

Unconstrained Optimization

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July 15, 2016

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Definition ((strict) max/min, (strict) local max/min)

Let $f : U \subset \mathbb{R}^n \rightarrow \mathbb{R}$

- ① A point \mathbf{x}^* is a (global, or absolute) max, maximizer, maximum point of f on U if $f(\mathbf{x}^*) \geq f(\mathbf{x}) \quad \forall \mathbf{x} \in U$
- ② $\mathbf{x}^* \in U$ is a strict (global, or absolute) max if \mathbf{x}^* is a max and $f(\mathbf{x}^*) > f(\mathbf{x}) \quad \forall \mathbf{x} \in U - \{\mathbf{x}^*\}$
- ③ $\mathbf{x}^* \in U$ is a local (relative) max of f if $\exists \epsilon > 0$ s.t.
 $f(\mathbf{x}^*) \geq f(\mathbf{x}) \quad \forall \mathbf{x} \in B_\epsilon(\mathbf{x}^*) \cap U$
- ④ $\mathbf{x}^* \in U$ is a strict local (relative) max of f if $\exists \epsilon > 0$ s.t.
 $f(\mathbf{x}^*) > f(\mathbf{x}) \quad \forall \mathbf{x} \in B_\epsilon(\mathbf{x}^*) \cap U$

- Definition of min: $>, \geq \rightarrow <, \leq$

Theorem (17.1)

Let $f : U \subset \mathbb{R}^n \rightarrow \mathbb{R}$ be a C^1 function. If \mathbf{x}^* is a local max or min of f and \mathbf{x}^* is an interior point of U , then

$$\frac{\partial f}{\partial x_i}(\mathbf{x}^*) = 0 \quad \forall i$$

In short,

$$Df_{\mathbf{x}}(\mathbf{x}^*) = \mathbf{0}$$

\mathbf{x}^* is a critical point of f

Note: Compare with one-var version FOC (Theorem 3.3)

Theorem (3.3: First Order Condition (FOC))

x_0 is an interior max or min of $f \Rightarrow x_0$ is a critical point of f . i.e.,
 $f'(x_0) = 0$ (Inverse is not always true)

SOC (Sufficient Conditions)

Theorem (17.2)

Let $f : U \subset \mathbb{R}^n \rightarrow \mathbb{R}$ be a C^2 function and U is open. Suppose \mathbf{x}^* is a critical point of f . (i.e., $Df_{\mathbf{x}}(\mathbf{x}^*) = \mathbf{0}$) Then,

- 1 If Hession ($D^2 f_{\mathbf{x}}(\mathbf{x}^*)$) is ND, then \mathbf{x}^* is a strict local max of f
- 2 If Hession ($D^2 f_{\mathbf{x}}(\mathbf{x}^*)$) is PD, then \mathbf{x}^* is a strict local min of f
- 3 If Hession is ID, \mathbf{x}^* is neither a local max nor local min of f . (saddle point)

Note: one-var version: (Theorem 3.4)

$$f'(x^*) = 0 \quad \wedge \quad f'' < 0 \quad \Rightarrow \quad x^* \text{ is a local max}$$

SOC (Necessary Conditions)

Theorem (17.6)

Let $f : U \subset \mathbb{R}^n \rightarrow \mathbb{R}$ be a C^2 function and U is open. Then,

- ① \mathbf{x}^* is a local min of $f \Rightarrow Df(\mathbf{x}^*) = \mathbf{0} \quad \wedge \quad D^2f(\mathbf{x}^*)$ is PSD
- ② \mathbf{x}^* is a local max of $f \Rightarrow Df(\mathbf{x}^*) = \mathbf{0} \quad \wedge \quad D^2f(\mathbf{x}^*)$ is NSD

Note: one-var version:

$$x^* \text{ is local max} \quad \Rightarrow \quad x' = 0 \quad \wedge \quad f'' \leq 0$$

Finding Global Max/Min

Different from one-var function, condition 1 (below) is not true when f is multi-var function

Sufficient Conditions for Global Max/Min ($f : I \in \mathbb{R} \rightarrow \mathbb{R}$)

- ① x^* is a local max/min and x^* is the only critical point of f in I
- ② $f'' \leq 0 \quad \forall I$. i.e., f is concave on I (max)
 - $f'' \leq 0 \quad \forall I$ (max)
 - $f'' \geq 0 \quad \forall I$ (min)

However, condition 2 is true even when f is multi-var function!

