Lecture 4: The Gradient Method

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Outline

Outline

Objective: find an optimal solution of the problem

$$\min\{f(\mathbf{x}) : \mathbf{x} \in \mathbb{R}^n\}$$

The iterative algorithms we consider are of the form

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

- $\mathbf{d}_k$ - direction.
- t_k - stepsize.

Limit ourselves to descent directions.

Definition

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

$$f'(\mathbf{x}; \mathbf{d}) = \nabla f(\mathbf{x})^\top \mathbf{d} < 0.$$

Lemma

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

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

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

Proof.

- Since $f'(\mathbf{x};\mathbf{d}) < 0$, it follows from the definition of the directional derivative that

$$\lim_{t \to 0^+} \frac{f(\mathbf{x} + t\mathbf{d}) - f(\mathbf{x})}{t} = f'(\mathbf{x};\mathbf{d}) < 0$$

- Therefore, $\exists \epsilon > 0$ such that

$$\frac{f(\mathbf{x} + t\mathbf{d}) - f(\mathbf{x})}{t} < 0$$

for any $t \in (0, \epsilon]$, which readily implies the desired result. $\square$

Algorithm 1 Schematic Descent Direction Method

1: **Initialization:** pick $\mathbf{x}_0 \in \mathbb{R}^n$ arbitrarily.
2: **for** $k = 0, 1, 2, \cdots$ **do**
3: pick a descent direction $\mathbf{d}_k$.
4: find a stepsize t_k satisfying $f(\mathbf{x}_k + t_k\mathbf{d}_k) < f(\mathbf{x}_k)$.
5: set $\mathbf{x}_{k+1} = \mathbf{x}_k + t_k\mathbf{d}_k$.
6: if a stopping criteria is satisfied, then STOP and $\mathbf{x}_{k+1}$ is the output.
7: **end for**

Many details are missing in the schematic algorithm:

- What is the starting point?
- How to choose the descent direction?
- What stepsize should be taken?
- What is the stopping criteria?

Stepsize Selection Rules

- **Constant stepsize** - $t_k = \bar{t}$ for any k.
- **Exact stepsize** - t_k is a minimizer of f along the ray $\mathbf{x}_k + t\mathbf{d}_k$:

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

- **Backtracking**[1] - requires three parameters:
  $s > 0, \alpha \in (0,1), \beta \in (0,1)$. Here start with an initial stepsize $t_k = s$. While

$$f(\mathbf{x}_k) - f(\mathbf{x}_k + t_k\mathbf{d}_k) < -\alpha t_k \nabla f(\mathbf{x}_k)^\top \mathbf{d}_k,$$

  set $t_k := \beta t_k$.
  Sufficient Decrease Property:

$$f(\mathbf{x}_k) - f(\mathbf{x}_k + t_k\mathbf{d}_k) \geq -\alpha t_k \nabla f(\mathbf{x}_k)^\top \mathbf{d}_k.$$

[1] also referred to as Armijo rule

Consider

$$f(\mathbf{x}) = \mathbf{x}^\top \mathbf{A}\mathbf{x} + 2\mathbf{b}^\top \mathbf{x} + c,$$

where $\mathbf{A}$ is an $n \times n$ positive definite matrix, $\mathbf{b} \in \mathbb{R}^n$ and $c \in \mathbb{R}$. Let $\mathbf{x} \in \mathbb{R}^n$ and let $\mathbf{d} \in \mathbb{R}^n$ be a descent direction of f at $\mathbf{x}$. The objective is to find a solution to

$$\min_{t \geq 0} f(\mathbf{x} + t\mathbf{d})$$

In class

- In the gradient method $\mathbf{d}_k = -\nabla f(\mathbf{x}_k)$.
- This is a descent direction as long as $\nabla f(\mathbf{x}_k) \neq 0$ since

$$f'(\mathbf{x}_k; -\nabla f(\mathbf{x}_k)) = -\nabla f(\mathbf{x}_k)^\top \nabla f(\mathbf{x}_k) = -\|\nabla f(\mathbf{x}_k)\|^2 < 0$$

- In addition for being a descent direction, minus the gradient is also the steepest direction method.

