Nonlinear Algebraic Equations Example

Continuous Stirred Tank Reactor (CSTR).

Look for steady state concentrations & temperature.

In: N_s spieces with concentrations $c_i^{(in)}$,

heat capacities $c_{p,i}^{(in)}$ and temperature $T^{(in)}$

Inside: N_r reactions with stoichiometric coefficients $\sigma_{\alpha,i}$

and reaction constants r_α.

Out: N_s spieces with concentrations $c_i^{(in)}$

(c-s may be equal to zero),

heat capacities $c_{p,i}$ and temperature T.

Nonlinear Algebraic Equations Example

$$(F/V)\left[c_i^{(in)} - c_i\right] + \sum_{\alpha=1}^{N_r} \sigma_{\alpha,i} r_\alpha = 0 \qquad i = 1, 2, \ldots, N_s$$

Mass balance for spieces $1, 2, \ldots, N_s$

$$(F/V)\sum_{i=1}^{N_s}\left[c_i^{(in)} c_{p,i}^{(in)} T^{(in)} - c_i c_{p,i} T\right] - \sum_{\alpha=1}^{N_r} \Delta H_\alpha r_\alpha = 0$$

Energy balance

Column of unknown variables : $x = [c_1, c_2, \ldots, c_{N_s}, T]^T$

Nonlinear Algebraic Equations Example

Each of the above equations may be written in the general form:

$f_i(x_1, x_2, ..., x_N) = 0$:

$$f_1(x_1, x_2, ..., x_N) = 0$$
$$f_2(x_1, x_2, ..., x_N) = 0$$
$$...$$
$$f_N(x_1, x_2, ..., x_N) = 0$$

In vector form:

f(x)=0

$$f(x)=\begin{bmatrix} f_1(x) \\ f_2(x) \\ ... \\ f_N(x) \end{bmatrix}$$

Let $\hat{x}$ be the solution staisfying f(x)=0.

We do not know $\hat{x}$ and take $x^{[0]}$ as initial guess.

Nonlinear Algebraic Equations

We need to form a sequence of estimates to the solution:

$x^{[1]}, x^{[2]}, x^{[3]}, \ldots$ that will hopehully converge to $\hat{x}$.

Thus we want: $\lim_{m\to\infty} x^{[m]} = \hat{x}$

$$\lim_{m\to\infty} \left\| \hat{x} - x^{[m]} \right\| = 0$$

Unlike with linear equations, we can't say much about existence or uniqueness of solutions, even for a single equation.

Single Nonlinear Equation

We assume f(x) is infinitely differentiable at the solution $\hat{x}$.

Then f(x) may be Taylor expanded around $\hat{x}$:

$$f(x) = f(\hat{x}) + (x - \hat{x})f'(x) + \frac{1}{2}(x - \hat{x})^2 f''(x) + \frac{1}{3!}(x - \hat{x})^3 f'''(x) + \ldots$$

Assume $x^{[0]}$ being close to $\hat{x}$ so that the series may be truncated:

