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Publications

The work presented in the thesis is fully documented in the form of following publications:

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Appendix A. Numerical Techniques for the Solution of Nonlinear Algebraic Equations

Newton Raphson Method

Solution of nonlinear algebraic equations encountered in steady state simulation is frequently carried out using the Newton Raphson method. The derivations of the Newton Raphson method for scalar (one variable) and vector (multivariable) functions are shown below:

<u>Scalar (one variable) Newton-Raphson method:</u>

The nonlinear algebraic equation is written as:

$$f(x) = 0 \qquad \text{Eq. A. 1}$$

Taylor series expansion of $f(x)$ around an initial (or guess) point x^k gives:

$$f(x) = 0 = f(x^k) + f^{'}(x^k)(x^{k+1} - x^k) \qquad \text{Eq. A. 2}$$

Accordingly, the value of x in the $k+1^{th}$ iteration is given as:

$$x^{k+1} = x^k - f(x^k) / f^{'}(x^k) \qquad \text{Eq. A. 3}$$

Where, $f^{'}(x^k)$ represents the derivative of $f(x)$ evaluated at x^k , as shown:

$$f'(x^k) = \frac{df(x)}{dx}|_{x^k} \qquad \text{Eq. A. 4}$$

Convergence is achieved when the error between the successively estimated values of the unknown variable is less than the specified tolerance, ε .

$$x^{k+1} - x^k \le \varepsilon \qquad \text{Eq. A. 5}$$

<u>Vector (multivariable) Newton-Raphson method:</u>

The set of simultaneous nonlinear algebraic equations (n equations in n unknowns) are written as:

$$\mathbf{f}(\mathbf{x}) = \mathbf{0} \qquad \text{Eq. A. 6}$$

Where, the (nx1) vector of (unknown) variables is defined as:

$$\mathbf{x} = (x_1, x_2, ..., x_i, ..., x_n)^T \qquad \text{Eq. A. 7}$$

And the (nx1) vector of functions is defined as:

$$\mathbf{f(x)} = (f_1, f_2, ..., f_i, ..., f_n)^T \qquad \text{Eq. A. 8}$$

The initial (or guess) value of the vector of variables is defined as:

$$\mathbf{x}^k = (x_1^k, x_2^k, ..., x_i^k, ..., x_n^k)^T \qquad \text{Eq. A. 9}$$

The Taylor series expansion of $\mathbf{f(x)}$ around the initial (or guess) point $\mathbf{x}^k$ gives:

$$\mathbf{x^{k+1} = x^k - J^{-1}(x^k)f(x^k)} \qquad \text{Eq. A. 10}$$

Where, $\mathbf{J(x^k)}$ represents the (nxn) jacobian matrix of derivatives evaluated at the point $\mathbf{x}^k$

Convergence is achieved when the error between the successively estimated values of the unknown variables is less than the specified tolerance vector, $\boldsymbol{\varepsilon}$.

$$\mathbf{x^{k+1} - x^k} \le \boldsymbol{\varepsilon} \qquad \text{Eq. A. 11}$$

Appendix B. Linear Regression

Linear Least Squares Parameter Estimation

Let the scalar dependent variable be denoted as: y . If y is dependent on a set of k independent variables, defined as:

$$\mathbf{x} = (x_1, x_2, x_3, ..., x_k)^T \quad \text{Eq.B. 1}$$

Then, the linear functionality of y and $\mathbf{x}$ is denoted as:

$$y = \mathbf{x}^{\mathbf{T}}\boldsymbol{\beta} \quad \text{Eq.B. 2}$$

Where, the vector of (unknown) parameters, $\boldsymbol{\beta}$ to be estimated, is given as:

$$\boldsymbol{\beta} = (\beta_1, \beta_2, \beta_3, ..., \beta_k)^T \quad \text{Eq.B. 3}$$

If the values of $\boldsymbol{\beta}$ are known exactly, y can be accurately predicted/inferred/estimated from the known values of $\mathbf{x}$.

