An existence criterion for the sum of squares

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Hrzz
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The general regression model is of the form:

$$y_i = f(t_i; \boldsymbol{\vartheta}) + \varepsilon_i, \quad \boldsymbol{\vartheta} \in \boldsymbol{\Theta}, \qquad i = 1, \dots, n,$$

- $\vartheta \mapsto f(t_i; \vartheta) =: f_i$ model-function given in advance, defined on parameter space $\boldsymbol{\Theta} \subseteq \mathbb{R}^m$
- t_i are independent variables
- y_i are observations
- ε_i are random errors, usually assumed to be normally distributed with mean zero and constant variance.

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Least squares (LS) problem

Least squares estimate (LSE)

Any point $\boldsymbol{\vartheta}^\star \in \boldsymbol{\Theta}$ that minimizes the sum of squares

$$S(\boldsymbol{\vartheta}) = \sum_{i=1}^{n} (f(t_i; \boldsymbol{\vartheta}) - y_i)^2$$

is called least squares estimate (LSE).

Existence question

Does there exist a point $\boldsymbol{\vartheta}^\star \in \boldsymbol{\Theta}$ (LSE) such that

$$S(\boldsymbol{\vartheta}^\star) = \min_{\boldsymbol{\vartheta} \in \boldsymbol{\Theta}} S(\boldsymbol{\vartheta})?$$

- If f is continuous and $\boldsymbol{\Theta}$ is compact, then LSE exists.
- Further we assume that f is continuous and $\boldsymbol{\Theta}$ is not compact.

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Motivation example - simple linear regression

Data points: $(t_i, y_i) \in \mathbb{R}^2 \colon i = 1, \ldots, n, \sum_{i=1}^n t_i^2 \neq 0$

$$y_i = \vartheta t_i + \varepsilon_i, \quad \vartheta \in \mathbf{\Theta} = \langle 0, \infty \rangle, \qquad i = 1, \ldots, n.$$

Sum of squares:

$$S(\vartheta) = \sum_{i=1}^{n} (\vartheta t_i - y_i)^2.$$

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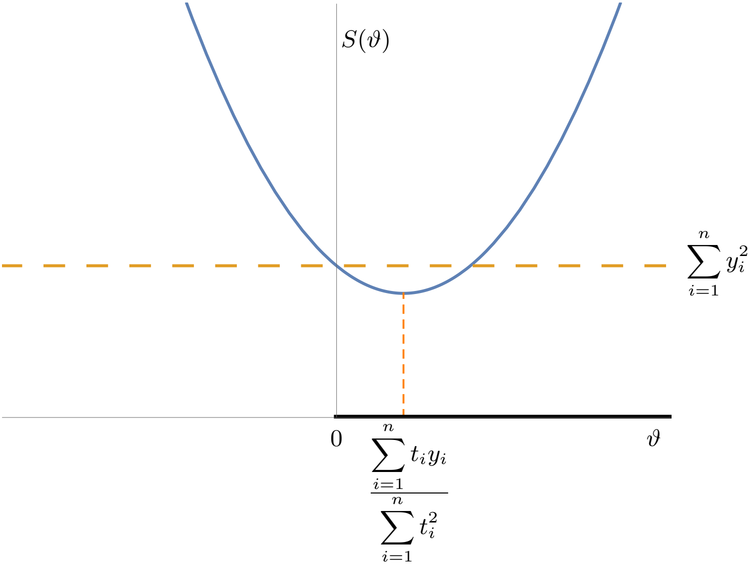
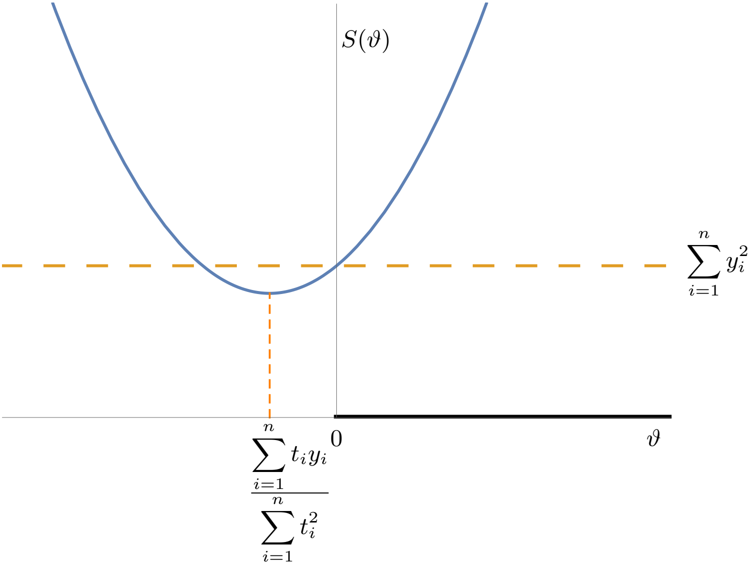
Case 1: $\sum_{i=1}^{n} t_i y_i > 0$



