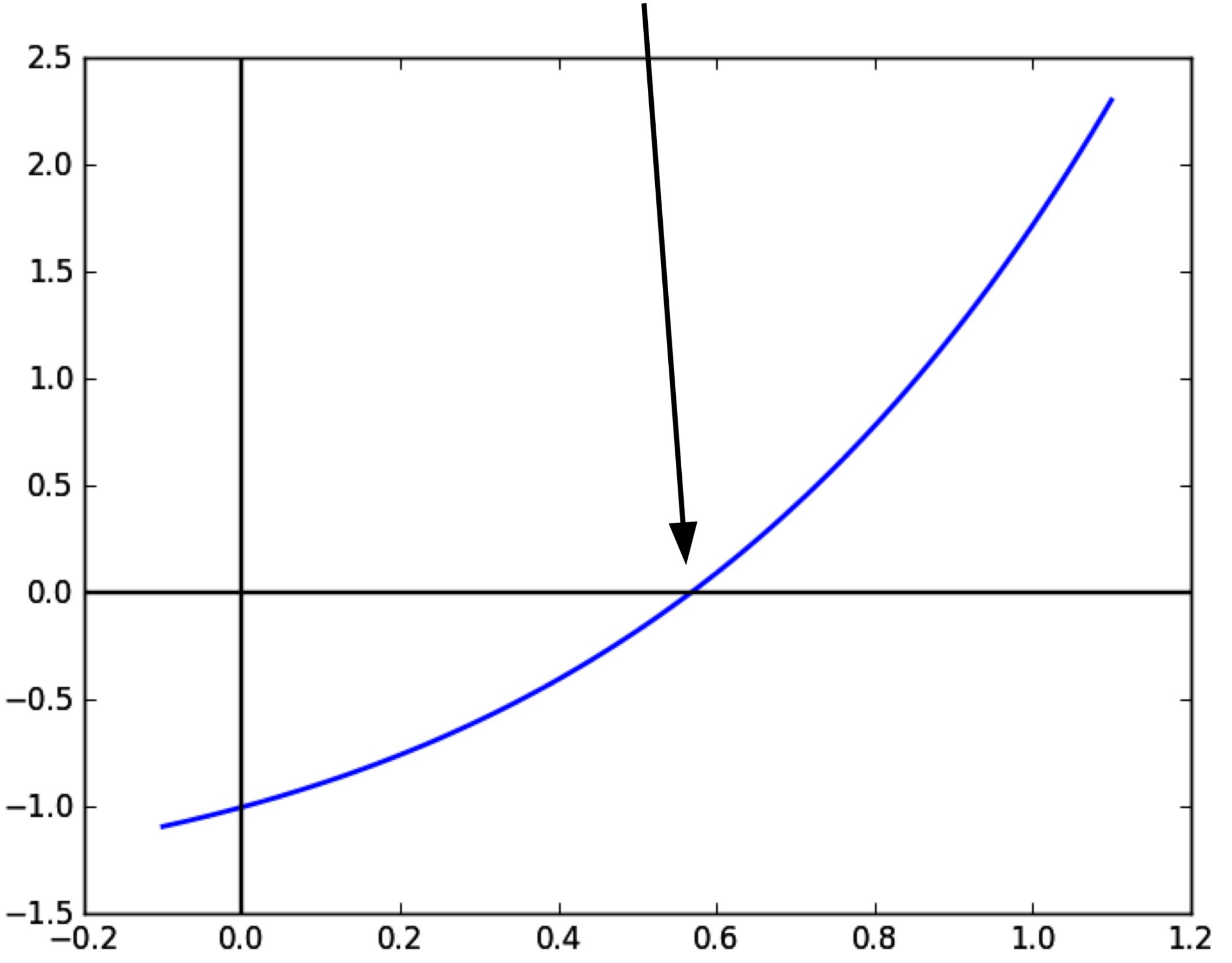
Ex. (1)

Fixed-point iterations

$$f(x) = xe^x - 1 \stackrel{!}{=} 0$$



Ex. (1)

Fixed-point iterations

$$f(x) = xe^x - 1 \overset{!}{=} 0$$

$$x^{(k+1)} = \phi(x^{(k)})\ ,\ k = 0, 1, ...$$

$$x = \phi_1(x) \quad \text{with} \quad \phi_1(x) = e^{-x}$$

$$x = \phi_2(x) \quad \text{with} \quad \phi_2(x) = \frac{x^2 e^x + 1}{e^x(1+x)}$$

$$x = \phi_3(x) \quad \text{with} \quad \phi_3(x) = x - xe^x + 1$$

Ex. (1)

Consistency

(i) $x \cdot e^x - 1 = 0$

$x \cdot e^x = 1$

$x = e^{-x} = \phi_1(x)$ fixed-point eq.

(consistent ✓.)

