Lecture 5

For steepest descent, (quadratic case)

$$E(X_{k+1}) \leq \left(\frac{A-a}{A+a}\right)^2 E(X_k)$$

$E(x) = f(x) - f(x^*) = f(x) - f_{min}$

A = largest e.v., a = smallest.

and $\left(\frac{A-a}{A+a}\right)^2 = \left(\frac{\frac{A}{a}-1}{\frac{A}{a}+1}\right)^2 = \left(\frac{r-1}{r+1}\right)^2$

condition number $\gg 1 \Rightarrow$ bad

$\approx 1 \Rightarrow$ good

Today, minimization method that performs better than steepest descent (for quadratic problems)

Today we minimize $f(x) = \frac{1}{2}x^TQx - b^Tx$

Definition: Two vectors $d_1, d_2 \in E^n$ are Q-orthogonal or conjugate with respect to Q if $d_1^TQd_2 = 0$.

Note: If $Q = I$ (Identity matrix)

then Q-orthogonal = orthogonal

A set $\{d_0, \cdots, d_n\}$ is Q-orthogonal if $d_i^TQd_j = 0$ whenever $i \neq j$.

Example: Let $Q = \begin{pmatrix} 1 & 0 \\ 0 & 100 \end{pmatrix}$ so $f(x,y) = \frac{x^2}{2} + 50y^2$

Recall: for steepest descent, for this f we saw that

if $(x_0, y_0) = (100, 1)$

then $(x_1, y_1) = \left(\frac{99}{101}\right)(100, -1)$

$(x_2, y_2) = \left(\frac{99}{101}\right)^2 (100, 1)$

Consider $d_0 = -100(1,1) = -\nabla f(x_0, y_0)^T$

Let's find d_1 which is Q-orthogonal to d_0

let $g_1 = -\nabla f(x_1, y_1) = -(x, 100y) = \frac{99}{101} 100(-1, 1)$ and $d_1 = g_1 - \beta d_0$

Where I choose β so that d_0, d_1 are Q-orthogonal.

This says: $0 \underset{\text{want}}{=} d_0^TQd_1 = d_0^TQg_1 - \beta d_0^TQd_0$

so $\beta = \frac{d_0^TQg_1}{d_0^TQd_0}$

and ~~this~~ I can check I get: $d_1 = g_1 - \beta d_0$ = multiple of $(-100, 1)$

Here's the point:

I'll try to minimize f by:

① Start at (x_0, y_0), minimize in direction d_0 as before, I end up at (x_1, y_1) as before.

② Now minimize in the d_1 direction (= gradient direction, modified to be Q-orthogonal to d_0)

The point is: d_1 points exactly toward the origin = global min of f.
So if I minimize in d_1 direction, I'll end up at the origin = global min in 2 steps

More generally.
To minimize $f(x) = \frac{1}{2}x^TQx - b^Tx$
proceed as follows:

① Assume that $d_0, d_1, \cdots, d_{n-1}$ are nonzero and Q-conjugate
② Start with guess x_0.
For $k = 1, 2, \cdots, n$
Let x_{k+1} = min pt of f on the line $\{x_k + sd_k : s \in \mathbb{R}\}$
Thm: This converges to minimum after at most n steps.

Remark:

$$\boxed{\begin{array}{l} x_{k+1} = x_k + \alpha_k d_k \\ \text{where } \alpha_k = \dfrac{-d_k^T g_k}{d_k^T Q d_k} \text{ and } g_k = Qx_k - b_k \end{array}} \quad (*)$$

To verify (*), we have to minimize $f(x_k + sd_k)$
Since this is definition of x_{k+1}
To minimize, expand and collect terms:

$$f(x_k + sd_k) = \tfrac{1}{2}(x_k + sd_k)^TQ(x_k + sd_k) - b^T(x_k + sd_k)$$

$$= \tfrac{1}{2}s^2 d_k^T Q d_k + s d_k^T \underbrace{(Qx_k - b)}_{g_k} + f(x_k)$$

so min occurs when $f'(s) = 0$ i.e.