Case 2: $\sum_{i=1}^{n} t_i y_i \leq 0$



LSE existence for linear regression

LSE $\vartheta^\star > 0$ for linear regression

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$$\Updownarrow$$

$$\sum_{i=1}^{n} t_i y_i > 0$$

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There exists $\vartheta_0 \in \Theta$ such that $S(\vartheta_0) \leq S_E^\star$, $\quad S_E^\star := \sum_{i=1}^{n} y_i^2$.

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Main goal

For any sum of squares

$$S(\boldsymbol{\vartheta}) = \sum_{i=1}^{n} (f(t_i; \boldsymbol{\vartheta}) - y_i)^2, \boldsymbol{\vartheta} \in \boldsymbol{\Theta}$$

to give necessary and sufficient criteria for the existence of the LSE.

Matrix notation:

$$S(\boldsymbol{\vartheta}) = \|\mathbf{f}(\boldsymbol{\vartheta}) - \mathbf{y}\|^2,$$

- $f_i(\boldsymbol{\vartheta}) := f(\boldsymbol{t}_i; \boldsymbol{\vartheta}), i = 1, \ldots, n.$
- $\mathbf{f}(\boldsymbol{\vartheta}) = (f_1(\boldsymbol{\vartheta}), \ldots, f_n(\boldsymbol{\vartheta}))^T$ and $\mathbf{y} = (y_1, \ldots, y_n)^T$.
- The set of all n-vectors $\mathbf{f}(\boldsymbol{\vartheta})$, i.e., the set

$$\mathcal{E} = \{\mathbf{f}(\boldsymbol{\vartheta}) : \boldsymbol{\vartheta} \in \boldsymbol{\Theta}\},$$

defines an m-dimensional surface: *expectation surface* or *solution locus*.

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- The LSE $\boldsymbol{\vartheta}^\star$, if it exists, corresponds to the point $\mathbf{f}(\boldsymbol{\vartheta}^\star)$ on $\mathcal{E}$ which is closest to $\mathbf{y}$.

Lemma 1

The least squares estimate exists if and only if there exists a point $\mathbf{f}(\boldsymbol{\vartheta}_0) \in \mathcal{E}$ such that

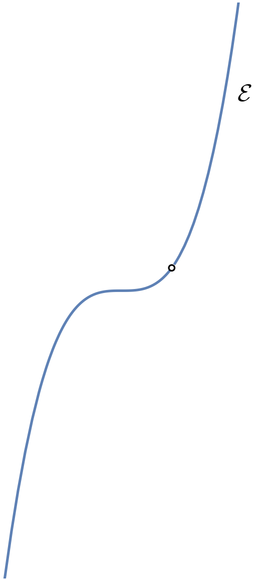
$$S(\boldsymbol{\vartheta}_0) = \|\mathbf{f}(\boldsymbol{\vartheta}_0) - \mathbf{y}\|^2 \leq \|\mathbf{e} - \mathbf{y}\|^2 \quad \text{for all } \mathbf{e} \in \mathrm{Cl}\,\mathcal{E} \backslash \mathcal{E},$$

or, equivalently,

$$\|\mathbf{f}(\boldsymbol{\vartheta}_0) - \mathbf{y}\|^2 \leq \inf_{\mathbf{e} \in \mathrm{Cl}\,\mathcal{E} \backslash \mathcal{E}} \|\mathbf{e} - \mathbf{y}\|^2,$$

where $\inf \emptyset := \infty$.