Lemma

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

$$\min_{\mathbf{d}} \left\{ f'(\mathbf{x}; \mathbf{d}) : \|\mathbf{d}\| = 1 \right\} \tag{1}$$

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

Proof. In class

The Gradient Method

Algorithm 2 The Gradient Method

Input: $\epsilon > 0$ - tolerance parameter.
Initialization: pick $\mathbf{x}_0 \in \mathbb{R}^n$ arbitrarily.
for $k = 0, 1, 2, \cdots$ **do**
    pick a stepsize t_k by a line search procedure on the function

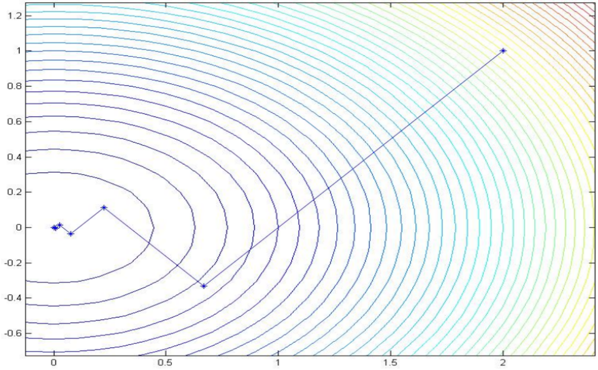
$$g(t) = f(\mathbf{x}_k - t\nabla f(\mathbf{x}_k)).$$

    set $\mathbf{x}_{k+1} = \mathbf{x}_k - t_k \nabla f(\mathbf{x}_k)$.
    if $\|\nabla f(\mathbf{x}_{k+1})\| \leq \epsilon$, then STOP and $\mathbf{x}_{k+1}$ is the output.
end for

Numerical Example

$$\min x^2 + 2y^2$$

$\mathbf{x}_0 = (2; 1), \epsilon = 10^{-5}$, exact line search.



13 iterations until convergence.

Lemma

Let $\{\mathbf{x}_k\}_{k\geq 0}$ be the sequence generated by the gradient method with exact line search for solving a problem of minimizing a continuously differentiable function f. Then for any $k = 0, 1, 2, \cdots$

$$(\mathbf{x}_{k+2} - \mathbf{x}_{k+1})^\top (\mathbf{x}_{k+1} - \mathbf{x}_k) = 0$$

Proof.

- $\mathbf{x}_{k+1} - \mathbf{x}_k = -t_k \nabla f(\mathbf{x}_k), \mathbf{x}_{k+2} - \mathbf{x}_{k+1} = -t_{k+1} \nabla f(\mathbf{x}_{k+1})$
- Therefore, need to prove $\nabla f(\mathbf{x}_k)^\top \nabla f(\mathbf{x}_{k+1}) = 0$.
- $t_k \in \arg\min_{t\geq 0}\{g(t) \equiv f(\mathbf{x}_k - t\nabla f(\mathbf{x}_k))\}$
- Hence, $g'(t_k) = 0$
- $-\nabla f(\mathbf{x}_k)^\top \nabla f(\mathbf{x}_k - t_k \nabla f(\mathbf{x}_k)) = 0$
- $\nabla f(\mathbf{x}_k)^\top \nabla f(\mathbf{x}_{k+1}) = 0$

$\square$

$$\min x^2 + 2y^2$$

$\mathbf{x}_0 = (2; 1)$, $\epsilon = 10^{-5}$, $\bar{t} = 0.1$

$$
\begin{aligned}
\text{iter\_number} &= 1, \ \text{norm\_grad} = 4.000000, \ \text{fun\_val} = 3.280000 \\
\text{iter\_number} &= 2, \ \text{norm\_grad} = 2.937210, \ \text{fun\_val} = 1.897600 \\
\text{iter\_number} &= 3, \ \text{norm\_grad} = 2.222791, \ \text{fun\_val} = 1.141888 \\
\vdots &= \vdots \\
\text{iter\_number} &= 56, \ \text{norm\_grad} = 0.000015, \ \text{fun\_val} = 0.000000 \\
\text{iter\_number} &= 57, \ \text{norm\_grad} = 0.000012, \ \text{fun\_val} = 0.000000 \\
\text{iter\_number} &= 58, \ \text{norm\_grad} = 0.000010, \ \text{fun\_val} = 0.000000
\end{aligned}
$$

quite a lot of iterations...

$$\min x^2 + 2y^2$$

$\mathbf{x}_0 = (2; 1)$, $\epsilon = 10^{-5}$, $\bar{t} = 10$.

$$\begin{aligned}
\text{iter_number} &= 1, \text{ norm_grad } = 1783, \text{ fun_val } = 476806 \\
\text{iter_number} &= 2, \text{ norm_grad } = 656210, \text{ fun_val } = 56962873606 \\
\text{iter_number} &= 3, \text{ norm_grad } = 256032703, \text{ fun_val } = 8318300807323452 \\
\vdots &= \vdots \\
\text{iter_number} &= 119, \text{ norm_grad } = \text{NaN}, \text{ fun_val } = \text{NaN}
\end{aligned}$$

- The sequence diverges :(
- Important question: how to choose the constant stepsize so that convergence is guaranteed?

