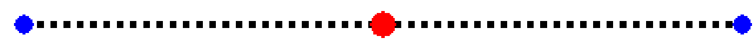
Estimates of the 1st Derivative (CRC)

2-point Forward Difference

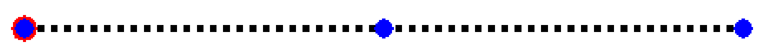
$$f'(x_0) = \frac{1}{h}\left(f_1 - f_0\right) - \frac{h}{2} f''\left(\xi\right)$$

2-point Central Difference



$$f'(x_0) = \frac{1}{2h}\left(f_1 - f_{-1}\right) - \frac{h^2}{6} f^{(3)}\left(\xi\right)$$

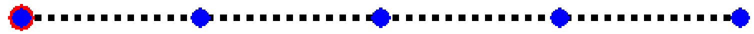
3-point Forward Difference



$$f'(x_0) = \frac{1}{2h}\left(-3f_0 + 4f_1 - f_2\right) + \frac{h^2}{3} f^{(3)}\left(\xi\right)$$

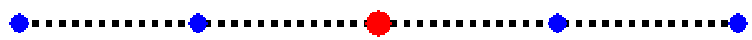
Some More "Exotic" Results(CRC)

5-point Forward Difference 1st Derivative:



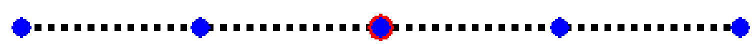
$$f'(x_0)=\frac{1}{12h}\left(-25f_0+48f_1-36f_2+16f_3-3f_4\right)-\frac{h^4}{5}f^{(5)}\left(\xi\right)$$

4-point Central Difference 3rd Derivative:



$$f^{(4)}(x_0)=\frac{1}{h^4}\left(f_2-4f_1+6f_0-4f_{-1}+f_{-2}\right)+O(h^2)$$

5-point Central Difference, 4th Derivative:

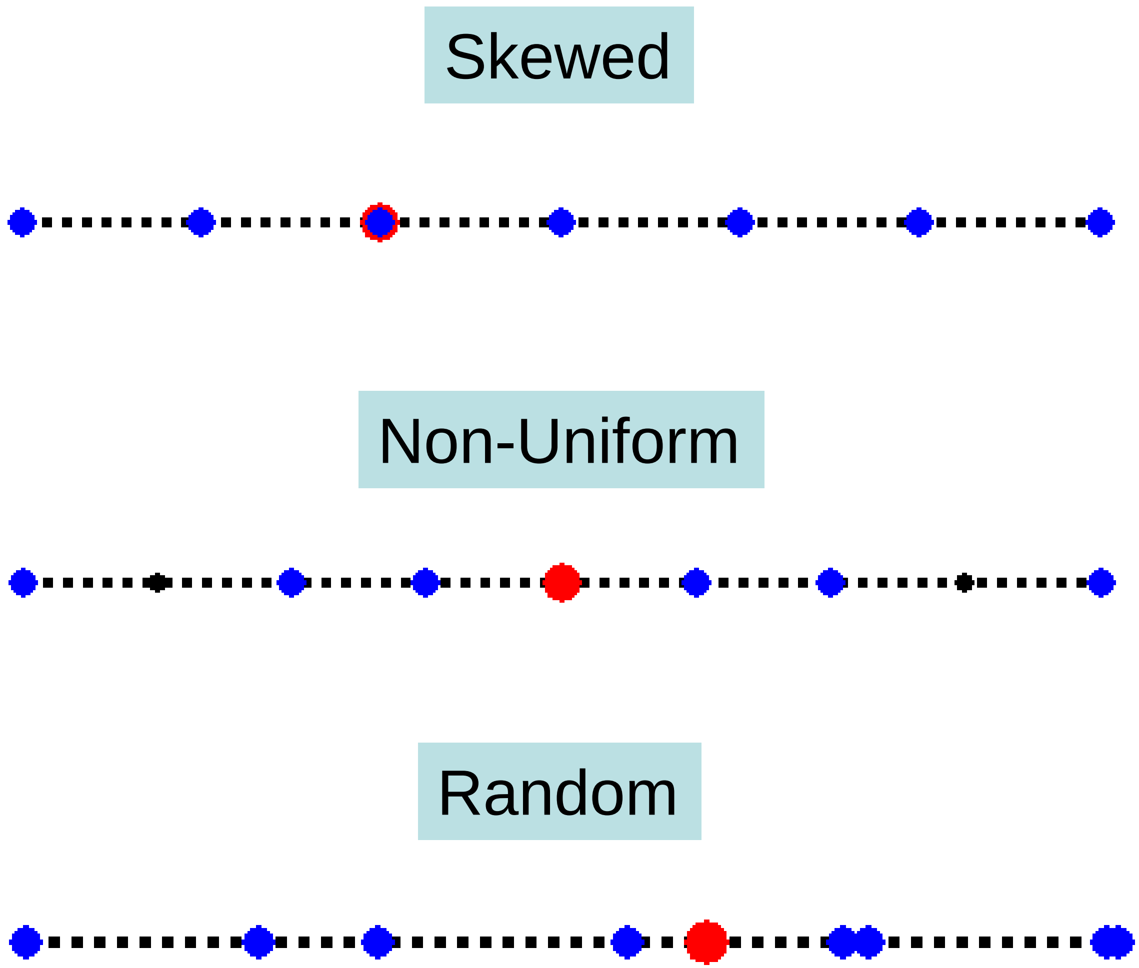


$$f^{(3)}(x_0)=\frac{1}{2h^3}\left(f_2-2f_1+2f_{-1}-f_{-2}\right)-O\left(h^2\right)$$

What's Missing?

		Derivative				
Grid Scheme	**# Points**	**1**	**2**	**3**	**4**	**>=5**
Forward/ Backward Difference	**2**		na	na	na	na
	3			na	na	na
	4	???	???		na	na
	5		???	???		
	>=6	???	???	???	???	???
Central Difference	**2**		na	na	na	na
	3	???		na	na	na
	4		???		na	na
	5	???	???	???		na
	>=6	???	???	???	???	???
Skewed Grid Schemes		???	???	???	???	???
Non-Uniform Grid Schemes		???	???	???	???	???
Random Grid Schemes		???	???	???	???	???

Non-Standard Grid Schemes



Question

Is there an expression that will generate an r-point finite difference approximation for an i^{th}-order derivative that will work equally well for both uniform and non-uniform grids as well as for asymmetric and random grids?

Derivation of 3-Point BD Equation for the 1st Derivative on a Uniform Grid

Start with Three 3-Term Taylor Series Expansions.

$$f_{-2} = \frac{(-2\delta)^0}{0!} f_o + \frac{(-2\delta)^1}{1!} f_o^{(1)} + \frac{(-2\delta)^2}{2!} f_o^{(2)} + \frac{(-2\delta)^3}{3!} f^{(3)}(\xi),$$

$$f_{-1} = \frac{(-\delta)^0}{0!} f_o + \frac{(-\delta)^1}{1!} f_o^{(1)} + \frac{(-\delta)^2}{2!} f_o^{(2)} + \frac{(-\delta)^3}{3!} f^{(3)}(\xi),$$

$$f_o = \frac{(0)^0}{0!} f_o + \frac{(0)^1}{1!} f_o^{(1)} + \frac{(0)^2}{2!} f_o^{(2)} + \frac{(0)^3}{3!} f^{(3)}(\xi),$$

$f_n = f(x_0 + n\delta)$ where δ is the grid spacing.
Note: Equation for f_0 is expanded for use in further derivation

Derivation of 3-Point BD Equation for the 1st Derivative on a Uniform Grid

Multiply Each Equation by a Weight ω_n .

$$\omega_{-2} f_{-2} \approx \omega_{-2} \frac{(-2\delta)^0}{0!} f_0 + \omega_{-2} \frac{(-2\delta)^1}{1!} f_0^{(1)} + \omega_{-2} \frac{(-2\delta)^2}{2!} f_0^{(2)},$$

$$\omega_{-1} f_{-1} \approx \omega_{-1} \frac{(-\delta)^0}{0!} f_0 + \omega_{-1} \frac{(-\delta)^1}{1!} f_0^{(1)} + \omega_{-1} \frac{(-\delta)^2}{2!} f_0^{(2)},$$

$$\omega_0 f_0 = \omega_0 \frac{(0)^0}{0!} f_0 + \omega_0 \frac{(0)^1}{1!} f_0^{(1)} + \omega_0 \frac{(0)^2}{2!} f_0^{(2)}.$$

Remainder terms have been dropped.

