GABRIEL MOISE

CONTINUOUS MATHEMATICS

HT 2019

PROBLEM SHEET 4

4.1. $f:\mathbb{R}\to\mathbb{R}$ has three continuous derivatives, and a double root: $f(x^*)=\frac{df}{dx}(x^*)=0$ and $\frac{d^2f}{dx^2}(x^*)\neq 0$. We find it using the relaxed Newton iteration:

$$x_{n+1}=x_n-\alpha\frac{f(x_n)}{\frac{df}{dx}(x_n)}, \text{ where } \alpha\in\mathbb{R} \text{ constant}$$

(a) We have $e_{n+1}=x_{n+1}-x^*=x_n-\alpha\frac{f(x_n)}{\frac{df}{dx}(x_n)}-x^*=e_n-\alpha\frac{f(x_n)}{\frac{df}{dx}(x_n)}=\frac{e_n\cdot\frac{df}{dx}(x_n)-\alpha f(x_n)}{\frac{df}{dx}(x_n)}$

(b) We'll now use:

- $\frac{df}{dx}(x_n)=\frac{df}{dx}(x^*)+(x_n-x^*)\frac{d^2f}{dx^2}(x^*)+\frac{(x_n-x^*)^2}{2}\frac{d^3f}{dx^3}(\varepsilon_2)$, for $\varepsilon_2\in(x_n,x^*)$

  $\frac{df}{dx}(x_n)=e_n\frac{d^2f}{dx^2}(x^*)+\frac{e_n^2}{2}\frac{d^3f}{dx^3}(\varepsilon_2)$

- $f(x_n)=f(x^*)+(x_n-x^*)\frac{df}{dx}(x^*)+\frac{(x_n-x^*)^2}{2}\frac{d^2f}{dx^2}(x^*)+\frac{(x_n-x^*)^3}{6}\frac{d^3f}{dx^3}(\varepsilon_3)$, for $\varepsilon_3\in(x_n,x^*)$

  $f(x_n)=\frac{e_n^2}{2}\frac{d^2f}{dx^2}(x^*)+\frac{e_n^3}{6}\frac{d^3f}{dx^3}(\varepsilon_3)$

- $\frac{df}{dx}(x_n)=\frac{df}{dx}(x^*)+(x_n-x^*)\frac{d^2f}{dx^2}(\varepsilon_1)$, for $\varepsilon_1\in(x_n,x^*)$

  $\frac{df}{dx}(x_n)=e_n\frac{d^2f}{dx^2}(\varepsilon_1)$

Substituting these 3 into the relation from (a) we get:

$$e_{n+1}=\frac{e_n\cdot\left(e_n\frac{d^2f}{dx^2}(x^*)+\frac{e_n^2}{2}\frac{d^3f}{dx^3}(\varepsilon_2)\right)-\alpha\left(\frac{e_n^2}{2}\frac{d^2f}{dx^2}(x^*)+\frac{e_n^3}{6}\frac{d^3f}{dx^3}(\varepsilon_3)\right)}{e_n\frac{d^2f}{dx^2}(\varepsilon_1)}$$

$$e_{n+1}=\frac{\left(e_n-\alpha\frac{e_n}{2}\right)\frac{d^2f}{dx^2}(x^*)+\frac{e_n^2}{2}\frac{d^3f}{dx^3}(\varepsilon_2)-\alpha\frac{e_n^2}{6}\frac{d^3f}{dx^3}(\varepsilon_3)}{\frac{d^2f}{dx^2}(\varepsilon_1)}$$

To have $e_{n+1}\leq|e_n|^2\cdot A$, we need to get rid of the term with e_n, so we need $e_n-\alpha\frac{e_n}{2}=0\Rightarrow$ $\boxed{\alpha=2}$. The equality then becomes:

$$e_{n+1} = \frac{\frac{e_n^2}{2}\frac{d^3f}{dx^3}(\varepsilon_2) - \frac{e_n^2}{3}\frac{d^3f}{dx^3}(\varepsilon_3)}{\frac{d^2f}{dx^2}(\varepsilon_1)}$$

Let $i = (x^* - c, x^* + c)$ where we have $\varepsilon_1, \varepsilon_2, \varepsilon_3 \in i$ (when x_n sufficiently close to x^*)

$$e_{n+1} = |e_n|^2 \frac{\frac{1}{2}\frac{d^3f}{dx^3}(\varepsilon_2) - \frac{1}{3}\frac{d^3f}{dx^3}(\varepsilon_3)}{\frac{d^2f}{dx^2}(\varepsilon_1)}$$

Let $A(c) = \dfrac{\frac{1}{2}\max_{\beta\in i}\left|\frac{d^3f}{dx^3}(\beta)\right| - \frac{1}{3}\min_{\gamma\in i}\left|\frac{d^3f}{dx^3}(\gamma)\right|}{\min_{\alpha\in i}\left|\frac{df}{dx}(\alpha)\right|}$, which is finite when x_n close to x^*

Then, $|e_{n+1}| \leq A(c)\,|e_n|^2$

(c) We'll assume that $x_0 \in (x^* - c, x^* + c)$ with sufficiently small to have $cA(c) < 1$.

