Rootfinding

Background
    Square roots

Convergence rates
    faster is better (if less costly)

Bracketing and bisection
    find the root and then zoom in

Secant, false position,
    faking derivatives

Brent's method
    improvements

Using derivatives: Newton-Raphson
    quadratic convergence

Fractals
    basins of attraction

Deflation of polynomials
    ??

n-dimensions: difficulties
    Newton-Raphson is all there is

To find Square root of N

Start with $x_0 = 1$

$$x_{i+1} = 1/2\ (x_i + N/x_i) \text{ until } |x_{i+1} - x_i| < \varepsilon$$

Samples $N = 2$	$N = 100$
$x_1 = 1.5000000000$	$x_1 = 50.5000000000$
$x_2 = 1.4166666667$	$x_2 = 26.2400990099$
$x_3 = 1.4142156863$	$x_3 = 15.0255301200$
$x_4 = 1.4142135624$	$x_4 = 10.8404346730$
	$x_5 = 10.0325785110$
	$x_6 = 10.0000528956$
	$x_7 = 10.0000000001$
	$x_8 = 10.0000000000$

Digits 1-->3-->6-->11+   Digits 0,0,1,2,3,6,11,12+

Once the methods get established the number of correct digits double.

But, if N = 1E-8

x0 = 0.5000000050
x1 = 0.2500000125
x2 = 0.1250000262
x3 = 0.0625000531
x4 = 0.0312501066
x5 = 0.0156252133
x6 = 0.0078129266
x7 = 0.0039071033
x8 = 0.0019548314
x9 = 0.0009799734
x10 = 0.0004950889
x11 = 0.0002576436
x12 = 0.0001482285
x13 = 0.0001078459
x14 = 0.0001002854
x15 = 0.0001000004
x16 = 0.0001000000

down by halves until close then by squaring

N = 2, start at -1

x0 = -1.5000000000
x1 = -1.4166666667
x2 = -1.4142156863
x3 = -1.4142135624

What if start at 0?

Issues in Root Finding

Choosing starting point
Assuring convergence
Rate of convergence.

Simple Idea -- Bracket a root

if $f(a) < 0 < f(b)$, there's a root in $[a,b]$

well maybe

This doesn't extend to higher than 1D.

Once you have a bracket -- Bisection

L = a, R = b;
compute M = (L+R)/2, and f(M);
if f(M) < 0 R = M; else L = M:

