Fundamentals of Unconstrained Optimization

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Outline

Optimization Problem

$$\min_{\boldsymbol{x} \in \Omega} f(\boldsymbol{x})$$

where $f(\boldsymbol{x})$ is a real-valued function

- The function $f : \mathbb{R}^n \to \mathbb{R}$ is called the objective function or cost function.
- The vector $\boldsymbol{x}$ is an n-vector of independent variables: $\boldsymbol{x} = [x_1, x_2, \cdots, x_n]^T \in \mathbb{R}^n$.
- The variables $x_1, x_2, \cdots, x_n$ are often referred to as decision variables.
- The set $\Omega \subset \mathbb{R}^n$ is called the *constraint set* or *feasible set*.

Type of extrema

- **Definition**: Suppose that $f : \mathbb{R}^n \to \mathbb{R}$ is a real-valued function defined on $\Omega \subset \mathbb{R}^n$. A point $\boldsymbol{x}^* \in \Omega$ is a *local minimizer* of f over Ω if there exists $\epsilon > 0$ such that $f(\boldsymbol{x}) \geq f(\boldsymbol{x}^*)$ for all $\boldsymbol{x} \in \Omega \setminus \{\boldsymbol{x}^*\}$ and $\|\boldsymbol{x} - \boldsymbol{x}^*\| < \epsilon$.
- **Definition**: Suppose that $f : \mathbb{R}^n \to \mathbb{R}$ is a real-valued function defined on $\Omega \subset \mathbb{R}^n$. A point $\boldsymbol{x}^* \in \Omega$ is a *global minimizer* of f over Ω if $f(\boldsymbol{x}) \geq f(\boldsymbol{x}^*)$ for all $\boldsymbol{x} \in \Omega \setminus \{\boldsymbol{x}^*\}$.
- Replacing $\geq$ with $>$ in the previous definitions we have a *strict local minimizer* and a *strict global minimizer*, respectively

Type of extrema

- If $\boldsymbol{x}^*$ is a global minimizer of f over Ω, we write

$$\begin{aligned} f(\boldsymbol{x}^*) &= \min_{\boldsymbol{x}\in\Omega} f(\boldsymbol{x}) \\ \boldsymbol{x}^* &= \arg\min_{\boldsymbol{x}\in\Omega} f(\boldsymbol{x}). \end{aligned}$$

- If $\boldsymbol{x}^*$ is a global minimizer of f over $\mathbb{R}^n$, i.e., unconstrained problem, we write

$$\begin{aligned} f(\boldsymbol{x}^*) &= \min_{\boldsymbol{x}} f(\boldsymbol{x}) \\ \boldsymbol{x}^* &= \arg\min_{\boldsymbol{x}} f(\boldsymbol{x}). \end{aligned}$$

- In general, global minimizers are difficult to find. So, in practice, we often are satisfied with finding local minimizers.

First order necessary conditions

Theorem: If $\boldsymbol{x}^*$ is a local minimizer (or maximizer) and f is continuously differentiable in an open neighborhood of $\boldsymbol{x}^*$, then $\nabla f(\boldsymbol{x}^*) = 0$.

First order necessary conditions

Theorem: If $\boldsymbol{x}^*$ is a local minimizer (or maximizer) and f is continuously differentiable in an open neighborhood of $\boldsymbol{x}^*$, then $\nabla f(\boldsymbol{x}^*) = 0$. **Proof (1)**: Suppose that $\nabla f(\boldsymbol{x}^*) \neq 0$. Therefore, we can find a direction $\boldsymbol{v} = -\frac{\nabla f(\boldsymbol{x}^*)}{\|\nabla f(\boldsymbol{x}^*)\|}$ for which $\nabla f(\boldsymbol{x}^*)^T \boldsymbol{v} < 0$. Let $h(\theta) = \nabla f(\boldsymbol{x}^* + \theta \boldsymbol{v})^T \boldsymbol{v}$. As $h(0) < 0$ there exits $\epsilon > 0$ for which $h(\theta) < 0$ for all $\theta \in (0, \epsilon)$. Using Taylor's Theorem, there exists $\tau \in (0, 1)$ such that for all $\hat{\epsilon} \in [0, \epsilon)$

$$f(\boldsymbol{x}^* + \hat{\epsilon}\boldsymbol{v}) \quad = \quad f(\boldsymbol{x}^*) + \hat{\epsilon} \nabla f(\boldsymbol{x}^* + \tau \hat{\epsilon} \boldsymbol{v})^T \boldsymbol{v}$$

Defining $\theta = \tau \hat{\epsilon}$ it holds that $\theta \in [0, \hat{\epsilon}) \subset [0, \epsilon)$. Therefore $\nabla f(\boldsymbol{x}^* + \tau \hat{\epsilon} \boldsymbol{v})^T \boldsymbol{v} < 0$ and as consequence $f(\boldsymbol{x}^* + \hat{\epsilon}\boldsymbol{v}) < f(\boldsymbol{x}^*)$ which contradict that $\boldsymbol{x}^*$ is a minimizer.

