Accelerating fixed point iterations with Newton's method

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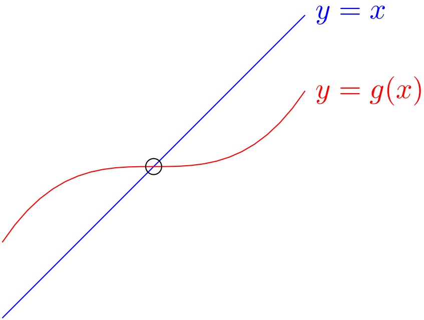
Fixed point iterations

Fixed points in 1D

The fixed point of a function $g(x)$ is a point x^* such that

$$g(x^*) = x^*.$$

These are also described as the intersection between the lines $y = g(x)$ and $y = x$.

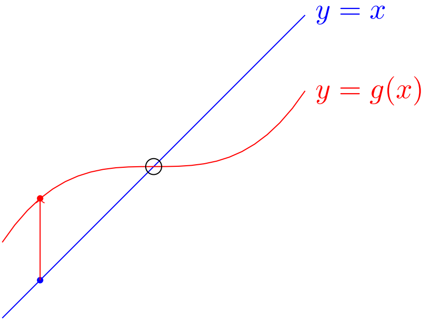


Fixed point iterations

To find fixed points of a given function $g(x)$, we can set up an iteration:

$$x_{n+1} = g(x_n).$$

This iteration stops at a fixed point. It converges if $g(x_n)$ is closer to x^* than x_n.



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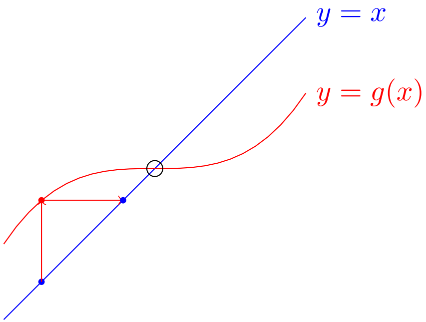

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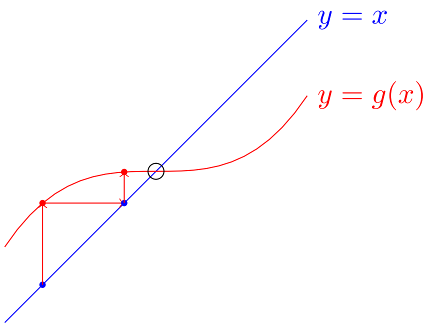

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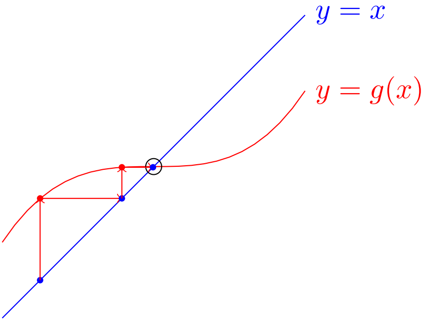


When does a fixed point iteration converge in 1D?

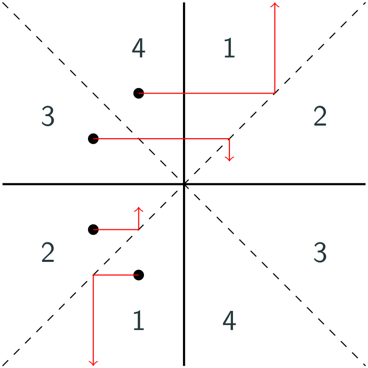
Convergence of the iteration $x_{n+1} = g(x_n)$ depends on which region $(x, g(x))$ lies.

1: Monotonic divergence

2: Monotonic convergence

3: Oscillatory convergence

4: Oscillatory divergence



Fixed point iterations in higher dimensions

Above 1D, fixed points of a vector-valued multivariate function $\boldsymbol{g}(\boldsymbol{x})$ satisfy

$$\boldsymbol{g}(\boldsymbol{x}^*) = \boldsymbol{x}^*.$$

Fixed point iterations are defined as

$$\boldsymbol{x}_{n+1} = \boldsymbol{g}(\boldsymbol{x}_n).$$

When does a fixed point iteration converge in nD?

Convergence can be shown with the Banach fixed-point theorem, which in this context requires

$$\|\boldsymbol{g}(\boldsymbol{x}) - \boldsymbol{g}(\boldsymbol{y})\| \leq q \, \|\boldsymbol{x} - \boldsymbol{y}\| \,, \quad q \in [0, 1).$$

In the 'regional' framework from 1D, we require

$$\|\boldsymbol{x}^* - \boldsymbol{g}(\boldsymbol{x}_n)\| < \|\boldsymbol{x}^* - \boldsymbol{x}_n\| \,.$$

This distinguishes between convergence and divergence, but monotonicity and oscillations are now harder to recognize.

