Numerical Methods

Last time: fixed point formulations: $f(x)=0 \iff \phi(x)=x$

Fixed point iteration: $x_{k+1} = \phi(x_k)$, $k=0,1,2,\ldots$

Global linear convergence: CMT ($\phi : [a,b] \to [a,b]$ strict contraction)

Local linear convergence: ϕ continuously differentiable and $|\phi'(\alpha)|<1$ ($\phi(\alpha)=\alpha$)

Correction: I forgot to prove linear convergence in my proof of CMT.

$$|x_{k+1}-\alpha| \underset{\text{defn}}{=} |\phi(x_k)-\phi(\alpha)| \underset{\text{fixed point}}{\leq} \Lambda |x_k-\alpha| .$$

In local convergence result we had

$$\lim_{k\to\infty} \frac{x_{k+1}-\alpha}{x_k-\alpha} = \phi'(\alpha) .$$

Q: If $\phi'(\alpha)=0$, is convergence super-linear?

A: Yes, if ϕ is smooth enough.

Theorem (local quadratic convergence)

Let $\phi : [a,b] \to \mathbb{R}$ be twice continuously differentiable and let $\alpha \in (a,b)$ be a fixed point of ϕ s.t. $\boxed{\phi'(\alpha)=0}$.
Then $\exists\, \delta>0$ s.t. $x_{k+1}=\phi(x_k)$ converges quadratically to α for any $x_0 \in [\alpha-\delta, \alpha+\delta]$. Furthermore,

$$\lim_{k\to\infty} \frac{x_{k+1}-\alpha}{(x_k-\alpha)^2} = \frac{\phi''(\alpha)}{2} .$$

Proof: Since $|\phi'(\alpha)| = 0 < 1$ we have local linear convergence.

Taylor expansion of $\phi(x_k)$ around α gives:

$$x_{k+1} - \alpha = \phi(x_k) - \phi(\alpha) = \underbrace{\phi'(\alpha)}_{\to 0}(x_k - \alpha) + \frac{\phi''(\xi_k)}{2}(x_k - \alpha)^2,$$

for some ξ_k between x_k and α.

Assuming $x_k \neq \alpha$ for any k,

$$\frac{x_{k+1} - \alpha}{(x_k - \alpha)^2} = \frac{\phi''(\xi_k)}{2} \longrightarrow \frac{\phi''(\alpha)}{2}$$

continuity of ϕ'' and convergence of $x_k \to \alpha$. (and hence of $\xi_k \to \alpha$)

Example: Newton's method. (for $f(x) = 0$)

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}, \quad k = 0, 1, \ldots$$

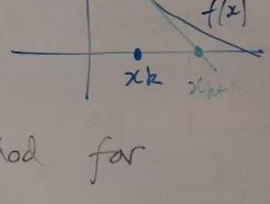
Where does this come from? assume $f(\alpha) = 0$.

- Taylor gives $0 = f(\alpha) = f(x_k) + f'(x_k)(\alpha - x_k) + R_1$ with $R_1(\alpha; x_k) = o(\alpha - x_k)$ as $\alpha \to x_k$.

Rearranging gives $\alpha = x_k - \dfrac{f(x_k)}{f'(x_k)} - \cancel{\dfrac{R_1(\alpha, x_k)}{f'(x_k)}}$

Newton comes from throwing away this term

- Another interpretation: x_{k+1} is the root of the best linear approximation to $f(x)$ at $x = x_k$.



Newton's method is a fixed point method for

$$\boxed{\phi(x) = x - \frac{f(x)}{f'(x)}}.$$

If f is twice differentiable and $f'(x) \neq 0$ then

$$\phi'(x) = \frac{f(x) f''(x)}{(f'(x))^2} \qquad \text{(quotient rule)}$$

Hence if $f(\alpha) = 0$ and $f'(\alpha) \neq 0$ then $\phi'(\alpha) = 0$.

Then iteration is locally linearly convergent, if f twice continuously diff.

If f is three times continuously differentiable then we expect quadratic convergence. (since then ϕ'' is cts)

But in fact this isn't necessary.

Theorem (local quadratic convergence of Newton)

Let $f : [a,b] \to \mathbb{R}$ be twice continuously differentiable.

Let $\alpha \in (a,b)$ satisfy $f(\alpha) = 0$ and $f'(\alpha) \neq 0$.

Then $\exists\, \delta > 0$ s.t. Newton iteration converges quadratically to α for all $x_0 \in [\alpha - \delta, \alpha + \delta]$, and

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

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

Proof: Since $f'(x)$ is continuous on $[a,b]$, and $f'(\alpha) \neq 0$, $\exists\, \rho > 0$ and $M > 0$ s.t.

$$x \in [\alpha - \rho, \alpha + \rho] \Rightarrow |f'(x)| \geq M > 0.$$

Also, since $f''(x)$ is continuous on $[a,b]$ $\exists\, C > 0$ s.t. $|f''(x)| \leq C$, $\forall x \in [a,b]$.

Define $\delta := \min\left(\rho, \frac{M}{C}\right) > 0$ and set $I_\delta = [\alpha - \delta, \alpha + \delta]$.

Claim: $x_0 \in I_\delta \Rightarrow x_k \in I_\delta$ for all $k \in \mathbb{N}$.

Proof by induction: if $x_k \in I_\delta$ then $|f'(x_k)| \geq M > 0$ since $\boxed{\delta \leq \rho}$.

Hence x_{k+1} is well defined.

Recall that $\alpha = \underbrace{x_k - \frac{f(x_k)}{f'(x_k)}}_{= x_{k+1}} - \frac{R_1(\alpha, x_k)}{f'(x_k)}$

Since f is twice diff., $R_1(\alpha, x_k) = \frac{f''(\xi_k)}{2}(\alpha - x_k)^2$, some ξ_k between α and x_k.

$\le C \qquad \le \delta \qquad \le 1$

Then $|x_{k+1} - \alpha| = \dfrac{\left|\frac{f''(\xi_k)}{2}\right| |\alpha - x_k|^2}{\underbrace{|f'(x_k)|}_{\ge M}} \le \dfrac{C\delta}{2M} |\alpha - x_k|$.

(*) $\le \frac{1}{2} |\alpha - x_k|$

Hence $x_{k+1} \in I_\delta$ so inductive step proved. $\le \frac{1}{2}\delta < \delta$.

Note that the inequality (*) gives $|x_{k+1} - \alpha| \le \frac{1}{2}|x_k - \alpha|$, giving linear convergence.

But furthermore we have $|x_{k+1} - \alpha| \le \frac{C}{2M}|x_k - \alpha|^2$, giving quadratic convergence.

And furthermore $\dfrac{x_{k+1} - \alpha}{(x_k - \alpha)^2} = \dfrac{f''(\xi_k)}{2f'(x_k)} \longrightarrow \dfrac{f''(\alpha)}{2f'(\alpha)}$ as $k \to \infty$.

(since $x_k \to \alpha \Rightarrow \xi_k \to \alpha$ and both f' and f'' are continuous, and $f'(\alpha) \neq 0$.)

Remark: Take-home message is that Newton is fast!

But:
- requires smoothness of f, and $f'(\alpha) \neq 0$.
- in general we can't compute δ.
  So we don't know whether a given x_0 is "close enough" to give convergence.

Examples of divergence of Newton: