Optimization Methods (CS1.404)
Spring 2025

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February 13th, 2025

Descent Direction Methods

- We consider the unconstrained minimization problem as follows:

$$\min_{\mathbf{x}\in\mathbb{R}^n} \quad f(\mathbf{x})$$

  where we assume that f is continuously differentiable over $\mathbb{R}^n$.
- In many cases, it might be very difficult to solve the equation $\nabla f(\mathbf{x}) = \mathbf{0}$ to find the stationary points.
- Even if it is possible to find the solutions of $\nabla f(\mathbf{x}) = \mathbf{0}$, if there are infinitely many solutions, finding the one corresponding to a local minima might be as difficult problem as original optimization problem.
- Due to these reasons, instead of finding the stationary points analytically, we consider adopting an iterative algorithm to find them.
- Iterative algorithms to find the stationary points are of the following form:

$$\mathbf{x}_{k+1} = \mathbf{x}_k + t_k \mathbf{d}_k, \quad k = 0, 1, 2, \ldots,$$

  where $\mathbf{d}_k$ is the so-called direction t_k is the stepsize.

Descent Direction

Definition

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a continuously differentiable function over $\mathbb{R}^n$. A vector $\mathbf{d} \in \mathbb{R}^n$ $(\mathbf{d} \neq \mathbf{0})$ is said a **descent direction** of f at $\mathbf{x}$ if the directional derivative of f at $\mathbf{x}$ along the direction $\mathbf{d}$ is negative, i.e.,

$$\nabla f(\mathbf{x})^T \mathbf{d} < 0$$

Remark: Taking small enough steps along descent directions lead to a decrease of the function f.

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Descent Property of Descent Directions

Lemma

Let f be a continuously differentiable function over an open set S of $\mathbb{R}^n$ and let $\mathbf{x} \in S$. Suppose that $\mathbf{d}$ is a descent direction of f at $\mathbf{x}$. Then there exist $\epsilon > 0$ such that

$$f(\mathbf{x} + \alpha \mathbf{d}) < f(\mathbf{x})$$

for any $\alpha \in (0, \epsilon]$.

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Schematic Descent Directions Method

Schematic Descent Directions Method

- **Initialization:** Pick $\mathbf{x}_0 \in \mathbb{R}^n$ arbitrarily
- **General Step:** For any $k = 0, 1, 2, \ldots$, set
  1. Pick a descent direction $\mathbf{d}_k$.
  2. Find a step size t_k satisfying $f(\mathbf{x}_k + t_k \mathbf{d}_k) < f(\mathbf{x}_k)$.
  3. Set $\mathbf{x}_{k+1} = \mathbf{x}_k + t_k \mathbf{d}_k$.
  4. STOP if the stopping condition is satisfied and Output $\mathbf{x}_{k+1}$. Else go to Step (1).

Challanges:

1. How to choose the initial point $\mathbf{x}_0$?
2. How to choose the descent direction $\mathbf{d}_k$?
3. How to choose the stepsize t_k?
4. What should be the stopping condition?
5. Does the algorithm converge? If yes, then how fast does it converge? Does the convergence depend on $\mathbf{x}_0$?

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Stopping Condition

1. Stopping condition for a minimization problem is $\nabla f(\mathbf{x}_k) = \mathbf{0}$ and $\nabla^2 f(\mathbf{x}_k)$ is positive semi-definite.
2. A practical stopping condition is $\|\nabla f(\mathbf{x}_k)\| \leq \epsilon$.
3. Other stopping conditions

$$\|\nabla f(\mathbf{x}_k)\| < \epsilon(1 + |f(\mathbf{x}_k)|)$$

$$\frac{f(\mathbf{x}_k) - f(\mathbf{x}_{k+1})}{|f(\mathbf{x}_k)|} \leq \epsilon$$

Finding Step Size t_k

- Step size t_k is chosen in such a way that $f(\mathbf{x}_{k+1}) < f(\mathbf{x}_k)$.
- The method of finding step size is called line search, since it a minimization of one dimensional function $g(t) = f(\mathbf{x}_k + t\mathbf{d}_k)$.
- Four popular choices for step size selection are as follows:
  - **Constant Step size:** $t_k = \eta$, $\forall k$. It is very simple approach, but it is unclear how to choose η. A large value of η might cause the algorithm to be nondecreasing and small η can cause very slow convergence.
  - **Diminishing Step Size:** $\alpha_k \to 0$, $\sum_{k=1}^{\infty} \alpha_k = \infty$. For example, $\alpha_k = \frac{1}{k}$.
    - Descent not guaranteed at each step; only later when becomes small.
    - $\sum_{k=1}^{\infty} \alpha_k = \infty$ imposed to guarantee progress does not become too slow.
    - Good theoretical guarantees, but unless the right sequence is chosen, can also be a slow method.

Finding Step Size t_k

- **Exact Line Search:** Here, t_k is the minimizer of f along the ray $\mathbf{x}_k + t\mathbf{d}_k$.

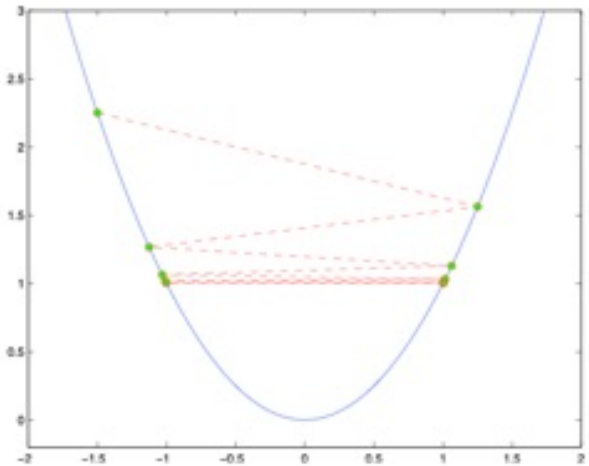
$$t_k = \arg\min_{t \geq 0} \; f(\mathbf{x}_k + t\mathbf{d}_k)$$

  It is an attractive approach, but it is not always possible to find the exact minimizer of $g(t) = f(\mathbf{x}_k + t\mathbf{d}_k)$.
- **Inexact Line Search:** This method iteratively finds t_k which minimizes f along the ray $\mathbf{x}_k + t\mathbf{d}_k$. It finds good enough step size which ensures sufficient decrease.

Example 1: How line search methods fail!

Large Step Sizes

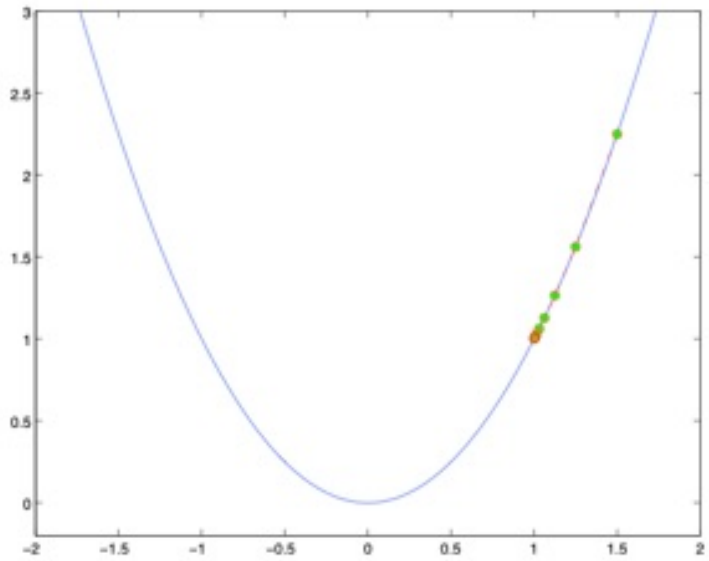
- The objective function $f(x) = x^2$. Global minimizer is $x^* = 0$ and optimal value of $f(x^*) = 0$.
- Iterates $x_{k+1} = x_k + \alpha_k d_k$ generated by the descent directions $d_k = (-1)^k$ and steps $\alpha_k = 2 + 3/2^k$ from $x_1 = 2$.
- $\{x\} = \{2, -3/2, 5/4, -9/8, \ldots\}$. As $k \to \infty$, x_k will oscillate between $+1$ and -1. Thus, the sequence x_k, $k = 1, 2, 3, \ldots$ does not converge.
- $\{f\} = \{4, 9/4, 25/16, 81/64, \ldots\}$. Thus, the function value decreases in each iteration. As $k \to \infty$, $f(x_k)$ will remain close to 1.
- **Key reason is a small decrease in function values relative to the step length.**



Example 2: How line search methods fail !

Small Step Sizes

- The objective function $f(x) = x^2$. Global minimizer is $x^* = 0$ and optimal value of $f(x^*) = 0$.
- Iterates $x_{k+1} = x_k + \alpha_k d_k$ generated by the descent directions $d_k = -1$, $\forall k$ and steps $\alpha_k = 1/2^k$ from $x_1 = 2$.
- $\{x\} = \{2, 3/2, 5/4, 9/8, \ldots\}$. As $k \to \infty$, x_k will converge to $+1$. But, $\lim_{k\to\infty} x_k \neq x^*$.
- $\{f\} = \{4, 9/4, 25/16, 81/64, \ldots\}$. Thus, the function value decreases in each iteration. As $k \to \infty$, $f(x_k)$ will remain close to 1.
- **Key reason is step sizes are too small compared to the initial rate of decrease of f.**



Sufficient Decrease Condition

Lemma

Let f be a continuously differentiable function over $\mathbb{R}^n$ and let $\mathbf{x} \in \mathbb{R}^n$. Suppose that $\mathbf{d} \in \mathbb{R}^n$ ($\mathbf{d} \neq \mathbf{0}$) is a descent direction of $\mathbf{d}$ at $\mathbf{x}$ and let $\alpha \in (0, 1)$. Then there exist $\epsilon > 0$ such that the inequality

$$f(\mathbf{x}) - f(\mathbf{x} + t\mathbf{d}) \geq -\alpha t \nabla f(\mathbf{x})^T \mathbf{d}$$

holds for all $t \in [0, \epsilon]$.

Armijo Line Search Method

- Armijo inexact line search condition stipulates that α_k should, first of all, give sufficient decrease in the objective function f, as measured by the following inequality:

$$f(\mathbf{x}_k + \alpha_k \mathbf{d}_k) \leq f(\mathbf{x}_k) + c_1 \alpha_k \nabla f(\mathbf{x}_k)^T \mathbf{d}_k$$

  for some constant $c_1 \in (0, 1)$.
- Thus, the reduction in f should be proportional to both the step length α_k and the directional derivative $\nabla f(\mathbf{x}_k)\mathbf{d}_k$.

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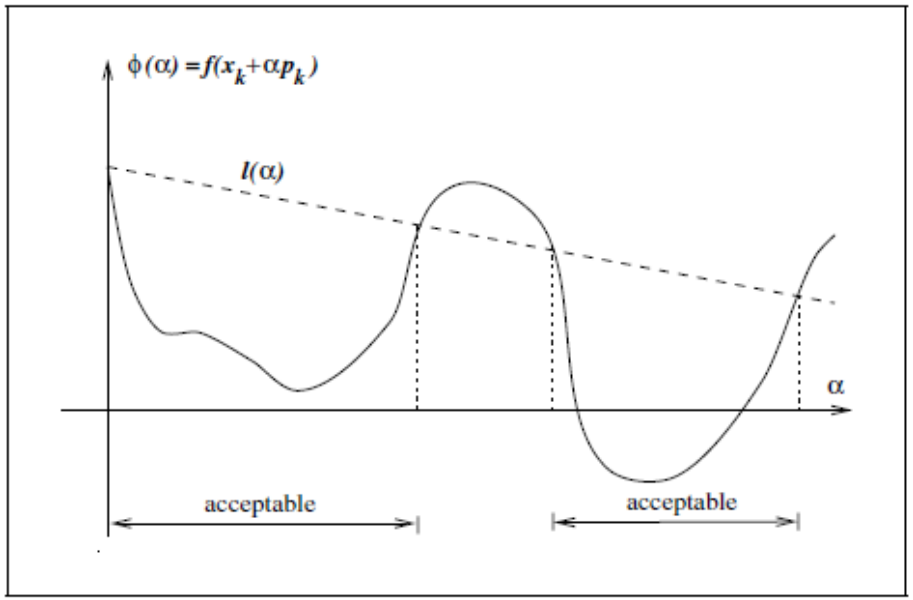
Geometric Interpretation of Armijo Condition



- Consider $\phi(\alpha) = f(\mathbf{x}_k + \alpha \mathbf{d}_k)$ and $l(\alpha) = f(\mathbf{x}_k) + c_1 \alpha_k \nabla f(\mathbf{x}_k)^T \mathbf{d}_k$.
- The function $l(\alpha)$ has negative slope $c_1 \nabla f(\mathbf{x}_k)^T \mathbf{d}_k$, but because $c_1 \in (0, 1)$, it lies above the graph of ϕ for small positive values of α.
- The sufficient decrease condition states that α is acceptable only if $\phi(\alpha) \leq l(\alpha)$. In practice, c_1 is chosen to be quite small, say $c_1 = 10^{-4}$.

Backtracking Line Search With Armijo

Backtracking

1. **Initialize:** $\alpha^{(0)} \in (0,1)$, $\tau \in (0,1)$, $l = 0$
2. Until $f(\mathbf{x}_k + \alpha^{(l)}\mathbf{d}_k) > f(\mathbf{x}_k) + c_1\alpha^{(l)}\nabla f(\mathbf{x}_k)^T\mathbf{d}_k$
   1. Set $\alpha^{(l+1)} = \tau\alpha^{(l)}$
   2. $l = l + 1$
3. $\alpha_k = \alpha^{(l)}$

In practice, the following choices are used

- $\tau \in (0.1, 0.5]$
- $c_1 \in [10^{-5}, 10^{-1}]$

Issue with Armijo's condition:

- It does not ensure that the step size is sufficiently large because Armijo's condition can be satisfied even with a very small step size.
- Backtracking partially addresses this by starting from large step sizes and checking Armijo's condition.
- But can we add some other condition to Armijo?