Analysis

You divide the size of the interval in half at each iteration

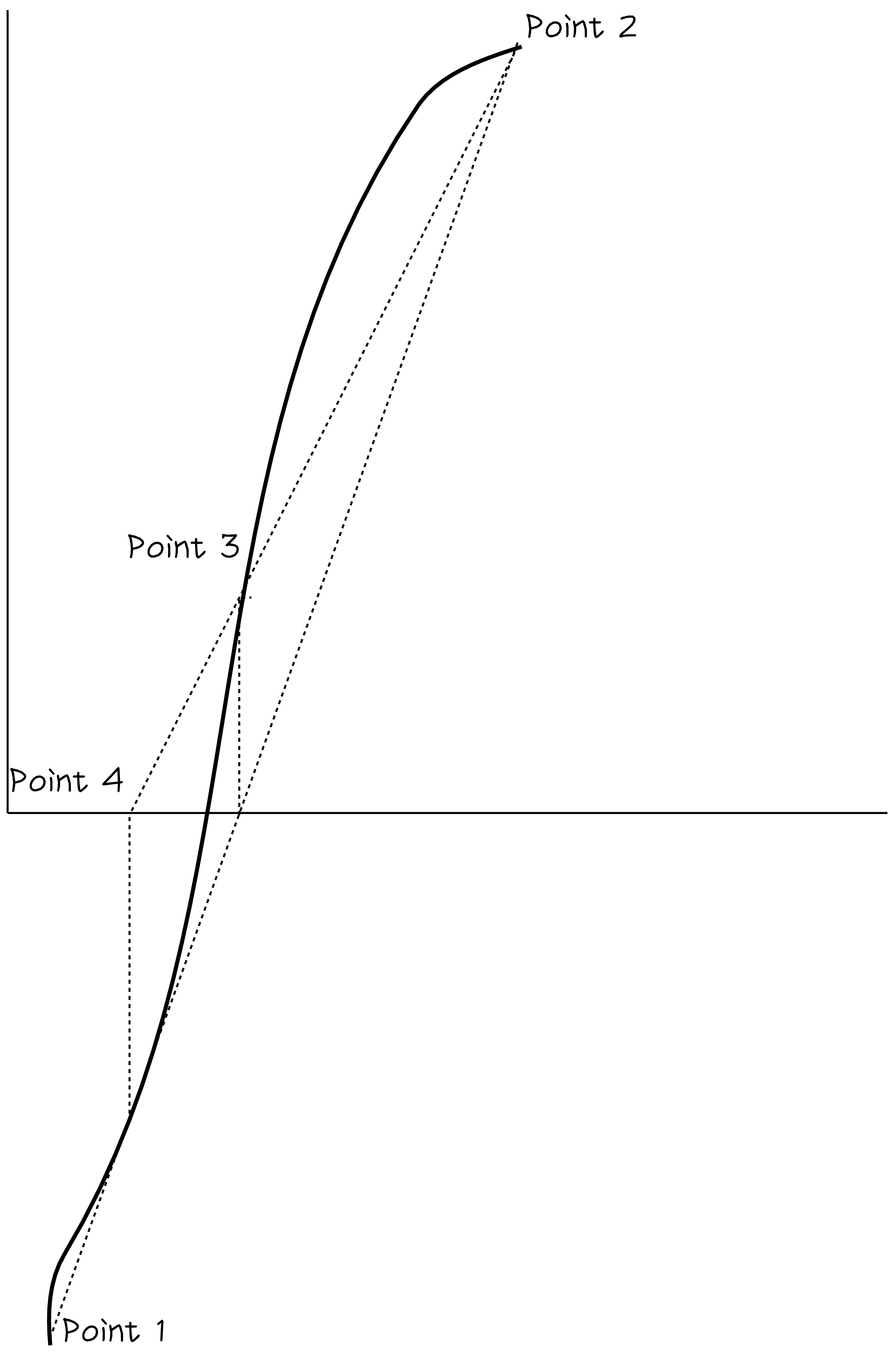
$e_{i+1} = e_i/2$

Linear convergence.