Ex. (1)

Fixed-point iterations

$$f(x) = xe^x - 1 \stackrel{!}{=} 0$$

$$x^{(k+1)} = \phi(x^{(k)})\ ,\ \ k = 0, 1, \dots$$

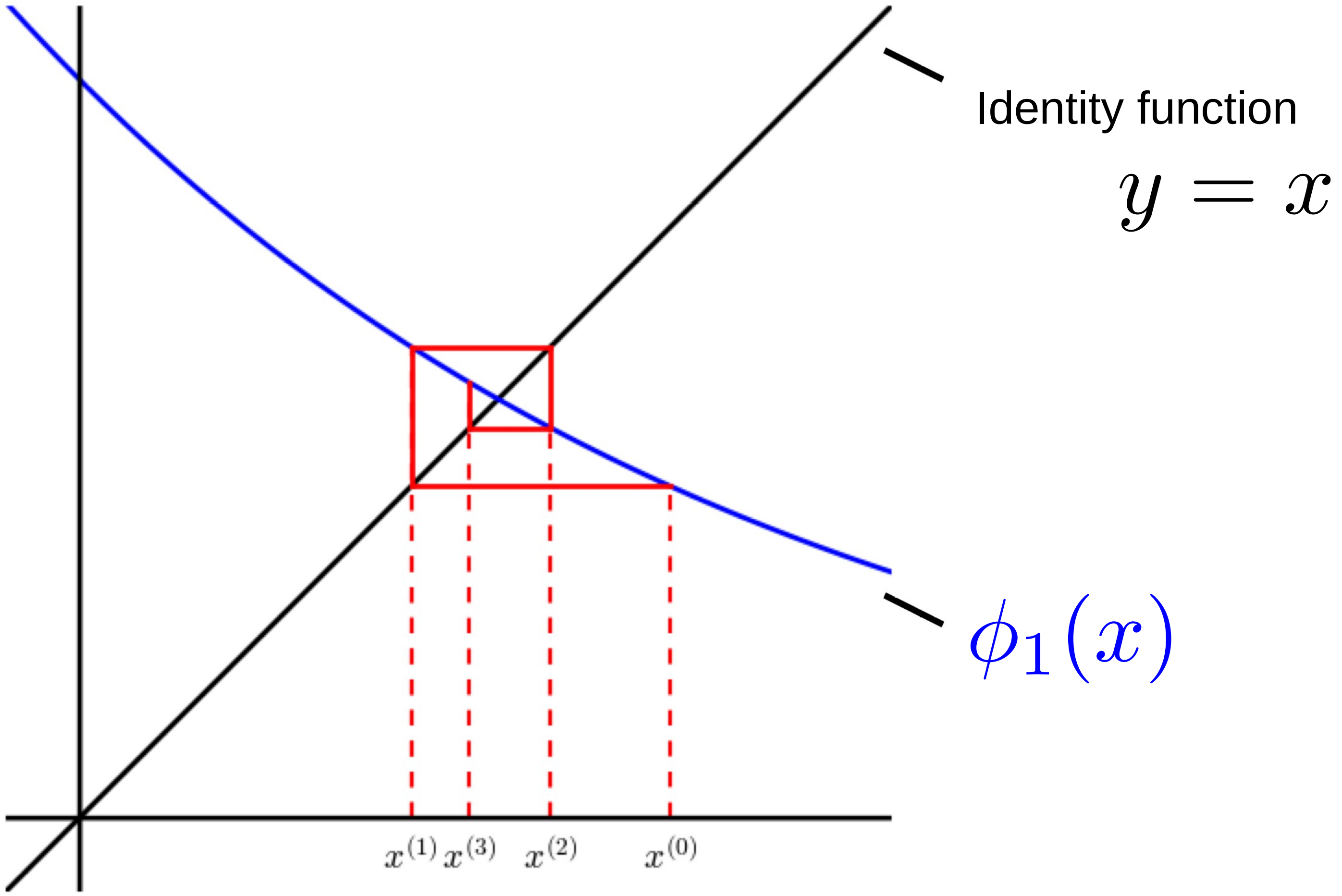
k	ϕ_1	ϕ_2	ϕ_3
0	0.8000000	0.9000000	0.6000000
1	0.4493290	0.6402998	0.5067287
2	0.6380562	0.5713091	0.6656338
3	0.5283184	0.5671575	0.3704946
4	0.5895956	0.5671433	0.8338514
5	0.5545515	0.5671433	-0.0858149
...	...	...	...

Ex. (1)