Derivation of 3-Point BD Equation for the 1st Derivative on a Uniform Grid

Sum up the Coefficients to Generate the 1st Derivative Expression .

$$\omega_{-2}\frac{(-2\delta)^0}{0!}+\omega_{-1}\frac{(-\delta)^0}{0!}+\omega_o\frac{0^0}{0!}=0,$$

$$\omega_{-2}\frac{(-2\delta)^1}{1!}+\omega_{-1}\frac{(-\delta)^1}{1!}+\omega_o\frac{0^1}{1!}=1,$$

$$\omega_{-2}\frac{(-2\delta)^2}{2!}+\omega_{-1}\frac{(-\delta)^2}{2!}+\omega_o\frac{0^2}{2!}=0.$$

Derivation of 3-Point BD Equation for the 1st Derivative on a Uniform Grid

Convert Equation in Matrix Form .

$$\begin{bmatrix} (-2)^0 & (-1)^0 & (0)^0 \\ (-2)^1 & (-1)^1 & (0)^1 \\ (-2)^2 & (-1)^2 & (0)^2 \end{bmatrix} \begin{bmatrix} \omega_{-2} \\ \omega_{-1} \\ \omega_0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1!/\delta \\ 0 \end{bmatrix}$$

Note: A Vandermonde Matrix

Solving for ω_{-2} Using Kramer's Rule

Cofactor Expansion

$$\omega_{-2} = \frac{\begin{vmatrix} 0 & (-1)^0 & (0)^0 \\ 1!/\delta & (-1)^1 & (0)^1 \\ 0 & (-1)^2 & (0)^2 \end{vmatrix}}{\begin{vmatrix} (-2)^0 & (-1)^0 & (0)^0 \\ (-2)^1 & (-1)^1 & (0)^1 \\ (-2)^2 & (-1)^2 & (0)^2 \end{vmatrix}} = \frac{(1!/\delta)(-1)^3 \begin{vmatrix} (-1)^0 & (0)^0 \\ (-1)^2 & (0)^2 \end{vmatrix}}{({}^{-}1 - {}^{-}2)(0 - {}^{-}2)(0 - {}^{-}1)} = \frac{1}{2\delta}$$

Determinant of a Vandermonde matrix

Derivation of 3-Point BD Equation for the 1st Derivative on a Uniform Grid

Solve for the Remaining Weights .

$$\omega_{-2} = \frac{1}{2\delta}, \quad \omega_{-1} = -\frac{4}{2\delta}, \quad \text{and} \quad \omega_{0} = \frac{3}{2\delta}.$$

Use Weights to Generate the Remainder Term

$$R = \begin{bmatrix} \omega_{-2} & \omega_{-1} & \omega_{0} \end{bmatrix} \begin{bmatrix} (-2)^3 \\ (-1)^3 \\ 0^3 \end{bmatrix} \frac{\delta^3}{3!} f^{(3)}(\xi) = -\frac{\delta^2}{3} f^{(3)}(\xi).$$

Derivation of 3-Point BD Equation for the 1st Derivative on a Uniform Grid

$$f_0^{(1)} = \frac{1}{2\delta}(f_{-2} - 4f_{-1} + 3f_0) + \frac{\delta^2}{3}f^{(3)}(\xi).$$

Derivation of 3-Point BD Equation for the 2nd Derivative on a Uniform Grid

Alter RHS Slightly ….

$$\begin{bmatrix} (-2)^0 & (-1)^0 & (0)^0 \\ (-2)^1 & (-1)^1 & (0)^1 \\ (-2)^2 & (-1)^2 & (-1)^2 \end{bmatrix} \begin{bmatrix} \omega_{-2} \\ \omega_{-1} \\ \omega_0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1!/\delta \\ 0 \end{bmatrix} \rightarrow \begin{bmatrix} 0 \\ 0 \\ 2!/\delta^2 \end{bmatrix}$$