Let $p = cA(c) < 1$. We'll show by induction on n that $|e_n| \leq p^n |e_0|$:

<u>Base case</u>: $|e_0| \leq |e_0|$ (YES)

<u>inductive step</u>: Given $|e_n| \leq p^n|e_0| < c$, we know that $x_n \in i$, so we have

$$|e_{n+1}| \leq A(c)|e_n^2| < cA(c)|e_n| = p|e_n| \leq p\cdot p^n|e_0| = p^{n+1}|e_0|$$

Therefore, we have $|e_{n+1}| < |e_n|$ for all $n \in \mathbb{N}$ and $|e_n| \geq 0$ $(\forall) n \in \mathbb{N} \Rightarrow (|e_n|)_{n\in\mathbb{N}}$ is convergent. ($|e_n| \leq p^n|e_0| \Rightarrow |e_n| \to 0$ as $n \to \infty$)

We have $\dfrac{|e_{n+1}|}{|e_n|^2} \leq A(c) \Rightarrow$ this is at least quadratic convergence.

(d) <u>Optional</u>:

Let x^* be a root of order m, where $f(x^*) = \frac{df}{dx}(x^*) = \dots = \frac{d^{m-1}f}{dx^{m-1}}(x^*) = 0$ and $\frac{d^mf}{dx^m}(x^*) \neq 0$

We then have to use:

- $\frac{df}{dx}(x_n) = \frac{df}{dx}(x^*) + (x_n - x^*)\frac{d^2f}{dx^2}(x^*) + \dots + \frac{(x_n-x^*)^{m-2}}{(m-2)!}\frac{d^{m-1}f}{dx^{m-1}}(x^*) + \frac{(x_n-x^*)^{m-1}}{(m-1)!}\cdot\frac{d^mf}{dx^m}(x^*) + \frac{(x_n-x^*)^m}{m!}\frac{d^{m+1}f}{dx^{m+1}}(\varepsilon$

$$\frac{df}{dx}(x_n) = \frac{e_n^{m-1}}{(m-1)!}\frac{d^mf}{dx^m}(x^*) + \frac{e_n^m}{m!}\frac{d^{m+1}f}{dx^{m+1}}(\varepsilon_m), \text{ where } \varepsilon_m \in (x_n, x^*)$$

- $f(x_n) = f(x^*) + (x_n - x^*)\frac{df}{dx}(x^*) + \dots + \frac{(x_n-x^*)^{m-1}}{(m-1)!}\frac{d^{m-1}f}{dx^{m-1}}(x^*) + \frac{(x_n-x^*)^m}{m!}\cdot\frac{d^mf}{dx^m} + \frac{(x_n-x^*)^{m+1}}{(m+1)!}\cdot\frac{d^{m+1}f}{dx^{m+1}}(\varepsilon_{m+1})$

$$f(x_n) = \frac{e_n^m}{m!}\frac{d^mf}{dx^m}(x^*) + \frac{e_n^{m+1}}{(m+1)!}\cdot\frac{d^{m+1}f}{dx^{m+1}}(\varepsilon_{m+1}), \text{ where } \varepsilon_{m+1} \in (x_n, x^*)$$

- $\frac{df}{dx}(x_n) = \frac{df}{dx}(x^*) + (x_n - x^*)\frac{d^2f}{dx^2}(x^*) + \dots + \frac{(x_n-x^*)^{m-2}}{(m-2)!}\frac{d^{m-1}f}{dx^{m-1}}(x^*) + \frac{(x_n-x^*)^{m-1}}{(m-1)!}\frac{d^mf}{dx^m}(\varepsilon_{m-1})$

$$\frac{df}{dx}(x_n) = \frac{e_n^{m-1}}{(m-1)!}\cdot\frac{d^mf}{dx^m}(\varepsilon_{m-1}), \text{ where } \varepsilon_{m-1} \in (x_n, x^*)$$

We use the three results in $e_{n+1}=\dfrac{e_n \frac{df}{dx}(x_n)-\alpha f(x_n)}{\frac{df}{dx}(x_n)}$ to get:

$$e_{n+1}=\frac{e_n\left(\frac{e_n^{m-1}}{(m-1)!}\frac{d^m f}{dx^m}(x^*)+\frac{e_n^m}{m!}\frac{d^{m+1}f}{dx^{m+1}}(\varepsilon_m)\right)-\alpha\left(\frac{e_n^m}{m!}\frac{d^m f}{dx^m}(x^*)+\frac{e_n^{m+1}}{(m+1)!}\cdot\frac{d^{m+1}f}{dx^{m+1}}(\varepsilon_{m+1})\right)}{\frac{e_n^{m-1}}{(m-1)!}\cdot\frac{d^m f}{dx^m}(\varepsilon_{m-1})}$$

$$e_{n+1}=\frac{e_n\frac{d^m f}{dx^m}(x^*)+\frac{e_n^2}{m}\frac{d^{m+1}f}{dx^{m+1}}(\varepsilon_m)-\alpha\frac{e_n}{m}\frac{d^m f}{dx^m}(x^*)-\alpha\frac{e_n^2}{m(m+1)}\frac{d^{m+1}f}{dx^{m+1}}(\varepsilon_{m+1})}{\frac{d^m f}{dx^m}(\varepsilon_{m-1})}$$

$$e_{n+1}=\frac{\left(e_n-\alpha\frac{e_n}{m}\right)\frac{d^m f}{dx^m}(x^*)+e_n^2\left(\frac{1}{m}\frac{d^{m+1}f}{dx^{m+1}}(\varepsilon_m)-\frac{\alpha}{m(m+1)}\frac{d^{m+1}f}{dx^{m+1}}(\varepsilon_{m+1})\right)}{\frac{d^m f}{dx^m}(\varepsilon_{m-1})}$$

