Newton's method has been around awhile, so there are many variants /extensions etc.

Outline:
- History /example
- Convergence revisited (multiple roots)
  - Modified Newton
  - Deflation
- Practical Newton's method
- Secant Method
- Pros/Cons of Newton

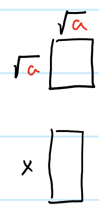
Ex. Babylonian Algo

2000+ years ago, Archimedes claimed $\underset{1.73202}{\frac{265}{153}} < \sqrt{3} < \underset{1.73205}{\frac{1351}{780}}$. Not bad!

How did he find it? Not sure, but maybe via the Babylonian Algorithm, aka Heron's method.

Algo: Find $x = \sqrt{a}$

Iterate $x_{k+1} = \frac{1}{2}\left(x_n + \frac{a}{x_n}\right)$ → motivation:



Square w/ area a

rectangle with same area a
If one side is x, other side must be a/x.

If $x > \sqrt{a}$ then $a/x < \sqrt{a}$
and vice-versa
(one side too short ⇒ other side too long)
So we have under and over approximations...
so average these

It turns out this is Newton's method applied to $f(x) = x^2 - a$ (i.e. $f'(x) = 2x$)

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

Convergence, revisited

Recall our result from last time:

Thm: (combining Thm 2.6 and Thm 2.9)

Let $f \in C^2([a,b])$ have a root $p \in (a,b)$ with multiplicity 1 (i.e. $f'(p) \neq 0$)
then if initialized sufficiently close to p, Newton's method will converge to p.

Furthermore, if additionally $|g''(x)|$ is bounded on some open interval around p,
then the convergence rate is quadratic. → $g(x) := x - \frac{f(x)}{f'(x)}$

Ok, but what if p isn't a simple root?
aka multiplicity 1

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Def Recall, a root p of f is $\boxed{\text{multiplicity}}$ m if the 1st $m-1$ derivatives of f are 0 at p

i.e., $f(p) = f'(p) = \dots = f^{m-1}(p) = 0$ and $f^{m}(p) \neq 0$

Equivalently, if $f(x) = (x-p)^m g(x)$ and $g(p) \neq 0$

Ex: $f(x) = x(x-1)(x-2)$ has a simple root at $x=0$ (and at $x=1, x=2$) $m=1$

$f(x) = x^2(x-1)$ has a double root at $x=0$ $m=2$

$f(x) = x^3$ has a triple root at $x=0$ $m=3$

Our theorem doesn't apply. Often we still get convergence but just not at a quadratic rate

Ex $f(x) = x^2$, $x=0$ is a double root. $f'(x) = 2x$

Newton's method is $x_{k+1} = x_k - \dfrac{f(x_k)}{f'(x_k)} = x_k - \dfrac{x_k^2}{2x_k} = \frac{1}{2}x_k$

ie., $x_{k+1} = \frac{1}{2}x_k$,

so, e.g., $x_0 = 1$, then we iterate $1, 1/2, 1/4, 1/8, 1/16, \dots$

error at step k is $\frac{1}{2^k}$, $e_k = \frac{1}{2^k}$. Is this quadratic?

Check: $\lim\limits_{k\to\infty} \dfrac{e_{k+1}}{e_k^2} = \lim \left(\dfrac{\frac{1}{2^{k+1}}}{\left(\frac{1}{2^k}\right)^2} = \dfrac{\frac{1}{2^{k+1}}}{\frac{1}{2^{2k}}} = \dfrac{2^{2k}}{2^{k+1}} = 2^{k-1} \right) = \infty$

No, not quadratic conv.

In fact, this is linear convergence since it fits the form ρ^k $(\rho = 1/2)$ which we've already discussed.

One fix to this multiplicity issue is...

