Practical Numerical Methods in Physics and Astronomy
Lecture 3 – Root Finding

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Slides available from
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Outline

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Solving equations

Everybody needs to solve an equation numerically eventually...

$$f(x) + a = g(x) + b$$

Solving equations

Everybody needs to solve an equation numerically eventually...

$$f(x) + a = g(x) + b$$

$$f(x) - g(x) + a - b = 0 \tag{1}$$

$$\text{i.e. } h(x) = 0 \tag{2}$$

Recast it as homogeneous and you have

The classic root-finding problem

For what x does $h(x) = 0$?

First. . .

Guess!

First. . .

Guess!

Then guess again!

First. . .

Guess!

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If your guesses have the same sign for $h(x)$, keep guessing. . .

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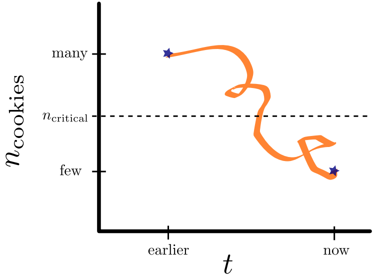
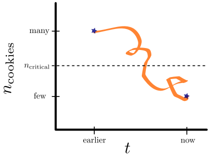


Bracketing

Intermediate value theorem $\Longrightarrow$ there must be some root between the guesses



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- Bracketing is essential.

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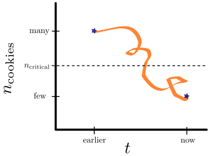

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- If *all* your guesses have the same sign for $h(x)$, you're a bit screwed – find something better than guessing. Actually, work out how to guess smarter.

Bracketing

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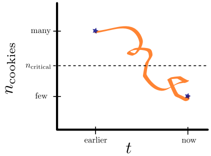

- The point of root-finding is to refine these ‘brackets’ as quickly as possible.
- Bracketing is essential.
- If *all* your guesses have the same sign for $h(x)$, you’re a bit screwed – find something better than guessing. Actually, work out how to guess smarter.
- Always eyeball your function before trying to find its roots, unless you know it very well.

Let's not get carried away. . .

Q

How do I bracket a root in more than 1D?

Let's not get carried away. . .

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Put it in a (hyper)box.

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But then how do I hunt it down?

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How do I bracket a root in more than 1D?

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But then how do I hunt it down?

A

With extreme difficulty. In general you can't. But of course you'll know it when (if) you find it :) Multi-D root finding is a dog – don't do it unless you really, really have to – or know the function really well.

Let's not get carried away. . .

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Why the hell does Pat only ask questions that have no real answers?

Outline

1. The problem
2. Solutions
   - Bisection
   - Brent's Method
   - Newton-Raphson

Outline

Bisection

Divide and conquer:

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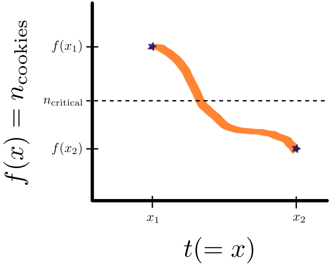

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Divide and conquer:

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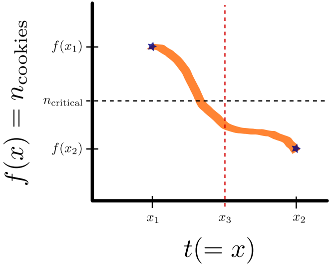

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Divide and conquer:

1. Start with a root bracketed by values x_1 and x_2
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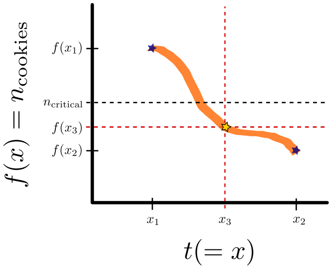

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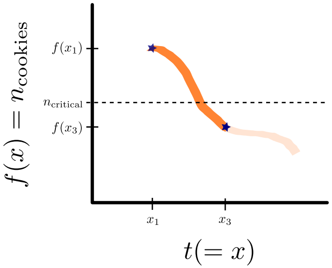

