

• Introduction

Root-finding: to find the value of x such that it satisfies equation $f(x) = 0$.

How to find the one-thirds power of 12, $x = 12^{1/3}$, by four operations (+, −, ×, /) calculator?

It is equivalent to find the root of $f(x) = x^3 - 12 = 0$.

Minimization of total energy:

$$\frac{\partial E(x)}{\partial x} = 0 \ .$$

Maximization of entropy:

$$\frac{\partial S(x)}{\partial x} = 0 \ .$$

Traveling sales person problem, etc.

• Polynomial

$$\begin{aligned} P_n(x) &= \sum_{k=0}^n a_k x^k \\ &= a_0 + a_1 x + \cdots + a_{n-1} x^{n-1} + a_n x^n . \end{aligned} \quad (1)$$

1. Quadratic Equation

$$a_0 + a_1 x + a_2 x^2 = 0 \quad (2)$$

Solution (**two** roots):

$$x_{\pm} = \frac{1}{2a_2} \left(a_1 \pm \sqrt{a_1^2 - 4a_0 a_2} \right) \quad (3)$$

Question: how do you get this solution?

2. Cubic Equation

$$a_0 + a_1 x + a_2 x^2 + a_3 x^3 = 0 \quad (4)$$

Solution: (first scale a_3 to 1).

$$\text{step 1 : } x = y - \frac{a_2}{3} \quad \Rightarrow \quad y^3 + py + q = 0 \quad (5)$$

$$p = -\frac{a_2^2}{3} + a_1, \quad q = \frac{2a_2^3}{27} - \frac{a_2 a_1}{3} + a_0 . \quad (6)$$

step 2: solve Eq. (5) (**three** roots)

$$y_1 = u + v; y_2 = \omega_1 u + \omega_2 v; y_3 = \omega_2 u + \omega_1 v \quad (7)$$

where

$$\omega_1 = \frac{-1 + \sqrt{3}i}{2}, \quad \omega_2 = \frac{-1 - \sqrt{3}i}{2} = \omega_1^2 , \quad (8)$$

$$u^3 = -\frac{q}{2} + \sqrt{\left(\frac{q}{2}\right)^2 + \left(\frac{p}{2}\right)^3} \quad (9)$$

$$v^3 = -\frac{q}{2} - \sqrt{\left(\frac{q}{2}\right)^2 + \left(\frac{p}{2}\right)^3} \quad (10)$$

3. *Quartic Equation*

$$a_0 + a_1x + a_2x^2 + a_3x^3 + a_4x^4 = 0 \quad (11)$$

Solution (**four** roots): see reference book.

For any order n , there *always* exists n roots such that

$$P_n(x) = a_n(x - x_1)(x - x_2) \cdots (x - x_{n-1})(x - x_n) . \quad (12)$$

x_i are complex numbers in general.

• Taylor Series

Assume function $f(x)$ has a continuous n th derivative in the interval of $a \leq x \leq b$. Then

$$\int_a^{x_1} dx_0 f^{[n]}(x_0) = f^{[n-1]}(x_1) - f^{[n-1]}(a) . \quad (13)$$

$$\begin{aligned} & \int_a^{x_2} \int_a^{x_1} dx_0 dx_1 f^{[n]}(x_0) \\ &= \int_a^{x_2} dx_1 \left(f^{[n-1]}(x_1) - f^{[n-1]}(a) \right) \\ &= f^{[n-2]}(x_2) - f^{[n-2]}(a) - (x_2 - a) f^{[n-1]}(a) . \end{aligned} \quad (14)$$

After n integrations, we have

$$\begin{aligned} & \int_a^{x_n} \cdots \int_a^{x_1} dx_0 \cdots dx_{n-1} f^{[n]}(x) \\ &= f(x_n) - f(a) - (x_n - a) f'(a) - \frac{(x_n - a)^2}{2!} f''(a) \\ & \quad - \frac{(x_n - a)^3}{3!} f'''(a) \cdots - \frac{(x_n - a)^{n-1}}{(n-1)!} f^{[n-1]}(a) . \end{aligned} \quad (15)$$