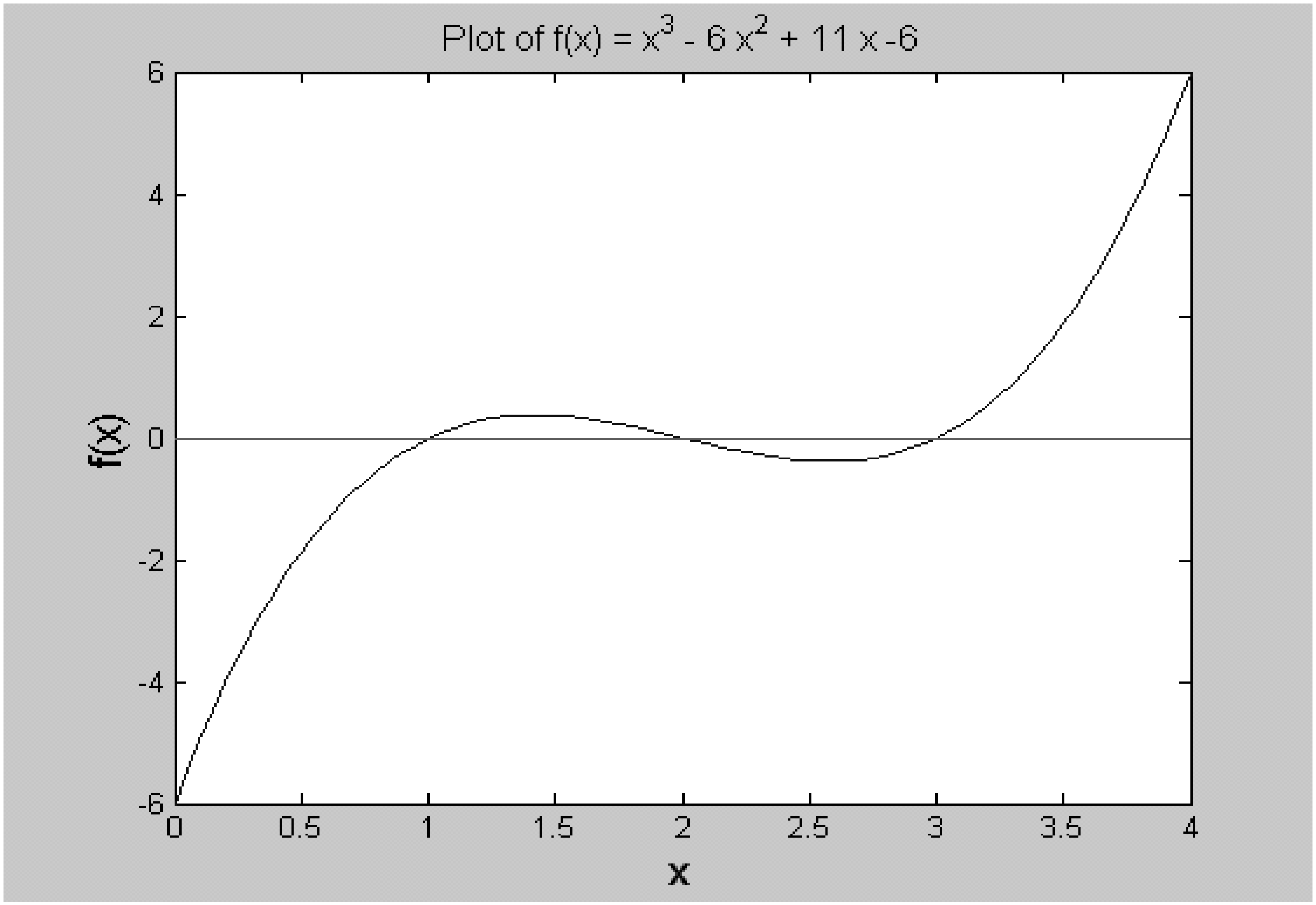
$$f(x^{[0]}) \approx (x^{[0]} - \hat{x})f'(x^{[0]}), \quad \text{or}$$

$$f(x^{[0]}) \approx (x^{[0]} - x^{[1]})f'(x^{[0]}) \qquad x^{[1]} = x^{[0]} - \frac{f(x^{[0]})}{f'(x^{[0]})} -$$

