Model Fitting

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Overview

- Model Fitting (Curve fitting)
- Functional Approach: Non-Linear Equation
- Algebraic Approach: Normal Equations
- Efficiency Indicators
- Polynomial Models
- Non-Polynomial Models
- Examples

Interpolation Problem

Popular choice is equidistant nodes:

$$x_j = a + jh$$
 $h = (b - a)/n$

Y-nodes are known

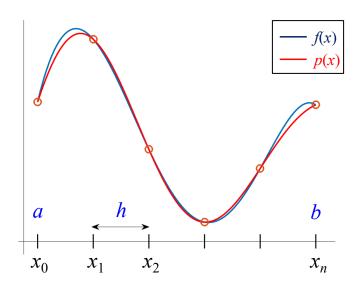
$$y_j = f(x_j)$$

Interpolate

$$f(x) \approx p_n(x)$$

• Define error

$$E_n = \max_{a \le x \le h} \left| f(x) - p_n(x) \right|$$



Two questions:

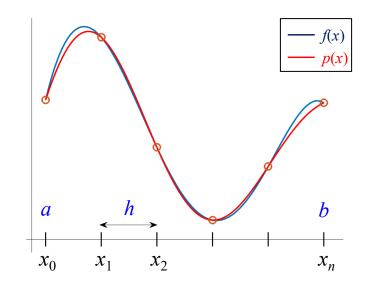
- Does it converge?
- How fast?

Nice Functions

Well-behaved functions such as $y = \sin(x)$ are well approximated by polynomials

Theorem

$$E_{n} \le \max_{a \le x \le b} \frac{\left| f^{(n+1)}(\xi) \right|}{4(n+1)} h^{n+1}$$



Numerical practice shows:

- Equidistant nodes are often worst
- Does not converge uniformly
- $p_n(x)$ strongly oscilates (Runge)

$$\frac{\left|f^{(n+1)}(\xi)\right|}{4(n+1)}h^{n+1} \xrightarrow[n\to\infty]{} \infty$$

Piecewise Linear

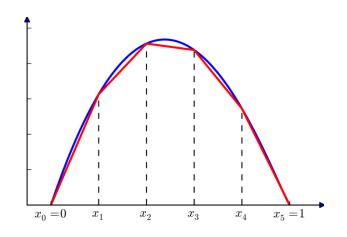
- Polynomial degree is limitted by 1.
- Does converge

Theorem

$$E_n \le Mh^2$$

$$h = \frac{b - a}{n}$$

$$M = \max_{a \le \xi \le h} \frac{|f''(\xi)|}{8}$$

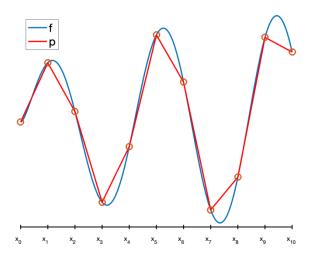


$$E_n \le Mh^2 \le tol \longrightarrow h \le \sqrt{tol/M}$$

$$n \ge (b-a)\sqrt{M/tol}$$

Piecewise Linear

- *M* does not depend on *h* (and *n*)
- Converges, $E_n \to 0$ as $O(h^2)$
- For small $h, E_n \approx Mh^2$



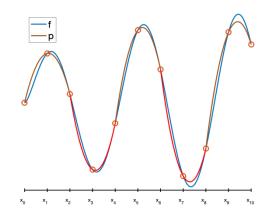
$$E_n \le Mh^2$$

$$h = \frac{b-a}{n}$$

$$M = \max_{a \le \xi \le b} \frac{|f''(\xi)|}{8}$$

Piecewise Polynomial

- Polynomial degree is limitted by *k*:
 - o Quadratic, k = 2;
 - \circ Cubic, k = 3 (splines)
- Converges faster with $n \to \infty$
- Beginning with k = 4 and higher, oscillations and instability
- Matlab, y = interp1 (xnod, ynod, x, method);
 - o method



$$\|f - S\|_{\infty} \le \frac{5}{384} h^4 \|f^{(4)}\|_{\infty}$$

Curve Fitting

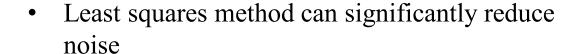
Constracting a curve (mathematical function) that has best fit to a series of data points.

