Mathematics for chemical engineers

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5. Numerical solutions of nonlinear equations

Mandatory material. It will be a part of writing tests and will be tested at the oral examination (no designation).

⭐ Examples of exercises - voluntary.

⭐ For students who want to know more. This material will not be lectured and it will not be a part of both writing and oral exams.

Outline

Numerical solutions of nonlinear equations

Numerical solution of nonlinear equations belongs together with solution of linear algebraic systems to the important problems of numerical analysis. Examples can be found in a variety of engineering applications, for example,

- Computation of a complex chemical equilibrium,
- Counter-current separation devices such as distillation and absorption columns
- Stationary simulation of a system of devices
- Replacement of parabolic or elliptic equations using finite differences,
- Finding stationary states of dynamical models described by ordinary differential equations

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Equation with one unknown

Equation with one unknown

For the solution of the equation

$$f(x) = 0 \tag{1}$$

several iteration methods have been developed. The main idea of these
methods is as follows:
Let us assume that we know a sufficiently small interval containing a single
root $x = x^*$ of the equation (1). We choose an initial approximation x_0 (close
to the root x^*) in this interval and we construct a sequence of points
$x_1, x_2, \ldots, x_n, \ldots$ according to the recurrent rule

$$x_k = \phi(x_0, x_1, \ldots, x_{k-1}). \tag{2}$$

The recurrent rule (2) is constructed in such a way that (under certain
assumptions) the sequence $\{x_n\}$ converges to x^*.

Various choices of the function ϕ_k (depending on the function f) give different
iterative methods.

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Equation with one unknown

★ **The choice of the function** ϕ_k

The function $\phi(x)$ is often designed so that the solution x^* is a fixed point of the function ϕ, i.e., it is also a solution of the equation

$$x = \phi(x), \tag{3}$$

where the sequence $\{x_k\}$ is constructed according to the rule

$$x_k = \phi(x_{k-1}), \quad k = 1, 2, \ldots. \tag{4}$$

Here, the ϕ does not depend on the increasing index k. Methods of this type are called stationary methods.

Let the function ϕ be differentiable. If

$$|\phi'(x^*)| \leq K < 1,$$

and if ϕ' is continuous then $|\phi'(x)| < 1$ also in some neighborhood of the root x^* and the successive approximations (4) converge, provided x_0 is close to x^*. The smaller is the constant K, the faster is the convergence.

If we want a solution x^* with the accuracy ϵ, then we stop the iterations when

$$\frac{K}{1-K}|x_k - x_{k-1}| < \epsilon.$$

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Equation with one unknown

The order of iterations is a measure of the rate of convergence of (4). We say that the iteration (4) is of order m, if

$$\phi'(x^*) = \phi''(x^*) = \cdots = \phi^{(m-1)}(x^*) = 0, \quad \phi^{(m)}(x^*) \neq 0. \quad (5)$$

If the function $\phi(x)$ has m continuous derivatives in a neighborhood of x^*, then the rest after the $m-1$ term of Taylor's expansion gives

$$x_k - x^* = \frac{1}{m!}(x_{k-1} - x^*)^m \phi^{(m)}(\xi_k).$$

Let us denote $M_m = \max |\phi^{(m)}(x)|$ in the neighborhood of x^*. Then

$$|x_k - x^*| \leq \frac{M}{m!}|x_{k-1} - x^*|^m. \qquad \text{If} \qquad (6)$$

$$|x_0 - x^*| < 1 \quad \text{and} \quad \frac{M_m}{m!}|x_0 - x^*| = \omega < 1,$$

then for $m > 1$ after some simplification we obtain

$$|x_k - x^*| \leq \omega^{\frac{m^k - 1}{m - 1}}, \quad (7)$$

which represents a fast convergence of x_k to x^*.

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Bisection method

Bisection method

Let us first examine the methods that allow us to fined a small interval in which the solution is located.

If the function $f(x)$ in (1) is continuous then it is sufficient to find two points x' and x'' such that $f(x')f(x'') < 0$, i.e., such points that the function f has different signs at these two points. Then, due to the continuity of f, there is at least one root between x' and x''. If there is exactly one root and not more in the given interval, we call this interval the separation interval.

The simplest method to decrease the interval $\langle x', x'' \rangle$ containing the root is the bisection method.

