Newton's method

For each iterate x_k, the function f is approximated by its tangent in x_k:

$$f(x) \approx f(x_k) + f'(x_k)(x - x_k)$$

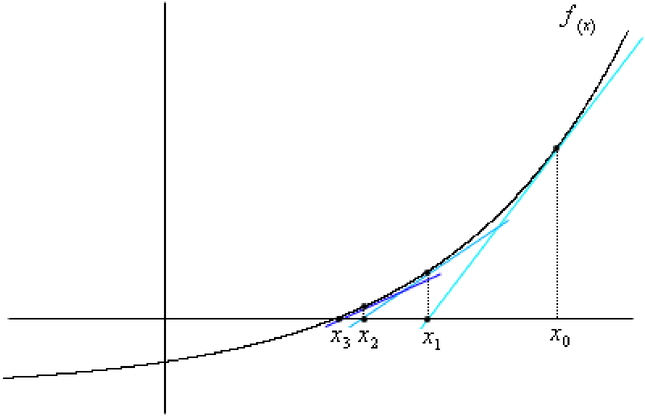
Then we impose that the right-hand side is 0 for $x = x_{k+1}$. Thus,

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$$

More assumptions needed on f:

- f must be differentiable, and f' must not vanish.
- the initial guess x_0 must be chosen well, otherwise the method might fail
- suitable stopping criteria have to be introduced to decide when to stop the procedure (no intervals here.......).

Example



Newton's method: Convergence theorem

Theorem

Let $f \in C^2([a,b])$ *such that:*

1. $f(a)f(b) < 0 \qquad (*)$
2. $f'(x) \neq 0 \quad \forall x \in [a,b] \qquad (**)$
3. $f''(x) \neq 0 \quad \forall x \in [a,b] \qquad (***)$

Let the initial guess x_0 *be a Fourier point (i.e., a point where* f *and* f'' *have the same sign). Then Newton sequence*

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} \qquad k = 0, 1, 2, \cdots \tag{1}$$

converges to the **unique** α *such that* $f(\alpha) = 0$*. Moreover, the order of convergence is* 2*, that is:*

$$\exists C > 0 : \quad |x_{k+1} - \alpha| \leq C|x_k - \alpha|^2. \tag{2}$$

Newton's method: Proof of the Theorem

Proof

Since f is continuous and has opposite signs at the endpoints then the equation $f(x) = 0$ has at least one solution, say α. Moreover condition (**) implies that α is unique (f is monotone).
To prove convergence, let us assume for instance that f is as follows: $f(a) < 0$, $f(b) > 0$, $f' > 0$, $f'' > 0$ (the other cases can be treated in a similar way), so that the initial guess x_0 is any point where $f(x_0) > 0$. We shall prove that Newton's sequence $\{x_n\}$ is a monotonic decreasing sequence bounded by below.

continue...

continuation of the proof

Use and evaluate in α the Taylor expansion centered in x_0, with Lagrange remainder[a]:

$$0 = f(\alpha) = f(x_0) + (\alpha - x_0)f'(x_0) + \underbrace{\frac{(\alpha - x_0)^2}{2} f''(z)}_{>0}$$

with z between α and x_0. Thus it holds

$$f(x_0) + (\alpha - x_0)f'(x_0) < 0 \qquad \text{i.e.} \qquad \alpha < x_0 - \frac{f(x_0)}{f'(x_0)} = x_1$$

Hence, $\alpha < x_1 < x_0$, implying, in particular, that $f(x_1) > 0$ so that x_1 is itself a Fourier point. Repeating the same argument as above we would get $\alpha < x_2 < x_1$, with $f(x_2) > 0$.

[a] see https://en.wikipedia.org/wiki/Taylor%27s_theorem#Explicit_formulas_for_the_remainder

continuation of the proof

Proceeding in this way we have

$$\alpha < x_k < x_{k-1} < \ldots < x_0$$

for all positive integer k.

Hence, $\{x_n\}$ being a monotonic decreasing sequence bounded by below, it has a limit, that is,

$$\exists\, \eta \quad \text{such that} \quad \lim_{k\to\infty} x_k = \eta.$$

Taking the limit in (1) for $k \to \infty$ (and remembering that both f and f' are continuous, and f' is always $\neq 0$), we have

$$\lim_{k\to\infty}(x_{k+1}) = \lim_{k\to\infty}\left(x_k - \frac{f(x_k)}{f'(x_k)}\right) \Longrightarrow \eta = \eta - \frac{f(\eta)}{f'(\eta)} \implies f(\eta) = 0$$

Then, η is a root of $f(x) = 0$, and since the root is unique, $\eta \equiv \alpha$.

continuation of the proof

It remains to prove (2). For this, use Taylor expansion centered in x_k, with Lagrange remainder

$$f(\alpha) = f(x_k) + (\alpha - x_k)f'(x_k) + \frac{(\alpha - x_k)^2}{2} f''(z), \quad z \text{ between } \alpha \text{ and } x_k.$$