First order necessary conditions

Theorem: If $\boldsymbol{x}^*$ is a local minimizer (or maximizer) and f is continuously differentiable in an open neighborhood of $\boldsymbol{x}^*$, then $\nabla f(\boldsymbol{x}^*) = 0$.

Proof (2):
Suppose that $\nabla f(\boldsymbol{x}^*) \neq 0$. Therefore, we can find a direction $\boldsymbol{h} = -\alpha \frac{\nabla f(\boldsymbol{x}^*)}{\|\nabla f(\boldsymbol{x}^*)\|} = -\alpha \boldsymbol{v}$ for which $\nabla f(\boldsymbol{x}^*)^T \boldsymbol{h} < 0$. Using Taylor's formula for $\boldsymbol{x} = \boldsymbol{x}^* + \boldsymbol{h}$

$$f(\boldsymbol{x}) \quad = \quad f(\boldsymbol{x}^*) + \boldsymbol{g}(\boldsymbol{x}^*)^T \boldsymbol{h} + o(\|\boldsymbol{h}\|)$$

if $\alpha \to 0$ then $\boldsymbol{h} \to 0$ and $\boldsymbol{g}(\boldsymbol{x}^*)^T \boldsymbol{h} + o(\|\boldsymbol{h}\|) < 0$ because $o(\|\boldsymbol{h}\|)$ goes to zero faster than $\boldsymbol{g}(\boldsymbol{x}^*)^T \boldsymbol{h}$, in fact $\lim_{\alpha \to 0} \frac{|\boldsymbol{g}(\boldsymbol{x}^*)^T \boldsymbol{h}|}{\|\boldsymbol{h}\|} = \frac{|\boldsymbol{g}(\boldsymbol{x}^*)^T \boldsymbol{v}|}{\|\boldsymbol{v}\|}$. Therefore $f(\boldsymbol{x}) < f(\boldsymbol{x}^*)$. This contradicts the assumption that $\boldsymbol{x}^*$ is a minimizer.

First order necessary conditions

Theorem: If $\boldsymbol{x}^*$ is a local minimizer (or maximizer) and f is continuously differentiable in an open neighborhood of $\boldsymbol{x}^*$, then $\nabla f(\boldsymbol{x}^*) = 0$.

- A point that satisfies that $\nabla f(\boldsymbol{x}^*) = 0$ is called *a stationary point*.
- According to the previous theorem, any local minimizer (or maximizer) must be a stationary point.

Second order necessary conditions

Theorem If $\boldsymbol{x}^*$ is a local minimizer (maximizer) of f and $\nabla^2 f$ exists and is continuous in an open neighborhood of $\boldsymbol{x}^*$, then $\nabla f(\boldsymbol{x}^*) = 0$ and $\nabla^2 f(\boldsymbol{x}^*)$ is positive semidefinite (negative semidefinite).

Second order necessary conditions

Theorem If $\boldsymbol{x}^*$ is a local minimizer (maximizer) of f and $\nabla^2 f$ exists and is continuous in an open neighborhood of $\boldsymbol{x}^*$, then $\nabla f(\boldsymbol{x}^*) = 0$ and $\nabla^2 f(\boldsymbol{x}^*)$ is positive semidefinite (negative semidefinite).

Proof:

- From the previous theorem $\nabla f(\boldsymbol{x}^*) = 0$
- (By contradiction) assume that $\nabla^2 f$ is not positive semidefinite.
- Then, we can choose a vector $\boldsymbol{v}$ such that $\boldsymbol{v}^T \nabla^2 f(\boldsymbol{x}^*) \boldsymbol{v}^T < 0$, and because $\nabla^2 f$ is continuous near $\boldsymbol{x}^*$, there is a scalar $\epsilon > 0$ such that $\boldsymbol{v}^T \nabla^2 f(\boldsymbol{x}^* + \hat{\epsilon}\boldsymbol{v})\boldsymbol{v}^T < 0$ for all $\hat{\epsilon} \in [0, \epsilon)$.

Second order necessary conditions

Theorem If $\boldsymbol{x}^*$ is a local minimizer (maximizer) of f and $\nabla^2 f$ exists and is continuous in an open neighborhood of $\boldsymbol{x}^*$, then $\nabla f(\boldsymbol{x}^*) = 0$ and $\nabla^2 f(\boldsymbol{x}^*)$ is positive semidefinite (negative semidefinite).