$$s d_k^T Q d_k + d_k^T \cdot g_k = 0$$

so α_k = minizing $s = \dfrac{-d_n^T g_k}{d_k^T Q d_k}$

So we can rewrite the algorithm: start with x_0

$$x_{k+1} = x_k + \alpha_k d_k, \quad \alpha_k = \frac{-d_k^T g_k}{d_k^T Q d_k}, \quad g_k = Qx_k - b$$

First:
Lemma: If $d_0, \cdots, d_{n-1}$ are Q-orthogonal, then they are linearly independent, hence a basis for E^n

Proof: We have to show:

if $\alpha_0 d_0 + \cdots + \alpha_{n-1} d_{n-1} = 0$ (1)
then $\alpha_0 = \alpha_1 = \cdots = \alpha_{n-1} = 0$

Assume (1) holds. All I know is $d_i^T Q d_j = 0$, $i \neq j$

So I'll multiply (1) from the left by $d_i^T Q$ for some i

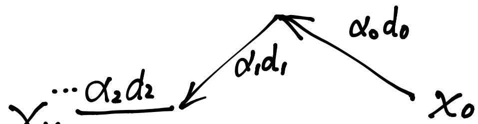
$$\alpha_0 d_i^T Q d_0 + \alpha_1 d_i^T Q d_1 + \cdots + \alpha_{n-1} d_i^T Q d_{n-1} = 0$$

All terms $= 0$ except :
$0 + 0 \cdots + 0 + \alpha_i d_i^T Q d_i + 0 + \cdots + 0 = 0$
$d_i^T Q d_i \to \neq 0$

so $\alpha_i = 0$

Since i was arbitrary, all α's $= 0$

Pf of Theorem:
Recall $f(x) = \frac{1}{2} x^T Q x - b^T x$
Let x^* = global min (which we know $= Q^{-1} b$)
b/c $d_0, \cdots, d_{n-1}$ form a basis for E^n, we can write
$x_0 - x_* = \alpha_0 d_0 + \cdots + \alpha_{n-1} d_{n-1}$ ②
for some coefficients $\alpha_0, \cdots, \alpha_{n-1}$
Moreover: multiply ② on left by $d_i^T Q$ and simplify we get:
$\alpha_i d_i^T Q d_i = d_i^T Q (x_0 - x_*) = d_i^T (Q x_0 - b)$
since $x_* = Q^{-1} b$
Compare to our algorithm: start with x_0
$x_{k+1} = x_k + a_k d_k$, $a_k = \dfrac{-d_k^T g_k}{d_k^T Q d_k}$, $g_k = Q x_k - b$
Claim: $x_k = x_0 - \alpha_0 d_0 - \cdots - \alpha_{k-1} d_{k-1}$



i.e.
$a_k = -\alpha_k \longrightarrow$ from expanding $x_0 - x^*$ in terms of basis $d_0, \cdots, d_{n-1}$
$\downarrow$
from iterative procedure

So we have to compare the formulas.
$\alpha_k = \dfrac{d_k^T (Q x_0 - b)}{d_k^T Q d_k}$ from above

vs
a_k defined above $= \dfrac{-d_k^T (Q x_0 - b)}{d_k^T Q d_k}$

Pf by induction: clear that $a_0 = -\alpha_0$.
Assume it's true for $j = 0, \cdots, k-1$. Want to prove for k.
If true for $j = 0, \cdots, k-1$.
$x_k = x_0 + a_0 d_0 + \cdots + a_{k-1} d_{k-1} = x_0 - \alpha_0 d_0 - \cdots - \alpha_{k-1} d_{k-1}$
So $\alpha_k = \dfrac{d_k^T (Q x_k - b)}{d_k^T Q d_k} = -d_k^T Q (x_0 -$??? $= -a_k$

Conclusion:
1. Algorithm works (for quadratic problems) much better than steepest descent.
2. So good idea to understand conjugate directions.

