Nonlinear Equations

(in 1D)

Numerical Analysis Spring 2021
A. Donev, Courant

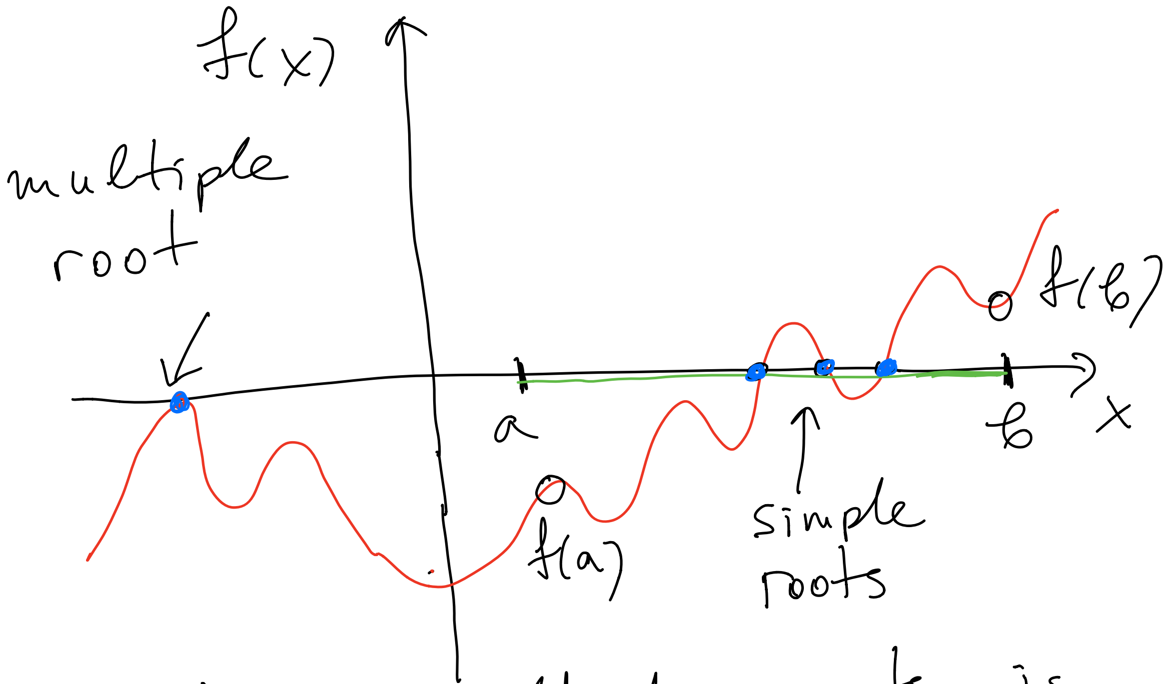
Consider solving a nonlinear equation like

$$\cos x + x^2 - 7 = 5$$

No closed form solution exists, so the only thing we can do is to solve numerically (on a computer)

Solve $f(x) = 0$ on $x \in [a, b]$

By this we mean find as accurately as possible at least one solution in $[a, b]$, assuming one exists.



Finding multiple roots is harder, so we focus on <u>simple roots</u> & assume there is at least one root in $[a,b]$ & f is <u>continuous</u>

<u>Theorem</u> If f is continuous on $[a,b]$ and $f(a)\cdot f(b) < 0$ (i.e., $f(a)$ & $f(b)$ have opposite sign) then $\exists\, x \in (a,b)$ s.t. $f(x)=0$

"Proof": It's "obvious" but if you insist apply the Intermediate Value Theorem $\square$