Modified* Newton's Method

* there are many ways to modify it, this is just our book's notation

Let p be a root of f w/ multiplicity m ($m=1$ is ok, but mostly interested in $m>1$)

Define $h(x) = \dfrac{f(x)}{f'(x)}$. Then claim p is a root of h also

proof: $m=1$ then $f'(p) \neq 0$ so immediately $h(p) = 0$

$m>1$ then $f'(p) = 0$, $\dfrac{f(p)}{f'(p)} = \dfrac{0}{0}$ ... use L'Hôpital

So $\lim\limits_{x\to p} \dfrac{f(x)}{f'(x)} = \lim\limits_{x\to p} \dfrac{f'(x)}{f''(x)} = \dots = \lim\limits_{x\to p} \dfrac{f^{m-1}(x)}{\underbrace{f^{m}(x)}_{\neq 0 \text{ at } p}} = 0$

Furthermore, p is a simple root of h

proof:

Can write $f(x) = (x-p)^m g(x)$ w/ $g(p) \neq 0$

then

$$h(x) = \frac{(x-p)^m g(x)}{m(x-p)^{m-1}g(x) + (x-p)^m g'(x)} = (x-p)\underbrace{\frac{g(x)}{m\cdot g(x) + (x-p)g'(x)}}_{\tilde{g}(x)},$$

$\tilde{g}(p) = \dfrac{g(p)}{m g(p) + \cancel{(p-p)}g'(p)} = 1/m \neq 0$

So $h(x) = (x-p)\tilde{g}(x)$ with $\tilde{g}(p) \neq 0$ $\Rightarrow$ is a simple root

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... back to the point.

p is a simple root of $h(x) = \frac{f(x)}{f'(x)}$

So run Newton on h instead of f.

Simplifying h', we get MODIFIED NEWTON

$$x_{n+1} = x_n - \frac{f(x_n)f'(x_n)}{\underbrace{f'(x_n)^2 - f(x_n)f''(x_n)}}$$

ugly quotient rule stuff

Not a perfect fix:

DRAWBACKS: ① must compute f''

② subtractive cancellations

Note: if m is known, $x_{n+1} = x_n - m\frac{f(x_n)}{f'(x_n)}$ will work and w/ quadratic convergence

example of a "stepsize"

Deflation

A related idea to dealing with roots of multiplicity > 1

Suppose f has simple roots at p_1 and p_2 (if $p_1 = p_2$ it's a double root)

If $|p_1 - p_2|$ is very small, starts to act like a double root, especially w/ roundoff errors. The condition number of the root-finding problem is large

One practical consequence:

Suppose we find p_1. How to find p_2? We have to start sufficiently close to it, which is hard since we don't know where it is! We might get "sucked into" the p_1 root.

... and a fix: deflation

Define $h(x) = \frac{f(x)}{x - p_1}$ so h doesn't have a root at p_1, but still has a root at p_2

(this is also the name for a broader class of techniques, eg. in eigenvalue problems)

Practical Newton's method, i.e. globalization strategies

We won't go into details

① combine w/ bracketing or another root-finding method

(our book mentions a special version called False Position / Regula Falsi)

② safeguarding / linesearch:

don't let x_{n+1} go too far

(ex: if we must keep $x_n \geq 0$)

or $x_{n+1} = x_n - \alpha \frac{f(x_n)}{f'(x_n)}$, $\alpha \leq 1$

Need $\alpha = 1$ for quadratic convergence but often take $\alpha < 1$ for the first few iterations

Don't worry about these, just use Matlab / Scipy libraries

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Secant Method

See demo: if you call scipy's 1D Newton and don't supply "fprime", it doesn't work as well (presumably it tries finite difference)

Idea: Newton's method is $x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$. What if we want to avoid calculating $f'(\,)$? *

*see lecture on "Automatic Differentiation" ($\neq$ Symbolic diff.) ex. backprop.

well, rule of thumb: when a step produces an approximate result, you are free to carry it out approximately.

Since Newton's method was derived via Taylor Series, ignoring higher-order terms, lets try approximating the derivative:

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{(x+h) - (x)}, \text{ i.e., } f'(x_k) \approx \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}} \text{ if } |x_k - x_{k-1}| \text{ small}$$

(re-use our old computation)

So

SECANT METHOD

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

Only needs 1 function evaluation per step, no derivative needed. Nice!

you can extend in 2 ways:

1. use more previous points, "inverse interpolation". Not very common
2. In multi-dimensional problems, there is "more freedom", and we actually have a whole class of QUASI-NEWTON METHODS. Very useful! often "state-of-the-art" (names like "Broyden class", "SR1", "BFGS")

Also, some extra computational savings that are irrelevant for scalar problems.