Proof:

- Applying Taylor's theorem around $\boldsymbol{x}^*$, there exits $\tau \in (0,1)$ for all $\hat{\epsilon} \in [0, \epsilon)$ for which

  $$f(\boldsymbol{x}^* + \hat{\epsilon}\boldsymbol{v}) \;\; = \;\; f(\boldsymbol{x}^*) + \hat{\epsilon}\nabla f(\boldsymbol{x}^*)^T \boldsymbol{v} + \frac{1}{2}\hat{\epsilon}^2 \boldsymbol{v}^T \nabla^2 f(\boldsymbol{x}^* + \tau\hat{\epsilon}\boldsymbol{v})\boldsymbol{v}$$

  using that $\nabla f(\boldsymbol{x}^*)^T \boldsymbol{v} = 0$ and $\boldsymbol{v}^T \nabla^2 f(\boldsymbol{x}^* + \tau\hat{\epsilon}\boldsymbol{v})\boldsymbol{v} < 0$ we obtain $f(\boldsymbol{x}^* + \hat{\epsilon}\boldsymbol{v}) < f(\boldsymbol{x}^*)$ which is a contradiction!

Second order sufficient conditions

Theorem: Suppose that $\nabla^2 f$ exists and is continuous in an open neighborhood of $\boldsymbol{x}^*$, and that $\nabla f(\boldsymbol{x}^*) = 0$ and $\nabla^2 f(\boldsymbol{x}^*)$ is positive definite (negative definite). Then $\boldsymbol{x}^*$ is a strict local minimizer (maximizer) of f.

Second order sufficient conditions

Proof:

- There exists a ball $B_r(\boldsymbol{x}^*) = \{\boldsymbol{x} | \, \|\boldsymbol{x} - \boldsymbol{x}^*\| < r\}$ for which $q(\theta) = \boldsymbol{h}^T D^2 f(\boldsymbol{z})\boldsymbol{h} > 0$ with $\|\boldsymbol{h}\| < r$, $\boldsymbol{z} = \boldsymbol{x}^* + \theta\boldsymbol{h}$ with $\theta \in (0, 1)$ (note that $\boldsymbol{z} \in B_r(\boldsymbol{x}^*)$) due to $q(\theta)$ is continuous and $q(0) > 0$.
- Using the Taylor's Theorem with $\boldsymbol{x} = \boldsymbol{x}^* + \boldsymbol{h} \in B_r(\boldsymbol{x}^*)$, i.e.,$\|\boldsymbol{h}\| < r$, and that $\nabla f(\boldsymbol{x}^*) = 0$, there exists $\theta \in (0, 1)$ such that

$$f(\boldsymbol{x}) \quad = \quad f(\boldsymbol{x}^*) + \frac{1}{2}\boldsymbol{h}^T D^2 f(\boldsymbol{x}^* + \theta\boldsymbol{h})\boldsymbol{h}.$$

- As $\boldsymbol{z} = \boldsymbol{x}^* + \theta\boldsymbol{h} \in B_r(\boldsymbol{x}^*)$ then $\boldsymbol{h}^T D^2 f(\boldsymbol{z})\boldsymbol{h} > 0$ and $f(\boldsymbol{x}) > f(\boldsymbol{x}^*)$ for all $\boldsymbol{x} \in B_r(\boldsymbol{x}^*)$ which gives the result.

Classification of stationary point

- **Definition**: A point $\boldsymbol{x}^*$ that satisfies $\boldsymbol{g}(\boldsymbol{x}^*) = 0$ is called a *stationary point*.
- **Definition**: A point $\boldsymbol{x}^*$ that is neither a maximizer nor a minimizer is called a *saddle point*.

Classification of stationary point

- At a point $\boldsymbol{x} = \boldsymbol{x}^* + \alpha \boldsymbol{d}$ in the neighborhood of a saddle point $\boldsymbol{x}^*$, the Taylor series gives

$$f(\boldsymbol{x}) = f(\boldsymbol{x}^*) + \frac{1}{2}\alpha^2 \boldsymbol{d}^T \mathbf{H}(\boldsymbol{x}^*)\boldsymbol{d} + o(\|\boldsymbol{d}\|^2)$$

  since $\boldsymbol{g}(\boldsymbol{x}^*) = 0$.

- As $\boldsymbol{x}^*$ is neither a maximizer nor a minimizer, there must be directions $\boldsymbol{d}_1$, $\boldsymbol{d}_2$ (or $\boldsymbol{x}_1$, $\boldsymbol{x}_2$) such that

$$\begin{array}{lclcl} f(\overbrace{\boldsymbol{x}^* + \alpha \boldsymbol{d}_1}^{\boldsymbol{x}_1}) & < & f(\boldsymbol{x}^*) & \Rightarrow & \boldsymbol{d}_1^T \mathbf{H}(\boldsymbol{x}^*)\boldsymbol{d}_1 < 0 \\ f(\underbrace{\boldsymbol{x}^* + \alpha \boldsymbol{d}_2}_{\boldsymbol{x}_2}) & > & f(\boldsymbol{x}^*) & \Rightarrow & \boldsymbol{d}_2^T \mathbf{H}(\boldsymbol{x}^*)\boldsymbol{d}_2 > 0 \end{array}$$

