Monday, ~~June~~ July 16 2012

From $m_0 \dots m_N$ we can obtain $s_{k,0}, s_{k,1}, s_{k,2}, s_{k,3}$ that are the coefficients of the splines.

We have

$$S(x) = s_{k,0} + s_{k,1}(x-x_k) + s_{k,2}(x-x_k)^2 + s_{k,3}(x-x_k)^3$$

Substituting $x = x_0$ in ⑩

$$S(x_0) = y_0 = s_{k,0} + s_{k,1}(x_k - x_k)^0 + s_{k,2}(x_k - x_k)^2 + s_{k,3}(x - x_k)^3$$

⑪ $\boxed{s_{k,0} = y_k}$

Derivating ⑩ twice

$$s'(x) = s_{k,1} + 2s_{k,2}(x-x_k) + 3s_{k,3}(x-x_k)^2$$

$$s''(x) = 2s_{k,2} + 6s_{k,3}(x-x_k)$$

From the definition $m_k = s''(x_k)$

Substitute in $s''(x)$ $x = x_k$

$$s''(x_k) = 2s_{k,2} + 6s_{k,3}(x_k - x_k)$$

$$s''(x_k) = 2s_{k,2} = m_k$$

⑫ $\boxed{s_{k,2} = \frac{m_k}{2}}$

By making $x = x_k$ in $s_k'(x)$

$s_k'(x_k) = s_{k,1}$.

From $\boxed{⑦ \ s_k'(x_k) = -\frac{m_k h_k}{3} - \frac{m_{k+1} h_k}{6} + d_k}$

Since $s_k'(x_k) = s_{k,1}$ then we have

$$s_{k,1} = s_k'(x_k) = -\frac{m_k h_k}{3} - \frac{m_{k+1} h_k}{6} + d_k$$

13 $\boxed{s_{k,1} = d_k - \frac{h_k(2m_k + m_{k+1})}{6}}$

Making $x = x_{k+1}$ in $s_k''(x)$

$$s_k''(x_{k+1}) = 2s_{k,2} + 6s_{k,3}\underbrace{(x_{k+1} - x)}_{h_k}$$

Since we have that $m_{k+1} = s_k''(x_{k+1})$

$$m_{k+1} = 2\frac{m_k}{2} + 6s_{k,3}h_k$$

$$m_{k+1} = m_k + 6s_{k,3}h_k \longrightarrow \boxed{s_{k,3} = \frac{m_{k+1} - m_k}{6h_k}}$$

## Other end point constraints

Equation ⑨ gives us N-1 equations to find $m_0 \dots m_N$ constraints (N+1) constants. We need two more equations to be able to find $m_0 \dots m_N$. The two other ~~of~~ equations can be found by choosing different end point constraints:

1) Clamped Spline

The first derivatives at the end ~~of~~ are given:

$s'(a)$, $s'(b)$

So we will have the following equations:

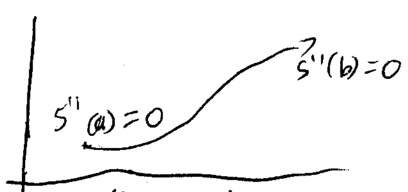
$$\left(\frac{3}{2}h_0 + h_1\right)m_1 + h_1 m_2 = U_1 - 3(d_0 - s'(x_0))$$

$$h_{k-1} m_{k-1} + 2(h_{k-1} + h_k) m_k + h_k m_{k+1} \qquad k = 2, 3 \dots N-2$$

$$h_{N-2} m_{N-2} + 2\left(h_{N-2} + \frac{3}{2} h_{N-1}\right) m_{N-1} = U_{N-1} - 3(s'(x_N) - d_{N-1})$$


2) Natural spline

The second derivatives at the ends are given




$m_0 = 0$
$m_N = 0$

$$2(h_0 + h_1) m_1 + h_1 m_2 = U_1$$

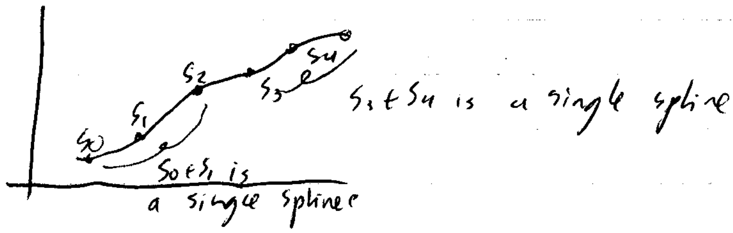
$$h_{k-1} + 2(h_{k-1} + h_k) m_k + h_k m_{k+1} = U_k$$

$k = 2, 3, n-2$

$$h_{N-2} m_{N-2} + 2(h_{N-2} + h_{N-1}) m_{N-1} = U_{N-1}$$

## 3) Extrapolated Spline

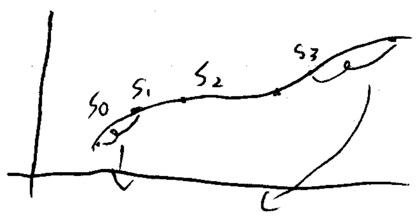
$S_0$ and $S_1$ are the same spline $S_{N-2}$, $S_{N-1}$ are the same spline
($S_1$ is an extension of $S_0$ and $S_{N-1}$ is an extension of $S_{N-1}$).




* For equations see the text book

## 4) Parabolic terminated Spline

$S_0$ and $S_{N-1}$ are quadratic instead of cubic.