Armijo-Goldstein Line Search

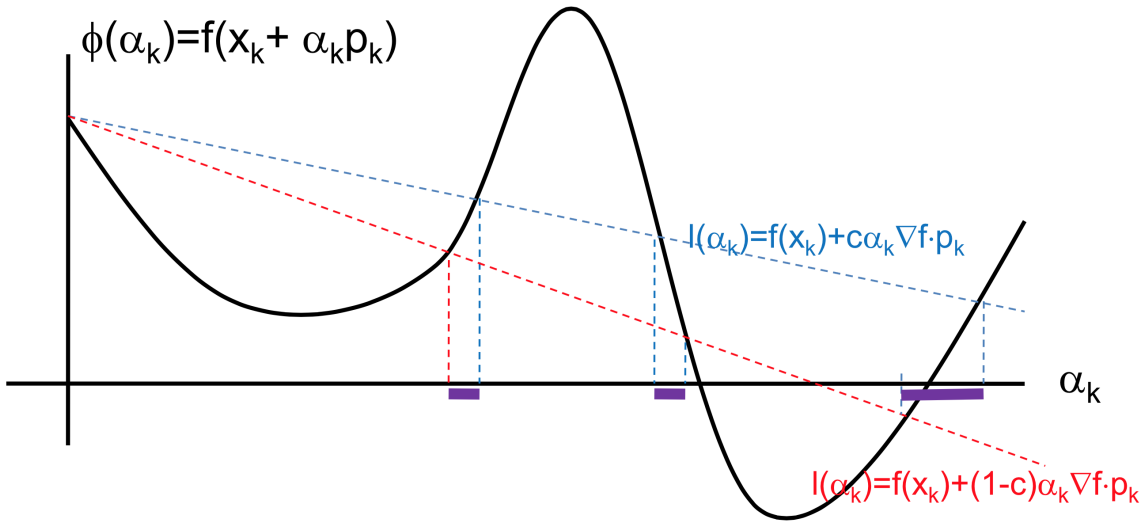
- Armijo-Goldstein inexact line search condition requires that α_k should be sufficiently large and it should give sufficient decrease in the objective function f as well.
- The condition is as follows.

  $$f(\mathbf{x}_k) + (1 - c_1)\alpha_k \nabla f(\mathbf{x}_k)^T \mathbf{d}_k \leq f(\mathbf{x}_k + \alpha_k \mathbf{d}_k) \leq f(\mathbf{x}_k) + c_1 \alpha_k \nabla f(\mathbf{x}_k)^T \mathbf{d}_k$$

  for some constant $c_1 \in (0, 1/2)$.
- The first inequality is introduced to control the step length from below.
- **Issue:** First inequality may exclude all minimizers of ϕ (see in figure). One can see that the Goldstein condition misses the first local minima.

Geometrical Interpretation of Goldstein Conditions

$$(1-c)\alpha_k \nabla f(x_k)^T p_k + f(x_k) \leq f(x_k + \alpha_k p_k) \leq c\alpha_k \nabla f(x_k)^T p_k + f(x_k)$$
$$(0 < c < 1/2)$$



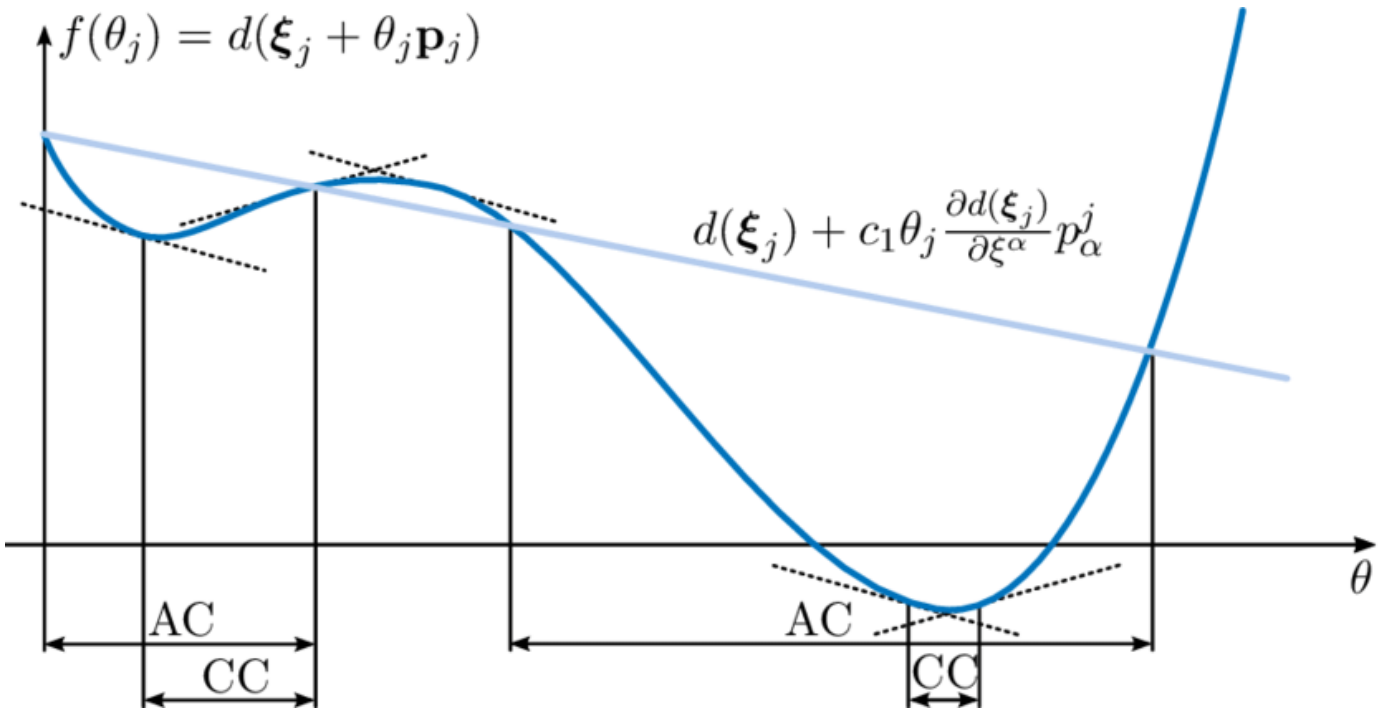
Armijo-Wolfe Condition

- Armijo-Wolfe condition is also used to rule out unacceptably short steps (called the curvature condition) and ensure sufficient decrease.
- The conditions are

$$f(\mathbf{x}_k + \alpha_k \mathbf{d}_k) \leq f(\mathbf{x}_k) + c_1 \alpha_k \nabla f(\mathbf{x}_k)^T \mathbf{d}_k$$
$$\nabla f(\mathbf{x}_k + \alpha_k \mathbf{d}_k)^T \mathbf{d}_k \geq c_2 \nabla f(\mathbf{x}_k)^T \mathbf{d}_k$$

  for some constants $0 < c_2 < c_1 < 1$.
- LHS in the curvature condition is simply the derivative $\phi'(\alpha_k)$. So, the curvature condition ensures that the slope of ϕ at α_k is greater than c_2 times the initial slope $\phi'(0)$.
- If the slope $\phi'(\alpha)$ is strongly negative, we have an indication that we can reduce f significantly by moving further along the chosen direction. if $\phi'(\alpha_k)$ is only slightly negative or even positive, then we cannot expect more decrease in f in this direction, so it makes sense to terminate the line search.
- Thus, Wolf condition ensures sufficient rate of decrease of function value in the given direction.
- **Issue:** A step length may satisfy the Armijo-Wolfe conditions without being particularly close to a minimizer of ϕ.

Armijo-Wolfe Condition



Optimization Methods (CS1.404), Spring 2025

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March 3rd, 2025

Armijo-Wolfe Condition

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- The conditions are

$$f(\mathbf{x}_k + \alpha_k \mathbf{d}_k) \leq f(\mathbf{x}_k) + c_1 \alpha_k \nabla f(\mathbf{x}_k)^T \mathbf{d}_k$$
$$\nabla f(\mathbf{x}_k + \alpha_k \mathbf{d}_k)^T \mathbf{d}_k \geq c_2 \nabla f(\mathbf{x}_k)^T \mathbf{d}_k$$

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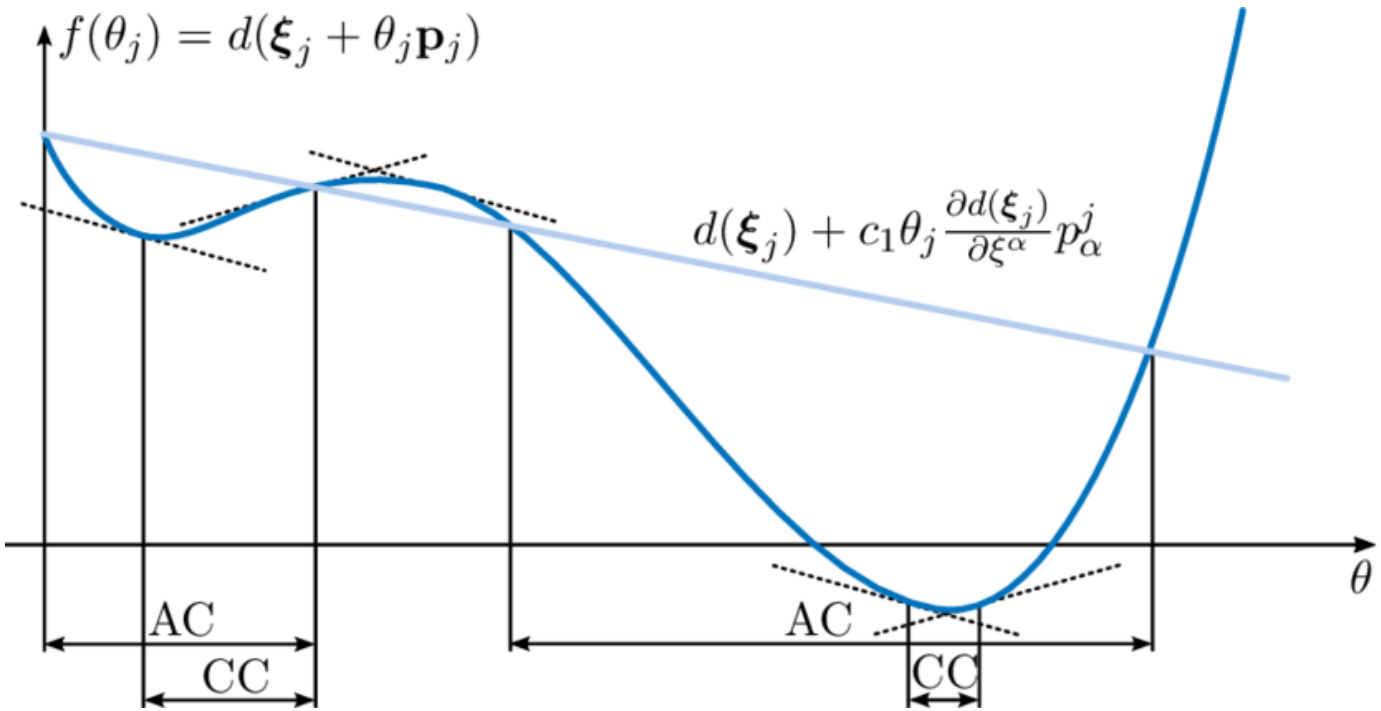
Armijo-Wolfe Condition



Exact Line Search

Here, α_k is the minimizer of f along the ray $\mathbf{x}_k + \alpha \mathbf{d}_k$.

$$\alpha_k = \arg\min_{\alpha \geq 0} f(\mathbf{x}_k + \alpha \mathbf{d}_k).$$

Example: Exact line search for quadratic function

- Let $f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T A\mathbf{x} + \mathbf{b}^T\mathbf{x} + c$, where A is an $n \times n$ symmetric positive definite matrix, $\mathbf{b} \in \mathbb{R}^n$ and $c \in \mathbb{R}$.
- Let $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{d} \in \mathbb{R}^n$ be a descent direction of f at $\mathbf{x}$.

Then

$$\arg\min_{t \geq 0} \; f(\mathbf{x} + t\mathbf{d}) = -\frac{\nabla f(\mathbf{x})^T \mathbf{d}}{\mathbf{d}^T A \mathbf{d}}$$

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Steepest Gradient Descent

- In the gradient method, the descent direction is chosen as the negative of the gradient at the current point: $\mathbf{d}_k = -\nabla f(\mathbf{x}_k)$. For such $\mathbf{d}_k$, we see that $\nabla f(\mathbf{x}_k)^T \mathbf{d}_k = -\|\mathbf{d}_k\|^2 < 0$.
- This is also called the steepest gradient descent direction.

Lemma: Optimality of the Steepest Gradient Descent Diirection

Let f be a continuously differentiable function, and let $\mathbf{x} \in \mathbb{R}^n$ be a non-stationary point (i.e., $\nabla f(\mathbf{x}) \neq \mathbf{0}$). Then, the optimal solution of

$$\min_{\mathbf{d} \in \mathbb{R}^n} \nabla f(\mathbf{x})^T \mathbf{d}$$
$$\text{s.t. } \|\mathbf{d}\| = 1$$

is $\mathbf{d} = -\frac{\nabla f(\mathbf{x})}{\|\nabla f(\mathbf{x})\|}$.