  Then, $\mathbf{H}(\boldsymbol{x}^*)$ is indefinite

Find and Classify Stationary points

We can find and classify stationary points as follows

- Find the points $\boldsymbol{x}^*$ at which $\boldsymbol{g}(\boldsymbol{x}^*) = 0$.
- Obtain the Hessian $\mathbf{H}(\boldsymbol{x})$.
- Determine the character of $\mathbf{H}(\boldsymbol{x}^*)$ for each point $\boldsymbol{x}^*$.
    - If $\mathbf{H}(\boldsymbol{x}^*)$ is positive (negative) definite then $\boldsymbol{x}^*$ is a minimizer (maximizer).
    - If $\mathbf{H}(\boldsymbol{x}^*)$ is indefinite, $\boldsymbol{x}^*$ is a saddle point.
    - If $\mathbf{H}(\boldsymbol{x}^*)$ is positive (negative) semidefinite, $\boldsymbol{x}^*$ can be a minimizer (maximizer). In this case, further work is necessary to classify the stationary point. A possible approach would be to deduce the third partial derivatives of $f(\boldsymbol{x}^*)$ and then calculate the corresponding term in the Taylor series. If this term is zero, then the next term needs to be calculated and so on (see next slide for 1D case).

Find and Classify Stationary points 1D

Assume that $f^{(1)}(x_0) = f^{(2)}(x_0) = \cdots = f^{(n-1)}(x_0) = 0$ and $f^{(n)}(x_0) \neq 0$, ie, $f^{(n)}(x_0) > 0$ or $f^{(n)}(x_0) < 0$.

1. Using Taylor's theorem $f(x) = f(x_0) + \frac{f^{(n)}(x_0+th)}{n!}(x - x_0)^n$, $h = x - x_0$, for some $t \in (0, 1)$. Therefore, one just needs to consider the sign of $q = \frac{f^{(n)}(x_0+th)}{n!}(x - x_0)^n$

Find and Classify Stationary points 1D

Assume that $f^{(1)}(x_0) = f^{(2)}(x_0) = \cdots = f^{(n-1)}(x_0) = 0$ and $f^{(n)}(x_0) \neq 0$, ie, $f^{(n)}(x_0) > 0$ or $f^{(n)}(x_0) < 0$.

1. Using Taylor's theorem $f(x) = f(x_0) + \frac{f^{(n)}(x_0+th)}{n!}(x - x_0)^n$, $h = x - x_0$, for some $t \in (0,1)$. Therefore, one just needs to consider the sign of $q = \frac{f^{(n)}(x_0+th)}{n!}(x - x_0)^n$
   - If the sign of $\frac{f^{(n)}(x_0+th)}{n!}(x - x_0)^n$ is positive for all $x \in (x_0 - \delta, x_0 + \delta)$ then $f(x) > f(x_0)$, and x_0 is a local minimum
   - If the sign of $\frac{f^{(n)}(x_0+th)}{n!}(x - x_0)^n$ is negative for all $x \in (x_0 - \delta, x_0 + \delta)$ then $f(x) < f(x_0)$, and x_0 is a local maximum
   - If the sign of $\frac{f^{(n)}(x_0+th)}{n!}(x - x_0)^n$ is positive and negative for $x \in (x_0 - \delta, x_0 + \delta)$ then $f(x) \lessgtr f(x_0)$, and x_0 is an inflection point

Find and Classify Stationary points 1D

1. Using Taylor's theorem $f(x) = f(x_0) + \frac{f^{(n)}(x_0+th)}{n!}(x - x_0)^n$ for some $t \in (0, 1)$.
   Which is the sign of $q = \frac{f^{(n)}(x_0+th)}{n!}(x - x_0)^n$?

Find and Classify Stationary points 1D

1. Using Taylor's theorem $f(x) = f(x_0) + \frac{f^{(n)}(x_0+th)}{n!}(x - x_0)^n$ for some $t \in (0, 1)$.

   Which is the sign of $q = \frac{f^{(n)}(x_0+th)}{n!}(x - x_0)^n$?

   - If n is even then the sign of q depends only of the factor $f^{(n)}(x_0 + th)$. Taking into account the *theorem of the sign preserving*, if $f^{(n)}(x_0) > 0$ then $q > 0$ in a neighborhood of x_0 and x_0 is a local minimum, on the contrary, if $f^{(n)}(x_0) < 0$ then $q < 0$ in a neighborhood of x_0 and x_0 is a local maximum.
   - If n is odd, q could be positive or negative independently of the sign of $f^{(n)}(x_0)$. The sign of q changes when $x > x_0$ or $x < x_0$. Then x_0 is an inflection point.