Derivation of 5-Point CD Equation for the 3rd Derivative on a Uniform GriD

(or, if I desire, anything up to the 4th Derivative)

$$\begin{bmatrix} (-2)^0 & (-1)^0 & (0)^0 & (1)^0 & (2)^0 \\ (-2)^1 & (-1)^1 & (0)^1 & (1)^1 & (2)^1 \\ (-2)^2 & (-1)^2 & (0)^2 & (1)^2 & (2)^2 \\ (-2)^3 & (-1)^3 & (0)^3 & (1)^3 & (2)^3 \\ (-2)^4 & (-1)^4 & (0)^4 & (1)^4 & (2)^4 \end{bmatrix} \begin{bmatrix} \omega_{-2} \\ \omega_{-1} \\ \omega_0 \\ \omega_1 \\ \omega_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 3!/\delta^3 \\ 0 \end{bmatrix} \rightarrow\rightarrow \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 4!/\delta^4 \end{bmatrix}$$

(or, if I desire, anything up to the 4th Derivative)

System will also Work for Skew Grid Schemes

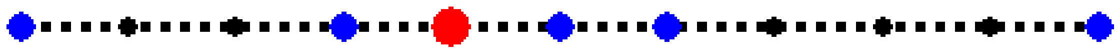
(i.e. use backward 1st and 4th point and forward 1st , 2nd, and 6th point to find the 3rd derivative on a uniform grid)

$$\begin{bmatrix} (-4)^0 & (-1)^0 & (1)^0 & (2)^0 & (6)^0 \\ (-4)^1 & (-1)^1 & (1)^1 & (2)^1 & (6)^1 \\ (-4)^2 & (-1)^2 & (1)^2 & (2)^2 & (6)^2 \\ (-4)^3 & (-1)^3 & (1)^3 & (2)^3 & (6)^3 \\ (-4)^4 & (-1)^4 & (1)^4 & (2)^4 & (6)^4 \end{bmatrix} \begin{bmatrix} \omega_{-2} \\ \omega_{-1} \\ \omega_0 \\ \omega_1 \\ \omega_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 3!/\delta^3 \\ 0 \end{bmatrix}$$

Note: The grid is “uniform”, the spacing between the points is not.

System Works for Asymmetric Schemes

(i.e. use backward 1st and 4th point and forward 1st, 2nd, and 6th point to find the 3rd derivative on a uniform grid)



$$\begin{bmatrix} (-4)^0 & (-1)^0 & (1)^0 & (2)^0 & (6)^0 \\ (-4)^1 & (-1)^1 & (1)^1 & (2)^1 & (6)^1 \\ (-4)^2 & (-1)^2 & (1)^2 & (2)^2 & (6)^2 \\ (-4)^3 & (-1)^3 & (1)^3 & (2)^3 & (6)^3 \\ (-4)^4 & (-1)^4 & (1)^4 & (2)^4 & (6)^4 \end{bmatrix} \begin{bmatrix} \omega_{-2} \\ \omega_{-1} \\ \omega_0 \\ \omega_1 \\ \omega_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 3!/\delta^3 \\ 0 \end{bmatrix}$$

Note: The grid is “uniform”, the spacing between the points is not.

A General Matrix System

(for an *r*-point approximation for the *i^th^ derivative*)

$$\begin{bmatrix} (a_1)^0 & \cdots & (a_i)^0 & \cdots & (a_r)^0 \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ (a_1)^i & \cdots & (a_i)^i & \cdots & (a_r)^i \\ \vdots & \ddots & \cdots & \ddots & \vdots \\ (a_1)^{r-1} & \cdots & (a_i)^{r-1} & \cdots & (a_r)^{r-1} \end{bmatrix} \begin{bmatrix} \omega_{a_1} \\ \vdots \\ \omega_{a_i} \\ \vdots \\ \omega_{a_r} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ i!/\delta^i \\ \vdots \\ 0 \end{bmatrix}$$

a_n: relative position of grid point with respect to center point.

Using Kramer's Rule to Solve for ω_{a_1}

$$
\omega_{a_1} = \frac{\begin{vmatrix} 0 & \cdots & (a_i)^0 & \cdots & (a_r)^0 \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ i!/\delta^i & \cdots & (a_i)^i & \cdots & (a_r)^i \\ \vdots & \ddots & \cdots & \ddots & \vdots \\ 0 & \cdots & (a_i)^{r-1} & \cdots & (a_r)^{r-1} \end{vmatrix}}{\begin{vmatrix} (a_1)^0 & \cdots & (a_i)^0 & \cdots & (a_r)^0 \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ (a_1)^i & \cdots & (a_i)^i & \cdots & (a_r)^i \\ \vdots & \ddots & \cdots & \ddots & \vdots \\ (a_1)^{r-1} & \cdots & (a_i)^{r-1} & \cdots & (a_r)^{r-1} \end{vmatrix}}
$$