However, in practice, such precision is almost never attainable and equation (B.2) is in error, since the parameter estimation problem is based on n number of experimental observations (measurements) of y and $\mathbf{x}$, as shown in Table B.1 below:

Table B. 1 Data of experimental observations

No. of Experimental observations, n	Experimental observations of the independent variables, $\mathbf{x}$					Experimental observations of the dependent variable, $\mathbf{y}$	Estimates/prediction of the dependent variable, $\hat{\mathbf{y}}$	Square of error $\mathbf{e}^2$
	x_1	x_2	x_3	$\cdots$	x_k			
1	x_{11}	x_{12}	x_{13}	$\cdots$	x_{1k}	y_1	$\hat{y}_1$	$(y_1 - \hat{y}_1)^2$
2	x_{21}	x_{22}	x_{23}	$\cdots$	x_{2k}	y_2	$\hat{y}_2$	$(y_2 - \hat{y}_2)^2$
3	x_{31}	x_{32}	x_{33}	$\cdots$	x_{3k}	y_3	$\hat{y}_3$	$(y_3 - \hat{y}_3)^2$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
n	x_{n1}	x_{n2}	x_{n3}	$\cdots$	x_{nk}	y_n	$\hat{y}_n$	$(y_n - \hat{y}_n)^2$
							SUM	$(\mathbf{e}^T\mathbf{e}) = \sum_{i=1}^{i=n} e_i^2$

Based on the experimental observations, the parameter estimation problem is framed as under:

Let the $(n\text{x}1)$ vector of observations of the dependent variable be denoted as:

$$\mathbf{y} = (y_1, y_2, y_3, ..., y_n)^T \qquad \text{Eq.B. 4}$$

The $(\text{kx}1)$ vector of (unknown) parameters to be estimated, is given as:

$$\boldsymbol{\beta} = (\beta_1, \beta_2, \beta_3, ..., \beta_k)^T \qquad \text{Eq.B. 5}$$

The $(\text{nx}k)$ matrix of n observations of the k independent variables is denoted as:

$$\mathbf{A} = \begin{bmatrix} x_{11} & x_{12} & x_{1k} \\ x_{21} & x_{22} & x_{2k} \\ & & \\ x_{n1} & x_{n2} & x_{nk} \end{bmatrix} \qquad \text{Eq.B. 6}$$

Let the (nx1) vector, $\hat{\mathbf{y}}$ denote the estimates of the dependent variable, based on the functionality of y and $\mathbf{x}$, as shown in equation B.2. $\hat{\mathbf{y}}$ is given as:

$$\hat{\mathbf{y}} = \mathbf{A\beta} \qquad \text{Eq.B. 7}$$

Let the (nx1) vector, $\mathbf{e}$ represent the error between the experimental and predicted values of the dependent variable, denoted as:

$$\mathbf{e = (y - \hat{y}) = (y - A\beta)} \qquad \text{Eq.B. 8}$$

A common method of estimating the parameters $\boldsymbol{\beta}$ is the method of Least Squares (LS), which is based on the following assumptions:

i. Since the error vector, $\mathbf{e}$ represents the error from various sources, $\mathbf{e}$ is assumed to have zero mean.

ii. The variance of $\mathbf{e}$ is constant and independent of the matrix $\mathbf{A}$.

The covariance of $\mathbf{e}$ is denoted as:

$$\text{cov}(e_i, e_j) = 0 \quad \forall \quad (i \neq j) \qquad \text{Eq.B. 9}$$

$$\text{cov}(e_i, e_j) = \text{var}(e_i, e_j) = \sigma^2 \quad \forall \quad (i = j) \qquad \text{Eq.B. 10}$$

The ($n$xn) variance-covariance matrix of errors is thus represented as:

$$\mathbf{P} = \sigma^2 \mathbf{I} = \begin{bmatrix} \sigma^2 & 0 & \cdots & 0 \\ 0 & \sigma^2 & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & \sigma^2 \end{bmatrix} \qquad \text{Eq.B. 11}$$

The assumptions imply that the error vector $\mathbf{e}$ has multivariate normal distribution, given as:

$$\mathbf{e} = N(0, \sigma^2 \mathbf{I}) \qquad \text{Eq.B. 12}$$

iii. The Matrix $\mathbf{A}$ is a set of fixed numbers and does not contain any error.

iv. The rank of matrix $\mathbf{A}$ is k, where, $k < n$. This implies that the k variables are linearly independent.

v. The number of experimental observations exceeds the number of parameters to be estimated.

