Nonlinear equations and root-finding

Given a univariate function

$$f : \mathbb{R} \to \mathbb{R} \ ,$$

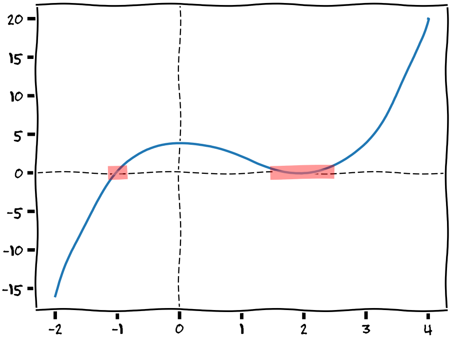
find x_* such that

$$f(x_*) = 0 \ .$$

Need to specify the problem: *all* roots or only some of them? (then which ones?) Real roots only or complex roots too (cf polynomials)?

Nonlinear equations and root-finding

Q: What does it mean that $f(x_*) = 0$ *numerically*?



Suppose that $f(x)$ is known with an uncertainty of Δ (e.g. roundoff)

$\exists\ \delta$ such that $|f(x)| < \Delta$ for $|x - x_*| \leqslant \delta$.

Nonlinear equations and root-finding

Assume $f(x)$ is differentiable at x_*. Then for x in the vicinity of x_*,

$$\begin{aligned} f(x) &= f(x_*) + f'(x_*)\,(x - x_*) + \dots \\ &= f'(x_*)\,(x - x_*) + \dots \end{aligned}$$

I.e.,

$$\delta = \frac{1}{|f'(x_*)|}\Delta$$

and any x such that $|x - x_*| \leqslant \delta x$ can be declated a root.

Notice that $1/|f'|$ serves as a *condition number*.

Q: $f'(x \to x_*) \to 0$?

Multiple roots

x_* is a *root of multiplicity* m if $f(x_*) = 0$ and $f^{(m)} \neq 0$ and

$$f'(x_*) = f''(x_*) = \cdots = f^{(m-1)}(x_*) = 0 \ .$$

For $m = 1$, x_* is called a *simple* root.

For $|x - x_*| \ll 1$

$$f(x) = 0 + \cdots + 0 + \frac{f^{(m)}(x_*)}{m!}(x - x)^m \ ,$$

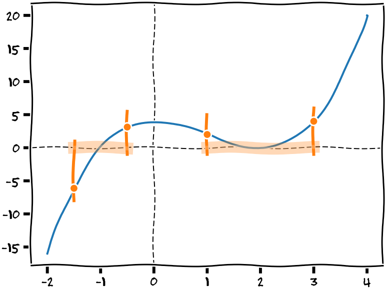
and

$$\delta = \left(\frac{m!}{|f^{(m)}|}\right)^{1/m} \Delta^{1/m} \ .$$

Solving non-linear equations

Proceed in two stages:

- Localization of roots. A root is localized on an interval $[a, b]$ if the interval contains only a single root.
- Iterative refinement (separately for each of the localization intervals.), until roots are localized to a predefined tolerance ϵ.



Bisection

Suppose that $f(x)$ is continuous on $[a, b]$. Let

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

Then there exist $x_* \in [a, b]$ such that $f(x_*) = 0$.

The main idea: Start with $a^{(0)} = a$ and $b^{(0)} = b$. Iteratively shrink the localization interval,

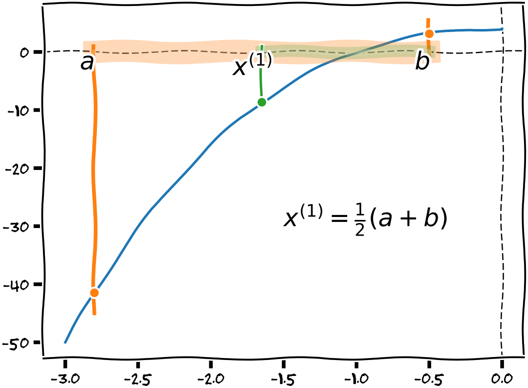
$$[a^{(n)}, b^{(n)}] \longrightarrow [a^{(n+1)}, b^{(n+1)}]$$

for $n = 0, 1, 2, \ldots$, until

$$|b^{(n)} - a^{(n)}| < \epsilon$$

for some *predefined* ϵ.

Bisection



Bisection

Clearly, *if* there is a root on $[a, b]$, bisection converges to it.

If there are several roots, bisection converges to one of them.

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If there are several roots, and x_* is found, one may try to separate it:

$$g(x) = \frac{f(x)}{x - x_*}$$

and repeat the process for $g(x)$.

