalent to $Ax = b$

Therefore minimizing $J(y) \Longleftrightarrow Ax = b$

Now take arbitrary point $y \in \mathbb{R}^n$ and take u - fixed vector of R^n. Form the function of one variable α

$\phi(\alpha) = J(y + \alpha u)$. Minimum of this quadratic function is achieved at

$\phi'(\alpha) = 0$



$$0 = \phi'(\alpha) = (Ay, y) - (b, y) + \alpha(Au, u)$$

$$\phi(\alpha) = \frac{1}{2}(A(y + \alpha u), y + \alpha u) - (b, y + \alpha u)$$

$$\phi(\alpha) = \frac{1}{2}(Ay, u) + \alpha[(Ay, u) - (b, u)] + \frac{\alpha^2}{2}(Au, u)$$

$\phi(\alpha) = J(y + \alpha u)$ is a parabola on the surface $J(y)$

$$\boxed{\alpha = \frac{(b - Ay, \ )}{(Au, u)}}$$

Let us face the situation $x^{(0)}$ is our first guess.

We are sitting on the surface $y^*_{n+1} = J(y)$ at point $J(x^{(0)})$. We would like to go down on the surface.

What would be the best direction?

The direction of the steepest descent is $-\nabla J(x^{(0)})$! And this is what we shall choose as u

$$x^{(0)} \quad \text{and direction } u = -\nabla J(x^0) = b - Ax^{(0)}$$

$$u = r^{(0)} \text{ the residual}$$

According to our formula above the minimum will be achieved for

$$\alpha_1 = \frac{(b - Ax^{(0)}, r^{(0)})}{(Ar^{(0)}, Ar^{(0)})} = \frac{(r^{(0)}, r^{(0)})}{(Ar^{(0)}, r^{(0)})}$$

$$x^{(1)} = x^{(0)} + \alpha_1 r^{(0)}$$

Steepest descent method for A SPD

$x^{(0)}$ given compute $r^{(0)} = b - Ax^{(0)}$

for $k = 1, 2, \ldots$ compute $\alpha_k = \dfrac{(r^{(k)}, r^{(k)})}{(Ar^{(k)}, r^{(k)})}$

$$\begin{cases} x^{(k+1)} = x^{(k)} + \alpha_k r^{(k)} \\ r^{k+1} = r^{(k)} - \alpha_k A r^{(k)} \end{cases} \qquad r^{(k+1)} = b - Ax^{(k+1)} = \underbrace{b - Ax^{(k)}}_{r^{(k)}} - \alpha_k A r^{(k)}$$

$$r^{(k)} = f - Ax^{(k)}$$

Lemma (Saad Book) Let $e^{(k+1)} = x^{(k+1)} - x$ & $\|x\|_A = (Ax, x)^{1/2}$
Then for the Steepest descent method we have

$$\|e^{(k+1)}\|_A^2 = \left(1 - \frac{(r^{(k)}, r^{(k)})^2}{(r^{(k)}, Ar^{(k)})(r^k, A^{-1}r^{(k)})}\right)\|e^{(k)}\|_A^2$$

Assume we have proved this equality. What can we say about the convergence of the SD method?

An easy result Let $\lambda \le \lambda_1 \le \lambda_2 \le \dots \le \lambda_n \le \Lambda$ be the eigenvalues of A. Then

$$\|e^{(k+1)}\|_A^2 \le \left(1 - \frac{\lambda}{\Lambda}\right)\|e^{(k)}\|_A^2$$

Indeed

$$1 - \frac{(r^{(k)}, r^{(k)})}{(r^{(k)}, Ar^{(k)})(r^{(k)}, A^{-1}r^{(k)})} \le 1 - \frac{1}{\sup\limits_{r} \frac{(r^{(k)}, Ar^{(k)})}{(r^{(k)}, r^{(k)})} \sup \frac{(r^{(k)}, A^{-1}r^{(k)})}{(r^{(k)}, r^{(k)})}}$$

$$\le 1 - \frac{1}{\Lambda \frac{1}{\lambda}} = 1 - \frac{\lambda}{\Lambda} = q < 1$$