Vandermonde matrix

Which "Simplifies" to:

$$\omega_{a_1} = \frac{(-1)^{(2+i)} \dfrac{i!}{\delta^i} \begin{vmatrix} (a_2)^0 & \cdots & (a_i)^0 & \cdots & (a_r)^0 \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ (a_2)^{i-1} & \cdots & (a_i)^{i-1} & \cdots & (a_r)^{i-1} \\ \vdots & \ddots & \cdots & \ddots & \vdots \\ (a_2)^{r-1} & \cdots & (a_i)^{r-1} & \cdots & (a_r)^{r-1} \end{vmatrix}}{\prod_{1 \le k < j \le r} \left(a_j - a_k\right)}$$

Cofactor Expansion About the 1st Column and The (i+1)th Row

Determinant of a Vandermonde matrix

Turning our Attention to the Numerator …

$$\det\left(M_{(i+1,n)}\right) = s_{r-i-1}\left(a_1,\ \ldots,\ a_{m\neq n},\ \ldots,\ a_r\right)\det\left(\bar{V}\right)$$

Minor of the Vandermonde Matrix With the *(i+1)*th row and *n*th column removed (from previous slide).

Schur polynomial of order *r-i-1*

Vandermonde Matrix with the rth row and *n*th column removed.

T. Ernst, Generalized Vendermonde Systems of Equations. *Mathematics of Computation,* ***24,*** (1970) 893-903.

I.G. Macdonald, *Symmetric Functions and Hall Polynomials*, Oxford Mathematical Mongraphs, Second Ed. 1995.

S.D. Marchi, Polynomials arising in factoring generalized Vandermonde determinants: An algorthm for computing their coefficients, *The Mathematical and Computer Modeling,* **34** (2003) 280-287.

Schur Polynomials

$$s_0(a_1,\ldots,a_n) = 1$$

$$s_1(a_1,\ldots,a_n) = \sum_{j=1}^{n} a_j$$

$$s_2(a_1,\ldots,a_n) = \sum_{1\le j<k\le n} a_j a_k$$

$$s_3(a_1,\ldots,a_n) = \sum_{1\le j<k<ln} a_j a_k a_l$$

$$\vdots \qquad \vdots \qquad \vdots$$

$$s_n(a_1,\ldots,a_n) = \prod_{j=1}^{n} a_j$$

Therefore …

$\det\left(\bar{V}\right)$

$$\omega_n = (-1)^{(1+i+n)} \frac{i!}{\delta^i} \left(\frac{s_{(r-i-1)}\left(a_1, \ldots, a_{m \neq n}, \ldots, a_r\right) \prod_{\substack{1 \le k < j \le r \\ j,k \neq n}} \left(a_j - a_k\right)}{\prod_{1 \le k < j \le r} \left(a_j - a_k\right)} \right)$$

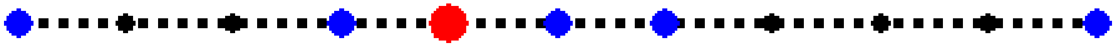
Finally …

$$\omega_n = (-1)^{(1+i+n)} \frac{i!}{\delta^i} \left(\frac{s_{(r-i-1)}\left(a_1, \ldots, a_{m \neq n}, \ldots, a_r\right)}{\prod_{1 \leq j \neq n \leq r} \left| \left(a_n - a_j\right) \right|} \right)$$

Where ω_n is the n^{th} weight for an r-point estimate of the i^{th} derivative with grid points whose relative position to the center is given by $\{a_1, \ldots, a_r\}$ and grid spacing is δ.