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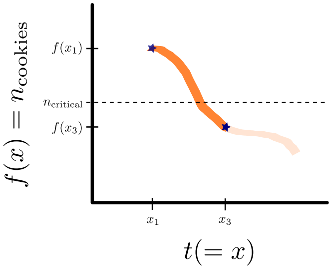

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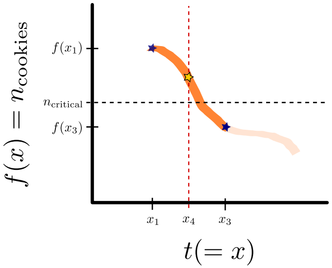

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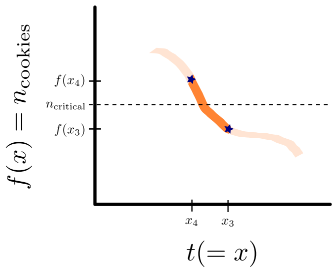


Improving on bisection

General idea for improving is to use some (convergent) approximation / guess function

- Linear interpolation = secant, false position method
- Exponential functions = Ridder's method
- Quadratic interpolation (+bisection) = Müller's method
- Inverse quadratic interpol (+bisection) = Brent's method
- Tangent extrapolation = Newton-Raphson

Outline

1. The problem
2. Solutions
   - Bisection
   - Brent's Method
   - Newton-Raphson

Richard Brent

- mathematician, ANU (Canberra)
- actually alive(!)

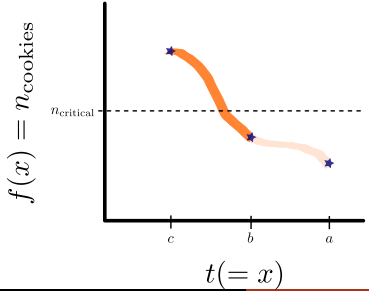
Features (of method, not Brent):

- Combines root bracketing, bisection, higher-order interpolation and careful error monitoring
  $\Longrightarrow$ Goldilocks Algorithm
- Inverse quadratic interpolation $+$ bisection
- Switches between, depending on which is performing better
- Pros: fast, über-reliable, accurate
  $\Longrightarrow$ the one-stop shop for 1D roots
- Cons: Reasonably complicated

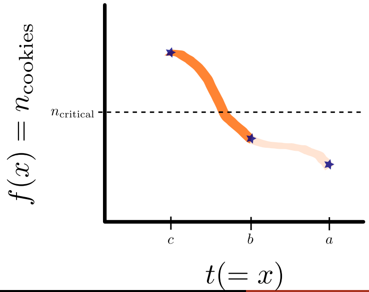
Let's begin with just the interpolation. . .

You work with 3 points: *a*, *b*, *c*

- *b* is your current best guess for the root, so $|f(b)| < |f(a)|, |f(c)|$
- *c* is the 'contrapoint' i.e. opposite side of *x* axis to *b*, so the root is always bracketed by *b* and *c*
- *a* is the previous best guess for the root (i.e. to first approximation $a_j = b_{j-1}$)

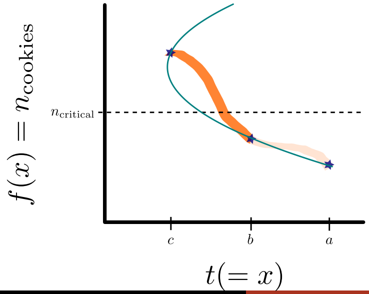


Stepping through inverse quadratic interpolation...