Fixed-point iterations

$$f(x) = xe^x - 1 \overset{!}{=} 0$$

$$x = \phi_1(x) \quad \text{with} \quad \phi_1(x) = e^{-x}$$

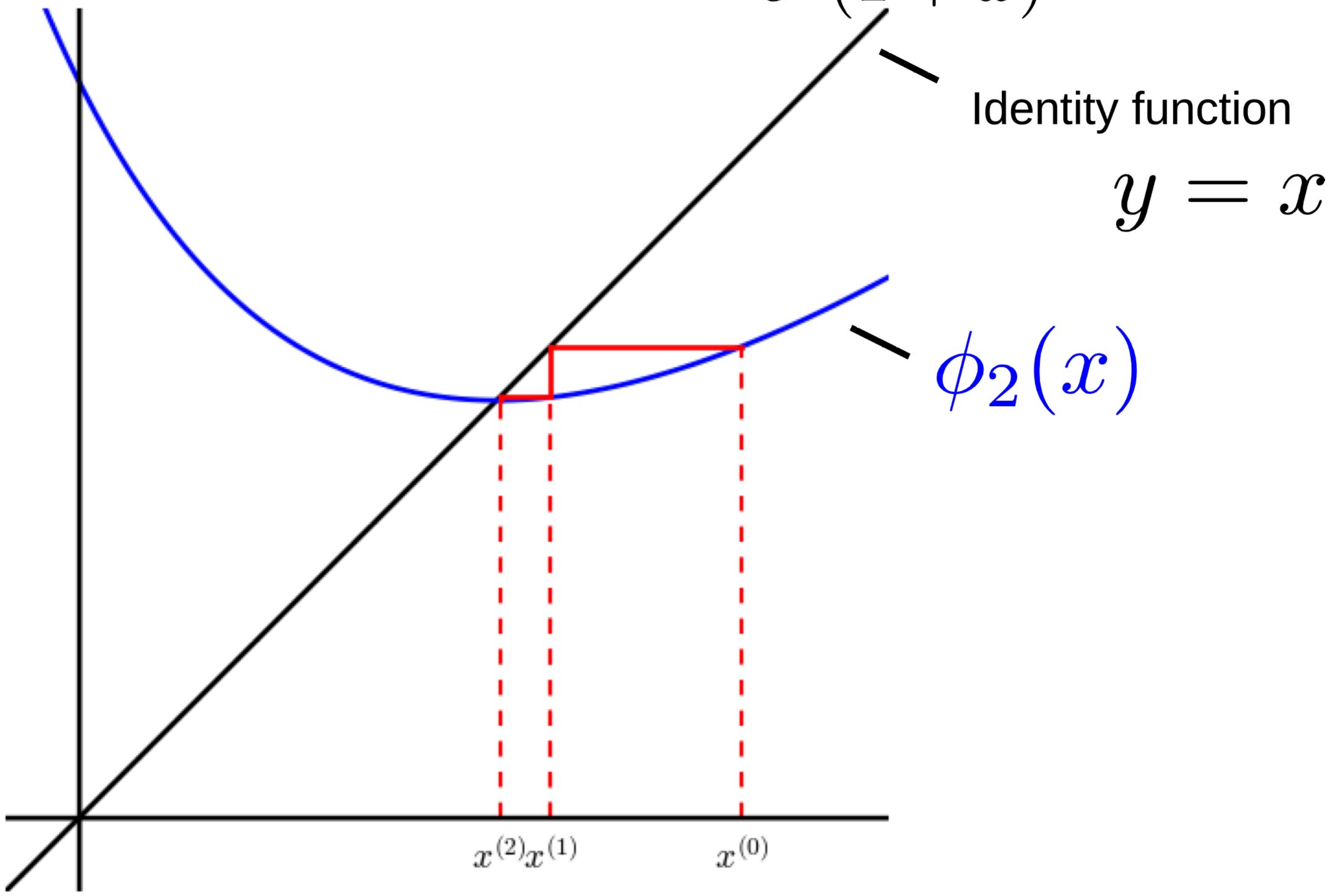


Ex. (1)

Fixed-point iterations

$$f(x) = xe^x - 1 \overset{!}{=} 0$$

$$x = \phi_2(x) \quad \text{with} \quad \phi_2(x) = \frac{x^2 e^x + 1}{e^x(1+x)}$$