$\boldsymbol{x}$ is a stationary point and $\mathbf{H}(\boldsymbol{x}^*) = \mathbf{0}$

- In the special case where $\mathbf{H}(\boldsymbol{x}^*) = \mathbf{0}$, $\boldsymbol{x}$ can be a minimizer or maximizer since the necessary conditions are satisfied in both cases.
- If $\mathbf{H}(\boldsymbol{x}^*)$ is semidefinite, more information is required for the complete characterization of a stationary point and further work is necessary in this case.

$\boldsymbol{x}$ is a stationary point and $\mathbf{H}(\boldsymbol{x}^*) = \mathbf{0}$

- A possible approach could be to compute the third partial derivatives of $f(\boldsymbol{x})$ and then calculate the corresponding term in the Taylor series, $D^3 f(\boldsymbol{x}^*)/3!$. If the this term is zero, then the next term $D^4 f(\boldsymbol{x}^*)/4!$ needs to be computed and so on...

$$
\begin{aligned}
f(\boldsymbol{x}+\boldsymbol{h}) &= f(\boldsymbol{x}) + \boldsymbol{g}(\boldsymbol{x})^T \boldsymbol{h} + \frac{1}{2}\boldsymbol{h}^T \mathbf{H}(\boldsymbol{x})\boldsymbol{h} + \frac{1}{3!} D^3 f(\boldsymbol{x}) + \cdots \\
D^r f(\boldsymbol{x}) &= \sum_{i_1=1}^{n} \sum_{i_2=1}^{n} \cdots \sum_{i_r=1}^{n} h_{i_1} h_{i_2} \cdots h_{i_r} \frac{\partial^r f(\boldsymbol{x})}{\partial x_{i_1} \partial x_{i_2} \cdots \partial x_{i_r}}
\end{aligned}
$$

- $P(\boldsymbol{h}) = D^r f(\boldsymbol{x}) : \mathbb{R}^r \to \mathbb{R}$ is a polynomial of grade r in the variable $\boldsymbol{h}$ (see, Multilinear form)

Example when $\mathbf{H}(\boldsymbol{x}^*) = \mathbf{0}$

$$\begin{aligned}
f(\boldsymbol{x}) &= \frac{1}{6}\left[(x_1-2)^3 + (x_2-3)^3\right] \\
\nabla f(\boldsymbol{x}) &= \frac{1}{2}\left[(x_1-2)^2, (x_2-3)^2\right]^T = 0, \Rightarrow \boldsymbol{x}^* = [2,3]^T \\
\mathbf{H}(\boldsymbol{x}) &= \begin{bmatrix} x_1 - 2 & 0 \\ 0 & x_2 - 3 \end{bmatrix}, \Rightarrow \mathbf{H}(\boldsymbol{x}^*) = \mathbf{0}
\end{aligned}$$

$\frac{\partial^2 f(\boldsymbol{x})}{\partial x_1^2} = x_1 - 2$, $\frac{\partial^2 f(\boldsymbol{x})}{\partial x_2^2} = x_2 - 3$, $\frac{\partial^2 f(\boldsymbol{x})}{\partial x_1 \partial x_2} = \frac{\partial^2 f(\boldsymbol{x})}{\partial x_2 \partial x_1} = 0.$
The third derivatives of f are all zero at $\boldsymbol{x}^*$ except
$\frac{\partial^3 f(\boldsymbol{x}^*)}{\partial x_1^3} = \frac{\partial^3 f(\boldsymbol{x}^*)}{\partial x_2^3} = 1.$

Example when $\mathbf{H}(\boldsymbol{x}^*) = \mathbf{0}$

The third derivatives of f are all zero at $\boldsymbol{x}^*$ except $\frac{\partial^3 f(\boldsymbol{x}^*)}{\partial x_1^3} = \frac{\partial^3 f(\boldsymbol{x}^*)}{\partial x_2^3} = 1$ then

$$
\begin{aligned}
D^3 f(\boldsymbol{x}^*) &= \sum_{i_1,i_2,i_3=1}^{2} h_{i_1} h_{i_2} h_{i_3} \frac{\partial^3 f(\boldsymbol{x}^*)}{\partial x_{i_1} \partial x_{i_2} \partial x_{i_3}} \\
&= h_1^3 \frac{\partial^3 f}{\partial x_1^3} + 3h_1^2 h_2 \frac{\partial^3 f}{\partial x_1^2 \partial x_2} + 3h_1 h_2^2 \frac{\partial^3 f}{\partial x_1 \partial x_2^2} + h_2^3 \frac{\partial^3 f}{\partial x_2^3} \\
&= h_1^3 \frac{\partial^3 f}{\partial x_1^3} + h_2^3 \frac{\partial^3 f}{\partial x_2^3} = h_1^3 + h_2^3 \lesseqqgtr 0
\end{aligned}
$$

that is positive if $h_1, h_2 > 0$ and negative if $h_1, h_2 < 0$. Then $\boldsymbol{x}^*$ is a saddle point due to $f(\boldsymbol{x}^* + \boldsymbol{h}) > f(\boldsymbol{x}^*)$ if $h_1, h_2 > 0$ and $f(\boldsymbol{x}^* + \boldsymbol{h}) < f(\boldsymbol{x}^*)$ if $h_1, h_2 < 0$.

