Summary so far

• Root finding versus Fixed Point finding:

\[ f(x) = 0 \iff x = g(x) \]

• We denote the solution by \( \alpha \).

• The corresponding fixed point iteration is

\[ x_0 \text{ given, } \quad x_{n+1} = g(x_n) \quad (1) \]

• The iteration (1) converges **linearly** (or of first order) if

\[ 0 < |g'(\alpha)| < 1. \]

• It converges of order \( p > 1 \) if

\[ g(\alpha) = \alpha, \quad g'(\alpha) = g''(\alpha) = g^{(p-1)}(\alpha) = 0, \quad g^{(p)}(\alpha) \neq 0. \]

• Convergence will occur if we start sufficiently close to \( \alpha \).

• Stop if

\[ \frac{1}{1 - L} |x_n - x_{n+1}| < \epsilon \]

where

\[ L = \begin{cases} |\frac{x_{n+1} - x_n}{x_n - x_{n-1}}| & \text{if } p = 1 \\ 0 & \text{if } p > 1. \end{cases} \]
• omit arguments for sake of simpler notation.

• For Newton’s Method:

\[ g = x - \frac{f}{f'} \]

\[ g' = 1 - \frac{f'^2 - ff''}{f'^2} = \frac{ff''}{f'^2} \]

\[ g'' = \frac{(f'f'' + ff''')f'^2 - 2f'f''f f''}{f'^4} \]

\[ = \frac{f'' f'^2 + ff'''}{f'^3} - \frac{2ff''}{f'^2} \]

and

\[ g''(\alpha) = \frac{f''}{f'}(\alpha) \]

• We get the following cases:

1. \( f'(\alpha) \neq 0, f''(\alpha) \neq 0 \). This is the standard case. NM converges quadratically.

2. \( f'(\alpha) \neq 0, f''(\alpha) = 0 \). NM converges of order at least 3. This is unlikely but it has a compelling geometric interpretation: NM is based on a first order Taylor Series. If \( f''(\alpha) = 0 \) then the quadratic term in the Taylor series is zero, and the linear Taylor approximation actually equals the quadratic Taylor approximation.

3. \( f'(\alpha) = 0 \). This is a special case of having a multiple root.
• $\alpha$ is a root of multiplicity $p$ if

\[ f(\alpha) = f'(\alpha) = \ldots = f^{(p-1)}(\alpha) = 0, \quad f^{(p)}(\alpha) \neq 0. \]

• Numerically, having a multiple root is similar to having several roots that are close together compared with the distance from the starting point.

\[
g = x - \frac{f}{f'} \quad \text{and} \quad g' = \frac{ff''}{f'^2}
\]

\[
f(\alpha) = f'(\alpha) = 0 \quad \Rightarrow \quad f'' + ff'' \frac{f'' + fff''}{2f'f''}
\]

\[
\Rightarrow \frac{1}{2}
\]
Example: $f(x) = x^2$

Figure 1. $f(x) = x^2$.

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

$x = 0$

It seems to work.
• Suppose
\[ f'(\alpha) = 0 \quad \text{and} \quad f''(\alpha) \neq 0 \]

• What happens to NM?
• We get
\[
g(x) = x - \frac{f}{f'}
\]
\[
g'(x) = \frac{ff''}{f'r^2} \quad \longrightarrow \quad 0
\]

• We need to use the Rule of L’Hopital:
\[
\frac{ff''}{f'r^2} \longrightarrow \frac{ff'''}{2f'f''}
\]
\[
\text{(again)} \quad \longrightarrow \quad \frac{ff^{iv} + f'f'''}{2(f''^2 + f'f''')}
\]

• Evaluating at \( \alpha \) gives
\[
g'(\alpha) = \frac{f''^2(\alpha)}{2f''^2(\alpha)} = \frac{1}{2}.
\]

• NM converges linearly with \( g'(\alpha) = \frac{1}{2} \).
Exercise: The modified Newton’s Method

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

covers of order 2.
• What about roots of multiplicity greater than 2?
• We could use the Rule of L’Hopital again.
• This gives rise to a mess (try it!)
• Here is a better idea:
• Write
  \[ f(x) = (x - \alpha)^p h(x) \]
  where
  \[ h(\alpha) \neq 0 \]
• Of course,
  \[ h(x) = \frac{f(x)}{(x - \alpha)^p} \]
• NM turns into

\[ g(x) = x - \frac{f(x)}{f'(x)} \]
\[ = x - \frac{(x - \alpha)^p h(x)}{(x - \alpha)^p h'(x) + p(x - \alpha)^{p-1} h(x)} \]
\[ = x - \frac{(x - \alpha) h(x)}{(x - \alpha) h'(x) + ph(x)} \]

where

\[ g'(x) = 1 - \frac{(h + (x - \alpha)h')((x - \alpha)h' + ph) - ((x - \alpha)h \times \text{denominator}')}{((x - \alpha)h' + ph)^2} \]
and

\[ g'(\alpha) = 1 - \frac{ph^2}{(ph)^2} = 1 - \frac{1}{p} = \frac{p - 1}{p} \]

• The iteration converges linearly, but \( g'(\alpha) \) goes to 1 as \( p \) goes to infinity.