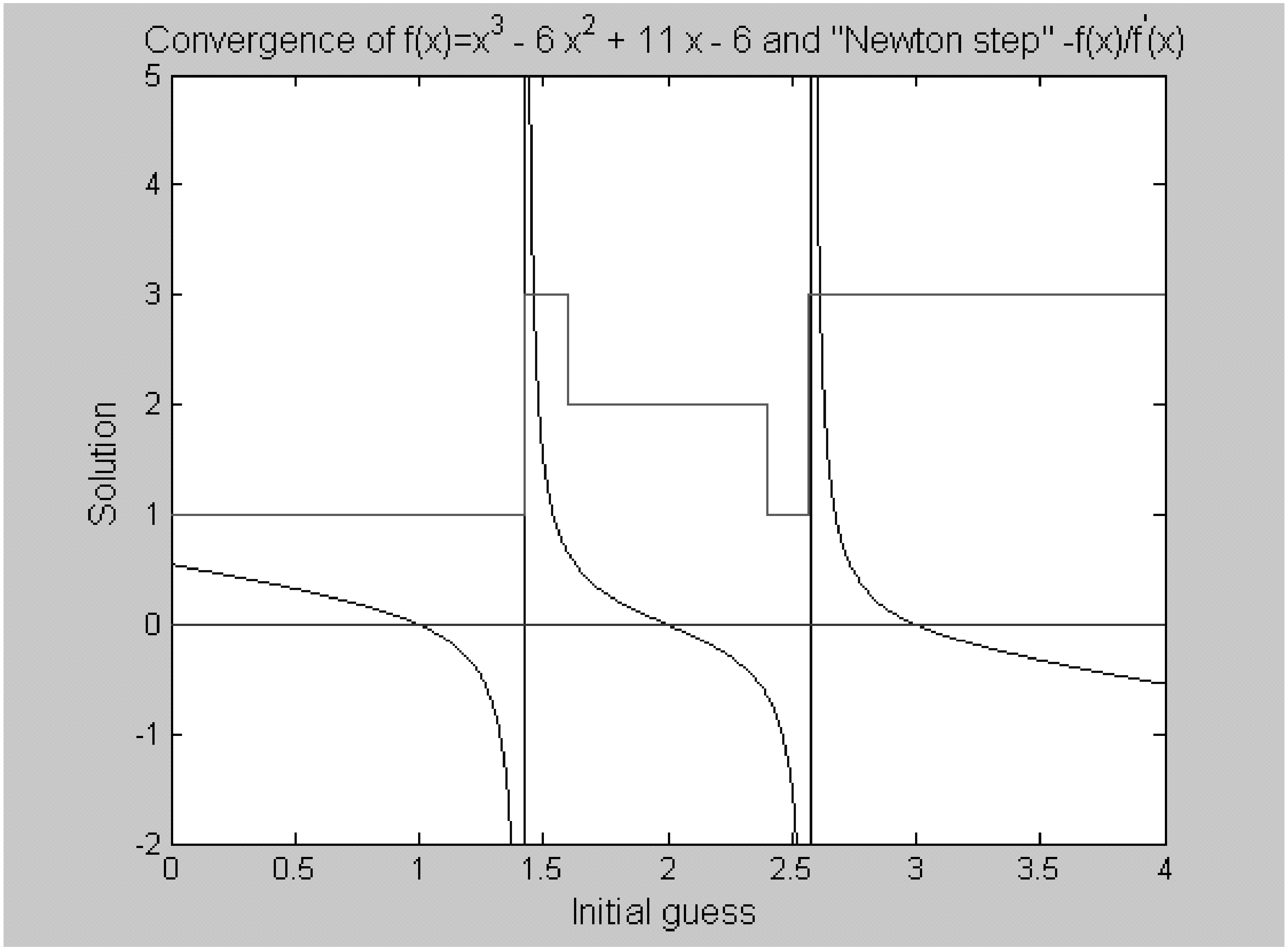
– Newton's method

$$\text{Example}: f(x) = (x-3)(x-2)(x-1) = x^3 - 6x^2 + 11x - 6$$

Single Nonlinear Equation



Single Nonlinear Equation



Single Nonlinear Equation

For $f(x)=(x-3)(x-2)(x-1)=x^3-6x^2+11x+6=0$, we se that Newton's method converges to the root at x=2 only if $1.6<x^{[0]}<2.4$.

We may look at the direction of the first step and see why: $x^{[1]}- x^{[0]}=-f(x^{[0]})/ f'(x^{[0]})$.

So, we have 2 "easy" roots: x=1, x=3 and a more difficult one.

We may "factorize out" the roots we already know.

Single Nonlinear Equation

Introduce $g(x) = \frac{f(x)}{(x-3)(x-1)}$

$$g'(x) = \frac{f'(x)}{(x-3)(x-1)} - \frac{f(x)}{(x-3)(x-1)}\left(\frac{1}{(x-3)} + \frac{1}{(x-1)}\right)$$

We now use Newton's method to find the roots of g(x):

$$x^{[i+1]} = x^{[i]} - \frac{g(x)}{g'(x)} \quad \rightarrow \text{ get } x = 2.$$

Systems of Nonlinear Equations

Let's extend the method to multiple equations:

$f_1(x_1,x_2,x,\ldots,x_N)=0$

$f_2(x_1,x_2,x,\ldots,x_N)=0$ => $f(x)=0$

….. Start from initial guess $x^{[0]}$

$f_N(x_1,x_2,x,\ldots,x_N)=0$

As before expand each equation at the solution $\hat{x}$ with $f(\hat{x})=0$:

$$f_i(x) = f_i(\hat{x}) + \sum_{j=1}^{N}(x_j - \hat{x}_j)\frac{\partial f_i(\hat{x})}{\partial x_j} + \frac{1}{2}\sum_{j=1}^{N}\sum_{k=1}^{N}(x_j - \hat{x}_j)\frac{\partial^2 f_i(\hat{x})}{\partial x_j \partial x_k}(x_k - \hat{x}_k) + \ldots$$