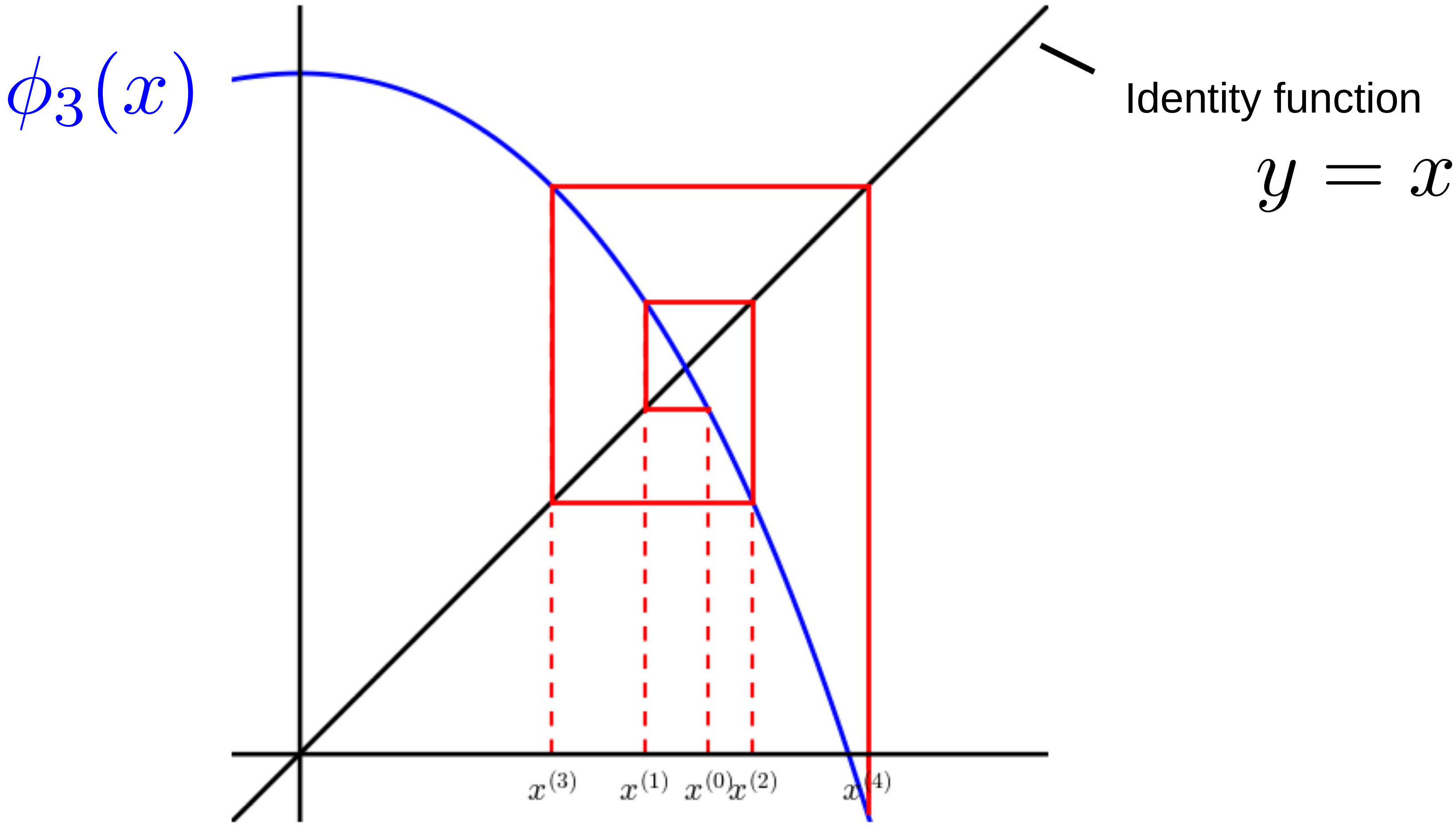


Ex. (1)

Fixed-point iterations

$$f(x) = xe^x - 1 \overset{!}{=} 0$$

$$x = \phi_3(x) \quad \text{with} \quad \phi_3(x) = x - xe^x + 1$$



Ex. (1)

Rem.: (i) Fixed-point iterations not unique

(ii) Fixed-point iterations may not converge

(iii) If they converge, they may do that with different speeds

Def.: A sequence $x^{(k)}$ with limit x^* converges with order $p \geq 1$, if there exists a constant $C > 0$ such that

$$|x^{(k+1)} - x^*| \leq C \, |x^{(k)} - x^*|^p$$

for all sufficiently large k.

For $p = 1$, it must $0 < C < 1$.
The constant C is called the rate of convergence.

In particular, convergence with order $\begin{Bmatrix} p = 1 \\ p = 2 \end{Bmatrix}$ is called $\begin{Bmatrix} \text{linear} \\ \text{quadratic} \end{Bmatrix}$.

It is often helpful, e.g. for code verification, to measure C and p in numerical experiments.

For this we define the error at the k-th iteration as

$$\varepsilon^{(k)} = |x^{(k)} - x^*|$$

Then we can write

$$\varepsilon^{(k)} = c \cdot \left(\varepsilon^{(k-1)}\right)^p$$

$$\varepsilon^{(k+1)} = c \cdot \left(\varepsilon^{(k)}\right)^p$$

Taking the log on both sides gives

$$\log\left(\varepsilon^{(k)}\right) = \log(c) + p \cdot \log\left(\varepsilon^{(k-1)}\right)$$

$$\log\left(\varepsilon^{(k+1)}\right) = \log(c) + p \cdot \log\left(\varepsilon^{(k)}\right)$$

This can be solved for C and p:

$$p = \frac{\log\left(\varepsilon^{(k+1)}\right) - \log\left(\varepsilon^{(k)}\right)}{\log\left(\varepsilon^{(k)}\right) - \log\left(\varepsilon^{(k-1)}\right)}$$

$$C = \frac{\varepsilon^{(k+1)}}{\left(\varepsilon^{(k)}\right)^{p}} = \frac{\varepsilon^{(k)}}{\left(\varepsilon^{(k-1)}\right)^{p}}$$

Ex. (2)

Fixed-point iterations

$$f(x) = xe^x - 1 \overset{!}{=} 0$$

$$x = \phi_1(x) \quad \text{with} \quad \phi_1(x) = e^{-x}$$

k	$x^{(k)}$	$\epsilon^{(k)}$	p	C
0	0.8000000	2.3285671e-01	-	-
1	0.4493290	1.1781433e-01	0.7451165	0.3489721
2	0.6380562	7.0912876e-02	1.1866067	0.8971140
3	0.5283184	3.8824901e-02	0.9091583	0.4305099
4	0.5895956	2.2452316e-02	1.0560201	0.6937276
5	0.5545515	1.2591794e-02	0.9697282	0.4999380
6	0.5743298	7.1865021e-03	1.0176407	0.6165178
7	0.5630821	4.0611662e-03	0.9901489	0.5382915
8	0.5694512	2.3079464e-03	1.0056361	0.5862095
9	0.5658359	1.3074270e-03	0.9968194	0.5556549

Ex. (2)

Fixed-point iterations

$$f(x) = xe^x - 1 \stackrel{!}{=} 0$$

$$x = \phi_2(x) \quad \text{with} \quad \phi_2(x) = \frac{x^2 e^x + 1}{e^x(1+x)}$$

k	$x^{(k)}$	$\epsilon^{(k)}$	p	C
0	0.8000000	3.3285671e-01	-	-
1	0.4493290	7.3156531e-02	1.8914068	0.5859477
2	0.6380562	4.1658100e-03	1.9832614	0.7450448
3	0.5283184	1.4171777e-05	1.9994808	0.8143094
4	0.5895956	1.6449608e-10	1.2503362	0.0001899
5	0.5545515	1.1102230e-16	-	-

Stopping criteria (SC):

(SC1) $|x^{(k)} - x^{(k-1)}| \leq atol$ (absolute-)

(SC2) $|x^{(k)} - x^{(k-1)}| \leq rtol \cdot |x^{(k)}|$ (relative-)

(SC3) $|x^{(k)} - x^{(k-1)}| \leq tol \cdot (1 + |x^{(k)}|)$ (hybrid-)

(SC4) $|f(x^{(k)})| \leq ftol$ (function-)

tolerance

Ex. (3)