Definition

Let f be a continuously differentiable function over $\mathbb{R}^n$. Say that f has a Lipschitz gradient if there exists $L \geq 0$ for which

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

L is called the Lipschitz constant.

- If ∇f is Lipschitz with constant L, then it is also Lipschitz with constant $\tilde{L}$ for all $\tilde{L} \geq L$.
- The class of functions with Lipschitz gradient with constant L is denoted by $C_L^{1,1}(\mathbb{R}^n)$ or just $C_L^{1,1}$

- **Linear functions** - Given $\mathbf{a} \in \mathbb{R}^n$, the function $f(\mathbf{x}) = \mathbf{a}^\top \mathbf{x}$ is in $C_0^{1,1}$.
- **Quadratic functions** - Let $\mathbf{A}$ be a symmetric $n \times n$ matrix, $\mathbf{b} \in \mathbb{R}^n$ and $c \in \mathbb{R}$. Then the function

$$f(\mathbf{x}) = \mathbf{x}^\top \mathbf{A}\mathbf{x} + 2\mathbf{b}^\top \mathbf{x} + c$$

is a $C^{1,1}$ function. The smallest Lipschitz constant of ∇f is $2\|\mathbf{A}\|_2$ – why? In class

Theorem

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

1. $f \in C_L^{1,1}(\mathbb{R}^n)$
2. $\|\nabla^2 f(\mathbf{x})\| \leq L$ *for any* $\mathbf{x} \in \mathbb{R}^n$

Proof on pages 73,74 of the book.

Example: $f(x) = \sqrt{1 + x^2} \in C_1^{1,1}$

In class

Outline

Convergence of the Gradient Method

Theorem

Let $\{\mathbf{x}_k\}_{k\geq 0}$ *be the sequence generated by GM 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* $s > 0$ *and* $\alpha, \beta \in (0, 1)$.

Assume that

- $f \in C_L^{1,1}(\mathbb{R}^n)$
- f *is bounded below over* $\mathbb{R}^n$ ($\exists m \in \mathbb{R}$ *s.t.* $f(\mathbf{x}) > m, \forall \mathbf{x} \in \mathbb{R}^n$)

Then,

1. *for any* k, $f(\mathbf{x}_{k+1}) < f(\mathbf{x}_k)$ *unless* $\nabla f(\mathbf{x}_k) = \mathbf{0}$
2. $\nabla f(\mathbf{x}_k) \to 0$ *as* $k \to \infty$

Theorem 4.25 in the book.

Lemma (descent lemma)

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

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

Proof. In class

Lemma (sufficient decrease lemma)

Suppose that $f \in C_L^{1,1}(D)$ *for some* $L > 0$. *Then for any* $\mathbf{x} \in \mathbb{R}^n$ *and* $t > 0$

$$f(\mathbf{x}) - f(\mathbf{x} - t\nabla f(\mathbf{x})) \geq t\left(1 - \frac{Lt}{2}\right) \|\nabla f(\mathbf{x})\|^2.$$

Proof. In class

Lemma (sufficient decrease of the gradient method)

Let $f \in C_L^{1,1}(D)$. *Let* $\{\mathbf{x}_k\}_{k\geq 0}$ *be the sequence generated by GM 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* $s > 0$ *and* $\alpha, \beta \in (0,1)$.

Then

$$f(\mathbf{x}_k) - f(\mathbf{x}_{k+1}) \geq M\|\nabla f(\mathbf{x}_k)\|^2,$$

where

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

Proof. In class

Theorem (rate of convergence of gradient norms)

Under the setting of Theorem 4.25, let f^* be the limit of the convergent sequence $\{f(\mathbf{x}_k)\}_{k\geq 0}$. Then for any $n = 0, 1, 2, \ldots$,

$$\min_{k=0,1,\ldots,n} \|\nabla f(\mathbf{x}_k)\| \leq \sqrt{\frac{f(\mathbf{x}_0) - f^*}{M(n+1)}}.$$

Proof. In class

Two Numerical Examples - Backtracking

$\min x^2 + 2y^2$, $\mathbf{x}_0 = (2;1), s = 2, \alpha = 0.25, \beta = 0.5, \epsilon = 10^{-5}$

$$\text{iter\_number} = 1, \ \text{norm\_grad} = 2.000000, \ \text{fun\_val} = 1.000000$$
$$\text{iter\_number} = 2, \ \text{norm\_grad} = 0.000000, \ \text{fun\_val} = 0.000000$$

- fast convergence (also due to luck!)
- no real disadvantage to exact line search.