1. Fit an inverse parabola through $f_{a,b,c} = f(a), f(b), f(c)$

$$x = \frac{(y-f_b)(y-f_c)}{(f_a-f_b)(f_a-f_c)}a + \frac{(y-f_a)(y-f_c)}{(f_b-f_a)(f_b-f_c)}b + \frac{(y-f_a)(y-f_b)}{(f_c-f_a)(f_c-f_b)}c \qquad (3)$$

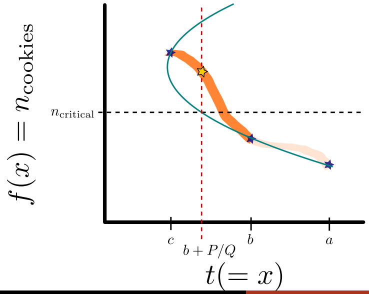


1. Fit an inverse parabola through $f_{a,b,c} = f(a), f(b), f(c)$
2. Find the point at which $y = 0$

$$x = b + P/Q \tag{4}$$

where

$$R \equiv f(b)/f(c), \quad S \equiv f(b)/f(a), \quad T \equiv f(a)/f(c)$$
$$P \equiv S[T(R - T)(c - b) - (1 - R)(b - a)]$$
$$Q \equiv (T - 1)(R - 1)(S - 1) \tag{5}$$



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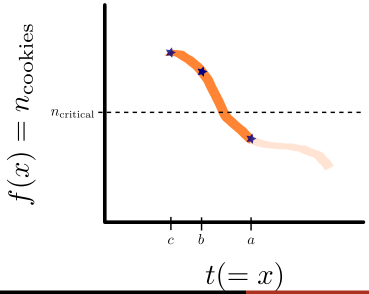
2. Find the point at which $y = 0$
3. This is your new b; the old b becomes a; discard the old a



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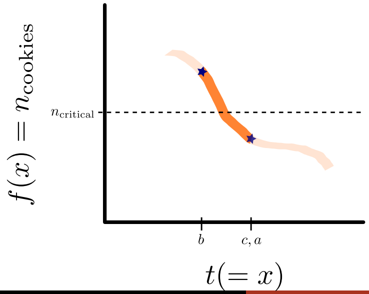

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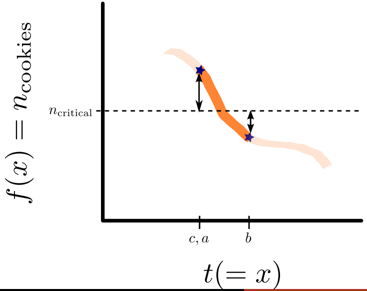

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Q

How do we proceed when we are down to only 2 points (e.g. here, and at the start of the search)?

A

Question 2.a) in Assignment 2 deals with this.

Inverse quadratic function vs. straight quadratic

- Quadratic
  - without bracketing: sometimes has no roots / complex roots
    $\Longrightarrow$ no new suggestion for b / or complex b
    $\Longrightarrow$ inefficient strategy for real roots - but good for complex roots (Müllers algo)
  - with bracketing: always has a root, always in brackets
- Inverse
  - inverse means no quadratic formula required for $y = 0$
    $\Longrightarrow$ no square root to take
    $\Longrightarrow$ less round-off error, quicker
  - fast if started near a root – BUT can end up outside the brackets
    $\Longrightarrow$ not robust
    $\Longrightarrow$ must be paired with careful bracket monitoring and bisection fallback

When to bisect I

(Brent's) Standard Condition

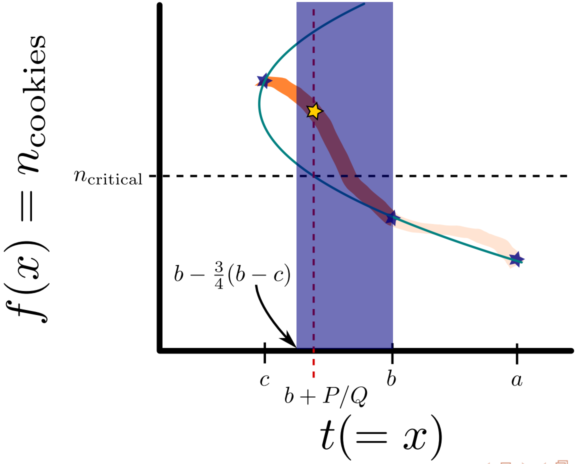
Trigger a bisection step instead of an interpolation step if:

Interpolation suggests a new point more than 3/4 of the way from b to c

$$\left|\frac{P}{Q}\right| \geq \frac{3}{4}|c - b| \tag{6}$$

(Remembering that $b_{\text{new}} = b + P/Q$)