We now need $e_n-\alpha\frac{e_n}{m}=0 \Rightarrow \boxed{\alpha=m}$. The equality becomes

$$e_{n+1}=\frac{|e_n|^2\left(\frac{1}{m}\frac{d^{m+1}f}{dx^{m+1}}(\varepsilon_m)-\frac{1}{m+1}\frac{d^{m+1}f}{dx^{m+1}}(\varepsilon_{m+1})\right)}{\frac{d^m f}{dx^m}(\varepsilon_{m-1})}$$

Let $A(c)=\dfrac{\frac{1}{m}\max_{\beta\in i}\left|\frac{d^{m+1}f}{dx^{m+1}}(\beta)\right|-\frac{1}{m+1}\min_{\gamma\in i}\left|\frac{d^{m+1}f}{dx^{m+1}}(\gamma)\right|}{\min_{\alpha\in i}\left|\frac{d^m f}{dx^m}(\alpha)\right|}$, which is finite when x_n close to x^* ($i=(x^*-c,\ x^*+c)$, where we have $\varepsilon_{m-1},\varepsilon_m,\varepsilon_{m+1}\in i$)

Then, $|e_{n+1}|\leq|e_n|^2\cdot A(c)$

As before, if $cA(c)<1$ (happens for sufficiently small c), we have at least quadratic convergence

$\boxed{4.2.}$ $Y\sim Geo(p)\Rightarrow \mathbb{P}(Y=k)=(1-p)^k p,\ k\geq 0;\ G_Y(s)=\dfrac{p}{1-(1-p)s}$

(a) $Y_{AA}\sim Geo(\frac{1}{2})$, $Y_{AB}\sim Geo(\frac{1}{2})$, $Y_{BA}\sim Geo(\frac{1}{3})$, $Y_{BB}\sim Geo(\frac{2}{3})$

We have to solve $\begin{cases} G_{AA}(x)\,G_{AB}(y)=x \\ G_{BA}(x)\,G_{BB}(y)=y\end{cases}$, on $\underline{f}(\underline{x})=\underline{0}$, where $\underline{f}=\begin{pmatrix}f_1\\f_2\end{pmatrix}$, $f_1=G_{AA}(x)\cdot G_{AB}(y)$ and $f_2=G_{BA}(x)\,G_{BB}(y)-y$.

We then have:

$$f_1(x,y)=0 \Rightarrow \frac{\frac{1}{2}}{1-\frac{1}{2}x}\cdot\frac{\frac{1}{2}}{1-\frac{1}{2}y} - x = 0 \Rightarrow \frac{1}{(2-x)(2-y)} - x = 0$$

$$f_2(x,y)=0 \Rightarrow \frac{\frac{1}{3}}{1-\frac{2}{3}x}\cdot\frac{\frac{2}{3}}{1-\frac{1}{3}y} - y = 0 \Rightarrow \frac{1}{(3-2x)}\cdot\frac{2}{(3-y)} - y = 0$$

The Jacobian of $\underline{f}$ is:

$$\underline{\underline{J}}(\underline{f}) = \begin{pmatrix} \frac{\partial f_1}{\partial x} & \frac{\partial f_1}{\partial y} \\ \frac{\partial f_2}{\partial x} & \frac{\partial f_2}{\partial y} \end{pmatrix} = \begin{pmatrix} \frac{1}{(2-x)^2(2-y)} - 1 & \frac{1}{(2-x)(2-y)^2} \\ \frac{4}{(3-2x)^2(3-y)} & \frac{2}{(3-2x)(3-y)^2} - 1 \end{pmatrix}$$

(b) Newton.scala

```
object Problem
{
  var tol = 1e-10
  var N = 100
  def [funct] (xn: Double, yn: Double) : (Double, Double) =   // f(x)
  {
    var x = 1.0 / ((2.0 - xn)*(2.0-yn)) - xn
    var y = 2.0 / ((3.0 - 2.0 * xn) * (3.0-yn)) - yn
    return (x,y)
  }
  def [system] (xn: Double, yn: Double) : (Double, Double) =   // Solving for Δx : J(f)(xn) Δx = -f(xn)
  {
    var A = 1.0 / ((2.0 - xn)*(2.0-xn)*(2.0-yn)) - 1.0
    var B = 1.0 / ((2.0 - xn)*(2.0-yn)*(2.0-yn))
    var C = 4.0 / ((3.0 - 2.0*xn)*(3.0-2.0*xn)*(3.0-yn))
    var D = 2.0 / ((3.0-2.0*xn)*(3.0-yn)*(3.0-yn)) - 1.0   // (A B; C D)(x; y) = (E; F)
    var E = xn - 1.0 / ((2.0 - xn)*(2.0 - yn))              // x = (de - bf)/(ad - bc)
    var F = yn - 2.0 / ((3.0 - 2.0* xn)*(3.0 - yn))
    var x = (D*E - B*F) / (A*D - B*C)                       // y = (af - ce)/(ad - bc)
    var y = (A*F - C*E) / (A*D - B*C)
    return (x,y)
  }
  def [size] (xn: Double, yn: Double): Double =   // (xn,yn) -> || f(xn, yn) ||
  {
    var (x,y) = funct (xn,yn)
    var aux = x*x + y*y
    return Math.pow (aux, 0.5)
  }
```

```
def Newton(arg1: Double, arg2: Double): (Double, Double, Int) =
                                         ↑xn     ↑yn     ↑m = #steps
{
  var m=0
  var xn = arg
  var yn = arg2
  while ((n!=N) && (size(xn,yn) > tol))
  {
    var (x,y) = system(xn,yn)   // Δx
    xn = xn + x
    yn = yn + y
    n = n+1
  }
  return (xn,yn,m)
}
def main(args: Array[String]) =
{
  var res = Newton(0.0, 0.0) // start with x0 = (0.0, 0.0)
  println(res)
}
```