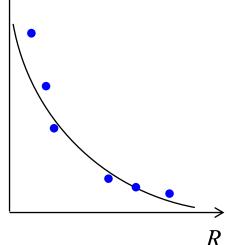
$$I = U/R$$

Ohm's law I = U/R Noise in each measurement $I_i = U/R_i + \varepsilon_i$

$$I_i = U/R_i + \varepsilon_i$$

Polynomyals give strong oscillations





Least Squares

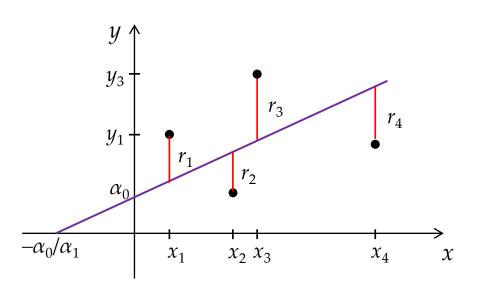
Least Squares Method, LSM, finds the straight line that minimizes the total distance from the given points.

Model function

$$f(x; \alpha_0, \alpha_1) = \alpha_0 + \alpha_1 x$$

$$r_i(\alpha_0, \alpha_1) = \alpha_0 + \alpha_1 x_i - y_i$$

$$R^{2}(\alpha_{0},\alpha_{1}) \equiv \sum_{i=1}^{n} r_{i}^{2}(\alpha_{0},\alpha_{1})$$



Solution may be found by

- Differential calculus
- Normal equations

$$\begin{cases} \partial_0 R^2(\alpha_0, \alpha_1) = \frac{\partial R(\alpha_0, \alpha_1)}{\partial \alpha_0} = 0 \\ \partial_1 R^2(\alpha_0, \alpha_1) = \frac{\partial R(\alpha_0, \alpha_1)}{\partial \alpha_1} = 0 \end{cases}$$

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Model Fitting

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Deriving System of Equations

$$R^{2}(\alpha_{0},\alpha_{1}) \equiv \sum_{i=1}^{n} r_{i}^{2}(\alpha_{0},\alpha_{1})$$

$$\begin{cases}
\frac{\partial R^{2}(\alpha_{0}, \alpha_{1})}{\partial \alpha_{0}} = \sum_{i=1}^{N} 2r_{i}(\alpha_{0}, \alpha_{1}) \frac{\partial r_{i}(\alpha_{0}, \alpha_{1})}{\partial \alpha_{0}} = 0 \\
\frac{\partial R^{2}(\alpha_{0}, \alpha_{1})}{\partial \alpha_{1}} = \sum_{i=1}^{N} 2r_{i}(\alpha_{0}, \alpha_{1}) \frac{\partial r_{i}(\alpha_{0}, \alpha_{1})}{\partial \alpha_{1}} = 0
\end{cases}$$

$$\frac{\partial R^{2}(\alpha_{0}, \alpha_{1})}{\partial \alpha_{1}} = \sum_{i=1}^{N} 2r_{i}(\alpha_{0}, \alpha_{1}) \frac{\partial r_{i}(\alpha_{0}, \alpha_{1})}{\partial \alpha_{1}} = 0$$

$$\begin{cases}
\frac{\partial r_i(\alpha_0, \alpha_1)}{\partial \alpha_0} = \frac{\partial}{\partial \alpha_0} \left(\alpha_0 + \alpha_1 x_i - y_i \right) = 1 \\
\frac{\partial r_i(\alpha_0, \alpha_1)}{\partial \alpha_1} = \frac{\partial}{\partial \alpha_1} \left(\alpha_0 + \alpha_1 x_i - y_i \right) = x_i
\end{cases}$$

$$\left| \frac{\partial r_i(\alpha_0, \alpha_1)}{\partial \alpha_1} = \frac{\partial}{\partial \alpha_1} (\alpha_0 + \alpha_1 x_i - y_i) = x_i \right|$$