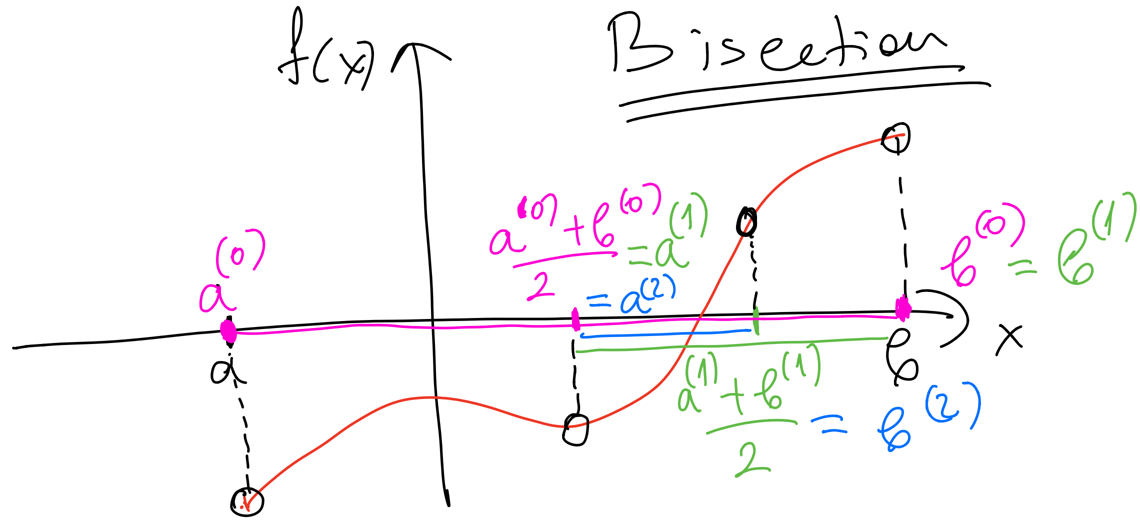
Now, assume that we are given an $f(x)$, meaning, given a real x we can evaluate $f(x)$ using some computer code, and an interval $[a,b]$ such that $f(a)\cdot f(b) < 0$

(Q1) Why don't I say $f(a)f(b) \leq 0$?

Can we devise an algorithm that will give us a root of f on $[a,b]$?

Answer: Yes, use bisection

Bisection



Algorithm Bisection

Input $[a, b]$, $n \in \mathbb{Z}^+$

Output x such that $f(x) \approx 0$

approximately equal

Set $a^{(0)} = a$, $b^{(0)} = b$

For $k = 0, 1, 2, \ldots, n-1$ do

$$x^{(k)} = \frac{a^{(k)} + b^{(k)}}{2}$$

$$f^{(k)} = f(x^{k})$$

If $f^{(k)} f(a^{(k)}) < 0$

$$b^{(k+1)} = x^{(k)}\ ; \ a^{(k+1)} = a^{(k)}$$

else

$$b^{(k+1)} = b^{(k)}\ ; \ a^{(k+1)} = x^{(k)}$$

end if

end for

Return $x \approx x^{(n)} = \dfrac{a^{(n)} + b^{(n)}}{2}$

or $x \in [a^{(n)}, b^{(n)}]$

[Matlab demo Bisection.m]

How accurate is x?

What is **absolute** error

$$\varepsilon^{(n)} = | x^{(n)} - x |$$

where $f(x) = 0$

We know

$$x \in [a^{(n)}, b^{(n)}]$$

$$\Rightarrow \quad |x^{(n)} - x| \leq \frac{b^{(n)} - a^{(n)}}{2}$$

Observe: $b^{(n)} - a^{(n)} = \dfrac{b^{(0)} - a^{(0)}}{2^n}$

$$\Rightarrow \quad \varepsilon^{(n)} = |x^{(n)} - x| \leq \frac{b-a}{2^{n+1}}$$

error estimate

This means the error approximately halves each iteration. This is guaranteed, which means the method is very robust, but it's not very fast.

given $\varepsilon < \dfrac{b-a}{2^{n+1}}$

$$2^{n+1} < \frac{b-a}{\varepsilon}$$

$$n+1 = \left\lfloor \log_2\left(\frac{b-a}{\varepsilon}\right)\right\rfloor$$

"floor" in Matlab

$$\Rightarrow \quad n = \left\lceil \log_2\left(\frac{b-a}{\varepsilon}\right)\right\rceil$$

ceil in Matlab

So given a target error tolerance ε we can directly estimate how many iterations to take.

[Numerical analyst job complete]

7

Newton & Secant methods

Can we do better than bisection? Bisection only used the sign of f, not the value of $f(x)$.

"Definition": A function $f(x)$ is a smooth function on $[a,b]$ if it can be approximated well by a low order polynomial (linear, quadratic, cubic) over the <u>whole</u> interval $[a,b]$

In most of this class, we will assume to work with functions that are sufficiently smooth. This is more than just being <u>sufficiently differentiable</u>, which we may <u>require</u> as an assumption. Smoothness also requires high-order derivatives not to be very large. In some sense [See Functional Analysis]

Our error / convergence estimates will only be accurate for smooth $f(x)$.