Result: (0.3667587252968 3695, 0.330 56621 34 785 6646, 4)

$\uparrow x$ $\quad \uparrow y$ $\quad \uparrow n$

5.3. First, we'll prove the Sherman-Morrison formula:

Let $\underline{\underline{A}}$ be an invertible $n \times n$ matrix, $\underline{u}, \underline{v} \in \mathbb{R}^n$, and $\underline{\underline{A}} + \underline{u}\,\underline{v}^T$ is invertible, then

$$\left(\underline{\underline{A}} + \underline{u}\,\underline{v}^T\right)^{-1} = \underline{\underline{A}}^{-1} - \frac{\underline{\underline{A}}^{-1}\underline{u}\,\underline{v}^T\underline{\underline{A}}^{-1}}{1+\underline{v}^T\underline{\underline{A}}^{-1}\underline{u}} \quad \Big| \cdot \left(\underline{\underline{A}} + \underline{u}\,\underline{v}^T\right)$$

$$\cancel{\underline{\underline{I_n}}} = \cancel{\underline{\underline{I_n}}} + \underline{\underline{A}}^{-1}\underline{u}\,\underline{v}^T - \frac{\underline{\underline{A}}^{-1}\underline{u}\,\underline{v}^T}{1+\underline{v}^T\underline{\underline{A}}^{-1}\underline{u}} - \frac{\underline{\underline{A}}^{-1}\underline{u}\,\underline{v}^T\underline{\underline{A}}^{-1}\underline{u}\,\underline{v}^T}{1+\underline{v}^T\underline{\underline{A}}^{-1}\underline{u}}$$

scalar

$$A \cdot \Big| \quad \underline{\underline{A}}^{-1}\underline{u}\,\underline{v}^T = \frac{\underline{\underline{A}}^{-1}\left(\underline{u}\,\underline{v}^T + \underline{u}\,\underline{v}^T\underline{\underline{A}}^{-1}\underline{u}\,\underline{v}^T\right)}{1+\underline{v}^T\underline{\underline{A}}^{-1}\underline{u}}$$

$$\underline{u}\,\underline{v}^T = \frac{\underline{u}\left(1+\underline{v}^T\underline{\underline{A}}^{-1}\underline{u}\right)\underline{v}^T}{1+\underline{v}^T\underline{\underline{A}}^{-1}\underline{u}}$$

$$\underline{u}\,\underline{v}^T = \underline{u}\,\underline{v}^T \quad \text{(YES)}$$

So, we proved Sherman-Morrison formula.

In Broyden's method we need to calculate

$$\underline{\underline{\hat{J}_n}} = \underline{\underline{\hat{J}_{n-1}}} + \frac{\Delta \underline{y} - \underline{\underline{\hat{J}_{n-1}}}\Delta \underline{x}}{\|\Delta \underline{x}\|^2} \Delta \underline{x}^T$$ and then to solve the system

$\underline{\underline{\hat{J}_n}} \Delta \underline{x} = -\underline{y_0}$ for $\Delta \underline{x}$, which would require $O(d^3)$ operations, where d is the dimension of the vector $\Delta \underline{x}$. To get rid of this, we can calculate $\underline{\underline{\hat{J}_n}}^{-1}$ at each step and the system would become $\Delta \underline{x} = -\underline{\underline{\hat{J}_n}}^{-1} \underline{y_0}$, with time complexity $O(d^2)$.

To do that, we'll use the Sherman-Morrison formula:

$$\underline{\underline{\hat{J}_n}} = \underline{\underline{\hat{J}_{n-1}}} + \frac{\Delta \underline{y} - \underline{\underline{\hat{J}_{n-1}}}\Delta \underline{x}}{\|\Delta \underline{x}\|^2} \Delta \underline{x}^T \quad \Big| \, (\,)^{-1}$$

$$\underline{\underline{\hat{J}_n}}^{-1} = \left(\underline{\underline{\hat{J}_{n-1}}} + \frac{\Delta \underline{y} - \underline{\underline{\hat{J}_{n-1}}}\Delta \underline{x}}{\|\Delta \underline{x}\|^2} \Delta \underline{x}^T\right)^{-1} \overset{\text{S-M}}{=} \underline{\underline{\hat{J}_{n-1}}}^{-1} - \frac{\underline{\underline{\hat{J}_{n-1}}}^{-1} \frac{\Delta \underline{y} - \underline{\underline{\hat{J}_{n-1}}}\Delta \underline{x}}{\|\Delta \underline{x}\|^2} \Delta \underline{x}^T \underline{\underline{\hat{J}_{n-1}}}^{-1}}{1 + \Delta \underline{x}^T \underline{\underline{\hat{J}_{n-1}}}^{-1} \frac{\Delta \underline{y} - \underline{\underline{\hat{J}_{n-1}}}\Delta \underline{x}}{\|\Delta \underline{x}\|^2}}$$

