Basic approach to solving nonlinear problems

Problem: find root of $f : \mathbb{R}^n \to \mathbb{R}^n$ (n eqs., n vars)

$\sim$ solve $f(x) = 0$

Newton iteration:

initial guess $x_0 \in \mathbb{R}^n$ ← Jacobian of f in x_k, $n \times n$ matrix

$x_{k+1} = x_k - Df(x_k)^{-1} f(x_k)$ (in Matlab "\")

until $\| x_k - x_{k-1} \| < tol$ & $\| f(x_k) \| < tol$

When does this work?

1) f has root x_* ($f(x_*) = 0$)
2) $Df(x_*)$ not singular / inverse exists) ← we don't know that, but most matrices are invertible
3) x_0 sufficiently close to x_* ← serious restriction if n is large

if 1)–3) are satisfied Newton converges fast

define $m(x) = \partial f(x)^{-1}$, $e_k = x_k - x_*$

$$f(x) = \underbrace{f(x_*)}_{=0} + m(x_*)^{-1}(x - x_*) + O((x - x_*)^2)$$

$$m(x) = m(x_*) + O(x - x_*)$$

$$x_{k+1} - x_* = x_k - x_* - m(x_k)\left[f(x_k) - \underbrace{f(x_*)}_{=0}\right]$$

$$e_{k+1} = e_k - [m(x_*) + O(e_k)][m(x_*)^{-1} e_k + O(e_k^2)]$$

$$= O(e_k^2)$$ quadratic convergence

Basic approach to overcoming problem (3): $x_0 \approx x_*$

In practice, problems depend on parameters

$$0 = f(x, p) \quad , \quad f : \mathbb{R}^{n_x} \times \mathbb{R}^{n_p} \to \mathbb{R}^{n_x}$$

we often know solution when p is special (e.g. $n_p = 1$, $p = 0$)

then (case $n_p = 1$):

0) we know x_0 s.t. $f(x_0, p_0) = 0$

choose $0 < h \ll 1$, $p_{k+1} = p_k + h$ for $k \geq 0$

k) use x_{k-1}, the solution of $f(x_{k-1}, p_{k-1}) = 0$ as initial guess when solving $f(x, p_k) = 0$

This works as long as $\partial_x f(x_k, p_k)$ is not singular.

Example: equilibria of AB reaction => Demo

$$\dot{x}_1 = -x_1 + \alpha\,(1 - x_1)\, e^{x_2}$$

$$\dot{x}_2 = -(1+\gamma)x_2 + \beta\alpha\,(1 - x_1)\, e^{x_2}$$

x_1 = concentration fraction

x_2 = temperature

⇒ Problem occurs when equilibria make curve that "turns around" (= fold) in parameter p

⇒ more general approach **Pseudoarclength continuation**

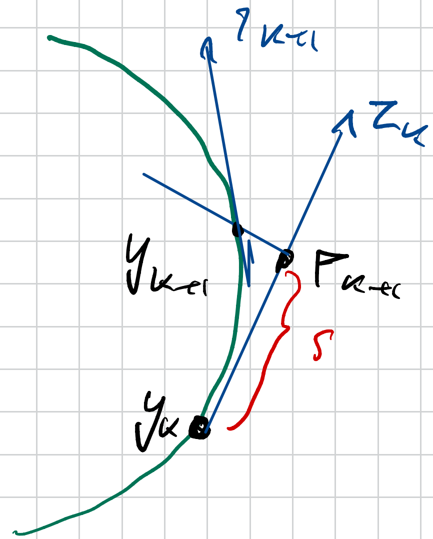
$(x,p) = y \in \mathbb{R}^{n+1}$, $f(x,p) = f(y)$, $f: \mathbb{R}^{n+1} \to \mathbb{R}^n$

set of solutions $Y = \{ y \in \mathbb{R}^{n+1} : f(y) = 0 \} \subseteq \mathbb{R}^{n+1}$ forms curve

We know one point y_0 with $f(y_0) = 0$, and tangent z_0 to Y in y_0. $(\|z_0\| = 1)$

Set $s \ll 1$ stepsize.

Step k1) predictor: $p_{k+1} = y_k + s z_k$



k2) corrector: apply Newton iteration to

$$f(y) = 0 \qquad n \text{ eqs.}$$

$$z_k^T (y - p_{k+1}) = 0 \qquad 1 \text{ eq.}$$

solution y_{k+1}

k3) new tangent: solve $\begin{bmatrix} f'(y_{k+1}) \\ z_k^T \end{bmatrix} z_{k+1} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}$

rescale $z_{k+1} \to z_{k+1} / \|z_{k+1}\|$

⇒ Demo