Deriving System of Equations

$$\begin{cases} \sum_{i=1}^{N} r_i(\alpha_0, \alpha_1) \frac{\partial r_i(\alpha_0, \alpha_1)}{\partial \alpha_0} = \sum_{i=1}^{N} r_i(\alpha_0, \alpha_1) \times 1 = 0 \\ \sum_{i=1}^{N} r_i(\alpha_0, \alpha_1) \frac{\partial r_i(\alpha_0, \alpha_1)}{\partial \alpha_1} = \sum_{i=1}^{N} r_i(\alpha_0, \alpha_1) \times x_i = 0 \end{cases}$$

$$r_i(\alpha_0, \alpha_1) = \alpha_0 + \alpha_1 x_i - y_i$$

$$\begin{cases} \sum_{i=1}^{N} (\alpha_0 + \alpha_1 x_i - y_i) = 0 \\ \sum_{i=1}^{N} (\alpha_0 + \alpha_1 x_i - y_i) x_i = 0 \end{cases}$$

System of Equations

$$\begin{cases} \alpha_0 N + \alpha_1 \sum_{i=1}^{N} x_i = \sum_{i=1}^{N} y_i \\ \alpha_0 \sum_{i=1}^{N} x_i + \alpha_1 \sum_{i=1}^{N} x_i^2 = \sum_{i=1}^{N} x_i y_i \end{cases}$$

$$\begin{cases} \alpha_{0}N + \alpha_{1}\sum_{i=1}^{N}x_{i} = \sum_{i=1}^{N}y_{i} \\ \alpha_{0}\sum_{i=1}^{N}x_{i} + \alpha_{1}\sum_{i=1}^{N}x_{i}^{2} = \sum_{i=1}^{N}x_{i}y_{i} \\ \alpha_{0}\sum_{i=1}^{N}x_{i} + \sum_{i=1}^{N}x_{i}^{2} = \sum_{i=1}^{N}x_{i}y_{i} \end{cases}$$

$$\alpha_{1} = \frac{\Delta_{1}}{\Delta} = \frac{N \sum_{i=1}^{N} x_{i} y_{i} - \sum_{i=1}^{N} x_{i} \cdot \sum_{i=1}^{N} y_{i}}{N \sum_{i=1}^{N} x_{i}^{2} - \left(\sum_{i=1}^{N} x_{i}\right)^{2}} \qquad \alpha_{0} = \frac{1}{N} \left[\sum_{i=1}^{N} y_{i} - \alpha_{1} \sum_{i=1}^{N} x_{i}\right]$$

$$\alpha_0 = \frac{1}{N} \left[\sum_{i=1}^N y_i - \alpha_1 \sum_{i=1}^N x_i \right]$$

Cramer's Rule

Gabriel Cramer, 1704 – 1752. Published 1750.

$$\begin{bmatrix} a_1 & b_1 \\ a_2 & b_2 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}$$

$$x = \frac{\begin{vmatrix} f_1 & b_1 \\ f_2 & b_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}} = \frac{f_1 b_2 - f_2 b_1}{a_1 b_2 - a_2 b_1}; \quad y = \frac{\begin{vmatrix} a_1 & f_1 \\ a_2 & f_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}} = \frac{a_1 f_2 - a_2 f_1}{a_1 b_2 - a_2 b_1}.$$

Algebraic Method

$$f(x; \alpha_0, \alpha_1) = y$$

Model function

$$\begin{cases} f(x_1; \alpha_0, \alpha_1) = \alpha_0 + \alpha_1 x_1 = y_1 \\ f(x_2; \alpha_0, \alpha_1) = \alpha_0 + \alpha_1 x_2 = y_2 \\ \vdots \\ f(x_N; \alpha_0, \alpha_1) = \alpha_0 + \alpha_1 x_N = y_N \end{cases}$$

