Numerical methods to solve $f(x) = 0$, $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$

$f$ is non-linear. Generally, pick $x_0 \in \mathbb{R}^n$, method generates $x_1, x_2, \ldots, x_n, \ldots$ and we hope $x_n$ converges to some $\overline{x}$, i.e. $\|x_n - \overline{x}\| \xrightarrow{n \to \infty} 0$, and $f(\overline{x}) = 0$.

Questions:

- How fast does $x_n$ converge?
- Do we obtain convergence for all $x_0$ in $\mathbb{R}^n$, or in smaller $S \subset \mathbb{R}^n$, or $x_0$ “close to” $\overline{x}$?

Classification of Speed of Convergence

**Definition 1 (The Rate of Convergence)** Know $\frac{\alpha_n}{\beta_n} \rightarrow 0$, and $\exists k > 0$ such that $|\alpha_n - \alpha| \leq k|\beta_n|$ for $n$ large enough, i.e. $\lim_{n \to \infty} \frac{|\alpha_n - \alpha|}{|\beta_n|} \leq k$, then we say $\alpha_n$ converges to $\alpha$ with the rate of convergence $O(\beta_n)$, also written as $\alpha_n = \alpha + O(\beta_n)$.

This can be considered that $\alpha_n$ converging to $\alpha$ is as fast as $\beta_n$ converging to 0. We often take $\beta_n$ as $p$-series: $\beta_n = \frac{1}{n^p}$ ($p > 0$).

**Definition 2 (The Order of Convergence)** Know $x_n \rightarrow \overline{x}$. If $\exists \alpha \geq 1$ and $\lambda > 0$ such that

$$\lim_{n \to \infty} \frac{\|x_{n+1} - \overline{x}\|}{\|x_n - \overline{x}\|^{\alpha}} = \lambda,$$

then we say “$x_n \rightarrow \overline{x}$ of order $\alpha$”.

Namely, the order above is described by comparing the current and next differences to the cluster point. If $x_n \rightarrow \overline{x}$ is of order $\alpha$, then for any given $\varepsilon > 0$, $\exists N \in \mathbb{N}$ such that

$$\lambda - \varepsilon \leq \frac{\|x_{n+1} - \overline{x}\|}{\|x_n - \overline{x}\|^{\alpha}} \leq \lambda + \varepsilon \quad \forall n \geq N,$$

$$\Rightarrow \|x_{n+1} - \overline{x}\| \leq c\|x_n - \overline{x}\|^{\alpha} \quad \forall n \geq N.$$

If $\alpha = 1$, usually we’d like to have $c \in (0, 1)$ so that $\|x_{n+1} - \overline{x}\|$’s keep shrinking:

$$\|x_{n+1} - \overline{x}\| \leq c\|x_n - \overline{x}\| \leq c^2\|x_{n-1} - \overline{x}\| \leq \cdots \leq c^{n+1}\|x_0 - \overline{x}\| \xrightarrow{n \to \infty} 0.$$
Definition 3 We say “\(x_n \rightarrow \bar{x}\) in at least order \(\alpha\)” if \(\exists c > 0\) such that
\[
\|x_{n+1} - \bar{x}\| \leq c\|x_n - \bar{x}\|^\alpha
\]
for large \(n\).

\(\alpha = 1\) with \(c \in (0, 1)\) : linear convergence
\(1 < \alpha < 2\) : super-linear convergence
\(\alpha = 2\) : quadratic convergence

In case \(\alpha = 1\), \(c \in (0, 1)\):
\[
\|x_{n+1} - \bar{x}\| \leq c^{n+1}\|x_0 - \bar{x}\| = k\beta_n \rightarrow 0,
\]
where \(k := c\|x_0 - \bar{x}\|\) and \(\beta_n := c^n\), i.e. \(x_n \rightarrow \bar{x}\) with \(O(\beta_n)\) rate.

Example 1 A simple “enclosure” method — bisection method, is a of order 1: \(f : \mathbb{R} \rightarrow \mathbb{R}\) is continuous on \([a, b]\) and \(f(a)f(b) < 0\), then, by Intermediate Value Theorem, \(\exists \) a real root \(\bar{x} \in [a, b]\).

