MEDUSA

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Grid Generation

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1 Introduction

In order to solve the partial differential equations that describe early diagenetic processes in MEDUSA, the domain of interest whcich we denote for simplicity by $[0, L]$, is overlaid with a grid or mesh of points denoted x_i ($i = 1, \ldots, n$), called *nodes*, such that $0 \leq x_1 < \ldots < x_i < \ldots < x_n \leq L$. Each node is representative of a small sub-interval of $[0, L]$, delimited by the mid-points between neigbouring nodes. These mid-points are called *vertices* and represent thus the boundaries between the sub-intervals called *finite volumes* or cells. Concentrations and reaction terms are evaluated at the nodes while the flux terms are evaluated at the vertices. Accordingly, in some instances it is necessary to have a vertex located at 0 or L (e.g., if boundary conditions involve fluxes only). In such cases, we call upon virtual grid points $x_0 < 0$ or $x_{n+1} > L$ outside the domain of interest to define the required vertices, such that $[0, L]$ always includes n nodes x_i. In other instances it is necessary or recommended to have nodes locates at 0 or L (e.g., if boundary conditions involve prescibed concentrations). In this case there are only half cells at 0 or L. Such nodes are thus virtual vertices (cell boundaries).

With a few exceptions, the strategy behind grid generation consists in choosing a function Q to remap a regular grid covering the interval $[0, 1]$ ($\xi_i = i/N, i = 0, \ldots, N$) onto an irregular grid $q_i = Q(\xi_i)$ ($i = 0, \ldots, N$) covering the same interval [0,1]. Accordingly, we always have $q_0 = 0$ and $Q_N = 1$. This q_i ($i = 0, \ldots, N$) grid is then scaled and shifted (moved by translation) to fulfil constraints set by the specific problem requirements:

- the extent L of the interval $[0, L]$;
- a vertex or a node is located at the starting point 0;
- a vertex or a node is located at the end point L;
- the number of nodes n to have on the grid.

The final grid x_i $(i = 1, \ldots, n)$, is then derived by

$$x_i = Sq_{i-m} + x_{\mathrm{td}},$$

where

- m denotes an index offset (possibly 0) to shift the transformed q_i grid if required;
- S is a scaling factor;
- x_{td} is the translation distance.

The finally generated grid only includes nodes. Vertices are, by definition, located mid-may between nodes, or at either end of the gridded domain.

In order to preserve second order truncation error that can be easily achieved on regular meshes, it is sufficient to use a mapping $Q : \xi_i \to q_i$ that is twice continuously differentiable on $[0, 1]$.

1.1 Node-to-node grids

For node-to-node grids, $x_1 = 0$ and $x_n = L$. Hence,

- q_0 must be remapped onto x_1, requiring that $m = 1$;
- q_N must be remapped onto x_n, requiring that $N + m = n$, i.e., $N = n - 1$
- $x_1 = 0$ and $x_1 = Sq_0 + x_{\mathrm{td}} = x_{\mathrm{td}}$ require that $x_{\mathrm{td}} = 0$
- $x_n = L$ and $x_n = Sq_{n-1} + x_{\mathrm{td}} = S$ require that $S = L$

1.2 Node-to-vertex grids

For node-to-vertex grids, $x_1 = 0$. x_n is inside the domain to be gridded and chosen so that with a virtual next point x_{n+1}, mapped from q_N would provide a vertex between x_n and x_{n+1} such that $\frac{1}{2}(x_n + x_{n+1}) = L$. Accordingly:

- q_0 must be remapped onto x_1, requiring that $m = 1$;

