Dynamical Systems Analysis I: Fixed Points & Linearization

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Michigan Chemical Process
Dynamics and Controls
Open Textbook

version 1.0

Creative commons

Problem: Given a large and complex system of ODEs describing the dynamics and control of your process, you want to know:

(1) Where will it go?

(2) What will it do?

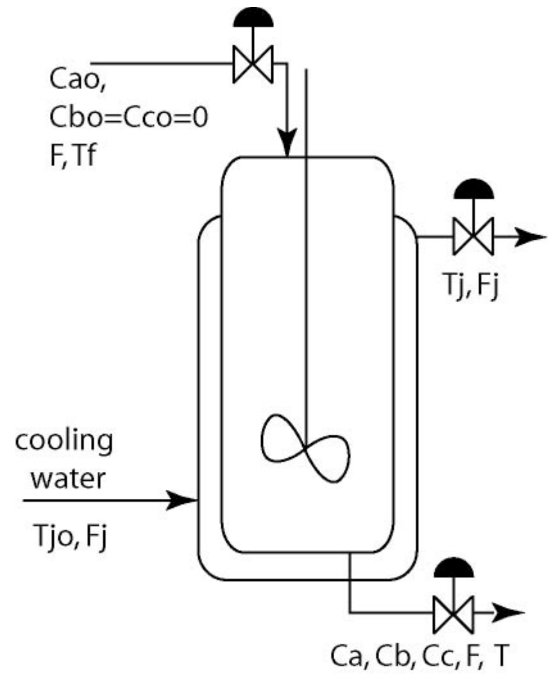
Is there anything fundamental you can say about it?

E.g. With my control architecture, this process will always _________.

Solution: Stability Analysis

Example: CSTR with cooling jacket and multiple reactions.

Reactions:
A+A --> B
B+ A --> C



$$\frac{dC_A}{dt} = \frac{F}{V}\left(C_{Af} - C_A\right) - k_1 Exp\left[\frac{-\Delta E_1}{RT}\right] C_A{}^2$$

$$\frac{dC_B}{dt} = \frac{F}{V}\left(0 - C_B\right) + k_1 Exp\left[\frac{-\Delta E_1}{RT}\right] C_A{}^2 - k_2 Exp\left[\frac{-\Delta E_2}{RT}\right] C_B C_A$$

$$\frac{dC_C}{dt} = \frac{F}{V}\left(0 - C_B\right) + k_2 Exp\left[\frac{-\Delta E_2}{RT}\right] C_B C_A$$

$$\frac{dT}{dt} = \frac{F}{V}\left(T_f - T\right) + \left[\frac{-\Delta H_1}{\rho c_p}\right] k_1 Exp\left[\frac{-\Delta E_1}{RT}\right] C_A{}^2 + \left[\frac{-\Delta H_2}{\rho c_p}\right] k_2 Exp\left[\frac{-\Delta E_2}{RT}\right] C_B C_A - \frac{UA}{V\rho c_p}\left(T - T_j\right)$$

$$\frac{dT_j}{dt} = \frac{F_j}{V_j}\left(T_{jin} - T_j\right) + \frac{UA}{V_j \rho c_p}\left(T - T_j\right)$$

Controls
PID on jacket cooling water

$$\frac{dF_j}{dt} = F_{jss} + K_c\left(T - T_{set}\right) + \frac{1}{\tau_I} x_I + \tau_D \frac{d(T - T_{set})}{dt}$$

$$\frac{dx_I}{dt} = T - T_{set}$$

What will happen?
What is possible?
What effect will my controller have?

Aside: Linear vs. Nonlinear

Linear systems are significantly easier to work with, and are the basis of stability analysis

Few physical systems are linear, but all can be locally approximated as linear.

Example:

$$\frac{dC_A}{dt} = \frac{F}{V}\left(\boxed{C_{Af}} - \boxed{C_A}\right) - \boxed{k_1 Exp\left[\frac{-\Delta E_1}{RT}\right]}\boxed{C_A^{\,2}}$$

$$\frac{dC_B}{dt} = \frac{F}{V}\left(0 - \boxed{C_B}\right) + \boxed{k_1 Exp\left[\frac{-\Delta E_1}{RT}\right]}\boxed{C_A^{\,2}} - \boxed{k_2 Exp\left[\frac{-\Delta E_2}{RT}\right]}\boxed{C_B C_A}$$

Feature: Any nonlinear terms in your model will render the whole system nonlinear, and as such harder to analyze.

