A Short Tutorial on Conjugate Gradient Method

FEM3220 Matrix Algebra Presentation

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  Adopt an iterative scheme to solve the optimization problem

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$$f(x_{k+1}) \approx f(x_k) + \alpha_k {d_k}^\top \nabla f(x_k)$$

  - Easy to see $f(x_{k+1}) < f(x_k)$ if ${d_k}^\top \nabla f(x_k) < 0$, and $\alpha_k > 0$

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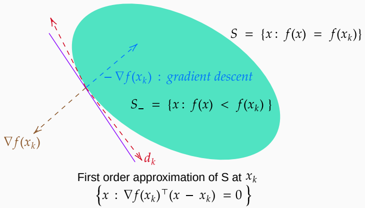

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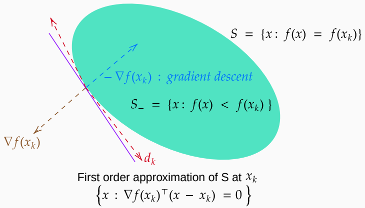

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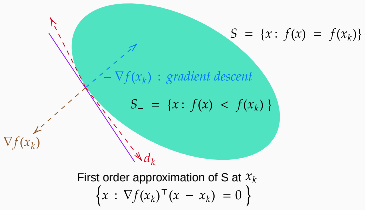

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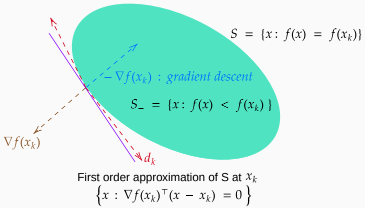

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- How do we find α_k?
  - Exact line search : step size $\alpha_k = \arg\min_{\alpha > 0} f(x_k + \alpha d_k)$

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- Recall:

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- Let $\{d_0, \ldots, d_{n-1}\}$ be a set of linearly independent directions. Note that this is a maximal linearly independent set in $\mathbb{R}^n$, and hence it forms a basis.

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- Let $D := (d_0 | d_1 | \ldots | d_{n-1})$

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- Now, $\Psi(\alpha) = \frac{1}{2}\alpha^\top \underbrace{D^\top A D}_{:=Q} \alpha + (Ax_0 - b)^\top D\alpha + \underbrace{\frac{1}{2}x_0{}^\top A x_0 - b^\top x_0}_{\text{constant}}$

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Definition

Let $A \in \mathbb{R}^{n\times n}$ be a symmetric posititve definite matrix. The vectors $\{d_0, \dots, d_{n-1}\}$ are $A - \textit{conjugate}$ if $d_i{}^T A d_j = 0, \forall\, i \neq j$.

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Proof.

$$\sum_{i=0}^{n-1} \mu_i d_i = 0 \implies d_i^\top A \sum_{j=0}^{n-1} \mu_j d_j = 0$$
$$\implies \sum_{j=0}^{n-1} \mu_j d_i^\top A d_j = 0$$
$$\implies \mu_i d_i^\top A d_i = 0 \, (\because d_i^\top A d_j = 0 \, \forall \, i \neq j (A - conjugacy))$$
$$\implies \mu_i = 0 \, (\because A \text{ is p.d. and } \therefore d_i^\top A d_i \neq 0)$$

Therefore, $\sum_{i=0}^{n-1} \mu_i d_i = 0 \implies \mu_i = 0$, and hence, $\{d_0, \ldots, d_{n-1}\}$ is a linearly independent set. □

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- If yes, how do we obtain them iteratively?

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- If yes, how do we obtain them iteratively?
- How does sequence x_k with $x_{k+1} = x_k + \alpha_k d_k$ converge to x^* in atmost n iterations?

Existence of Conjugate Directions

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$\therefore$ Conjugate directions exist!

Convergence of Conjugate Descent: Expanding Subspace Theorem

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Let us try to prove this claim. We shall denote the gradient $\nabla f(x_k)$ by g_k.

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In other words, $g_k \perp \mathcal{B}_k$.

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$$f(x_0 + \sum_{j=0}^{k-1} \alpha_j d_j) \leq f(x_0 + \sum_{j=0}^{k-1} \mu_j d_j), \quad \mu_j \in \mathbb{R}$$

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So, at n^{th} iteration, $f(x_n) \leq f(x) \, \forall\, x \in x_0 + \mathcal{B}_n$.

Convergence of Conjugate Descent

Claim

${g_j}^\top d_j = {g_0}^\top d_j,\ \forall j$

Proof.

$x_j = x_0 + \sum_{i=0}^{j-1} \alpha_i d_i$

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Hence, $x_n = x^*$

Procedure to Obtain Conjugate Directions: Gram-Schmidt Procedure

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$$d_i{}^\top A d_k = -d_i{}^\top A g_k + \sum_{j=0}^{k-1} \beta_i d_i{}^\top A d_j, \quad i = 0, \ldots, k-1$$

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The above update is called Fletcher-Reeves update

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- The curse of inverse computation can be avoided if the Hessian matrix is positive definite
- Conjugate gradient (descent) method finds the optimal solution in at most n iterations

References

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