$x \rightarrow x_n$, we obtain **Taylor series**:

$$\begin{aligned} f(x) &= f(a) + (x - a) f'(a) + \frac{(x - a)^2}{2!} f''(a) \\ & \quad + \frac{(x - a)^3}{3!} f'''(a) + \cdots + \frac{(x - a)^{n-1}}{(n-1)!} f^{[n-1]}(a) \\ & \quad + R_n(x) . \end{aligned} \quad (16)$$

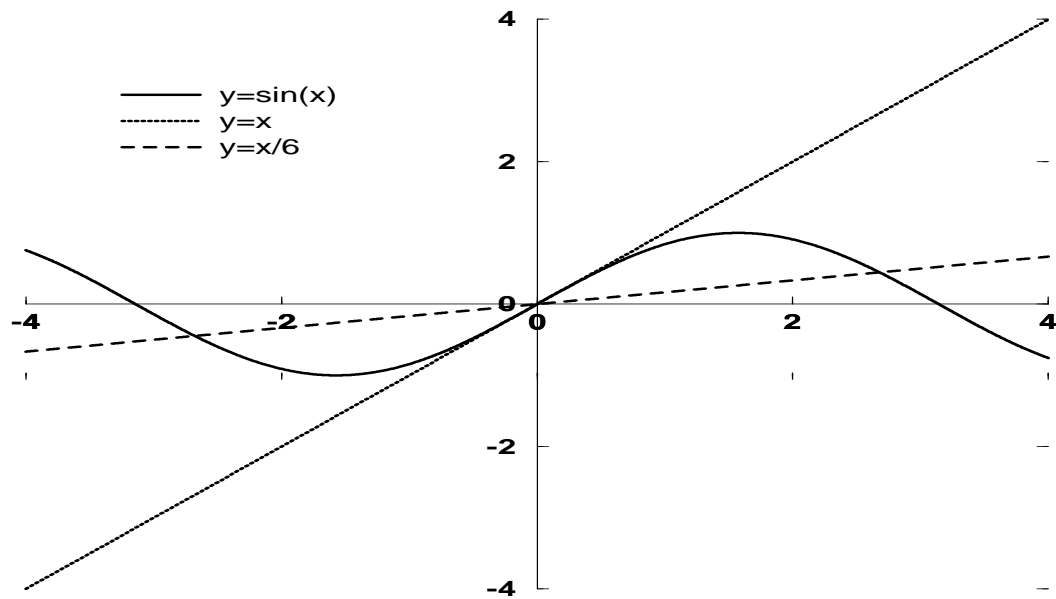
Remainder $R_n(x)$ can be written as

$$R_n(x) = \frac{(x - a)^n}{n!} f^{[n]}(\xi), \quad a \leq \xi \leq x . \quad (17)$$