Basically, begin with \(f(a)f(b) < 0\):
do {
\(t := \frac{a+b}{2}\).
If \(f(t) \approx 0\) or \(a \approx b\), then break. (subject to change)
If \(f(a)f(t) < 0\), then \(b := t\),
else, \(a := t\).
}

At each step, define \(x_n := \frac{a_n + b_n}{2}\) and know \(\exists \bar{x} \in (a_n, b_n)\) is a real root of \(f\).

\[
|x_n - \bar{x}| \leq \frac{1}{2}|b_n - a_n| \leq \cdots \leq \left(\frac{1}{2}\right)^n \frac{|b_0 - a_0|}{\beta_n k}.
\]

Usually we use bisection method for one dimensional problems to get a good starting \(x_0\) for other faster method.

Iterating Methods for Finding Roots

Most sophisticated methods for finding roots are based on “fixed point iteration” method:

Idea: Convert the original problem \(f(x) = 0\) holds at \(\bar{x}\)
into a new problem \(\Phi(x) = x\) holds at \(\bar{x}\)
and use \(\Phi\) to define the method:
starting from some \(x_0\), then \(x_1 := \Phi(x_0), x_2 := \Phi(x_1), \ldots\)

Questions:

- How to construct \(\Phi\)?
- Once \(\Phi\) is obtained, does the method converge?
- If the method converges, does it converge for all \(x_0\)? How fast?
Example 2  \( f : \mathbb{R} \to \mathbb{R}, \ f \in C^1(\mathbb{R}) \) with \( f' \neq 0 \), define \( \Phi(x) := x - [f'(x)]^{-1}f(x) \), iteration: \( x_{n+1} = \Phi(x_{n}) = x_{n} - [f'(x_{n})]^{-1}f(x_{n}) \) —— iterator of Newton’s method, seen later.

Note that NOT EVERY \( \Phi \) for which \( \overline{x} \) is a fixed point works:

Example 3  \( f(x) = x^2 - 3, \ \overline{x} = \sqrt{3} \) is a root.

1. \( \Phi_1(x) := f(x) + x = x^2 - 3 + x \ (\Phi_1(\sqrt{3}) = \sqrt{3}) \)
   \( x_{n+1} := \Phi_1(x_{n}) = x_{n}^2 - 3 + x_{n}, \ n = 0, 1, 2, \ldots. \)
2. \( \Phi_2(x) := \frac{3}{x} \ (\Phi_2(\sqrt{3}) = \sqrt{3}) \)
   \( x_{n+1} := \Phi_2(x_{n}) = \frac{3}{x_{n}}, \ n = 0, 1, 2, \ldots. \)
3. \( \Phi_3(x) := \frac{1}{2}(x + \frac{3}{x}) \ (\Phi_3(\sqrt{3}) = \sqrt{3}) \)
   \( x_{n+1} := \Phi_3(x_{n}) = \frac{1}{2}(x_{n} + \frac{3}{x_{n}}), \ n = 0, 1, 2, \ldots. \)

<table>
<thead>
<tr>
<th></th>
<th>(1)</th>
<th>(2)</th>
<th>(3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( x_0 )</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
</tr>
<tr>
<td>( x_1 )</td>
<td>3.0</td>
<td>1.5</td>
<td>1.75</td>
</tr>
<tr>
<td>( x_2 )</td>
<td>9.0</td>
<td>2.0</td>
<td>1.732143</td>
</tr>
<tr>
<td>( x_3 )</td>
<td>81.0</td>
<td>1.5</td>
<td>1.732051</td>
</tr>
<tr>
<td>( x_4 )</td>
<td>6639.0</td>
<td>2.0</td>
<td>1.73205088</td>
</tr>
</tbody>
</table>
\[ \downarrow \] \[ \downarrow \] \[ \sqrt{3} \]

Not every root being a fixed point of \( \Phi \) is a cluster.