Two Numerical Examples - Backtracking

$\min x^2 + 2y^2$, $\mathbf{x}_0 = (2;1), s = 2, \alpha = 0.25, \beta = 0.5, \epsilon = 10^{-5}$

$$\begin{aligned} \text{iter\_number} &= 1, \ \text{norm\_grad} = 2.000000, \ \text{fun\_val} = 1.000000 \\ \text{iter\_number} &= 2, \ \text{norm\_grad} = 0.000000, \ \text{fun\_val} = 0.000000 \end{aligned}$$

- fast convergence (also due to luck!)
- no real disadvantage to exact line search.

ANOTHER EXAMPLE:

min $0.01x^2 + 2y^2, \mathbf{x}_0 = (2;1), s = 2, \alpha = 0.25, \beta = 0.5, \epsilon = 10^{-5}$

$$\begin{aligned} \text{iter\_number} &= 1, \ \text{norm\_grad} = 0.028003, \ \text{fun\_val} = 0.009704 \\ \text{iter\_number} &= 2, \ \text{norm\_grad} = 0.027730, \ \text{fun\_val} = 0.009324 \\ \text{iter\_number} &= 3, \ \text{norm\_grad} = 0.027465, \ \text{fun\_val} = 0.008958 \\ &\vdots \quad \vdots \\ \text{iter\_number} &= 201, \ \text{norm\_grad} = 0.000010, \ \text{fun\_val} = 0.000000 \end{aligned}$$

Important Question: can we detect key properties of the objective function that imply slow/fast convergence?

Theorem

Let $\{\mathbf{x}_k\}_{k\geq 0}$ *be the sequence generated by the gradient method with exact line search for solving the problem*

$$\min_{\mathbf{x}\in\mathbb{R}^n} \mathbf{x}^\top \mathbf{A}\mathbf{x} \quad (\mathbf{A} \succ \mathbf{0})$$

Then for any $k = 0, 1, \cdots,$

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

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

Proof.

We have $\mathbf{x}_{k+1} = \mathbf{x}_k - t_k \mathbf{d}_k$, where $t_k = \frac{\mathbf{d}_k^\top \mathbf{d}_k}{2\mathbf{d}_k^\top \mathbf{A}\mathbf{d}_k}$, $\mathbf{d}_k = 2\mathbf{A}\mathbf{x}_k$. Hence

$$
\begin{aligned}
f(\mathbf{x}_{k+1}) &= \mathbf{x}_{k+1}^\top \mathbf{A}\mathbf{x}_{k+1} = (\mathbf{x}_k - t_k\mathbf{d}_k)^\top \mathbf{A}(\mathbf{x}_k - t_k\mathbf{d}_k) \\
&= \mathbf{x}_k^\top \mathbf{A}\mathbf{x}_k - 2t_k\mathbf{d}_k^\top \mathbf{A}\mathbf{x}_k + t_k^2\mathbf{d}_k^\top \mathbf{A}\mathbf{d}_k \\
&= \mathbf{x}_k^\top \mathbf{A}\mathbf{x}_k - t_k\mathbf{d}_k^\top \mathbf{d}_k + t_k^2\mathbf{d}_k^\top \mathbf{A}\mathbf{d}_k
\end{aligned}
$$

Plugging in the expression for t_k,

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

□

Proof continued.

By Kantorovich:

$$f(\mathbf{x}_{k+1}) \leq \left(1 - \frac{4Mm}{(M+m)^2}\right) f(\mathbf{x}_k) = \left(\frac{M-m}{M+m}\right)^2 f(\mathbf{x}_k)$$
$$= \left(\frac{\kappa(\mathbf{A})-1}{\kappa(\mathbf{A})+1}\right)^2 f(\mathbf{x}_k),$$

where $\kappa(\mathbf{A}) = \frac{M}{m}$. □

Lemma (Kantorovich Inequality)

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

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

holds.

Kantorovich Inequality

Proof.