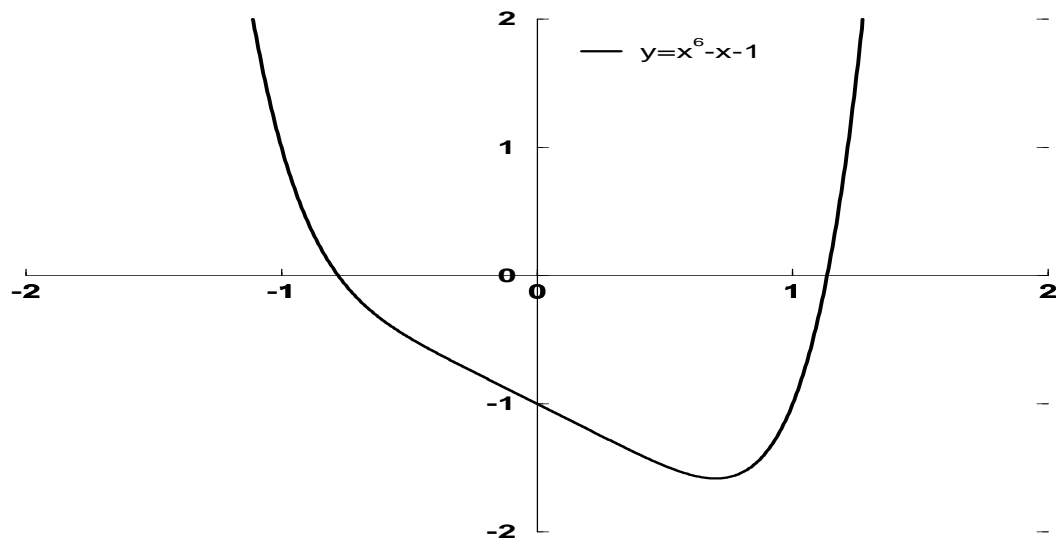
• Graphic Solution

The simplest way, unaccurate, but very powerful.

Example 1: $\sin(x) = ax$.



Example 2: $f(x) = x^6 - x - 1$.



• The Bisection Algorithm

Probably the simplest method, but very powerful.

Task: find the root x such that $f(x) = 0$.

1. Choose two values, x_{left} and x_{right} , with $x_{left} < x_{right}$, such that $f(x_{left})f(x_{right}) < 0$. There must be a value of x such that $f(x) = 0$ in the interval $[x_{left}, x_{right}]$.
2. Choose the midpoint, $x_{mid} = x_{left} + \frac{1}{2}(x_{right} - x_{left}) = \frac{1}{2}(x_{right} + x_{left})$, as the guess for x .
3. If $f(x_{mid})$ has the same sign as $f(x_{left})$, then replace x_{left} by x_{mid} ; otherwise, replace x_{right} by x_{mid} . Thus, we halved the interval for the location of the root.
4. Repeat steps 2 and 3 until the desired level of precision is achieved.

Error Bounds: let $a = x_{left}$ and $b = x_{right}$ at beginning with error tolerance ϵ and number of iterations n , then (see **Error Analysis**)

$$\frac{1}{2^n}(b - a) \leq \epsilon .$$

• Error Analysis

Absolute error

$$= \left| \text{true value} - \text{approximate value} \right| .$$

Relative error

$$= \left| \frac{\text{true value} - \text{approximate value}}{\text{true value}} \right| .$$

Approximate relative error

$$= \left| \frac{\text{best approximation} - \text{approximate value}}{\text{best approximation}} \right| .$$

Example: the bisection method

$$\begin{aligned} |x - x_{mid}| &\leq x_{mid} - x_{left} = x_{right} - x_{mid} \\ &= \frac{1}{2}(x_{right} - x_{left}) = \dots = \frac{1}{2^n}(b - a) . \end{aligned}$$

$$|x - x_{mid}^n| \leq \frac{1}{2^n}(b - a) \leq \epsilon .$$

$$n \geq \frac{\log((b - a)/\epsilon)}{\log 2} .$$

• The Newton-Raphson Method

Assume that we have a good “guess” of solution x^* so that $(x - x^*)$ is a small number. By Taylor expansion, we have

$$0 = f(x^*) \approx f(x) + (x^* - x)f'(x) .$$

Thus

$$x^* = x - \frac{f(x)}{f'(x)} \quad \Rightarrow \quad x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} . \quad (18)$$

Example 1: $f(x) = x^6 - x - 1, f'(x) = 6x^5 - 1$.

n	x_n	$f(x_n)$	$x_n - x_{n-1}$
0	1.5	8.89E+1	
1	1.30049088	2.54E+1	-2.00E-1
2	1.18148042	5.38E-1	-1.19E-1
3	1.13945559	4.92E-2	-4.20E-2
4	1.13477763	5.50E-4	-4.68E-3
5	1.13472415	7.11E-8	-5.35E-5
6	1.13472414	1.55E-15	-6.91E-9

Example 2: $f(x) = x^2 + 1, f'(x) = 2x$.

n	x_n	$f(x_n)$	$x_n - x_{n-1}$
0	0.57735027	1.3333	
1	-0.57735027	1.3333	-1.1547
2	0.57735027	1.3333	1.1547
3	-0.57735027	1.3333	-1.1547
4	0.57735027	1.3333	1.1547
5	-0.57735027	1.3333	-1.1547
6	0.57735027	1.3333	1.1547