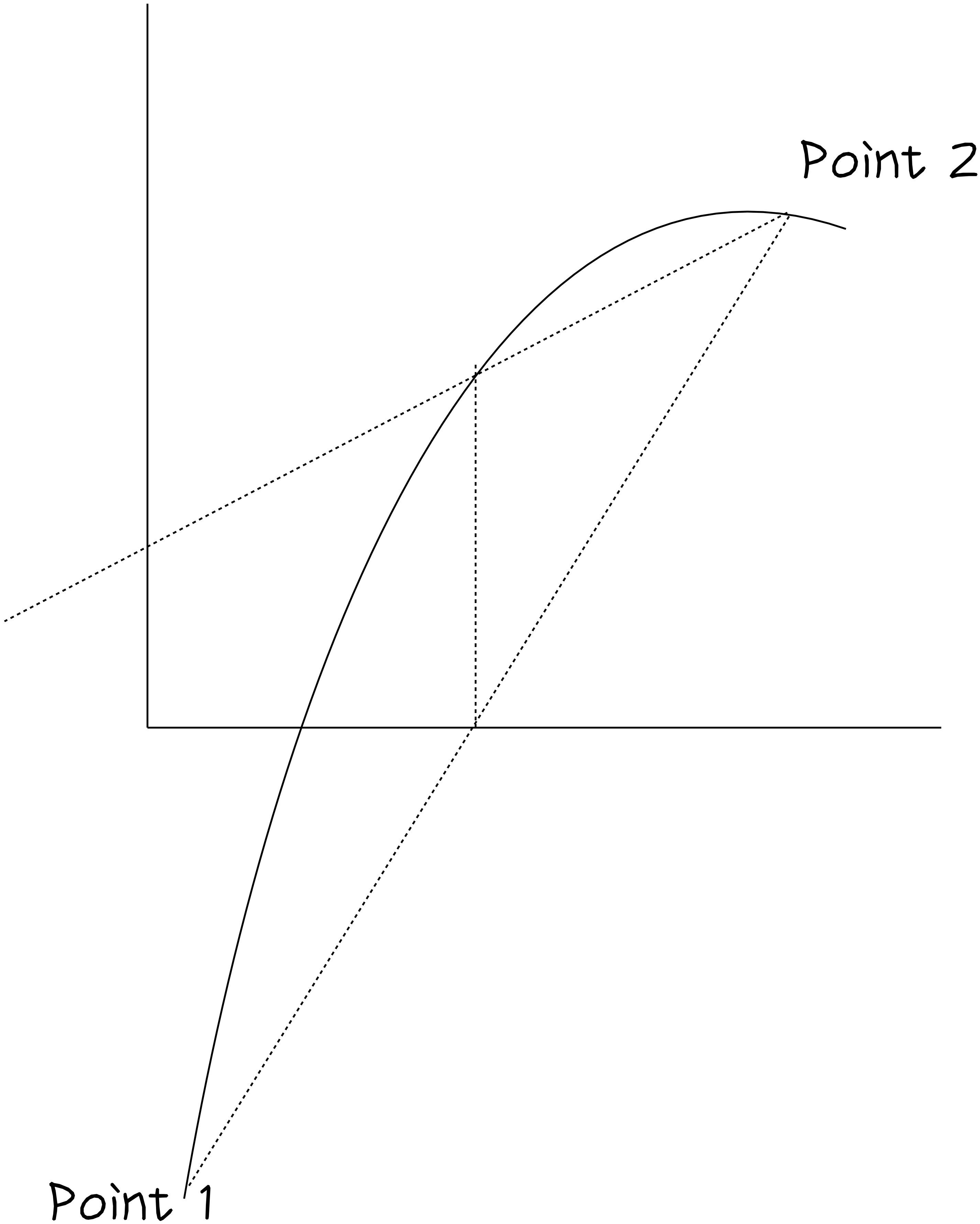
Square root method seemed to have

$e_{i+1} = e_i^2$ **quadratic convergence**

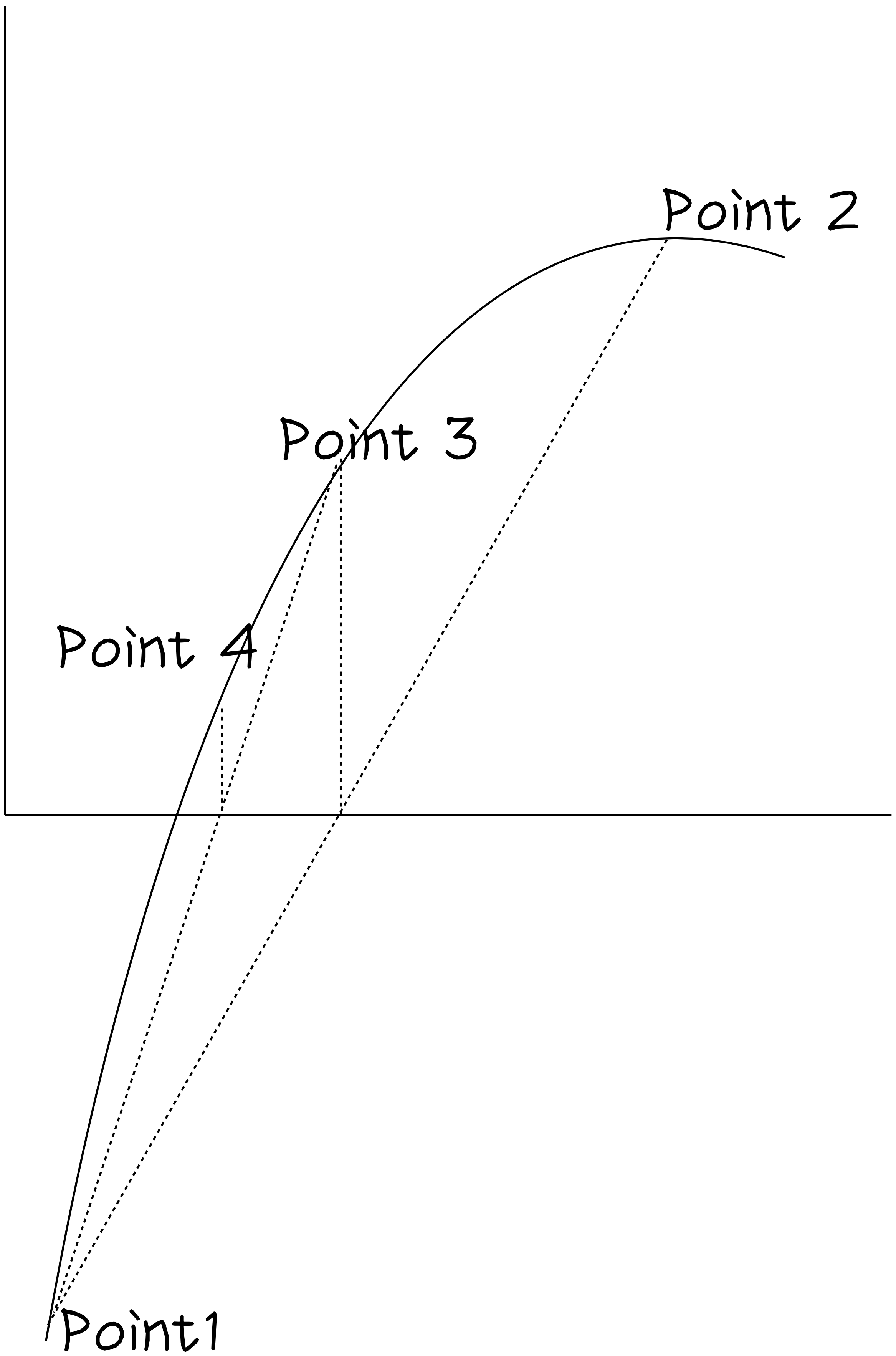
Secant Method Convergence 1.618



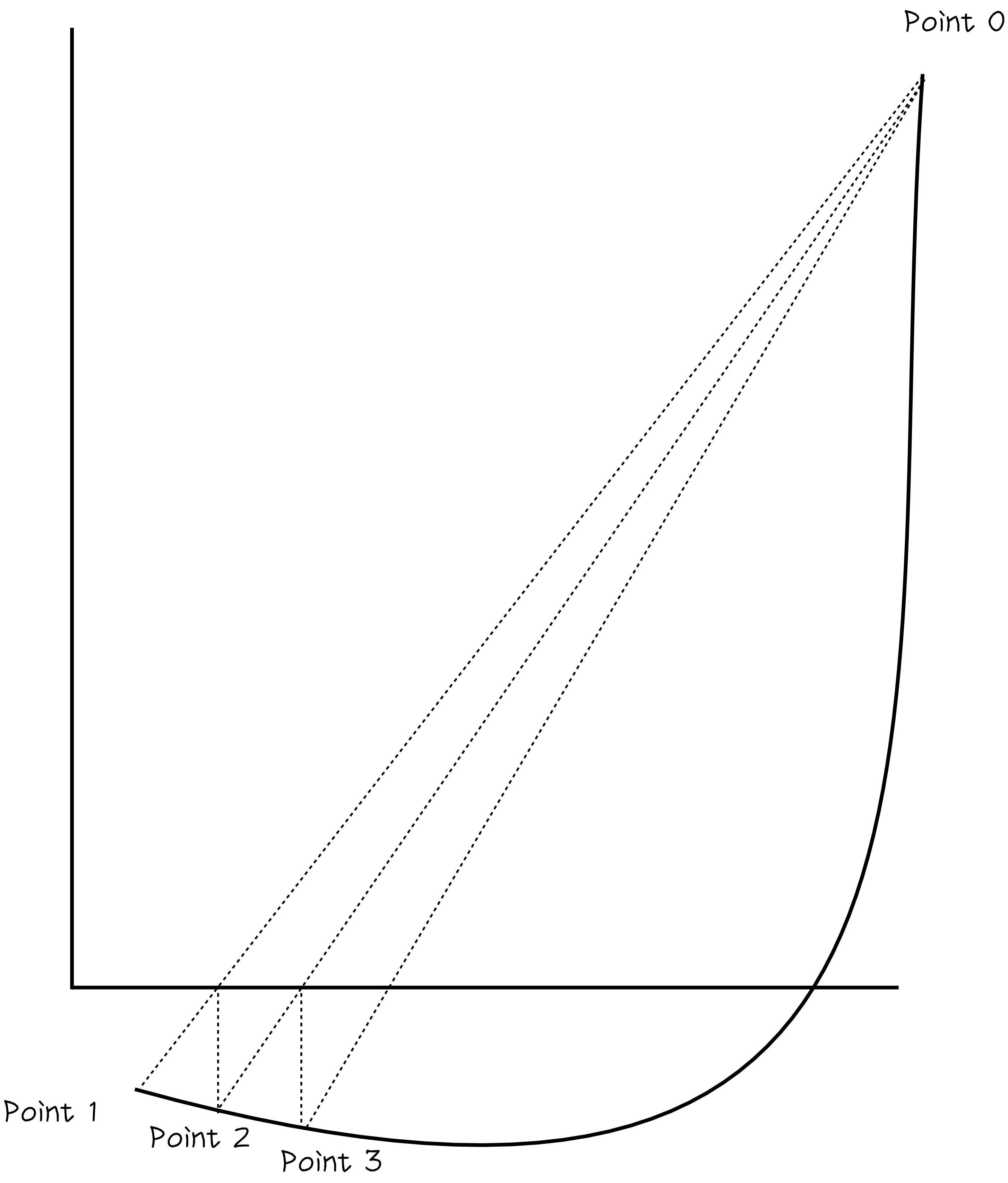
Secant Method -- Bad Case



Method of False Position (Regula Falsi)
Rate of Convergence 1.618



Bad case for Method of False Position



Improvement -- Brent's Method

Combine

- root bracketing
- bisection
- inverse quadratic interpolation

Inverse quadratic interpolation

Instead of fitting a line thru 2 points,
fit a quadratic thru 3 points.

Find the zero.

If it's in the bracket, use it

Otherwise use the midpoint.

The quadratic goes thru (a,f(a)),(b,f(b)),(c,f(c)) and has a root (ie y=0) at

$$x = b + P/Q \text{ where}$$
$$P = S(t(R-T)(c-b) - (1-R)(b-a))$$
$$Q = (T-1)(R-1)(S-1)$$

and $R = f(B)/f(c)$, $S = f(b)/f(a)$, $T = f(a)/f(c)$

P/Q should be small and in all cases, the new x should lie in the bracketed interval.

If there's a problem, just take a bisection step.

Brent's method is recommended if derivatives are not easily available.