x^* is a stationary point and $\mathbf{H}(x^*) \neq \mathbf{0}$

- In this case, and from the previous discussion, the problem of classifying stationary points of the function $f(\boldsymbol{x})$ becomes the problem of characterizing the Hessian $\mathbf{H}(\boldsymbol{x})$ at $\boldsymbol{x} = \boldsymbol{x}^*$, i.e., one needs to determine if $\mathbf{H}(\boldsymbol{x}^*)$ is positive, negative, positive semidefinite or negative semidefinite.

x^* is a stationary point and $\mathbf{H}(x^*) \neq \mathbf{0}$

Theorem *Characterization of symmetric matrices*: A real symmetric $n \times n$ matrix $\mathbf{H}$ is positive definite, positive semidefinite, etc., if for every nonsingular matrix $\mathbf{B}$ of the same order, the $n \times n$ matrix $\hat{\mathbf{H}}$ given by $\hat{\mathbf{H}} = \mathbf{B}^T\mathbf{H}\mathbf{B}$ is positive definite, positive semidefinite, etc.

Proof: Let $\boldsymbol{x} \neq \mathbf{0}$

$$\boldsymbol{x}^T\hat{\mathbf{H}}\boldsymbol{x} \;=\; \boldsymbol{x}^T\mathbf{B}^T\mathbf{H}\mathbf{B}\boldsymbol{x} = \boldsymbol{y}^T\mathbf{H}\boldsymbol{y},$$

where $\boldsymbol{y} = \mathbf{B}\boldsymbol{x} \neq \mathbf{0}$ since $\mathbf{B}$ is no singular. Then $\boldsymbol{x}^T\hat{\mathbf{H}}\boldsymbol{x} = \boldsymbol{y}^T\mathbf{H}\boldsymbol{y} > 0$ or ≥ 0, $\cdots$ and therefore $\hat{\mathbf{H}}$ is positive definite, positive semidefinite, etc.

Theorem *Characterization of symmetric matrices via diagonalization*

1. If the $n \times n$ matrix $\mathbf{B}$ is nonsingular and $\hat{\mathbf{H}} = \mathbf{B}^T\mathbf{H}\mathbf{B}$ is a diagonal matrix with diagonal **real elements** $\hat{h}_1, \hat{h}_2, \cdots, \hat{h}_n$ then $\mathbf{H}$ is positive definite, positive semidefinite, negative semidefinite, negative definite, if $\hat{h}_i > 0, \geq 0, \leq 0, < 0$ for $i = 1, 2, \cdots, n$. Otherwise, if some $\hat{h}_i$ are positive and some are negative, $\mathbf{H}$ is indefinite.
2. The converse of the previous part is also true, that is, if $\mathbf{H}$ is positive definite, positive semidefinite, etc., then $\hat{h}_i > 0, \geq 0$, etc., and if $\mathbf{H}$ is indefinite, then some $\hat{h}_i$ are positive and some are negative.

Theorem *Characterization of symmetric matrices via diagonalization*
Proof (Part 1):

$$\boldsymbol{x}^T \hat{\mathbf{H}} \boldsymbol{x} = \hat{h}_1 x_1^2 + \hat{h}_2 x_2^2 + \cdots + \hat{h}_n x_n^2$$

if $\hat{h}_i > 0, \geq 0, \leq 0, < 0$ for $i = 1, 2, \cdots, n$ then $\boldsymbol{x}^T \hat{\mathbf{H}} \boldsymbol{x} > 0, \geq 0, \leq 0, < 0$. Therefore $\hat{\mathbf{H}}$ is positive definite, positive semidefinite, negative semidefinite, negative definite. If some $\hat{h}_i$ are positive and some are negative, one can find a vector $\boldsymbol{x}$ that yields a positive or negative $\boldsymbol{x}^T \hat{\mathbf{H}} \boldsymbol{x}$ and then $\hat{\mathbf{H}}$ is indefinite. Using the previous theorem (slide 24) one concludes that $\mathbf{H} = \mathbf{B}^{-T} \hat{\mathbf{H}} \mathbf{B}^{-1}$ is also positive definite, positive semidefinite, negative semidefinite or indefinite.

Theorem *Characterization of symmetric matrices via diagonalization*

Proof (Part 2):

Suppose that $\mathbf{H}$ is positive definite, positive semidefinite, etc. Since $\hat{\mathbf{H}} = \mathbf{B}^T\mathbf{H}\mathbf{B}$, it follows from the previous theorem (slide 24) that $\hat{\mathbf{H}}$ is positive definite, positive semidefinite, etc. If $\boldsymbol{x}$ is a vector of the canonical base, i.e. $\boldsymbol{x} = \boldsymbol{e}_i$

$$\boldsymbol{x}^T\hat{\mathbf{H}}\boldsymbol{x} = \boldsymbol{e}_i^T\hat{\mathbf{H}}\boldsymbol{e}_i = \hat{h}_i > 0, \geq 0, \leq, <$$

for $i = 1, 2, \cdots, n$.