Example:
$f(x) = \frac{1}{2} (\lambda_1 x_1^2 + \cdots + \lambda_n x_n^2) - b^T x$
so $Q = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix}$ Then the standard basis for E^n is conjugate
i.e. $d_0 = (1, 0, \cdots, 0)^T$, $d_1 = (0, 1, 0, \cdots, 0)^T$ etc.

Minimizer: $x^* = Q^{-1} b = \begin{pmatrix} b_1/\lambda_1 \\ \vdots \\ b_n/\lambda_n \end{pmatrix}$

Consider conjugate direction method, starting at 0.

$x_0 = 0$

$d_0 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$ $\quad x_1 = x_0 + \alpha_0 d_0$, $\alpha_0 = \dfrac{-d_0^T(Qx_0 - b)}{d_0^T Q d_0} = \dfrac{b_1}{\lambda_1}$

$x_1 = \begin{pmatrix} b_1/\lambda_1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$

$x_2 = x_1 + \alpha_1 d_1$, $\alpha = \dfrac{-d_1^T g_1}{d_1^T Q d_1} = \dfrac{b_2}{\lambda_2}$

$x_2 = \begin{pmatrix} b_1/\lambda_1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \dfrac{b_2}{\lambda_2}\begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} b_1/\lambda_1 \\ b_2/\lambda_2 \\ \vdots \\ 0 \end{pmatrix}$ This is ~~What the proof~~ showed.

More facts about conjugate directions method = the algorithm discussed above.

Expanding sub space theorem

Let f(x)$= \frac{1}{2} x^T Q x - b^T x$ $\quad$ Q pos def, and Let $d_0, \cdots, d_{n-1}$ be nonzero Q-conj vectors

start with x_0 & define x_k as above. for $k=1,2,\cdots,n$.
Then x_k minimizes f in the set. $\{x_0 + s_0 d_0 + \cdots + s_{k-1} d_{k-1} : s_0, \cdots, s_{k-1}$, real numbers$\}$
This is a k-dim plane containing x_0, and with $d_0, \cdots, d_{k-1}$ all tangent vectors.

Idea of proof

1. Since f is convex, it suffices to show that $\boxed{\nabla f(x_k) d_j = 0 \text{ for } j = 0, \cdots, k-1}$ ✯
2. This can be done by induction (details omitted)

Must show that ✯ $\Longrightarrow x_k$ minimizes f in the set described above

i.e. consider
$\phi(s_0, \cdots, s_{k-1}) \stackrel{def}{=} f(x_0 + s_0 d_0 + \cdots + s_{k-1} d_{k-1})$
Note $x_k = x_0 + \alpha_0 d_0 + \cdots + \alpha_{k-1} d_{k-1}$
So we want to show
if ✯ then ϕ minimized at $(s_0, \cdots, s_{k-1}) = (\alpha_0, \cdots, \alpha_{k-1})$ corresponding to x_k

First, note that ϕ is convex, since f is convex.
So every point where $\frac{\partial \phi}{\partial s} = 0$ (for all i) is a global minimum point (by convexity)

Also, $\dfrac{\partial \phi}{\partial s_i} = \nabla f(x_0 + s_0 d_0 + \cdots + s_{k-1} d_{k-1}) d_i$

so $\dfrac{\partial \phi}{\partial s_i} = 0 \ \forall i \Longleftrightarrow \nabla f(\quad) d_i = 0, \forall i.$ $\quad$ ϕ has a global min at the pt which is x_k

so putting this together: $\nabla f(x_k) d_i = 0 \ \forall i$:
$\Downarrow \dfrac{\partial \phi}{\partial s_i}(x_0 + \alpha_0 d_0 + \cdots + \alpha_{k-1} d_{k-1}) = 0 \ \forall i$

Next : How to find directions d_k ?

Idea: Again · I want to minimize $f(x) = \frac{1}{2}x^TQx - b^Tx$ but I don't know directions d_k ...