<u>Note</u>: If $f(x)$ is continuously differentiable, it will be almost linear over a sufficiently small interval $[a,b]$ (think calculus as $b-a \to dx$)

Idea for "all" of NA: Approximate smooth functions by low-degree polynomials

If $f(x) \approx p(x)$ on $[a,b]$ then we can solve

$$p(x) = 0$$

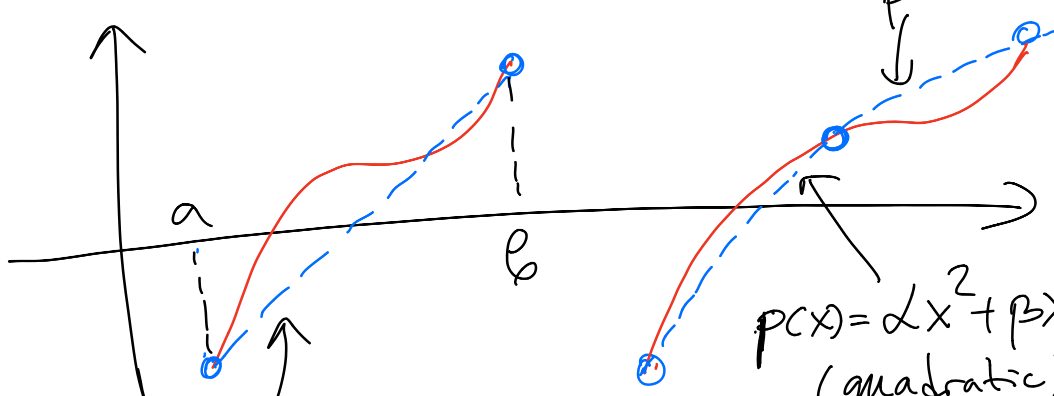
instead. If p is a <u>linear</u> or <u>quadratic</u> function then we have explicit solution!

How do we approximate $f(x)$ by $p(x)$?

Two <u>ideas</u> common in all of numerical analysis:

(1) Evaluate $f(x)$ at a few points & fit a polynomial through them:

parabola



$p(x) = \alpha x^2 + \beta x + \gamma$
(quadratic)

$$p(x) = f(a) + \frac{x-a}{b-a} f(b)$$

linear

(2) Approximate $f(x)$ by it's Taylor series around the current guess for the answer

Reminder

If $f(x)$ is infinitely differentiable at x_0,

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x_0)}{n!}(x-x_0)^n$$

$$= f(x_0) + f'(x_0)(x-x_0) + \frac{1}{2} f''(x_0)(x-x_0)^2 + \dots$$

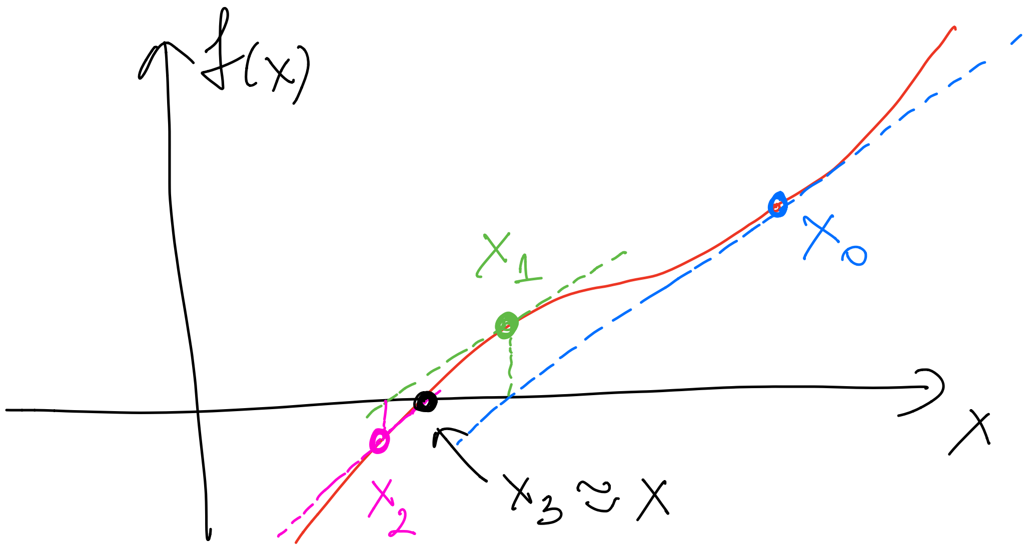
Taylor series with remainder

$$f(x) = \sum_{n=0}^{k} \frac{f^{(n)}(x_0)}{n!}(x-x_0)^n + \frac{f^{(k+1)}(\xi)}{(k+1)!}(x-x_0)^{n+1}$$