<u>The method of Least Squares (LS)</u>

The method of Least Squares (LS) based on the minimization of the sum of squares of errors. The (scalar) objective function, $\phi(\boldsymbol{\beta})$ is therefore represented as:

Minimize: $\phi(\boldsymbol{\beta}) = \mathbf{e}^T\mathbf{e}$ Eq.B. 13

Applying the necessary condition for optimality:

The Jacobin vector (first partial derivatives of $\phi(\boldsymbol{\beta})$ with respect to $\boldsymbol{\beta}$) must be zero:

$$\frac{\partial \phi}{\partial \boldsymbol{\beta}} = 0 \qquad \text{Eq.B. 14}$$

$$\frac{\partial \phi}{\partial \boldsymbol{\beta}} = \left[-\mathbf{A}^T(\mathbf{y} - \mathbf{A}\boldsymbol{\beta}) + (\mathbf{y} - \mathbf{A}\boldsymbol{\beta})^T(-\mathbf{A})\right] = 0 \qquad \text{Eq.B. 15}$$

Using the matrix –vector identity, $\mathbf{A}^T\mathbf{v} = \mathbf{v}^T\mathbf{A}$, the above equation is simplified as:

$$\left[-2\mathbf{A}^T(\mathbf{y} - \mathbf{A}\boldsymbol{\beta})\right] = 0 \qquad \text{Eq.B. 16}$$

Further simplification of equation B.16 gives:

$$(\mathbf{A}^T\mathbf{A})\boldsymbol{\beta} = \mathbf{A}^T\mathbf{y} \qquad \text{Eq.B. 17}$$

Equation B.17 represents a set of k number of simultaneous linear algebraic equations, called the normal equations. Solution of equation B.17 is given as:

$$\boldsymbol{\beta} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{y} \qquad \text{Eq.B. 18}$$

The matrix ($\mathbf{A}^T\mathbf{A}$) is symmetric matrix of dimension (kxk).

The assumption (iv) guarantees that ($\mathbf{A}^T\mathbf{A}$) is non-singular and hence its inverse exists.

Statistical Performance Indices (SPI)

Once the parameters are estimated using equation B.18, the following Statistical Performance Indices (SPI) are used to provide a quantitative measure of the goodness of the estimates of the dependent variable.

a. Mean and variance / standard deviation

b. Sum of Square of Error (SSE)

c. Root Mean Square Error (RMSE)

d. Mean Absolute Percentage Error (MAPE)

e. Coefficient of Multiple Determination (CMD)

f. Covariance-Correlation matrix and Correlation Coefficient

The Sum of Square of Error (SSE) is defined as:

$$SSE = \mathbf{e}^T \mathbf{e} \qquad \text{Eq.B. 19}$$

The absolute value of error is given as:

$$abs(\mathbf{e}) \qquad \text{Eq.B. 20}$$

The percentage error is given as:

$$\mathbf{p} = 100.*abs(\mathbf{e})./\,\mathbf{y} \qquad \text{Eq.B. 21}$$

The Mean Absolute Percentage Error (MAPE) is given as:

$$MAPE = (\mathbf{j}^T * \mathbf{p})./\,n \qquad \text{Eq.B. 22}$$

Where, the (nx1) vector $\mathbf{j}$ is defined as:

$$\mathbf{j} = (1,1,\cdots,1)^T \qquad \text{Eq.B. 23}$$

Appendix C. Tridiagonal Matrix Algorithm

The steady-state process model of counter current flow equilibrium staged processes is represented by a system of n linear (or linearized nonlinear) algebraic equations in n unknowns, as shown:

$$\begin{pmatrix} b_1 x_1 + c_1 x_2 = d_1 \\ a_2 x_1 + b_2 x_2 + c_2 x_3 = d_2 \\ a_3 x_2 + b_3 x_3 + c_3 x_4 = d_3 \\ \vdots \\ a_i x_{i-1} + b_i x_i + c_i x_{i+1} = d_i \\ \vdots \\ a_{n-1} x_{n-2} + b_{n-1} x_{n-1} + c_{n-1} x_n = d_{n-1} \\ a_n x_{n-1} + b_n x_n = d_n \end{pmatrix} \qquad \text{Eq. C. 1}$$