System of equations

Matrix Form

$$\begin{cases} \alpha_0 + \alpha_1 x_1 = y_1 \\ \alpha_0 + \alpha_1 x_2 = y_2 \\ \vdots \\ \alpha_0 + \alpha_1 x_N = y_N \end{cases}$$

$$\begin{cases} \alpha_0 + \alpha_1 x_1 = y_1 \\ \alpha_0 + \alpha_1 x_2 = y_2 \\ \vdots \\ \alpha_0 + \alpha_1 x_N = y_N \end{cases} \qquad \mathbf{A}\boldsymbol{\alpha} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_N \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \alpha_1 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} = \mathbf{b}$$

Normal Equations

$$\mathbf{A}^T \mathbf{A} \boldsymbol{\alpha} = \mathbf{A}^T \mathbf{b}$$

$$\mathbf{A}^{\mathsf{T}}\mathbf{A} = \begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_N \end{bmatrix} \cdot \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_N \end{bmatrix} = \begin{bmatrix} N & \sum x_i \\ \sum x_i & \sum x_i^2 \end{bmatrix}$$

$$\mathbf{A}^{\mathsf{T}}\mathbf{b} = \begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_N \end{bmatrix} \cdot \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} = \begin{bmatrix} \sum y_i \\ \sum x_i y_i \end{bmatrix}$$

Sample Statistics

Two data sets can be characterised by:

$$\mathbf{x} \equiv \left\{ x_1, x_2, \dots, x_N \right\}$$
$$\mathbf{y} \equiv \left\{ y_1, y_2, \dots, y_N \right\}$$

$$\overline{\mathbf{x}} \equiv \frac{1}{N} \sum_{i=1}^{N} x_i$$

Samples, observations, measurements etc.

$$S_{\mathbf{x}} \equiv \sqrt{\frac{1}{N}} \sum_{i=1}^{N} \left(x_i - \overline{\mathbf{x}} \right)^2$$

$$Var(\mathbf{x}) = S_{\mathbf{x}}^{2} \equiv \frac{1}{N} \sum_{i=1}^{N} (x_{i} - \overline{\mathbf{x}})^{2}$$

$$Cov(\mathbf{x}, \mathbf{y}) = \frac{1}{N} \sum_{i=1}^{N} (x_i - \overline{\mathbf{x}}) (y_i - \overline{\mathbf{y}})$$

$$Corr(\mathbf{x}, \mathbf{y}) = \rho(\mathbf{x}, \mathbf{y}) \equiv \frac{Cov(\mathbf{x}, \mathbf{y})}{S_{\mathbf{x}} \cdot S_{\mathbf{y}}}$$

Link to Sample Statistics

$$\begin{bmatrix} N & \sum_{i=1}^{N} x_i \\ \sum_{i=1}^{N} x_i & \sum_{i=1}^{N} x_i^2 \end{bmatrix} \cdot \begin{bmatrix} \alpha_0 \\ \alpha_1 \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{N} y_i \\ \sum_{i=1}^{N} x_i y_i \end{bmatrix}$$

$$\mathbf{y} = \{y_1, y_2, \dots, y_N\}$$

$$\mathbf{x} = \{x_1, x_2, \dots, x_N\}$$

$$\mathbf{x}^2 = \{x_1^2, x_2^2, \dots, x_N^2\}$$

$$\mathbf{x} = \{x_1, x_2, \dots, x_N^2\}$$

$$\mathbf{y} = \{y_1, y_2, \dots, y_N\}$$

$$\mathbf{x} = \{x_1, x_2, \dots, x_N\}$$

$$\mathbf{x}^2 = \{x_1^2, x_2^2, \dots, x_N^2\}$$

$$\mathbf{xy} = \{x_1 y_1, \dots, x_N y_N\}$$

$$\begin{bmatrix} 1 & \overline{\mathbf{x}} \\ \overline{\mathbf{x}} & \overline{\mathbf{x}^2} \end{bmatrix} \cdot \begin{bmatrix} \alpha_0 \\ \alpha_1 \end{bmatrix} = \begin{bmatrix} \overline{\mathbf{y}} \\ \overline{\mathbf{x}} \end{bmatrix}$$

$$\begin{bmatrix} 1 & \overline{\mathbf{x}} \\ \overline{\mathbf{x}} & \overline{\mathbf{x}^2} \end{bmatrix} \cdot \begin{bmatrix} \alpha_0 \\ \alpha_1 \end{bmatrix} = \begin{bmatrix} \overline{\mathbf{y}} \\ \alpha_1 \end{bmatrix} = \begin{bmatrix} \overline{\mathbf{y}} \\ \alpha_1 \end{bmatrix} = \begin{bmatrix} \overline{\mathbf{y}} \\ \alpha_1 \end{bmatrix} = \begin{bmatrix} \alpha_0 \\ \overline{\mathbf{x}} \end{bmatrix}$$

