At x_s: n_2 free parameters that must be specified at x_s leading to different values for the n_2 constraints $B_{fk}(x; \vec{y})$ at x_f.

The n_2 parameters are gathered into the n_2-dimensional vector $\vec{v}$.

We consider the subspace of $\vec{y}$ such that

$$y_i(x_s) = y_i(x_s; \vec{v}), \quad i = 1, \dots, n_2$$

fulfills

$$B_{sj}(x_s; \vec{y}) = 0 \quad \text{for } j = 1, \dots, n_1.$$

We now define an <u>error vector</u>

$$F_k = B_{fk}(x_f; \vec{y}(x_f; \vec{v})) = F_k(\vec{v})$$

Our problem is thus transformed into solving the equation

$$\boxed{\vec{F}(\vec{v}) = 0}$$

For this, we use the Newton-Raphson formula.

In one dimension, this works as follows:

Find x such that $f(x)=0$.

$$f(x_i) + f'(x_i)\,\delta x = 0$$

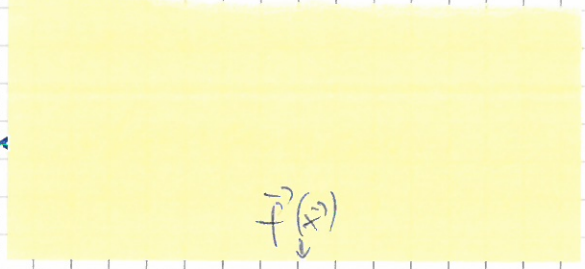
$$x = x_i + \delta x$$

$$\delta x = -\frac{f(x_i)}{f'(x_i)} = x - x_i \quad \Rightarrow$$

Iteration:

$$\boxed{x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}}$$

In higher



$$\vec{f}(\vec{x}) = 0 \Rightarrow f(\vec{x}_i) + \vec{\vec{J}}(\vec{x}_i) \cdot d\vec{x} = 0$$

Jacobi matrix:

$$\vec{\vec{J}} = \left\{ \frac{\partial f_i}{\partial x_j} \right\}$$

$\Rightarrow$

$$\boxed{\vec{x}_{i+1} = \vec{x}_i - \vec{\vec{J}}^{-1}(\vec{x}_i) \cdot \vec{f}(\vec{x}_i)}$$

In our case: $\vec{F}(\vec{v}) = 0$

$$J_{ij} = \frac{\partial F_i}{\partial V_j} = \frac{F_i(V_1, \ldots, V_j + \Delta V_j, \ldots, V_{n_2}) - F_i(\vec{V})}{\Delta V}$$

$$\vec{V}_{i+1} = \vec{V}_i - \vec{\vec{J}}^{-1}(\vec{V}_i) \cdot \vec{F}(\vec{V}_i)$$

Example: Laplace equation.

$$\left.\begin{aligned} \frac{dy_1}{dx} &= y_2 \\ \frac{dy_2}{dx} &= 0 \end{aligned}\right\}$$

$$\begin{cases} B_{s1}(x, \vec{y}) = y_1(x) \\ B_{f1}(x, \vec{y}) = y_1(x) - 1 \end{cases}$$

Analytical solution for y_1 and y_2:

$$\begin{cases} y_1 = C_2 x + C_1 \\ y_2 = C_2 \end{cases}$$

$$B_{s1}(0, \vec{y}) = 0 = C_1 \Rightarrow \underline{C_1 = 0}$$

$$F(C_2) = B_{f1}(1, \vec{y}) = C_2 - 1 = 0$$

$$\Rightarrow \underline{C_2 = 1}.$$

$$\Rightarrow \quad \left.\begin{aligned} y_1(x) &= x \\ y_2(x) &= 1 \end{aligned}\right\} \Rightarrow \underline{\phi(x) = x.}$$

(B) Relaxation

Differential equations $\Rightarrow$

Finite difference equations.

Grid points $x_1, \ldots, x_M$

Unknowns:

$$M \times N$$

M: # grid points

N: # equations.

$$\vec{y}(x_k) = \vec{y}_k$$

$$y'(x_k) = \frac{\vec{y}_k - \vec{y}_{k-1}}{x_k - x_{k-1}}$$

$$\vec{y}' = \vec{f}(\vec{y}) \Rightarrow$$

$$\vec{E}_k = \vec{y}_k - \vec{y}_{k-1} - (x_k - x_{k-1}) \cdot \vec{f}\left(\frac{1}{2}(x_k + x_{k-1}); \frac{1}{2}(\vec{y}_k + \vec{y}_{k-1})\right) = 0$$

$k = 2, \dots, M.$

gives $N \times (M-1)$ equations.