$$\boxed{\underline{\underline{\hat{J}_n}}^{-1} = \underline{\underline{\hat{J}_{n-1}}}^{-1} - \frac{\frac{\underline{\underline{\hat{J}_{n-1}}}^{-1}\Delta \underline{y} - \Delta \underline{x}}{\|\Delta \underline{x}\|^2} \Delta \underline{x}^T \underline{\underline{\hat{J}_{n-1}}}^{-1}}{1 + \Delta \underline{x}^T \frac{\underline{\underline{\hat{J}_{n-1}}}^{-1}\Delta \underline{y} - \Delta \underline{x}}{\|\Delta \underline{x}\|^2}}} = \underline{\underline{\hat{J}_{n-1}}}^{-1} - \frac{A}{B},$$ where

$$A = \frac{\underline{\underline{\hat{J}_{n-1}}}^{-1}\Delta \underline{y} - \Delta \underline{x}}{\|\Delta \underline{x}\|^2} \Delta \underline{x}^T \underline{\underline{\hat{J}_{n-1}}}^{-1}$$

- $\underline{\underline{\hat{J}_{n-1}}}^{-1} \Delta \underline{y}$ needs $O(d^2)$ operations $\Rightarrow (d\times 1)$ vector
- $\Delta \underline{x}^T \underline{\underline{\hat{J}_{n-1}}}^{-1}$ needs $O(d^2)$ operations $\Rightarrow (1\times d)$ vector
- $\left(\frac{\underline{\underline{\hat{J}_{n-1}}}^{-1}\Delta \underline{y} - \Delta \underline{x}}{\|\Delta \underline{x}\|^2}\right) \cdot \left(\Delta \underline{x}^T \underline{\underline{\hat{J}_{n-1}}}^{-1}\right)$ needs $O(d^2)$ operations

$\Rightarrow A$ is a $(d\times d)$ matrix which needs $O(d^2)$ operations

$$B = 1 + \Delta \underline{x}^T \frac{\underline{\underline{\hat{J}_{n-1}}}^{-1}\Delta \underline{y} - \Delta \underline{x}}{\|\Delta \underline{x}\|^2}$$

- $\underline{\underline{\hat{J}_{n-1}}}^{-1} \Delta \underline{y}$ needs $O(d^2)$ operations $\Rightarrow (d\times 1)$ vector
- $\Delta \underline{x}^T \frac{\underline{\underline{\hat{J}_{n-1}}}^{-1}\Delta \underline{y} - \Delta \underline{x}}{\|\Delta \underline{x}\|^2}$ needs $O(d^2)$ operations $\Rightarrow$ scalar

$\Rightarrow B$ is a scalar which needs $O(d^2)$ operations

So, the complexity of each iteration becomes $O(d^2)$ from $O(d^3)$ as the linear system $\underline{\underline{\hat{J}_n}} \Delta \underline{x} = -\underline{y_0}$ becomes $\Delta \underline{x} = -\underline{\underline{\hat{J}_n}}^{-1} \underline{y_0}$, which is $O(d^2)$.

4.4. We will first find the function $\hat{f}$ that interpolates the points $(a, f(a))$, $(b, f(b))$, $(c, f(c))$, where $\hat{f}$ is quadratic by using the Lagrange Interpolation formula:

$$\hat{f}(x) = \frac{(x-b)(x-c)}{(a-b)(a-c)} f(a) + \frac{(x-a)(x-c)}{(b-a)(b-c)} f(b) + \frac{(x-a)(x-b)}{(c-a)(c-b)} f(c)$$

__Problem 1__: This requires dividing by $(a-b)$, $(b-c)$ and $(c-a)$, but when we get to very small numbers, the catastrophic cancellation phenomenon might occur from roundoff errors.

__Problem 2__: If we get to a bracket (a,b,c) where $f(a)=f(b)=f(c)$, then $\hat{f}(x)$ will be equal to $f(a)$, so we don't know what z from the interval to choose.

As $a < b < c$ and $f(a) > f(b) < f(c) \Rightarrow \hat{f}(a) > \hat{f}(b) < \hat{f}(c) \Rightarrow \hat{f}$ is convex and its minimum is the only stationary point.

$$\hat{f}'(x) = \frac{f(a)}{(a-b)(a-c)}(2x-b-c) + \frac{f(b)}{(b-a)(b-c)}(2x-a-c) + \frac{f(c)}{(c-a)(c-b)}(2x-a-b)$$

$$\hat{f}'(x) = 2\left(\frac{f(a)}{(a-b)(a-c)} + \frac{f(b)}{(b-a)(b-c)} + \frac{f(c)}{(c-a)(c-b)}\right)x - \left(\frac{b+c}{(a-b)(a-c)}f(a) + \frac{a+c}{(b-a)(b-c)}f(b) + \frac{a+b}{(c-a)(c-b)}f(c)\right)$$

$$\hat{f}'(z) = 0 \iff z = \frac{\frac{b+c}{(a-b)(a-c)}f(a) + \frac{a+c}{(b-a)(b-c)}f(b) + \frac{a+b}{(c-a)(c-b)}f(c)}{2\left(\frac{f(a)}{(a-b)(a-c)} + \frac{f(b)}{(b-a)(b-c)} + \frac{f(c)}{(c-a)(c-b)}\right)}$$

$$\boxed{z = \frac{1}{2}\cdot\frac{(b^2-c^2)f(a) + (c^2-a^2)f(b) + (a^2-b^2)f(c)}{(b-c)f(a) + (c-a)f(b) + (a-b)f(c)}} \quad (*)$$