Expectation surface illustration



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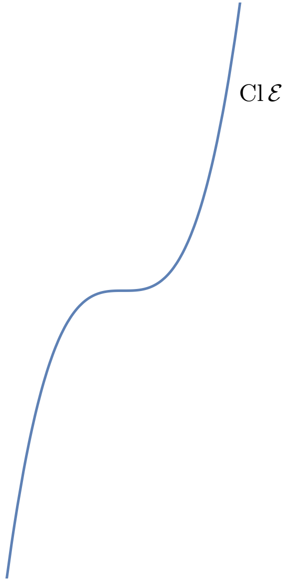

Expectation surface illustration

- $\mathbf{e}, \quad \{\mathbf{e}\} = \mathrm{Cl}\,\mathcal{E} \setminus \mathcal{E}$

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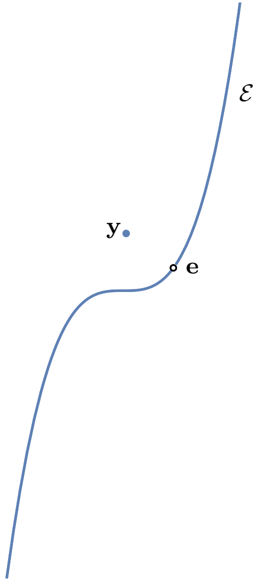

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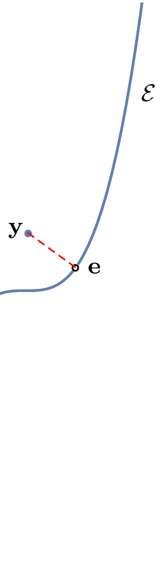

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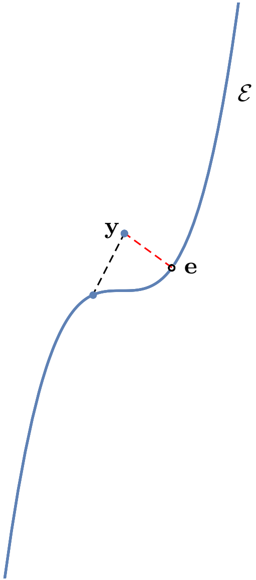

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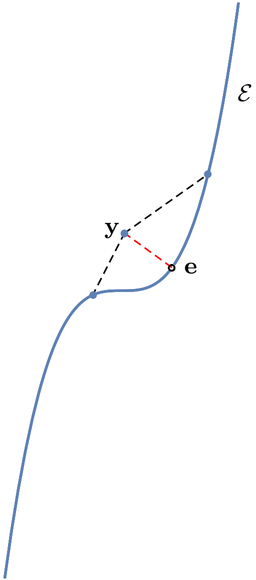

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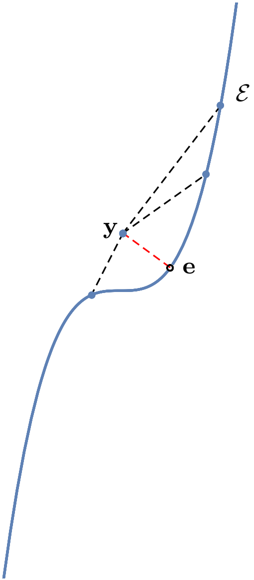