Convergence Analysis of Secant method [possibly skip in lecture]

Recall for Newton $\lim \frac{|e_{k+1}|}{|e_k^2|} < \infty$ i.e. $\alpha = 2$

where $e_k = p - x_k$ is the error.

For the secant method, assuming e_k is small, we can do a Taylor expansion of our secant method iteration (tedious but straightforward) to get

$$e_{k+1} \approx \underbrace{-\tfrac{1}{2}\frac{f''(p)}{f'(p)}}_{\text{some constant}} e_k e_{k-1} \qquad (*)$$

Let's guess/hope that we have α convergence and can write

$(\forall k)$ $\underbrace{e_{k+1} = c \cdot e_k^{\alpha}}_{\text{like an "ansatz"}}$ and solve for α

then $e_{k+1} = c \cdot e_k^{\alpha} = c \cdot (c \cdot e_{k-1}^{\alpha})^{\alpha} = \text{const} \cdot e_{k-1}^{\alpha^2}$

and $e_k e_{k-1} = c \cdot e_{k-1}^{\alpha} e_k = c \cdot e_{k-1}^{\alpha+1}$

Plugging into $(*)$ gives $e_{k-1}^{\alpha^2} = (\text{some constant})\, e_{k-1}^{\alpha+1}$

involves c and $-\frac{1}{2}\frac{f''(p)}{f'(p)}$

this should be true for all e_{k-1} (when e_{k-1} is near 0)

So need (constant) $= 1$

and $\boxed{\alpha^2 = \alpha + 1}$, $\alpha > 0$ $\longrightarrow$ solution is the Golden Ratio $\alpha = \frac{1+\sqrt{5}}{2} \approx 1.618$

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So... Newton's method has rate $\alpha = 2$

Secant method has rate $\alpha = 1.62$

... and in fact if you say that Newton's method takes <u>twice</u> as much work as the secant method (since you must evaluate $f(x_n)$ <u>and</u> $f'(x_n)$) then we can do <u>2</u> iterations of the secant method and count the rate as $(1.62)^2 = 2.62$

(or, keep as 1.62 but call Newton's rate $\sqrt{2} = 1.41$)

... meaning the secant method is <u>better</u> than Newton, in this sense.

Summary of Pros / Cons

Newton's method:

PROS

+ No need for bracketing interval $[a,b]$. Doesn't need $f(a) \cdot f(b) < 0$ (which excludes $f(x) = x^2$)

+ Very fast convergence eventually (the gold-standard)

+ Simple

+ extends to dimensions ≥ 1

CONS

− x_0 must be close to root, and hard to know how close. If not close enough, may diverge or converge to wrong root

− Slower convergence for multiple roots $m > 1$. Some fixes but not perfect

− practical implementations need more information, more complicated

− must supply $f'(\ )$

Secant method

same pros / cons except no longer need to provide $f'(\ )$, slightly slower convergence rate

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Skip in lecture

Addendum

Theorems 2.6 and 2.8 in the book are not stated in the most useful way, especially 2.8. Notation: let p denote a fixed pt.

Book's Thm 2.8: $g \in C[a,b]$, $g(x) \in [a,b]$ $\forall x \in [a,b]$, g' continuous on (a,b), and $|g'(x)| \le k$ $\forall x \in (a,b)$ for some $k < 1$.

Then unless p_0 is a fixed point, the sequence (p_n), defined by $p_{n+1} = g(p_n)$, converges only linearly if $g'(p) \neq 0$.

(They state it this way since Thm 2.9 gives quadratic convergence if $g'(p) = 0$)

⚠ First, recall

① root-finding, $f(p) = 0$, here $f'(p) = 0$ is BAD

② fixed-pt. iter, eg. Newton

$$g(x) = x - \frac{f(x)}{f'(x)}, \quad g(p) = p$$

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

$$= \frac{f(x)f''(x)}{(f'(x))^2}$$

$g'(p) = 0$ is GOOD

We can strengthen Thm 2.8 by looking at its proof:

Better Thm 2.8 (same assumptions ...)

... then if $g'(p) \neq 0$, (p_n) converges to p linearly at rate $|g'(p)|$.