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Steepest Gradient Descent Algorithm

- **Input:** $\epsilon > 0$ - tolerance parameter
- **Initialization:** Pick $\mathbf{x}_0 \in \mathbb{R}^n$ arbitrarily.
- **General Step:** For any $k = 0, 1, 2, \ldots$ execute the following steps
  1. Fix $\mathbf{d}_k = -\nabla f(\mathbf{x}_k)$
  2. Pick stepsize t_k by a line search on the function

$$g(t) = f(\mathbf{x}_k + t\mathbf{d}_k)$$

  3. Set $\mathbf{x}_{k+1} = \mathbf{x}_k + t_k\mathbf{d}_k$
  4. If $\|\nabla f(\mathbf{x}_k)\| \leq \epsilon$, then stop and $\mathbf{x}_{k+1}$ is the output.

Example 1: Gradient Descent with Exact Line Search on Quadratic Function

- Consider function $f(x, y) = x^2 + 2y^2$, whose optimal solution is $(0, 0)$ with optimal value 0.
- Let $(x_0, y_0) = (2, 1)$, $\epsilon = 10^{-5}$.
- The Gradient descent approach stops in 13 iterations and finds a solution that is pretty close to the optimal value. $(x^*, y^*) = (0.1254 * 10^{-5}, -0627 * 10^{-5})$.

```
iter_number =   1 norm_grad = 1.885618 fun_val = 0.666667
iter_number =   2 norm_grad = 0.628539 fun_val = 0.074074
iter_number =   3 norm_grad = 0.209513 fun_val = 0.008230
iter_number =   4 norm_grad = 0.069838 fun_val = 0.000914
iter_number =   5 norm_grad = 0.023279 fun_val = 0.000102
iter_number =   6 norm_grad = 0.007760 fun_val = 0.000011
iter_number =   7 norm_grad = 0.002587 fun_val = 0.000001
iter_number =   8 norm_grad = 0.000862 fun_val = 0.000000
iter_number =   9 norm_grad = 0.000287 fun_val = 0.000000
iter_number =  10 norm_grad = 0.000096 fun_val = 0.000000
iter_number =  11 norm_grad = 0.000032 fun_val = 0.000000
iter_number =  12 norm_grad = 0.000011 fun_val = 0.000000
iter_number =  13 norm_grad = 0.000004 fun_val = 0.000000
```

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Example 1: Gradient Descent with Constant Step Size on Quadratic Function

- Consider function $f(x, y) = x^2 + 2y^2$, whose optimal solution is $(0, 0)$ with optimal value 0.
- Let $(x_0, y_0) = (2, 1)$, $\epsilon = 10^{-5}$, $t_k = 0.1$.
- The Gradient descent approach stops in 58 iterations.
- The stepsize was too small, which caused slow convergence.

```
iter_number =   1 norm_grad = 4.000000 fun_val = 3.280000
iter_number =   2 norm_grad = 2.937210 fun_val = 1.897600
iter_number =   3 norm_grad = 2.222791 fun_val = 1.141888
      :                :                :
iter_number =  56 norm_grad = 0.000015 fun_val = 0.000000
iter_number =  57 norm_grad = 0.000012 fun_val = 0.000000
iter_number =  58 norm_grad = 0.000010 fun_val = 0.000000
```

Example 1: Gradient Descent with Backtracking Line Search on Quadratic Function

- Consider function $f(x, y) = x^2 + 2y^2$, whose optimal solution is $(0, 0)$ with optimal value 0.
- Let $(x_0, y_0) = (2, 1)$, $\epsilon = 10^{-5}$, $\tau = 0.5$, $s = 2$, $c_1 = 0.25$.
- The Gradient descent approach stops in 2 iterations and outputs the exact optimal solution.
- **For this example, inexact line search performs better than exact line search.**

```
iter_number =   1 norm_grad = 2.000000 fun_val = 1.000000
iter_number =   2 norm_grad = 0.000000 fun_val = 0.000000
```

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Example 2: Gradient Descent with Backtracking Line Search on Quadratic Function

- Consider function $f(x, y) = x^2 + \frac{1}{100}y^2$, whose optimal solution is $(0, 0)$ with optimal value 0.
- Let $(x_0, y_0) = (\frac{1}{100}, 1)$, $\epsilon = 10^{-5}$, $\tau = 0.5$, $s = 2$, $c_1 = 0.25$.
- The Gradient descent approach stops in 201 iterations.

```
iter_number =   1 norm_grad = 0.028003 fun_val = 0.009704
iter_number =   2 norm_grad = 0.027730 fun_val = 0.009324
iter_number =   3 norm_grad = 0.027465 fun_val = 0.008958
      :                   :                  :
iter_number = 201 norm_grad = 0.000010 fun_val = 0.000000
```

Convergence of Steepest Gradient Descent

- For different quadratic functions, we observe that the convergence time varies for gradient descent.
- Can we find a measure that can predict how many iterations are needed for the convergence of the Gradient method?
- This measure would quantify, in some sense, the hardness of the problem.
- One such measure that can partially answer the above question is **condition number**.

Convergence of Steepest Gradient Descent with Exact Line Search for Quadratic Function

- Let $f(\mathbf{x}) = \mathbf{x}^T A\mathbf{x}$, where A is a symmetric positive definite matrix.
- For Steepest descent, $\mathbf{d}_k = -\nabla f(\mathbf{x}_k) = -2A\mathbf{x}_k$.
- Exact line search will result in $t_k = \arg\min_{t\geq 0} \; f(\mathbf{x}_k + t\mathbf{d}_k) = \frac{\mathbf{d}_k^T\mathbf{d}_k}{2\mathbf{d}_k^T A\mathbf{d}_k}$. Using this, we get

$$
\begin{aligned}
f(\mathbf{x}_k + t_k\mathbf{d}_k) &= f(\mathbf{x}_k) + t_k^2\mathbf{d}_k^T A\mathbf{d}_k + 2t_k\mathbf{d}_k^T A\mathbf{x}_k \\
&= \mathbf{x}_k^T A\mathbf{x}_k + \frac{(\mathbf{d}_k^T\mathbf{d}_k)^2}{4\mathbf{d}_k^T A\mathbf{d}_k} + \frac{\mathbf{d}_k^T\mathbf{d}_k}{2\mathbf{d}_k^T A\mathbf{d}_k}\mathbf{d}_k^T(-\mathbf{d}_k) \\
&= \mathbf{x}_k^T A\mathbf{x}_k - \frac{1}{4}\frac{(\mathbf{d}_k^T\mathbf{d}_k)^2}{\mathbf{d}_k^T A\mathbf{d}_k} = \mathbf{x}_k^T A\mathbf{x}_k\left(1 - \frac{1}{4}\frac{(\mathbf{d}_k^T\mathbf{d}_k)^2}{(\mathbf{d}_k^T A\mathbf{d}_k)(\mathbf{x}_k^T A\mathbf{x}_k)}\right) \\
&= \mathbf{x}_k^T A\mathbf{x}_k\left(1 - \frac{1}{4}\frac{(\mathbf{d}_k^T\mathbf{d}_k)^2}{(\mathbf{d}_k^T A\mathbf{d}_k)(\mathbf{x}_k^T AA^{-1}A\mathbf{x}_k)}\right) \\
&= \left(1 - \frac{(\mathbf{d}_k^T\mathbf{d}_k)^2}{(\mathbf{d}_k^T A\mathbf{d}_k)(\mathbf{d}_k^T A^{-1}\mathbf{d}_k)}\right) f(\mathbf{x}_k)
\end{aligned}
$$

Convergence of Steepest Gradient Descent with Exact Line Search for Quadratic Function

Kantorovich Inequality

Let A be a positive definite $n \times n$ matrix. Then for any $\mathbf{x} \in \mathbb{R}^n$ ($\mathbf{x} \neq \mathbf{0}$), the inequality

$$\frac{(\mathbf{x}^T\mathbf{x})^2}{(\mathbf{x}^TA\mathbf{x})(\mathbf{x}^TA^{-1}\mathbf{x})} \geq \frac{4\lambda_{max}(A)\lambda_{min}(A)}{(\lambda_{max}(A)+\lambda_{min}(A))^2}$$

holds.

Lemma

Let $\{\mathbf{x}_k\}_{k\geq 0}$ be the sequence generated by the gradient descent method with exact line search for finding the minimizer of $f(\mathbf{x}) = \mathbf{x}^TA\mathbf{x}$. Then, for any $k = 0, 1, 2, \ldots$

$$f(\mathbf{x}_{k+1}) \leq \left(\frac{M-m}{M+m}\right)^2 f(\mathbf{x}_k)$$

where $M = \lambda_{max}(A)$ and $m = \lambda_{min}(A)$.

Condition Number and Convergence

Condition Number

Let A be an $n \times n$ positive definite matrix. Then the **condition number** of A is defined as

$$\chi(A) = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)}$$

- For quadratic functions with large condition numbers, the gradient method might require a large number of iterations to converge.
- Matrices with large condition numbers are called **ill conditioned**.
- Matrices with small condition numbers are called **well conditioned**.
- In the case of non-quadratic functions, the rate of convergence of $\mathbf{x}_k$ to a given stationary point $\mathbf{x}^*$ depends on the condition number of $\nabla^2 f(\mathbf{x}^*)$.

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Example: Rosenbrock Function

- The Rosenbrock function is the following function

$$f(x_1, x_2) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$

- The optimal solution is $(1, 1)$ with the optimal value 0.
- The Rosenbrock function is extremely ill-conditioned at the optimal solution.

$$\nabla f(\mathbf{x}) = \begin{pmatrix} -400x_1(x_2 - x_1^2) - 2(1 - x_1) \\ 200(x_2 - x_1^2) \end{pmatrix}$$

$$\nabla^2 f(\mathbf{x}) = \begin{pmatrix} -400x_2 + 1200x_1^2 + 2 & -400x_1 \\ -400x_1 & 200 \end{pmatrix}$$

- $(1, 1)$ is unique stationary point.
- $\nabla^2 f(1, 1) = \begin{pmatrix} 802 & -400 \\ -400 & 200 \end{pmatrix}$
- Condition number of $\nabla^2 f(1, 1)$ is 2.508×10^3

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Example: Steepest Descent with Backtracking on Rosenbrock Function

- Starting point $\mathbf{x}_0 = [2, 5]^T$. The run required 6890 iterations. So, ill-conditioning of $\nabla^2 f(1, 1)$ has significant impact.

```
iter_number =    1 norm_grad = 118.254478 fun_val = 3.221022
iter_number =    2 norm_grad = 0.723051 fun_val = 1.496586
      :                :                :
iter_number = 6889 norm_grad = 0.000019 fun_val = 0.000000
iter_number = 6890 norm_grad = 0.000009 fun_val = 0.000000
```

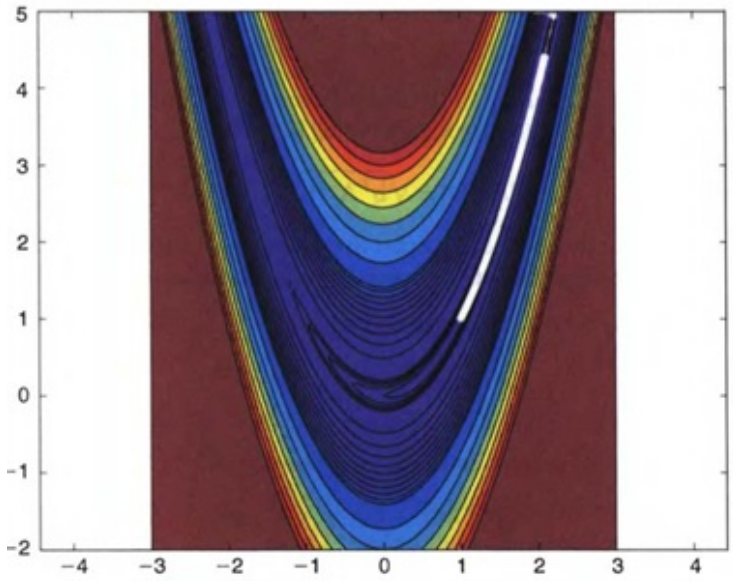

Figure: Banana-shaped contour lines of the Rosenbrock function surrounding the unique stationary point $(1, 1)$. Along with it thousands of iterations of steepest descent.

Convergence Analysis of Gradient Descent

L-Smooth Functions

An L-smooth function is continuously differentiable and that its gradient ∇f is Lipschitz continuous over $\mathbb{R}^n$, meaning that there exists $L > 0$ for which

$$\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\| \leq L\|\mathbf{x} - \mathbf{y}\|, \quad \text{for any } \mathbf{x}, \mathbf{y} \in \mathbb{R}^n.$$

The class of functions with Lipschitz gradient with constant L are denoted by $\mathcal{C}_L^1$.

Examples:

- **Linear Functions:** Given $\mathbf{a} \in \mathbb{R}^n$, the function $f(\mathbf{x}) = \mathbf{a}^T\mathbf{x}$ is in $\mathcal{C}_0^1$.
- **Quadratic Functions:** Let A be an $n \times n$ symmetric matrix, $\mathbf{b} \in \mathbb{R}^n$ and $c \in \mathbb{R}$. Then,

$$\|f(\mathbf{x}) - f(\mathbf{y})\| = 2\|A(\mathbf{x} - \mathbf{y})\| \leq 2\|A\|.\|\mathbf{x} - \mathbf{y}\|$$

Thus, the Lipschitz constant of ∇f is $2\|A\|$.

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Interpretation of L-Smoothness

- The gradient of a function measures how the function changes when we move in a particular direction from a point.
- If the gradient were to change arbitrarily quickly, the old gradient does not give us much information at all, even if we take a small step.
- In contrast, smoothness assures us that the gradient cannot change too quickly. Therefore, we have an assurance that the gradient information is informative within a region around where it is taken. The implication is that we can decrease the function's value by moving in the direction opposite of the gradient.

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Properties of L-Smooth Function

Theorem 4.20 (Chapter 4: Introduction to Nonlinear Optimization by Amir Beck)

Let f be a twice continuously differentiable function over $\mathbb{R}^n$. Then the following two claims are equivalent.