• What if we don’t know \( p \) but \( p < \infty \)?

• A root of multiplicity \( p \) of \( f \) is a root of multiplicity 1 of

\[ \phi = \frac{f}{f'} \]

• Run NM of \( \Phi \).
Inverse Interpolation

- Here is a nifty trick by which you can build iterations of arbitrarily high order of convergence.

- Suppose $F$ is the inverse of $f$.

  $$F(f(x)) = x.$$  

- Then

  \[
  \begin{align*}
  f(\alpha) &= 0 \\
  F(f(\alpha)) &= F(0) \\
  \alpha &= F(0)
  \end{align*}
  \]

- Idea: expand $F$ into a Taylor series about $f(x_n) = y_n$.

- Evaluate the truncated Taylor series at $y = 0$.

  $$F(y) = F(y_n) + F'(y_n)(y-y_n) + \frac{1}{2}F''(y_n)(y-y_n)^2 + \ldots$$

  $$x_n - f(x_n)$$

- Of course, $F(y_n) = x_n$.

- What’s $F'(y)$?

  We have

  $$F(\nu) = x_n - \frac{f(x_n)}{f'(x_n)}$$

  $$F(f(x)) = x \implies F'(f(x))f'(x) = 1$$

  $$\implies F'(f(x)) = \frac{1}{f'(x)}$$
Evaluating the Taylor Series for $F(y)$ and truncating after the linear term gives

$$x_{n+1} = F(0) = x_n - \frac{f(x_n)}{f'(x_n)},$$

i.e., Newton’s Method again.

- Exercise: Work out the second derivative of $F$, truncate after the quadratic term in the Taylor Series, and obtain a third order method.
Newton’s Method for Systems

• Suppose $F$ is function from $\mathbb{R}^n$ to $\mathbb{R}^n$:

$$F : \mathbb{R}^n \longrightarrow \mathbb{R}^n$$

and we want to solve

$$F(x) = 0$$  \hspace{1cm} (2)

Here

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

and

$$F(x) = \begin{bmatrix} F_1(x) \\ F_2(x) \\ \vdots \\ F_n(x) \end{bmatrix}$$

• We are going to construct a sequence of vectors

$$x^{(0)}, x^{(1)}, x^{(2)}, \ldots$$

that hopefully converges to the solution of (2). (We use superscripts in parentheses because subscripts would refer to components of a vector, and plain superscripts would denote exponents.)
• As in the case of one variable, Newton’s Method for (2) can be obtained by linearizing $F$ and solving the linear problem.

$$F(x) = F(x^{(0)}) + \nabla F(x^{(0)}) (x - x^{(0)}) + \text{HOT}$$

where HOT means “higher order terms” (which we ignore) and

$$\nabla F = \left[ \frac{\partial F_i}{\partial x_j} \right]_{i,j=1,2,...,n}$$

is the Jacobian of $F$.

• Solving

$$F(x^0) + \nabla F(x^{(0)}) (x - x^{(0)}) = 0$$

for $x$ gives

$$x = x^{(1)} = x^{(0)} - \left( \nabla F(x^{(0)}) \right)^{-1} F(x^{(0)})$$

• This gives rise to Newton’s Method:

$$x^{(0)} \text{ given } x^{(k+1)} = x^{(k)} - \left( \nabla F(x^{(k)}) \right)^{-1} F(x^{(k)})$$

where $k = 0, 1, 2, \ldots$

• Note that in the case that $n = 1$ this reduces to the ordinary scalar Newton’s method.
• As a practical matter, we never invert a matrix (more on that later in the semester).

• Instead we can implement Newton’s Method as follows:

\[ x^{(0)} \text{ given} \]

• For \( k = 0, 1, 2, \ldots \) do:
  1. Compute \( F(x^{(k)}) \) and \( A = \nabla F(x^{(k)}) \)
  2. Solve \( As = -F(x^{(k)}) \) \( s = -A^{-1}F(x^{(k)}) \)

  (The vector \( s \) is called the \textbf{Newton Step}).
  3. Let \( x^{(k+1)} = x^{(k)} + s \)
  4. Repeat until \( \|s\| < 0.01 \)

  (We stop when the length of the Newton step is less than 1 cm.)