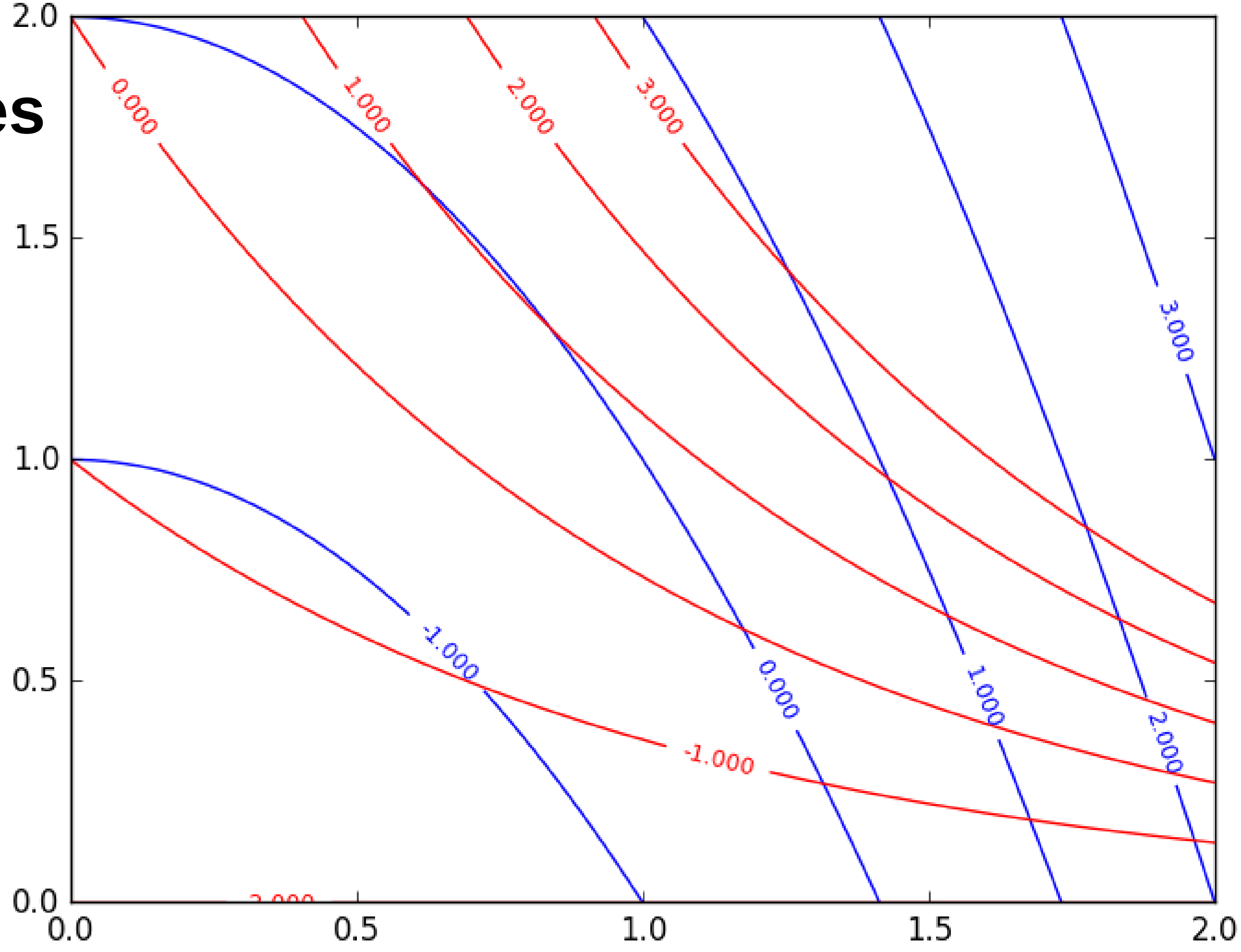
Newton Method

$$
\begin{aligned}
f_1(x_1, x_2) &= x_1^2 + x_2 - 2 &&= 0 \\
f_2(x_1, x_2) &= x_2 e^{x_1} - 2 &&= 0
\end{aligned}
$$

Ex. (3)

Newton method

Level curves



$\mathrm{f}_1(x_1, x_2) = x_1^2 + x_2 - 2$

$f_2(x_1, x_2) = x_2 e^{x_1} - 2$

Newton method

Idea: linearize $\vec{f}$

Taylor at $\vec{x}^{(k)}$

Jacobian Matrix

$$Df(\vec{x}) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & & \\ \frac{\partial f_n}{\partial x_1} & \cdots & \frac{\partial f_n}{\partial x_n} \end{pmatrix}$$

$$\vec{f}(\vec{x}) = \vec{f}(\vec{x}^{(k)}) + D\vec{f}(\vec{x}^{(k)})(\vec{x} - \vec{x}^{(k)}) + \dots$$

$$\underset{\sim}{\vec{f}} = \vec{f}(\vec{x}^{(k)}) + D\vec{f}(\vec{x}^{(k)})(\vec{x} - \vec{x}^{(k)}) \overset{!}{=} 0$$

$$\rightsquigarrow \quad \vec{x}^{(k+1)} = \vec{x}^{(k)} - D\vec{f}(\vec{x}^{(k)})^{-1} \, \vec{f}(\vec{x}^{(k)})$$

inverse of Jacobian

Ex. (4)

Newton method

$$f_1(x_1, x_2) = x_1^2 + x_2 - 2 \quad = 0$$
$$f_2(x_1, x_2) = x_2 e^{x_1} - 2 \quad = 0$$

$$\mathbf{f}(\mathbf{x}) = \begin{pmatrix} x_1^2 + x_2 - 2 \\ x_2 e^{x_1} - 2 \end{pmatrix} = 0$$