- $f \in \mathcal{C}_L^1(\mathbb{R}^n)$
- $\|\nabla^2 f(\mathbf{x})\| \leq L$ for any $\mathbf{x} \in \mathbb{R}^n$.

See the proof in the book.

Example: Let $f : \mathbb{R} \to \mathbb{R}$ be given by $f(x) = \sqrt{1+x^2}$. Then,

$$0 \leq f''(x) = \frac{1}{(1+x^2)^{3/2}} \leq 1$$

for any $x \in \mathbb{R}$. Thus, $f \in \mathcal{C}_1^1$.

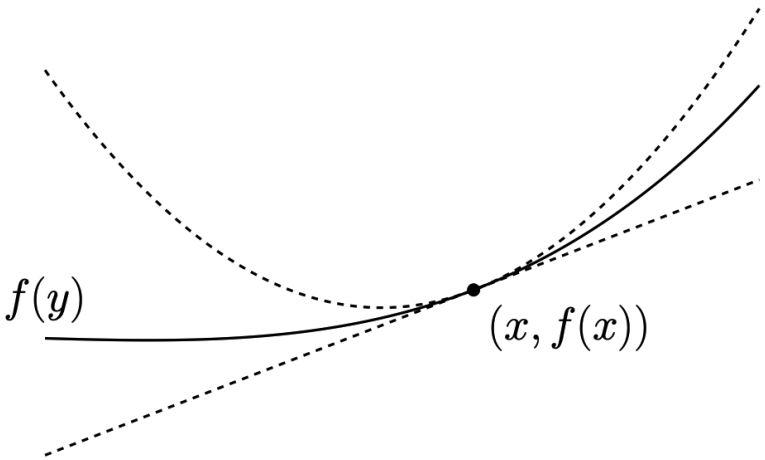
Descent Property of L-Smooth Functions

Lemma 4.22 (Chapter 4: Introduction to Nonlinear Optimization by Amir Beck)

Let $f \in C_L^1(\mathbb{R}^n)$ for some $L > 0$. Then, for any $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$, it holds that

$$f(\mathbf{y}) \leq f(\mathbf{x}) + \nabla f(\mathbf{x})^T(\mathbf{y} - \mathbf{x}) + \frac{L}{2}\|\mathbf{x} - \mathbf{y}\|^2$$

See the proof in the book.



Comments:

1. This result shows that an L-smooth function can be bounded above by a quadratic function over the entire space.
2. This result is very useful in the convergence proofs of gradient-based methods.

Descent Property of Steepest Descent for L-Smooth Functions

Lemma (Sufficient Decrease of the Gradient Method)

Suppose that $f \in \mathcal{C}_L^1(\mathbb{R}^n)$. Let $\{\mathbf{x}_k\}_{k\geq 0}$ be the sequence generated by the gradient method for solving $\min_{\mathbf{x}\in\mathbb{R}^n} f(\mathbf{x})$ with one of the following stepsize strategies:

- constant stepsize $\bar{t} \in (0, \frac{2}{L})$
- exact line search
- backtracking procedure with parameters $s \in \mathbb{R}_{++}$, $\alpha \in (0,1)$, $\beta \in (0,1)$.

Then for any $\mathbf{x} \in \mathbb{R}^n$ and $t > 0$

$$f(\mathbf{x}) - f(\mathbf{x} - t\nabla f(\mathbf{x})) \geq M\|\nabla f(\mathbf{x})\|^2$$

where

$$M = \begin{cases} \bar{t}\left(1 - \frac{\bar{t}L}{2}\right), & \text{constant stepsize} \\ \frac{1}{2L}, & \text{exact line search} \\ \alpha \min\left\{s, \frac{2(1-\alpha)\beta}{L}\right\}, & \text{backtracking} \end{cases}$$

- Above result shows that at each iteration the decrease in the function value is at least a constant times the squared norm of the gradient.

Convergence of the Steepest Descent for L-Smooth Functions

Lemma (Sufficient Decrease of the Gradient Method)

Suppose that $f \in \mathbb{C}_L^{1,1}(\mathbb{R}^n)$. Let $\{\mathbf{x}_k\}_{k\geq 0}$ be the sequence generated by the gradient method for solving $\min_{\mathbf{x}\in\mathbb{R}^n} f(\mathbf{x})$ with one of the following stepsize strategies:

- constant stepsize $\bar{t} \in (0, \frac{2}{L})$
- exact line search
- backtracking procedure with parameters $s \in \mathbb{R}_{++}$, $\alpha \in (0,1)$, $\beta \in (0,1)$.

Assume that f is bounded below over $\mathbb{R}^n$, that is, there exists $m \in \mathbb{R}$ such that $f(\mathbf{x}) > m$ for all $\mathbf{x} \in \mathbb{R}^n$. Then we have the following:

1. The sequence $\{f(\mathbf{x}_k)\}_{k\geq 0}$ is non-increasing. In addition, for any $k \geq 0$, $f(\mathbf{x}_{k+1}) < f(\mathbf{x}_k)$ unless $\nabla f(\mathbf{x}_k) = \mathbf{0}$.
2. $\nabla f(\mathbf{x}_k) \to \mathbf{0}$ as $k \to \infty$.

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Optimization Methods (CS1.404), Spring 2025

Naresh Manwani

Machine Learning Lab, IIIT-H

March 5th, 2025

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Diagonal Scaling to Improve Condition Number

- Consider the problem $\min_{\mathbf{x}} \frac{1}{2}\mathbf{x}^T\mathbf{H}\mathbf{x} - \mathbf{c}^T\mathbf{x}$, where $\mathbf{H}$ is a symmetric positive definite matrix.
- Condition number of Hessian matrix controls the convergence rate of steepest descent.
- Faster convergence if Hessian is closer to a scalar multiple of the identity matrix.
- Can we transform the problem into another space in which the condition number of the Hessian becomes Identity?
- Let $\mathbf{H} = \mathbf{L}\mathbf{L}^T$ be the Cholesky decomposition of H.
- Define $\mathbf{y} = \mathbf{L}^T\mathbf{x}$.
- Consider the transformed function $h(\mathbf{y}) = f(\mathbf{L}^{-T}\mathbf{y})$.

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Diagonal Scaling to Improve Condition Number

$$h(\mathbf{y}) = f(\mathbf{L}^{-T}\mathbf{y}) = \frac{1}{2}\mathbf{y}^T\mathbf{L}^{-1}\mathbf{H}\mathbf{L}^{-T}\mathbf{y} - \mathbf{c}^T(\mathbf{L}^{-T}\mathbf{y})$$
$$= \frac{1}{2}\mathbf{y}^T\mathbf{L}^{-1}\mathbf{L}\mathbf{L}^T\mathbf{L}^{-T}\mathbf{y} - \mathbf{c}^T(\mathbf{L}^{-T}\mathbf{y})$$
$$= \frac{1}{2}\mathbf{y}^T\mathbf{y} - \mathbf{c}^T(\mathbf{L}^{-T}\mathbf{y})$$

- The hessian of $h(\mathbf{y})$ is identity matrix.
- Let us apply steepest descent on $\mathbf{y}$ space.

$$\mathbf{y}^{k+1} = \mathbf{y}^k - \nabla h(\mathbf{y}^k) = \mathbf{y}^k - \mathbf{L}^{-1}\nabla f(\mathbf{L}^{-T}\mathbf{y}^k)$$

- Applying transformation $\mathbf{L}^{-T}$ on both sides

$$\mathbf{L}^{-T}\mathbf{y}^{k+1} = \mathbf{L}^{-T}\mathbf{y}^k - \mathbf{L}^{-T}\mathbf{L}^{-1}\nabla f(\mathbf{L}^{-T}\mathbf{y}^k)$$
$$\Rightarrow \quad \mathbf{x}^{k+1} = \mathbf{x}^k - \mathbf{H}^{-T}\nabla f(\mathbf{x}^k) = \mathbf{x}^k - \mathbf{H}^{-1}\nabla f(\mathbf{x}^k)$$

- This method is called **Newton Method**.

Newton Method

- Consider $\min_{\mathbf{x}\in\mathbb{R}^n} f(\mathbf{x})$, where $f \in \mathcal{C}^2(\mathbb{R}^n)$.
- Newton's method used second-order information to determine the descent direction.
- At each iteration, it uses a second-order Taylor series approximation of f at $\mathbf{x}_k$ and finds the minimum of it to get $\mathbf{x}_{k+1}$.

$$\mathbf{x}_{k+1} = \arg\min_{\mathbf{x}\in\mathbb{R}^n} \left\{ f(\mathbf{x}_k) + \nabla f(\mathbf{x}_k)^T(\mathbf{x}-\mathbf{x}_k) + \frac{1}{2}(\mathbf{x}-\mathbf{x}_k)^T\nabla^2 f(\mathbf{x}_k)(\mathbf{x}-\mathbf{x}_k) \right\}$$

- The above formula is well defined only if we further assume that $\nabla^2 f(\mathbf{x}_k)$ is positive definite. Under this assumption, the unique minimizer is

$$\mathbf{x}_{k+1} = \mathbf{x}_k - (\nabla^2 f(\mathbf{x}_k))^{-1}\nabla f(\mathbf{x}_k)$$

- **Newton Direction:** $\mathbf{d}_N = -(\nabla^2 f(\mathbf{x}_k))^{-1}\nabla f(\mathbf{x}_k)$.

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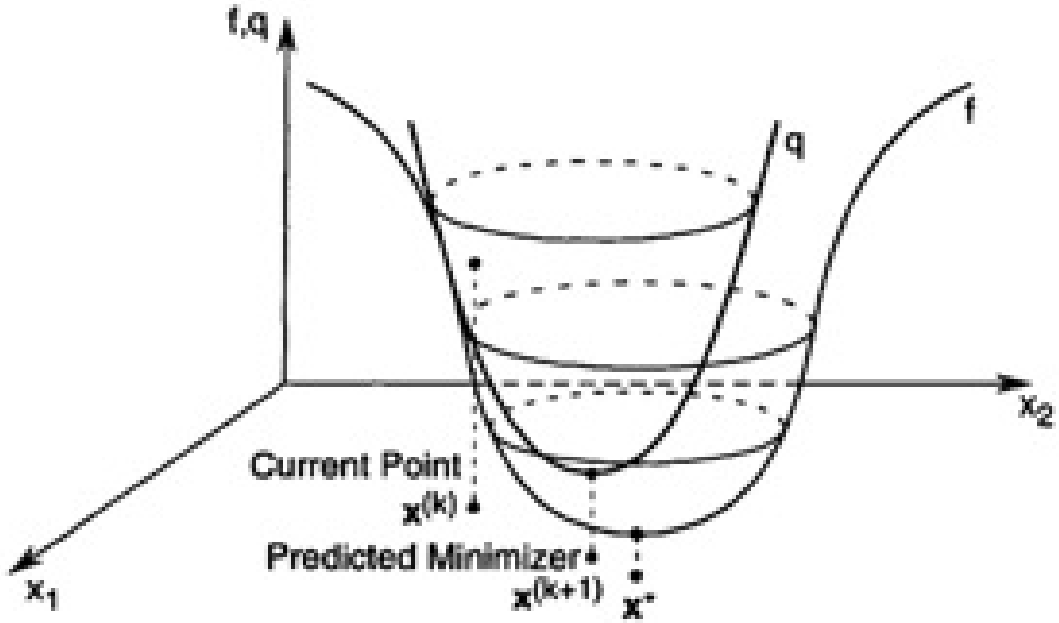
Geometry of Newton Method



Pure Newton Method

- **Input:** $\epsilon > 0$ -tolerance parameter
- **Initialization:** Pick $\mathbf{x}_0 \in \mathbb{R}^n$ arbitrarily
- **General Step :** For any $k = 0, 1, 2, \ldots$ execute the following steps:
  1. Compute the Newton's direction, which is the solution to the linear system: $\nabla^2 f(\mathbf{x}_k)\mathbf{d}_k = -\nabla f(\mathbf{x}_k)$.
  2. Set $\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{d}_k$
  3. If $\|\nabla f(\mathbf{x}_{k+1})\| \leq \epsilon$, then STOP and output $\mathbf{x}_{k+1}$.

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Convergence of Newton Method for Quadratic Functions

- Newton method requires that $\nabla^2 f(\mathbf{x})$ is positive definite for every $\mathbf{x}$ (strict convexity).
- Consider quadratic function $f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathbf{H}\mathbf{x} - \mathbf{c}^T\mathbf{x}$ such that matrix $\mathbf{H}$ is real symmetric and positive definite matrix.
- We know that the unique global minimizer of f is $\mathbf{x}^* = \mathbf{H}^{-1}\mathbf{c}$.
- We see that $\nabla f(\mathbf{x}) = \mathbf{H}\mathbf{x} - \mathbf{c}$ and $\nabla^2 f(\mathbf{x}) = \mathbf{H}$.
- Applying Newton method on this function for $\mathbf{x}_0$ as initial point, we see that

$$\mathbf{x}_1 = \mathbf{x}_0 - \nabla^2 f(\mathbf{x}_0)^{-1}\nabla f(\mathbf{x}_0) = \mathbf{x}_0 - \mathbf{H}^{-1}(\mathbf{H}\mathbf{x}_0 - \mathbf{c}) = \mathbf{H}^{-1}\mathbf{c}$$

- Thus, using Newton's method, we reach to the global minima of a quadratic and strictly convex function in one step.

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Convergence of Newton Method for General Functions

- Newton method requires that $\nabla^2 f(\mathbf{x})$ is positive definite for every $\mathbf{x}$ (strict convexity).
- Which implies a unique optimal solution $\mathbf{x}^*$ exists.
- However, this is not enough to guarantee convergence.
- Consider the following example.