We want \( \Phi \) to be a COTRACTION:

Definition 4  Let \( \Phi : \mathbb{R}^n \to \mathbb{R}^n, \ S \subset \mathbb{R}^n \). \( \Phi : S \to S \) is called a contraction mapping on \( S \) if \( \exists k \in [0, 1) \) such that

\[
\|\Phi(x) - \Phi(y)\| \leq k\|x - y\| \ \forall \ x, y \in S.
\]

This definition suggests the continuity of \( \Phi \) on \( S \), but not necessarily the differentiability.

Example 4  If \( \Phi \) is differentiable on \( \mathbb{R}^n \) ( \( D\Phi = (\frac{\partial \Phi}{\partial x})_{i,j} \) ), then, by Mean Value Theorem in \( \mathbb{R}^n \),
\( \Phi(x) - \Phi(y) = D\Phi(z)(x - y) \) for some \( z \in \) line segment \([x, y]\) : \( \|\Phi(x) - \Phi(y)\| \leq \|D\Phi(z)\| \|x - y\| \),
where \( \|D\Phi(z)\| \) is the induced matrix norm\(^1\). But for \( x, y \in S \subset \mathbb{R}^n \), \( z \in [x, y] \) may not be in \( S \). So, if \( \sup_{z \in S} \|D\Phi(z)\| = k < 1 \) and if \( S \) contains all line segments between arbitrary \( x, y \) in \( S \) ( \( \iff \ S \) is convex), then, \( \Phi \) is a contraction on \( S \).

\(^1\)Linear transformation \( A : \mathbb{R}^m \to \mathbb{R}^n \). Induced matrix norm of \( A \):
\( \|A\| \overset{\text{def}}{=} \sup_{\|x\| \leq 1} \|Ax\| = \sup_{\|x\|=1} \|Ax\| = \sup_{0 \neq x} \frac{\|Ax\|}{\|x\|} \),
\( x \in \mathbb{R}^m, Ax \in \mathbb{R}^n \), so \( \|x\| \) and \( \|Ax\| \) are in their space norms respectively.
Theorem 1 (Contraction Mapping Theorem) \( S \subset \mathbb{R}^n \) is closed and \( \Phi \) is a contraction on \( S \), i.e. \( \forall x, y \in S, \|\Phi(x) - \Phi(y)\| \leq k\|x - y\| \) for some \( k \in [0, 1) \), then \( \exists \) a unique \( \bar{x} \in S \) such that \( \Phi(\bar{x}) = \bar{x} \).

Furthermore, for any \( x_0 \in S \), define \( x_{n+1} := \Phi(x_n), n = 0, 1, 2, \cdots \) (fixed point iteration). This gives a sequence \( \{x_n\} \subset S \) satisfying \( \|x_n - \bar{x}\| \xrightarrow{n \to \infty} 0. \)

(proof) \( \Phi : S \to S, : \{x_n\} \subset S. \) Must show \( \{x_n\} \) is Cauchy:

\[
\|x_{n+1} - x_n\| = \|\Phi(x_n) - \Phi(x_{n-1})\| \leq k\|x_n - x_{n-1}\| = \cdots = k^n\|x_1 - x_0\|,
\]

therefore \( \|x_{n+p} - x_n\| \leq \|x_{n+p} - x_{n+p-1}\| + \cdots + \|x_{n+1} - x_n\| \leq (k^{n+p-1} + \cdots + k^n)\|x_1 - x_0\| \leq k^n \frac{1}{1-k}\|x_1 - x_0\| \xrightarrow{n \to \infty} 0 \).

\( S \) is closed, \( x_n \) sequence will converge to some point in \( S \), say \( \bar{x} \), i.e. \( x_n \xrightarrow{n \to \infty} \bar{x} \in S \). Must show

- Cluster point \( \bar{x} \) is a fixed point of \( \Phi \):
  \[
  \|\Phi(\bar{x}) - \bar{x}\| \leq \|\Phi(\bar{x}) - x_n\| + \|x_n - \bar{x}\| \leq \|\Phi(\bar{x}) - \Phi(x_{n-1})\| + \|x_n - \bar{x}\| \leq k\|\bar{x} - x_{n-1}\| + \|x_n - \bar{x}\| \xrightarrow{n \to \infty} 0,
  \]

  therefore \( \Phi(\bar{x}) = \bar{x} \).