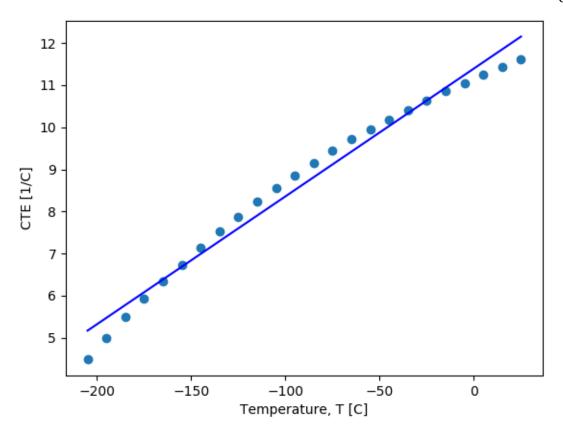
$$\alpha_1 = \frac{\Delta_1}{\Delta} = \frac{\overline{\mathbf{x}} \mathbf{y} - \overline{\mathbf{x}} \cdot \overline{\mathbf{y}}}{\overline{\mathbf{x}^2} - \overline{\mathbf{x}}^2} = \frac{\operatorname{Cov}(\mathbf{x}, \mathbf{y})}{S_{\mathbf{x}}^2}$$

$$\alpha_0 = \overline{\mathbf{y}} - \overline{\mathbf{x}} \cdot \alpha_1$$

$$y = f(x; \alpha_0, \alpha_1) = \alpha_0 + \alpha_1 x = \alpha_1 \left(x - \overline{\mathbf{x}} \right) + \overline{\mathbf{y}} = \frac{S_{\mathbf{y}}}{S_{\mathbf{x}}} \rho(\mathbf{x}, \mathbf{y}) \left(x - \overline{\mathbf{x}} \right) + \overline{\mathbf{y}}$$

Coefficient of Thermal Exp.

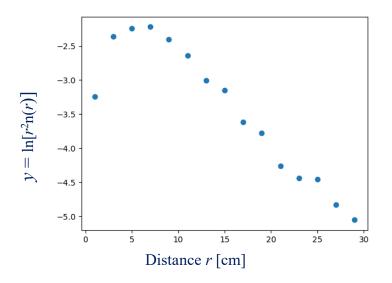
$$\alpha_{\rm L}(T) = \frac{1}{L} \frac{dL}{dT}$$
 $(L_1 - L_0)/L_0 \ll 1$ $\alpha_{\rm L}(T_0) \approx \frac{1}{L_0} \frac{L_1 - L_0}{T_1 - T_0}$



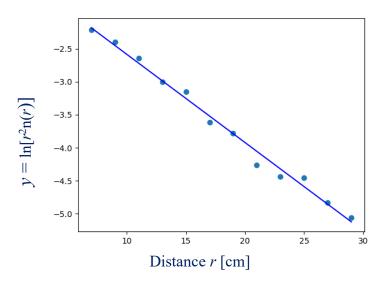
Non-Linear Problems

Reactor physics predicts that the density of fast neutrons in water from a point neutron source behaves with distance *r* from the source as

$$n(r) = \frac{A}{r^2} e^{-r/\lambda}$$



$$y \equiv \ln \left[r^2 n(r) \right] = \ln A - r/\lambda$$



Regression Model

$$\mathbf{x} = \{x_1, x_2, \dots, x_N\} \qquad \boldsymbol{\alpha} = (\alpha_0, \alpha_1, \dots, \alpha_M)$$
$$\mathbf{y} = \{y_1, y_2, \dots, y_N\} \qquad y(x) = f(x; \boldsymbol{\alpha})$$