Let us denote by x the center of the interval $\langle x', x'' \rangle$, i.e., $x = (x' + x'')/2$. Then either $f(x') \cdot f(x) < 0$ or $f(x) \cdot f(x'') < 0$. In the former case we decrease the interval to $\langle x', x \rangle$, in the latter case the new interval will be $\langle x, x'' \rangle$. After n bisection steps the size of the interval is
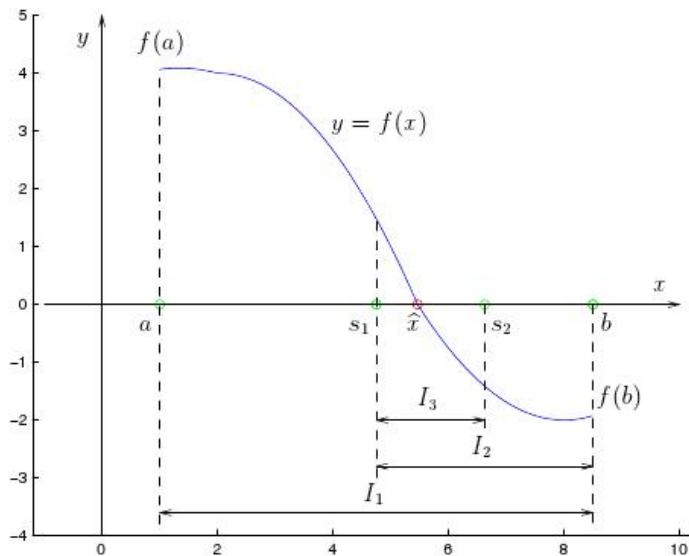
$$|x' - x''| = 2^{-n}r, \tag{8}$$

where r is the size of the original interval. After 10 bisection steps the interval shrinks 1024 times.

This method converges slowly but it is reliable and it is good when we have not enough information about the precise location of the root.

Bisection method

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Newton method

Newton method

One of the most frequently used methods for solving nonlinear equations is the Newton method. The Newton method is sometimes called the method of tangents due to its geometrical meaning.

At first, we have to find the separation interval, i.e., the interval in which precisely one root of the equation (1) is located.

Let us assume that the function f is continuous and twice continuously differentiable on interval $\langle a, b \rangle$. Moreover, let

(a) $f(a) \cdot f(b) < 0$,

(b) $f'(x) \neq 0 \; \forall x \in \langle a, b \rangle$,

(c) $f''(x) \neq 0 \; \forall x \in \langle a, b \rangle$,

(d) as the initial approximation x_0 of the root α, we choose that one of the end points a, b for which it is valid

$$f(x_0) \cdot f''(x_0) > 0 \,.$$

Let us note that the interval $\langle a, b \rangle$ is a separation interval if and only if the conditions (a) and (b) are satisfied. Conditions (c) and (d) guarantee convergence of the Newton method to the root α.

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Newton method

Let us choose the zero approximation x_0 of the root α. Geometrically, the Newton method can be described as follows: At the point $[x_0, f(x_0)]$ we construct the tangent to the graph of the function $f(x)$. The first iteration is the intersection of this tangent with the x axis. Hence, for the first iteration we have

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}.$$

Now, we construct the tangent at the point $[x_1, f(x_1)]$ and the intersection of this tangent with the x is the second approximation of the root α and so on. In general, for $(n+1)-$ iteration we have the formula

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_{n-1})}, \ n = 1, 2, \dots.$$
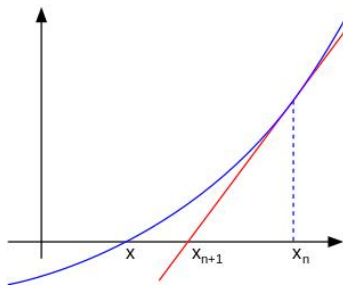
If we prescribe the accuracy of the calculation in advance, for example $\varepsilon = 10^{-4}$, then we will end the calculation if

$$|x_{n+1} - x_n| < const \cdot 10^{-4}.$$

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Newton method

★ Quadratic convergence of Newton's method

We are looking for a root α of the equation $f(x) = 0$, i.e. for such α that $f(\alpha) = 0$. Let x_0 be a starting approximation. Then $(k+1)-$st step gives

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}, \quad k = 1, 2, \dots.$$

The error of computation in $k-$th step is $e_k = \alpha - x_k \Rightarrow \alpha = x_k + e_k$.
If we apply Taylor's expansion to the function f at the point x_k we obtain

$$f(x) = f(x_k) + f'(x_k)(x - x_k) + \frac{f''(x_k)}{2!}(x - x_k)^2 + \mathcal{O}(x - x_k)^3,$$