- Uniqueness of fixed point \( \bar{x} \):
  Suppose \( \bar{y} \in S \) and \( \Phi(\bar{y}) = \bar{y} \). Then \( \|\bar{x} - \bar{y}\| = \|\Phi(\bar{x}) - \Phi(\bar{y})\| \leq k\|\bar{x} - \bar{y}\| \Rightarrow \bar{x} = \bar{y} \). \( \blacksquare \)

Example 5 Let \( \Phi : \mathbb{R} \to \mathbb{R} \) be differentiable. If graphs of \( y = \Phi(x) \) and \( y = x \) intersect at \( \bar{x} \) and \( |\Phi'(\bar{x})| < 1 \), then \( \Phi \) is a contraction on \( [\bar{x} - \delta, \bar{x} + \delta] \) for \( \delta > 0 \) small enough.

\[
\begin{align*}
\text{a contraction} & \quad & \text{not a contraction} \\
\end{align*}
\]

Corollary 1 When the conditions of Theorem 1 hold, this method converges at least in linear order.

(proof) \( \|x_{n+1} - \bar{x}\| = \|\Phi(x_n) - \Phi(\bar{x})\| \leq k\|x_n - \bar{x}\|^1 \). \( \text{(Definition 3)} \) \( \blacksquare \)

Theorem 2 \( \Phi : \mathbb{R} \to \mathbb{R}, \Phi(\bar{x}) = \bar{x}, I \) is an open interval containing \( \bar{x} \), and

- \( \Phi'' \in \mathcal{C}(I) \) (twice differentiable on \( I \)),
- \( \exists M > 0 \ s.t. \ |\Phi''(x)| \leq M \forall x \in I \),
- \( \Phi'(\bar{x}) = 0 \).

Then for \( x_0 \) close enough to \( \bar{x} \), \( x_n \to \bar{x} \) at least quadratically.
(pf.) By the continuity of $\Phi'$, $\exists I_0 \subset I$ s.t. $\exists \in I_0$ and $|\Phi'(x)| < 1 \ \forall \ x \in I_0$. $\Rightarrow \Phi'$ is a contract on $I_0$.

To show “converges at least quadratically”: expand $\Phi$ about $\xi$:

$$\Phi(x) = \Phi(\xi) + \Phi'(\xi)(x - \xi) + \frac{\Phi''(\xi)}{2!}(x - \xi)^2$$

on $I_0$ for some $\xi$ between $x$ and $\xi$. Pick $x = x_n$:

$$\Rightarrow \Phi(x_n) = x_{n+1} = \xi + 0(x_n - \xi) + \frac{\Phi''(\xi)}{2!}(x_n - \xi)^2,$$

$\therefore |x_{n+1} - \xi| = \left| \frac{\Phi''(\xi)}{2!} \right| |x_{n+1} - \xi|^2 \leq \frac{M}{2} |x_n - \xi|^2$. $\blacksquare$

**Theorem 3** $\Phi : \mathbb{R}^n \to \mathbb{R}^n$, $\Phi(\xi) = R$, $B := B(\xi, r)$, and if

- $\frac{\partial^2 \Phi_i}{\partial x_j \partial x_k}$ is continuous on $B \ \forall \ i, j, k = 1, \ldots, n$ ($\Phi$ is twice differentiable on $B$),
- $\exists M > 0 \ s.t. \ |\frac{\partial^2 \Phi_i}{\partial x_j \partial x_k}| \leq M$ on $B$,
- $D\Phi(\xi) = 0_{n \times n}$.

Then for $x_0$ close enough to $\xi$, $x_n \to \xi$ at least quadratically.