- q_N must be remapped onto x_{n+1}, requiring that $N + m = n + 1$, i.e., $N = n$;
- $x_1 = 0$ and $x_1 = Sq_0 + x_{\text{td}} = x_{\text{td}}$ require that $x_{\text{td}} = 0$;
- noting that

$$\begin{aligned} x_n + x_{n+1} &= Sq_{n-1} + Sq_n + 2x_{\text{td}} \\ &= Sq_{N-1} + Sq_N \\ &= SQ(\xi_{N-1}) + S \\ &= S(Q(\xi_{N-1}) + 1) \end{aligned}$$

the vertex condition $\frac{1}{2}(x_n + x_{n+1}) = L$ finally leads to

$$S = L\frac{2}{Q(\xi_{N-1}) + 1} = L\frac{2}{Q(\frac{n-1}{n}) + 1}.$$

1.3 Vertex-to-node grids

For vertex-to-node grids, $x_n = L$. x_1 is inside the domain to be gridded and chosen so that with a virtual preceding point x_0, mapped from q_0 would provide a vertex between x_0 and x_1 such that $\frac{1}{2}(x_0 + x_1) = 0$. Accordingly:

- q_1 must be remapped onto x_1, requiring that $m = 0$;
- q_N must be remapped onto x_n, requiring that $N + m = n$, i.e., $N = n$;
- $x_n = L$ and $x_n = Sq_N + x_{\text{td}} = S + x_{\text{td}}$ require that $x_{\text{td}} = L - S$;
- noting that

$$\begin{aligned} x_0 + x_1 &= Sq_0 + Sq_1 + 2x_{\text{td}} \\ &= Sq_1 + 2(L - S) \\ &= SQ(\xi_1) + 2(L - S) \\ &= S(Q(\xi_1) - 2) + 2L \end{aligned}$$

the vertex condition $\frac{1}{2}(x_0 + x_1) = 0$ finally then leads to

$$S = L\frac{2}{2 - Q(\xi_1)} = L\frac{2}{2 - Q(\frac{1}{n})}.$$

Hence,

$$x_{\text{td}} = L - S = L\left(1 - \frac{2}{2 - Q(\frac{1}{n})}\right) = -L\frac{Q(\frac{1}{n})}{2 - Q(\frac{1}{n})}$$

1.4 Vertex-to-vertex grids

For vertex-to-vertex grids grids, x_1 is inside the domain to be gridded and chosen so that with a virtual preceding point x_0, mapped from q_0 would provide a vertex between x_0 and x_1 such that $\frac{1}{2}(x_0 + x_1) = 0$; x_n is also inside the domain to be gridded and chosen so that with a virtual next point x_{n+1}, mapped from q_N would provide a vertex between x_n and x_{n+1} such that $\frac{1}{2}(x_n + x_{n+1}) = L$. Accordingly:

- q_1 must be remapped onto x_1, requiring that $m = 0$;
- q_{N-1} must be remapped onto x_n, requiring that $N - 1 + m = n$, i.e., $N = n + 1$;
- noting, as above, that

  $$x_0 + x_1 = SQ(\xi_1) + 2x_{\mathrm{td}}$$

  and that

  $$\begin{aligned} x_n + x_{n+1} &= Sq_{n-1} + Sq_n + 2x_{\mathrm{td}} \\ &= Sq_{N-1} + Sq_N + 2x_{\mathrm{td}} \\ &= S(Q(\xi_{N-1}) + 1) + 2x_{\mathrm{td}} \end{aligned}$$

  the vertex conditions $\frac{1}{2}(x_0 + x_1) = 0$ and $\frac{1}{2}(x_n + x_{n+1}) = L$ require that S and x_{td} obey to a linear system

  $$\left\{ \begin{array}{rcrcl} Q(\xi_1)S & + & 2x_{\mathrm{td}} & = & 0 \\ (Q(\xi_{N-1}) + 1)S & + & 2x_{\mathrm{td}} & = & 2L \end{array} \right.$$

  i.e.,

  $$\left\{ \begin{array}{rcrcl} Q(\frac{1}{n+1})S & + & 2x_{\mathrm{td}} & = & 0 \\ (Q(\frac{n}{n+1}) + 1)S & + & 2x_{\mathrm{td}} & = & 2L \end{array} \right.$$