Now: $f(\alpha) = 0$, $f'(x)$ is always $\neq 0$ so we can divide by $f'(x_k)$ and get

$$0 = \underbrace{\frac{f(x_k)}{f'(x_k)} - x_k}_{-x_{k+1}} + \alpha + \frac{(\alpha - x_k)^2}{2f'(x_k)} f''(z)$$

We found

$$0 = \underbrace{\frac{f(x_k)}{f'(x_k)} - x_k}_{-x_{k+1}} + \alpha + \frac{(\alpha - x_k)^2}{2f'(x_k)} f''(z)$$

end of the proof

that we re-write as

$$x_{k+1} - \alpha = \frac{(\alpha - x_k)^2}{2f'(x_k)} f''(z).$$

Thus,

$$|x_{k+1} - \alpha| = \frac{(\alpha - x_k)^2}{2} \frac{|f''(z)|}{|f'(x_k)|} \leq \frac{(\alpha - x_k)^2}{2} \frac{\max |f''(x)|}{\min |f'(x)|}$$

Therefore (2) holds with

$$C = \frac{\max |f''(x)|}{\min |f'(x)|}$$

which exists since both $|f'(x)|$ and $|f''(x)|$ are continuous on the closed interval, and $f'(x)$ is always different from zero.

Newton's method: Practical use of the theorem

The practical use of the above Convergence theorem is not easy.

• Often difficult, if not impossible, to check that all the assumptions are verified.

In practice, we interpret the Theorem as: *if x_0 is "close enough" to the (unknown) root, the method converges, and converges fast*.

• Suggestions: the graphics of the function (if available), and a few bisection steps help in locating the root with a rough approximation. Then choose x_0 in order to start Newton's method and obtain a much more accurate evaluation of the root.

If α is a multiple root ($f'(\alpha) = 0$) the method is in troubles.

Newton's method: Stopping criteria 1

Unlike with bisection method, here there are no intervals that become smaller and smaller, but just the sequence of iterates.
A reasonable criterion could be

- **test on the iterates**: stop at the first iteration n such that

$$|x_n - x_{n-1}| \leq Tol,$$

  and take x_n as "root".

This would work, unless the function is very **steep** in the vicinity of the root (that is, if $|f'(\alpha)| >> 1$): the tangents being almost vertical, two iterates might be very close to each other but not close enough to the root to make $f(x_n)$ also small, and the risk is to stop when $f(x_n)$ is still big.

Newton's method: Stopping criteria 2

In this situation it would be better to use the

- **test on the residual**: stop at the first iteration n such that

$$|f(x_n)| \leq Tol,$$

and take x_n as "root".

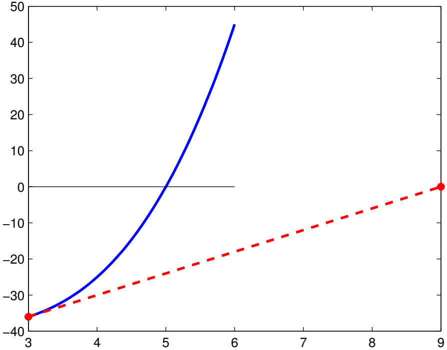
In contrast to the previous criterion, this one would fail if the function is very **flat** in the vicinity of the root (that is, if $|f'(\alpha)| << 1$). In this case $|f(x_n)|$ could be small, but x_n could still be far from the root.

What to do then??

Safer to use both criteria, and stop when both of them are verified.

Newton's method: Examples of choices of x_0

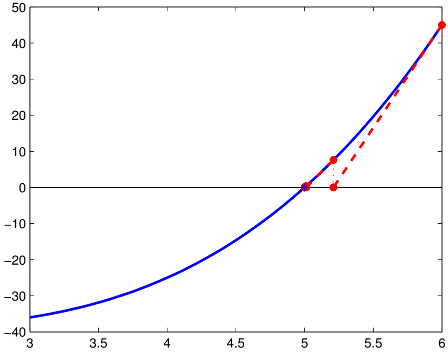
$$f(x) = x^3 - 5x^2 + 9x - 45 \quad \text{in } [3,6] \quad \alpha = 5$$



Bad x_0: $x_0 = 3 \Rightarrow x_1 = 9$ outside $[3,6]$

Newton's method: Examples of choices of x_0

$$f(x) = x^3 - 5x^2 + 9x - 45 \quad \text{in } [3,6] \quad \alpha = 5$$



Good x_0: 3 iterations with $Tol = 1.e-3$

Newton's method: Solution of nonlinear systems

We have to solve a system of N nonlinear equations:

$$\begin{cases} f_1(x_1, x_2, \cdots, x_N) = 0 \\ f_2(x_1, x_2, \cdots, x_N) = 0 \\ \qquad \vdots \\ f_N(x_1, x_2, \cdots, x_N) = 0 \end{cases}$$

or, in compact form,

$$\underline{F}(\underline{x}) = \underline{0},$$

having set

$$\underline{x} = (x_1, x_2, \cdots, x_N), \quad \underline{F} = (f_1, f_2, \cdots, f_N)$$

Newton method

We mimic what done for a single equation $f(x) = 0$: starting from an initial guess x_0 we constructed a sequence by linearizing f at each point and replacing it by its tangent, i.e., its Taylor polynomial of degree 1.