We need in addition N equations:

m_1 constraints at $x_1 = x_{l_1}$

m_2 constraints at $x_f = x_M$

$m_1 + m_2 = N.$

At x_1:

$$\vec{E}_1 = \vec{\beta}_s(x_1; \vec{y}_1) = 0$$

At x_M:

$$\vec{E}_{M+1} = \vec{\beta}_f(x_M; \vec{y}_M) = 0$$

We set up the vectors $\vec{E}_1$ and $\vec{E}_{M+1}$ in the following way:

$$\begin{cases} E_{j,1} \equiv 0 & \text{for } j = 1, \dots, m_2 \\ E_{j,1} = B_{s,j-m_2}(x_1, \vec{y}_1) & \text{for } j = m_2+1, \dots, N \end{cases}$$

$$\begin{cases} E_{j,M+1} = B_{f,j}(x_M; \vec{y}_M) & \text{for } j = 1, \dots, m_2 \\ E_{j,M+1} \equiv 0 & \text{for } j = m_2+1, \dots, N \end{cases}$$

We have thus constructed the following set of equations:

$$\boxed{E_{j,k} = 0 \quad \text{for} \quad \begin{matrix} j = 1, \dots, N \\ k = 1, \dots, M+1 \end{matrix}}$$

with respect to $y_{j,k}$

$j = 1, \dots, N$ $\quad$ $k = 1, \dots, M$

In practice, start with an initial guess for $y_{j,k}$.

Construct a sequence $\{y_{j,k}\}$ that converges on the solution of

$$E_{j,k}(y_{j,k}, y_{j,k-1}) = 0$$

We construct an iterative procedure

$$\vec{y}_k \to \vec{y}_k + \Delta\vec{y}_k$$

$$\vec{E}_k(\vec{y}_k + \Delta\vec{y}_k,\ \vec{y}_{k-1} + \Delta\vec{y}_{k-1})$$

$$= \vec{E}_k(\vec{y}_k, \vec{y}_{k-1}) + \sum_{n=1}^{N} \frac{\partial \vec{E}_k}{\partial y_{n,k-1}} \Delta y_{n,k-1}$$

1st order Taylor expansion

$$+ \sum_{n=1}^{N} \frac{\partial \vec{E}_k}{\partial y_{n,k}} \Delta y_{n,k}$$

We define

$$S^{k}_{j,m} = \frac{\partial E_{j,k}}{\partial y_{m,k-1}}$$

$$S^{k}_{j,m+N} = \frac{\partial E_{j,k}}{\partial y_{m,k}} \qquad m = 1, \ldots, N.$$

We may then write the 1st order expansion as:

$$(1) \quad \sum_{m=1}^{N} S^{k}_{j,m} \Delta y_{m,k-1} + \sum_{m=N+1}^{2N} S^{k}_{j,m} \Delta y_{m-N,k}$$

$$= - E_{j,k}$$

for $j = 1, \ldots, N$.

$\{ S^{k}_{j,m} \}$ is an $N \times 2N$ matrix at each point k.

Each internal k ($\neq 1, M+1$) produces a block of N equations that couples $2N$ variables at k and $k-1$.

At the boundaries:

$\underline{k=1:}$

$\vec{E}_1$ depends only on $\vec{y}_1$.

$$(2) \quad \sum_{m=1}^{N} S^{1}_{j,m} \Delta y_{m,1} = - E_{j,1}$$

$$j = M_2 + 1, \ldots, N$$

$$S^{1}_{j,m} = \frac{\partial E_{j,1}}{2 y_{m,1}} \qquad m = 1 \ldots N$$

$k = M+1$

$$(3) \quad \sum_{m=1}^{N}{}' S_{j,m}^{M+1} \Delta y_{m,M} = -E_{j,M+1}$$

$$j = 1, \ldots, n_2$$

$$S_{j,m}^{M+1} = \frac{\partial E_{j,M+1}}{\partial y_{m,M}} \qquad m = 1, \ldots, N.$$

Equations (1), (2) and (3) form a block diagonal system of equations for $\Delta y_{j,k}$.

We solve this set by iteration (see chapter on linear algebra).