Quadratic equations instead of cubic

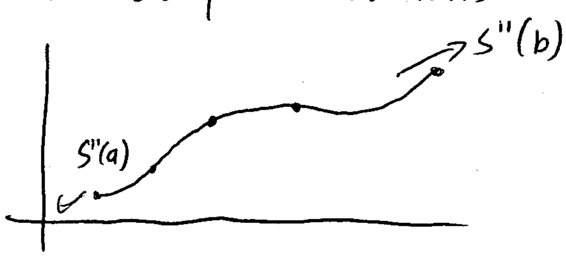
$Y = ax^2 + bx + c$

See books for equations

## 5) End-point curvature adjusted spline

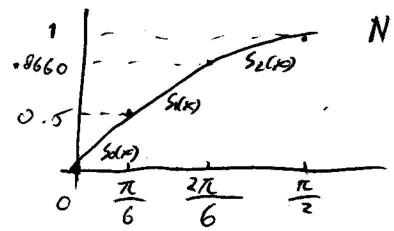
$S''(a)$ and $S''(b)$ are given

See book for equations



· Example of spline

Find the natural spline that approximates $Y = \sin(x)$ in the interval $0 \to \frac{\pi}{2}$ with 4 points, equally spaced




$N = 3$

| X | Y |
|---|---|
| 0 | 0 |
| $\frac{\pi}{6} = .5230$ | .5 |
| $\frac{\pi}{3} = 1.0478$ | .866 |
| $\frac{\pi}{2} = 1.570$ | 1 |

$$S_0(x) = S_{0,0} + S_{0,1}(x - x_k) + S_{0,2}(x - x_k)^2 + S_{0,3}(x - x_k)^3$$
$$0 \le x \le \frac{\pi}{6}$$

$$S_1(x) = S_{1,0} + S_{1,1}(x - x_k) + S_{1,2}(x - x_k)^2 + S_{1,3}(x - x_k)^3$$
$$\frac{\pi}{6} \le x \le \frac{\pi}{3}$$

$$S_2(x) = S_{2,0} + S_{2,1}(x - x_k) + S_{2,2}(x - x_k)^2 + S_{2,3}(x - x_k)^3$$
$$\frac{\pi}{3} \le x \le 1$$

We have that

$S_{k,0} = Y_k$ , $S_{k,1} = d_k - \frac{h_k(2m_k + m_{k+1})}{6}$

$S_{k,2} = \frac{m_k}{2}$ , $S_{k,3} = \frac{m_{k+1} - m_k}{h_k}$

Since this is a natural spline we have that $m_0 = 0$ and $m_3 = 0$

$h_0 = x_1 - x_0 = \frac{\pi}{6}$ $\quad$ $h_k = x_{k+1} - x_k$

$h_1 = \frac{\pi}{6}$

$h_2 = \frac{\pi}{6}$

$d_0 = \frac{Y_1 - Y_0}{h_0} = \frac{.5 - 0}{\pi/6} = .9549$ $\quad$ $d_k = \frac{Y_{k+1} - Y_k}{h_k}$

$d_1 = \frac{Y_2 - Y_1}{h_1} = \frac{.8660 - .5}{\pi/6} = .6990$

$d_2 = \frac{Y_3 - Y_2}{h_2} = \frac{1 - .8660}{\pi/6} = .2559$

$U_1 = 6(d_1 - d_0)$ $\qquad\qquad$ $U_k = 6(d_k - d_{k-1})$

$= 6(.6990 - .9549) = -1.5354$

$U_2 = 6(d_2 - d_1)$

$= 6(.2559 - .6990) = -2.6586$

From 2) Natural spline

$2(h_0 + h_1) m_1 + h_1 m_2 = U_1$

$h_{k-1} m_{k-1} + 2(h_{k-1} + h_k) m_k + h_k m_{k+1} = U_k$

$k = 2, 3 \ldots N-2$ $\quad h_{N-2} m_{N-2} + 2(h_{N-2} + h_{N-1}) m_{N-1} = U_{N-1}$

So we have

From a) $2\left(\frac{\pi}{6} + \frac{\pi}{6}\right) m_1 + \frac{\pi}{6} m_2 = -1.5354$

$\Downarrow$

① $2.0944\, m_1 + .5236\, m_2 = -1.5354$

~~From $k = 2$~~

~~b) $\frac{\pi}{6} m_1 + 2\left(\frac{\pi}{6} + \frac{\pi}{6}\right) m_2 + \frac{\pi}{6} m_3 = 2.6586$~~

~~$.5236\, m_1 + 2.0944\, m_2$~~

Since $N=3$ and equations in b) go from $2, 3 \ldots N-2$ so there are no equations for b)

From c) ② $\frac{\pi}{6} m_1 + 2\left(\frac{\pi}{6} + \frac{\pi}{6}\right) m_2 = -2.6586$

From ① and ② we can find $m_1, m_2$

So we have the following system

$$\begin{array}{c} A \\ B \end{array}\begin{bmatrix} 2.0944 & .5236 & -1.5354 \\ .5236 & 2.0944 & -2.6586 \end{bmatrix}$$

Using Gauss Elimination

$$\begin{array}{c} A \\ B + A\frac{(-.5236)}{2.0944} \end{array}\begin{bmatrix} 2.0944 & .5236 & -1.5354 \\ 0 & 1.9635 & -2.2748 \end{bmatrix}$$

Tuesday, 7/17/2012

**Back Substitution**

$$\boxed{m_2 = \frac{-2.2748}{1.9635} = -1.1585}$$

$$m_1 = \frac{-1.5354 - .5236\,(-1.1585)}{2.0944}$$

$$\boxed{m_1 = -.4435}$$

Also we have from natural spline that $m_0 = 0$ and $m_2 = 0$

$k = 0$

$h_0, h_1, h_2 = \frac{\pi}{6}$

$d_0 = .9549$

$d_1 = .6990$

$d_2 = .2559$

$u_1 = -1.5354,\ u_2 = -2.6586$

$$S_k(x) = S_{k,0} + S_{k,1}(x - x_k) + S_{k,2}(x - x_k)^2 + S_{k,3}(x - x_k)^3$$