For systems we do the same:
starting from a point $\underline{x}^{(0)} = (x_1^{(0)}, x_2^{(0)}, \cdots, x_N^{(0)})$ we construct a sequence $\{\underline{x}^{(k)}\}$ by

- linearising $\underline{F}$ at each point through its Taylor expansion of degree 1:

$$\underline{F}(\underline{x}) \simeq \underline{F}(\underline{x}^{(k)}) + J_F(\underline{x}^{(k)})(\underline{x} - \underline{x}^{(k)})$$

- and then defining $\underline{x}^{(k+1)}$ as the solution of

$$\underline{F}(\underline{x}^{(k)}) + J_F(\underline{x}^{(k)})(\underline{x}^{(k+1)} - \underline{x}^{(k)}) = \underline{0}.$$

$J_F(\underline{x}^{(k)})$ is the **jacobian matrix** of $\underline{F}$ evaluated at the point $\underline{x}^{(k)}$:

$$J_F(\underline{x}) = \begin{bmatrix} \frac{\partial f_1(\underline{x})}{\partial x_1} \; \frac{\partial f_1(\underline{x})}{\partial x_2} \cdots\cdots \frac{\partial f_1(\underline{x})}{\partial x_N} \\ \frac{\partial f_2(\underline{x})}{\partial x_1} \; \frac{\partial f_2(\underline{x})}{\partial x_2} \cdots\cdots \frac{\partial f_2(\underline{x})}{\partial x_N} \\ \vdots \\ \vdots \\ \frac{\partial f_N(\underline{x})}{\partial x_1} \; \frac{\partial f_N(\underline{x})}{\partial x_2} \cdots\cdots \frac{\partial f_N(\underline{x})}{\partial x_N} \end{bmatrix},$$

System $\underline{F}(\underline{x}^{(k)}) + J_F(\underline{x}^{(k)})(\underline{x}^{(k+1)} - \underline{x}^{(k)}) = \underline{0}$ can obviously be written as: $\underline{x}^{k+1} = \underline{x}^{(k)} - (J_F(\underline{x}^{(k)}))^{-1}\underline{F}(\underline{x}^{(k)})$.
In the actual computation of $\underline{x}^{k+1}$ we **do not** compute the inverse matrix $(J_F(\underline{x}^{(k)}))^{-1}$, but we solve the system

$$J_F(\underline{x}^{(k)})\underline{x}^{k+1} = J_F(\underline{x}^{(k)})\underline{x}^{(k)} - \underline{F}(\underline{x}^{(k)}).$$

Newton's method: Algorithm

Given $\underline{x}^{(0)} \in \mathbb{R}^N$, for $k = 0, 1, \cdots$

solve $J_F(\underline{x}^{(k)})\underline{x}^{k+1} = J_F(\underline{x}^{(k)})\underline{x}^{(k)} - \underline{F}(\underline{x}^{(k)})$ by the following steps

- solve $J_F(\underline{x}^{(k)})\underline{\delta}^{(k)} = -\underline{F}(\underline{x}^{(k)})$
- set $\underline{x}^{(k+1)} = \underline{x}^{(k)} + \underline{\delta}^{(k)}$

At each iteration k we have to solve a linear system with matrix $J_F(\underline{x}^{(k)})$ (that is the most expensive part of the algorithm).

Note that by introducing the unknown $\underline{\delta}^{(k)}$ we pay an extra sum ($\underline{x}^{(k+1)} = \underline{x}^{(k)} + \underline{\delta}^{(k)}$) but we save the (much more expensive) matrix-vector multiplication $J_F(\underline{x}^{(k)})\underline{x}^{(k)}$.

Newton's method: Stopping criteria

They are the same two criteria that we saw for scalar equations:

- **test on the iterates**: stop at iteration k such that

$$\|\underline{x}^{(k)} - \underline{x}^{(k-1)}\| \leq Tol$$

for some vector norm, and take $\underline{x}^{(k)}$ as "root".

- **test on the residual**: stop at iteration k such that

$$\|\underline{F}(\underline{x}^{(k)})\| \leq Tol,$$

and take $\underline{x}^{(k)}$ as "root".

Here too, it would be wise in practice to use **both** criteria, and stop when both of them are satisfied.