Recall the Earlier Example …

(i.e. use the grid below to approximate the 3rd derivative)



$$\begin{bmatrix} (-4)^0 & (-1)^0 & (1)^0 & (2)^0 & (6)^0 \\ (-4)^1 & (-1)^1 & (1)^1 & (2)^1 & (6)^1 \\ (-4)^2 & (-1)^2 & (1)^2 & (2)^2 & (6)^2 \\ (-4)^3 & (-1)^3 & (1)^3 & (2)^3 & (6)^3 \\ (-4)^4 & (-1)^4 & (1)^4 & (2)^4 & (6)^4 \end{bmatrix} \begin{bmatrix} \omega_{-2} \\ \omega_{-1} \\ \omega_0 \\ \omega_1 \\ \omega_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 3!/\delta^3 \\ 0 \end{bmatrix}$$

Solving for the First Weight

$$\omega_1 = -\frac{3!}{\delta^3}\left(\frac{s_1\left(a_2,\ldots,a_5\right)}{\prod\limits_{1\le j\ne 1\le r}\left|\left(a_1-a_j\right)\right|}\right)\rightarrow$$

$$\omega_1 = -\frac{6}{\delta^3}\left(\frac{-1+1+2+6}{\left|\left(-4+1\right)\left(-4-1\right)\left(-4-2\right)\left(-4-6\right)\right|}\right) = -\frac{4}{75\delta^3}$$

Solutions for Remaining Weights

$$\omega_2 = -\frac{6}{\delta^3}\left(\frac{-4+1+2+6}{\left|(-1+4)(-1-1)(-1-2)(-1-6)\right|}\right) = \frac{5}{21\delta^3}$$

$$\omega_3 = -\frac{6}{\delta^3}\left(\frac{-4-1+2+6}{\left|(1+4)(1+1)(1-2)(1-6)\right|}\right) = -\frac{9}{25\delta^3}$$

$$\omega_4 = -\frac{6}{\delta^3}\left(\frac{-4-1+1+6}{\left|(2+4)(2+1)(2-1)(2-6)\right|}\right) = \frac{5}{24\delta^3}$$

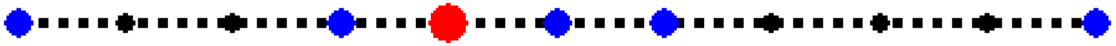
$$\omega_5 = -\frac{6}{\delta^3}\left(\frac{-4-1+1+2}{\left|(6+4)(6+1)(6-1)(6-2)\right|}\right) = \frac{3}{350\delta^3}$$

Determining an Error Term

$$\left[-\frac{4}{75\delta^3}, \frac{5}{21\delta^3}, -\frac{9}{25\delta^3}, \frac{5}{24\delta^3}, \frac{3}{350\delta^3}\right] \begin{bmatrix} (-4\delta)^5 \\ (-\delta)^5 \\ (\delta)^5 \\ (2\delta)^5 \\ (6\delta)^5 \end{bmatrix} f^{(5)}(\xi)$$

Putting it all Together

$$f^{(3)} = \frac{1}{\delta^3}\left(-\frac{4}{75}f_{-4} + \frac{5}{21}f_{-1} - \frac{9}{25}f_1 + \frac{5}{24}f_2 + \frac{3}{350}f_6\right) - \frac{21}{20}\delta^2 f^{(5)}(\xi)$$



… but with equal ease this grid scheme and can be used to generate the following approximation formula ….

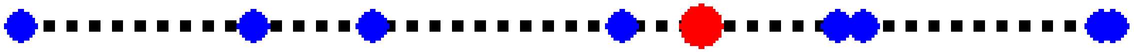
The 1st, 2nd, and 4th Derivatives …

$$f^{(1)} = \frac{1}{\delta}\left(-\frac{2}{225}f_{-4} - \frac{34}{63}f_{-1} + \frac{14}{25}f_{1} - \frac{1}{36}f_{2} - \frac{1}{200}f_{6}\right) + \frac{1}{6}\delta^4 f^{(5)}(\xi)$$

$$f^{(2)} = \frac{1}{\delta^2}\left(\frac{11}{450}f_{-4} + \frac{16}{63}f_{-1} - \frac{24}{25}f_{1} + \frac{25}{36}f_{2} - \frac{9}{700}f_{6}\right) + \frac{13}{15}\delta^3 f^{(5)}(\xi)$$

$$f^{(4)} = \frac{1}{\delta^4}\left(\frac{2}{75}f_{-4} - \frac{4}{21}f_{-1} + \frac{12}{25}f_{1} - \frac{1}{3}f_{2} + \frac{3}{175}f_{6}\right) - \frac{4}{5}\delta f^{(5)}(\xi)$$

The Extension to Random Grids…



… is simply accomplished,
but undoubtedly I am out of time

Questions?