A hard proof (Kantorovich lemma) $\frac{(Ax, x)(x, A^{-1}x)}{(x,x)\ (x,x)} \le \frac{(\lambda+\Lambda)^2}{4\lambda\Lambda}$

$$1 - \frac{4\lambda\Lambda}{(\lambda+\Lambda)^2} = \frac{(\Lambda-\lambda)^2}{(\lambda+\Lambda)^2}$$

$$\|e^{(k+1)}\|_A^2 \le \left(\frac{\Lambda-\lambda}{\Lambda+\lambda}\right)^2\|e^{(k)}\|_A^2 \qquad \frac{\Lambda-\lambda}{\Lambda+\lambda} = \frac{1-\xi}{1+\xi}$$

$$\|e^{(k+1)}\|_A \le \frac{1-\xi}{1+\xi}\|e^{(k)}\|_A$$

<u>Proof</u>

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

$$e^{(k)} = x^{(k)} - x$$

$$\alpha_k = \frac{(r^{(k)}, r^{(k)})}{(Ar^{(k)}, r^{(k)})}$$

SD: $$x^{(k+1)} = x^{(k)} + \alpha_k r^{(k)}$$

apply A

$$A x^{(k+1)} - \underbrace{Ax}_{\substack{-b \\ -Ax}} = A x^{(k)} - \underbrace{Ax}_{\substack{-b \\ -Ax}} + \alpha_k A r^{(k)}$$

$$\Rightarrow \boxed{-r^{(k+1)} = -r^{(k)} + \alpha_k A r^{(k)}}$$

$$\Rightarrow \boxed{Ae^{(k+1)} = Ae^{(k)} + \alpha_k A r^{(k)}}$$

$$\Downarrow$$

$$\boxed{e^{(k+1)} = e^{(k)} + \alpha_k r^{(k)}}$$

These three are fundamental equalities we shall use

$$(\underbrace{Ae^{(k+1)}}, e^{(k+1)}) = (-r^{(k+1)}, e^{(k)} + \alpha_k r^{(k)}) = -(r^{(k+1)}, e^{(k)})$$

$$= (-r^{(k)} + \alpha_k A r^{(k)}, e^{(k)})$$

$$e^{(k)} = x^{(k)} - x = A^{-1} A (x^{(k)} - x) = -A^{-1} r^{(k)}$$

$$\|e^{(k+1)}\|_A^2 = (r^{(k)}, A^{-1} r^{(k)}) - \alpha_k (\cancel{A} r^{(k)}, A^{-1} r^{(k)})$$

$$= (r^{(k)}, A^{-1} r^{(k)}) \left[1 - \frac{\alpha_k (r^{(k)}, r^{(k)})}{(r^{(k)}, A^{-1} r^{(k)})} \right]$$

$$(Ae^{(k)}, e^{(k)}) \left[1 - \frac{(r^{(k)}, r^{(k)})^2}{(r^{(k)}, A r^{(k)})(r^{(k)}, A^{-1} r^{(k)})} \right] \quad \boxtimes$$

Alternative proof via comparison

What do we know about the optimal Richardson method

$$\tau = \frac{2}{\lambda+\lambda} \qquad \|e^{(k+1)}_{Rich}\|_2 \le \frac{1-\xi}{1+\xi}\|e^{(k)}_{Rich}\|_2$$

Can we proof convergence of Richardson in the A-norm?