for some ξ between x_0 & x

Newton's method

Approximate $f(x)$ by it's tangent at x_k, i.e., first-order Taylor series



$$f(x) \simeq f_k(x) = f(x_k) + f'(x_k)(x - x_k)$$

Solve $f_k(x) = 0 \Rightarrow$

$$x \approx x_k - \frac{f(x_k)}{f'(x_k)}$$

Newton's method

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

E.g. $f(x) = x^2 - c$

(square root calculation)

$f'(x) = 2x \Rightarrow$

$$x_{k+1} = x_k - \frac{x_k^2 - c}{2x_k}$$

$$= \frac{x_k}{2} + \frac{c}{2x_k}$$

which is the Babylonian method!

Remember that the method converged fast. Why?

General idea: When analyzing the error / convergence of method based on Taylor series, use Remainder Theorem

Error $\quad e_k = x_k - x$

$$f(x) = 0 = f(x_k) + (x - x_k) f'(x_k)$$

remainder $\longrightarrow$ $$+ \frac{1}{2}(x - x_k)^2 f''(\xi)$$

ξ between x_k and x

Divide both sides by $f'(x_k) \neq 0$

& rearrange

$$\underbrace{\left(x_k - \frac{f(x_k)}{f'(x_k)}\right)}_{x_{k+1}} - x = -\frac{1}{2}(x - x_k)^2 \frac{f''(\xi)}{f'(x_k)}$$

$$x_{k+1} - x = e_{k+1} = -\frac{1}{2} e_k^2 \cdot \frac{f''(\xi)}{f'(x_k)}$$

$$\frac{e_{k+1}}{e_k^2} = -\frac{f''(\xi)}{2 f'(x_k)}$$

If the method converges,

$$x_k \to x$$

and $\xi \to x$ $\Rightarrow$

$$\frac{|e_{k+1}|}{e_k^2} \longrightarrow \frac{f''(x)}{2f'(x)} = C$$

$$\Rightarrow |e_{k+1}| \approx C \cdot e_k^2$$

Error gets squared every iteration, not halved like for bisection. This leads to fast convergence after the error is small

If $e_k \ll 1 \Rightarrow e_k^2 \ll e_k$

much less than

This explains why the Babylonian method converged fast.

But when does Newton method converge?

General answer hard to give but we can give a sufficient condition

We want $|e_{k+1}| < |e_k|$

(error decreases)

$$\left|\frac{f''(\xi)}{2f'(x_k)}\right| e_k^2 < |e_k|$$

If $|e_k| < \left|\frac{2f'(x_k)}{f''(\xi)}\right|$

then error decreases

Imagne that

$$\left|\frac{f''(y_1)}{f'(y_2)}\right| \leq A \quad \forall y_1, y_2 \in I$$

$$I = [x-\delta, x+\delta]$$

(see Theorem 1.8 in Suli)

and $x_0 \in I \Rightarrow$

$$|e_0| = |x_0 - x| < \delta$$

If $|e_0| < \frac{1}{A} < \left|\frac{f'(x_h)}{f''(\xi)}\right|$

$\Rightarrow |e_1| < \frac{|e_0|}{2}$ and error decreases strictly by at least half and eventually much faster

Conclusion:

If we give Newton's method an initial guess closer to a simple root x than $\approx \left| \frac{f'(x)}{f''(x)} \right|$, it will converge rapidly.

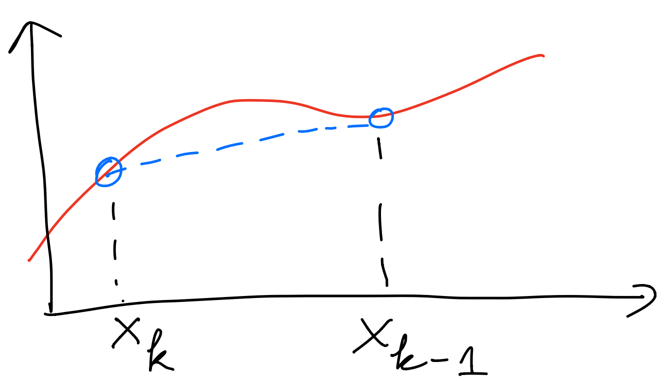
Otherwise, it may converge very slowly, erratically, or diverge.