On the other hand, if $\mathbf{H}$ is indefinite then by theorem in slide 24, $\hat{\mathbf{H}}$ is indefinite and therefore some $\hat{h}_i$ must be positive and some must be negative. (on the contrary $\mathbf{H}$ would be positive definite, positive semidefinite, etc.)

Theorem *Eigen decomposition of symmetric matrices*

1. If $\mathbf{H}$ is a real symmetric matrix, then there exists a real unitary (or orthogonal) matrix $\mathbf{U}$ such that

$$\mathbf{\Lambda} = \mathbf{U}^T \mathbf{H} \mathbf{U}$$

   is a diagonal matrix whose diagonal elements are the eigenvalues of $\mathbf{H}$.

2. The eigenvalues of $\mathbf{H}$ are real.

Comments..

Theorem *Eigen decomposition of symmetric matrices*

1. If $\mathbf{H}$ is a real symmetric matrix, then there exists a real unitary (or orthogonal) matrix $\mathbf{U}$ such that

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is a diagonal matrix whose diagonal elements are the eigenvalues of $\mathbf{H}$.

Comments: According to the *Schur decomposition*, any real matrix $\mathbf{A}$ can be written as $\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{U}^T$, where $\mathbf{A}, \mathbf{U}, \mathbf{D}$ contain only real numbers, $\mathbf{D}$ is a block upper triangular matrix and $\mathbf{U}$ is an orthogonal matrix. Using the *Schur decomposition* $\mathbf{H} = \mathbf{U}\mathbf{D}\mathbf{U}^T$, then $\mathbf{U}^T\mathbf{H}\mathbf{U} = \mathbf{D}$, as $\mathbf{H}$ is symmetric then $\mathbf{U}^T\mathbf{H}\mathbf{U}$ is also symmetric, therefore $\mathbf{D}$ is a symmetric triangular matrix this implies that $\mathbf{D}$ is necessarily diagonal.

Comments...

Theorem *Eigen decomposition of symmetric matrices*

1. The eigenvalues of $\mathbf{H}$ are real.

Comments: If $\mathbf{H}\boldsymbol{x} = \lambda\boldsymbol{x}$ then $\mathbf{H}\bar{\boldsymbol{x}} = \bar{\lambda}\bar{\boldsymbol{x}}$. The symbol $^{-}$ represents the complex conjugate.
$\lambda\boldsymbol{x}^T\bar{\boldsymbol{x}} = \boldsymbol{x}^T\mathbf{H}\bar{\boldsymbol{x}} = \bar{\lambda}\boldsymbol{x}^T\bar{\boldsymbol{x}}$ then $\lambda = \bar{\lambda}$. This implies that λ is real.

Summary

- If the Hessian is positive definite (positive eigenvalues) at $\boldsymbol{x}^*$, then $\boldsymbol{x}^*$ is a **local minimum**.
- If the Hessian is negative definite (negative eigenvalues) at $\boldsymbol{x}^*$, then $\boldsymbol{x}^*$ is a **local maximum**.
- If the Hessian has both positive and negative eigenvalues then $\boldsymbol{x}^*$ is a **saddle point**.
- Otherwise the test is inconclusive.
- At a local minimum (local maximum), the Hessian is positive semidefinite (negative semidefinite).
- For positive semidefinite and negative semidefinite Hessians the test is inconclusive.

Approximation problem

Example 1. Suppose, that through an experiment the value of a function g is observed at m points, $x_1, x_2, \cdots, x_m$, which mean that values $g(x_1), g(x_2), \cdots, g(x_m)$ are known. We want to approximate the function by a polynomial

$$h(x) \quad = \quad a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$$

with $n < m$.
The error at each observation point is

$$\epsilon_k \quad = \quad g(x_k) - h(x_k), \; k = 1, 2, \cdots, m$$

Then we obtain the following optimization problem

$$\min \sum_{k=1}^{m} (\epsilon_k)^2$$

Approximation problem

Let $\boldsymbol{x}_k = [1, x_k, x_k^2, \cdots, x_k^n]^T$, $\boldsymbol{g} = [g(x_1), g(x_2), \cdots, g(x_m)]^T$ and $\mathbf{X} = [\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_m]^T$

$$
\begin{aligned}
f(\boldsymbol{a}) &= \sum_{k=1}^{m} (\epsilon_k)^2 = \sum_{k=1}^{m} [g(x_k) - h(x_k)]^2 \\
&= \sum_{k=1}^{m} [g(x_k) - a_0 + a_1 x_k + a_2 x_k^2 + \cdots + a_n x_k^n]^2 \\
&= \sum_{k=1}^{m} [g(x_k) - \boldsymbol{x}_k^T \boldsymbol{a}]^2 = \|\boldsymbol{g} - \mathbf{X}\boldsymbol{a}\|_2^2 \\
&= \boldsymbol{a}^T \mathbf{Q} \boldsymbol{a} - 2\boldsymbol{b}^T \boldsymbol{a} + c
\end{aligned}
$$

with $\mathbf{Q} = \mathbf{X}^T\mathbf{X}$, $\boldsymbol{b} = \mathbf{X}^T\boldsymbol{g}$ and $c = \|\boldsymbol{g}\|_2^2$