**Generically Construct a Fixed Point Iterator $\Phi$ for $f : \mathbb{R}^n \to \mathbb{R}^n$**

Define an iterator $\Phi(x) = x - [A(x)]^{-1}f(x)$ with some $A(x)_{n \times n}$ to be determined. Let $B(x) = \begin{pmatrix} b_{ij}(x) \end{pmatrix} = [A(x)]^{-1}$, then $\Phi_i(x) = x_i - \sum_{j=1}^n b_{ij}(x)f_j(x)$, and

$$\frac{\partial \Phi_i}{\partial x_k}(x) = \delta_{ik} - \sum_{j=1}^n \frac{\partial b_{ij}}{\partial x_k}(x)f_j(x) - \sum_{j=1}^n b_{ij}(x)\frac{\partial f_j}{\partial x_k}(x).$$

Suppose $\xi$ is a root of $f(x) = [f_1(x), \ldots, f_n(x)]^T$, then

$$\frac{\partial \Phi}{\partial x_k}(\xi) = \delta_{ik} - \sum_{j=1}^n b_{ij}(\xi)\frac{\partial f_j}{\partial x_k}(\xi).$$

If we want $D\Phi(\xi) = \begin{pmatrix} \frac{\partial \Phi_i}{\partial x_k} \end{pmatrix}_{i,k}(\xi) = 0_{n \times n}$, i.e. $I = B(\xi)Df(\xi)$, $\iff A(\xi) = Df(\xi)$. Notice that the singularity of $Df(x)$ is not discussed yet.

If $f(x)$ is “smooth enough” and if $Df(x)$ is non-singular for $x$ “sufficiently close” to $\xi$ (true if, for example, $Df(\xi)$ is non-singular, but, who knows?), then we can take $A(x) := Df(x)$, so $\Phi(x) = x - [Df(x)]^{-1}f(x)$ iteration can have quadratic convergence, by the previous theorem.

What if $Df(\xi)$ is singular(not invertible)?
Example 6 \( f(x) := (x-a)^mg(x) \), and \( g(a) \neq 0 \). Fix \( x_0 \) sufficiently close to \( a \) and apply Newton’s iteration \( \Phi(x) = x - f'(x)^{-1}f(x) \).

If the multiplicity \( m \) of root \( a \) is 1 and if the continuity of \( f'' \) at \( a \) is assumed, then \( f'(a) = g(a) + (a-a)g'(a) \neq 0 \) (the graph of \( f \) around \( a \) is “slant”), \( \Phi'(a) = 1 - (1 - \frac{f'(a)f''(a)}{f'(a)^2}) = 0 \), and the Newton’s iteration has at least quadratic convergence by Theorem 2.

Visualize that if \( m \) is bigger, then the graph of \( f \) around \( a \) is kind of “flatter”, so that the Newton’s iteration is slower, but, at least has linear convergence:

If the multiplicity \( m \) of root \( a \) is > 1, then \( f'(a) = 0 \), singular, \( \Phi'(a) \) not existing, possibly no quadratic convergence. \( \Phi(x) = x - \frac{f(x)}{f'(x)} = x - \frac{(x-a)g(x)}{mg(x)+(x-a)g'(x)} \). Obviously, if \( g' \) continuous at \( a \), then \( \lim_{x \to a} \frac{(x-a)g(x)}{mg(x)+(x-a)g'(x)} = 0 \) so \( x_n \to a \) consequently. Let \( h(x) := \frac{g(x)}{mg(x)+(x-a)g'(x)} \), i.e. \( \Phi(x) = (x-a)h(x) \).