$$S_{k,0} = y_k,\quad S_{k,1} = d_k - \frac{h_k(2m_k - m_1)}{6}$$

$$S_{k,2} = \frac{m_k}{2},\quad S_{k,3} = \frac{m_{k+1} - m_k}{6h_k}$$

$k = 0$

$x_0 = 0$

$y_0 = 0$

$$S_{0,0} = y_0 = 0$$

$$S_{0,1} = d_0 - \frac{h_0(2m_0 - m_1)}{6}$$

$$= .9549 - \frac{.5236\,(2(0) - (-.4435))}{6}$$

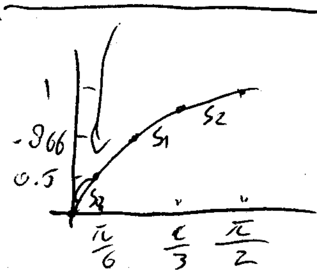
$$= .9936$$

$$S_{0,2} = \frac{m_0}{2} = \frac{0}{2} = 0$$

$$S_{0,2} = \frac{m_1 - m_0}{6h_0} = \frac{-.4435 - 0}{6(.5236)} = -.1412$$

$$S_0(x) = 0 + .9936(x - 0) + 0\,(x - 0)^2 - .1412(x - 0)^3$$

$$\boxed{S_0(x) = .9936x - .1412x^3}$$




So we have that

$$S_0(0) = .9936(0) - .1412(0)^3$$

$$= 0$$

$$S_0\left(\frac{\pi}{6}\right) = .9936\,(.5236) - .1412(.5236)^3$$

$$= .52084 - .08026$$

$$= .49948 \approx .5$$

verify splines are correct → check the points → derivative → 2nd derivative

$k = 1$

$S_{1,0} = Y_1 = .5$

$S_{1,1} = d_1 - \frac{h_1(2m_1 + m_2)}{6}$

$= .6990 - \frac{.5236\,(2(-.4435) + (-1.1585))}{6}$

$= .8775$

$S_{1,2} = \frac{m_1}{2} = \frac{-.4435}{2} = -.2218$

$S_{1,3} = \frac{m_2 - m_1}{6h_1} = \frac{-1.1585 - (-.4435)}{6(.5236)}$

$= -.2276$

$S_1(x) = .5 + .8775\,(x - \overset{x_1}{.5236}) - .2218\,(x - .5236)^2 - .2376\,(x - .5236)^2$

$k = 2$

$S_{2,0} = Y_2 = .8660$

$S_{2,1} = d_2 - \frac{h_2\,(2m_2 + m_3)}{6}$

$= .2559 - \frac{.5236\,(2(-1.1585) + 0)}{6}$

$= .4581$

$S_{2,2} = \frac{m_2}{2} = \frac{-1.1585}{2} = -.5793$

$S_{2,3} = \frac{m_3 - m_2}{6 \cdot h_2} = \frac{0 - (-1.1585)}{6(.5236)} = .3688$

$S_2(x) = .8660 + .4581\,(x - 1.0472) - .5793(x - 1.0472)^2 + .3688\,(x - 1.0472)^3$

verify splines are correct → check the points → derivative → 2nd derivative

$k=1$

$$S_{1,0} = y_1 = .5$$

$$S_{1,1} = d_1 - \frac{h_1(2m_1+m_2)}{6}$$

$$= .6990 - \frac{.5236\,(2(-.4435)+(-1.1585))}{6}$$

$$= .8775$$

$$S_{1,2} = \frac{m_1}{2} = \frac{-.4435}{2} = -.2218$$

$$S_{1,3} = \frac{m_2-m_1}{6h_1} = \frac{-1.1585-(-.4435)}{6(.5236)}$$

$$= -.2276$$

$$S_1(x) = .5 + .8775\,(x - \overset{x_1}{.5236}) - .2218\,(x-.5236)^2 - .2376\,(x-.5236)^2$$

$k=2$

$$S_{2,0} = y_2 = .8660$$

$$S_{2,1} = d_2 - \frac{h_2\,(2m_2+m_3)}{6}$$

$$= .2559 - \frac{.5236\,(2(-1.1585)+0)}{6}$$

$$= .4581$$

$$S_{2,2} = \frac{m_2}{2} = \frac{-1.1585}{2} = -.5793$$

$$S_{2,3} = \frac{m_3-m_2}{6 \cdot h_2} = \frac{0-(-1.1585)}{6(.5236)} = .3688$$

$$S_2(x) = .8660 + .4581\,(x-1.0472) - .5793(x-1.0472)^2 + .3688\,(x-1.0472)^3$$

• <u>Numerical Differentiation</u>

We can use the definition of a derivative to compute it numerically

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

So we can estimate a derivative as

$$D(x) = \frac{f(x+h) - f(x)}{h} \quad \text{for a small } h$$

How small h should be?
That depends on $f(x)$.
You can start with some value of h and decrease it until $D(x)$ stares to loose precision.

Example: $f(x) = e^x$

$$D(x) = \frac{e^{x+h} - e^x}{h}$$

Let

$$D(1) = \frac{e^{1+h} - e^1}{h}$$

| | h | D(1) |
|---|---|---|
| 0 | .1 | 2.8588 |
| 1 | .01 | 2.7319 |
| 2 | .001 | 2.7196 |
| 3 | .0001 | 2.7184 |
| 4 | .00001 | 2.7183 |
| 5 | .000001 | 2.7183 |

Example we can stop when $|D_k - D_{k-1}| < \epsilon$

Wednesday, 7/19/2012

There are other more precise formulas to obtain derivatives

• Central Difference Formula

Also called Centered Formula of order $O(h^2)$.

A more accurate way to obtain derivative.

Start with Taylor expansion $f(x+h)$ and $f(x-h)$

① $f(x+h) = f(x) + f'(x)h + \frac{f''(x)h^2}{2!} + \ldots$ error $\frac{f'''(c_1)h^3}{3!}$

② $f(x-h) = f(x) + f'(x)(-h) + \frac{f''(x)(-h)^2}{2!} \ldots$ $\frac{f'''(c_2)h^3}{3!}$

$= f(x) - f'(x)h + \frac{f''(x)h^2}{2!}$

Subtracting ① - ②

$$f(x+h) - f(x-h) \cong f(x) + f'(x)h + \frac{f''(x)h^2}{2!} - f(x) + f'(x)h - \frac{f''(x)h^2}{2!}$$

$$\cong 2f'(x)h + \frac{f'''(c_1)h^3 - f'''(c_2)h^3}{3!}$$

$$f(x+h) - f(x-h) - \frac{f'''(c_1) - f'''(c_2)}{3!}h^3 = 2f'(x)h$$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{f'''(c_1) - f'''(c_2)}{3!}\frac{h^{\not 3\, 2}}{2\not h}$$

truncation error $ch^2$ $O(h^2)$

$$\boxed{f'(x) \cong \frac{f(x+h) - f(x-h)}{2h}}$$

Central difference formula of order $O(h^2)$

Example:

$f(x) = e^x \qquad h = .001$

$f'(x) = e^x$

$$f'(1) = \frac{e^{1+.0001} - e^{1-.0001}}{2(.0001)}$$

$= 2.7183$

$e^1 = 2.718281$

Centered formula of order $O(h^4)$ $\quad h = .01 = 10^{-2} \quad h^4 = 10^{-8} = .00000001$

Do Taylor Expansion

① $f(x+h) = f(x) + f'(x)h + \frac{f''(x)h^2}{2!} + \frac{f'''(x)h^3}{3!} + \frac{f''''(x)h^4}{4!} + \underbrace{\frac{f'''''(x)h^5}{5!}}_{\text{error}}$

② $f(x-h) = f(x) - f'(x)h + \frac{f''(x)h^2}{2!} - \frac{f'''(x)h^3}{3!} + \frac{f''''(x)h^4}{4!} - \frac{f'''''(x)h^5}{5!}$

Using step size 2h instead of h in ①

③ $f(x+2h) = f(x) + f'(x)2h + \frac{f''(x)4h^2}{2!} + \frac{f'''(x)8h^3}{3!} + \frac{f''''(x)16h^4}{4!} + \frac{f'''''(x)32h^5}{5!}$

④ $f(x-2h) = f(x) - f'(x)2h + \frac{f''(x)4h^2}{2!} - \frac{f'''(x)8h^3}{3!} + \frac{f''''(x)16h^4}{4!} - \frac{f'''''(x)32h^5}{5!}$

$f(x+2h) - f(x-2h) = 4f'(x)h + 16\frac{f'''(x)h^3}{3!} + c_3 h^5$

Now multiply ① and ② by 8 and substract them from it

$$8f(x+h) - 8f(x-h) - f(x+2h) + f(x-2h) =$$

$$8f(x) + 8f'(x)h + \frac{8f''(x)h^2}{2!} + \frac{8f'''(x)h^3}{3!} + \frac{8f''''(x)h^4}{4!} + 8ch^5$$

$$-8f(x) + 8f'(x)h - \frac{8f''(x)h^2}{2!} + \frac{8f'''(x)h^3}{3!} - \frac{8f''''(x)h^4}{4!} + 8ch^5$$

$$-f(x) - f'(x)2h - \frac{f''(x)4h^2}{2!} - \frac{f'''(x)8h^3}{3!} - \frac{f''''(x)16h^4}{4!} + ch^5$$

$$+f(x) - f'(x)2h + \frac{f''(x)4h^2}{2!} - \frac{f'''(x)8h^3}{3!} + \frac{f''''(x)16h^4}{4!} + c_0h^5$$

$$16f'(x)h - 4f'(x)h + c_E h^5 = 8f(x+h) - 8f(x-h) - f(x+2h) + f(x-2h)$$

$$= 8f(x+h) - 8f(x-h) - f(x+2h) + f(x-2h)$$

$$f'(x)(12)h + c_E h^5 = 8f(x+h) - 8f(x-h) - f(x+2h) + f(x-2h)$$

$$f'(x) = 8f(x+h) - 8f(x-h) - f(x+2h) + f(x-2h) + c_E h^5$$

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + \frac{c_E h^4}{12}$$

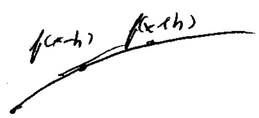
error

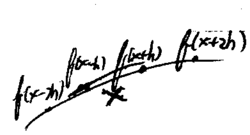
$h = .01$

$h^2 = .0001$

$h^4 = .00000001$

$$\frac{c_E h^4}{12} = O(h^4)$$



Let $f(x) = \sin(x)$ $h = .001$

- Centered formula $O(h^4)$

$$f'\left(\frac{\pi}{3}\right) \cong \frac{-\sin\left(\frac{\pi}{3}+.002\right)+8\sin\left(\frac{\pi}{3}+.001\right) - 8\sin\left(\frac{\pi}{3}-.001\right)+\sin\left(\frac{\pi}{3}-.002\right)}{12(.001)}$$

$$\cong \frac{-.8670 + 6.9322 - 6.9242 + .8650}{.012}$$

$$= .5$$

$f(x) = \sin(x)$

$f'(x) = \cos(x)$

$f'\left(\frac{\pi}{3}\right) = \cos\left(\frac{\pi}{3}\right) = .5$

Using centered formula $O(h^2)$

$$f'(x) \cong \frac{\sin\left(\frac{\pi}{3}+.001\right) - \sin\left(\frac{\pi}{3}-.001\right)}{2(.001)}$$

$$= \frac{.8665 - .8655}{.002}$$

$$= .49999\,9917$$

Using difference quotient

$$f'(x) = \frac{\sin\left(\frac{\pi}{3}+.001\right) - \sin\left(\frac{\pi}{3}\right)}{~~(.001)~~ .001}$$

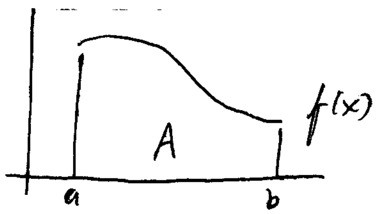
$$= \frac{~~.8665 - .8655~~}{.002}$$

$$= ~~.49999\,9917~~ \; .49956\,6904$$

Thursday, 19 July 2012

## • Numerical Integration

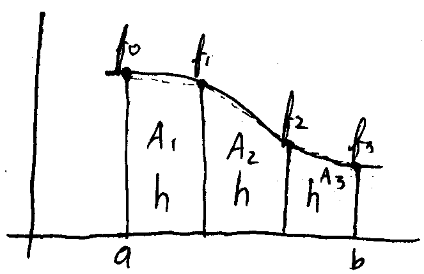
Integration is the area under the curve $f(x)$.




$$A = \int_a^b f(x)\,dx$$

### · Trapezoidal rule

- Approximates the area using trapezoids.