We start with an initial bracket (a_0, b_0, c_0). Then, at each step we calculate z given $(*)$ and compare $f(z)$ with $f(b)$: if $f(b) < f(z)$, then the new bracket will be (a, b, z), otherwise, the new bracket will be (b, z, c). Repeat this until $(c-a) < tol$.

4.5. We want to find $\arg\min_{\underline{x}} f(\underline{x})$, where $H(f)$ is positive definite everywhere

- $\kappa(H(f)) = \frac{\lambda_{max}}{\lambda_{min}}$, lower condition numbers $\Rightarrow$ faster convergence
- M symmetric positive definite $\Rightarrow M^T = M$

We use Gradient Descent for $\arg\min_{\underline{y}} f(M\underline{y})$ to generate $(\underline{y}_0, \underline{y}_1, \dots, \underline{y}_n)$, then recover $\underline{x}_n = M\underline{y}_n$

(a) $$\frac{df(M\underline{y})}{d\underline{y}}(\underline{y}_n) = \frac{d(f\circ \overset{g(\underline{y}) = M\underline{y}}{\underline{g}})}{d\underline{y}}(\underline{y}_n) \underset{\text{Partial Chain Rule}}{=} J(\underline{g})^T\left(\frac{df}{d\underline{x}}\circ \underline{g}(\underline{y}_n)\right) = J(M\underline{y})^T \cdot \frac{df}{d\underline{x}}(\underline{x}_n) \overset{M^T=M}{=} M\frac{df}{d\underline{x}}(\underline{x}_n)$$

Using Gradient Descent for $\arg\min_{\underline{y}} f(M\underline{y})$, we get:

$$\underline{y_{n+1}} = \underline{y_n} - \alpha_n \frac{df(M\underline{y})}{d\underline{y}}(\underline{y_n})$$

$$M\cdot \Big|\ M^{-1}\underline{x_{n+1}} = M^{-1}\underline{x_n} - \alpha_n M \frac{df}{d\underline{x}}(\underline{x_n})$$

$$\underline{x_{n+1}} = \underline{x_n} - \alpha_n M^2 \frac{df}{d\underline{x}}(\underline{x_n}) \quad (*)$$

(b) $$H(f(M\underline{y}))(\underline{y_n}) = J\left(\frac{df(M\underline{y})}{d\underline{y}}\right)^T(\underline{y_n}) = J\left(\overset{\text{same } \underline{g}}{\frac{d(f\circ\underline{g})}{d\underline{y}}}\right)(\underline{y_n}) \overset{\text{Partial chain Rule}}{=} J\left(J(\underline{g})^T\cdot\left(\frac{df}{d\underline{x}}\circ\underline{g}\right)\right)^T(\underline{y_n}) =$$

$$\overset{M^T=M}{=} J\left(M\cdot\left(\frac{df}{d\underline{x}}\circ\underline{g}\right)\right)^T(\underline{y_n}) = M\cdot J\left(\frac{df}{d\underline{x}}\circ\underline{g}\right)(\underline{y_n}) \overset{\text{Partial Chain Rule}}{=} M\cdot\left(J\left(\frac{df}{d\underline{x}}\right)\circ\underline{g}\right)(\underline{y_n})\cdot J(\underline{g}) = M\cdot J\left(\frac{df}{d\underline{x}}\right)(\underline{g}(\underline{y_n}))\cdot M \Rightarrow$$

$$\Rightarrow \boxed{H(f(M\underline{y}))(\underline{y_n}) = M\cdot H(f)(\underline{x_n})\cdot M}$$

(c) We want to obtain the lowest possible condition number for the first step of $(*)$, so we want to minimize

$$\kappa(H(f(M\underline{y}))(\underline{y_0})) = \kappa(M\cdot H(f)(\underline{x_0})\cdot M) = \frac{\lambda_{max}}{\lambda_{min}} \geq 1 \text{ (page 31 - lecture notes - (vi)(e))}$$

To have $\frac{\lambda_{max}}{\lambda_{min}} = 1$, we will choose M such that

$$M^{-1}\Big|\ M\cdot H(f)(\underline{x_0})\cdot M = I\ \Big|\ M^{-1}$$

$$H(f)(\underline{x_0}) = M^{-2}$$

$$Q^{-1}\Delta^2 Q = M^{-2} \Rightarrow \boxed{M = Q^{-1}\Delta^{-1}Q}$$

We have $M^2 = H(f)(\underline{x_0})$ and if we compare Newton's method's first step:

$$\underline{x_1} = \underline{x_0} - \alpha_0 H^{-1}(f)(\underline{x_0}) \frac{df}{d\underline{x}}(\underline{x_0})$$

with the first step from our method:

$\underline{x_1} = \underline{x_0} - \alpha_0 M^2 \frac{df}{d\underline{x}}(\underline{x_0})$, and replace M^2 by $(Q^{-1}\Delta^{-1}Q)^2 = (Q^{-1}\Delta^2 Q)^{-1} = H^{-1}(f)(\underline{x_0})$, we observe that they are equivalent!