Theorem (17.8)

Let $f : U \in \mathbb{R}^n \rightarrow \mathbb{R}$ be a C^2 function with convex open domain U .

- ① $DF(\mathbf{x}^*) = \mathbf{0}$ and $D^2f_{\mathbf{x}}$ is PSD on $U \Rightarrow \mathbf{x}^*$ is a global max of f on U
- ② $DF(\mathbf{x}^*) = \mathbf{0}$ and $D^2f_{\mathbf{x}}$ is NSD on $U \Rightarrow \mathbf{x}^*$ is a global min of f on U

Ordinary Least Squares (OLS)

OLS

Find $y = \mathbf{x}\beta + c$ for given N data $X = \begin{pmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_N \end{pmatrix}$, $Y = \begin{pmatrix} y_1 \\ \vdots \\ y_N \end{pmatrix}$ satisfying:

$$\arg \min_{\beta, c} \sum_i^N ((\mathbf{x}_i \beta + c) - y_i)^2 \quad (\text{Least Square})$$

$$y = \mathbf{x}\beta + c = x_1\beta_1 + \cdots + x_m\beta_m + c$$

Note: given points – $(y_1, \mathbf{x}_1) = (y_1, x_{11}, x_{12}, \cdots, x_{1m})$,
 $(y_2, \mathbf{x}_2), \cdots, (y_N, \mathbf{x}_N)$ – are not variables. Our object is to find β^*, c^*
(linear equation) from given data X, Y .

OLS: Solution

Let our object function $f(\beta_1, \dots, \beta_n, c) := \sum_i^N ((\mathbf{x}_i\beta + c) - y_i)^2$. Then FOC is:

$$Df_{\beta,c}(\beta^*, c^*) = \mathbf{0} \quad (\text{FOC})$$

This leads to $m + 1$ equations:

$$\frac{\partial f}{\partial \beta_1}(\beta^*, c^*) = 2(\mathbf{x}_1\beta^* + c^* - y_1)x_{11} + 2(\mathbf{x}_2\beta^* + c^* - y_2)x_{21} + \dots + 2(\mathbf{x}_N\beta^* + c^* - y_N)x_{N1}$$

...

$$\frac{\partial f}{\partial \beta_m}(\beta^*, c^*) = 2(\mathbf{x}_1\beta^* + c^* - y_1)x_{1m} + 2(\mathbf{x}_2\beta^* + c^* - y_2)x_{2m} + \dots + 2(\mathbf{x}_N\beta^* + c^* - y_N)x_{Nm}$$

$$\Rightarrow 2(\mathbf{x}_1\beta^* + c^* - y_1)\mathbf{x}_1^T + 2(\mathbf{x}_2\beta^* + c^* - y_2)\mathbf{x}_2^T + \dots + 2(\mathbf{x}_N\beta^* + c^* - y_N)\mathbf{x}_N^T = \mathbf{0} \quad (\text{B})$$

$$\frac{\partial f}{\partial c}(\beta^*, c^*) = 2(\mathbf{x}_1\beta^* + c^* - y_1)1 + 2(\mathbf{x}_2\beta^* + c^* - y_2)1 + \dots + 2(\mathbf{x}_N\beta^* + c^* - y_N)1 = 0 \quad (\text{C})$$

Remember

$$X = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1m} \\ x_{21} & x_{22} & \cdots & x_{2m} \\ \vdots & \vdots & \vdots & \vdots \\ x_{N1} & x_{N2} & \cdots & x_{Nm} \end{pmatrix} = (C_1 \quad \cdots \quad C_m) = \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \vdots \\ \mathbf{x}_N \end{pmatrix}$$