  Hence,

  $$\begin{aligned} S &= L\frac{2}{Q(\frac{n}{n+1}) - Q(\frac{1}{n+1}) + 1} \\ x_{\mathrm{td}} &= -L\frac{Q(\frac{1}{n+1})}{Q(\frac{n}{n+1}) - Q(\frac{1}{n+1}) + 1} \end{aligned}$$

2 Linear grids

For linear grids, the fundamental remapping function is simply

$$Q(\xi_i) = \xi.$$

3 Quadratic-linear grids

For quadratic-linear grids, the fundamental remapping function is

$$Q(\xi_i) = \frac{(\xi_i^2 + \xi_c^2)^{\frac{1}{2}} - \xi_c}{(1 + \xi_c^2)^{\frac{1}{2}} - \xi_c}.$$

4 Geometric progression grids

For geometric progression grids in general, there are several parameters of importance, besides the number of grid points, which we assume fixed a priori:

- the thickness of the first interval, δ;
- the geometric progression ratio, r;
- the extent of the interval to be gridded, L.

The three parameters are not independent of each other. However, the relationships are different from one grid type to another.

To take advantage of the developments presented in the introduction, let us start to derive the remapping $\xi_i \to q_i$. For any initial scale factor σ and progression ratio r, we have

$$\begin{aligned}
q_0 &= 0 \\
q_1 &= \sigma \\
q_2 &= q_1 + \sigma r = \sigma(1 + r) \\
q_3 &= q_2 + \sigma r^2 = \sigma(1 + r + r^2) \\
&\vdots \\
q_i &= \sigma(1 + r + r^2 + \ldots + r^{i-1}) \\
&\vdots \\
q_N &= \sigma(1 + r + r^2 + \ldots + r^{N-1})
\end{aligned}$$

Notice that $q_i = \sigma(1 + r + r^2 + \ldots + r^{i-1}) = \sigma(1 - r^i)/(1 - r)$. Hence, if $q_N = 1$ then $\sigma = \frac{1-r}{1-r^N}$, leading to the remapping function

$$Q(\xi_i) = \frac{1 - r^i}{1 - r^N} = \frac{r^i - 1}{r^N - 1} = \frac{r^{N\xi_i} - 1}{r^N - 1}$$

4.1 Grid types

4.1.1 Node-to-node

Characteristics: $m = 1$, $N = n - 1$, $S = L$, $x_{\mathrm{td}} = 0$. Hence,

$$x_i = L \cdot Q(\xi_{i-1}) = L\frac{r^{i-1} - 1}{r^{n-1} - 1}, \quad i = 1, \ldots, n$$

Since

$$x_2 = \delta = L\frac{r - 1}{r^{n-1} - 1}$$

we can rewrite this as

$$x_i = \delta\frac{r^{i-1} - 1}{r - 1}, \quad i = 1, \ldots, n$$

and we furthermore have

$$L = \delta\frac{r^{n-1} - 1}{r - 1}$$

4.1.2 Node-to-vertex

Characteristics: $m = 1$, $N = n$, $S = L\frac{2}{Q(\xi_{N-1})+1}$, $x_{\mathrm{td}} = 0$.

$$x_i = L\frac{2}{Q(\xi_{N-1}) + 1} \cdot Q(\xi_{i-1}) = L\frac{2}{\frac{r^{n-1}-1}{r^n-1} + 1}\frac{r^{i-1} - 1}{r^n - 1}, \quad i = 1, \ldots, n$$

and again

$$x_2 = \delta = L\frac{2}{\frac{r^{n-1}-1}{r^n-1} + 1}\frac{r - 1}{r^n - 1} = L\frac{2(r - 1)}{r^n - 1 + r^{n-1} - 1}.$$

