
Kaiserwetter - Mobbtrix

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FB3 Mathematik / Informatik
AG analoge Digitaltechnik

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EIDESSTATTLICHE ERKLÄRUNG

Hiermit versichere ich, dass ich die vorliegende Arbeit im Sinne der Prüfungsordnung nach §24(5) ohne fremde Hilfe selbstständig verfasst und nur die angegebenen Hilfsmittel benutzt habe.

Bremen, 10. Dezember 2007

Ort, Datum

Unterschrift

ZUSAMMENFASSUNG

Hier steht die Zusammenfassung bzw. **das abstract**

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KAPITEL 1

Einführung

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KAPITEL 2

State of the Art

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TOLLER INDEX

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APPENDIX A

Least squares fit of response surface models by multiple linear regression

If the number of experiments, n , exceed the number of model parameters, p , there will always be some aberrations between the model and the experimental data, i.e. there will be at least some residuals which are different from zero. Here is shown that the relation

$$(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} = \mathbf{b} \quad (\text{A.1})$$

will always give the least squares estimate of the model parameters.

Let \mathbf{X} be the model matrix for a series of n experiments; let \mathbf{b} be the vector of model parameters to be estimated; let \mathbf{y} be the vector of measured responses, such that $\mathbf{y}^T = [y_1, y_2, \dots, y_n]$; and let \mathbf{e} be the vector of unknown residuals, $\mathbf{e}^T = [e_1, e_2, \dots, e_n]$. For the series of experiments, the following relation applies

$$\mathbf{y} = \mathbf{Xb} + \mathbf{e}, \quad (\text{A.2})$$

i.e.

$$\mathbf{e} = \mathbf{y} - \mathbf{Xb}. \quad (\text{A.3})$$

$$\sum e_i^2 = \mathbf{e}^T \mathbf{e} \text{ (a scalar product)}. \quad (\text{A.4})$$

Develop the right part of (Eq. A.3) as a scalar product. This gives

$$\sum e_i^2 = (\mathbf{y} - \mathbf{Xb})^T (\mathbf{y} - \mathbf{Xb}) \quad (\text{A.5})$$

$$\sum e_i^2 = \mathbf{y}^T \mathbf{y} - 2\mathbf{y}^T \mathbf{Xb} + (\mathbf{Xb})^T \mathbf{Xb} \quad (\text{A.6})$$

$$\sum e_i^2 = \mathbf{y}^T \mathbf{y} - 2\mathbf{y}^T \mathbf{Xb} + \mathbf{b}^T \mathbf{X}^T \mathbf{Xb}. \quad (\text{A.7})$$

We wish to determine which set of model parameters minimizes the sum of squared residuals. This minimum can be found by solving the following systems of equations

$$\frac{\partial}{\partial \beta_j} \sum e_i^2 = 0, \text{ for all parameters } \beta_j. \quad (\text{A.8})$$

In matrix notation (see Appendix: Matrix calculus), the above expression can be written

$$\frac{\partial \mathbf{e}^T \mathbf{e}}{\partial \boldsymbol{\beta}} = \mathbf{0}, \quad (\text{A.9})$$

which corresponds to

$$\frac{\partial}{\partial \boldsymbol{\beta}} (\mathbf{y}^T \mathbf{y} - 2\mathbf{y}^T \mathbf{X} \boldsymbol{\beta} + \boldsymbol{\beta}^T \mathbf{X}^T \mathbf{X} \boldsymbol{\beta}) = \mathbf{0}. \quad (\text{A.10})$$

This gives

$$2(\mathbf{y}^T \mathbf{X})^T + [\mathbf{X}^T \mathbf{X} + (\mathbf{X}^T \mathbf{X})^T] \mathbf{b} = \mathbf{0}. \quad (\text{A.11})$$

The matrix $\mathbf{X}^T \mathbf{X}$ is symmetric and $\mathbf{X}^T \mathbf{X} = (\mathbf{X}^T \mathbf{X})^T$ and the above expression is equivalent to

$$\mathbf{X}^T \mathbf{y} = \mathbf{X}^T \mathbf{X} \mathbf{b}. \quad (\text{A.12})$$

Provided that $(\mathbf{X}^T \mathbf{X})^{-1}$ exists, a multiplication of both sides by $(\mathbf{X}^T \mathbf{X})^{-1}$ affords the least squares relation

$$(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} = \mathbf{b}. \quad (\text{A.13})$$

Q.E.D.