- Denote $m = \lambda_{\min}(\mathbf{A})$ and $M = \lambda_{\max}(\mathbf{A})$.
- The eigenvalues of the matrix $\mathbf{A} + Mm\mathbf{A}^{-1}$ are $\lambda_i(\mathbf{A}) + \frac{Mm}{\lambda_i(\mathbf{A})}$.
- The maximum of the $1-D$ function $\phi(t) = t + \frac{Mm}{t}$ over $[m, M]$ is attained at the endpoints m and M with a corresponding value of $M + m$.
- Thus, the eigenvalues of $\mathbf{A} + Mm\mathbf{A}^{-1}$ are smaller than $(M + m)$.
- $\mathbf{A} + Mm\mathbf{A}^{-1} \preceq (M + m)\mathbf{I}$
- $\mathbf{x}^\top\mathbf{A}\mathbf{x} + Mm(\mathbf{x}^\top\mathbf{A}^{-1}\mathbf{x}) \leq (M + m)(\mathbf{x}^\top\mathbf{x})$.
- Therefore,

$$
\begin{aligned}
(\mathbf{x}^\top\mathbf{A}\mathbf{x})\left[Mm(\mathbf{x}^\top\mathbf{A}^{-1}\mathbf{x})\right] \leq & \frac{1}{4}\left[(\mathbf{x}^\top\mathbf{A}\mathbf{x}) + Mm(\mathbf{x}^\top\mathbf{A}^{-1}\mathbf{x})\right]^2 \\
\leq & \frac{(M + m)^2}{4}(\mathbf{x}^\top\mathbf{x})^2.
\end{aligned}
$$

□

Definition

Let $\mathbf{A}$ be a positive definite $n \times n$ matrix. Then the condition number of $\mathbf{A}$ is defined by

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

- Matrices (or quadratic functions) with large condition number are called ill-conditioned.
- Matrices with small condition number are called well-conditioned.
- Large condition number implies large number of iterations of the gradient method.
- Small condition number implies small number of iterations of the gradient method.
- For a non-quadratic function, the asymptotic rate of convergence of $\mathbf{x}_k$ to a stationary point $\mathbf{x}^*$ is usually determined by the condition number of $\nabla^2 f(\mathbf{x}^*)$.

A Severely Ill-Condition Function - Rosenbrock

Consider

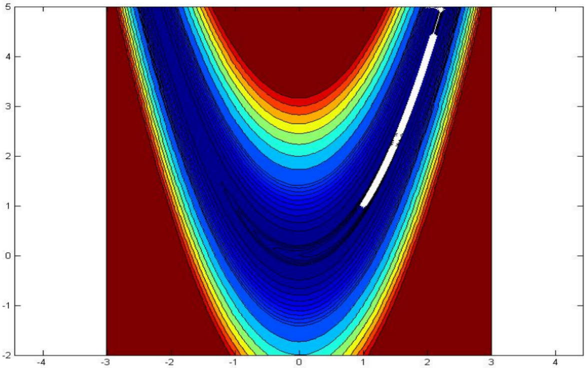
$$\min \left\{ f(x_1, x_2) = 100(x_1 - x_2^2)^2 + (1 - x_1)^2 \right\}.$$

- Optimal solution: $(x_1, x_2) = (1, 1)$, optimal value: 0.
- $$\begin{aligned} \nabla f(\mathbf{x}) &= \begin{pmatrix} -400x_1(x_2 - x_1^2) - 2(1 - x_1) \\ 200(x_2 - x_1^2) \end{pmatrix}, \\ \nabla^2 f(\mathbf{x}) &= \begin{pmatrix} -400x_2 + 1200x_1^2 + 2 & -400x_1 \\ -400x_1 & 200 \end{pmatrix}, \end{aligned}$$

$$\nabla^2 f(1, 1) = \begin{pmatrix} 802 & -400 \\ -400 & 200 \end{pmatrix}.$$

condition number: 2508

$\mathbf{x}_0 = (2;5), s = 2, \alpha = 0.25, \beta = 0.5, \epsilon = 10^{-5}$, backtracking stepsize selection.



6890(!!!) iterations.

- Suppose that we are given the linear system

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

  where $\mathbf{A} \succ 0$ and assume that $\mathbf{x}$ is indeed the solution of the system ($\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$).
- Suppose that the right-hand side is perturbed $\mathbf{b} + \Delta\mathbf{b}$. What can be said on the solution of the new system $\mathbf{x} + \Delta\mathbf{x}$?
- $\Delta\mathbf{x} = \mathbf{A}^{-1}\Delta\mathbf{b}$.
- Result (derivation in class):

$$\frac{\|\Delta\mathbf{x}\|}{\|\mathbf{x}\|} \leq \kappa(\mathbf{A})\frac{\|\Delta\mathbf{b}\|}{\|\mathbf{b}\|}$$