Error in Newton-Raphson

Let $\epsilon_n = x^* - x_n$ and from Eq. (18), we have

$$\epsilon_{n+1} = \epsilon_n + \frac{f(x_n)}{f'(x_n)} .$$

Do Taylor expansion to second order, we have

$$\begin{aligned} f(x^*) &= f(x_n) + (x^* - x_n)f'(x_n) \\ &\quad + \frac{(x^* - x_n)^2}{2!}f''(x_n) + \cdots . \end{aligned} \tag{19}$$

Since $0 = f(x^*)$ so we have

$$f(x_n) = -\epsilon_n f'(x_n) - \frac{\epsilon_n^2}{2} f''(x_n) .$$

$$\frac{f(x_n)}{f'(x_n)} = -\epsilon_n - \frac{\epsilon_n^2 f''(x_n)}{2f'(x_n)} .$$

$$\epsilon_{n+1} = -\frac{\epsilon_n^2 f''(x_n)}{2f'(x_n)} . \tag{20}$$

The error in x_{n+1} is proportional to the *square* of the error in x_n ($p = 2$). Convergence could be very rapid!

Error Estimation

$$x^* - x_n \approx x_{n+1} - x_n \quad f'(x^*) \neq 0 . \tag{21}$$

This method fails if $f'(x^*) = 0$! Now what?

• Rates of Convergence

One must concern the speed of convergence of an iteration method. We say that a sequence $x_n; n \geq 0$ converges to x^* with an *order of convergence* $p > 0$ if

$$|x^* - x_{n+1}| \leq c|x^* - x_n|^p, \quad n \geq 0 \quad (22)$$

for some constant $c \geq 0$.

1. *Linear convergence*: $p = 1$, $c < 1$?

e.g., Bisection method.

2. *Quadratic convergence*: $p = 2$.

e.g., Newton-Raphson method.

3. *Cubic convergence*: $p = 3$.

• The Secant Method

It could be difficult to calculate $f'(x)$.

By Taylor expansion

$$f(x_n) \approx f(x_{n-1}) + (x_n - x_{n-1})f'(x_n) .$$

$$f'(x_n) \approx \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}} ,$$

$$\begin{aligned} x_{n+1} &= x_n - \frac{f(x_n)}{f'(x_n)} \\ &\approx x_n - f(x_n) \frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})} \end{aligned} \quad (23)$$

Error Analysis

One can show that $|x^* - x_{n+1}| \leq c|x^* - x_n|^p$, with $p = (\sqrt{5} + 1)/2 = 1.62$.

Example 1: $f(x) = x^6 - x - 1, x_0 = 2.0, x_1 = 1.0$.

n	x_n	$f(x_n)$	$x_n - x_{n-1}$
2	1.01612903	-9.15E-1	1.61E-2
3	1.19057777	6.57E-2	1.74E-1
4	1.11765583	-1.68E-1	-7.29E-2
5	1.13253155	-2.24E-2	1.49E-2
6	1.13481681	9.54E-4	2.29E-3
7	1.13472365	-5.07E-6	-9.32E-5
8	1.13472414	-1.13E-8	4.92E-7

• The False Position Method

Approximate

$$f(x) \approx \frac{x-b}{a-b}f(a) + \frac{x-a}{b-a}f(b) ,$$

then

$$f'(x) = \frac{f(b) - f(a)}{b - a} ,$$

and (Newton-Raphson)

$$\bar{x} = x - \frac{f(x)}{f'(x)} = \frac{af(b) - bf(a)}{f(b) - f(a)} .$$

If $f(a)f(\bar{x}) < 0$, replace b by \bar{x} ;

If $f(b)f(\bar{x}) < 0$, replace a by \bar{x} .

Continue \dots .

• The Hybrid Bisection/Newton-Raphson Method

Bisection – *always* gives solution but *slowly* converges.

Newton-Raphson – converges *fast* but could *fail*.

Naturally, hybridize both of them.