The (nx1) vector of (unknown) output variables is defined as:

$$\mathbf{x} = (x_1, x_2, x_3, ..., x_n)^T \qquad \text{Eq. C. 2}$$

The vector of n (known) inputs is defined as:

$$\mathbf{d} = (d_1, d_2, d_3, ..., d_n)^T \qquad \text{Eq. C. 3}$$

The (n x n) tridiagonal matrix of (known) coefficients is defined as:

$$\mathbf{U} = \begin{bmatrix} b_1 & c_1 & 0 & 0 & \ldots 0 & 0 & 0 \\ a_2 & b_2 & c_2 & 0 & \ldots 0 & 0 & 0 \\ 0 & a_3 & b_3 & c_3 & \cdots 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 \cdots & a_{n-1} & b_{n-1} & c_{n-1} \\ 0 & 0 & 0 & 0 \cdots & 0 & a_n & b_n \end{bmatrix} \qquad \text{Eq. C. 4}$$

The equation C.1 is conveniently expressed in vector-matrix notation as:

$$\mathbf{Ux} = \mathbf{d} \qquad \text{Eq. C. 5}$$

The first equation of equation C.1 is written as:

$$x_1 + p_1 x_2 = q_1 \qquad \text{Eq. C. 6}$$

Where, p_1 and q_1 are defined as:

$$p_1 = c_1 / b_1 \qquad \text{Eq. C. 7}$$

$$q_1 = d_1 / b_1 \qquad \text{Eq. C. 8}$$

Combining the second equation of equation C.1 with equation C.6 gives:

$$x_2 + p_2 x_3 = q_2 \qquad \text{Eq. C. 9}$$

Where, p_2 and q_2 are defined as:

$$p_2 = [c_2 / (b_2 - p_1 a_2)] \qquad \text{Eq. C. 10}$$

$$q_2 = [(d_2 - q_1 a_2) / (b_2 - p_1 a_2)] \qquad \text{Eq. C. 11}$$

Similarly, any general i^{th} equation of equation C.1 is written as:

$$x_i + p_i x_{i+1} = q_i \qquad (\forall\, i = 1 : n) \qquad \text{Eq. C. 12}$$

Where, p_i and q_i are defined as:

$$p_i = [c_i / (b_i - p_{i-1} a_i)] \qquad \text{Eq. C. 13}$$

$$q_i = [(d_i - q_{i-1} a_i) / (b_i - p_{i-1} a_i)] \qquad \text{Eq. C. 14}$$

$$p_0 = q_0 = 0 \qquad \text{Eq. C. 15}$$

The $n-1^{th}$ equation of equation C.1 is written as:

$$x_{n-1} + p_{n-1} x_n = q_{n-1} \qquad \text{Eq. C. 16}$$

And since x_{n+1} does not exist, the n^{th} equation of equation C.1 is written as:

$$x_n = q_n \qquad \text{Eq. C. 17}$$

Based on equations C.6 to C.17, the system of equations represented by equation in C.1 are transformed as:

$$\begin{pmatrix} x_1 + p_1 x_2 = q_1 \\ x_2 + p_2 x_3 = q_2 \\ \vdots \\ x_i + p_i x_{i+1} = q_i \\ \vdots \\ x_n = q_n \end{pmatrix} \quad \text{Eq. C. 18}$$

The tridiagonal algorithm is implemented as a sequential numerical solution. The computational steps in the tridiagonal algorithm are written as:

Step 1 : Input Specification

Read all specified data ((nx1) vector of coefficients $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}$ in equation C.1)

$$\mathbf{a} = (0, a_2, a_3, ..., a_n)^T \quad \text{Eq. C. 19}$$

$$\mathbf{b} = (b_1, b_2, b_3, ..., b_n)^T \quad \text{Eq. C. 20}$$

$$\mathbf{c} = (c_1, c_2, c_3, ..., c_{n-1}, 0)^T \quad \text{Eq. C. 21}$$

$$\mathbf{d} = (d_1, d_2, d_3, ..., d_n)^T \quad \text{Eq. C. 22}$$

Step 2:Forward substitution

For $(i = 1, 2, \cdots, n)$, compute p_i and q_i using equations C.13-C.15.

Step 3: Assignment

For $(i = n)$, assign:

$$x_n = q_n \quad \text{Eq. C. 23}$$

Step 4: Backward substitution

For $(i = n-1, n-2, \cdots, 1)$, compute:

$$x_{n-1} = q_{n-1} - p_{n-1} x_n \quad \text{Eq. C. 24}$$

$$x_i = q_i - p_i x_{i+1} \quad \text{Eq. C. 25}$$

$$x_1 = q_1 - p_1 x_2 \quad \text{Eq. C. 26}$$