- Consider the ill-conditioned matrix:

$$\mathbf{A} = \begin{pmatrix} 1+10^{-5} & 1 \\ 1 & 1+10^{-5} \end{pmatrix}$$

$\gg$ A=[1+1e-5,1;1,1+1e-5];
$\gg$ cond(A)
ans = 2.000009999998795e+005

- We have
  $\gg$ A\[1;1]
  ans = 0.499997500018278
  0.499997500006722
- However, $\gg$ A\[1.1;1]
  ans = 1.0e+003 *
  5.000524997400047
  -4.999475002650021

Outline

1. The Gradient Method
2. Convergence of The Gradient Method
3. Scaled Gradient Method

Scaled Gradient Method

- Consider the minimization problem

$$(P) \qquad \min\{f(\mathbf{x}) : \mathbf{x} \in \mathbb{R}^n\}.$$

- For a given nonsingular matrix $\mathbf{S} \in \mathbb{R}^{n\times n}$, we make the linear change of variables $\mathbf{x} = \mathbf{S}\mathbf{y}$, and obtain the equivalent problem

$$(P') \qquad \min\{g(\mathbf{y}) \equiv f(\mathbf{S}\mathbf{y}) : \mathbf{y} \in \mathbb{R}^n\}.$$

- Since $\nabla g(\mathbf{y}) = \mathbf{S}^\top \nabla f(\mathbf{S}\mathbf{y}) = \mathbf{S}^\top \nabla f(\mathbf{x})$, the gradient method for (P') is

$$\mathbf{y}_{k+1} = \mathbf{y}_k - t_k \mathbf{S}^\top \nabla f(\mathbf{S}\mathbf{y}_k)$$

- Multiplying the latter equality by $\mathbf{S}$ from the left, and using the notation $\mathbf{x}_k = \mathbf{S}\mathbf{y}_k$:

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

- Defining $\mathbf{D} = \mathbf{S}\mathbf{S}^\top$, we obtain the scaled gradient method:

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

Scaled Gradient Method

- $\mathbf{D} \succ \mathbf{0}$, so the direction $-\mathbf{D}\nabla f(\mathbf{x}_k)$ is a descent direction:

$$f'(\mathbf{x}_k; -\mathbf{D}\nabla f(\mathbf{x}_k)) = -\nabla f(\mathbf{x}_k)^\top \mathbf{D}\nabla f(\mathbf{x}_k) < 0$$

We allow different scaling matrices at each iteration.

Algorithm 3 Scaled Gradient Method

Input: $\epsilon > 0$ - tolerance parameter.
Initialization: pick $\mathbf{x}_0 \in \mathbb{R}^n$ arbitrarily.
for $k = 0, 1, 2, \cdots$ execute the following steps: **do**
    pick a scaling matrix $\mathbf{D}_k \succ 0$
    pick a stepsize t_k by a line search procedure on the function

$$g(t) = f(\mathbf{x}_k - t\mathbf{D}_k\nabla f(\mathbf{x}_k))$$

    set $\mathbf{x}_{k+1} = \mathbf{x}_k - t_k\mathbf{D}_k\nabla f(\mathbf{x}_k)$.
    if $\|\nabla f(\mathbf{x}_{k+1})\| \le \epsilon$, then STOP and $\mathbf{x}_{k+1}$ is the output.
end for

- The scaled gradient method with scaling matrix $\mathbf{D}$ is equivalent to the gradient method employed on the function $g(\mathbf{y}) = f(\mathbf{D}^{1/2}\mathbf{y})$.
- Note that the gradient and Hessian of g are given by

$$\nabla g(\mathbf{y}) = \mathbf{D}^{1/2}\nabla f(\mathbf{D}^{1/2}\mathbf{y}) = \mathbf{D}^{1/2}\nabla f(\mathbf{x})$$
$$\nabla^2 g(\mathbf{y}) = \mathbf{D}^{1/2}\nabla^2 f(\mathbf{D}^{1/2}\mathbf{y})\mathbf{D}^{1/2} = \mathbf{D}^{1/2}\nabla^2 f(\mathbf{x})\mathbf{D}^{1/2}$$

- The objective is usually to pick $\mathbf{D}_k$ so as to make $\mathbf{D}_k^{1/2}\nabla^2 f(\mathbf{x}_k)\mathbf{D}_k^{1/2}$ as well-conditioned as possible.
- A well known choice (Newton's method): $\mathbf{D}_k = (\nabla^2 f(\mathbf{x}_k))^{-1}$.
- Diagonal scaling: $\mathbf{D}_k$ is picked to be diagonal. For example,

$$(\mathbf{D}_k)_{ii} = \left(\frac{\partial^2 f(\mathbf{x}_k)}{\partial x_i^2}\right)^{-1}$$

- Diagonal scaling can be very effective when the decision variables are of different magnitudes.