Linear part

Nonlinear part

Goal: convert nonlinear system to a simpler linear system

Linear System Notation

__Linear approximation__

$$\frac{dC_A}{dt} = k_{11}C_A + k_{12}C_B + k_{13}C_C + k_{14}T + k_{15}T_j + k_{16}$$

$$\frac{dC_B}{dt} = k_{21}C_A + k_{22}C_B + k_{23}C_C + k_{24}T + k_{25}T_j + k_{26}$$

$$\frac{dC_C}{dt} = k_{31}C_A + k_{32}C_B + k_{33}C_C + k_{34}T + k_{35}T_j + k_{36}$$

$$\frac{dT}{dt} = k_{41}C_A + k_{42}C_B + k_{43}C_C + k_{44}T + k_{45}T_j + k_{46}$$

$$\frac{dT_j}{dt} = k_{51}C_A + k_{52}C_B + k_{53}C_C + k_{54}T + k_{55}T_j + k_{56}$$

$$\Rightarrow \begin{bmatrix} C'_A \\ C'_B \\ C'_C \\ T' \\ T'_J \end{bmatrix} = \begin{bmatrix} k_{11} & k_{12} & k_{13} & k_{14} & k_{15} \\ k_{21} & k_{22} & k_{23} & k_{24} & k_{25} \\ k_{31} & k_{32} & k_{33} & k_{34} & k_{35} \\ k_{41} & k_{42} & k_{43} & k_{44} & k_{45} \\ k_{51} & k_{52} & k_{53} & k_{54} & k_{55} \end{bmatrix} \begin{bmatrix} C_A \\ C_B \\ C_C \\ T \\ T_J \end{bmatrix} + \begin{bmatrix} k_{16} \\ k_{26} \\ k_{36} \\ k_{46} \\ k_{56} \end{bmatrix}$$

__Identical linear system in matrix form__

$\Uparrow$ ***How do we do this??***

__Nonlinear system__

$$\frac{dC_A}{dt} = \frac{F}{V}\left(C_{Af} - C_A\right) - k_1 Exp\left[\frac{-\Delta E_1}{RT}\right]C_A{}^2$$

$$\frac{dC_B}{dt} = \frac{F}{V}\left(0 - C_B\right) + k_1 Exp\left[\frac{-\Delta E_1}{RT}\right]C_A{}^2 - k_2 Exp\left[\frac{-\Delta E_2}{RT}\right]C_B C_A$$

$$\frac{dC_C}{dt} = \frac{F}{V}\left(0 - C_B\right) + k_2 Exp\left[\frac{-\Delta E_2}{RT}\right]C_B C_A$$

$$\frac{dT}{dt} = \frac{F}{V}\left(T_f - T\right) + \left[\frac{-\Delta H_1}{\rho c_p}\right]k_1 Exp\left[\frac{-\Delta E_1}{RT}\right]C_A{}^2 + \left[\frac{-\Delta H_2}{\rho c_p}\right]k_2 Exp\left[\frac{-\Delta E_2}{RT}\right]C_B C_A - \frac{UA}{V\rho c_p}\left(T - T_j\right)$$