In this case $h = \frac{b-a}{3}$

$A_1 = \left(\frac{f_0 + f_1}{2}\right) h$ | $A_2 = \left(\frac{f_1 + f_2}{2}\right) h$ | $A_3 = \left(\frac{f_2 + f_3}{2}\right) h$

$$A_1 + A_2 + A_3 = \frac{f_0 + f_1}{2} h + \frac{f_1 + f_2}{2} h + \frac{f_2 + f_3}{2} h$$

$$A = \frac{f_0}{2} h + f_1 h + f_2 h + \frac{f_3}{2} h$$

In general

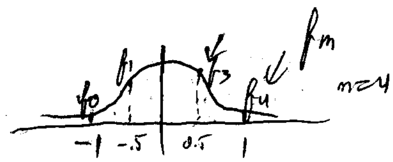
$$A = \frac{f_0}{2} h + f_1 h + f_2 h + \dots f_{m-1} h + \frac{f_m}{2} h$$

$$\int_a^b f(x)\,dx = h\left(\frac{f(x_0) + f(x_m)}{2} + \sum_{k=1}^{m-1} f(x_k)\right)$$

Trapezoidal Rule

Example:

$\int_{-1}^{1} e^{-x^2}\,dx$




$$h = \frac{b-a}{m} = \frac{1-(-1)}{4} = \frac{2}{4} = .5$$

$$\int_{-1}^{1} e^{-x^2} \approx .5\left(\frac{e^{-(-1)^2}+e^{-(1)^2}}{2} + e^{-(-.5)^2} + e^{-(0)^2} + e^{-(.5)^2}\right)$$

$$\approx .5\,\left(e^{-1} + e^{-(-.5)^2} + 1 + e^{-(.5)^2}\right)$$

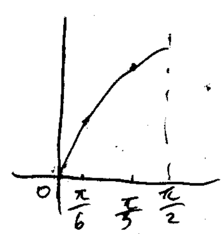
$$\approx .5\,(.36788 + 1.5576 + 1)$$

$$\boxed{\int_{-1}^{1} e^{-x^2}\,dx \approx 1.46274}$$

---

$\int_0^{\pi/2} \sin(x)$

$m=3$




$$\int_0^{\frac{\pi}{2}} \sin(x) \cong \frac{\pi}{6}\left[\frac{\sin(0)+\sin(\frac{\pi}{2})}{2} + \sin\left(\frac{\pi}{6}\right) + \sin\left(\frac{\pi}{3}\right)\right]$$

$$h = \frac{\frac{\pi}{2}-0}{3} = \frac{\pi}{6}$$

$$\cong \frac{\pi}{6}\left[\frac{0+1}{2} + .5 + .866025\right]$$

$$= \frac{\pi}{6}\left[1.866025\right]$$

$$\boxed{\int_0^{\pi/2} \sin(x)\,dx \cong .9770486}$$ Trapezoid Rule

Exact solution

$$\int_0^{\pi/2} \sin(x)\,dx = -\cos(x)\Big|_0^{\pi/2}$$

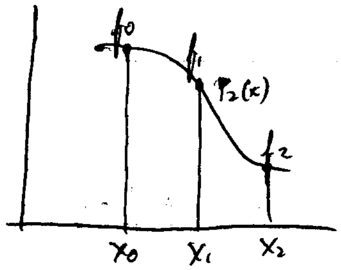
$$= -\left[\cos\left(\frac{\pi}{2}\right) - \cos(0)\right]$$

$$= -[0-1]$$

$$\boxed{\int_0^{\pi/2} \sin(x)\,dx = 1}$$

## • Simpson Rule

Approximate $f(x)$ using a quadratic polynomial every 3 points




We use Lagrange polynomials to obtain $P_2(x)$

$$P_2(x) = f_0 \frac{(x-x_1)(x-x_2)}{\underset{-h}{(x_0-x_1)}\underset{-2h}{(x_0-x_2)}} + f_1 \frac{(x-x_0)(x-x_2)}{\underset{h}{(x_1-x_0)}\underset{-h}{(x_1-x_2)}} + f_2 \frac{(x-x_0)(x-x_1)}{\underset{2h}{(x_2-x_0)}\underset{h}{(x_2-x_1)}}$$

$$\int_{x_0}^{x_2} P_2(x)\,dx = \int_{x_0}^{x_2} f_0 \frac{(x-x_1)(x-x_2)}{2h^2} + f_1 \frac{(x-x_0)(x-x_2)}{-h^2} + f_2 \frac{(x-x_0)(x-x_1)}{2h^2}\,dx$$

We will do a change of variables

Let $x = x_0 + ht$

$dx = h\,dt$

$$t = \frac{x-x_0}{h} \qquad t_0 = \frac{x_0-x_0}{h} = 0$$

$$t_2 = \frac{x_2-x_0}{h} = \frac{2h}{h} = 2$$

$$\int_{x_0}^{x_2} P_2(x)\,dx = \int_{t_0=0}^{t_2=2} \Bigg( f_0 \frac{\overbrace{(x_0+ht-x_1)}^{-h+ht}\overbrace{(x_0+ht-x_2)}^{-2h+ht}}{2h^2}$$

$$+ f_1 \frac{\overbrace{(x_0+ht-x_0)}^{ht}\overbrace{(x_0+ht-x_2)}^{-2h+ht}}{-h^2}$$

$$+ f_2 \frac{(x_0+ht-x_0)\overbrace{(x_0+ht-x_1)}^{-h+ht}}{2h^2} \Bigg) h\,dt$$

$$= \int_0^2 \frac{f_0(ht-h)(ht-2h)}{2h^2}h\,dt$$

$$+ \int_0^2 f_1 \frac{(ht)(ht-2h)}{-h^2}h\,dt + \int_0^2 f_2 \frac{(ht)(ht-h)}{2h^2}h\,dt$$

$$= \frac{h f_0}{2} \int_0^2 (t-1)(t-2)\,dt + f_1 h \int_0^2 t(t-2)\,dt$$

$$+ \frac{f_2 h}{2} \int_0^2 t(t-1)\,dt$$

$$= \frac{h f_0}{2} \int_0^2 (t^2 - 3t + 2)\,dt - f_1 h \int_0^2 (t^2 - 2t)\,dt$$

$$+ \frac{f_2 h}{2} \int_0^2 (t^2 - t)\,dt$$

$$= \frac{f_0 h}{2} \left[ \frac{t^3}{3} - \frac{3t^2}{2} + 2t \right]_0^2 - f_1 h \left[ \frac{t^3}{3} - \frac{2t}{2} \right]_0^2$$

$$+ \frac{f_2 h}{2} \left[ \frac{t^3}{3} - \frac{t^2}{2} \right]_0^2$$

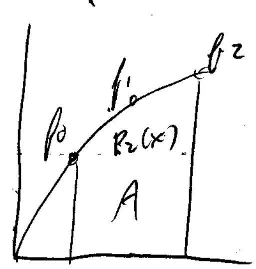
$$= \frac{f_0 h}{2} \left[ \frac{8}{3} - 6 + 4 \right] - f_1 h \left[ \frac{8}{3} - 4 \right] + \frac{f_2 h}{2} \left[ \frac{8}{3} - \frac{4}{2} \right] \ldots$$

$$= \frac{f_0 h}{2} \left[ \frac{2}{3} \right] - f_1 h \left[ -\frac{4}{3} \right] + \frac{f_2 h}{2} \left[ \frac{2}{3} \right]$$