Example

- Consider the function $f(x) = \sqrt{1+x^2}$. The minimizer of f is $x = 0$.
- $f'(x) = \frac{x}{\sqrt{1+x^2}}$, $f''(x) = \frac{1}{(1+x^2)^{3/2}}$.
- Therefore, the Pure Newton method update equations are

$$x_{k+1} = x_k - (1+x_k^2)^{3/2} \frac{x_k}{\sqrt{1+x_k^2}} = x_k - x_k(1+x_k^2) = -x_k^3$$

- Newton method converges to $x^* = 0$ when $|x_0| < 1$. For $|x_0| > 1$, it diverges.

Quadratic Local Convergence of Newton's Method

Theorem

Let f be a twice continuously differentiable function defined over $\mathbb{R}^n$. Assume that

- There exists $m > 0$ for which $\nabla^2 f(\mathbf{x}) \succeq m\mathbf{I}$ for any $\mathbf{x} \in \mathbb{R}^n$,
- There exists $L > 0$ for which $\|\nabla^2 f(\mathbf{x}) - \nabla^2 f(\mathbf{y})\| \leq L\|\mathbf{x} - \mathbf{y}\|$ for any $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$.

Let $\{\mathbf{x}_k\}_{k \geq 0}$ be the sequence generated by Newton's Method, and let $\mathbf{x}^*$ be the unique minimizer of f over $\mathbb{R}^n$. Then for any $k = 0, 1, 2, \ldots$ the inequality

$$\|\mathbf{x}_{k+1} - \mathbf{x}^*\| \leq \frac{L}{2m}\|\mathbf{x}_k - \mathbf{x}^*\|^2$$

holds. In addition, if $\|\mathbf{x}^* - \mathbf{x}_0\| \leq \frac{m}{L}$, then

$$\|\mathbf{x}^* - \mathbf{x}_k\| \leq \frac{2m}{L}\left(\frac{1}{2}\right)^{2^k}, \ k = 0, 1, 2, \ldots$$

- Thus, near the optimal solution, the error $e_k = \|\mathbf{x}^* - \mathbf{x}_k\|$ satisfies the inequality $e_{k+1} \leq Me_k^2$ for some positive $M > 0$.

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Example 2: $\nabla f(\mathbf{x}) \succeq m\mathbf{I}$ not satisfied

- Consider the problem $\min_{x_1,x_2} \sqrt{1+x_1^2} + \sqrt{1+x_2^2}$. The optimal solution is $(0,0)$.
- Hessian of the function is $\nabla^2 f(\mathbf{x}) = \begin{pmatrix} \frac{1}{(1+x_1^2)^{3/2}} & 0 \\ 0 & \frac{1}{(1+x_2^2)^{3/2}} \end{pmatrix} \succeq \mathbf{0}$.
- Even though the Hessian is positive definite, there does not exist an $m > 0$ for which $\nabla^2 f(\mathbf{x}) \succeq m\mathbf{I}$. As $x_1, x_2 \to \infty$, $\nabla^2 f(\mathbf{x})$ becomes a zero matrix.
- Basic assumption for convergence is not satisfied.
- This is reflected in implementation also.
- Newton's method with initial vector $\mathbf{x}_0 = (1,1)$ and tolerance parameter $\epsilon = 10^{-8}$ we obtain convergence after 37 iterations.
- Newton's method with initial vector $\mathbf{x}_0 = (10,10)$ diverges.

```
iter=  1 f(x)=2.8284271247
iter=  2 f(x)=2.8284271247
   :                :
iter= 30 f(x)=2.8105247315
iter= 31 f(x)=2.7757389625
iter= 32 f(x)=2.6791717153
iter= 33 f(x)=2.4507092918
iter= 34 f(x)=2.1223796622
iter= 35 f(x)=2.0020052756
iter= 36 f(x)=2.0000000081
iter= 37 f(x)=2.0000000000
```

(a) Starting point (1,1). Not much progress in 30 iterations. Converges in 37 iterations.

```
iter=  1 f(x)=2000.0009999997
iter=  2 f(x)=1999999999.9999990000
iter=  3 f(x)=19999999999999973000000000.0000000
iter=  4 f(x)=199999999999999230000000000000000000....
iter=  5 f(x)=       Inf
```

(b) Starting point (10,10). Newton's method diverges.

Issues with the Newton Method

- Requires computing inverse of hessian in each iteration. It can be computationally intensive if the number of variables is large.
- No guarantee that $\mathbf{d}_N = -\nabla^2 f(\mathbf{x})^{-1} \nabla f(\mathbf{x})$ is descent direction as the algorithm does not check if the hessian is positive definite.
- Problem happens when hessian is singular in some iteration.
- No guarantee that the function value decreases in each iteration (as no line search is used).
- Convergence is sensitive to the initial point.

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Newton method with Backtracking Line Search

Damped Newton Method

- **Input:** $\alpha, \beta \in (0,1)$ - parameters for the backtracking procedure. $\epsilon > 0$ -tolerance parameter
- **Initialization:** Pick $\mathbf{x}_0 \in \mathbb{R}^n$ arbitrarily
- **General Step :** For any $k = 0, 1, 2, \ldots$ execute the following steps:
  1. Compute the Newton's direction, which is the solution to the linear system: $\nabla^2 f(\mathbf{x}_k)\mathbf{d}_k = -\nabla f(\mathbf{x}_k)$.
  2. Set $t_k = 1$. While,
  $$f(\mathbf{x}_k) - f(\mathbf{x}_k + t_k \mathbf{d}_k) < -\alpha t_k \nabla f(\mathbf{x}_k)^T \mathbf{d}_k$$
  Set $t_k = \beta t_k$.
  3. $\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{d}_k$
  4. If $\|\nabla f(\mathbf{x}_{k+1})\| \leq \epsilon$, then STOP and output $\mathbf{x}_{k+1}$.

One can also use other step-size selection methods.

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Newton Method with Backtracking on Example 2

- Consider the problem $\min_{x_1,x_2} \sqrt{1+x_1^2} + \sqrt{1+x_2^2}$. The optimal solution is $(0,0)$.
- Take initial point (10,10).
- Using backtracking line search with $\alpha = \beta = 0.5$ and $\epsilon = 10^{-8}$ Newton method converges in 17 iterations.

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Levenberg Marquardt Algorithm

- If the hessian matrix $\nabla^2 f(\mathbf{x}_k)^{-1}$ is not positive definite, the Newton direction $\mathbf{d}_N = -\nabla^2 f(\mathbf{x})^{-1} \nabla f(\mathbf{x})$ may not remain a descent direction.
- This issue can be resolved by updating the Newton update in the following way.

$$\mathbf{x}_{k+1} = \mathbf{x}_k - (\nabla^2 f(\mathbf{x}_k) + \mu_k \mathbf{I})^{-1} \nabla f(\mathbf{x}_k)$$

  where $\mu_k \geq 0$.
- The idea is as follows.
  - Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of $\nabla^2 f(\mathbf{x}_k)$ and $\mathbf{v}_1, \ldots, \mathbf{v}_n$ be the corresponding eigenvectors.
  - If $\nabla^2 f(\mathbf{x}_k)$ is not positive definite, then some of the eigenvalues of it are negative.
  - Matrix $\nabla^2 f(\mathbf{x}_k) + \mu_k \mathbf{I}$ has eigenvalues $\lambda_1 + \mu_k, \ldots, \lambda_n + \mu_k$ with $\mathbf{v}_1, \ldots, \mathbf{v}_n$ be the corresponding eigenvectors.
  - if μ_k is chosen sufficiently large, all eigenvalues of $\nabla^2 f(\mathbf{x}_k) + \mu_k \mathbf{I}$ can become positive.
  - In that case $-(\nabla^2 f(\mathbf{x}_k) + \mu_k \mathbf{I})^{-1} \nabla f(\mathbf{x}_k)$ becomes a descent direction.

Choosing μ_k

Choosing μ_k

1. Start with some μ_k (a small value)
2. Do the Cholesky factorization of $\nabla^2 f(\mathbf{x}_k) + \mu_k \mathbf{I}$.
3. If Unsuccessful, increase the value of μ_k and go to step 2,

- If μ_k is very large, then this method becomes same as steepest descent.
- If μ_k is very small, then this method becomes same as Newton method.

Levenberg Marquardt Algorithm

- **Input:** Tolerance parameter $\epsilon > 0$, lower bound on minimum eigenvalue $\delta > 0$
- **Initialization:** Pick $\mathbf{x}_0 \in \mathbb{R}^n$ arbitrarily. Set $k = 0$.
- While $(\|\nabla f(\mathbf{x}_k)\| > \epsilon)$
  1. Find the smallest $\mu_k \geq 0$ such that the smallest eigenvalue of $\nabla^2 f(\mathbf{x}_k) + \mu_k \mathbf{I}$ is greater than δ.
  2. Set $\mathbf{d}_k = -(\nabla^2 f(\mathbf{x}_k) + \mu_k \mathbf{I})^{-1} \nabla f(\mathbf{x}_k)$
  3. Find $\alpha_k > 0$ using backtracking
  4. Update $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$
  5. $k = k + 1$
- **Output:** $\mathbf{x}^* = \mathbf{x}_k$ as stationary point of $f(\mathbf{x})$.

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Need for Cholesky Factorization

- In Levenberg Marquardt algorithm, it is required to validate the positive definiteness of the matrix $\nabla^2 f(\mathbf{x}_k) + \mu_k \mathbf{I}$.
- Another issue is to solve the equation $\nabla^2 f(\mathbf{x}_k)\mathbf{d} = -\nabla f(\mathbf{x}_k)$ in general for Newton method.
- These two issues are resolved using Cholesky factorization.

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Solving $\mathbf{Ax} = \mathbf{b}$ using Cholesky Factorization

- Let $\mathbf{A}$ be $n \times n$ positive definite matrix. Cholesky factorization of $\mathbf{A}$ has the form $\mathbf{A} = \mathbf{L}\mathbf{L}^T$, where $\mathbf{L}$ is a lower triangular $n \times n$ matrix whose diagonal is positive
- Given the Cholesky factorization, equation $\mathbf{Ax} = \mathbf{b}$ can be solved in following two steps.
  - Find the solution $\mathbf{u}$ of $\mathbf{Lu} = \mathbf{b}$
  - Find the solution $\mathbf{x}$ of $\mathbf{L}^T\mathbf{x} = \mathbf{u}$.

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Optimization Methods (CS1.404), Spring 2025

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Machine Learning Lab, IIIT-H

March 13th, 2025

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  - Find the solution $\mathbf{u}$ of $\mathbf{Lu} = \mathbf{b}$
  - Find the solution $\mathbf{x}$ of $\mathbf{L}^T\mathbf{x} = \mathbf{u}$.

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Cholesky Factorization Algorithm

- The computation of Cholesky factorization is done using a simple recursive approach.
- Consider the following block matrix partitioning of the matrices A and L.

$$\mathbf{A} = \begin{pmatrix} A_{11} & \mathbf{A}_{21} \\ \mathbf{A}_{12} & \mathbf{A}_{22} \end{pmatrix} \qquad \mathbf{L} = \begin{pmatrix} L_{11} & \mathbf{0} \\ \mathbf{L}_{21} & \mathbf{L}_{22} \end{pmatrix}$$

  where $A_{11} \in \mathbb{R}, \mathbf{A}_{21} \in \mathbb{R}^{(n-1)\times 1}, \mathbf{A}_{22} \in \mathbb{R}^{(n-1)\times(n-1)}, L_{11} \in \mathbb{R}$, $\mathbf{L}_{21} \in \mathbb{R}^{(n-1)\times 1}, \mathbf{L}_{22} \in \mathbb{R}^{(n-1)\times(n-1)}$.
- Since $\mathbf{A} = \mathbf{L}\mathbf{L}^T$, we have

$$\begin{pmatrix} A_{11} & \mathbf{A}_{21} \\ \mathbf{A}_{12} & \mathbf{A}_{22} \end{pmatrix} = \begin{pmatrix} L_{11}^2 & L_{11}\mathbf{L}_{21}^T \\ L_{11}\mathbf{L}_{21} & \mathbf{L}_{21}\mathbf{L}_{21}^T + \mathbf{L}_{22}\mathbf{L}_{22}^T \end{pmatrix}$$

Cholesky Factorization Algorithm: Continue

- Therefore, in particular $L_{11} = \sqrt{A_{11}}$, $\mathbf{L}_{21} = \frac{1}{\sqrt{A_{11}}}\mathbf{A}_{12}^T$.
- $\mathbf{L}_{22}\mathbf{L}_{22}^T = \mathbf{A}_{22} - \mathbf{L}_{21}\mathbf{L}_{21}^T = \mathbf{A}_{22} - \frac{1}{A_{11}}\mathbf{A}_{12}^T\mathbf{A}_{12}$.
- We are left with the task of Cholesky factorization of $(n-1) \times (n-1)$ matrix $\mathbf{A}_{22} - \frac{1}{A_{11}}\mathbf{A}_{12}^T\mathbf{A}_{12}$.
- We keep following the above procedure and we can get the complete Cholesky factorization.
- The algorithm for Cholesky factorization will find a solution only if all the diagonal elements l_{ii} that are computed during the process are positive, so that computing their square root is possible.
- The positiveness of these elements is equivalent to the property that the matrix to be factored is positive definite.
- Therefore, the Cholesky factorization process can be viewed as a criteria for positive definiteness.

Coordinate Descent Method

- Consider the problem $\min_{\mathbf{x}\in\mathbb{R}^n} f(\mathbf{x})$, where $f : \mathbb{R}^n \to \mathbb{R}$ is a continuously differentiable function.
- Coordinate descent method works as follows.
  1. For every coordinate variable x_i, $i \in \{1, \ldots, n\}$, minimize $f(\mathbf{x})$ with respect to x_i, keeping other variables x_j, $j \neq i$ constant.
  2. Repeat the above process in step 1 until some stopping condition is satisfied.