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Q: What is the rate of convergence?

The rate of convergence

At each bisection step,

$$\begin{aligned} |b^{(n+1)} - a^{(n+1)}| &= \frac{1}{2}|b^{(n)} - a^{(n)}| \\ &= \frac{1}{2^{n+1}}|b - a| \end{aligned}$$

i.e., the localization interval shrinks as a geometric series with the common ratio of $1/2$.

Fixed-point iteration

Fixed-point iteration

Given $f(x) = 0$, rewrite it identically as

$$x = \phi(x)$$

So that

$$f(x_*) = 0 \qquad \Longleftrightarrow \qquad x_* = \phi(x_*)$$

There are multiple ways of constructing $\phi(x)$. The simplest one is

$$\phi(x) = x - f(x) \ .$$

Or $\phi(x) = x - \alpha\, f(x)$, where α is arbitrary. (More below)

Fixed-point iteration

Start from some $x^{(0)}$, and iterate

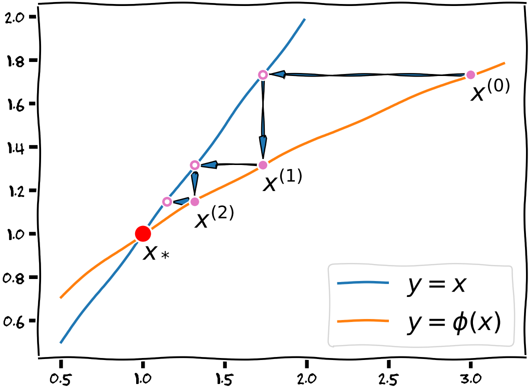
$$x^{(n+1)} = \phi\left(x^{(n)}\right) \ , \qquad n = 0, 1, 2, \ldots$$

If the limit

$$\lim_{n\to\infty} x^{(n)} = x_*$$

exists, then

$$x_* = f(x_*)$$



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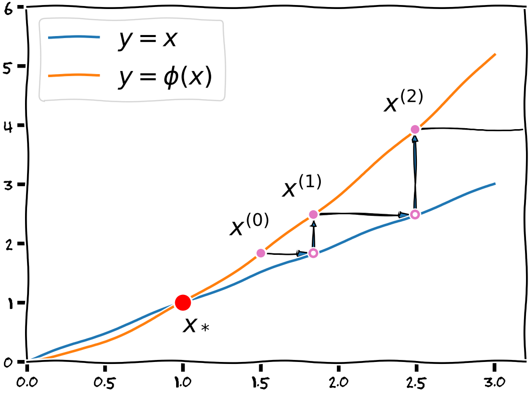

Fixed-point iteration

- What are the convergence criteria?
- What is the rate of convergence?
- What is the condition number?

Detour: The rate of convergence.
Some definitions and useful results.

The rate of convergence

Consider a sequence

$$x^{(0)}, x^{(1)}, \dots, x^{(n)}, \dots ,$$

Unless specified otherwise, we will assume that $x^{(n)}$ only depends on $x^{(n-1)}$.

Define $x_* \equiv \lim_{n\to\infty} x^{(n)}$, if this limit exists.

Definition: The sequence $\{x^{(n)}\}$ converges with a rate of a geometric series with a common ratio q, $0 < q < 1$, if

$$|x^{(n)} - x_*| \leqslant \text{const} \times q^n$$

for all n.

The rate of convergence

Define $U = \{x : |x - x_*| < R\}$.

Suppose that a sequence $\{x^{(n)}\}$ is such that for all $x^{(n)} \in U$

$$|x^{(n+1)} - x_*| \leqslant q \times |x^{(n)} - x_*|^p \ .$$

where $0 < q < 1$ and $p \geqslant 1$ are constants.

Definition: p is called the *rate of convergence*.

If $p = 1$, the convergence is *linear*; $p > 1$: *superlinear* convergence.

The rate of convergence

Lemma A. Suppose that the sequence $\{x^{(n)}\}$ is linearly convergent in a some region $U = \{x : |x - x_*| < R\}$. Then for all $x^{(0)} \in U$

1. $x^{(n)} \in U$ for all n;
2. the sequence converges with the rate of a geometric series with the common ratio q;
3. the following error bound holds for $n \geqslant 0$:

$$\left|x^{(n)} - x_*\right| \leqslant q^n \left|x^{(0)} - x_*\right| .$$

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Clearly, item 2 follows from 3. Item 1 also follows from 3 since $q < 1$.