The Gauss-Newton Method

- Nonlinear least squares problem:

$$\text{(NLS):} \qquad \min_{\mathbf{x}\in\mathbb{R}^n}\{g(\mathbf{x}) \equiv \sum_{i=1}^{m}(f_i(\mathbf{x}) - c_i)^2\}.$$

  $f_1, \cdots, f_m$ are continuously differentiable over $\mathbb{R}^n$ and $c_1, \cdots, c_m \in \mathbb{R}$.

- Denote:

$$F(\mathbf{x}) = \begin{pmatrix} f_1(\mathbf{x}) - c_1 \\ f_2(\mathbf{x}) - c_2 \\ \vdots \\ f_m(\mathbf{x}) - c_m \end{pmatrix}$$

- Then the problem becomes:

$$\min \|F(\mathbf{x})\|^2$$

Given the k-th iterate $\mathbf{x}_k$, the next iterate is chosen to minimize the sum of squares of the linearized terms, that is,

$$\mathbf{x}_{k+1} = \arg\min_{\mathbf{x}\in\mathbb{R}^n} \left\{ \sum_{i=1}^{m} \left[f_i(\mathbf{x}_k) + \nabla f_i(\mathbf{x}_k)^\top (\mathbf{x} - \mathbf{x}_k) - c_i \right]^2 \right\}$$

- The general step actually consists of solving the linear LS problem

$$\min \|\mathbf{A}_k \mathbf{x} - \mathbf{b}_k\|^2$$

where

$$\mathbf{A}_k = \begin{pmatrix} \nabla f_1(\mathbf{x}_k)^\top \\ \nabla f_2(\mathbf{x}_k)^\top \\ \vdots \\ \nabla f_m(\mathbf{x}_k)^\top \end{pmatrix} = J(\mathbf{x}_k)$$

is the so-called Jacobian matrix, assumed to have full column rank.

$$\mathbf{b}_k = \begin{pmatrix} \nabla f_1(\mathbf{x}_k)^\top \mathbf{x}_k - f_1(\mathbf{x}_k) + c_1 \\ \nabla f_2(\mathbf{x}_k)^\top \mathbf{x}_k - f_2(\mathbf{x}_k) + c_2 \\ \vdots \\ \nabla f_m(\mathbf{x}_k)^\top \mathbf{x}_k - f_m(\mathbf{x}_k) + c_m \end{pmatrix} = J(\mathbf{x}_k)\mathbf{x}_k - F(\mathbf{x}_k)$$

- The Gauss-Newton method can thus be written as:

$$\mathbf{x}_{k+1} = (J(\mathbf{x}_k)^\top J(\mathbf{x}_k))^{-1} J(\mathbf{x}_k)^\top \mathbf{b}_k$$

- The gradient of the objective function $g(\mathbf{x}) = \|F(\mathbf{x})\|^2$ is

$$\nabla g(\mathbf{x}) = 2J(\mathbf{x})^\top F(\mathbf{x})$$

- The GN method can be rewritten as follows:

$$\begin{aligned}
\mathbf{x}_{k+1} &= (J(\mathbf{x}_k)^\top J(\mathbf{x}_k))^{-1} J(\mathbf{x}_k)^\top (J(\mathbf{x}_k)\mathbf{x}_k - F(\mathbf{x}_k)) \\
&= \mathbf{x}_k - (J(\mathbf{x}_k)^\top J(\mathbf{x}_k))^{-1} J(\mathbf{x}_k)^\top F(\mathbf{x}_k) \\
&= \mathbf{x}_k - \frac{1}{2}(J(\mathbf{x}_k)^\top J(\mathbf{x}_k))^{-1} \nabla g(\mathbf{x}_k)
\end{aligned}$$

- That is, it is a scaled gradient method with a special choice of scaling matrix:

$$\mathbf{D}_k = \frac{1}{2}(J(\mathbf{x}_k)^\top J(\mathbf{x}_k))^{-1}$$

The Gauss-Newton method does not incorporate a stepsize, which might cause it to diverge. A well known variation of the method incorporating stepsizes is the damped Gauss-newton Method.