We can rewrite this as

$$x_i = \delta\frac{r^{i-1} - 1}{r - 1}, \quad i = 1, \ldots, n$$

and we furthermore have

$$L = \delta\frac{r^n - 1 + r^{n-1} - 1}{2(r - 1)}$$

4.1.3 Vertex-to-node

Characteristics: $m = 0$, $N = n$, $S = L\frac{2}{2-Q(\frac{1}{n})}$, $x_{\text{td}} == -L\frac{Q(\frac{1}{n})}{2-Q(\frac{1}{n})}$.

$$\begin{aligned}
x_i &= L\frac{2}{2-Q(\frac{1}{n})} \cdot Q(\xi_i) - L\frac{Q(\frac{1}{n})}{2-Q(\frac{1}{n})} \\
&= L\frac{1}{2-Q(\frac{1}{n})} \cdot (2Q(\xi_i) - Q(\tfrac{1}{n})) \\
&= L\frac{1}{2-\frac{r-1}{r^n-1}} \cdot (2\frac{r^i-1}{r^n-1} - \frac{r-1}{r^n-1}) \\
&= L\frac{2r^i - r - 1}{2r^n - r - 1}
\end{aligned}$$

In this case,

$$\delta = x_1 - x_0 = 2L\frac{r-1}{2r^n - r - 1}$$

and we can rewrite the sequence as

$$x_i = \frac{\delta}{2}\frac{2r^i - r - 1}{r-1}$$

and we furthermore have

$$L = \delta\frac{2r^n - r - 1}{2(r-1)}$$

4.1.4 Vertex-to-vertex

Characteristics: $m = 0$, $N = n+1$, $S = 2L/(Q(\xi_{N-1}) - Q(\xi_1) + 1)$, $x_{\text{td}} = -LQ(\xi_1)/(Q(\xi_{N-1}) - Q(\xi_1) + 1)$

$$\begin{aligned}
x_i &= L\frac{2}{Q(\xi_{N-1}) - Q(\xi_1) + 1} \cdot Q(\xi_i) - L\frac{Q(\xi_1)}{Q(\xi_{N-1}) - Q(\xi_1) + 1} \\
&= L\frac{2Q(\xi_i) - Q(\xi_1)}{Q(\xi_{N-1}) - Q(\xi_1) + 1} \\
&= L\frac{2\frac{r^i-1}{r^{n+1}-1} - \frac{r-1}{r^{n+1}-1}}{\frac{r^n-1}{r^{n+1}-1} - \frac{r-1}{r^{n+1}-1} + 1} \\
&= L\frac{2r^i - r - 1}{r^{n+1} - r + r^n - 1} \\
&= L\frac{2r^i - r - 1}{(r+1)(r^n - 1)}
\end{aligned}$$

In this case,

$$\delta = x_1 - x_0 = 2L\frac{r-1}{(r+1)(r^n-1)}$$

and we can rewrite the sequence as

$$x_i = \frac{\delta}{2}\frac{2r^i - r - 1}{r-1}$$

and we have

$$L = \delta\frac{(r+1)(r^n-1)}{2(r-1)}.$$

Furthermore,

$$x_{n+1} + x_n = L\frac{2r^{n+1} - 2r + 2r^n - 2}{(r+1)(r^n-1)} = 2L\frac{(r+1)(r^n-1)}{(r+1)(r^n-1)} = 2L$$

as expected.

4.2 Derived quantities

As mentioned above, the three parameters of interest, δ, r and L are interdependent. For each of the four grid-types, we have shown that the three parameters are related by one relationship. Accordingly, one of the three parameters can be derived from the two others. There are two cases that are straightforward to handle:

- for given r and δ, L can be directly derived;
- for given r and L, δ can be directly derived;

The third case, where δ and L are given, is more complicated to handle as it involves a non-linear equation to solve for r. The equation to solve depends on the grid type adopted.