Proof of Lemma A

Establish the error bound by induction.

base of induction: take $n = 0$.
The error bound obviously holds.

inductive step: suppose the error bound holds for $n - 1$. Then

$$
\begin{aligned}
|x^{(n)} - x_*| &\leqslant q\,|x^{(n-1)} - x_*| && \text{linear convergence} \\
&\leqslant q\,q^{n-1}\,|x^{(0)} - x_*| && \text{assumption} \\
&= q^n\,|x^{(0)} - x_*|
\end{aligned}
$$

Back to the fixed-point iteration

$$x = \phi(x) \quad \Longrightarrow \quad x^{(n+1)} = \phi(x^{(n)}) \;, \quad n \geqslant 0 \;.$$

Theorem 1: Suppose that in some neighborhood U of the root x_*, the right-hand side $\phi(x)$ is differentiable and the derivative is bounded:

$$|\phi'(x)| \leqslant q \;,$$

with $0 \leqslant q < 1$.

Then $\forall\, x^{(0)} \in U$

- $x^{(n)} \in U$ for all $n \geqslant 0$;
- the sequence converges with the rate of a geometric series;
- $$|x^{(n)} - x_*| \leqslant q^n \, |x^{(0)} - x_*| \;.$$

Proof of theorem 1

We use the mean value theorem

$$\begin{aligned} x^{(n+1)} - x_* &= \phi(x^{(n)}) - \phi(x_*) \\ &= \phi'(\xi)\,(x^{(n)} - x_*) \qquad \text{mean value theorem} \end{aligned}$$

where $\xi \in [x^{(n+1)}, x_*]$.

By assumption, $|\phi'(\xi)| \leqslant q$, thus

$$|x^{(n+1)} - x_*| \leqslant q|x^{(n)} - x_*| \ ,$$

and the theorem follows from Lemma A.

When to stop iterations: *a priori* vs *a posteriori*

We want to find the fixed point, $x_* = \phi(x_*)$ with an absolute tolerance ϵ.
We construct a sequence $x^{(n+1)} = \phi\left(x^{(n)}\right)$, with $n = 0, 1, 2, \ldots$.

Q: When do we stop? How do we know that we have achieved the target tolerance?

Theorem 1 gives an *a priori* error bound. But we do not know x_*.

We need an *a posteriori* error bound.

The *a posteriori* error bound

Theorem 2: Suppose that Theorem 1 holds, and the starting point $x^{(0)} \in U$. Then,

$$|x^{(n)} - x_*| \leqslant \frac{q}{1-q} \left| x^{(n)} - x^{(n-1)} \right| , \qquad n \geqslant 1$$

Roughly speaking, the l.h.s. is what we need to achieve, and the r.h.s. is what we have when iterating.

Proof of Theorem 2

Using the mean value theorem,

$$
\begin{aligned}
x^{(n)} - x_* &= \phi\left(x^{(n-1)}\right) - \phi(x_*) \\
&= \phi'(\xi)\,\left(x^{(n-1)} - x_*\right)\ , \qquad \text{with} \quad \xi \in [x^{(n-1)}, x_*] \\
&= \phi'(\xi)\,\left(x^{(n-1)} - x^{(n)}\right) + \phi'(\xi)\,\left(x^{(n)} - x_*\right)
\end{aligned}
$$

Therefore,

$$
x^{(n)} - x_* = \frac{\phi'(\xi)}{1 - \phi'(\xi)}\,\left(x^{(n-1)} - x^{(n)}\right)
$$

And,

$$
\left|x^{(n)} - x_*\right| \leqslant \frac{q}{1-q}\,\left|x^{(n-1)} - x^{(n)}\right|\ .
$$

The stopping criterion

Therefore, to achieve $\left|x^{(n)} - x_*\right| \leqslant \epsilon$, we stop when

$$\left|x^{(n-1)} - x^{(n)}\right| \leqslant \frac{1-q}{q}\epsilon \ .$$

In practice, we often drop the factor in the r.h.s., and use simply

$$\left|x^{(n-1)} - x^{(n)}\right| \leqslant \epsilon \ .$$

This is justified as long as $q < 1/2$, since then $(1-q)/q > 1$.

Fine-tuning the fixed-point function

The key ingredient is converting the original equation $f(x) = 0$ into the equivalent one, $x = \phi(x)$. We use

$$\phi(x) = x - \alpha\, f(x)$$

where α is an arbitrary constant.

Fixed-point iterations converge if $|\phi'(x)| \leqslant q < 1$.

Idea: choose α to minimize q.

Fine-tuning the fixed-point function

Suppose that $f(x)$ is continuously differentiable on the localization interval $[a, b]$.

Further, suppose that for $x \in [a, b]$

$$m \leqslant f'(x) \leqslant M$$

for some constants $m \geqslant 0$ and M.