Coordinate Descent Method

Algorithm

- **Input:** $\epsilon > 0$ (tolerance parameter)
- **Initialize:** $\mathbf{x}_1$, $k = 1$
- **Step 1:** Set $\mathbf{d}_k = \mathbf{e}_k$, where $\mathbf{e}_k$ is k^{th} basis vector of standard basis of $\mathbb{R}^n$
- **Step 2:** Set $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$, where $\alpha_k = \arg\min_{\alpha \in \mathbb{R}} f(\mathbf{x}_k + \alpha \mathbf{d}_k)$.
- **Step 3:**
  - If $(\|\nabla f(\mathbf{x}_k)\| \leq \epsilon)$
    - then output $\mathbf{x}^* = \mathbf{x}_k$
  - Else if $(k = n)$
    - Set $\mathbf{x}_1 = \mathbf{x}_{k+1}$ and repeat from Step 2.
  - Else,
    - Set $k = k + 1$ and repeat from Step 2.

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Coordinate Descent Method on Quadratic Functions

- **For convex quadratic functions of n variables, above algorithm converges in n-steps.**
  - Example 1: $\min_{\mathbf{x}\in\mathbb{R}^2}\ 4x_1^2 + x_2^2$ (spherical contours). Take $\mathbf{x}_0 = (-1, -1)$. Coordinate descent method finds minimizer in two steps.
  - Example 2: $\min_{\mathbf{x}\in\mathbb{R}^2}\ 4x_1^2 + x_2^2 - 2x_1x_2$ (elliptical contours) . Take $\mathbf{x}_0 = (-1, -1)$. Coordinate descent method does not converge in two steps.
- In other words, when the objective function is separable in terms of variables (hessian is diagonal), then coordinate descent method will find $\mathbf{x}^*$ in n-steps if there are n-variables.
- When objective function is not separable in variables, then Hessian is not diagonal. Coordinate descent method will not find minimizer in n-steps.
- Can we choose $\mathbf{d}_1, \ldots, \mathbf{d}_n$ in such a way that it converges in n-steps?

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Conjugate Directions

Definition

Let Q be a real symmetric $n \times n$ matrix. The directions $\mathbf{d}_0, \ldots, \mathbf{d}_{n-1}$ are Q-conjugate if, for all $i \neq j$, we have $\mathbf{d}_i^T Q \mathbf{d}_j = 0$.

Lemma

Let Q be a symmetric positive definite $n \times n$ matrix. Let directions $\mathbf{d}_0, \mathbf{d}_1, \ldots, \mathbf{d}_k \in \mathbb{R}^n$ $(k \leq n-1)$ are Q-conjugate, then they are linearly independent.

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Conjugate Directions: Example 1

- Let $f(x_1, x_2) = 4x_1^2 + x_2^2 - 2x_1x_2$
- Hessian $H = \begin{pmatrix} 8 & -2 \\ -2 & 2 \end{pmatrix}$
- Let $\mathbf{d}_0 = (1, 0)^T$
- Then the conjugate direction $\mathbf{d}_1 = (a, b)^T$ would satisfy $\mathbf{d}_0^T H \mathbf{d}_1 = 0$.
- This results in relation $8a - 2b = 0$. Thus, we can take $\mathbf{d}_1 = (1, 4)^T$.

Conjugate Directions: Example 2

- Let $Q = \begin{pmatrix} 3 & 0 & 1 \\ 0 & 4 & 2 \\ 1 & 2 & 3 \end{pmatrix}$
- Let $\mathbf{d}_0 = (1, 0, 0)^T$.
- Now, we want to find $\mathbf{d}_1 = (a, b, c)^T$ which is Q-conjugate to $\mathbf{d}_0$. We require $\mathbf{d}_0^T H \mathbf{d}_1 = 0$. Which results in relation $3a + c = 0$. So, we can choose $\mathbf{d}_1 = (1, 0, -3)^T$.
- Now, we want to find $\mathbf{d}_2 = (e, f, g)^T$ which is Q-conjugate to $\mathbf{d}_0$ and $\mathbf{d}_1$. So, we get the conditions $3e + g = 0$ and $-6f - 8g = 0$. We can choose $\mathbf{d}_2 = (1, 4, -3)^T$.

Choosing Conjugate Directions

- A systematic procedure for finding Q-conjugate directions can be developed using the idea of Gram-Schmidt algorithm of transforming a given basis of $\mathbb{R}^n$ into an orthogonal basis of $\mathbb{R}^n$.
- For a symmetric matrix matrix H, orthogonal eigenvectors of H itself are H-conjugate.
  - Let $\mathbf{v}_1$ and $\mathbf{v}_2$ are mutually orthonormal eigenvectors of H corresponding to eigenvalues λ_1 and λ_2.
  - Then $\mathbf{v}_1^T H \mathbf{v}_2 = \lambda_2 \mathbf{v}_1^T \mathbf{v}_2 = 0$.

Conjugate Direction Method

- Consider minimization problem $\min_{\mathbf{x}\in\mathbb{R}^n} \ \frac{1}{2}\mathbf{x}^T H\mathbf{x} + \mathbf{c}^T\mathbf{x}$, where H is symmetric positive definite matrix.
- Let $\mathbf{x}_0$ be the initial parameters.
- Let $\mathbf{d}_0, \mathbf{d}_1, \ldots, \mathbf{d}_{n-1} \in \mathbb{R}^n$ be H-conjugate directions.
- As we know that these conjugate directions are linearly independent. We can write any $\mathbf{x} - \mathbf{x}_0 \in \mathbb{R}^n$ as a linear combination of these conjugate directions. Thus,

$$\mathbf{x} - \mathbf{x}_0 = \sum_{i=0}^{n-1} \alpha_i \mathbf{d}_i$$

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Conjugate Direction Method - Continue

- Given $\mathbf{d}_0, \mathbf{d}_1, \ldots, \mathbf{d}_{n-1} \in \mathbb{R}^n$ and $\mathbf{x}_0 \in \mathbb{R}^n$, the above minimization problem becomes

$$\begin{aligned}
\phi(\boldsymbol{\alpha}) &= \frac{1}{2}\left(\mathbf{x}_0 + \sum_{i=0}^{n-1}\alpha_i\mathbf{d}_i\right)^T H\left(\mathbf{x}_0 + \sum_{i=0}^{n-1}\alpha_i\mathbf{d}_i\right) + \mathbf{c}^T\left(\mathbf{x}_0 + \sum_{i=0}^{n-1}\alpha_i\mathbf{d}_i\right) \\
&= \frac{1}{2}\mathbf{x}_0^T H\mathbf{x}_0 + \frac{1}{2}\left(\sum_{i=0}^{n-1}\alpha_i\mathbf{d}_i\right)^T H\left(\sum_{i=0}^{n-1}\alpha_i\mathbf{d}_i\right) + \left(\sum_{i=0}^{n-1}\alpha_i\mathbf{d}_i\right) H\mathbf{x}_0 \\
&\quad + \mathbf{c}^T\left(\mathbf{x}_0 + \sum_{i=0}^{n-1}\alpha_i\mathbf{d}_i\right) \\
&= \frac{1}{2}\mathbf{x}_0^T H\mathbf{x}_0 + \frac{1}{2}\sum_{i=0}^{n-1}\alpha_i^2\mathbf{d}_i^T H\mathbf{d}_i + \sum_{i=0}^{n-1}\alpha_i\mathbf{d}_i^T H\mathbf{x}_0 + \mathbf{c}^T\left(\mathbf{x}_0 + \sum_{i=0}^{n-1}\alpha_i\mathbf{d}_i\right) \\
&= \sum_{i=0}^{n-1}\left(\frac{1}{2}(\mathbf{x}_0 + \alpha_i\mathbf{d}_i)^T H(\mathbf{x}_0 + \alpha_i\mathbf{d}_i) + \mathbf{c}^T(\mathbf{x}_0 + \alpha_i\mathbf{d}_i)\right) \\
&\quad - (n-1)\left(\frac{1}{2}\mathbf{x}_0^T H\mathbf{x}_0 + \mathbf{c}^T\mathbf{x}_0\right)
\end{aligned}$$

Conjugate Direction Method - Continue

- Ignoring the constant term, we define a new function

$$\psi(\boldsymbol{\alpha}) = \sum_{i=0}^{n-1} \left(\frac{1}{2}(\mathbf{x}_0 + \alpha_i \mathbf{d}_i)^T H(\mathbf{x}_0 + \alpha_i \mathbf{d}_i) + \mathbf{c}^T(\mathbf{x}_0 + \alpha_i \mathbf{d}_i) \right)$$

- ψ is separable in terms of $\alpha_0, \alpha_1, \ldots, \alpha_{n-1}$, which are our new optimization variables.
- Minimizing ψ with respect to α_i, we get

$$\alpha_i^* = -\frac{\mathbf{d}_i^T(H\mathbf{x}_0 + \mathbf{c})}{\mathbf{d}_i^T H \mathbf{d}_i}$$

- $\mathbf{x}^* = \mathbf{x}_0 + \sum_{i=0}^{n-1} \alpha_i^* \mathbf{d}_i$

Basic Conjugate Direction Algorithm

Given starting point $\mathbf{x}_0$ and H conjugate directions $\mathbf{d}_0, \mathbf{d}_1, \ldots, \mathbf{d}_{n-1} \in \mathbb{R}^n$, the Conjugate Direction Algorithm works as follows:

- For $(k = 0, 1, \ldots, n-1)$
  - $\nabla f(\mathbf{x}_k) = H\mathbf{x}_k + \mathbf{c}$
  - $\alpha_k = -\frac{\nabla f(\mathbf{x}_k)^T \mathbf{d}_k}{\mathbf{d}_k^T H \mathbf{d}_k}$
  - $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$

Theorem

Consider minimization problem $\min_{\mathbf{x} \in \mathbb{R}^n} \ \frac{1}{2}\mathbf{x}^T H \mathbf{x} + \mathbf{c}^T \mathbf{x}$, where H is symmetric positive definite matrix. For any starting point $\mathbf{x}_0$ and H conjugate directions $\mathbf{d}_0, \mathbf{d}_1, \ldots, \mathbf{d}_{n-1} \in \mathbb{R}^n$, the **Basic Conjugate Direction Algorithm** converges to the unique $\mathbf{x}^*$ (that solves $H\mathbf{x}^* + \mathbf{c} = \mathbf{0}$) in n-steps; that is $\mathbf{x}_n = \mathbf{x}^*$.

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Optimization Methods (CS1.404), Spring 2025

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March 28, 2025

Conjugate Gradient Algorithm for Non-Quadratic Problems

- To minimize a non-quadratic function, we first find a quadratic approximation at $\mathbf{x}_k$ using Taylor series and minimize it using conjugate descent to find $\mathbf{x}_{k+1}$.
- We replace H by Hessian at that iteration.
- The conjugate descent algorithm requires computation of Hessian at each iteration which makes it computationally expensive.
- An efficient implementation of conjugate descent eliminates the evaluation of Hessian at each step.
- Note that in conjugate descent algorithm, Hessian appears in the expression of α_k and β_k.
- Because $\alpha_k = \arg\min_{\alpha \geq 0} \ f(\mathbf{x}_k + \alpha \mathbf{d}_k)$, closed form formula for α_k can be replaced by numerical line search method.
- To eliminate Hessian from the formula of β_k, there are three possible ways.

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Hestenes-Stiefel Formula

- Recall that $\beta_k = \frac{\mathbf{g}_{k+1}^T H \mathbf{d}_k}{\mathbf{d}_k^T H \mathbf{d}_k}$.
- Here, we replace $H\mathbf{d}_k$ by the term $\frac{\mathbf{g}_{k+1} - \mathbf{g}_k}{\alpha_k}$.
  $\left(\frac{\mathbf{g}_{k+1} - \mathbf{g}_k}{\alpha_k} = \frac{H\mathbf{x}_{k+1} + \mathbf{c} - H\mathbf{x}_k - \mathbf{c}}{\alpha_k} = \frac{H(\mathbf{x}_{k+1} - \mathbf{x}_k)}{\alpha_k} = H\mathbf{d}_k\right)$
- Using this in the β_k formula, we get $\beta_k = \frac{\mathbf{g}_{k+1}^T (\mathbf{g}_{k+1} - \mathbf{g}_k)}{\mathbf{d}_k^T (\mathbf{g}_{k+1} - \mathbf{g}_k)}$.
- **For quadratic functions, $\beta_k = \frac{\mathbf{g}_{k+1}^T (\mathbf{g}_{k+1} - \mathbf{g}_k)}{\mathbf{d}_k^T (\mathbf{g}_{k+1} - \mathbf{g}_k)}$ is same as $\beta_k = \frac{\mathbf{g}_{k+1}^T H \mathbf{d}_k}{\mathbf{d}_k^T H \mathbf{d}_k}$.**

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Hestenes-Stiefel Approach

Initialize: The starting point $\mathbf{x}_0$ and the tolerance parameter $\epsilon > 0$, Set $k = 0$
Assign $\mathbf{d}_0 = -\mathbf{g}_0$
while $\|\mathbf{g}_k\| > \epsilon$ **do**
  $\alpha_k = \arg\min_{\alpha>0} f(\mathbf{x}_k + \alpha \mathbf{d}_k)$
  $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$
  Compute $\mathbf{g}_{k+1} = \nabla f(\mathbf{x}_{k+1})$
  if $(k < n-1)$ **then**
    $\beta_k = \frac{\mathbf{g}_{k+1}^T(\mathbf{g}_{k+1}-\mathbf{g}_k)}{\mathbf{d}_k^T(\mathbf{g}_{k+1}-\mathbf{g}_k)}$
    $\mathbf{d}_{k+1} = -\mathbf{g}_{k+1} + \beta_k \mathbf{d}_k$
    $k = k+1$
  else
    $\mathbf{x}_0 = \mathbf{x}_{k+1}$
    $\mathbf{d}_0 = -\mathbf{g}_{k+1}$
    $k = 0$
  end if
end while
Output: $\mathbf{x}^* = \mathbf{x}_k$, a stationary point of f.