Idea: Use bisection first to find an initial guess that is good & then switch to Newton

This is called safe guarded Newton method but we will not go into the details in class.

Secant method

Newton's method was based on approximating $f(x)$ with its first-order Taylor series (tangent). How about approximating $f(x)$ based on two points?



$$f(x) \simeq p(x) = f(x_k) + \frac{x - x_k}{x_{k-1} - x_k}\left(f(x_{k-1}) - f(x_k)\right)$$

<u>Check</u>: $\begin{cases} p(x_k) = f(x_k) \\ p(x_{k-1}) = f(x_{k-1}) \end{cases}$

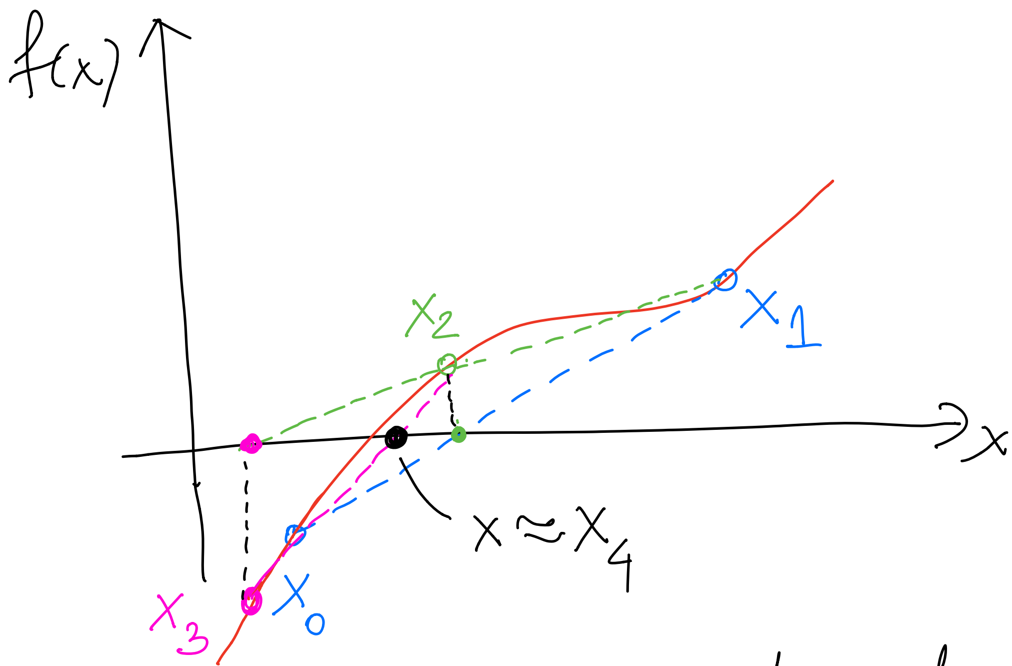
$$f(x_{k+1}) \simeq p(x_{k+1}) = 0$$

Solve for x_{k+1} (<u>linear</u> eq.)

$$x_{k+1} = x_k - f_k \left(\frac{x_k - x_{k-1}}{f_k - f_{k-1}}\right)$$

Secant method

Here $f_k = f(x_k)$ (notation)



One way to think of secant method is as Newton's method with the approximation

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

which is good if f is smooth and $x_{k-1} \approx x_k$.

Called finite-difference approximation

Note we need <u>two</u> points to start the iteration.

It is therefore very natural to combine secant with bisection: instead of using midpoint use secant point as new guess.

This method of Regula Falsi is <u>guaranteed</u> to converge to a root but maybe it is faster than bisection?

[Demo Secant.m]

Conclusion: True secant converges faster than bisection or Regula Falsi.

But <u>how much faster</u>?

Bisection: $|e_{k+1}| \le \frac{|e_k|^1}{2}$

(linear)

Newton: $|e_{k+1}| \to \left|\frac{f''(x)}{2f'(x)}\right| |e_k|^2$

(quadratic)

Secant (we will not prove):

$$|e_{k+1}| \to \mu \cdot |e_k|^q$$

where $q = \frac{1}{2}(1+\sqrt{5}) \simeq 1.6$ is Golden Ratio

We say bisection converges at a linear rate, Newton at quadratic rate, and secant at order of convergence ~1.6

<u>Aside</u>: For secant method, one can prove (see (4.17) in "Practice" book)

$$|e_{k+1}| \to \left|\frac{f''(x)}{2f'(x)}\right| |e_k e_{k-1}|$$

which makes the relationship with Newton's method more obvious.