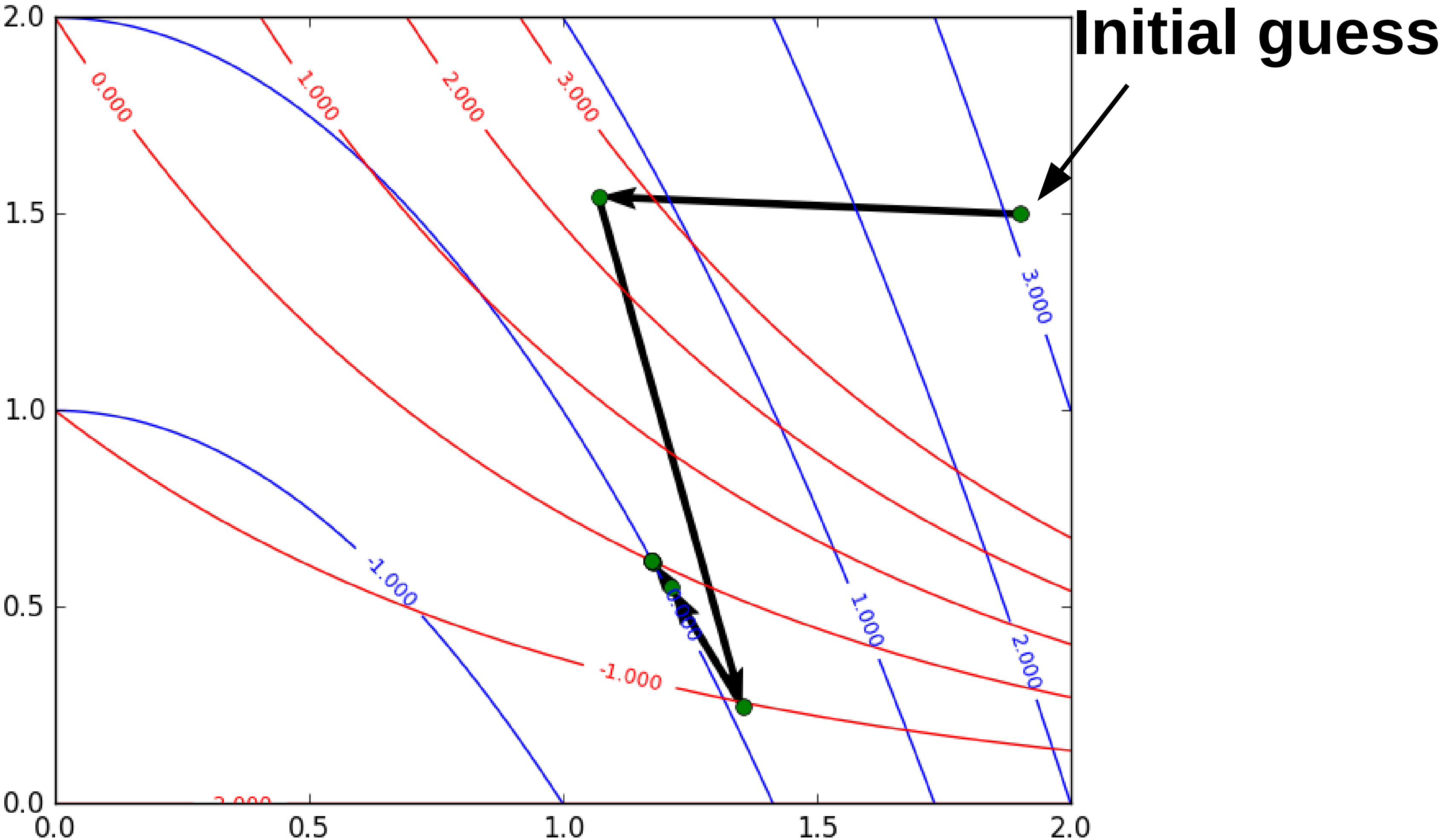
$$\mathrm{D}\mathbf{f}(\mathbf{x}) = \begin{pmatrix} 2x_1 & 1 \\ x_2 e^{x_1} & e^{x_1} \end{pmatrix} \quad \mathrm{D}\mathbf{f}^{-1}(\mathbf{x}) = \frac{1}{(2x_1 - x_2)e^{x_1}} \begin{pmatrix} e^{x_1} & -1 \\ -x_2 e^{x_1} & 2x_1 \end{pmatrix}$$

$$\mathrm{A} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

$$\mathrm{A}^{-1} = \frac{1}{ad - cb} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

Ex. (4)