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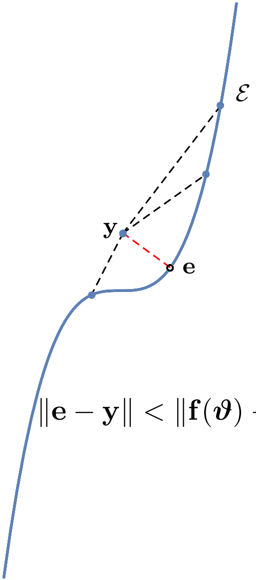
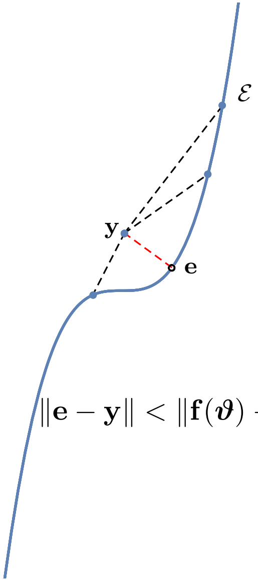


$\|\mathbf{e} - \mathbf{y}\| < \|\mathbf{f}(\boldsymbol{\vartheta}) - \mathbf{y}\|$ for all $\boldsymbol{\vartheta} \in \boldsymbol{\Theta} \Rightarrow$ LSE doesn't exist.

Expectation surface illustration



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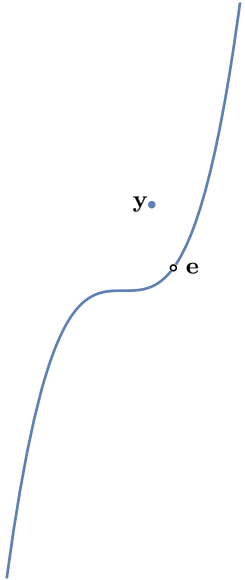

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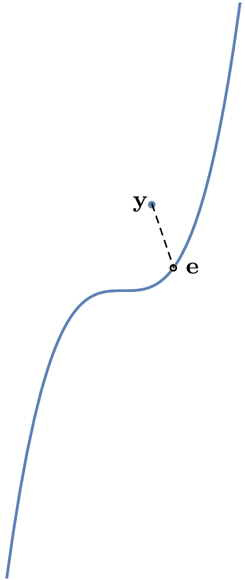

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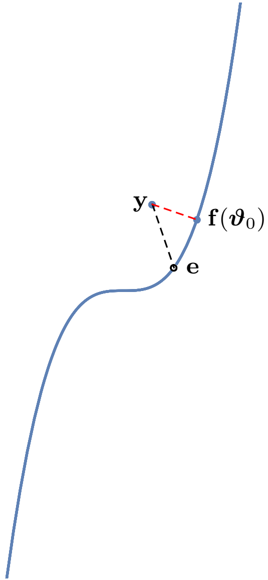

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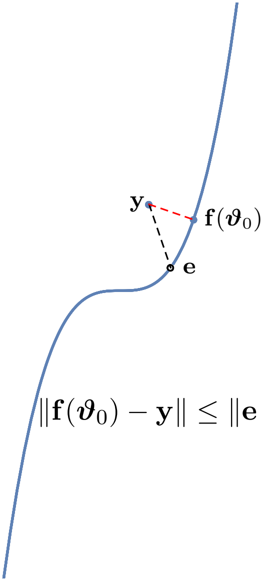

$$\|\mathbf{f}(\boldsymbol{\vartheta}_0) - \mathbf{y}\| \le \|\mathbf{e} - \mathbf{y}\| \Rightarrow \text{LSE exists.}$$

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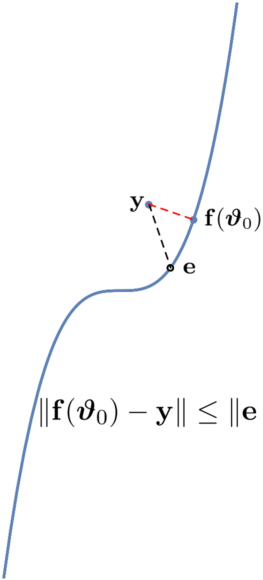

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Extendend boundary

$$\partial_\infty \boldsymbol{\Theta} = \begin{cases} \partial\boldsymbol{\Theta}, & \text{if } \boldsymbol{\Theta} \text{ is bounded} \\ \partial\boldsymbol{\Theta} \cup \{\infty\}, & \text{if } \boldsymbol{\Theta} \text{ is unbounded} \end{cases}$$

is the so-called *extended boundary* of the set $\boldsymbol{\Theta}$.

