Computation of bifurcation diagrams

1. Fixed points

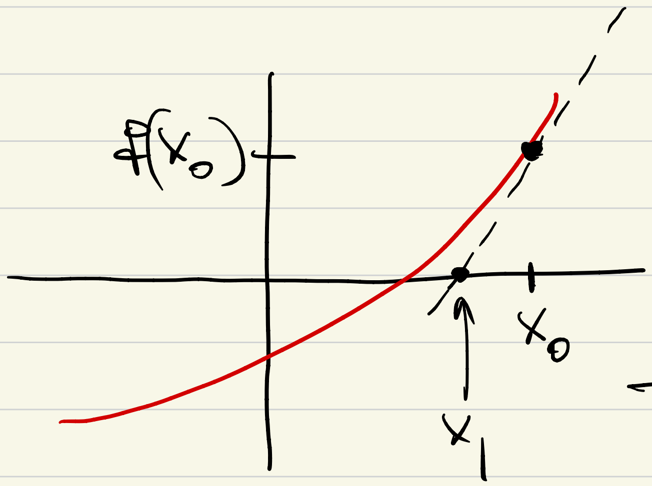
a) 1D : $f(\bar{x}, \lambda) = 0$

zeroes of nonlinear eq.

Method: Newton-Raphson (NR)

iterate k

initial guess: x_0



$y = f'(x_0)x + b$

intersect with $y = 0$ is x_1

$$\rightarrow \begin{cases} 0 = f'(x_0)x_1 + b \\ f(x_0) = f'(x_0)x_0 + b \end{cases}$$

$$\rightarrow \quad f'(x_0)(x_1 - x_0) = -f(x_0)$$

assume $f'(x_0) \neq 0$

$$\rightarrow \quad x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

iteration k

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$$

NR converges quadratically under 'mild' conditions to $\bar{x}$.

b) More generally:

$$\underline{f}(\bar{\underline{x}}, \lambda) = 0$$

$$J(\underline{x}_k)\underbrace{(\underline{x}_{k+1} - \underline{x}_k)}_{\Delta \underline{x}_{k+1}} = -\underline{f}(\underline{x}_k)$$

$\rightarrow$ system of linear equations ($A\underline{x} = \underline{b}$ type)

Stability of fixed points $\underline{\bar{x}}$

$$\underline{x} = \underline{\bar{x}} + \underline{\tilde{x}} \quad , \quad \underline{\dot{x}} = \underline{f}(\underline{x}, \lambda)$$

$$\rightarrow \quad \underline{\dot{\tilde{x}}} = J(\underline{\bar{x}})\,\underline{\tilde{x}} \qquad (\text{page } \boxed{25})$$

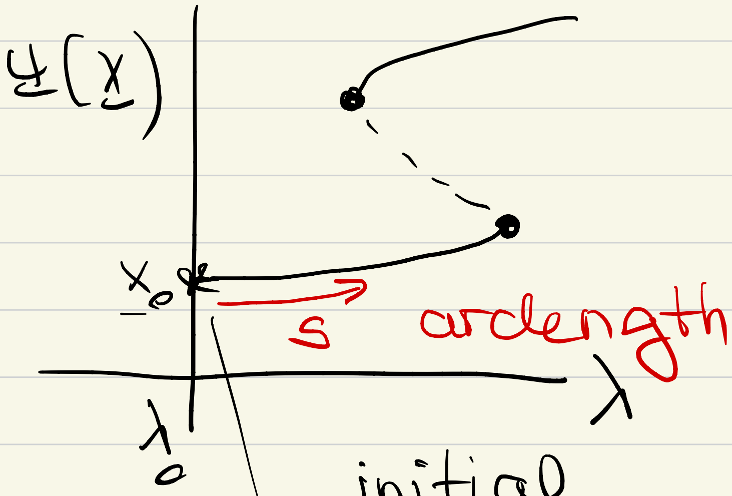
Let $\underline{\tilde{x}} = e^{\sigma t}\,\underline{\hat{x}}$

$$\rightarrow \quad \sigma e^{\sigma t}\,\underline{\hat{x}} = J(\underline{\bar{x}})\,e^{\sigma t}\,\underline{\hat{x}}$$

$$\rightarrow \quad J(\underline{\bar{x}})\,\underline{\hat{x}} = \sigma\,\underline{\hat{x}}$$

eigenvalue problem for the matrix $J(\underline{\bar{x}})$.