Algorithm 4 Damped Gauss-Newton Method

Input: $\epsilon > 0$ - tolerance parameter.
Initialization: pick $\mathbf{x}_0 \in \mathbb{R}^n$ arbitrarily.
for $k = 0, 1, 2, \cdots$ execute the following steps: **do**
    set $\mathbf{d}_k = -(J(\mathbf{x}_k)^\top J(\mathbf{x}_k))^{-1} J(\mathbf{x}_k)^\top F(\mathbf{x}_k)$
    set t_k by a line search procedure on the function

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

    set $\mathbf{x}_{k+1} = \mathbf{x}_k + t_k \mathbf{d}_k$.
    if $\|\nabla f(\mathbf{x}_{k+1})\| \le \epsilon$, then STOP and $\mathbf{x}_{k+1}$ is the output.
end for

Fermat-Weber Problem: Given m points in $\mathbb{R}^n$: $\mathbf{a}_1, \cdots, \mathbf{a}_m$ – also called "anchor point" – and m weights $\omega_1, \omega_2, \cdots, \omega_m > 0$, find a point $\mathbf{x} \in \mathbb{R}^n$ that minimizes the weighted distance of $\mathbf{x}$ to each of the points $\mathbf{a}_1, \cdots, \mathbf{a}_m$:

$$\min_{\mathbf{x} \in \mathbb{R}^n} \left\{ f(\mathbf{x}) \equiv \sum_{i=1}^{m} \omega_i \|\mathbf{x} - \mathbf{a}_i\| \right\}$$

- The objective function is not differentiable at the anchor points $\mathbf{a}_1, \cdots, \mathbf{a}_m$.
- One of the simplest instances of facility location problems.

Weiszfeld's Method (1937)

- Start from the stationarity condition $\nabla f(\mathbf{x}) = \mathbf{0}$.[2]
- $\sum_{i=1}^{m} \omega_i \frac{\mathbf{x}-\mathbf{a}_i}{\|\mathbf{x}-\mathbf{a}_i\|} = \mathbf{0}$
- $\left(\sum_{i=1}^{m} \frac{\omega_i}{\|\mathbf{x}-\mathbf{a}_i\|}\right) \mathbf{x} = \sum_{i=1}^{m} \frac{\omega_i \mathbf{a}_i}{\|\mathbf{x}-\mathbf{a}_i\|}$
- $\mathbf{x} = \frac{1}{\sum_{i=1}^{m} \frac{\omega_i}{\|\mathbf{x}-\mathbf{a}_i\|}} \sum_{i=1}^{m} \frac{\omega_i \mathbf{a}_i}{\|\mathbf{x}-\mathbf{a}_i\|}$
- The stationarity condition can be written as $\mathbf{x} \equiv T(\mathbf{x})$, where T is the operator

$$T(\mathbf{x}) \equiv \frac{1}{\sum_{i=1}^{m} \frac{\omega_i}{\|\mathbf{x}-\mathbf{a}_i\|}} \sum_{i=1}^{m} \frac{\omega_i \mathbf{a}_i}{\|\mathbf{x} - \mathbf{a}_i\|}$$

- Weiszfeld's method is a fixed point method:

$$\mathbf{x}_{k+1} = T(\mathbf{x}_k)$$

[2] We implicitly assume here that $\mathbf{x}$ is not an anchor point.

Weiszfeld's Method
Initialization: pick $\mathbf{x}_0 \in \mathbb{R}^n$ arbitrarily.
General step: for any $k = 0, 1, 2, \cdots$ compute:

$$\mathbf{x}_{k+1} = T(\mathbf{x}_k) = \frac{1}{\sum_{i=1}^m \frac{\omega_i}{\|\mathbf{x}_k - \mathbf{a}_i\|}} \sum_{i=1}^m \frac{\omega_i \mathbf{a}_i}{\|\mathbf{x}_k - \mathbf{a}_i\|}$$

- Weiszfeld's method is a gradient method since

$$\begin{aligned} \mathbf{x}_{k+1} &= \mathbf{x}_k - \frac{1}{\sum_{i=1}^m \frac{\omega_i}{\|\mathbf{x}_k - \mathbf{a}_i\|}} \sum_{i=1}^m \omega_i \frac{\mathbf{x}_k - \mathbf{a}_i}{\|\mathbf{x}_k - \mathbf{a}_i\|} \\ &= \mathbf{x}_k - \frac{1}{\sum_{i=1}^m \frac{\omega_i}{\|\mathbf{x}_k - \mathbf{a}_i\|}} \nabla f(\mathbf{x}_k) \end{aligned}$$

- A gradient method with a special choice of stepsize: $t_k = \frac{1}{\sum_{i=1}^m \frac{\omega_i}{\|\mathbf{x}_k - \mathbf{a}_i\|}}$.