As $H(f)(\underline{x_0})$ is symmetric $\Rightarrow Q^{-1} = Q^T \Rightarrow M^T = (Q^{-1}\Delta^{-1}Q)^T = Q^T(\Delta^{-1})^T(Q^{-1})^T = Q^{-1}\Delta^{-1}Q \Rightarrow$

$\Rightarrow M$ is symmetric

$\boxed{5.6.}$ The quadratic function $g(\alpha)$ interpolates the points $(0, f(\underline{x_n}))$ and $(\alpha', f(\underline{x_n} + \alpha'\underline{d}))$ and satisfies $\frac{dg}{d\alpha}(0) = \frac{df(\underline{x_n} + \alpha\underline{d})}{d\alpha}(0)$

$$\frac{df(\underline{x_n} + \alpha\underline{d})}{d\alpha}(0) = \left(\frac{df}{d\underline{x}}\circ(\underline{x_n} + \alpha\underline{d})\right)\left(\frac{d(\underline{x_n} + \alpha\underline{d})}{\alpha}\right)(0) = \underline{g_n}\cdot\underline{d}$$

$g(\alpha) = A\alpha^2 + B\alpha + C$

We have $g(0) = f(\underline{x_n}) \Rightarrow \boxed{C = f(\underline{x_n})}$

$g(\alpha') = A\alpha'^2 + B\alpha' + f(\underline{x_n}) = f(\underline{x_n} + \alpha\underline{d})$

and

$\frac{dg}{d\alpha}(0) = \underline{g_n^T d} \Rightarrow 2\alpha A + B\Big|_{\alpha=0} = \underline{g_n^T d} \Rightarrow \boxed{B = \underline{g_n^T d}}$

$\Rightarrow \boxed{A = \frac{f(\underline{x_n} + \alpha\underline{d}) - f(\underline{x_n}) - \alpha' \underline{g_n^T d}}{\alpha'^2}}$

- Why is this a good choice?

If we want to be able to choose how much we want to go in a direction, we need to approximate the function $f(\underline{x_n} + \alpha\underline{d})$ with a quadratic function g. It's important that g agrees with $f(\underline{x_n} + \alpha\underline{d})$ at the two points: $\alpha = 0$ (when we make no progress) and $\alpha = \alpha'$ (the predefined length from the previous step (we can't go more than that)).

Also, as we approach the minimum, g will have a smaller codomain and the minimum of g will become closer and closer to 0 (as we will get $f(\underline{x_n})$ closer to the minimum), so we need to have the error as small as possible (from Taylor's theorem, the error will be the term with degree $= 2$), so we choose $\frac{dg}{d\alpha}(0) = \frac{df(\underline{x_n} + \alpha\underline{d})}{d\alpha}(0)$.

- What should be the conditions on $\underline{d}$ and/or α'?

First, we need that $\boxed{A > 0}$, to be sure that α_n is a minimum (and not a maximum). So: $f(\underline{x_n} + \alpha\underline{d}) - f(\underline{x_n}) - \alpha'\underline{g_n^T d} > 0$. Second, we need to have a descent direction, so we need $\underline{g_n^T d_n} < 0 \Rightarrow \boxed{B < 0}$.

Finally, we have the next step length is α_n, which is the minimum of g, but if we get an $\alpha_n > \alpha'$, we basically "undo" what we did at the previous step, so we want the minimum to fall between 0 and α', so we need that $\frac{dg}{d\alpha}(0) < 0$ and $\frac{dg}{d\alpha}(\alpha') > 0$, so that we have an α_n with $\frac{dg}{d\alpha}(\alpha_n) = 0$: $B < 0$ - already established and

$$2\alpha' \cdot \frac{f(\underline{x_n}' + \alpha\underline{d}) - f(\underline{x_n}) - \alpha'\underline{g_n^T d}}{\alpha'^2} + \underline{g_n^T}\,\underline{d} > 0.$$

- Find a formula for α_n:

$$\frac{dg}{d\alpha}(\alpha_n) = 0 \iff 2\alpha_n A + B = 0 \iff \alpha_n = -\frac{B}{2A} = -\frac{\alpha'^2 \underline{g_n^T d}}{f(\underline{x_n} + \alpha\underline{d}) - f(\underline{x_n}) - \alpha'\underline{g_n^T d}}.$$

4.7. $\underline{f}: \mathbb{R}^d \to \mathbb{R}^m$, $m > d \Rightarrow$ finding $\underline{w} \in \mathbb{R}^d$ s.t. $\underline{f}(\underline{w})$ is as close as possible to $\underline{0}$ is an overdetermined system.