Rearrange FOCs:

$$(\mathbf{x}_1^T \quad \mathbf{x}_2^T \quad \cdots \quad \mathbf{x}_N^T) \begin{pmatrix} \mathbf{x}_1 \beta^* + c^* - y_1 \\ \vdots \\ \mathbf{x}_N \beta^* + c^* - y_N \end{pmatrix} = X^T (X \beta^* + \mathbf{1}_{N \times 1} c^* - Y) = \mathbf{0}_N \quad (\text{B2})$$

$$c^* = \frac{1}{N} (1 \quad 1 \quad \cdots \quad 1) \begin{pmatrix} y_1 - \mathbf{x}_1 \beta^* \\ \vdots \\ y_N - \mathbf{x}_N \beta^* \end{pmatrix} = \frac{1}{N} \mathbf{1}_{1 \times N} (Y - X \beta^*) \quad (\text{C2})$$

From (C2) and (B2),

$$X^T \left(X\beta^* + \mathbf{1}_{N \times 1} \frac{1}{N} \mathbf{1}_{1 \times N} (Y - X\beta^*) - Y \right) = \mathbf{0}_{m \times 1} \quad (\text{D})$$

Rearrange (D) with regard to β^* yields:

$$X^T \left(X - \frac{1}{N} \mathbf{1}_{N \times 1} \mathbf{1}_{1 \times N} X \right) \beta^* = X^T \left(I_N - \frac{1}{N} \mathbf{1}_{N \times 1} \mathbf{1}_{1 \times N} \right) Y$$

Let $\mathbf{1}_{N \times 1} \mathbf{1}_{1 \times N} = \mathbf{1}_N$. ($N \times N$ matrix with all elements are 1)

$$\begin{aligned} \beta^* &= \left(X^T \left(X - \frac{1}{N} \mathbf{1}_N X \right) \right)^{-1} \left(X^T \left(Y - \frac{1}{N} \mathbf{1}_N Y \right) \right) \\ &= \left(X^T \left(I_N - \frac{1}{N} \mathbf{1}_N \right) X \right)^{-1} \left(X^T \left(I_N - \frac{1}{N} \mathbf{1}_N \right) Y \right) \end{aligned}$$

Sample Mean \bar{X}, \bar{Y}

$$\frac{1}{N} \mathbf{1}_N X = \frac{1}{N} \begin{pmatrix} 1 & \cdots & 1 \\ 1 & \cdots & 1 \\ \vdots & \vdots & \vdots \\ 1 & \cdots & 1 \end{pmatrix} \begin{pmatrix} x_{11} & \cdots & x_{1m} \\ x_{21} & \cdots & x_{2m} \\ \vdots & \vdots & \vdots \\ x_{N1} & \cdots & x_{Nm} \end{pmatrix} = \begin{pmatrix} \bar{x}_1 & \cdots & \bar{x}_m \\ \bar{x}_1 & \cdots & \bar{x}_m \\ \cdots & & \\ \bar{x}_1 & \cdots & \bar{x}_m \end{pmatrix} = \bar{X}$$

$$\frac{1}{N} \mathbf{1}_N Y = \frac{1}{N} \begin{pmatrix} 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & \cdots & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ \vdots \\ y_N \end{pmatrix} = \begin{pmatrix} \bar{y} \\ \vdots \\ \bar{y} \end{pmatrix} = \bar{Y}$$

Here \bar{x}_j, \bar{y} means sample mean of x_{ij}, y_i

$$\bar{x}_j := \frac{1}{N} \sum_i^N x_{ij}, \quad \bar{y} := \frac{1}{N} \sum_i^N y_i$$

Therefore, β^* is:

$$\beta^* = (X^T(X - \bar{X}))^{-1}X^T(Y - \bar{Y})$$

Note1: If $N \rightarrow \infty$, then $I_N - \frac{1}{N}\mathbf{1}_N \rightarrow I_N$ and

$$\beta^* \rightarrow (X^T X)^{-1}X^T Y$$

Note2: We should check SOC: whether $H = D^2 f_{\beta,c}(\beta^*, c^*)$ is PD or not. Our object function has quadratic form with positive sign with regard to β, c when \mathbf{x}_j is independent with each other and this means f is PD (when \mathbf{x}_j is independent with each other: covariance with other variables are 0).

Note3: Some researchers denote X^T by X'