4.2.1 Node-to-node

The equation to solve is

$$f_{\mathrm{nn}}(r) \equiv \frac{r^{n-1} - 1}{r-1} - \frac{L}{\delta} = 0$$

$r = 1$ appears to be a critical value: for $r = 1$, the equation function evaluates to

$$f_{\mathrm{nn}}(1) = (n-1) - \frac{L}{\delta}$$

4.2.2 Node-to-vertex

The equation to solve is

$$f_{\mathrm{nv}}(r) \equiv \frac{r^n - 1 + r^{n-1} - 1}{2(r-1)} - \frac{L}{\delta} = 0$$

For $r = 1$, the function evaluates to

$$f_{\mathrm{nv}}(1) = \frac{2n-1}{2} - \frac{L}{\delta}$$

4.2.3 Vertex-to-node

The equation to solve is

$$f_{\mathrm{vn}}(r) \equiv \frac{2r^n - r - 1}{2(r-1)} - \frac{L}{\delta} = 0.$$

For $r = 1$, the function evaluates to

$$f_{\mathrm{vn}}(1) = \frac{2n-1}{2} - \frac{L}{\delta}$$

4.2.4 Vertex-to-vertex

The equation to solve is

$$f_{\mathrm{vv}}(r) \equiv \frac{(r+1)(r^n-1)}{2(r-1)} - \frac{L}{\delta} = 0.$$

For $r = 1$, the function evaluates to

$$f_{\mathrm{vv}}(1) = n - \frac{L}{\delta}$$

4.3 Solving for r

4.3.1 Preliminaries

For $r > 1$, $r^2 = r \cdot r > r$, ..., $r^i = r \cdot r^{i-1} > r$ and thus

$$\begin{aligned} \frac{r^p - 1}{r - 1} &= r^{p-1} + \ldots + r + 1 \\ &> r + \ldots + r + 1 \\ &> (p-1)r + 1 \\ &> (p-1)r \end{aligned}$$

Accordingly, for $r = a/(p-1)$, where $a > (p-1)$,

$$\frac{r^p - 1}{r-1} - a > (p-1) \cdot r - a = (p-1) \cdot a/(p-1) - a = 0.$$

For $r > 1$, and n sufficiently large, we thus have for the different equation functions:

$$f_{\mathrm{nn}}(r) = \frac{r^{n-1} - 1}{r-1} - \frac{L}{\delta} > (n-2)r - \frac{L}{\delta}$$

$$f_{\mathrm{nv}}(r) = \frac{r^n - 1 + r^{n-1} - 1}{2(r-1)} - \frac{L}{\delta} > (\frac{n-1}{2} + \frac{n-2}{2})r - \frac{L}{\delta} = \frac{2n-3}{2}r - \frac{L}{\delta}$$

$$f_{\mathrm{vn}}(r) = \frac{2r^n - r - 1}{2(r-1)} - \frac{L}{\delta} = \frac{r^n - 1 + r(r^{n-1} - 1)}{2(r-1)} - \frac{L}{\delta} > \frac{2n-3}{2}r - \frac{L}{\delta}$$

$$f_{\mathrm{vv}}(r) = \frac{(r+1)(r^n - 1)}{2(r-1)} - \frac{L}{\delta} > \frac{r^n - 1}{r-1} - \frac{L}{\delta} > (n-1)r - \frac{L}{\delta}$$

This inequalities can be used to derive bounds, so that a Newton method safe-guarded by a bisection method can be used.

4.3.2 Solution algorithm

Simple cases:

- $n = 2$
  - $f_{\mathrm{nn}}(r) = \frac{r-1}{r-1} - \frac{L}{\delta} = 1 - \frac{L}{\delta}$. No condition on r, but it is required that $L = \delta$
  - $f_{\mathrm{nv}}(r) = \frac{r^2+r-2}{2(r-1)} - \frac{L}{\delta} = \frac{1}{2}(r+2) - \frac{L}{\delta}$ and thus $r = 2(\frac{L}{\delta} - 1)$. Since $r > 0$, this is only possible if $L > \delta$.
  - $f_{\mathrm{vn}}(r) = \frac{2r^2-r-1}{2(r-1)} - \frac{L}{\delta} = \frac{1}{2}(r + \frac{1}{2}) - \frac{L}{\delta}$ and thus $r = 2\frac{L}{\delta} - \frac{1}{2}$, requiring that $L > 4\delta$.
  - $f_{\mathrm{vv}}(r) = \frac{(r+1)(r^2-1)}{2(r-1)} - \frac{L}{\delta} = \frac{1}{2}(r+1)^2 - \frac{L}{\delta}$ and thus $r = \sqrt{2\frac{L}{\delta}} - 1$ (the negative square root leads to negative r), requiring that $L > 2\delta$.

- $n = 3$
  - $f_{\mathrm{nn}}(r) = \frac{r^2-1}{r-1} - \frac{L}{\delta} = (r+1) - \frac{L}{\delta}$ and thus $r = \frac{L}{\delta} - 1$, requiring that $L > \delta$.

– $f_{\mathrm{nv}}(r) = \frac{r^3-1+r^2-1}{2(r-1)} - \frac{L}{\delta} = \frac{1}{2}(r^2+2r+2) - \frac{L}{\delta}$. The equation to solve is then $r^2+2r+2(1-\frac{L}{\delta})$. This equation has a real solution only if $4-8\cdot(1-\frac{L}{\delta}) \geq 0$, i.e., if $1-\frac{L}{\delta} \leq \frac{1}{2}$, i.e., if $L \geq \frac{1}{2}\delta$. In this case, $r = -1+\sqrt{2\frac{L}{\delta}-1}$. That root r is only positive if $L > \delta$.

– $f_{\mathrm{vn}}(r) = \frac{2r^3-r-1}{2(r-1)} - \frac{L}{\delta} = (r^2+r+\frac{1}{2}) - \frac{L}{\delta}$. The equation to solve is then $r^2+r+(\frac{1}{2}-\frac{L}{\delta})$. This equation has only a solution if $1-4\cdot(\frac{1}{2}-\frac{L}{\delta}) \geq 0$, i.e., if $\frac{1}{2}-\frac{L}{\delta} \leq \frac{1}{4}$, i.e., if $L \geq \frac{1}{4}\delta$. In this case, $r = -\frac{1}{2}+\frac{1}{2}\sqrt{4\frac{L}{\delta}-1}$. That root r is only positive if $L > \frac{1}{2}\delta$.

– $f_{\mathrm{vv}}(r) = \frac{(r+1)(r^3-1)}{2(r-1)} - \frac{L}{\delta} = \frac{1}{2}(r+1)(r^2+r+1) - \frac{L}{\delta}$. The equation to solve is then $(r+1)(r^2+r+1) - 2\frac{L}{\delta} = 0$. The first term is a monotonously increasing polynomial. The equation has thus only one real solution; the other two must be complex conjugate. The product of the three solutions is equal to $-(1-2\frac{L}{\delta})$. The real solution can therefore only be positive if $L > \frac{1}{2}\delta$.
$f_{\mathrm{vv}}(0) = \frac{1}{2} - \frac{L}{\delta}$: always negative
$f_{\mathrm{vv}}(1) = 3 - \frac{L}{\delta}$: positive or zero if $\frac{L}{\delta} \leq 3$
$f_{\mathrm{vv}}(\frac{L}{\delta}/2) > 0$ if $\frac{L}{\delta} > 2$

General case ($n > 3$)

- $f_{\mathrm{nn}}(r) = \frac{r^{n-1}-1}{r-1} - \frac{L}{\delta} = GP_{n-1}(r) - \frac{L}{\delta}$

  $f_{\mathrm{nn}}(0) = 1 - \frac{L}{\delta}$: $f_{\mathrm{nn}}(0) \leq 0$ if $\frac{L}{\delta} \geq 1$