Assume the root is bounded between $x = a$ and $x = b$, and the best current guess is $x = r$, then we want to know if the *next Newton-Raphson guess* is within the bounds, i.e.,

$$\begin{aligned} a &\leq \tilde{r} = r - \frac{f(r)}{f'(r)} \leq b \\ \Rightarrow 0 &\leq (r - a)f'(r) - f(r) = A(r) \\ 0 &\geq (r - b)f'(r) - f(r) = B(r) . \end{aligned} \tag{24}$$

Thus, if $A(r) \times B(r) \leq 0$, Newton-Raphson.

if $A(r) \times B(r) > 0$, Bisection.

Alternatively, just calculate $(\tilde{r} - a) \times (\tilde{r} - b)$.

The Hybrid Bisection/Secant Method

Same idea: if $a < x_{n+1} < b$ (Secant), no (Bisection).

Or make a simple replacement in the Hybrid

Bisection/Newton-Raphson routine.

• Iteration in General

Consider solving the equation $f(x) = 0$. One can rewrite it in various form such that

$$x = G(x) \quad \Rightarrow \quad x_{n+1} = G(x_n) ,$$

and iterative x_n with given error tolerance ϵ , say,

$$|x_{n+1} - x_n| \leq \epsilon.$$

The solution is also called *fixed point*: $x^* = G(x^*)$.

Convergence

1. Let $G(x)$ be a continuous function for an interval $[a, b]$, and suppose G satisfies the property

$$a \leq x \leq b \Rightarrow a \leq G(x) \leq b . \quad (25)$$

Then the equation $x = G(x)$ has at least one solution x^* in the interval $[a, b]$.

Proof: Define the function $f(x) = x - G(x)$. It is continuous for $a \leq x \leq b$. Moreover, $f(a) \leq 0$ and $f(b) \geq 0$. By the intermediate value theorem, there exists a point x^* in $[a, b]$ at which $f(x^*) = 0$.

2. Assume $G(x)$ and $G'(x)$ are continuous for $[a, b]$, and assume G satisfies Eq. (25). Further assume that $\lambda \equiv \text{Maximum}_{a \leq x \leq b} |G'(x)| < 1$. Then

(a) There is a unique solution x^* of $x = G(x)$ in the interval $[a, b]$.

(b) For any initial estimate x_0 in $[a, b]$, the iterates x_n will converge to x^* .

$$(c) \quad |x^* - x_n| \leq \frac{\lambda^n}{1 - \lambda} |x_0 - x_1|, \quad n \geq 0. \quad (26)$$

$$(d) \quad \lim_{n \rightarrow \infty} \frac{x^* - x_{n+1}}{x^* - x_n} = G'(x^*). \quad (27)$$

Proof: By using the mean value theorem, we have that for any two points w and z in $[a, b]$,

$$G(w) - G(z) = G'(c)(w - z)$$

for some c between w and z . Then

$$|G(w) - G(z)| = |G'(c)| |w - z| \leq \lambda |w - z|.$$

(a) Suppose that there are two solutions, α and β , then

$$\alpha - \beta = G(\alpha) - G(\beta).$$

$$|\alpha - \beta| \leq \lambda |\alpha - \beta|$$

$$(1 - \lambda)|\alpha - \beta| \leq 0$$

Since $\lambda < 1$, we must have $\alpha = \beta$.

(b) For any initial guess x_0 , the iterates x_n will all remain in $[a, b]$. Then

$$x^* - x_{n+1} = G(x^*) - G(x_n) = G'(c)(x^* - x_n)$$

$$|x^* - x_{n+1}| \leq \lambda |x^* - x_n| \leq \lambda^n |x^* - x_0|$$

Since $\lambda < 1$, $x_n \rightarrow x^*$ as $n \rightarrow \infty$.