Model function with parameters

Degree of Freedom, DoF:

$$DoF \equiv N - (M+1)$$

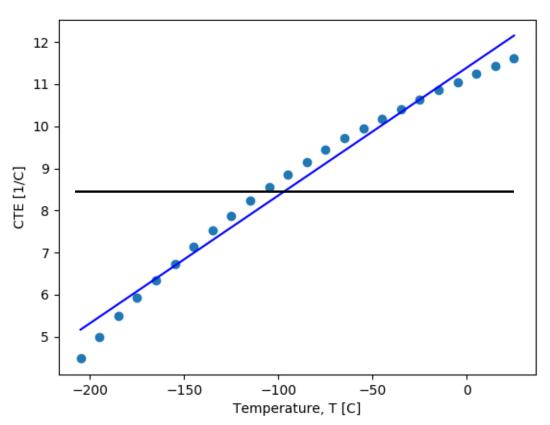
$$f(x; \boldsymbol{\alpha}) = \alpha_0 + \alpha_1 x + \alpha_2 x^2 + \dots + \alpha_M x^M$$

Baseline model M = 0:

$$y = f(x; \boldsymbol{\alpha}) = \overline{\mathbf{y}}$$
 $\overline{\mathbf{y}} = (y_1 + y_2 + ... + y_N)/N$

Baseline for Thermal Exp.

$$\alpha_{\rm L}(T) = \frac{1}{L} \frac{\mathrm{d}L}{\mathrm{d}T} \quad \alpha_{\rm L}(T_0) \approx \frac{1}{L_0} \frac{L_1 - L_0}{T_1 - T_0}$$

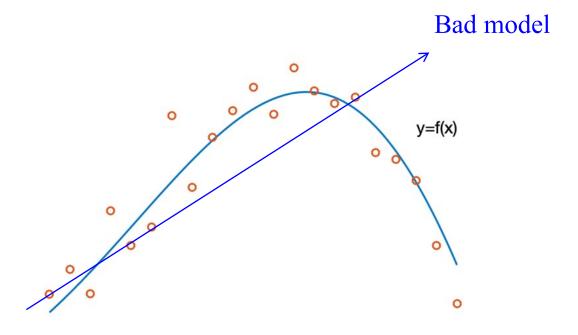


Selecting Model

A particular choice of the model may stem from:

- Physical model such as Ohm's law;
- Numerical simulation such as solving numerically Neutron Diffusion Equation, NDE;
- Previous experience e.g. the current conditions are similar to the previous ones;
- Educated guess;
- Visual inspection;
- Assumption subject to confirm or reject.

Visual Inspection



Sum of Squared Residuals

When parameter vector α is found, the model function is defined

$$y = f(x; \boldsymbol{\alpha})$$

Predicted (computed) values: $\hat{y}_i = f(x_i; \alpha)$

$$\hat{y}_i = f(x_i; \boldsymbol{\alpha})$$

$$r_i \equiv \hat{y}_i - y_i$$

SSR =
$$R^2 = \sum_{i=1}^{N} r_i^2 = \sum_{i=1}^{N} [\hat{y}_i - y_i]^2 = \sum_{i=1}^{N} [f(x_i; \alpha) - y_i]^2$$

Also, Sum of Squared Errors, SSE; Residual Sum of Squares, RSS.

Root Mean Square Error

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left[\hat{y}_i - y_i \right]^2}$$

$$S_{y} \equiv \sqrt{\frac{1}{N} \sum_{i=1}^{N} (y_{i} - \overline{y})^{2}}$$

$$RMSN \equiv RMSE/S_y \qquad \text{(normalised)}$$

Coefficient of Determination

CoD, is a popular choice to characterize the quality of the regression model.