2. Pseudo-arclength methods

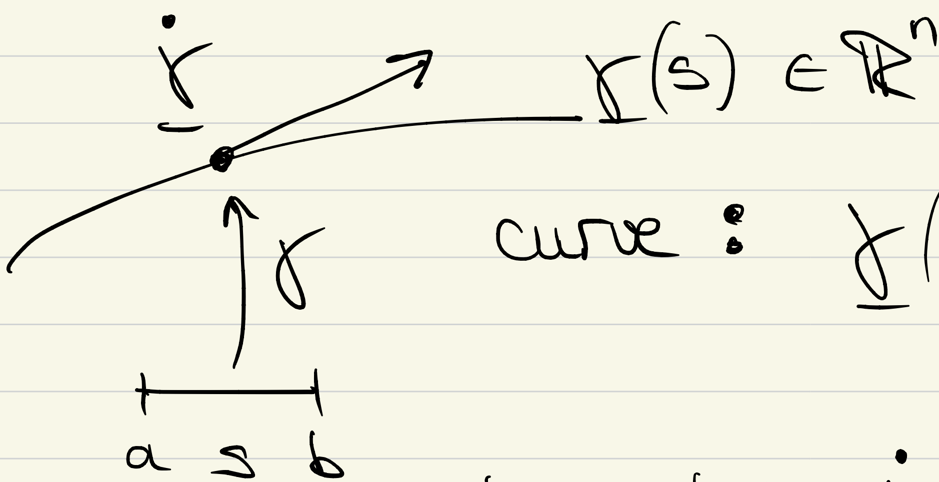


direct comp of bif. diagrams

initial fixed point $(\underline{x}_0, \lambda_0)$

a) – Solutions: $(\underline{x}(s), \lambda(s))$
of $\underline{f}(\underline{x}(s), \lambda(s)) = 0$

– Extra degree of freedom s
need extra condition Σ



curve: $\underline{\gamma}(s) = \begin{pmatrix} \gamma_1(s) \\ \vdots \\ \gamma_n(s) \end{pmatrix}$

tangent: $\dot{\underline{\gamma}}(s)$

$\underline{\text{Ex}}$
$\overline{n=2}$

$$\underline{\gamma}(s) = \begin{pmatrix} \cos 2\pi s \\ \sin 2\pi s \end{pmatrix} \quad s \in [0,1)$$

$\longrightarrow$ circle $\square$

$$\underline{\gamma}(s) = \begin{pmatrix} \underline{x}(s) \\ \lambda(s) \end{pmatrix}$$

$$\Sigma\left(\underline{x}(s), \lambda(s)\right) = \|\underline{\gamma}'(s)\|^2 - 1$$
$$= 0$$

$\longrightarrow$ normalization of the tangent.

Total system of equations:

$$\underline{f}(\underline{\gamma}(s)) = \underline{f}\left(\underline{x}(s), \lambda(s)\right) = 0$$

$$\dot{\underline{x}}^T \dot{\underline{x}} + \dot{\lambda}^2 = 1$$

b) Computation initial tangent

$$\dot{\gamma}(s_0) = \begin{pmatrix} \dot{x}_0 \\ \dot{\lambda}_0 \end{pmatrix}$$

Differentiate $\underline{f}(\underline{\gamma}(s)) = 0$ to s:

$$\begin{array}{cc} & n+1 \\ n & \begin{bmatrix} J & \underline{f}_\lambda \end{bmatrix} \end{array} \underline{\dot{\gamma}}(s) = 0$$

$$n \times n \quad n \times 1 \quad (n+1) \times 1$$

- If $(\underline{x}_0, \lambda_0)$ is not a bif. point then rank $[J \ \underline{f}_\lambda] = n$

- we can determine $(\underline{\dot{x}}_0, \dot{\lambda}_0)$ from

$$\begin{array}{cc} & n+1 \\ n+1 & \begin{pmatrix} J(x_0) & \underline{f}_\lambda \\ \underline{0} & 1 \end{pmatrix} \end{array} \begin{pmatrix} \underline{\dot{x}}_0 \\ \dot{\lambda}_0 \end{pmatrix} = \begin{pmatrix} \underline{0} \\ 1 \end{pmatrix}$$