Then

\[
\Phi'(x) = 1 - h(x) - (x-a)h'(x) = 1 - \frac{1}{m+(x-a)\frac{g'(x)}{g(x)}} - (x-a)h(x),
\]

Further more, if \( g' \) is continuous at \( a \), then for \( x \) very close to \( a \), roughly speaking, \( \Phi'(x) \approx 1 - \frac{1}{m} \) since \( (x-a)\frac{g'(x)}{g(x)} \) and \( (x-a)h(x) \) will be very small, \( |\Phi'(x)| < 1 \) for \( x \approx a \), therefore \( \Phi \) is a contraction on a small neighborhood of \( a \), by previous corollary, \( x_n \to a \) at least linearly for \( x_0 \) close to \( a \). ■

**Tangent Line Method = Newton’s Method**

Taylor expansion of \( f \) at \( x_0 \)

\[
f(x) = f(x_0) + f'(x_0)(x-x_0) + \frac{f''(x_0)}{2!}(x-x_0)^2 + \frac{f'''(x_0)}{3!}(x-x_0)^3 + \cdots
\]

i.e. \( f(x) \approx f(x_0) + f'(x_0)(x-x_0) \) for \( x \approx x_0 \). It is believed that root of \( f(x) \) is also close to root of \( f(x_0) + f'(x_0)(x-x_0) \). Tangent line

\[
y = f(x_0) + f'(x_0)(x-x_0),
\]

will intersect \( x \)-axis at

\[
x_1 := x_0 - f'(x_0)^{-1}f(x_0),
\]

therefore \( \Phi(x) := x - f'(x)^{-1}f(x) \) is taken as the iterator. Obviously, \( \Phi(\bar{x}) = \bar{x} \iff f(\bar{x}) = 0 \).

**Secant Line Method**

For \( x_0 \approx x_1 \), replace tangent line by secant line in Newton’s method, i.e. regard secant line as an approximation, as \( x \approx x_0, x_1 \):

\[
f(x) \approx f(x_0) + f'(x_0)(x-x_0) \\
\approx f(x_0) + \frac{f(x_0) - f(x_1)}{x_0 - x_1} (x-x_0) \left( = f(x_1) + \frac{f(x_0) - f(x_1)}{x_0 - x_1} (x-x_1) \right)
\]

the slope of the tangent is replaced by the slope of the secant, much easier to evaluate in most of the cases.

\[
\therefore f(x_i) + \frac{f(x_0) - f(x_1)}{x_0 - x_1} (x-x_i) = 0 \iff x := x_i - \frac{x_0 - x_1}{f(x_0) - f(x_1)} f(x_i).
\]
Though \( i = 0 \) or \( i = 1 \) gives the same \( x \)-intercept, to do it regularly, we'll take \( i = 1 : x_2 := x_1 - \frac{x_0 - x_1}{f(x_0) - f(x_1)} f(x_1) \), i.e. the iterator is defined as

\[
x_{n+2} = \Phi(x_{n+1}) := x_{n+1} - \frac{x_n - x_{n+1}}{f(x_n) - f(x_{n+1})} f(x_{n+1})
\]

\( x_{n+2} \) is where secant \( x_n x_{n+1} \) and \( x \)-axis intersect. If \( (x_n) \) converges, say, to \( \bar{x} \), then \( \bar{x} \) must be a fixed point of \( \Phi \):

\[
\begin{align*}
x_{n+2} &= x_{n+1} - \frac{x_n - x_{n+1}}{f(x_n) - f(x_{n+1})} f(x_{n+1}) & n \to \infty \quad \downarrow \quad \downarrow \quad \downarrow \quad \downarrow \\
\bar{x} &= \bar{x} - f'(\bar{x})^{-1} f(\bar{x})
\end{align*}
\]

the same as in Newton’s method.

**False Position Method**

In the secant line method, if we pick \( i = 0 \), \( x_2 := x_0 - \frac{x_0 - x_1}{f(x_0) - f(x_1)} f(x_0) \) “by mistake”, follow this regularity, the sequence should be

\[
\begin{align*}
x_2 &= x_0 - \frac{x_0 - x_1}{f(x_0) - f(x_1)} f(x_0), \\
x_3 &= x_0 - \frac{x_0 - x_2}{f(x_0) - f(x_2)} f(x_0), \\
x_4 &= x_0 - \frac{x_0 - x_3}{f(x_0) - f(x_3)} f(x_0), \\
&\quad \vdots \\
x_{n+1} &= x_0 - \frac{x_0 - x_n}{f(x_0) - f(x_n)} f(x_0),
\end{align*}
\]