Newton's (Raphsen) Method

If f() well-behaved, can write as Taylor series

$$f(x) = f(x_0) + (x-x_0)\, f'(x_0) + \ldots$$

If we want to find x such that $f(x) = 0$,

$$x = x_0 - f(x_0)/f'(x_0)\,.$$

So, iteration is $\quad x_{i+1} = x_i - f(x_i)/f'(x_i)$

Imagine $f(x) = x^2 - N$,
So $f'(x) = 2x$,
So

$$x_{i+1} = x_i - (x_i^2 - N)/(2x_i) = 1/2\ (x_i + N/x_i)$$

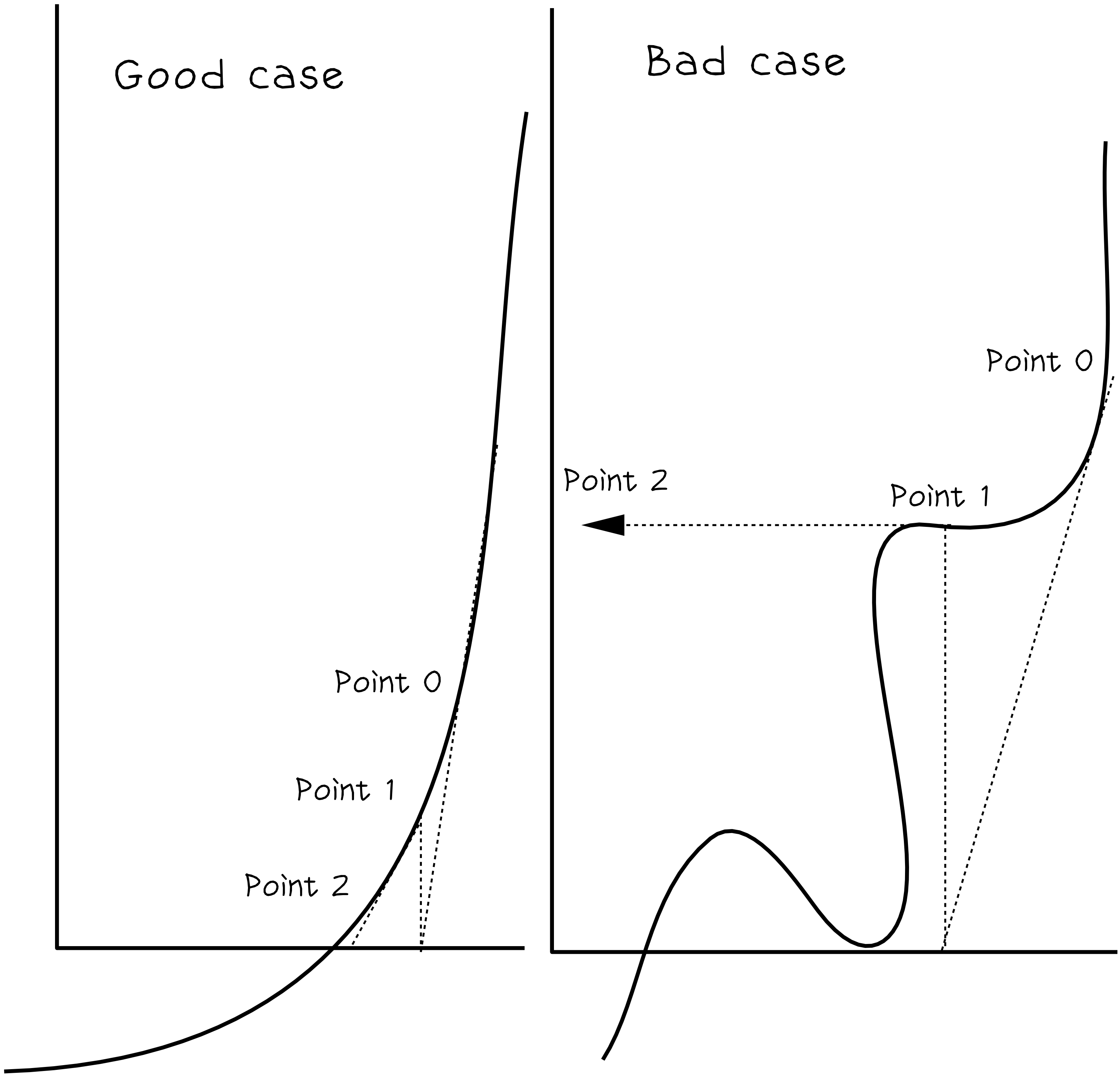
Cube roots, $f(x) = x^3 - N$

$$x_{i+1} = x_i - (x_i^3 - N)/(3x_i^2) = 1/3\ (2x_i^2 + N)/x_i^3$$

For cube roots, could also carry Taylor series to one extra term....

Taylor series -- Pros and Cons

+ Quadratic convergence
+ Extends to higher dimensions
- Can be unstable



Showing the quadratic convergence

$f(x+\varepsilon) = f(x) + \varepsilon f'(x) + \varepsilon^2 f''(x)/2 + \ldots$
$f'(x+\varepsilon) = f'(x) + \varepsilon f''(x) + \ldots$

$x_{i+1} = x_i - f(x_i)/f'(x_i),$

so $\varepsilon_{i+1} = \varepsilon_i - f(x_i)/f'(x_i)$

$= \quad \varepsilon_i - (\varepsilon f'(x_i) + \varepsilon^2 f''(x_i)/2)/(f'(x_i) + \varepsilon f''(x_i))$

$= \quad -e_i^2 f''(x_i) / 2f'(x_i)$

Near the root, it converges quadratically.
==> double the digits of precision per iteration

If you can't get the derivative, you could approximate by $(f(x+dx) - f(x))/dx$.

In a flat region, you can keep using the same derivative.

Basins of convergence

Whether you converge and to which root you converge is determined by where you start.

We saw this in the square root example

Iterating in complex plane to solve a cubic

$z^3 - 1 = 0$ leads to the iteration

$$z_{j+1} = z_j - (z_j^3 - 1)/(3z_j^2)$$

Mark the points that converge to z=1

Pretty pictures, fractal mountain, Julia sets, Hollywood Special effects, ...

Deflation of polygons

How to find all roots rather than just finding the first root.

Straightforward method

Locate the root r of $P(x)$.
Do synthetic division $P(x) = (x-r)Q(x)$
Repeat

For complex roots (with real coefficients),
they come in pairs $(a+bi, a-bi)$.
so divide by

$$(x-(a+bi))(x-(a-bi)) = x^2 - 2ax + (a^2 + b^2).$$

Things to worry about.