Newton method



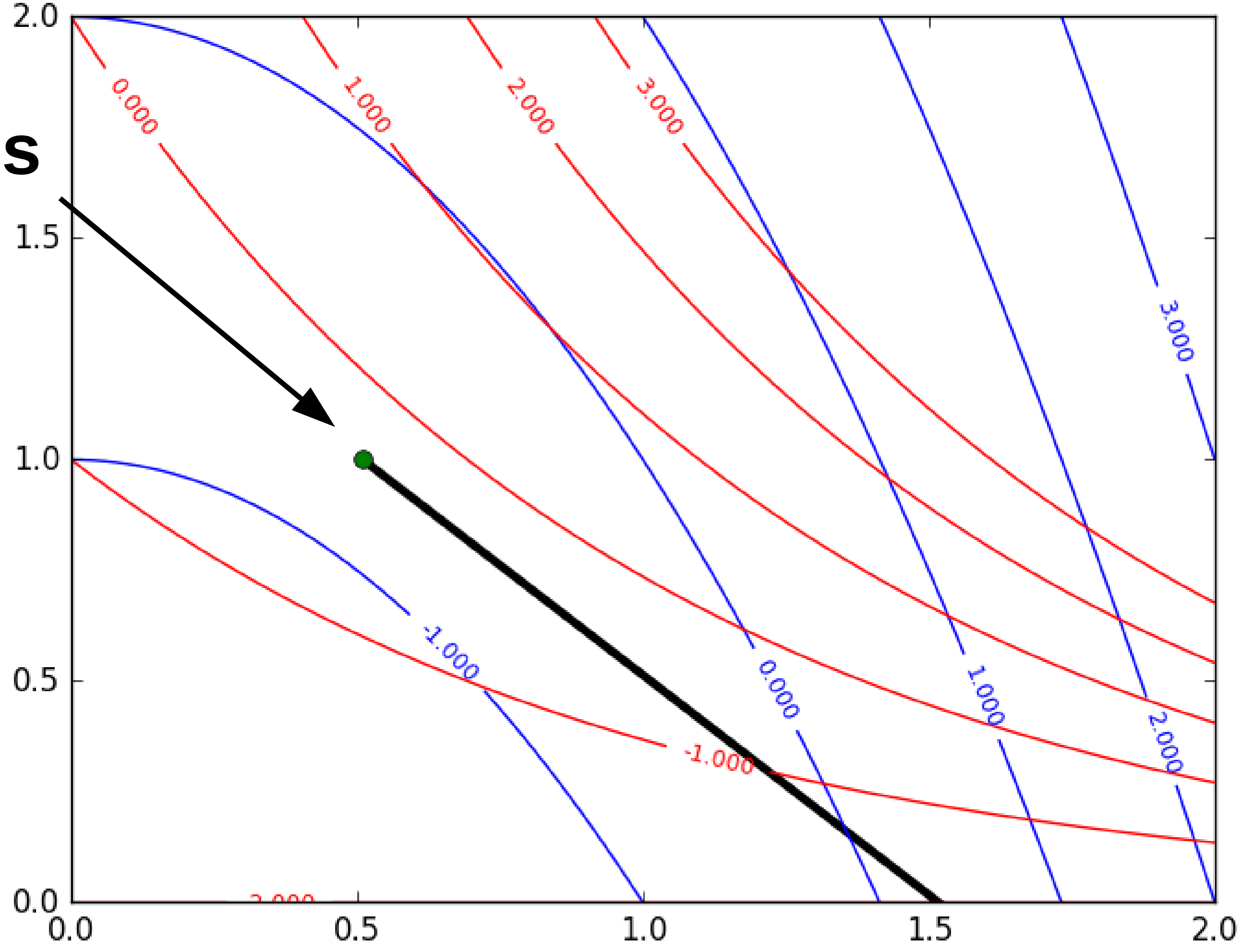
$$\mathrm{f}_1(x_1, x_2) = x_1^2 + x_2 - 2$$

$$f_2(x_1, x_2) = x_2 e^{x_1} - 2$$

Ex. (4)