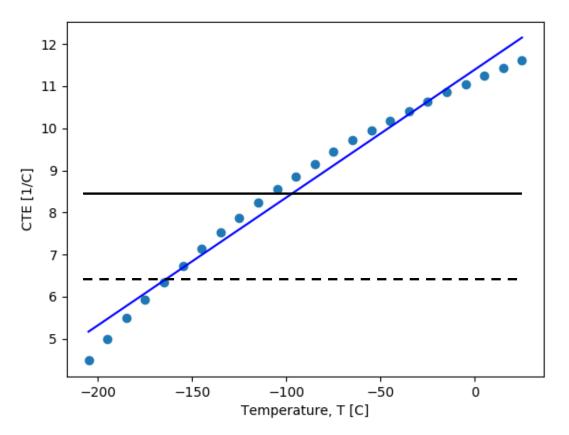
$$CoD = r^{2} = R^{2} = 1 - RMSN^{2} = 1 - \frac{\sum_{i=1}^{N} \left[\hat{y}_{i} - y_{i}\right]^{2}}{\sum_{i=1}^{N} \left[\overline{\mathbf{y}} - y_{i}\right]^{2}}$$

Baseline
$$\hat{y}_i = \overline{\mathbf{y}}$$
 $0 \le \text{CoD} \le 1$ $\hat{y}_i = y_i$ Best

It may happen CoD < 0 Pathology!!

Unacceptable Baseline

$$\alpha_{\rm L}(T) = \frac{1}{L} \frac{\mathrm{d}L}{\mathrm{d}T} \quad \alpha_{\rm L}(T_0) \approx \frac{1}{L_0} \frac{L_1 - L_0}{T_1 - T_0}$$



$$CoD = 0$$

Polynomial Model Function

$$f(x; \boldsymbol{\alpha}) = \alpha_0 + \alpha_1 x + \alpha_2 x^2 + \cdots + \alpha_M x^M$$

$$\begin{cases} f(x_1; \boldsymbol{\alpha}) = \alpha_0 + \alpha_1 x_1 + \alpha_2 x_1^2 + \cdots + \alpha_M x_1^M = y_1 \\ f(x_2; \boldsymbol{\alpha}) = \alpha_0 + \alpha_1 x_2 + \alpha_2 x_2^2 + \cdots + \alpha_M x_2^M = y_2 \\ \vdots \\ f(x_N; \boldsymbol{\alpha}) = \alpha_0 + \alpha_1 x_N + \alpha_2 x_N^2 + \cdots + \alpha_M x_N^M = y_N \end{cases}$$

Functional Approach

$$r_i(\boldsymbol{\alpha}) \equiv r_i \equiv f(x_i; \boldsymbol{\alpha}) - y_i$$
 $R^2(\boldsymbol{\alpha}) \equiv R^2 \equiv \sum_{i=1}^N r_i^2 = \sum_{i=1}^N \left[f(x_i; \boldsymbol{\alpha}) - y_i \right]^2$

$$\min_{\alpha} R^{2}(\alpha) = \min_{\alpha} \sum_{i=1}^{N} \left[f(x_{i}; \alpha) - y_{i} \right]^{2}$$

$$\begin{cases} \frac{\partial R^2(\boldsymbol{\alpha})}{\partial \alpha_m} = 0 & m = 0, 1, 2, \dots, M \end{cases}$$

$$\left\{ \sum_{i=1}^{N} 2 \left[f(x_i; \boldsymbol{\alpha}) - y_i \right] \frac{\partial f(x_i; \boldsymbol{\alpha})}{\partial \alpha_m} = 0 \qquad m = 0, 1, \dots, M \right\}$$

Linear Equations

$$g_m(\boldsymbol{\alpha}) \equiv \sum_{i=1}^N \left[f(x_i; \boldsymbol{\alpha}) - y_i \right] \frac{\partial f(x_i; \boldsymbol{\alpha})}{\partial \alpha_m} = 0 \qquad m = 0, 1, \dots, M$$

$$\mathbf{G}(\boldsymbol{\alpha}) \equiv \begin{bmatrix} g_0(\boldsymbol{\alpha}) \\ \vdots \\ g_M(\boldsymbol{\alpha}) \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix} = \mathbf{0}$$

