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## Midterm Project

Due date: Sunday, 12 May 2024, 11:59 PM

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### Exercise 1

Let  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  be given by  $f(x) = \frac{1}{2}x^T Ax - b^T x$  with  $A$  symmetric positive definite. Let  $x_m$  be the minimizer of the function  $f$ . Let  $v$  be an eigenvector of  $A$ , and let  $\lambda$  be the associated eigenvalue. Suppose that we use Steepest Descent (SD) method to minimize  $f$  and the starting point for the SD algorithm is  $x_0 = x_m + v$ .

1. Prove that the gradient at  $x_0$  is  $\nabla f(x_0) = \lambda v$ .

To begin with the proof, it is required to remark the gradient formula of the quadratic form function which is the following:

$$\nabla f(x) = Ax - b$$

Then, considering the starting point  $x_0 = x_m + v$ , it is possible to write the gradient at that position as :

$$\nabla f(x_0) = Ax_0 - b \tag{1}$$

$$= A(x_m + v) - b \tag{2}$$

$$= Ax_m + Av - b \tag{3}$$

We know from the hypothesis that  $x_m$  is the minimizer of the function  $f$ , thus, it means that its gradient must be equal to zero according to the first necessary condition for a minimizer:

$$\nabla f(x_m) = 0$$

$$Ax_m - b = 0$$

$$Ax_m = b$$

Substituting  $Ax_m$  inside the expression (3), we obtain that :

$$\nabla f(x_0) = b - Av - b = -Av$$

In addition, we know beforehand the definition of eigenvalues and eigenvectors which affirms

that :

$$Av = \lambda v \quad (4)$$

Hence it is possible to write that :

$$\nabla f(x_0) = \lambda v$$

Consequently, we have proved that  $\nabla f(x_0) = \lambda v$ .

2. How many iterations does the SD method take to minimize the function  $f$  if we use the optimal step length? Show the computations behind your reasoning.

First of all, we know that the Steepest Descent method uses the negative value of the gradient of function at the given point as the step direction to reach its minimizer. Therefore, that direction, starting from  $x_0$ , is equal to the following value as we proved previously:

$$p = -\nabla f(x_0) = -\lambda v$$

Now, we can show that the subsequent iteration  $x_1$  is computed as following:

$$x_1 = x_0 - \alpha \lambda v \quad (5)$$

$$= x_m + v - \alpha \lambda v \quad \text{where } x_0 = x_m + v \quad (6)$$

Secondly, we want to know the number of iterations of the gradient method in the case in which it is used the optimal step length, thus, we can write that:

$$\alpha_{opt} = \frac{\nabla f(x_i)^T \nabla f(x_i)}{\nabla f(x_i)^T A \nabla f(x_i)}$$

Hence, the optimal step size of the starting point  $x_0$  is:

$$\alpha_{opt} = \frac{\nabla f(x_0)^T \nabla f(x_0)}{\nabla f(x_0)^T A \nabla f(x_0)} \quad (7)$$

$$= \frac{\cancel{\lambda} v^T v}{\cancel{\lambda} v^T A v} \quad (8)$$

$$= \frac{v^T v}{v^T \lambda v} \quad Av = \lambda v \quad (4) \quad (9)$$

$$= \frac{1 \cancel{v^T} v}{\lambda \cancel{v^T} v} \quad (10)$$

$$= \frac{1}{\lambda} \quad (11)$$

Knowing that l'optimal step size is equal to  $\frac{1}{\lambda}$  we can simplify the expression 6, thus we achieve that:

$$x_1 = x_m + v - \frac{1}{\cancel{\lambda}} \cancel{\lambda} v$$

$$x_1 = x_m + v - v$$

$$x_1 = x_m$$

Then, knowing that  $x_m$  is the function minimizer as initial hypothesis, its gradient is equal to zero according to the first necessary condition for minimizer point and given this information we can write the next equation:

$$\nabla f(x_m) = \nabla f(x_1) = 0$$

In conclusion, it is possible to notice that the Steepest Descent method converges in only 1 iteration.

In particular, the single iteration that brings the iterative method to converge, directly depends on the fact that we are using the optimal step lenght in the process,  $\alpha_{opt} = \frac{1}{\lambda}$ . This information lets the steepest method to find the best step size in order to get closer towards the minimizer of the function. On the other hand, if  $\alpha \neq \frac{1}{\lambda}$ , the method could have required at least 1 iteration concluding that:

$$x_1 \neq x_m \wedge \nabla f(x_m) \neq \nabla f(x_1) \implies f(x_1) > f(x_m) \wedge \nabla f(x_1) > \nabla f(x_m)$$

## Exercise 2

Given a starting point  $x_0 \in \mathbb{R}^n$  and a set of conjugate directions  $\{p_0, p_1, \dots, p_{n-1}\}$ , we generate the sequence  $\{x_k\}$  by setting

$$x_{k+1} = x_k + \alpha_k p_k \quad (12)$$

where

$$\alpha_k = -\frac{r_k^T p_k}{p_k^T A p_k} \quad (13)$$

and  $r_k$  is the residual, as defined in class.