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Polak-Ribiere Formula

- Starting from Hestenes-Stiefel formula, we multiply out the denominator to get $\beta_k = \frac{\mathbf{g}_{k+1}^T(\mathbf{g}_{k+1}-\mathbf{g}_k)}{\mathbf{d}_k^T\mathbf{g}_{k+1}-\mathbf{d}_k^T\mathbf{g}_k}$.
- But, we know that $\mathbf{d}_k^T\mathbf{g}_{k+1} = 0$.
- Also, since $\mathbf{d}_k = -\mathbf{g}_k + \beta_{k-1}\mathbf{d}_{k=1}$, we get

$$\mathbf{g}_k^T\mathbf{d}_k = -\mathbf{g}_k^T\mathbf{g}_k + \beta_{k-1}\mathbf{g}_k^T\mathbf{d}_{k-1} = -\mathbf{g}_k^T\mathbf{g}_k$$

- Thus, we get $\beta_k = \frac{\mathbf{g}_{k+1}^T(\mathbf{g}_{k+1}-\mathbf{g}_k)}{\mathbf{g}_k^T\mathbf{g}_k}$.
- This expression for β_k is called Polak-Ribiere Formula.
- **For quadratic functions, $\beta_k = \frac{\mathbf{g}_{k+1}^T(\mathbf{g}_{k+1}-\mathbf{g}_k)}{\mathbf{g}_k^T\mathbf{g}_k}$ is same as $\beta_k = \frac{\mathbf{g}_{k+1}^T H\mathbf{d}_k}{\mathbf{d}_k^T H\mathbf{d}_k}$.**

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Polak-Ribiere Approach

Initialize: The starting point $\mathbf{x}_0$ and the tolerance parameter $\epsilon > 0$, Set $k = 0$
Assign $\mathbf{d}_0 = -\mathbf{g}_0$
while $\|\mathbf{g}_k\| > \epsilon$ **do**
  $\alpha_k = \arg\min_{\alpha>0} f(\mathbf{x}_k + \alpha \mathbf{d}_k)$
  $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$
  Compute $\mathbf{g}_{k+1} = \nabla f(\mathbf{x}_{k+1})$
  if $(k < n-1)$ **then**
    $\beta_k = \frac{\mathbf{g}_{k+1}^T(\mathbf{g}_{k+1} - \mathbf{g}_k)}{\mathbf{g}_k^T \mathbf{g}_k}$
    $\mathbf{d}_{k+1} = -\mathbf{g}_{k+1} + \beta_k \mathbf{d}_k$
    $k = k + 1$
  else
    $\mathbf{x}_0 = \mathbf{x}_{k+1}$
    $\mathbf{d}_0 = -\mathbf{g}_{k+1}$
    $k = 0$
  end if
end while
Output: $\mathbf{x}^* = \mathbf{x}_k$, a stationary point of f.

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Fletcher Reeves Formula

- Starting with the Polak-Ribiere Formula, we get $\beta_k = \frac{\mathbf{g}_{k+1}^T \mathbf{g}_{k+1} - \mathbf{g}_{k+1}^T \mathbf{g}_k}{\mathbf{g}_k^T \mathbf{g}_k}$.
- We know that $\mathbf{d}_k = -\mathbf{g}_k + \beta_k \mathbf{d}_{k-1}$. Thus, $\mathbf{g}_{k+1}^T \mathbf{d}_k = -\mathbf{g}_{k+1}^T \mathbf{g}_k + \beta_k \mathbf{g}_{k+1}^T \mathbf{d}_{k-1}$.
- But, we know that $\mathbf{g}_{k+1}^T \mathbf{d}_k = \mathbf{g}_{k+1}^T \mathbf{d}_{k-1} = 0$.
- Thus, $\mathbf{g}_{k+1}^T \mathbf{g}_k = 0$.
- This leads to $\beta_k = \frac{\mathbf{g}_{k+1}^T \mathbf{g}_{k+1}}{\mathbf{g}_k^T \mathbf{g}_k}$.
- This is called Fletcher Reeves formula.
- **For quadratic functions, $\beta_k = \frac{\mathbf{g}_{k+1}^T \mathbf{g}_{k+1}}{\mathbf{g}_k^T \mathbf{g}_k}$ is same as $\beta_k = \frac{\mathbf{g}_{k+1}^T H \mathbf{d}_k}{\mathbf{d}_k^T H \mathbf{d}_k}$.**

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Fletcher Reeves Approach

Initialize: The starting point $\mathbf{x}_0$ and the tolerance parameter $\epsilon > 0$, Set $k = 0$
Assign $\mathbf{d}_0 = -\mathbf{g}_0$
while $\|\mathbf{g}_k\| > \epsilon$ **do**
  $\alpha_k = \arg\min_{\alpha>0} f(\mathbf{x}_k + \alpha \mathbf{d}_k)$
  $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$
  Compute $\mathbf{g}_{k+1} = \nabla f(\mathbf{x}_{k+1})$
  if $(k < n-1)$ **then**
    $\beta_k = \frac{\mathbf{g}_{k+1}^T \mathbf{g}_{k+1}}{\mathbf{g}_k^T \mathbf{g}_k}$
    $\mathbf{d}_{k+1} = -\mathbf{g}_{k+1} + \beta_k \mathbf{d}_k$
    $k = k + 1$
  else
    $\mathbf{x}_0 = \mathbf{x}_{k+1}$
    $\mathbf{d}_0 = -\mathbf{g}_{k+1}$
    $k = 0$
  end if
end while
Output: $\mathbf{x}^* = \mathbf{x}_k$, a stationary point of f.

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Summary: Conjugate Gradient Methods

- Conjugate direction methods can be regarded as being between the method of steepest descent (first-order method that uses gradient) and Newton's method (second-order method that uses Hessian as well).
  - Steepest descent is slow.
  - Newton method is fast, but we need to calculate the inverse of the Hessian matrix.
  - **Conjugate gradient uses gradient only and faster than steepest descent.**
- Conjugate gradient method attempts to accelerate gradient descent by building in momentum.
  - Recall $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$
  - Using $\mathbf{d}_k = -\mathbf{g}_k + \beta_{k-1}\mathbf{d}_{k-1}$, we get

$$\begin{aligned}\mathbf{x}_{k+1} &= \mathbf{x}_k + \alpha_k \mathbf{d}_k \\ &= \mathbf{x}_k - \alpha_k \mathbf{g}_k + \alpha_k \beta_{k-1}\mathbf{d}_{k-1}\end{aligned}$$

  - Using $\mathbf{d}_{k-1} = \frac{\mathbf{x}_k - \mathbf{x}_{k-1}}{\alpha_{k-1}}$, we get

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k \mathbf{g}_k + \frac{\alpha_k \beta_{k-1}}{\alpha_{k-1}}(\mathbf{x}_k - \mathbf{x}_{k-1})$$

momentum term

Quasi Newton Methods

- **Newton Method:** Given a function $f \in \mathcal{C}^2(\mathbb{R}^n)$, Newton method finds the descent direction by solving $H_k \mathbf{d}_k = -\mathbf{g}_k$, where $H_k = \nabla^2 f(\mathbf{x}_k)$ and $\mathbf{g}_k = \nabla f(\mathbf{x}_k)$.
- **Quasi Newton Method:** Given a function $f \in \mathcal{C}^1(\mathbb{R}^n)$, quasi-Newton method finds descent direction as $\mathbf{d}_k = -B_k \mathbf{g}_k$, where B_k is a positive definite matrix.
  - B_k^{-1} is either H_k or its approximation.
  - $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k^{QN} = \mathbf{x}_k - \alpha_k B_k \mathbf{g}_k$
  - Given $\mathbf{x}_k$, $\mathbf{x}_{k+1}$, $\mathbf{g}_k$, $\mathbf{g}_{k+1}$ and B_k, how to get symmetric positive definite B_{k+1}?
  - Are there any conditions that B_{k+1} needs to satisfy?

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Quasi-Newton Method

- We find quadratic approximation of f at $\mathbf{x}_{k+1}$ using B_{K+1} as follows.
  $f_{k+1}(\mathbf{x}) = f(\mathbf{x}_{k+1}) + \mathbf{g}_{k+1}^T(\mathbf{x} - \mathbf{x}_{k+1}) + \frac{1}{2}(\mathbf{x} - \mathbf{x}_{k+1})^T B_{k+1}^{-1}(\mathbf{x} - \mathbf{x}_{k+1})$
- We require that $\nabla f_{k+1}(\mathbf{x}_k) = \mathbf{g}_k$ and $\nabla f_{k+1}(\mathbf{x}_{k+1}) = \mathbf{g}_{k+1}$.
- Therefore, using the first condition, we require
  $\nabla f_{k+1}(\mathbf{x}_k) = \mathbf{g}_k = \mathbf{g}_{k+1} + B_{k+1}^{-1}(\mathbf{x}_k - \mathbf{x}_{k-1})$.
- Letting $\gamma_k = \mathbf{g}_{k+1} - \mathbf{g}_k$ and $\boldsymbol{\delta}_k = \mathbf{x}_{k+1} - \mathbf{x}_k$, we get $B_{k+1}\gamma_k = \boldsymbol{\delta}_k$.
- This condition is also called **Quasi-Newton condition**.
- B_{k+1} should be positive definite. Thus, $\gamma_k^T B_{k+1}\gamma_k = \gamma_k^T \boldsymbol{\delta}_k > 0$.
  - From Wolfe line search condition

$$\mathbf{g}_{k+1}^T \mathbf{d}_k \geq c_2 \mathbf{g}_k^T \mathbf{d}_k, \quad \text{where } c_2 \in (0,1)$$

$$\Rightarrow (\mathbf{g}_{k+1} - \mathbf{g}_k)^T \mathbf{d}_k \geq (c_2 - 1)\mathbf{g}_k^T \mathbf{d}_k$$

We know that $c_2 - 1 < 0$ and $\mathbf{g}_k^T \mathbf{d}_k = -\mathbf{g}_k^T B_k \mathbf{g}_k < 0$ as B_k is positive definite matrix. Thus, we get

$$(\mathbf{g}_{k+1} - \mathbf{g}_k)^T \mathbf{d}_k \geq (c_2 - 1)\mathbf{g}_k^T \mathbf{d}_k > 0 \Rightarrow \gamma_k^T \mathbf{d}_k > 0$$

$$\Rightarrow \gamma_k^T \boldsymbol{\delta}_k > 0, \quad \text{using } \mathbf{d}_k = \frac{1}{\alpha_k}(\mathbf{x}_{k+1} - \mathbf{x}_k) = \frac{1}{\alpha_k}\boldsymbol{\delta}_k$$

  - When Wolfe condition is satisfied in a line search, $\exists B_{k+1}$ which satisfies Quasi-Newton condition.

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Symmetric Rank One Correction

- Here, we want to update B_k to B_{k+1} by adding a rank one matrix $a_k \mathbf{z}_k \mathbf{z}_k^T$, where $a_k \in \mathbb{R}(a \neq 0)$ and $\mathbf{z}_k \in \mathbb{R}^n(\mathbf{z} \neq \mathbf{0})$. Thus,

$$B_{k+1} = B_k + a_k \mathbf{z}_k \mathbf{z}_k^T$$

- Now, we choose a_k and $\mathbf{z}_k$ such that B_{k+1} satisfies Quasi-Newton condition. Thus, we want

$$\begin{aligned} & B_{k+1}\gamma_k = \boldsymbol{\delta}_k \\ \Rightarrow & (B_k + a_k \mathbf{z}_k \mathbf{z}_k^T)\gamma_k = \boldsymbol{\delta}_k \\ \Rightarrow & a_k \mathbf{z}_k \mathbf{z}_k^T \gamma_k = \boldsymbol{\delta}_k - B_k \gamma_k \end{aligned}$$

- Let $\mathbf{z}_k = \boldsymbol{\delta}_k - B_k \gamma_k$. Therefore, $a_k \mathbf{z}_k^T \gamma_k = 1$.
- That gives $\alpha_k = \frac{1}{(\boldsymbol{\delta}_k - B_k \gamma_k)^T \gamma_k}$.

Thus, using $\mathbf{x}_k$, $\mathbf{x}_{k+1}$, $\mathbf{g}_{k+1}$ and $\mathbf{g}_k$, we get

$$B_{k+1}^{SR1} = B_k + \frac{(\boldsymbol{\delta}_k - B_k \gamma_k)(\boldsymbol{\delta}_k - B_k \gamma_k)^T)}{(\boldsymbol{\delta}_k - B_k \gamma_k)^T \gamma_k}$$

Quasi-Newton Method (Rank One Correction)

1: **Initialize:** The starting point $\mathbf{x}_0$, Symmetric positive definite matrix B_0 and the tolerance parameter $\epsilon > 0$, Set $k = 0$
2: **while** $\|\mathbf{g}_k\| > \epsilon$ **do**
3: $\mathbf{d}_k = -B_k \mathbf{g}_k$
4: Find α_k along $\mathbf{d}_k$ such that

- $f(\mathbf{x}_k + \alpha_k \mathbf{d}_k) < f(\mathbf{x}_k)$
- α_k satisfies Armijo-Wolfe condition

5: $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$
6: Find B_{k+1} as

$$B_{k+1} = B_k + \frac{(\boldsymbol{\delta}_k - B_k \boldsymbol{\gamma}_k)(\boldsymbol{\delta}_k - B_k \boldsymbol{\gamma}_k)^T)}{(\boldsymbol{\delta}_k - B_k \boldsymbol{\gamma}_k)^T \boldsymbol{\gamma}_k}$$

7: $k = k + 1$
8: **end while**
9: **Output:** $\mathbf{x}^* = \mathbf{x}_k$, a stationary point of f.