When to bisect I



When to bisect II

Further conditions (these are apparently Brent's main addition):

- If the previous step $j-1$ was a bisection:

  Allow an interpolation at step j so long as both

  a) $\left|\frac{P}{Q}\right|_j < \frac{1}{2}\left|\frac{P}{Q}\right|_{j-1}$

  b) $\left|\frac{P}{Q}\right|_{j-1} > \frac{\delta}{2}$

- If the previous step $j-1$ was an interpolation:

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  a) $\left|\frac{P}{Q}\right|_j < \frac{1}{2}\left|\frac{P}{Q}\right|_{j-2}$

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These ensure

- we don't get bogged down in little steps – either comparable to the required accuracy, or $\ll$ than provided by bisection
- at worst interpolation halves bracket in **2** steps (vs **1** step for bisection)

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Note: A few other subtleties in the algorithm are not mentioned here – you will find them as you program it for your assignment. NR is pretty sparse on explanation – Wikipedia is surprisingly good, but still misses a few things.

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   - Bisection
   - Brent's Method
   - Newton-Raphson

The Newton-Raphson method

- Very famous routine
- Requires ability to evaluate both function and derivative

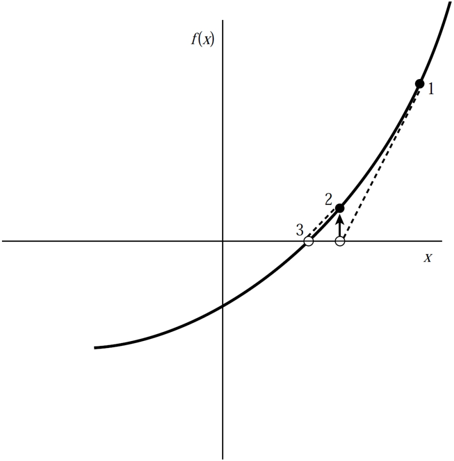
How-to, from a first guess a:

1. Linearise $f(x)$ around $x = a$
   (Taylor expansion to linear order)
2. Take y-intercept of linearised function as next guess

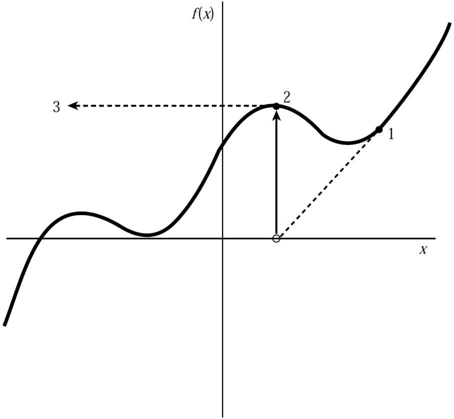
$$a_j = a_{j-1} + \delta = a_{j-1} + -\frac{f(a_{j-1})}{f'(a_{j-1})} \tag{7}$$

3. Repeat

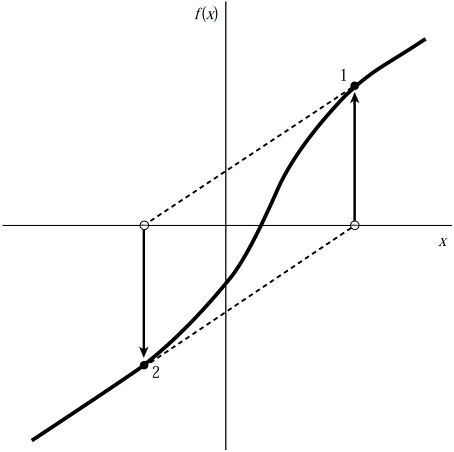
Example 1 – good



Example 2 – bad



Example 3 – ugly



Comments on Newton-Raphson:

- Fast!! Not robust though
- Like everything else, can be made more robust by embedding bisection and good bracketing
- Not worth using in 1D unless you have analytic derivatives (but even then Brent's just about as good)
- Good for multi-D though as there is little else!!

Housekeeping

- Issues with Assignment 1?
- Next lecture: Random Numbers (Monday Jan 28)