With steplength Δs, Σ is then approximated by

$$\Sigma = \dot{\underline{x}}_0^T \frac{\underline{x} - \underline{x}_0}{\Delta s} + \dot{\lambda}_0 \frac{\lambda - \lambda_0}{\Delta s} - 1$$

where $(\underline{x}, \lambda)$ is the next fixed point to be computed. The system for $(\underline{x}(s), \lambda(s))$ is

$$(*) \begin{cases} \underline{f}(\underline{x}(s), \lambda(s)) = 0 \\ \dot{\underline{x}}_0^T (\underline{x} - \underline{x}_0) + \dot{\lambda}_0 (\lambda - \lambda_0) = \Delta s \end{cases}$$

where Δs is chosen and $\underline{x}_0$, $\dot{\underline{x}}_0$, λ_0, $\dot{\lambda}_0$ are known

c) Euler-Newton method

- initial guess

$$\underline{x}_1 = \underline{x}_0 + \Delta s \, \dot{\underline{x}}_0$$
$$\lambda_1 = \lambda_0 + \Delta s \, \dot{\lambda}_0$$

- NR on (*) $\quad \underline{x}_{k+1} = \underline{x}_k + \Delta \underline{x}_{k+1}$

$$\overbrace{\begin{pmatrix} \underline{\underline{J}} & \underline{f}_\lambda \\ \dot{\underline{x}}_0^T & \dot{\lambda}_0 \end{pmatrix}}^{\tilde{\underline{\underline{J}}}} \begin{pmatrix} \Delta \underline{x}_{k+1} \\ \Delta \lambda_{k+1} \end{pmatrix} = \begin{pmatrix} \underline{I} \\ \alpha \end{pmatrix}$$

$$\begin{pmatrix} \underline{I} \\ \alpha \end{pmatrix} = \begin{pmatrix} -\underline{f}(\underline{x}_k, \lambda_k) \\ \Delta s - \dot{\underline{x}}_0^T (\underline{x}_k - \underline{x}_0) - \dot{\lambda}_0 (\lambda_k - \lambda_0) \end{pmatrix}$$

Advantage: at bif points $\underline{\underline{J}}$ becomes singular but $\tilde{\underline{\underline{J}}}$ does not.

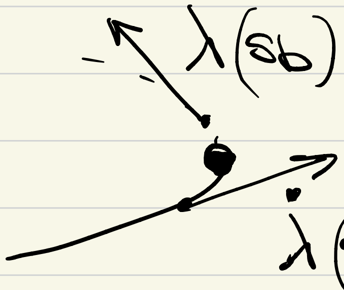
Converged solution gives next fixed point $\left(\underline{x}(s_1), \lambda(s_1) \right)$ with $s_1 = s_0 + \Delta s$; when

$$\left\| \begin{pmatrix} \Delta x_{k+1} \\ \Delta \lambda_{k+1} \end{pmatrix} \right\| < \varepsilon_{NR} \left\| \begin{pmatrix} \underline{x}_0 \\ \lambda_0 \end{pmatrix} \right\|$$

- NR determines fixed points regardless of their stability

3. Detection of bifurcation points

- saddle-node:



$$\dot{\lambda}(s_a)\,\dot{\lambda}(s_b) < 0$$

$$s_b > s_a$$

- pitchfork / transcritical

1) $\left(\det J(s_a)\right) \cdot \left(\det J(s_b)\right) < 0$

2) solve stability problem

$$J\left(\underline{x}(s), \lambda(s)\right) \hat{\underline{x}} = \sigma \hat{\underline{x}}$$