Approximation problem

Then

$$\min_{\boldsymbol{a}} f(\boldsymbol{a}) = \boldsymbol{a}^T \mathbf{Q} \boldsymbol{a} - 2\boldsymbol{b}^T \boldsymbol{a} + c$$

with $\boldsymbol{q}_k = [1, x_k, x_k^2, \cdots, x_k^n]^T$, $\boldsymbol{g} = [g(x_1), g(x_2), \cdots, g(x_m)]^T$, $\mathbf{X} = [\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_m]^T$, $\mathbf{Q} = \mathbf{X}^T \mathbf{X}$, $\boldsymbol{b} = \mathbf{X}^T \boldsymbol{g}$ and $c = \|\boldsymbol{g}\|_2^2$

$$\begin{aligned} \nabla_{\boldsymbol{a}} f(\boldsymbol{a}) &= 2\mathbf{Q}\boldsymbol{a} - 2\boldsymbol{b} = 0 \\ \boldsymbol{a} &= \mathbf{Q}^{-1}\boldsymbol{b} \end{aligned}$$

Approximation problem

Example 2

Given a continuous $f(x)$ in $[a,b]$. Find the approximation polynomial of degree n

$$p(x) \quad = \quad a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$$

such that minimizes

$$\int_a^b [f(x) - p(x)]^2 dx$$

Maximum likelihood

Suppose there is a sample $x_1, x_2, \cdots, x_n$ of n independent and identically distributed observations, coming from a distribution with an unknown probability density function $f(\cdot)$. If $f(\cdot)$ belongs to a certain family of distributions $\{f(\cdot|\theta), \theta \in \Theta\}$ (where θ is a vector of parameters for this family), called the parametric model, so that $f_0 = f(|\theta_0)$. The value θ_0 is unknown and is referred to as the true value of the parameter vector. It is desirable to find an estimator $\hat{\theta}$ which would be as close to the true value θ_0 as possible. For example

$$f(x|\mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

where $\theta = [\mu, \sigma]^T$

Maximum likelihood Method

In the method of maximum likelihood, one first specifies the joint density function for all observations. For an independent and identically distributed sample, this joint density function is

$$f(x_1, x_2, \ldots, x_n \mid \theta) = f(x_1 \mid \theta) f(x_2|\theta) \cdots f(x_n \mid \theta)$$

The observed values $x_1, x_2, \cdots, x_n$ are known whereas θ is the variable of the function. This function is called the **likelihood**:

$$\mathcal{L}(\boldsymbol{x}; \theta) = f(\boldsymbol{x} \mid \theta) = \prod_{i=1}^{n} f(x_i \mid \theta)$$

The problem es to maxime the **log-likelihood**, i.e., $\ell(\boldsymbol{x}; \theta) = \log \mathcal{L}(\boldsymbol{x}; \theta)$. This method of estimation defines a **maximum-likelihood estimator**.

Maximum likelihood Method: Example

For the normal distribution $\mathcal{N}(\mu, \sigma^2)$ which has probability density function

$$f(x \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right),$$

the corresponding probability density function for a sample of n independent identically distributed normal random variables (the likelihood) is

$$\begin{aligned} f(x_1, \ldots, x_n \mid \mu, \sigma^2) &= \prod_{i=1}^{n} f(x_i \mid \mu, \sigma^2) \\ &= \left(\frac{1}{2\pi\sigma^2}\right)^{n/2} \exp\left(-\frac{\sum_{i=1}^{n}(x_i-\mu)^2}{2\sigma^2}\right), \end{aligned}$$

Maximum likelihood Method: Example

The **log likelihood** can be written as follows:

$$\log(\mathcal{L}(\mu,\sigma)) = (-n/2)\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(x_i-\mu)^2$$

Computing the derivatives of this log likelihood as follows.

$$0 = \frac{\partial}{\partial\mu}\log(\mathcal{L}(\mu,\sigma)) = 0 - \frac{-2n(\bar{x}-\mu)}{2\sigma^2}. \tag{1}$$

This is solved by $\hat{\mu} = \bar{x} = \sum_{i=1}^{n}\frac{x_i}{n}$.
Similarly for σ and one obtains $\widehat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i-\mu)^2$.