Let us put $x := \alpha$ and $x - x_k = \alpha - x_k = e_k$. Then

$$0 = f(\alpha) = f(x_k + e_k) = f(x_k) + f'(x_k) \cdot e_k + \frac{1}{2} f''(x_k) \cdot e_k^2 + \mathcal{O}(e_k^3)$$

$$-f(x_k) = f'(x_k) \cdot e_k + \frac{1}{2} f''(x_k) \cdot e_k^2 + \mathcal{O}(e_k^3) \quad | : f'(x_k) \neq 0$$

$$\underbrace{-\frac{f(x_k)}{f'(x_k)}}_{x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}} = e_k + \frac{1}{2} \frac{f''(x_k)}{f'(x_k)} e_k^2 + \mathcal{O}(e_k^3)$$

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We obtain

$$e_{k+1} = \alpha - x_{k+1} = \alpha - \left(x_k - \frac{f(x_k)}{f'(x_k)} \right) = \underbrace{\alpha - x_k}_{e_k} + \frac{f(x_k)}{f'(x_k)} \quad \Rightarrow$$

$$e_{k+1} = e_k + \frac{f(x_k)}{f'(x_k)} = e_k - e_k - \frac{1}{2} \frac{f''(x_k)}{f'(x_k)} \cdot e_k^2 + \mathcal{O}(e_k^3)$$

Thus,

$$e_{k+1}^1 = -\frac{1}{2} \frac{f''(x_k)}{f'(x_k)} \cdot e_k^2 + \mathcal{O}(e_k^3), \quad \Rightarrow$$

the method converges quadraticaly, i.e., the number of correct decimal places doubles with each iteration.

Remark Let us recall that $\mathcal{O}(e_k^3)$ characterizes the remainder of Taylor's expansion of f at x_k:

$$\exists const. \; \alpha > 0, A > 0 : |\text{reminder}| \leq A \cdot e_k^3 \; \forall |e_k| < \alpha \, .$$

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Newton method

★ **Examples for practicing**

1. Verify that the interval $\langle 1, \sqrt{3} \rangle$ is the separation interval for solution of the equation

$$x + \arctan x - 2 = 0 \,,$$

and that at this interval, the Newton method can be used to solve this equation. Select the zero approximation x_0 and calculate at least one other approximation of the root.

2. Verify that the interval $\langle \frac{\pi}{2}, \pi \rangle$ is the separation interval for solution of the equation

$$x = 6 \sin x \,,$$

and that at this interval, the Newton method can be used to solve this equation. Select the zero approximation x_0 and calculate at least one other approximation of the root. How many other solutions does this equation have?

3. Use an appropriate figure to find out how many roots has the equation

$$x \ln x - 3 = 0$$

and for the smallest root specify a separation interval of a length of at most 1 and the initial approximation x_0 for the Newton method. Calculate at least one additional approximation by the Newton method.

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Numerical solution of systems of nonlinear equations

A very common problem arising when dealing with practical problems in chemical engineering is the task to find n unknowns $x_1, x_2, \ldots, x_n$, which satisfy the following system of nonlinear equations:

$$
\begin{aligned}
f_1(x_1, x_2, \ldots, x_n) &= 0 \\
f_2(x_1, x_2, \ldots, x_n) &= 0 \\
&\vdots \\
f_n(x_1, x_2, \ldots, x_n) &= 0.
\end{aligned}
\tag{9}
$$

For solving of systems of nonlinear equations, there were developed several iterative methods of the type

$$
\mathbf{x}_{k+1} = \Phi(\mathbf{x}_k), \quad k = 0, 1, \ldots,
\tag{10}
$$

where $\mathbf{x}_k$ is the $k-$th aproximation of the vector of unknowns $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$. Newton's method is the most frequent one.

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Newton's method for systems of nonlinear equations

Newton's method for systems of nonlinear equations

Let us denote $\mathbf{f} = (f_1, \ldots, f_n)^{\mathrm{T}}$. We define Jacobi matrix of functions f_i (partial derivatives are evaluated at the point $\mathbf{x}$) as:

$$\mathbf{J}(\mathbf{x}) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \cdots & & \\ \vdots & & & \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_n}{\partial x_n} \end{pmatrix}. \tag{11}$$

For Newton's method, we choose in the equation (10) Φ as

$$\Phi(\mathbf{x}) = \mathbf{x} - \lambda \mathbf{J}^{-1}(\mathbf{x})\mathbf{f}(\mathbf{x}).$$

Thus,

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \lambda_k \mathbf{J}^{-1}(\mathbf{x}_k)\mathbf{f}(\mathbf{x}_k). \tag{12}$$

We multiply the equation (12) by the matrix $\mathbf{J}(\mathbf{x}_k)$ and we obtain the final form of the Newton method, as it is practically used:

$$\mathbf{J}(\mathbf{x}_k)\triangle\mathbf{x}_k = -\mathbf{f}(\mathbf{x}_k) \tag{13}$$

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \lambda_k\triangle\mathbf{x}_k. \tag{14}$$

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Newton's method for systems of nonlinear equations

Remarks

- The relation (13) is a system of *n* linear algebraic equations for *n* unknowns (increments) $\triangle \mathbf{x}_k$. This system we solve by linear algebra methods.