$$\sigma = \sigma_r \pm i\,\sigma_i$$

then bif when: $\sigma_r(s_a) \cdot \sigma_r(s_b) < 0$

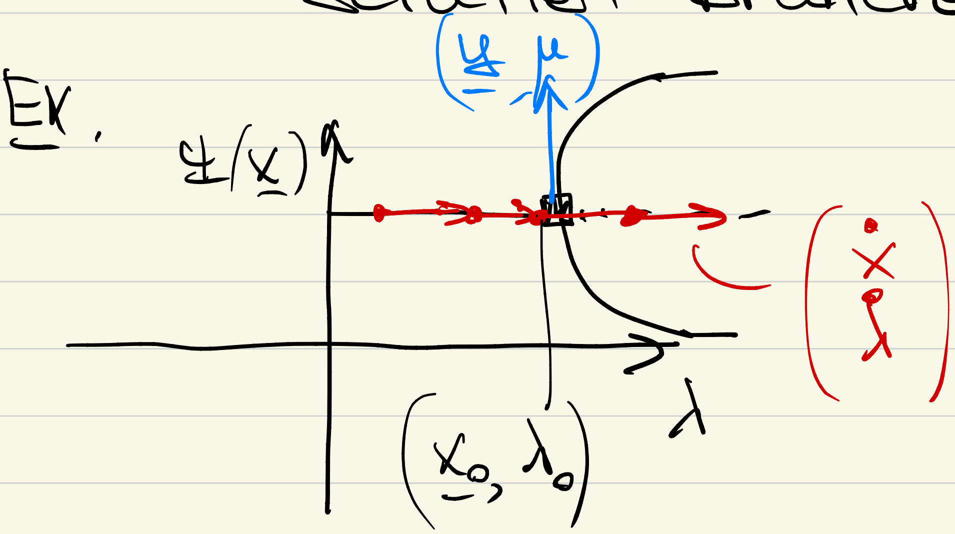
After a sign change in any indicator $\phi(s)$ has been found, the precise location of the bif point can be computed through a secant iteration:

$$\begin{cases} s_{\ell+1} = s_\ell - \phi(s_\ell) \dfrac{s_\ell - s_{\ell-1}}{\phi(s_\ell) - \phi(s_{\ell-1})} \\ s_0 = s_a \, , \quad s_1 = s_b \end{cases}$$

until $|s_{\ell+1} - s_\ell| < \varepsilon_s \, s_0$

4. Detection of additional solution branches.

Ex.



- Branch switching near BP solution $(\underline{x}_0, \lambda_0)$

  - compute $\begin{pmatrix} \underline{y} \\ \mu \end{pmatrix} \perp \begin{pmatrix} \dot{\underline{x}}_0 \\ \dot{\lambda}_0 \end{pmatrix}$ and $\underline{\underline{J}}\, \underline{v} = 0$

$$\rightarrow \begin{pmatrix} \underline{\underline{J}} & \underline{f}_\lambda \\ \dot{\underline{x}}_0^T & \dot{\lambda}_0 \end{pmatrix} \begin{pmatrix} \underline{y} \\ \mu \end{pmatrix} = \begin{pmatrix} \underline{0} \\ 0 \end{pmatrix}$$

$$\rightarrow (**) \quad \begin{cases} \underline{\underline{J}}\,\underline{y} + \mu \underline{f}_\lambda = 0 \\ \dot{\underline{x}}_0^T \underline{y} + \mu \dot{\lambda}_0 = 0 \end{cases}$$

Let $\underline{z}$ be the solution of

$$J \underline{z} = \underline{f}_\lambda$$

which can be solved as the kernel $\underline{v}$ is known

$\longrightarrow$

$$\begin{cases} \underline{y} = \underline{v} - \mu \underline{z} \\ \underline{\dot{x}}_0^T \underline{v} - \mu \underline{\dot{x}}_0 \underline{z} + \mu \dot{\lambda}_0 = 0 \end{cases}$$

$\longrightarrow$ $$\mu = \frac{- \underline{\dot{x}}_0^T \underline{v}}{\dot{\lambda}_0 - \underline{\dot{x}}_0^T \underline{z}}$$

Start Euler - Newton with

$$\begin{cases} \underline{x}_1 = \underline{x}_0 + \Delta s \, \underline{y} \\ \lambda_1 = \lambda_0 + \Delta s \, \mu \end{cases}$$

In practise, other methods are often used.

5. Stability of branches

- solve $J\left(\underline{x}(s), \lambda(s)\right)\hat{\underline{x}} = \sigma\,\hat{\underline{x}}$
  standard QR method.