- whenever we write $\boldsymbol{\vartheta}_k \to \infty$, we will mean that $\|\boldsymbol{\vartheta}_k\| \to \infty$.

Existence level

$$S_E^\star = \inf_{\substack{\{\boldsymbol{\vartheta}_k\}\subseteq\boldsymbol{\Theta} \\ \boldsymbol{\vartheta}_k\to\boldsymbol{\vartheta}_0\in\partial_\infty\boldsymbol{\Theta}\setminus\boldsymbol{\Theta}}} \underline{\lim_k} S(\boldsymbol{\vartheta}_k),$$

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Theorem 1: Necessary and sufficient criterion for the existence of the LSE

The LSE exists if and only if there exists $\boldsymbol{\vartheta}_0 \in \boldsymbol{\Theta}$ such that

$$S(\boldsymbol{\vartheta}_0) \leq S_E^{\star}.$$

We will say that $\bar{\mathbf{f}}(\boldsymbol{\beta})$ is *limit regression* of $\mathbf{f}(\boldsymbol{\vartheta})$ if

$$\bar{\mathbf{f}}(\boldsymbol{\beta}) = \lim_{k\to\infty} \mathbf{f}(\boldsymbol{\vartheta}_k)$$

for some sequence $\{\boldsymbol{\vartheta}_k\} \subset \boldsymbol{\Theta}$ with a limit in $\partial_\infty\boldsymbol{\Theta}\backslash\boldsymbol{\Theta}$. If we denote by LR the set of all limit regressions, then, by definition of $S_E^\star$, it is easy to check that

$$S_E^\star = \inf_{\bar{\mathbf{f}}(\boldsymbol{\beta})\in LR} \|\bar{\mathbf{f}}(\boldsymbol{\beta}) - \mathbf{y}\|^2.$$

Theorem 1: reformulated

The LSE exists if and only if there is at least one point $\boldsymbol{\vartheta}_0 \in \boldsymbol{\Theta}$ with the sum of squares less than or equal to the corresponding sum of squares for any limit regression.

Modified Biggs EXP2 Function

M.C. Biggs, A new variable metric technique taking account of non-quadratic behaviour of the objective function, IMA Journal of Applied Mathematics, 8 (1971), 315-327.

$$f_i(\boldsymbol{\vartheta}) = e^{at_i} + 5e^{bt_i},\ \boldsymbol{\vartheta} = (a,b) \in \boldsymbol{\Theta} = \{(a,b) \in \mathbb{R}^2 : a,b \geq 0\},$$

$$t_i = 0.1\, i, \quad y_i = e^{t_i} + 5e^{10t_i},\ i = 1,\ldots,10.$$

Sum of squares:

$$S(\boldsymbol{\vartheta}) = \sum_{i=1}^{10} \left(e^{at_i} + 5e^{bt_i} - y_i\right)^2$$

$$\min_{\boldsymbol{\vartheta}\in\boldsymbol{\Theta}} S(\boldsymbol{\vartheta}) = S(\hat{\boldsymbol{\vartheta}}) = 0, \quad \hat{\boldsymbol{\vartheta}} = (1,10).$$

Illustrative example 1

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$$\partial_\infty \mathbf{\Theta} \setminus \mathbf{\Theta} = \{\infty\}$$

$$\{\boldsymbol{\vartheta_k}\} = \{(a_k, b_k)\} \subset \mathbf{\Theta} \Rightarrow \boldsymbol{\vartheta_k} \to \infty \Rightarrow S(a_k, b_k) \to \infty \Rightarrow$$

$$S_E^\star = \infty$$

Since $S(\boldsymbol{\vartheta_0}) < S_E^\star$, for any $\boldsymbol{\vartheta_0} \in \mathbf{\Theta}$, in accordance with Theorem 1 the LSE exists

