Numerical Methods

§3.8 Stopping criteria: when to stop iteration?

We'd like to stop when

$$|e_k| := |x_k - \alpha| \leq tol$$

absolute error

kth iteration of numerical method

exact soln of $f(\alpha)=0$, or $\phi(\alpha)=\alpha$

user-specified tolerance

Last time: If we have a priori bound e.g. $|e_k| \leq C\Lambda^k$, $0<\Lambda<1$, we can stop when $C\Lambda^k \leq tol$.

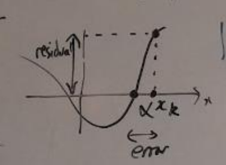
Other options:

Residual-based criterion:

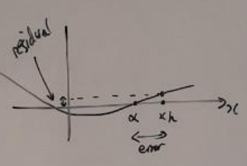
Stop when $|f(x_k)|$ is sufficiently small.

residual ← how well does x_k satisfy the equation $f(x)=0$?

For smooth f, relationship between error and residual depends on $f'(x)$ near α.



$|f'(\alpha)|$ large $\Rightarrow \dfrac{\text{residual}}{\text{error}}$ is large.



$|f'(\alpha)|$ small $\Rightarrow \dfrac{\text{residual}}{\text{error}}$ is small

If $|f'(\alpha)| \approx 1$ then stopping when $|f(x_k)| \leq tol$ will ensure $|e_k|$ is approximately $\leq tol$.

If we know more about f', we can be more precise:

Theorem: Suppose $f : [a,b] \to \mathbb{R}$ is differentiable.

Suppose $\exists \, \alpha \in [a,b]$ s.t. $f(\alpha) = 0$

Suppose also that $\exists \, L, U > 0$ s.t.

$$0 < L \leq |f'(x)| \leq U \qquad \forall x \in [a,b].$$

Then
$$\frac{1}{U} \underbrace{|f(x)|} \leq \underbrace{|x - \alpha|}_{\text{error at } x} \leq \frac{1}{L} \underbrace{|f(x)|}_{\text{residual at } x} \qquad \forall x \in [a,b]$$

Proof: By MVT $\exists \, \xi$ between x and α s.t.

$$f(x) = f(x) - f(\alpha) = f'(\xi)(x - \alpha).$$

Then
$$|x - \alpha| = \frac{|f(x)|}{|f'(\xi)|} \in \left[\frac{1}{U} |f(x)|, \frac{1}{L} |f(x)| \right].$$

So if we can find such an L, we know that stopping when $\boxed{\frac{1}{L} |f(x_k)| \leq tol}$ $(*)$ will guarantee that $|e_k| \leq tol$.

$|e_k| \leq \frac{1}{L} |f(x_k)|$ is an "a posteriori" error bound (because the RHS involves x_k)

Another option: increment-based stopping criteria.

Here we might stop the algorithm when $|x_k - x_{k+1}|$ is sufficiently small.

For a fixed point method $x_{k+1} = \phi(x_k)$ with smooth ϕ, it holds that

$$e_k \approx \frac{x_k - x_{k+1}}{1 - \phi'(\alpha)}$$

so this is reasonable provided $\phi'(\alpha)$ is not close to 1.

Matlab tips: 1e-3 means 1×10^{-3}

2e-3 ..... 2×10^{-3}

Ctrl-Enter runs the current section.

; suppresses output

In command window, Ctrl-c terminates current process!

If $e_k = C \Lambda^k$ then $\log_{10}(e_k) = \log_{10} C + k \log_{10} \Lambda$

If $e_{k+1} = C e_k^2$ then $\log_{10}(e_{k+1}) = \log_{10} C + 2 \log_{10} e_k$