(c) Let $n = 1$, we have

$$|x^* - x_0| \leq |x^* - x_1| + |x_1 - x_0|$$

$$| \leq \lambda |x^* - x_0| + |x_1 - x_0|$$

$$(1 - \lambda)|x^* - x_0| \leq |x_1 - x_0|$$

$$|x^* - x_0| \leq \frac{1}{1 - \lambda} |x_1 - x_0|$$

(d) Use previous results to write

$$\lim_{n \rightarrow \infty} \frac{x^* - x_{n+1}}{x^* - x_n} = \lim_{n \rightarrow \infty} G'(c) = G'(x^*)$$

3. If $|G'(x^*)| > 1$, then the iteration $x_{n+1} = G(x_n)$ will not converge to x^* .

Atiken's error estimate

From

$$x^* - x_n = G(x^*) - G(x_{n-1}) \approx G'(x^*)(x^* - x_{n-1})$$

we have

$$x^* - x_n \approx \lambda(x^* - x_{n-1})$$

then

$$x^* = x_n + \frac{\lambda}{1 - \lambda}(x_n - x_{n-1})$$

Let's estimate λ ,

$$\lambda_n = \frac{x_n - x_{n-1}}{x_{n-1} - x_{n-2}}, \quad n \geq 2 .$$

Then we get

$$x^* - x_n \approx \frac{\lambda_n}{1 - \lambda_n}(x_n - x_{n-1}) .$$

Example: $f(x) = x^2 - 5 = 0$, $x = \pm\sqrt{5} = \pm 2.2361$.

We can write

$$(I1) \quad x_{n+1} = 5 + x_n - x_n^2$$

$$(I2) \quad x_{n+1} = 5/x_n$$

$$(I3) \quad x_{n+1} = 1 + x_n - \frac{1}{5}x_n^2$$

$$(I4) \quad x_{n+1} = \frac{1}{2} \left(x_n + \frac{5}{x_n} \right) .$$

Start from $x_0 = 2.5$,

n	$x_n(I1)$	$x_n(I2)$	$x_n(I3)$	$x_n(I4)$
0	2.5	2.5	2.5	2.5
1	1.25	2.0	2.25	2.25
2	4.6875	2.5	2.2375	2.2361
3	-12.2852	2.0	2.2362	2.2361
$G'(\sqrt{5})$	$1 - 2\sqrt{5}$	-1.0	$1 - \frac{2}{5}\sqrt{5}$	0

Start from $x_0 = -2.5$,

n	$x_n(I1)$	$x_n(I2)$	$x_n(I3)$	$x_n(I4)$
0	-2.5	-2.5	-2.5	-2.5
1	-3.75	-2.0	-2.75	-2.25
2	-12.8125	-2.5	-3.2625	-2.2361
3	-171.9726	-2.0	-4.3913	-2.2361
$G'(\sqrt{5})$	$1 + 2\sqrt{5}$	-1.0	$1 + \frac{2}{5}\sqrt{5}$	0

What have we learned here?

- Continue ...

1. Accelerating the rate of convergence

In the Hybrid Bisection/Secant method, a *linear approximation* of the function is used to obtain the next approximation to the root, and then the end-points of the interval are *adjusted* to keep the root *bounded*. How about higher order approximation? Consider three points x_0, x_1 , and x_2 , and function evaluated at these points. Then approximate $f(x)$ by a *quadratic* function (2nd order)

$$f(x) \approx p(x) = a_2(x - x_2)^2 + a_1(x - x_2) + a_0 .$$

Let $f(x_3) \approx p(x_3) = 0$, we get

$$x_3 - x_2 = \frac{-a_1 \pm \sqrt{a_1^2 - 4a_2a_0}}{2a_2}$$

We expect x_3 approaches x_2 , thus

$$x_3 = x_2 - \frac{2a_0}{a_1 + \sqrt{a_1^2 - 4a_2a_0}}, \quad a_1 \geq 0 .$$

$$x_3 = x_2 - \frac{2a_0}{a_1 - \sqrt{a_1^2 - 4a_2a_0}}, \quad a_1 \leq 0 .$$

It is *robust, virtually failsafe, and no derivatives*.

2. Multiple Root

$$f(x) = (x - a)^m h(x)$$

When the Newton and Secant methods are applied to the calculation of a multiple root, the convergence of $x^* - x_n$ to zero is much slower than it would be for a simple root. In addition, there is a large *interval of uncertainty* as to where the root actually lies, because of the *noise* in evaluating $f(x)$.