① Start as with steepest descent: $d_0 = \nabla f(x_0)^T = Qx_0 - b$

Then : $x_1 = x_0 + \alpha_0 d_0$ $\quad \alpha_0 =$ same formula

How to find d_1?

2 case: case 1: $\nabla f(x_1) = 0$

case 2: $\nabla f(x_1) \neq 0$

case 1: x_1 is already global min. We can stop. — don't need d_1

case 2: let $g_1 = \nabla f(x_1)^T = Qx_1 - b$, $d_1 = g_1$, adjusted to be Q-orthogonal to d_0.

Concretely :

$d_1 = g_1 + \beta_0 d_0$ where β_0 chosen so that $d_0^T Q d_0 = 0$, so β_0 should satisfy

$0 \overset{\text{want}}{=} d_0^T Q d_1 = d_0^T Q g_1 + \beta_0 d_0^T Q d_0$

$$\boxed{\beta_0 = -d_0^T Q g_1 / d_0^T Q d_0}$$

Having found d_1, I can find $x_2 = x_1 + \alpha_1 d_1$, $\alpha_1 =$ usual formula

Then. repeat

Idea is at each step:

1. Find gradient direction
2. Correct to make it Q-orthogonal to previous direction.

This is called **conjugate gradient direction**

3. Minimize in conjugate gradient direction then repeat.

In general

$x_{k+1} = x_k + \alpha_k d_k$, α_k same formula and $d_k = g_k + \beta_{k-1} d_{k-1}$.

β_{k-1} chosen so that $d_{k-1}^T Q d_k = 0$

i.e. $\beta_{k-1} = \dfrac{-d_{k-1}^T Q g_k}{d_{k-1}^T Q d_{k-1}}$ and $g_{k-1} = \nabla f(x_{k-1}) = Qx_{k-1} - b$

(if g_{k-1} ever $= 0$ then x_{k-1} is a global min and we've done)

Theorem: The directions $d_0, d_1, \cdots, d_{n-1}$ chosen as above are Q-conjugate. So the method converges in at most n steps.

Proof of theorem:

Interesting, because: we chose d_k to be Q-orthogonal to d_(k-1)

Not obvious that it is also Q-orthogonal to d_(k-2), d_(k-3)...

But in fact this is true. This is "magical"

Proof goes by induction details omitted (see book section 9.3 if interested)

Question: let Q be positive definite, symmetric matrix.
Let p_0, ..., p_(n-1) be linearly independent.
Define d_0=p_0

$$d_k = p_k - \sum_{j=0}^{k-1} \left(\frac{d_j^T Q\, d_k}{d_j^T Q\, d_j}\right) d_j \qquad \text{for } k=1,\dots,n-1$$

Show that $d_0, \dots, d_{n-1}$ are Q-orthogonal.
Remark: this gives a way of producing sets of Q-orthogonal vectors.
Remark 2: more complicated that conjugate gradients ← "magic"

This is like Gram-Schmidt, with orthogonality with respect to Q, rather than ordinary innerproduct.

Proof by induction.
Assume $d_0, \dots, d_{k-1}$ are Q-orthogonal and we must show that $\boxed{d_0, \dots, d_k \text{ are Q-orthogonal}}$ (*)

Note: the base case $k=1$, which is obvious since then there is only one vector.
To prove (*), I must show that $d_i^T Q d_j = 0$ if $i \neq j$ and $i, j \in \{0, \dots, k\}$

This follows by induction hypothesis if both $i, j \leq k-1$
So we only need need to show that, $d_k^T Q d_i = 0$ if $i \leq k-1$

So we check: $d_i^T Q\, d_k = d_i^T Q\, p_k - \sum_{j=0}^{k-1} \left(\frac{d_j^T Q\, p_k}{d_j^T Q\, d_j}\right) d_i^T Q d_j$
by induction hypothesis $d_i^T Q d_j = 0$ when $j = i$
So $d_i^T Q\, d_k - d_i^T Q\, p_k - \frac{d_i^T Q\, p_k}{d_i^T Q d_i} \cdot d_i^T Q\, d_i = 0$