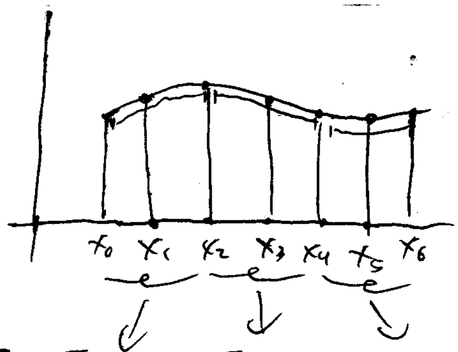
$$= \frac{f_0 h}{3} + f_1 h \frac{4}{3} + \frac{f_2 h}{3}$$

$$\int_{x_0}^{x_2} P_2(x) = \frac{h}{3} \left[ f_0 + 4 f_1 + f_2 \right]$$

Simpson Rule



Now if the interval $[a, b]$ is subdivided into $2m$ intervals $[x_k, x_{k+1}]$ of equal width $h = \frac{b-a}{2m}$




Example

$2M = 6$

$$I = I_{0,1,2} + I_{2,3,4} + I_{4,5,6}$$

$$= \frac{h}{3}[f_0 + 4f_1 + f_2] + \frac{h}{3}[f_2 + 4f_3 + f_4] + \frac{h}{3}[f_4 + 4f_5 + f_6]$$

$$= \frac{h}{3}[f_0 + 4f_1 + f_2 + f_2 + 4f_3 + f_4 + f_4 + 4f_5 + f_6]$$

$$I = \frac{h}{3}[f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + 4f_5 + f_6]$$

In general

$$I = \frac{h}{3}[f_0 + 4f_1 + 2f_2 + 4f_3 \cdots + 4f_{2m-1} + f_{2m}]$$

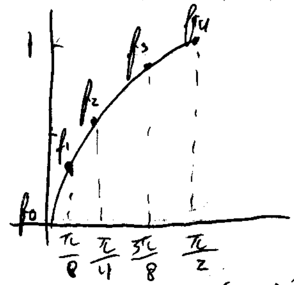
Simpson Rule for $2m$ intervals

Friday, 7/20/2012

Example

$\int_0^{\pi/2} \sin(x)$

$2m = 4$




$h = \frac{b-a}{2m} = \frac{\frac{\pi}{2}-0}{4} = \frac{\pi}{8}$

$I = \frac{\pi/8}{3}\left[\sin(0) + 4\sin\left(\frac{\pi}{8}\right) + 2\sin\left(\frac{\pi}{4}\right) + 4\sin\left(\frac{3\pi}{8}\right) + \sin\left(\frac{\pi}{2}\right)\right]$

$= \frac{\pi}{24}\left[0 + 1.53073 + 1.414213 + 3.6955 + 1\right]$

$= \frac{\pi}{24}\, 7.640443$

$= 1.0001316$ ($2m=4$)

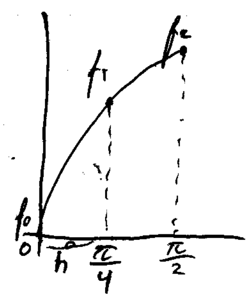
The exact value is

$\int_0^{\pi/2} \sin(x) = 1$

$I = .9770486$ Simpson Rule

With $2m = 2$

$h = \frac{\frac{\pi}{2} - 0}{2} = \frac{\pi}{4}$



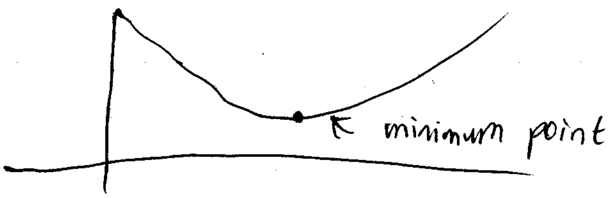

$I = \frac{\left(\frac{\pi}{4}\right)}{3}\left[\sin(0) + 4\sin\left(\frac{\pi}{4}\right) + \sin\left(\frac{\pi}{2}\right)\right]$

$= \frac{\pi}{12}\left[0 + 2.828427 + 1\right]$

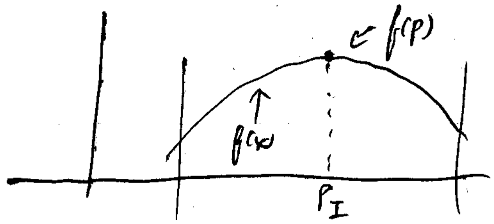
$I = 1.00$[illegible]$2798$ ($2m=2$)

· Numerical Optimization

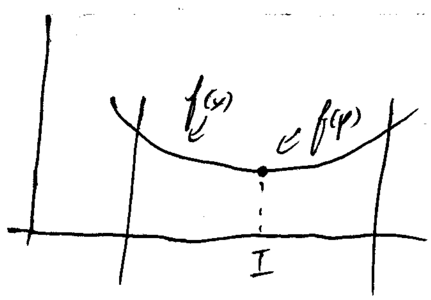
Minimization of an equation



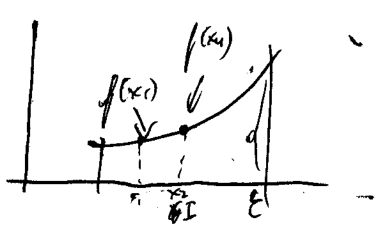

Local maximum value at $x = p$ in interval $I$ if $f(x) \le f(p)$ for all $x \in I$