Consider the following theorem:

**Theorem 1** For any  $x_0 \in \mathbb{R}^n$ , the sequence  $\{x_k\}$  generated by the conjugate gradient direction algorithm converges to the solution  $x^*$  of the linear system  $Ax = b$  in at most  $n$  steps.

Prove the theorem and explain carefully every step of your reasoning.

*Proof:*

To begin with, it can be noticed from the hypothesis that the final solution  $x^*$  can be written directly in term of the iterative process (12) where the step size is computed according to the formula (13). Thus,  $x^*$  is equal to:

$$x^* = \underbrace{x_0 + \alpha_0 p_0}_{x_1} + \alpha_1 p_1 + \alpha_2 p_2 + \dots + \alpha_{n-1} p_{n-1}; \quad (14)$$

$$\underbrace{\hspace{10em}}_{x_2}$$

$$\underbrace{\hspace{15em}}_{x_3}$$

Since, the directions  $\{p_0, p_1, p_2, \dots, p_{n-1}\}$  are linearly independent and orthogonal due to the conjugacy property between each other :

$$\langle p_i, A p_j \rangle = 0 \quad \forall i \neq j \text{ where } A \text{ is s.p.d} \quad (15)$$

They must be a span of the whole  $n$  real space:

$$\mathbb{R}^n = \{p_0, p_1, p_2, \dots, p_{n-1}\}$$

This affirmation allows to write a generic vector  $x \in \mathbb{R}^n$  merely as a linear combination of these directions:

$$x = \sum_{i=0}^{n-1} \gamma_i p_i$$

Especially, this definition can also be extended to the vectors defined by the difference between the final solution  $x^*$  and the initial value  $x_0$  given that also these vectors are part of the same real space  $\mathbb{R}^n$ :

$$\underbrace{e}_{\text{Initial error}} = x^* - x = \sum_{i=0}^{n-1} \sigma_i p_i$$

for some coefficients  $\sigma_i$ .

Now, I want to proof that the coefficients  $\sigma_i$  of the basis  $p_i$  match exactly the the optimal step sizes. To achieve this condition, I need to multiply the initial error with the quantity  $p_k^T A$ , then:

$$p_k^T A e = p_k^T A (x^* - x_0) \quad (16)$$

$$= p_k^T A \sum_{i=0}^{n-1} \sigma_i p_i \quad (17)$$

$$= \sum_{i=0}^{n-1} p_k^T A \sigma_i p_i \quad (18)$$

$$= \sum_{i=0}^{n-1} \sigma_i p_k^T A p_i \quad (19)$$

$$= \sigma_k p_k^T A p_k \quad \text{Conjugacy property (15)} \quad (20)$$

Hence, it is possible to write that :

$$p_k^T A (x^* - x_0) = \sigma_k p_k^T A p_k \implies \sigma_k = \frac{p_k^T A (x^* - x_0)}{p_k^T A p_k}$$

However, it is still required to prove that  $A(x^* - x_0) = -r_k$  (where  $-r_k = b - Ax_k$ ) in order to confirm that the coefficients  $\sigma_i$  correspond to the optimal step sizes.

The generic iteration  $x_k$ , if it is generated by the iterative procedure (12), then we have that :

$$x_k = \underbrace{x_0 + \alpha_0 p_0}_{x_1} + \underbrace{\alpha_1 p_1}_{x_2} + \underbrace{\alpha_2 p_2 + \dots + \alpha_{k-1} p_{k-1}}_{x_3}$$

Subsequently, we aim to pre-multiply the expression with  $p_k^T A$  and using the conjugacy property we obtain that:

$$p_k^T A p_k = p_k^T A x_0$$

Then, substituting the previous expression to the formula  $\sigma_k$  we obtain that:

$$\begin{aligned}
\sigma_k &= \frac{p_k^T A(x^* - x_0)}{p_k^T A p_k} \\
&= \frac{p_k^T A(x^* - x_k)}{p_k^T A p_k} \quad (p_k^T A x_0 = p_k^T A p_k) \\
&= \frac{p_k^T A x^* - p_k^T A x_k}{p_k^T A p_k} \\
&= \frac{p_k^T b - p_k^T A x_k}{p_k^T A p_k} \quad (A x^* = b) \\
&= \frac{p_k^T \overbrace{(b - A x_k)}^{-r_k}}{p_k^T A p_k} \\
&= -\frac{r_k p_k}{p_k^T A p_k} \\
&= \alpha_k
\end{aligned}$$

In conclusion, we prove that the coefficients  $\sigma_k = \alpha_k$  and consequently we verified that the algorithm converges in at most  $n$  steps:

$$\begin{aligned}
x^* - x_0 &= \sum_{i=0}^{n-1} \sigma_i p_i = \sum_{i=0}^{n-1} \alpha_i p_i \\
x^* &= x_0 + \sum_{i=0}^{n-1} \alpha_i p_i
\end{aligned}$$