\( x_{n+1} \) is where secant \( x_0 x_{n+1} \) and \( x \)-axis intersect. Iterator: \( \Phi(x) = x_0 - \frac{x_0 - x}{f(x_0) - f(x)} f(x_0) \). Obviously, \( \Phi(p) = p \iff f(p) = 0 \). If \( x_n \to p \), then

\[
p = x_0 - \frac{x_0 - p}{f(x_0) - f(p)} f(x_0),
\]

i.e. \( x_0 p \) intersects \( x \)-axis at \( p \), which implies \( (p, f(p)) \) is actually on the \( x \)-axis, i.e. \( f(p) = 0 \).

**Questions:**

- Is it always expected that iteration will produce a monotonic sequence to converge?
- If secant line method works for two initial inputs \( x_0 \) and \( x_1 \), so does false position method? Ask yourself the converse question.
- If initially, \( f(x_0) f(x_1) < 0 \), how do you compare bisection with secant line and false position?

**Müller’s Method** for finding a complex root of \( f \)

Three distinct points \((x_0, f(x_0)), (x_1, f(x_1)), (x_2, f(x_2))\) uniquely determine a quadratic function \( q(x) \), viewed as an approximation of \( f \). Root of \( q \), \( x_3 \), trivially, can be computed by the quadratic formula, maybe complex. Overwrite \( x_0 \) by \( x_1 \), \( x_1 \) by \( x_2 \), \( x_2 \) by new root \( x_3 \), start all over again until the \( \{x_n\} \) sequence converges:
Given distinct $x_0, x_1, x_2$, let $f_i := f(x_i)$ and $q(x) := a(x - x_2)^2 + b(x - x_2) + c$ with $q(x_i) = f_i$. Then trivially $c = f_2$, and

$$a = \frac{(f_0 - f_1) - (f_1 - f_2)}{x_0 - x_2} = \frac{(x_1 - x_2)(f_0 - f_2) - (x_0 - x_2)(f_1 - f_2)}{(x_0 - x_1)(x_1 - x_2)(x_0 - x_2)},$$

$$b = \frac{(f_1 - f_2)}{x_0 - x_2} + (x_2 - x_1)a = \frac{(x_0 - x_2)^2(f_1 - f_2) - (x_1 - x_2)^2(f_0 - f_2)}{(x_0 - x_1)(x_1 - x_2)(x_0 - x_2)},$$

$$q(x_3) = 0 \iff x_3 - x_2 = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} = \frac{-2c}{b \mp \sqrt{b^2 - 4ac}}.$$  

For the sake of accuracy, pick the one whose denominator $D$ has larger absolute value: $x_3 := x_2 + \frac{-2c}{b}$. 

**Polynomial equation \(\leadsto\) eigenvalue problem**

For example, given a polynomial $f(x) := x^4 + a_3x^3 + a_2x^2 + a_1x + a_0$, and define

its companion matrix $A := \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -a_0 & -a_1 & -a_2 & -a_3 \end{bmatrix}$. Then

$$f(\lambda) = 0 \iff \det(A - \lambda I) = 0 \iff \exists \mathbf{v} = [v_1 \ v_2 \ v_3 \ v_4]^T \neq 0 \text{ such that } A\mathbf{v} = \lambda \mathbf{v}$$

$$v_2 = \lambda v_1, \quad (1)$$

$$v_3 = \lambda v_2, \quad (2)$$

$$v_4 = \lambda v_3, \quad (3)$$

$$-a_0v_1 - a_1v_2 - a_2v_3 - a_3v_4 = \lambda v_4, \quad (4)$$

\[. \] $v_3 = \lambda^2v_1, \ v_4 = \lambda^3v_1$, and (4) becomes $v_1(a_0 + a_1\lambda + a_2\lambda^2 + a_3\lambda^3 + \lambda^4) = 0$, i.e. a root of $f$ is an eigenvalue of $A$.

Instead of solving characteristic equation of $A$ (equivalent to $f(x) = 0$), we can apply other methods to solve for eigenvalues of $A$, for example, the homotopy continuation method.