Algebraic Approach

$$\begin{cases} f(x_1; \boldsymbol{\alpha}) = \alpha_0 + \alpha_1 x_1 + \alpha_2 x_1^2 + \dots + \alpha_M x_1^M = y_1 \\ f(x_2; \boldsymbol{\alpha}) = \alpha_0 + \alpha_1 x_2 + \alpha_2 x_2^2 + \dots + \alpha_M x_2^M = y_2 \\ \vdots \\ f(x_N; \boldsymbol{\alpha}) = \alpha_0 + \alpha_1 x_N + \alpha_2 x_N^2 + \dots + \alpha_M x_N^M = y_N \end{cases}$$

$$\begin{bmatrix} 1 & x_1 & \cdots & x_1^M \\ 1 & x_2 & \cdots & x_2^M \\ 1 & x_3 & \cdots & x_3^M \\ \vdots & \vdots & & \vdots \\ 1 & x_{N-1} & \cdots & x_N^M \\ 1 & x_N & \cdots & x_N^M \end{bmatrix} \cdot \begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_M \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{N-1} \\ y_N \end{bmatrix}$$

$$\mathbf{V}\boldsymbol{\alpha} = \mathbf{y}$$

$$\mathbf{V}^T \mathbf{V}\boldsymbol{\alpha} = \mathbf{V}^T \mathbf{y}$$

Trigonometric Functions

(1) Assume model function

$$f(x; c_0, c_1) = c_0 \sin(x) + c_1 \cos(x)$$

(2) Find coefficients c_0 and c_1 that minimize residual

$$R(\mathbf{c}) = \sum_{j=1}^{n} \left[f(x_j; c_0, c_1) - y_j \right]^2 \qquad R'_{c_0}(\mathbf{c}) = 0 \quad R'_{c_1}(\mathbf{c}) = 0$$

(3) Form linear equations

$$f(x_1) = c_0 \sin(x_1) + c_1 \cos(x_1) = y_1$$

$$f(x_2) = c_0 \sin(x_2) + c_1 \cos(x_2) = y_2$$

$$\vdots$$

$$f(x_N) = c_0 \sin(x_N) + c_1 \cos(x_N) = y_N$$

Matrix Form

$$\begin{bmatrix} \sin(x_1) & \cos(x_1) \\ \sin(x_2) & \cos(x_2) \\ \vdots & \vdots \\ \sin(x_N) & \cos(x_N) \end{bmatrix} \cdot \begin{bmatrix} c_0 \\ c_1 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} \qquad \mathbf{V} = \begin{bmatrix} \sin(x_1) & \cos(x_1) \\ \sin(x_2) & \cos(x_2) \\ \vdots & \vdots \\ \sin(x_N) & \cos(x_N) \end{bmatrix}$$

$$\mathbf{V}^{T} = \begin{bmatrix} \sin(x_0) & \sin(x_1) & \cdots & \sin(x_n) \\ \cos(x_0) & \cos(x_1) & \cdots & \cos(x_n) \end{bmatrix}$$

$$\mathbf{V}^{T}\mathbf{V}\mathbf{c} = \begin{bmatrix} \sum \sin^{2}(x_{i}) & \sum \sin(x_{i})\cos(x_{i}) \\ \sum \sin(x_{i})\cos(x_{i}) & \sum \cos^{2}(x_{i}) \end{bmatrix} \cdot \begin{bmatrix} c_{0} \\ c_{1} \end{bmatrix} = \begin{bmatrix} \sum y_{i}\sin(x_{i}) \\ \sum y_{i}\cos(x_{i}) \end{bmatrix} = \mathbf{V}^{T}\mathbf{y}$$

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Matlab

Backslash command

$$>> x = A b$$

solves:

- $\mathbf{A}\mathbf{x} = \mathbf{b}$ in ordinary sense when n = m
- $\mathbf{A}\mathbf{x} = \mathbf{b}$ in least squares sense when $n \neq m$

$$>> c = polyfit(x,y,m)$$

finds:

• Coefficients c of polynomial of degree m that is the best fit.

Important

- Model Fitting (Curve fitting)
- Functional Approach: Non-Linear Equation
- Algebraic Approach: Normal Equations
- Efficiency Indicators
- Polynomial Models
- Non-Polynomial Models