One can show that when we use Newton's method to calculate a root of multiplicity m , the ratio of the error in successful iteration

$$\frac{x^* - x_n}{x^* - x_{n-1}} \rightarrow \lambda = \frac{m-1}{m},$$

so the error decreases at about the constant rate.

$$f(x) = (x - 1.1)^3(x - 2.1)$$

n	x_n	$f(x_n)$	$x^* - x_n$	Ratio
0	0.800000	0.03510	0.300000	
1	0.892857	0.01073	0.207143	0.690
2	0.958176	0.00325	0.141824	0.685
3	1.00344	0.00099	0.09656	0.681
4	1.03486	0.00029	0.06514	0.675
5	1.05581	0.00009	0.04419	0.678
6	1.07028	0.00003	0.02972	0.673
7	1.08092	0.00000	0.01908	0.642

Thus, with any root of multiplicity $m \geq 2$, the Bisection method is always better!

The only way to obtain accurate values for multiple roots is to analytically remove the multiplicity, obtaining a new function for which x^* is a simple root. How to proceed?

Determine m experimentally, then work on

$$F(x) = f^{(m-1)}(x) .$$

3. Stability of Roots

Ill-conditioned or *unstable* problems.

Very small errors in evaluating $f(x)$ will lead to very large changes in the roots of the function.

Example

$$\begin{aligned}f(x) &= (x-1)(x-2)(x-3)(x-4)(x-5)(x-6)(x-7) \\&= x^7 - 28x^6 + \dots\end{aligned}$$

$$F(x) = x^7 - 28.002x^6 + \dots$$

Root of f(x)	Root of F(x)
1	1.0000028
2	1.9989382
3	3.0331253
4	3.8195692
5	5.4586758 + 0.54012578 i
6	5.4586758 - 0.54012578 i
7	7.2330128

There is not much that can be done except to go to higher precision arithmetic. Or find other ways to formulate the problem.

4. Exhaustive Searching

Find all roots?

5. Function of n Variables

e.g., spin glass $E(\{S_i\}) = \sum_{ij} J_{ij} S_i S_j$, Hartree-Fock (mean-field) solution of many-body problems.

The task is to find out the roots of the row vector function

$$F(X) = [f_1(X), f_2(X), \dots, f_n(X)]$$

with $X = [x_1, x_2, \dots, x_n]$.

Using the Taylor expansion,

$$F(X^*) = F(X_n) - \delta X D(X_n) + O(\delta X^2) ,$$

where D is called the Jacobian matrix,

$$D_{ij}(X) = \frac{\partial f_j(X)}{\partial x_i} .$$

Thus Newton's method (matrix form)

$$X_{n+1} = X_n - \delta X = X_n - F(X_n) D^{-1}(X_n) .$$

One can apply other iteration schemes.

6. *There are many other root-finding methods!*

e.g., Chapter 9 of *Numerical Recipes*.

⋮

Mean Value Theorems

- **Intermediate Value Theorem**

Let $f(x)$ be a continuous function on the interval $a \leq x \leq b$. Let

$$M = \max\{f(x)\}, \quad m = \min\{f(x)\}$$

Then for every value v satisfying $m \leq v \leq M$, there is at least one point c in $[a, b]$ for which $f(c) = v$.

It is rather easy to understand this *intuitive result* graphically.

- **Mean Value Theorem**

Let $f(x)$ be continuous on the interval $a \leq x \leq b$, and also let it be differentiable for $a < x < b$. Then there is at least one point c in (a, b) for which

$$f(b) - f(a) = f'(c)(b - a)$$

• Integral Mean Theorem

Let $\omega(x)$ be a nonnegative integrable function on $[a, b]$, and let $f(x)$ be continuous on $[a, b]$. Then there is at least one point c in $[a, b]$ for which

$$\int_a^b dx \omega(x) f(x) = f(c) \int_a^b dx \omega(x)$$

In particular, if we take $\omega(x) = 1$, then

$$\int_a^b dx f(x) = f(c)(b - a)$$

for some c in $[a, b]$.