**Evaluation of Polynomials**

When solving for roots of a function $f$ by any iterative method, we need to evaluate, unavoidably, the function value $f$ or its derivative $f'$ many times. To save do that efficiently, we should always take advantages of the specialty of $f$ itself. If $f$ is a univariate polynomial, then $f(a)$, by the so-called Chinese Remainder Theorem equals the remainder of $f(x)$ divided by $(x - a)$:

If $f(x) = r + (x - a)q(x)$, then $f(a) = r$,

$$\Rightarrow f'(x) = q(x) + (x - a)q'(x),$ \ and \ $f'(a) = q(a)$ —— evaluation of a polynomial still.

Therefore, we need to reduce the computation of evaluating polynomials. This can be done easily with *Synthetic Division*: $q_0(x)$ is a polynomial written in the power of $x$ in ascending order

$$q_0(x) = a_n x^n + \cdots + a_1 x + a_0.$$  

Let $b_i$ be the remainder quotient of $q_i(x)$ divided by $(x - a)$ for $i = 0, 1, 2, \cdots$:

$$q_i(x) = b_i + (x - a)q_{i+1}(x).$$
Keep doing synthetic division to the quotient, \( q_0(x) \) can be written as a polynomial in \( (x - a) \):

\[
q_0(x) = b_0 + (x-a)q_1(x) \\
= b_0 + (x-a)[b_1 + (x-a)q_2(x)] \\
\ldots \\
= b_0 + (x-a)[b_1 + (x-a)[b_2 \cdots + (x-a)\cdots]]
\]

Evaluating \( a_0 + a_1\Delta + \cdots + a_{n-1}\Delta^{n-1} + a_n\Delta^n \) by \( a_0 + \Delta(a_1 + \Delta(a_{n-1} + \Delta(a_n)\cdots)) \) is called the “Horner’s Scheme”.

**Accelerating Convergence — Aitken’s \( \Delta^2 \) method**

If \( p_n \to p \), then, for large \( n \), roughly we have

\[
P_{n+1} - p \approx \frac{P_{n+2} - p}{P_{n+1} - p} \\
\Rightarrow (P_{n+1} - p)^2 \approx (P_n - p)(P_{n+2} - p), \\
\Rightarrow P_{n+2} - 2P_{n+1}p + p^2 \approx P_nP_{n+2} - (P_n + P_{n+2})p + p^2,
\]

\[
\Rightarrow p \approx \frac{P_nP_{n+2} - P_{n+1}^2}{P_{n+2} - 2P_{n+1} + P_n} \\
\approx \frac{P_n(P_{n+2} - 2P_{n+1} + P_n) + 2P_nP_{n+1} - P_n^2}{P_{n+2} - 2P_{n+1} + P_n} \\
\approx P_n - \frac{(P_{n+1} - P_n)^2}{P_{n+2} - 2P_{n+1} + P_n} \overset{\text{def}}{=} \hat{p}_n
\]

i.e. if \( p_n \to p \), then \( \hat{p}_n \to p \), and, “faster”.

The following is why called “\( \Delta^2 \)” (second difference):

\[
\begin{array}{ccc}
p_n & \Delta p_n & \Delta^2 p_n \\
p_0 & \Delta p_0 & \Delta p_0 \\
p_1 & \Delta p_1 & \Delta^2 p_0 \\
p_2 & \Delta p_2 & \Delta^2 p_1 \\
p_3 & \vdots & \vdots \\
\end{array}
\]

\( \Delta p_n \) \overset{\text{def}}{=} p_{n+1} - p_n,

\( \Delta^2 p_n = \Delta(\Delta p_n) = \Delta(p_{n+1} - p_n) = p_{n+2} - p_{n+1} - (p_n - p) = p_{n+2} - 2p_{n+1} + p_n \).

The new sequence is built upon the first and the second differences of the original: \( \hat{p}_n = p_n - \frac{(\Delta p_n)^2}{\Delta^2 p_n} \).