<u>Homework</u>

Try & (maybe) analyze Steffensen's method

$$x_{k+1} = x_k - \frac{f_k^2}{f(x_k + f_k) - f_k}$$

Fixed-point iteration

Every iterative method of the form

$$x_{k+1} = g(x_k)$$

that converges to $x_k \to x$ satisfies

$$x = g(x)$$

which for <u>consistency</u> must be equivalent (imply) $f(x)=0$

For example, Babylonian method for $x^2 - c = 0$ has

$$g(x) = \frac{1}{2}\left(x + \frac{c}{x}\right)$$

$$x = g(x) \Rightarrow \frac{x}{\cancel{2}} = \frac{1}{\cancel{2}} \frac{c}{x}$$

$$\Rightarrow x^2 = c \quad \text{as desired}$$

But also

$x = x^2 + x - c = g(x)$ is equivalent to $x = \sqrt{c}$.

So we have lot's of options to choose $g(x)$.

Every $g(x)$ gives us an iterative fixed-point method

$$x_{k+1} = g(x_k)$$

When does this method converge, and how fast?

For example, relaxation method

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

where $\lambda \neq 0$ has

$$g(x) = x - \lambda f(x) = x$$
iff $f(x) = 0$

What is a good choice of λ?

Full analysis of fixed-point in theory textbook. We will follow a quicker analysis (less general & precise).

Let's use Taylor series

$$x_{k+1} = g(x_k) = g(x) + (x_k - x)g'(\xi_k)$$

$$= x + (x_k - x)g'(\xi_k)$$

$$\Rightarrow e_{k+1} = x_{k+1} - x = g'(\xi_k)\, e_k$$

If we want error to <u>decrease</u> (converge to zero) we want $|g'(\xi_k)| < 1$

$$|e_{k+1}| = |g'(\xi_k)|\,|e_k|$$

Theorem

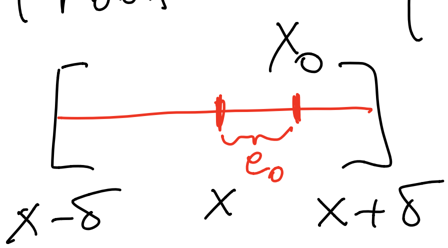
continuously differentiable

If $g \in C^1$ and

$$|g'(y)| < 1 \quad \forall y \in [x-\delta, x+\delta]$$

where $g(x) = x$ is a fixed point,
then fixed point iteration starting with $x_0 \in [x-\delta, x+\delta]$ converges to x.

"Proof": $|e_0| < \delta$ and



$$|e_1| = |g(\xi_h)|\,|e_0|$$

$$\Rightarrow |e_1| < \delta \text{ and}$$

$$x_1 \in [x-\delta, x+\delta]$$

By induction, iterates remain inside interval $[x-\delta, x+\delta]$

and $|e_{k+1}| < L|e_k|$

where (Lipshitz constant)

$$L = \max_{y \in [x-\delta, x+\delta]} |g'(y)| < 1$$

$$\Rightarrow |e_k| < L^k |e_0|$$

with $0 \leq L < 1$

and thus $|e_k| \to 0$.

As we get closer to root

$$\frac{|e_{k+1}|}{|e_k|} \to |g'(x)|$$

Convergence is fastest if

$$|g'(x)| << 1$$

Ideally $g'(x) = 0 \Rightarrow$

super-linear convergence

Go back to relaxation method

$$g(x) = x - \lambda f(x)$$

$$g'(x) = 1 - \lambda f'(x) = 0$$

$$\Rightarrow \lambda = \frac{1}{f'(x)} \Rightarrow$$

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

But of course we don't know x but if we converge $x_k \to x$ so do

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

which is Newton's method!

Newton's: $g = x - \frac{f(x)}{f'(x)}$

$$g'(x) = \cancel{1} - \cancel{\frac{f'(x)}{f'(x)}} + \frac{f(x) f''(x)}{(f'(x))^2}$$

$g'(x) = 0$ if $f(x) = 0$ and $f'(x) \neq 0$