Numerical methods as fixed point iterations

Almost every iterative method can be expressed as a fixed point iteration.

For example, consider Gauss-Seidel applied to:

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{v} \end{bmatrix} = \begin{bmatrix} \boldsymbol{a} \\ \boldsymbol{b} \end{bmatrix}$$

$$\boldsymbol{u}_{n+1} = A^{-1}\left(\boldsymbol{a} - B\boldsymbol{v}_n\right), \quad \boldsymbol{v}_{n+1} = D^{-1}\left(\boldsymbol{b} - C\boldsymbol{u}_{n+1}\right)$$

$$\implies \boldsymbol{v}_{n+1} = D^{-1}\Big(\boldsymbol{b} - CA^{-1}\left(\boldsymbol{a} - B\boldsymbol{v}_n\right)\Big) = \boldsymbol{g}(\boldsymbol{v}_n)$$

Continuous fixed point iterations

We can represent a fixed point iteration as the numerical integration of a function:

$$\frac{\boldsymbol{x}_{n+1} - \boldsymbol{x}_n}{\Delta t} = \boldsymbol{g}(\boldsymbol{x}_n) - \boldsymbol{x}_n, \quad \Delta t = 1,$$

$$\implies \frac{d\boldsymbol{x}}{dt} = \boldsymbol{g}(\boldsymbol{x}) - \boldsymbol{x}.$$

Newton's method

Newton's method (in 1D)

Newton's method is used to find a root of a given function $f(x)$:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}.$$

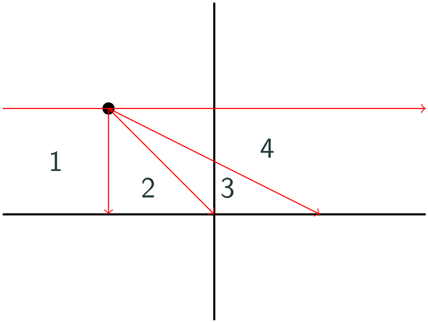
This can be viewed as a fixed point iteration:

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

then a fixed point of $g_f(x)$ is a root of $f(x)$.

When does Newton's method converge in 1D?

For Newton's method the regions of $g_f(x)$ depend on the slope of $f(x)$.
Most of the boundaries between the regions are known problems for Newton's method: a slope of zero divides regions 1 and 4, and an infinite slope divides 1 and 2.

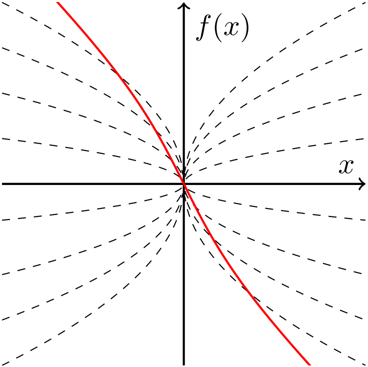


Cycles in Newton's method

The line between regions 3 and 4 can cause cycles in fixed point iterations. For Newton's method, this happens when $f(x)$ is parallel to

$$f_C(x) = C\sqrt{|x - x^*|}$$

for some constant $C \in \mathbb{R}$.



Continuous Newton's method

We can represent Newton's method as the numerical integration of an ODE:

$$\frac{x_{n+1} - x_n}{\Delta t} = -\frac{f(x_n)}{f'(x_n)}, \quad \Delta t = 1,$$

$$\implies \frac{\partial f}{\partial x}\frac{dx}{dt} = -f(x) \implies f(x(t)) = f(x(0))e^{-t}.$$

Newton's method in higher dimensions

Newton's method in higher dimensions requires the Jacobian of the function, $J_f(\boldsymbol{x})$:

$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n - J_f^{-1}(\boldsymbol{x}_n)\boldsymbol{f}(\boldsymbol{x}_n).$$

The Kantorovich Theorem tells us this method converges as long as the initial guess is sufficiently close to the root (amongst other assumptions).

Davidenko-Branin trick

Davidenko (1953) and Branin (1972) suggest an update to Newton's method:

$$\frac{d\boldsymbol{x}}{dt} = \frac{\operatorname{adj} J_f}{|\det J_f|} \boldsymbol{f}(\boldsymbol{x}),$$

using some numerical integration scheme (the update is the absolute value around $\det J_f$).

Because $\det J_f$ only changes sign when passing over a root, this version of Newton's method will always travel in the same direction between roots. This allows the method to go over 'humps' in the function that would cause Newton to diverge otherwise.

Acceleration

Reposing a fixed point as a root

Given a function $\boldsymbol{g}(\boldsymbol{x})$ with a fixed point $\boldsymbol{x}^*$, we can make a function with a root:

$$\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{g}(\boldsymbol{x}) - \boldsymbol{x}.$$

There are an infinite number of ways to construct such a function, but this is the simplest.