- We usually choose $\lambda_k = 1$ but we test whether the residua have been reduced, i.e., weather

$$\sum_{i=1}^{n} f_i^2(\mathbf{x}_{k+1}) < \sum_{i=1}^{n} f_i^2(\mathbf{x}_k).$$

  If this condition is not satisfied, we diminish λ_k.

- The Newton method for the system of equations is also the method of the second order. The method converges to the root $\mathbf{x}^*$ for which $\mathbf{J}(\mathbf{x}^*)$ is regular under the condition that the initial approximation $\mathbf{x}_0$ is chosen close enough to this root $\mathbf{x}^*$.

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Geometric concept in $\mathbb{R}^2$

Geometric concept in $\mathbb{R}^2$

Let us consider a system of two equations for two unknowns x, y:

$$
\begin{aligned}
f_1(x, y) &= 0, \\
f_2(x, y) &= 0.
\end{aligned}
$$

Let (x_k, y_k) be an approximation of the root (α, β).

At the point $(x_k, y_k, f_1(x_k, y_k))$ we construct the tangent plane to the graph of the function $f_1(x, y)$ and similarly, at the point $(x_k, y_k, f_2(x_k, y_k))$ we construct the tangent plane to the graph of the function $f_2(x, y)$.

These two tangent planes intersect the plane $z = 0$ in two lines of the intersection.

The intersection of these lines is the next approximation (x_{k+1}, y_{k+1}) of the root (α, β).

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Example

★ **Example**

Let us solve the following system of nonlinear equations:

$$\begin{aligned} f_1(\mathbf{x}) &= 16x_1^4 + 16x_2^4 + x_3^4 - 16 = 0 \\ f_2(\mathbf{x}) &= x_1^2 + x_2^2 + x_3^2 - 3 = 0 \\ f_3(\mathbf{x}) &= x_1^3 - x_2 = 0. \end{aligned} \qquad (15)$$

Let us choose the initial approximation $\mathbf{x}_0 = (1, 1, 1)$.
Then

$$\mathbf{f}(\mathbf{x}_0) = \begin{pmatrix} 17 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{J}(\mathbf{x}_0) = \begin{pmatrix} 64 & 64 & 4 \\ 2 & 2 & 2 \\ 3 & -1 & 0 \end{pmatrix},$$

$$\mathbf{x}_1 = \mathbf{x}_0 - \mathbf{J}^{-1}(\mathbf{x}_0)\mathbf{f}(\mathbf{x}_0) = \left(\frac{223}{240}, \frac{63}{80}, \frac{79}{60} \right).$$

For clarity, all iterations are listed in the following table. The fourth approximation has already the precision to six decimal places.

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Example

Iterations in the Example(15)

Newton's method for system (15)

k	$x_1^{(k)}$	$x_2^{(k)}$	$x_3^{(k)}$	$f_1(\mathbf{x}_k)$	$f_2(\mathbf{x}_k)$	$f_3(\mathbf{x}_k)$
0	1	1	1	17	0	0
1	0, 929167	0, 787500	1, 283333	4, 791917	0, 130451	0, 014697
2	0, 887075	0, 693176	1, 320865	0, 645310	0, 012077	0, 004864
3	0, 878244	0, 677195	1, 330610	0, 001845	0, 000428	0, 000207
4	0, 877966	0, 676757	1, 330855	0, 000015	0, 000000	0, 000000
5	0, 877966	0, 676757	1, 330855	0, 000000	0, 000000	0, 000000

Recommended literature

- Kubíček M., Dubcová M., Janovská D.: Numerical Methods and Algorithms, http://old.vscht.cz/mat/Ang/NM-Ang/NM-Ang.pdf
- Rasmuson A., Andersson B., Olsson L., Andersson R.: Mathematical Modeling in Chemical Engineering. Cambridge University Press, 2014.
- Recktenwald G.: Numerical Integration of Ordinary Differential Equations for Initial Value Problems. Portland State University 2007, gerry@me.pdx.edu.
- Shampine L. F., Allen R, C, Jr., and Pruess S.: Fundamentals of Numerical Computing. J. Wiley, New York 1997.
- Upreti S. R.: Process Modeling and Simulation for Chemical Engineers. John Wiley & Sons Ltd. 2017.