  $f_{\mathrm{nn}}(1) = n-1-\frac{L}{\delta}$: $f_{\mathrm{nn}}(1) > 0 \Leftrightarrow \frac{L}{\delta} < n-1$

  $f_{\mathrm{nn}}(\frac{L}{\delta}/(n-2))) > 0$ if $\frac{L}{\delta} > n-2$

- $f_{\mathrm{nv}}(r) = \frac{r^n-1+r^{n-1}-1}{2(r-1)} - \frac{L}{\delta} = \frac{1}{2}(GP_n(r)+GP_{n-1}(r)) - \frac{L}{\delta} = \frac{1}{2}((r+1)GP_{n-1}(r)+1) - \frac{L}{\delta}$

  $f_{\mathrm{nv}}(0) = 1 - \frac{L}{\delta}$: $f_{\mathrm{nv}}(0) \leq 0$ if $\frac{L}{\delta} \geq 1$

  $f_{\mathrm{nv}}(1) = n-\frac{1}{2}-\frac{L}{\delta}$: $f_{\mathrm{nv}}(1) > 0 \Leftrightarrow \frac{L}{\delta} < n-\frac{1}{2}$

  $f_{\mathrm{n}}(\frac{L}{\delta}/(n-\frac{3}{2})) > 0$ if $\frac{L}{\delta} > n-\frac{3}{2}$

- $f_{\mathrm{vn}}(r) = \frac{2r^n-r-1}{2(r-1)} - \frac{L}{\delta} = \frac{1}{2}(GP_n(r)+rGP_{n-1}(r)) - \frac{L}{\delta} = rGP_{n-1}(r)+\frac{1}{2}-\frac{L}{\delta}$

  $f_{\mathrm{vn}}(0) = \frac{1}{2} - \frac{L}{\delta}$: $f_{\mathrm{nv}}(0) \leq 0$ if $\frac{L}{\delta} \geq \frac{1}{2}$

  $f_{\mathrm{vn}}(1) = n-\frac{1}{2}-\frac{L}{\delta}$: $f_{\mathrm{nv}}(1) > 0 \Leftrightarrow \frac{L}{\delta} < n-\frac{1}{2}$

  $f_{\mathrm{vn}}(\frac{L}{\delta}/(n-\frac{3}{2})) > 0$ if $\frac{L}{\delta} > n-\frac{3}{2}$

- $f_{\mathrm{vv}}(r) = \frac{(r+1)(r^n-1)}{2(r-1)} - \frac{L}{\delta} = \frac{1}{2}(r+1)GP_n(r) - \frac{L}{\delta}$
  $f_{\mathrm{vv}}(0) = \frac{1}{2} - \frac{L}{\delta}$: $f_{\mathrm{nv}}(0) \leq 0$ if $\frac{L}{\delta} \geq \frac{1}{2}$
  $f_{\mathrm{vv}}(1) = n - \frac{L}{\delta}$: $f_{\mathrm{nv}}(1) > 0 \Leftrightarrow \frac{L}{\delta} < n$
  $f_{\mathrm{vv}}(\frac{L}{\delta}/(n-1)) > 0$ if $\frac{L}{\delta} > n-1$

So for each case, it is possible to derive lower and upper bounds for the root r of the equation: $r = 0$ can always provides a lower bound and the third bound listed for each grid type above an upper bound for the root of the equation; $r = 1$ may be used to override either of them, depending on whether it is a lower ($f_{\mathrm{xx}}(1) < 0$) or an upper bound ($f_{\mathrm{xx}}(1) > 0$) of the root.

5 General series-based grids

For general series-based grids, we assume that we have a sequence $\delta_i > 0$ ($i = 1, \ldots N$) and that

$$q_i = \frac{1}{\Delta}\sum_{j=1}^{i}\delta_i \quad i = 1, \ldots N$$

where

$$\Delta = \sum_{j=1}^{N}\delta_i$$

is a normalizing scale such that $q_N = 1$. Furthermore, $q_0 = 0$.