$$\|e^{(k+1)}_{Rich}\|_A \le \frac{1-\xi}{1+\xi}\|e^{(k)}_{Rich}\|_A \quad ?$$

$$e^{(k+1)}_{Rich} = (I-\tau A)e^{(k)}_{Rich}$$

$$Ae^{(k+1)}_{Rich} = (I-\tau A)Ae^{(k)}_{Rich}$$

$A\psi_j = \lambda_j\psi_j$ (λ_j, ψ_j) Eigenpairs of A

$$e^{(k)}_R = \sum c_j\psi_j \qquad Ae^{(k)}_R = \sum c_j\lambda_j\psi_j$$

$$(Ae^{(k)}_R, e^{(k)}_R) = \sum_{j=1}^{n} c_j^2\lambda_j \equiv \|e^{(k)}_R\|_A^2$$

$$e^{(k+1)}_R = (I-\tau A)e^{(k)}_R = \sum_{j=1}^{n}(1-\tau\lambda_j)c_j\psi_j$$

$$(Ae^{k+1}_R, e^{k+1}) = \sum_{j=1}^{n}(1-\tau\lambda_j)^2 c_j^2\lambda_j \le \frac{\overbrace{\max(|1-\tau\lambda_1|^2, |1-\tau\lambda_n|^2)}^{\left(\frac{1-\xi}{1+\xi}\right)^2}}{\sum c_j^2\lambda_j}$$

$$\boxed{\|e^{k+1}_R\|_A^2 \le \left(\frac{1-\xi}{1+\xi}\right)^2\|e^{(k)}_R\|_A^2}$$

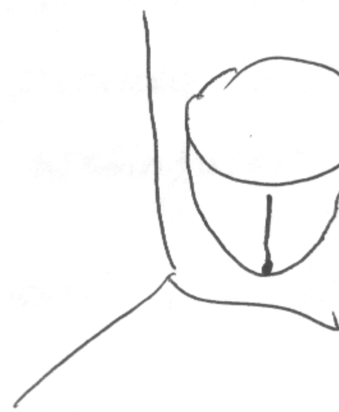
But in A-norm SD is the best method

$$\|e^{(1)}_{SD}\|_A \le \|e^{(1)}_R\|_A \le \frac{1-\xi}{1+\xi}\|e^{(0)}\|_A$$

Why SD is slow? Consider ill conditioned system (in 2-D this will be a very splashed paraboloid)

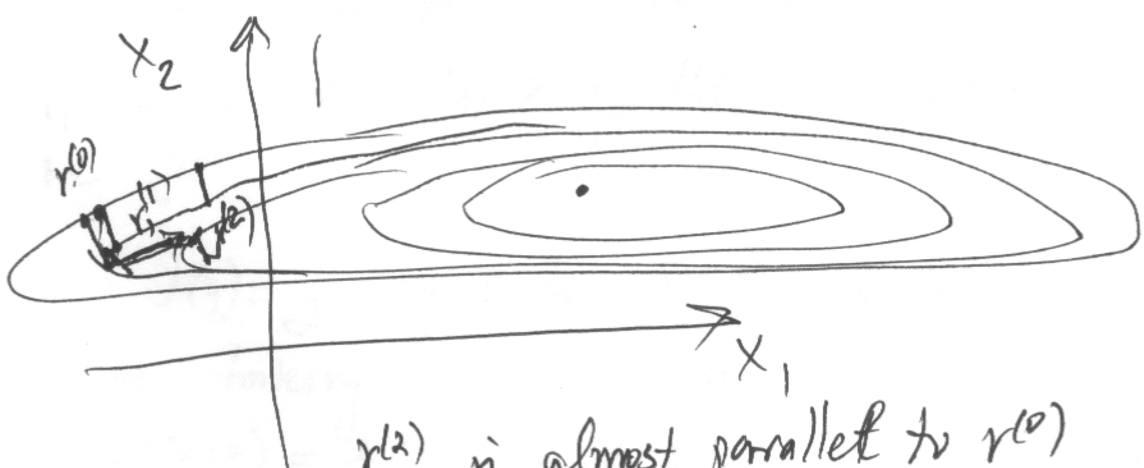
$$(Ax, x) = a_{11}x_1^2 + 2a_{12}x_1x_2 + a_{22}x_2^2$$

$$a_{12} = 0 \quad a_{11} = a_{22} = a$$



circle

Isolines $J(x) = c$



$r^{(2)}$ is almost parallel to $r^{(0)}$

So you are repeating very often the same search (minimization direction)

This is very SLOW!