Simple example: Laplace equation in one dimension.

$$\frac{d^2\phi}{dx^2} = 0 \; ; \quad \phi(0) = 1 \, , \quad \phi(1) = 2$$

$\Rightarrow$

$$\begin{cases} \dfrac{dy_1}{dx} = y_2 & y_1(0) = 0 \\ & y_1(1) = 2 \\ \dfrac{dy_2}{dx} = 0 \end{cases}$$

$$\Rightarrow \begin{cases} y_{1,k} - y_{1,k-1} = \dfrac{\Delta x}{2}\left(y_{2,k} + y_{2,k-1}\right) \\ \qquad\qquad k = 2, \dots, M \\ y_{2,k} - y_{2,k-1} = 0 \end{cases}$$

Set of equations for internal points

$k = 2, \dots, M$ after discretizing x.

$$\begin{cases} E_{1,k} = y_{1,k} - y_{1,k-1} - \frac{\Delta x}{2}(y_{2,k} + y_{2,k-1}) \\ E_{2,k} = y_{2,k} - y_{2,k-1} \end{cases}$$

$$S^k_{j,m} = \frac{\partial E_{j,k}}{\partial y_{m,k-1}} \qquad S^k_{j,m+1} = \frac{\partial E_{j,k}}{\partial y_{m,k}}$$

$\Rightarrow$

$$S^k_{1,1} = -1 \qquad S^k_{2,1} = 0$$

$$S^k_{1,2} = -\frac{\Delta x}{2} \qquad S^k_{2,2} = -1$$

$$S^k_{1,3} = 1 \qquad S^k_{2,3} = 0$$

$$S^k_{1,4} = -\frac{\Delta x}{2} \qquad S^k_{2,4} = 1$$

$$\sum_{m=1}^{2} S^k_{j,m}\,\Delta y_{m,k-1} + \sum_{m=3}^{4} S^k_{j,m}\,\Delta y_{m-2,k} = -E_{j,k}$$

- $-\Delta y_{1,k-1} - \frac{\Delta x}{2}\Delta y_{2,k-1} + \Delta y_{1,k}$

$$-\frac{\Delta x}{2}\Delta y_{2,k} = -y_{1,k} + y_{1,k-1} + \frac{\Delta x}{2} y_{2,k} + \frac{\Delta x}{2} y_{2,k-1}$$

- $-\Delta y_{2,k-1} + \Delta y_{2,k} = 0$

$k = 2, \dots, M.$

Constraints at the boundaries:

$\underline{k = 1:}$

$y_{1,1} = 0$ $\qquad E_{1,1} = 0$

$E_{2,1} = y_{1,1}$

$$S'_{j,m} = \frac{\partial E_{j,1}}{\partial y_{m,1}}, \quad m = 1, 2$$

$S'_{1,1} = 0$ $\qquad S'_{1,2} = 0$

$S'_{2,1} = 1$ $\qquad S_{2,2} = 0$

$$\sum_{m=1}^{2} S'_{j,m}\, \Delta y_{m,1} = - E_{j,1}$$

$\Rightarrow$

$$\boxed{\bullet \quad \Delta y_{2,1} = - y_{1,1}}$$

$\underline{k = M+1}$

$$E_{1,M+1} = y_{1,m} - 1$$

$$E_{2,M+1} = 0$$

$$S^{M+1}_{j,m} = \frac{\partial E_{j,M+1}}{\partial y_{m,m}} \qquad m = 1, 2$$

$$S^{M+1}_{1,1} = 1 \qquad S^{M+1}_{1,2} = 0$$

$$S^{M+1}_{2,1} = 0 \qquad S^{M+1}_{2,2} = 0$$

$$\sum_{m=1}^{2} S^{M+1}_{1,M}\, \Delta y_{m,m} = - E_{j,M+1} \qquad j = 1$$

$$\Delta y_{1,M} = -y_{1,M} + 1$$

(B) Initial value problems

$$\begin{cases} y_i'(x) = f_i(x; \vec{y}) & i = 1, \dots, N \\ y_i(x_0) \text{ are all given} \end{cases}$$

Basic idea:

$$\Delta y_i = \Delta x \, f_i$$

All algorithms have this as starting point.

Simplest method:

Euler integration

$$y_i(x+\Delta x) = y_i(x) + \Delta x\, f_i(x, \vec{y}(x))$$

This is the most unstable and least accurate method.

3 main classes of algorithms to improve the accuracy:

① Runge-Kutta

Combining more Euler steps to form a higher-order Taylor series.

(2) Richardson extrapolation

Integrate system with different Δx. Extrapolate result to $\Delta x \to 0$ limit.

(3) Predictor - Corrector

Integrate from $x \to x + \Delta x$ using simple scheme.
Then use result as input for more accurate scheme.

Numerical Recipes:

prefers (1) for simplicity
(2) for speed.