We will find $\arg\min_{\underline{w}} \ell(\underline{w})$, where $\ell(\underline{w}) = \|\underline{f}(\underline{w})\|^2 = \underline{f}(\underline{w})^T \underline{f}(\underline{w})$

(a) $$\frac{d\ell}{d\underline{w}} = \frac{d\|\underline{f}(\underline{w})\|^2}{d\underline{w}} = J(\underline{f})^T(2\cdot\underline{f}) = 2J(\underline{f})\underline{f}$$

We approximate $H(\ell)$ by $2J(\underline{f})^T J(\underline{f})$ as we have

here we approximate $J(\underline{f})$ to be a constant matr

$$H(\ell) = J\left(\frac{d\ell}{d\underline{w}}\right)^T = J\left(J(\underline{f})\cdot 2\underline{f}\right) = 2J\left(J(\underline{f})\underline{f}\right) \approx 2J(\underline{f})^T J(\underline{f})$$

We fix the step length of the quasi-Newton iterative step to $1 \Rightarrow \alpha_n = 1$.

From Newton's method we have

$$\Delta\underline{w} = -\left(H(\ell)(\underline{w_n})\right)^{-1}\frac{d\ell}{d\underline{w}}(\underline{w_n})$$

$$-H(\ell)(\underline{w_n})\cdot\Delta\underline{w} = \frac{d\ell}{d\underline{w}}(\underline{w_n})$$

And we can approximate $H(\ell)(\underline{w_n})$ by $2J(\underline{f})^T J(\underline{f})$:

$$-\cancel{2}J(\underline{f})^T J(\underline{f})\,\Delta\underline{w} = \cancel{2}J(\underline{f})\,\underline{f}$$

$$\boxed{-J(\underline{f})^T J(\underline{f})\,\Delta\underline{w} = J(\underline{f})\,\underline{f}}$$

Linear regression: $\underline{f}(\underline{w}) = X\underline{w} - \underline{y}$, $\underline{X} \in \mathbb{R}^{m\times d}$ and $\underline{y} \in \mathbb{R}^m$.

(b) To find the minimum of $\underline{f}$, we use ℓ and find it's arg min:

$$\ell(\underline{w}) = \|\underline{f}(\underline{w})\|^2 = (X\underline{w} - \underline{y})^T(X\underline{w} - \underline{y}) = \underline{w}^T X^T X\underline{w} - \underline{y}^T X\underline{w} - \underline{w}^T X^T\underline{y} + \underline{y}^T\underline{y}$$

$$\frac{d\ell}{d\underline{w}} = 2X^T X\underline{w} - X^T\underline{y} - X^T\underline{y} = 2X^T(X\underline{w} - \underline{y})$$

We need a minimum for this, so

$$\cancel{2}X^T(X\underline{w} - \underline{y}) = 0$$

$$X^T X\underline{w} = X^T\underline{y} \Rightarrow \underline{w} = (X^T X)^{-1}X^T\underline{y} \quad \circledast$$

The answer needs (to be well-defined) that $X^T X$ is non-singular (otherwise we have infinitely many stationary points, but we only want the minimum of ℓ).

In order for us to determine that this solution is a minimum, we need to show that the Hessian of ℓ in $\underline{w_0}$ is positive definite ($\underline{w_0}$ is the solution from $\circledast$)

$$H(\ell)(\underline{w_0}) = J\left(\frac{d\ell}{d\underline{w}}\right)(\underline{w_0}) = J\left(\frac{d\ell}{d\underline{w}}\right)^T(\underline{w_0}) = J(2J(f)^T f)(\underline{w_0}) = J\left(2(X\underline{w} - \underline{y})^T(X\underline{w} - \underline{y})\right)(\underline{w_0})$$

$$2J(X^T(X\underline{w} - \underline{y})) = 2X^T X$$

We now have for any vector $\underline{v} \in \mathbb{R}^d$:

$$2\,\underline{v}^T X^T X \underline{v} = 2(X\underline{v})^T (X\underline{v}) = 2\|X\underline{v}\|^2 \geq 0 \Rightarrow H(\ell)(\underline{w_0})$$ is positive semi-definite and because the Hessian does not depend on $\underline{w}$, we have the Hessian positive semi-definite everywhere $\Rightarrow$

$\Rightarrow \ell$ is a convex function $\Rightarrow$ the stationary point we found is a global minimum.

(c) $\|\underline{w}\| < 1$ (ridge regression)

As $\|w\| > 0$, we can use $\|\underline{w}\|^2 < 1$ instead.

The constraint is $h(\underline{w}) = 1 - \|\underline{w}\|^2 > 0$

We want to find the stationary points of

$\Lambda(\mu, \underline{w}) = \ell(\underline{w}) - \mu h(\underline{w})$, where

$$\frac{d\ell}{d\underline{w}} = \mu \frac{dh}{d\underline{w}}$$

$$2X^T(X\underline{w} - \underline{y}) = \mu \frac{d(\underline{w}^T\underline{w})}{d\underline{w}} = \mu \cdot 2\underline{w}$$

$$X^T(X\underline{w} - \underline{y}) = \mu \underline{w}$$

$$X^T X \underline{w} - X^T \underline{y} = \mu \underline{w}$$

$$(X^T X - \mu I)\underline{w} = X^T \underline{y}$$

$$\boxed{\underline{w} = (X^T X - \mu I)^{-1} X^T \underline{y}}$$

The formula is well-defined because for some μ as the constrained region is $\|\underline{w}\| < 1$, which means that it is a closed region, where we have a minimum that is finite. On the contour we have the region as a circle, so the minimum is inside it or on the margin.