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Michaelis-Menten regression model

L. Michaelis, M.L. Menten, Die Kinetik der Invertinwirkung, Biochem. Z. 49 (1913) 333–369

$\boldsymbol{D} = \{(a,b) : a > 0, b > 0\}$ and

$$f_i(a,b) = \frac{a\,t_i}{b+t_i},\ i = 1,\ldots,n.$$

$0 < t_1 \leq t_2 \ldots \leq t_n$ and $y_1,\ldots,y_n > 0$.
Reparametrization: $f_i(\boldsymbol{\vartheta}) = \frac{\alpha\,t_i}{\beta+\gamma t_i}$, $i = 1,\ldots,n$,

$$\alpha := \frac{a}{\sqrt{1+b^2}},\ \beta := \frac{b}{\sqrt{1+b^2}},\ \gamma := \frac{1}{\sqrt{1+b^2}}.$$

Sum of squares:

$$S(\boldsymbol{\vartheta}) = \sum_{i=1}^{n}(f_i(\boldsymbol{\vartheta}) - y_i)^2 = \sum_{i=1}^{n}\left(\frac{\alpha\,t_i}{\beta+\gamma t_i} - y_i\right)^2.$$

Illustrative example 2

Michaelis-Menten regression model

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$$f_i(a,b) = \frac{a\, t_i}{b + t_i},\ i = 1,\ldots,n.$$

$0 < t_1 \leq t_2 \ldots \leq t_n$ and $y_1,\ldots,y_n > 0$.

Reparametrization: $f_i(\vartheta) = \frac{\alpha\, t_i}{\beta + \gamma t_i},\ i = 1,\ldots,n,$

$$\alpha := \frac{a}{\sqrt{1+b^2}},\ \beta := \frac{b}{\sqrt{1+b^2}},\ \gamma := \frac{1}{\sqrt{1+b^2}}.$$

Sum of squares:

$$S(\vartheta) = \sum_{i=1}^{n}(f_i(\vartheta) - y_i)^2 = \sum_{i=1}^{n}\left(\frac{\alpha\, t_i}{\beta + \gamma t_i} - y_i\right)^2.$$

Illustrative example 2

Michaelis-Menten regression model

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$$\overline{y} = \frac{1}{n} \sum_{i=1}^{n} y_i.$$

$$S_E^\star = \min \left\{ \sum_{i=1}^{n} y_i^2, \sum_{i=1}^{n} (y_i - \overline{y})^2, \sum_{i=1}^{n} (\hat{\kappa} t_i - y_i)^2 \right\}$$
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- *If the data* (t_i, y_i), $i = 1, \ldots, n$, $n \geq 3$, *are such that* $0 < t_1 \leq t_2 \leq \ldots \leq t_n$, $y_i > 0$, *and if they fulfill one of the two sets of inequalities*

$$n\left(\sum_{i=1}^{n} t_i\, y_i\right)^2 \leq \sum_{i=1}^{n} t_i^2 \left(\sum_{i=1}^{m} y_i\right)^2$$

$$\sum_{i=1}^{n} \frac{1}{t_i} \sum_{i=1}^{m} y_i > n \sum_{i=1}^{m} \frac{y_i}{t_i}$$

or

$$n\left(\sum_{i=1}^{n} t_i\, y_i\right)^2 \geq \sum_{i=1}^{n} t_i^2 \left(\sum_{i=1}^{n} y_i\right)^2$$

$$\sum_{i=1}^{n} t_i\, y_i \sum_{i=1}^{n} y_i^3 > \sum_{i=1}^{n} t_i^2 \sum_{i=1}^{n} t_i^2 y_i,$$

then there exists $\boldsymbol{\vartheta}_0 \in \boldsymbol{\Theta}$ *such that* $S(\boldsymbol{\vartheta}_0) \leq S_E^\star$, *i.e., there exists an LSE for the Michaelis-Menten function.*