Newton method

Initial guess



$\mathrm{f}_1(x_1, x_2) = x_1^2 + x_2 - 2$

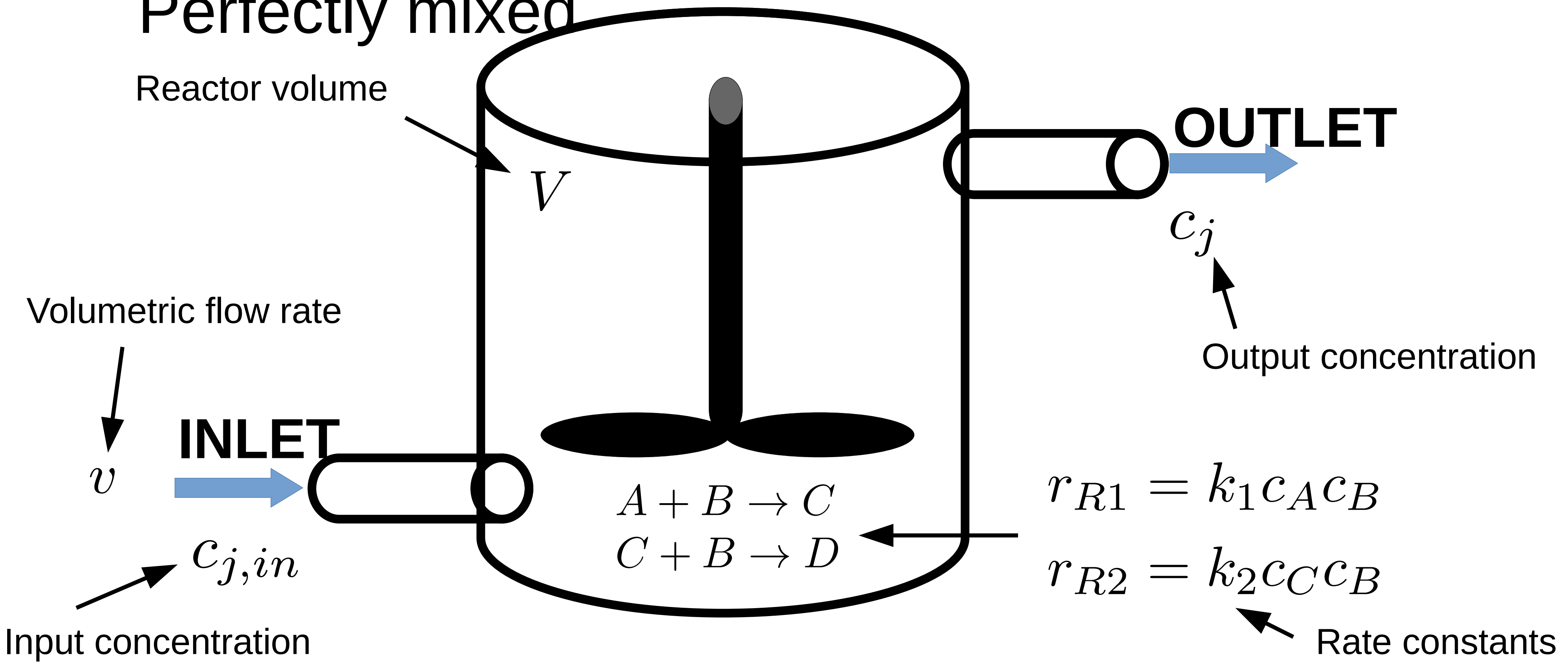
$f_2(x_1, x_2) = x_2 e^{x_1} - 2$

Ex. (5)

CSTR

Continuously Stirred-Tank Reactor

- CSTR operated isothermally, with negligible volume change, in inflow mode with constant fluid volume, and with two elementary reactions Perfectly mixed



Ex. (5)

CSTR

- Concentration of each species governed by set of mass balances

$$\frac{d}{dt}(Vc_A) = v\left(c_{A,in} - c_A\right) \quad + V\left(-k_1 c_A c_B\right)$$

$$\frac{d}{dt}(Vc_B) = v\left(c_{B,in} - c_B\right) \quad + V\left(-k_1 c_A c_B - k_2 c_C c_B\right)$$

$$\frac{d}{dt}(Vc_C) = v\left(c_{C,in} - c_C\right) \quad + V\left(+k_1 c_A c_B - k_2 c_C c_B\right)$$

$$\frac{d}{dt}(Vc_D) = v\left(c_{D,in} - c_D\right) \quad + V\left(+k_2 c_C c_B\right)$$

Inflow/Outflow Reactions

CSTR

- Concentration of each species governed by set of mass balances

Steady state $\frac{d}{dt}(Vc_j) \rightarrow 0$

$$
\begin{aligned}
0 &= v\left(c_{A,in} - c_A\right) \quad + V\left(-k_1 c_A c_B\right) \\
0 &= v\left(c_{B,in} - c_B\right) \quad + V\left(-k_1 c_A c_B - k_2 c_C c_B\right) \\
0 &= v\left(c_{C,in} - c_C\right) \quad + V\left(+k_1 c_A c_B - k_2 c_C c_B\right) \\
0 &= v\left(c_{D,in} - c_D\right) \quad + V\left(+k_2 c_C c_B\right)
\end{aligned}
$$

Set of coupled nonlinear Equations

Ex. (5)

CSTR

$$c_A = x_1 \qquad c_B = x_2 \qquad c_C = x_3 \qquad c_D = x_4$$

$$\begin{aligned}
v\left(c_{A,in} - x_1\right) + V\left(-k_1 x_1 x_2\right) &= 0 \\
v\left(c_{B,in} - x_2\right) + V\left(-k_1 x_1 x_2 - k_2 x_3 x_2\right) &= 0 \\
v\left(c_{C,in} - x_3\right) + V\left(+k_1 x_1 x_2 - k_2 x_3 x_2\right) &= 0 \\
v\left(c_{D,in} - x_4\right) + V\left(+k_2 x_3 x_2\right) &= 0
\end{aligned}$$

$$\mathbf{f}(\mathbf{x}) = \begin{pmatrix} v\left(c_{A,in} - x_1\right) + V\left(-k_1 x_1 x_2\right) \\ v\left(c_{B,in} - x_2\right) + V\left(-k_1 x_1 x_2 - k_2 x_3 x_2\right) \\ v\left(c_{C,in} - x_3\right) + V\left(+k_1 x_1 x_2 - k_2 x_3 x_2\right) \\ v\left(c_{D,in} - x_4\right) + V\left(+k_2 x_3 x_2\right) \end{pmatrix}$$

Ex. (5)

CSTR

$$c_A = x_1 \qquad c_B = x_2 \qquad c_C = x_3 \qquad c_D = x_4$$

$$\mathbf{f}(\mathbf{x}) = \begin{pmatrix} v\left(c_{A,in} - x_1\right) + V\left(-k_1 x_1 x_2\right) \\ v\left(c_{B,in} - x_2\right) + V\left(-k_1 x_1 x_2 - k_2 x_3 x_2\right) \\ v\left(c_{C,in} - x_3\right) + V\left(+k_1 x_1 x_2 - k_2 x_3 x_2\right) \\ v\left(c_{D,in} - x_4\right) + V\left(+k_2 x_3 x_2\right) \end{pmatrix}$$

$$\mathrm{D}\mathbf{f}(\mathbf{x}) = \begin{pmatrix} -v - V k_1 x_2 & -V k_1 x_1 & 0 & 0 \\ -V k_1 x_2 & -v - V k_1 x_1 - V k_2 x_3 & -V k_2 x_2 & 0 \\ V k_1 x_2 & V k_1 x_1 - V k_2 x_3 & -v - V k_2 x_2 & 0 \\ 0 & V k_2 x_3 & V k_2 x_2 & -v \end{pmatrix}$$

… Solve with Newton method!