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Example: Rank One Correction

- Consider the problem min $f(x, y) = 4x^2 + y^2 - 2xy$
- For this problem, $\mathbf{x}^* = [0 \;\; 0]^T$, $H = \begin{bmatrix} 8 & -2 \\ -2 & 2 \end{bmatrix}$, $H^{-1} = \begin{bmatrix} 0.1667 & 0.1667 \\ 0.1667 & 0.6667 \end{bmatrix}$
- We run **rank one correction** approach with $\mathbf{x}_0 = [-2 \;\; -2]^T$ and B_0 as identity matrix.
- We see that the algorithm converges in 3 steps. Below are the updates in each step.

k	x_k	y_k	B_k	$\|\mathbf{g}_k\|$
0	-2	-2	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	12.0
1	0	-2	$\begin{bmatrix} 0.1833 & 0.2333 \\ 0.2333 & 0.9333 \end{bmatrix}$	5.65
2	0.1538	0.1536	$\begin{bmatrix} 0.1667 & 0.1667 \\ 0.1667 & 0.6667 \end{bmatrix}$	0.92
3	0	0	H^{-1}	0

Quasi-Newton Algorithm Applied on Quadratic Functions

- Consider the problem $\min_{\mathbf{x}} \frac{1}{2}\mathbf{x}^T H\mathbf{x} + \mathbf{c}^T\mathbf{x}$, where H is a symmetric positive definite matrix.
- To solve this problem using rank one correction method, at every iteration k
  - B_{k+1} is symmetric positive definite.
  - B_{k+1} is obtained from $\mathbf{x}_k$, $\mathbf{x}_{k+1}$, $\mathbf{g}_{k+1}$ and $\mathbf{g}_k$.
  - B_{k+1} satisfies Quasi-Newton condition, $B_{k+1}\gamma_k = \delta_k$
- Note that $\mathbf{g}_{k+1} - \mathbf{g}_k = H\mathbf{x}_{k+1} + \mathbf{c} - H\mathbf{x}_k - \mathbf{c} = H(\mathbf{x}_{k+1} - \mathbf{x}_k)$. Which means, $\gamma_k = H\delta_k$.

Lemma: Hereditary Property

SR1 correction approach applied to quadratic function with positive definite Hessian H, we have

$$B_{k+1}\gamma_i = \delta_i,\ 0 \leq i \leq k.$$

When f is quadratic, the hereditary property is satisfied by SR1 regardless of how the line search is performed.

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Convergence of SR1 Applied on Quadratic Functions

Theorem1: For Quadratic Functions

Consider SR1 quasi-Newton algorithm applied to a quadratic function with positive definite Hessian H. Then, for any starting point $\mathbf{x}_0$ and any symmetric starting matrix B_0, the sequence of iterates $\mathbf{x}_k$ generated by SR1 converges to the minimizer in n-steps, provided $(\boldsymbol{\delta}_k - B_k\boldsymbol{\gamma}_k)^T\boldsymbol{\gamma}_k \neq 0, \forall k$. Moreover, if n-steps are performed and $\boldsymbol{\delta}_0, \boldsymbol{\delta}_1, \ldots, \boldsymbol{\delta}_{n-1}$ are linearly independent, then $B_n = H^{-1}$.

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Convergence of SR1 Applied on General Functions

- For general nonlinear functions, the SR1 update continues to generate good Hessian approximations under certain conditions.

Theorem

Suppose that f is twice continuously differentiable, and that its Hessian is bounded and Lipschitz continuous in a neighborhood of a point x^*. Let $\mathbf{x}_k,\ k = 0, 1, \ldots$ be any sequence of iterates such that $\mathbf{x}_k \to \mathbf{x}^*$ for some $\mathbf{x}^* \in \mathbb{R}^n$. Suppose in addition that the $|(\boldsymbol{\delta}_k - B_k\boldsymbol{\gamma}_k)^T\boldsymbol{\gamma}_k| \geq r\|\boldsymbol{\delta}_k - B_k\boldsymbol{\gamma}_k\|.\|\boldsymbol{\gamma}_k\|$ holds for all k, for some $r \in (0, 1)$, and that $\boldsymbol{\delta}_0, \boldsymbol{\delta}_1, \ldots, \boldsymbol{\delta}_{n-1}$ are linearly independent. Then, the matrices B_k generated by the SR1 updating formula satisfy

$$\lim_{k\to\infty} \|B_k - \nabla^2 f(\mathbf{x}^*)\| = 0$$

SR1: Some Remarks

- SR1 is a simple and elegant way to use the information gathered during two consecutive iterations to update B_k.
- B_{k+1} is positive definite if $(\boldsymbol{\delta}_k - B_k\boldsymbol{\gamma}_k)^T\boldsymbol{\gamma}_k >$ which can not be guaranteed for every k.
- Numerical difficulties happen if $(\boldsymbol{\delta}_k - B_k\boldsymbol{\gamma}_k)^T\boldsymbol{\gamma}_k$ is close to 0.

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Issues with SR1

- The main drawback of SR1 updating is that the $(\boldsymbol{\delta}_k - B_k\boldsymbol{\gamma}_k)^T\boldsymbol{\gamma}_k$ can vanish.
- Even when the objective function is a convex quadratic, there may be steps on which no symmetric rank-1 update satisfies the Quasi-Newton condition.
- By reasoning in terms of B_k, we see that there are three cases:
  - If $(\boldsymbol{\delta}_k - B_k\boldsymbol{\gamma}_k)^T\boldsymbol{\gamma}_k \neq 0$, then there is a unique rank-one updating formula which satisfies Quasi-Newton condition.
  - If $\boldsymbol{\delta}_k - B_k\boldsymbol{\gamma}_k = \mathbf{0}$, then the only updating formula satisfying Quasi-Newton condition is $B_{k+1} = B_k$.
  - If $\boldsymbol{\delta}_k - B_k\boldsymbol{\gamma}_k \neq \mathbf{0}$ and $(\boldsymbol{\delta}_k - B_k\boldsymbol{\gamma}_k)^T\boldsymbol{\gamma}_k = 0$, then there is no symmetric rank-one updating formula satisfying the Quasi-Newton Condition.

Strategy to Handle the Case $\boldsymbol{\delta}_k - B_k\boldsymbol{\gamma}_k \neq \mathbf{0}$ and $(\boldsymbol{\delta}_k - B_k\boldsymbol{\gamma}_k)^T\boldsymbol{\gamma}_k = 0$

- It has been observed in practice that SR1 performs well simply by skipping the update if the denominator is small.
- More specifically, the SR1 update is applied only if $(\boldsymbol{\delta}_k - B_k\boldsymbol{\gamma}_k)^T\boldsymbol{\gamma}_k \geq r\|\boldsymbol{\delta}_k - B_k\boldsymbol{\gamma}_k\|\,\|\boldsymbol{\gamma}_k\|$ where $r \in (0,1)$ is a small number, say $r = 10^{-8}$.
- If this condition is not satisfied, then we update it as $B_{k+1} = B_k$.
- The condition $(\boldsymbol{\delta}_k - B_k\boldsymbol{\gamma}_k)^T\boldsymbol{\gamma}_k = 0$ occurs infrequently since it requires certain vectors to be aligned in a specific way. When it does occur, skipping the update appears to have no negative effects on the iteration.

Optimization Methods (CS1.404), Spring 2024
Lecture 17

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March 14th, 2024

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Rank Two Correction Quasi newton Method

- Given that B_k is symmetric and positive definite matrix, let

$$B_{k+1} = B_k + \alpha \mathbf{u}\mathbf{u}^T + \beta \mathbf{v}\mathbf{v}^T$$

- B_{k+1} is required to satisfy Quasi-Newton condition. Thus,

$$\alpha \mathbf{u}^T \gamma_k \mathbf{u} + \beta \mathbf{v}^T \gamma_k \mathbf{v} = \boldsymbol{\delta}_k - B_k \gamma_k$$

- Letting $\alpha \mathbf{u}^T \gamma_k = \beta \mathbf{v}^T \gamma_k = 1$, we get $\mathbf{u} + \mathbf{v} = \boldsymbol{\delta}_k - B_k \gamma_k$. Taking $\mathbf{u} = \boldsymbol{\delta}_k$ and $\mathbf{v} = -B_k \gamma_k$, we get

$$\alpha^{-1} = \mathbf{u}^T \gamma_k = \boldsymbol{\delta}_k^T \gamma_k$$
$$\beta^{-1} = \mathbf{v}^T \gamma_k = -\gamma_k^T B_k \gamma_k$$

- Therefore, we get the following update for B_{k+1}:

$$B_{k+1} = B_k + \frac{\boldsymbol{\delta}_k \boldsymbol{\delta}_k^T}{\boldsymbol{\delta}_k^T \gamma_k} - \frac{B_k \gamma_k \gamma_k^T B_k}{\gamma_k^T B_k \gamma_k}$$

- This update is called DFP named after Davidson, Fletcher and Powell.

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Rank Two Correction Quasi newton Method

Theorem

Given that B_k is symmetric and positive definite, B_{k+1} generated by DFP is symmetric and positive definite.

DFP Quasi-Newton Algorithm

1: **Initialize:** The starting point $\mathbf{x}_0$, Symmetric positive definite matrix B_0 and the tolerance parameter $\epsilon > 0$, Set $k = 0$
2: **while** $\|\mathbf{g}_k\| > \epsilon$ **do**
3: $\mathbf{d}_k = -B_k \mathbf{g}_k$
4: Find α_k along $\mathbf{d}_k$ such that

- $f(\mathbf{x}_k + \alpha_k \mathbf{d}_k) < f(\mathbf{x}_k)$
- α_k satisfies Armijo-Wolfe condition

5: $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$
6: Find B_{k+1} as

$$B_{k+1} = B_k + \frac{\boldsymbol{\delta}_k \boldsymbol{\delta}_k^T}{\boldsymbol{\delta}_k^T \boldsymbol{\gamma}_k} - \frac{B_k \boldsymbol{\gamma}_k \boldsymbol{\gamma}_k^T B_k}{\boldsymbol{\gamma}_k^T B_k \boldsymbol{\gamma}_k}$$

7: $k = k + 1$
8: **end while**
9: **Output:** $\mathbf{x}^* = \mathbf{x}_k$, a stationary point of f.

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BFGS Algorithm

- Quasi Newton condition requires $B_{k+1}\gamma_k = \delta_k$ to hold for all k.
- Assume that we want to approximate the Hessian H_{k+1} rather than its inverse. Let $G_{k+1} = B_{k+1}^{-1}$ which approximates Hessian H_{k+1}.
- Then, Quasi-Newton condition would result into $G_{k+1}\delta_k = \gamma_k$.
- Rank two update of G_{k+1} will have the form

$$G_{k+1} = G_k + \alpha \mathbf{u}\mathbf{u}^T + \beta \mathbf{v}\mathbf{v}^T$$

- G_{k+1} is required to satisfy Quasi-Newton condition. Thus,

$$\alpha \mathbf{u}^T \delta_k \mathbf{u} + \beta \mathbf{v}^T \delta_k \mathbf{v} = \gamma_k - G_k \delta_k$$

- Letting $\alpha \mathbf{u}^T \delta_k = \beta \mathbf{v}^T \delta_k = 1$, we get $\mathbf{u} + \mathbf{v} = \gamma_k - G_k \delta_k$. Taking $\mathbf{u} = \gamma_k$ and $\mathbf{v} = -G_k \delta_k$, we get

$$\alpha^{-1} = \mathbf{u}^T \delta_k = \gamma_k^T \delta_k$$
$$\beta^{-1} = \mathbf{v}^T \delta_k = -\delta_k^T G_k \delta_k$$

- Therefore, we get the following update for B_{k+1}:

$$G_{k+1} = G_k + \frac{\gamma_k \gamma_k^T}{\gamma_k^T \delta_k} - \frac{G_k \delta_k \delta_k^T G_k}{\delta_k^T G_k \delta_k}$$

BFGS Algorithm

- Next step is to find B_{k+1} as G_{k+1}^{-1}.
- We use Sherman-Morrison Formula to find G_{k+1}^{-1}.
  $(A + \mathbf{u}\mathbf{v}^T)^{-1} = A^{-1} - \frac{A^{-1}\mathbf{u}\mathbf{v}^T A^{-1}}{1+\mathbf{v}^T A^{-1}\mathbf{u}}$
- Applying this formula twice to G_{k+1}, we get

$$B_{k+1}^{BFGS} = B_k^{BFGS} + \left(1 + \frac{\gamma_k^T B_k^{BFGS} \gamma_k}{\delta_k^T \gamma_k}\right) \frac{\delta_k \delta_k^T}{\delta_k^T \gamma_k} - \left(\frac{\delta_k \gamma_k^T B_k^{BFGS} + B_k^{BFGS} \gamma_k \delta_k^T}{\delta_k^T \gamma_k}\right)$$

Broyden Family

- $B_{k+1}(\phi) = \phi B_{k+1}^{BFGS} + (1-\phi) B_{k+1}^{DFP}$, where $\phi \in [0,1]$

Broyden Familty Quasi-Newton Algorithm

1: **Initialize:** The starting point $\mathbf{x}_0$, Symmetric positive definite matrix B_0 and the tolerance parameter $\epsilon > 0$, Set $k = 0$
2: **while** $\|\mathbf{g}_k\| > \epsilon$ **do**
3: $\mathbf{d}_k = -B_k \mathbf{g}_k$
4: Find α_k along $\mathbf{d}_k$ such that

- $f(\mathbf{x}_k + \alpha_k \mathbf{d}_k) < f(\mathbf{x}_k)$
- α_k satisfies Armijo-Wolfe condition

5: $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{d}_k$
6: Find B_{k+1} as

$$B_{k+1}(\phi) = \phi B_{k+1}^{BFGS} + (1 - \phi) B_{k+1}^{DFP}$$

where $\phi \in [0, 1]$.
7: $k = k + 1$
8: **end while**
9: **Output:** $\mathbf{x}^* = \mathbf{x}_k$, a stationary point of f.