Assume $x^{[0]}$ is close to $\hat{x}$ and discard quadratic terms:

$$f_i(x) \approx \sum_{j=1}^{N}(x_j - \hat{x}_j)\frac{\partial f_i(\hat{x})}{\partial x_j}$$

Systems of Nonlinear Equations

Let 's define the Jacobian matrix $J(\hat{x})$ with the elements:

$$J_{ij}(\hat{x}) = \frac{\partial f_i(\hat{x})}{\partial x_j}$$

Then our approximate expansion may be written as:

$$f_i(x) \approx \sum_{j=1}^{N} J_{ij}(\hat{x})(x_j - \hat{x}_j) = \left(J(\hat{x})(x - \hat{x}) \right)_i$$

This gives us the linear system:

$$f(x) \approx J(\hat{x})(x - \hat{x})$$

Systems of Nonlinear Equations

$$f(x^{[i]}) = J(x^{[i]})(x^{[i]} - x^{[i+1]}) = \left(J(\hat{x})(x - \hat{x}) \right)_i$$

Note, Jacobian is evaluated at the position of an old iteration, not at an unknown solution

Defining $\Delta x^{[i]} = x^{[i+1]} - x^{[i]}$, we rewrite the equation as

$J(x^{[i]})\Delta x^{[i]} = -f(x^{[i]})$ or just $J^{[i]}\Delta x^{[i]} = -f^{[i]}$

The iterations are continued untill some convergence criteria are met:

relative error $\left\| f^{[i]} \right\| \le \delta_{rel} \left\| f^{[0]} \right\|$

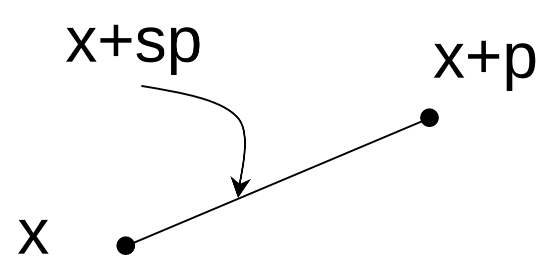
absolute error $\left\| f^{[i]} \right\| \le \delta_{abs}$

Systems of Nonlinear Equations

Newton's method does not always converge. If it does, can we estimate the error?

Let our function f(x) be continuously differentiable in the vicinity of x and the vector connecting x and x +p all lies inside this vicinity.

$$J(x+sp) = \left.\frac{\partial f}{\partial x^T}\right|_{x+sp}$$



$$f(x+p) = f(x) + \int_0^1 J(x+sp)\, p\, ds$$

– use path integral along the line x - x+p, parametrized by s.

Systems of Nonlinear Equations

Add and subtract J(x)p to RHS:

$$\underbrace{f(x+p) = f(x) + J(x)\,p}_{} + \int_0^1 \left[J(x+sp) - J(x)\right] p\, ds$$

In Newton's method we ignore the integral term and choose p to estimate f(x+p). Thus the error in this case is:

$$\int_0^1 \left[J(x+sp) - J(x)\right] p\, ds = f(x+p)$$

What is the upper bound on this error?

f(x) and J(x) are continuous:

$\left\| J(x+sp)\text{-}J(x) \right\| \rightarrow 0$ as $p \rightarrow 0$ for all $0 \le s \le 1$.

Systems of Nonlinear Equations

The norm of the matrix is defined as: $\|A\| = \max\limits_{v \neq 0} \dfrac{\|Av\|}{\|v\|}$,

so for any y $\|A\| \geq \dfrac{\|Ay\|}{\|y\|}$, or $\|Ay\| \leq \|A\| \|y\|$, therefore

$$\left\| \int_0^1 \left[J(x+sp) - J(x) \right] p \, ds \right\| \leq \left\| \int_0^1 \left[J(x+sp) - J(x) \right] ds \right\| \|p\|$$

The error goes down at least as fast as $\|p\|$ because for a continuous Jacobian $\|J(x\text{+}sp)\text{-}J(x)\| \to 0$ as $p \to 0$.