Then,

$$|\phi'(x)| \leqslant q(\alpha) = \max_{\alpha} \left(|1 - \alpha\, m|, |1 - \alpha\, M|\right)$$

The best value of $\alpha = 2/(m + M)$, so that $q(\alpha) = \dfrac{M - m}{M + m}$.

Fixed-point iteration and Newton's method

In fact, α need not be constant.

Consider the fixed-point function

$$\phi_N(x) = x - \frac{f(x)}{f'(x)} \ ,$$

so that the iterations have the form

$$x^{(n+1)} = x^{(n)} - \frac{f(x^{(n)})}{f'(x^{(n)})} \ .$$

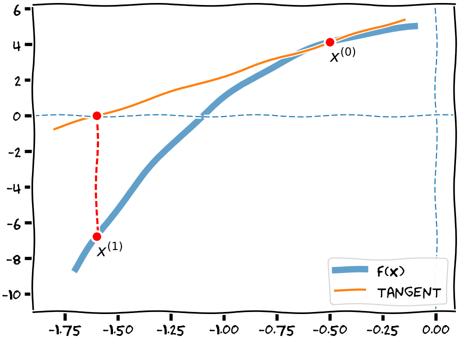
Newton’s method

Newton's method

The equation of the tangent line to $f(x)$ at $x^{(n)}$ is

$$y = \left(x - x^{(n)}\right)\ f'(x^{(n)}) + f(x^{(n)})\ .$$

We take as $x^{(n+1)}$ the zero crossing of the tangent line.



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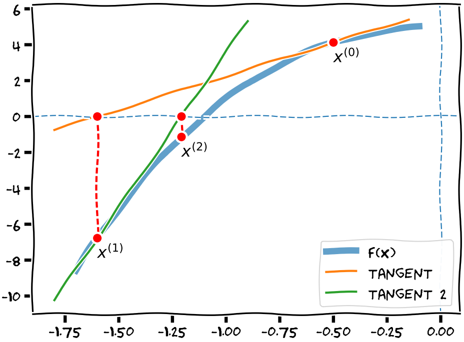


Newton's method: the rate of convergence

Theorem 1 asserts linear convergence for fixed-point iterations, including the Newton's method.

Convergence is controlled by $\phi'(x)$ for $x \in U$.

However,

$$\phi_N'(x) = f(x)\frac{f''(x)}{f'(x)^2} \to 0 \qquad \text{as} \quad x \to x_* \ ,$$

so that we can expect a *superlinear* convergence.

Newton's method: The rate of convergence

Theorem N: Let x_* is a simple real root of $f(x)$. Let $f'(x) \neq 0$ for all $x \in U = \{|x - x_*| < R\}$.
Futher, suppose that $f''(x)$ is continuous for $x \in U$, and

$$q = \frac{M_2}{2m_1} |x_0 - x_*| < 1 \, ,$$

where

$$0 < m_1 = \min_{x \in U} |f'(x)| \, , \qquad M_2 = \max_{x \in U} |f''(x)|$$

Then for $x_0 \in U$, the Newton's method converges to x_*, and

$$|x^{(n)} - x_*| \leqslant q^{2n-1} |x_0 - x_*| \, .$$

Newton's method: Quadratic convergence

To lighten the notation, define $\delta_n \equiv x^{(n+1)} - x_*$, and $f' \equiv f'(x_*)$, $f'' \equiv f''(x_*)$. Assume that $f''(x)$ exists and is continuous for $x \in U$.

For $\delta \ll 1$, use Taylor expansions around x_*:

$$
\begin{aligned}
f(x) &= 0 + f'\,\delta + f''\,\frac{\delta^2}{2} + \dots \\
f'(x) &= f' + f''\,\delta + \dots
\end{aligned}
$$

Newton's method: Quadratic convergence

Then the Newton's iteration takes the form

$$\begin{aligned}
\delta_{n+1} &= \delta_n - \frac{f(x_n)}{f'(x_n)} \\
&= \delta_n - \delta_n \frac{f' + f''\,\dfrac{\delta_n}{2} + \dots}{f' + f''\,\delta_n + \dots} \\
&= \delta_n \frac{f' + f''\,\delta_n - (f' + f''\,\dfrac{\delta_n}{2}) + \dots}{f' + f''\,\delta_n + \dots} \\
&= \delta_n^2\,\frac{f''}{2f'} + \dots
\end{aligned}$$