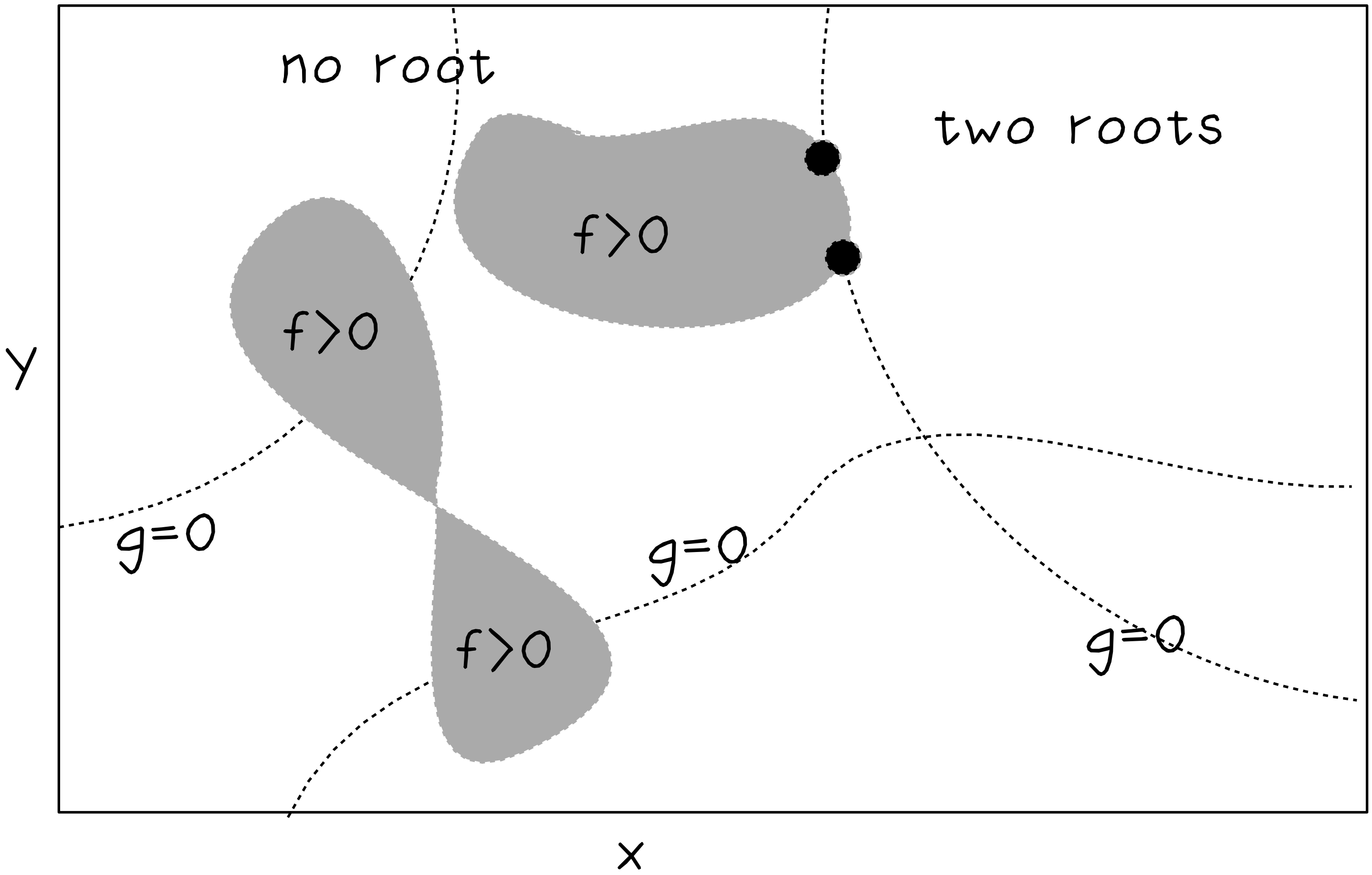
1. You don't get the root exactly, so each new $Q(x)$ is less accurate.

2. Multiple roots are a nuisance.

Newton-Raphson in higher dimensions

It's an ugly scene

$f(x,y) = 0,\ g(x,y) = 0$



Imagine $F_i(x_1, x_2, \ldots, x_n) = 0 \quad i = 1, \ldots, n$

Taylor series

$$F_i(\mathbf{x}+d\mathbf{x}) = F_i(\mathbf{x}) + \sum_{j=1,n} \mathrm{partial}(F_j \ \mathrm{wrt}\, x_j)\ dx_j \ +O((d\mathbf{x})^2)$$

$$\mathbf{F}(\mathbf{x}+d\mathbf{x}) = \mathbf{F}(\mathbf{x}) + \mathbf{J}d\mathbf{x} + O((d\mathbf{x})^2).$$

Solve $\mathbf{j}d\mathbf{x} = \mathbf{F}$ by inverting Jacobian