Systems of Nonlinear Equations

If we suggest that there exist some L>0 such that

$$\left\| J(y)\text{-}J(z) \right\| \le L \left\| y - z \right\|$$

or there is some upper bound on the "stretching" effect of J.

$$\left\| f(x+sp) \right\| = \left\| \int_0^1 [J(x+sp) - J(x)]p\, ds \right\| \le \left\| \int_0^1 [J(x+sp) - J(x)]\, ds \right\| \left\| p \right\|$$

and $\left\| \int_0^1 [J(x+sp) - J(x)]\, ds \right\| \le L|s|\left\| p \right\|$, so in this case

$$\left\| f(x+sp) \right\| = \left\| \int_0^1 [J(x+sp) - J(x)]\, pds \right\| \le \left(L|s|\left\| p \right\| \right) \left\| p \right\|$$

$$\le \left(L|s| \right) \left\| p \right\|^2 = O\left(\left\| p \right\|^2 \right)$$

Systems of Nonlinear Equations

Thus if we are at distance p from the solution, our error scales as $||p||^2$.

What about convergence? How the error scales with the number of iterations?

The answer is:

$$\left\| x^{[i+1]} - \hat{x} \right\| = O\left(\left\| x^{[i]} - \hat{x} \right\|^2 \right)$$ - local quadratic convergence,

a very fast one! Works when you are close enough to the solution.

Systems of Nonlinear Equations

$$\left\| x^{[i]} - \hat{x} \right\| \sim 0.1 = 10^{-1}$$

$$\left\| x^{[i+1]} - \hat{x} \right\| \sim 0.01 = 10^{-2}$$

$$\left\| x^{[i+2]} - \hat{x} \right\| \sim 0.00001 = 10^{-4}$$

$$\left\| x^{[i+3]} - \hat{x} \right\| \sim 0.000000001 = 10^{-8}$$

Works if we are close enough to an isolated (non-singular) solution: $\det\left[J(\hat{x}) \right] \neq 0.$

Systems of Nonlinear Equations, Example

Let's examine how Newton's method works for a simple system:

$$f_1 = 3x_1^3 + 4x_2^2 - 145 = 0 \qquad \hat{x} = \begin{bmatrix} 3 \\ 4 \end{bmatrix}$$
$$f_2 = 4x_1^2 - x_2^3 + 28 = 0$$

The Jacobian is:

$$J = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 9x_1^2 & 8x_2 \\ 8x_1 & -3x_2^2 \end{bmatrix}$$

Systems of Nonlinear Equations, Example

At each step we have the following system to solve:

$$J^{[i]} = \begin{bmatrix} 9\left(x_1^{[i]}\right)^2 & 8x_2^{[i]} \\ 8x_1^{[i]} & -3\left(x_2^{[i]}\right)^2 \end{bmatrix}$$

$$f^{[i]} = \begin{bmatrix} 3\left(x_1^{[i]}\right)^3 + 4\left(x_2^{[i]}\right)^2 - 145 \\ 4\left(x_1^{[i]}\right)^2 - \left(x_2^{[i]}\right)^3 + 28 \end{bmatrix}$$

$$J^{[i]}\Delta x^{[i]} = -f^{[i]} \qquad x^{[i+1]} = x^{[i]} + \Delta x^{[i]}$$

Systems of Nonlinear Equations, Example

Let us examine performance of

Newton's method with the convergence

criterion $\|f\| = \max\{|f_1|, |f_2|\} < \delta_{abs}$

$\delta_{bs} = 10^{-10}$

Newton's Method

Newton's method works well close to the solution, but otherwise takes large erratic steps, shows poor performance and reliability.

Let's try to avoid such large steps: employ reduced step Newton's algorithm.

"Full" Newton's step gives $x^{[i+1]}=x^{[i]}+p^{[i]}$. We'll use only fraction of of the step: $x^{[i+1]}=x^{[i]}+\lambda_i\, p^{[i]}$, $0<\lambda_i<1$.

Newton’s Method

How do we choose λ_i ?
Simplest way - weak line search:
- start with $\lambda_i = 2^{-m}$ for m=0,1,2,…

As we reduce the value of λ_i bya a factor of 2 at each step, we accept the first one that satisfies a descent criterion: $\left\| f\left(x^{[i]} + \lambda_i p^{[i]}\right) \right\| < \left\| f\left(x^{[i]}\right) \right\|$

It can be proven that if the Jacobian is not singular, the correct solution will be found by the reduced step Newton’s algorithm.