Newton's method: local convergence only

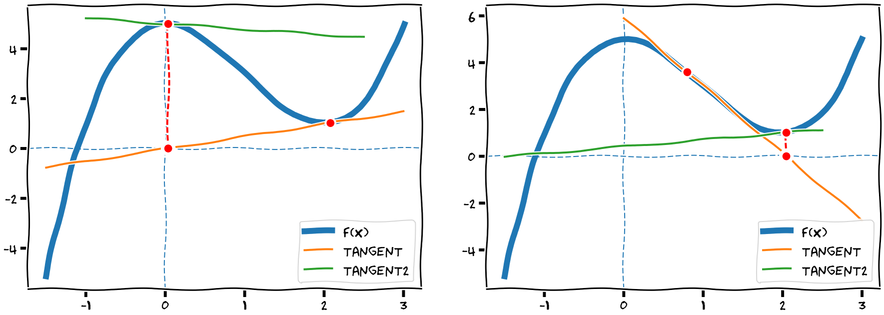
Practical matters for using the Newton's method:

- Need to be able to compute the derivative $f'(x)$.
- The starting point needs to be close to x_*. Note that Theorem N relates x_0 and bounds on both first and second derivatives.
- Localization interval is not honored.

In practice, it's best suited for *polishing* roots obtained by some other method.

Newton's method: local convergence only

$$f(x) = x^3 - 3x^2 + 5\ .$$



For $0 < x_0 < 2$, it may or may not converge.

In the complex plane, *basins of attraction* of the roots are fractal.

Multiple roots

Modified Newton's method

Multiple roots

Let x_* is a double root, i.e. $f(x_*) = f'(x_*) = 0$ and $f''(x_*) \neq 0$.

What is the rate of convergence of the Newton's iteration?

The previous estimate, $\delta_{n+1} = \delta_n^2 \dfrac{f''}{2f'}$, breaks down because the denominator is zero.

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The leading order of the Taylor expansion becomes

$$\delta_{n+1} = \delta_n - \frac{f'' \dfrac{\delta_n^2}{2} + \dots}{f'' \, \delta_n + \dots}$$

so that the convergence is only *linear*.

Multiple roots: modified Newton's method

Let x_* is an m-fold root.

Suppose $f(x)$ is $m+1$ times continuously differentiable.

The *modified Newton's method*

$$x^{(n+1)} = x^{(n)} - m\,\frac{f(x^{(n)})}{f'(x^{(n)})}$$

converges quadratically to x_*.

Multiple roots: modified Newton's method

The *modified Newton's method*

$$x^{(n+1)} = x^{(n)} - m \, \frac{f(x^{(n)})}{f'(x^{(n)})}$$

converges quadratically to x_*.

To show it, Taylor expand $f(x)$ in the vicinity of x_*:

$$\begin{aligned} f(x) &= 0 + f^{(m)} \, \frac{\delta^m}{m!} + f^{(m+1)} \, \frac{\delta^{m+1}}{(m+1)!} + \dots \\ f'(x) &= f^{(m)} \, \frac{\delta^{m-1}}{(m-1)!} + f^{(m+1)} \, \frac{\delta^m}{m!} + \dots \end{aligned}$$

Related methods: secants, false position

Related methods: False position

Fixed-point transformations can be used to generate a variety of related iterative schemes.

Fix some c, and use

$$\phi(x) = x - \frac{c - x}{f(c) - f(x)}\, f(x)$$

Convergence is linear. The root is not kept localized.

Related methods: Secants

Replace the tangent at $x^{(n)}$ by the secant passing through $x^{(n)}$ and $x^{(n-1)}$.

$$x^{(n+1)} = x^{(n)} - \frac{x^{(n-1)} - x^{(n)}}{f(x^{(n-1)}) - f(x^{(n)})} f(x^{(n)})$$

Convergence is superlinear with $p \approx 1.6$. The root is not kept localized.

Inverse quadratic interpolation

Inverse quadratic interpolation

Suppose we know three consequtive iterates, x_0, x_1 and x_2. Suppose further that $y_j = f(x_j)$, $j = 0, 1, 2$ are all different.

Construct a unique parabola which passes through (x_j, y_j), $j = 0, 1, 2$. Take as a next approximation, x_3, the root of this parabola.

In fact, use an *inverse interpolation*: interpolate x_j vs y_j where $y_j = f(x_j)$. I.e., construct a second order polynomial $Q(y)$ such that $Q(y_j) = x_j$. Then, $x_3 = Q(0)$.

This method is locally convergent, with the convergence rate of $p \approx 1.8$.

Hybrid algorithms

Brent's method

In practice, use a combination of a fast, locally convergent method (e.g. inverse parabolic interpolation), and a robust method which keeps track of the localization interval (bisection).