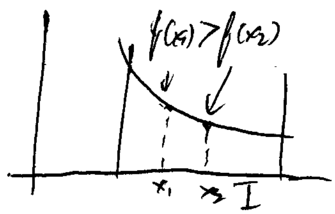

There is a local minimum value at $x = p$ in interval $I$ if $f(x) \ge f(p)$ for all $x \in I$



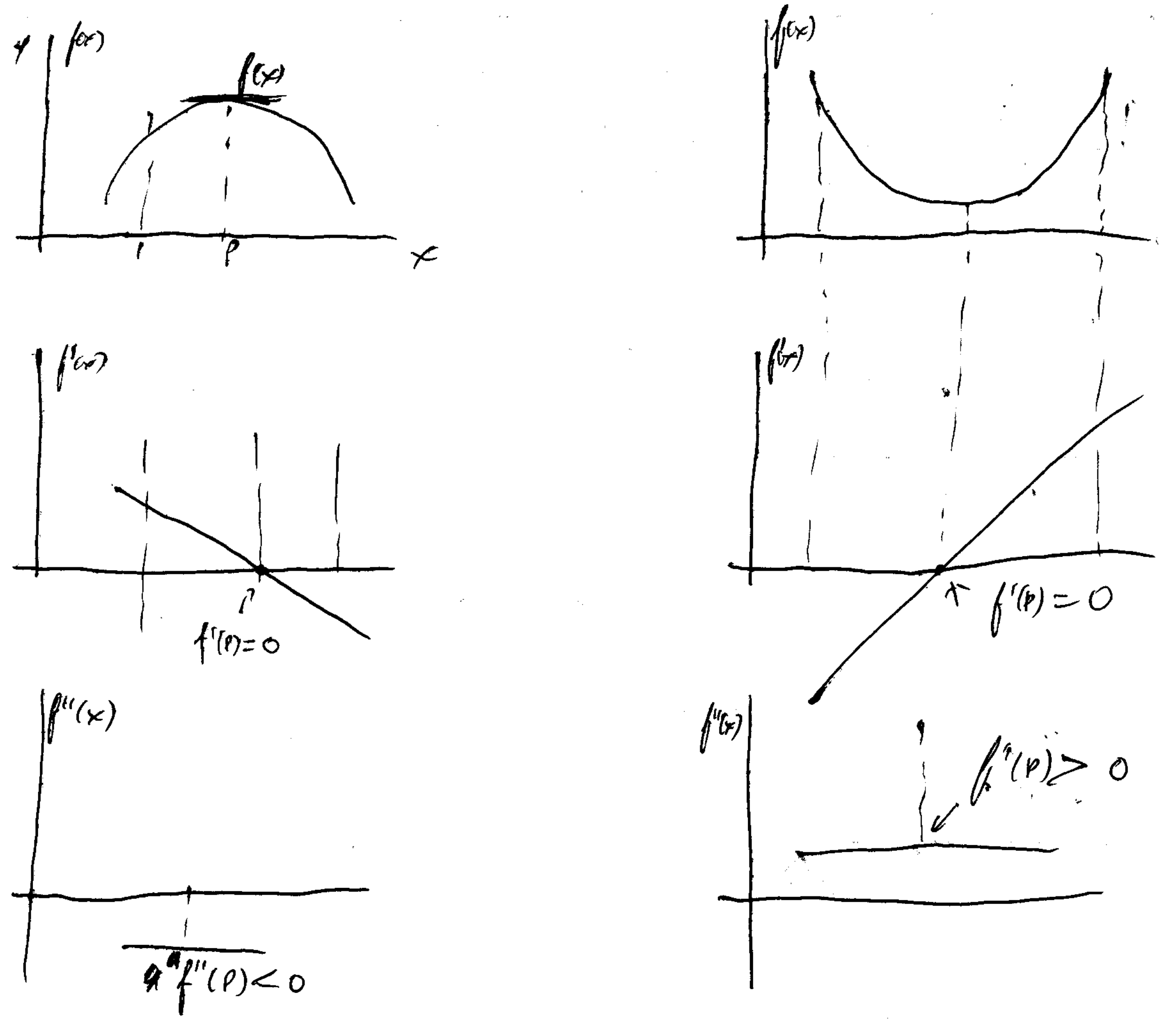

A function is increasing on $I$ if $x_1 < x_2$ and $f(x_1) < f(x_2)$ for all $x_1, x_2 \in I$



A function is decreasing on $I$ if $x_1 < x_2$ and $f(x_1) < f(x_2)$ for all $x_1, x_2 \in I$




- Suppose $f(x)$ is continuous in $I = [a, b]$ and it is differentiable then
- If $f'(x) > 0$ for all $x = (a, b)$ then $f(x)$ is increasing on $I$
- If $f'(x) < 0$ for all $x = (a, b)$ then $f(x)$ is decreasing on $I$
- If there is a maximum or minimum value at $x = p$, then $f'(p) = 0$

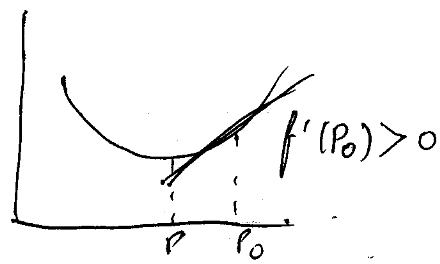


· Minimization using Derivatives

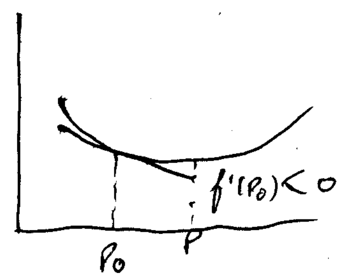
Assume we want to minimize $f(x)$ and it has a unique minimum $P$, $a \le p \le b$.

If we start at $P_0$

If $f'(P_0) > 0$ then $p$ is at the left




If $f'(P_0) < 0$ then $p$ is at the right




Any method used to solve non-linear equations can be used to find the minimum by finding $f'(x) = 0$

- From $f(x)$ find $f'(x)$
- You could use bisection, regula falsi, newton to find $f'(x) = 0$
- If the exact solution of $f'(x)$ is not available the estimate the derivatives using the formulas for numerical differentiation.

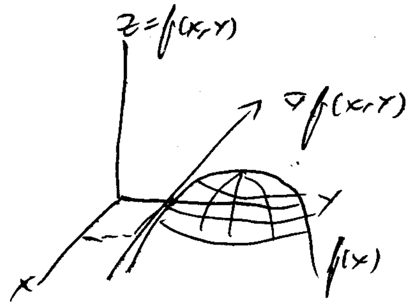
Another way to obtain the minimum is using the Steepest Descent method or Gradient Method

Assume that we want to minimize $f(x)$ where $(x = x_1, x_2 \ldots x_N)$

The gradient f(x) is a vector function defined as:

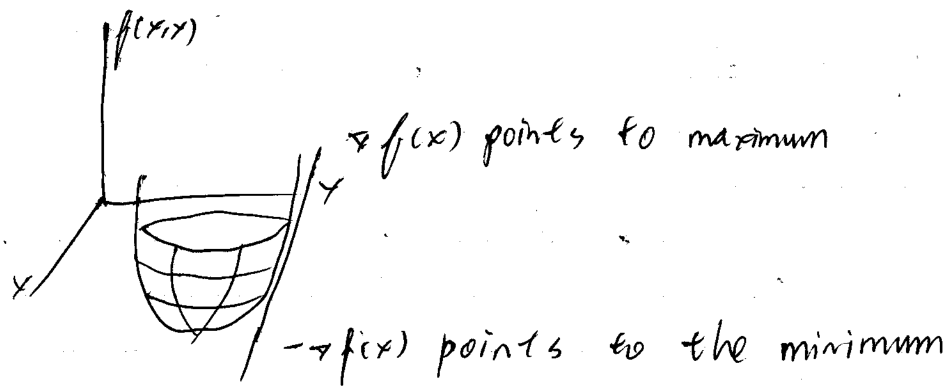
$$\text{grad } f(x) = \left( \frac{\partial f(x)}{\partial x_1}, \frac{\partial f(x)}{\partial x_2} \ldots \frac{\partial f(x)}{\partial x_n} \right)$$

$\nabla f(x)$




- From the concept of gradient, we know that the gradient vector points in the direction of greatest increase of f(x)

- We want to find the minimum




Then $-\text{grad}(f(x))$ or $-\nabla f(x)$ points to the direction of greater decrease

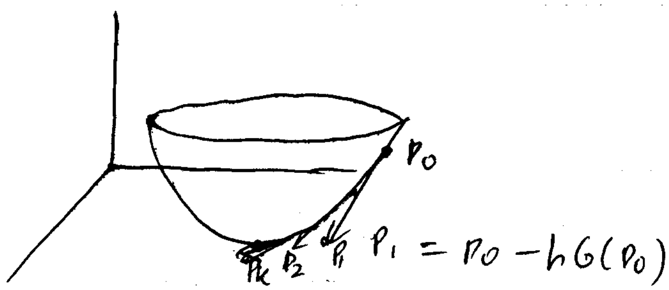
- Gradient Method

- Start at point $P_0$ and move along the line $-G_0$ where $G_0 = \nabla f(P_0)$

$P_1 = P_0 - Gh$ where $h$ is a small increment

In general
$P_{k+1} = P_k - G_k h \qquad G_k = \nabla f(x_k)$

Stop when $|P_{k+1} - P_k| < \varepsilon$ or when $|f(x_k)| < \varepsilon$

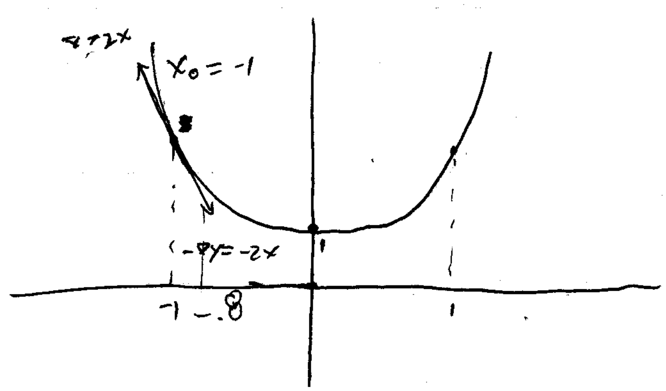



Monday, 23 July 2012

Example

$y = x^2 + 1$

$\nabla y = 2x \qquad G = 2x$




$P_{k+1} = P_k - G_k h \qquad h = .1$

$x_0 = -1$

$x_1 = -1 - (-2)(.1) = -1 + .2 = -.8$

$x_2 = -.8 - (-1.6)(.1) = -.8 + .16 = -.64$

$x_3 = -.64 - (-1.28)(.1) = -.64 + .128 = -.512$

$G = 2x$

$G_0 = 2(-1) = -2$

$G_1 = 2(-.8) = -1.6$

$G_2 = 2(-.64) = -1.28$

$G_3 = 2(.512) = -1.024$

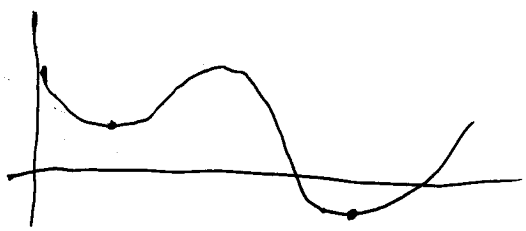
$x_4 = -.512 - (.1)(-1.024)$
$= -.4096$
$x_5 = -.4096 - (.1)(-.8196)$
$= -.3278$
$\vdots$

$G_4 = 2(.4096) = -.8192$

Improved gradient method

$$P_{k+1} = P_k + \frac{G_k}{|G_k|} h$$

Gradient method is only useful for local minimums.



Other techniques like "Simulated annealing" can be used to obtain global minimum.

· Numerical Solution of Differential Equations

$$\frac{dy}{dt} = kY$$

Solution:

$$\int \frac{dy}{y} = \int k_1 \, dt$$

$$\log Y = k_1 t + k_2$$

$$Y = e^{k_1 t + k_2} = e^{k^2} e^{kt}$$

$$\boxed{Y = k_3 e^{k_1 t}}$$

Some differential equations are impossible to solve analytically so they have to ~~app~~ be approximated with numerical methods.