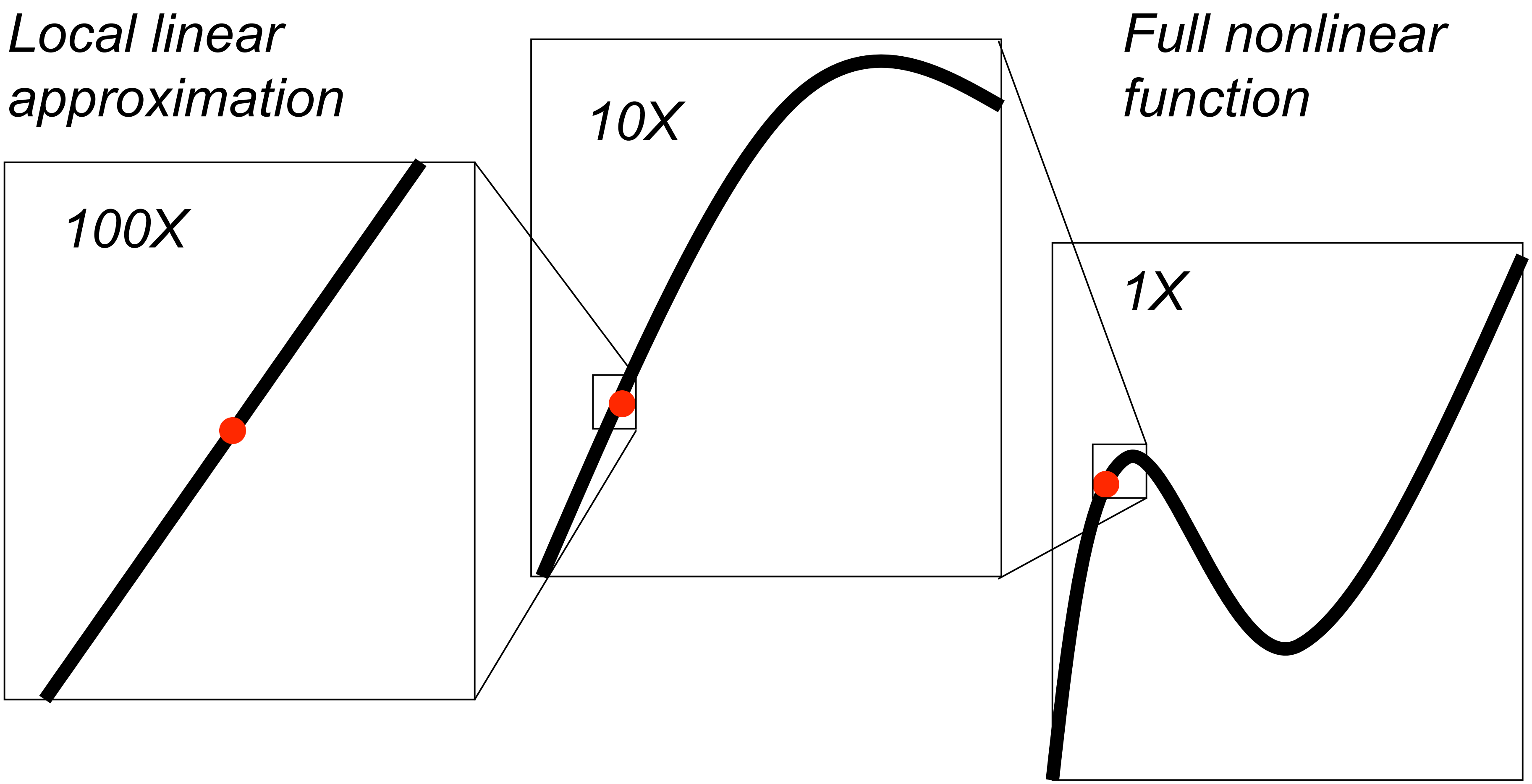
$$\frac{dT_j}{dt} = \frac{F_j}{V_j}\left(T_{jin} - T_j\right) + \frac{UA}{V_j \rho c_p}\left(T - T_j\right)$$

Linearization

1. Choose a relevant point to make your linear approximation.
2. Calculate the Jacobian matrix at that point
3. Solve to find the unknown constants

Linearization

1. Choose a relevant point to make your linear approximation.

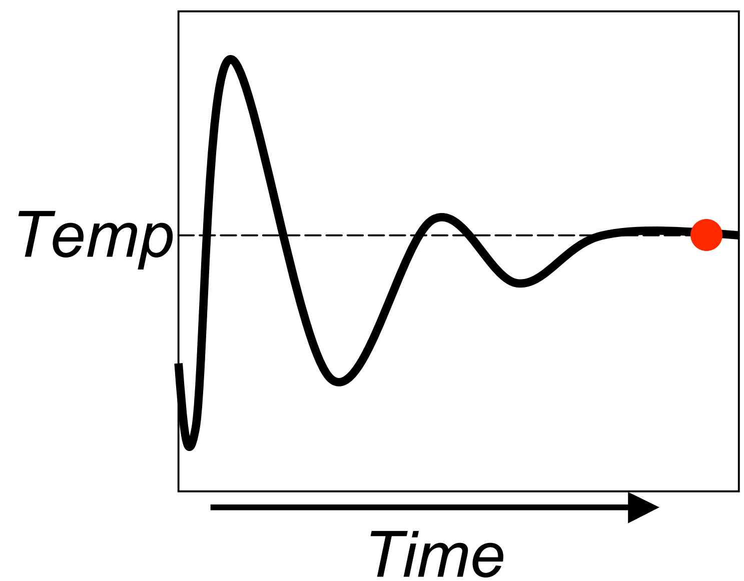


Linearization

1. Choose a relevant point to make your linear approximation.

Possible relevant points:

- ***Steady state value:*** *points where the system does not change*
- ***Current location****: given where I am now, where will I go next.*



Calculating Steady State Values

Given a system of ODEs, steady state values can be found by setting all time derivatives equal to zero and solving.

Kinetics example:

$$\frac{dA}{dt} = 3A - A^2 - AB$$

$$\frac{dB}{dt} = 2B - AB - 2B^2$$

Set derivatives equal to zero

$$0 = 3A - A^2 - AB$$

$$0 = 2B - AB - 2B^2$$

Solve for steady state values of A and B

Four solutions

{A=0,B=0} *{A=3,B=0}*

{A=0,B=1} *{A=4,B=-1}*

Calculating Steady State Values

$$0 = 3A - A^2 - AB$$

$$0 = 2B - AB - 2B^2$$

Mathematica function Solve[ ]: solves a system of algebraic expressions analytically or numerically.

```
eqns = {0 == 3 * A - A^2 - A * B, 0 == 2 * B - A * B - 2 * B^2}
Solve[eqns, {A, B}]
```

$\{0 == 3\,A - A^2 - A\,B,\ 0 == 2\,B - A\,B - 2\,B^2\}$

$\{\{A \to 0,\ B \to 0\},\ \{A \to 0,\ B \to 1\},\ \{A \to 3,\ B \to 0\},\ \{A \to 4,\ B \to -1\}\}$

Or with variables…

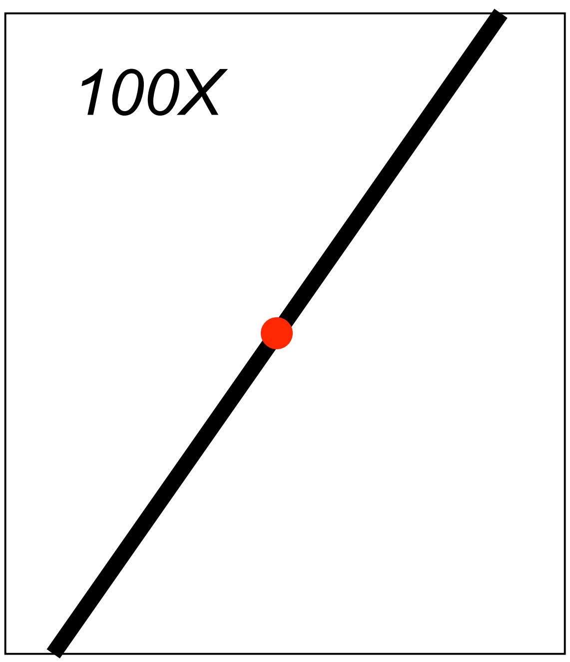
```
eqns = {0 == k1 * A - A^2 - A * B, 0 == 2 * B - A * B - k3 * B^2}
Solve[eqns, {A, B}]
```

$\{0 == -A^2 - A\,B + A\,k1,\ 0 == 2\,B - A\,B - B^2\,k3\}$

$$\left\{\{A \to 0,\ B \to 0\},\ \{A \to k1,\ B \to 0\},\ \left\{A \to -\frac{2 - k1\,k3}{-1 + k3},\ B \to -\frac{-2 + k1}{-1 + k3}\right\},\ \left\{B \to \frac{2}{k3},\ A \to 0\right\}\right\}$$

Linearization

1. Choose a relevant point to make your linear approximation.
2. Calculate the Jacobian matrix at that point



Jacobian matrix is essentially a Tailor series expansion around a point.

$$\underbrace{f(x)}_{\text{Possibly nonlinear}} \approx \underbrace{f(a) + f'(a)(x-a)}_{\text{Linear approximation}} + \text{higher order terms}$$

Calculating a Jacobian matrix

$$J = \left. \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} \end{bmatrix} \right|_{x_{1f}, x_{2f}}$$

Jacobian shows how every variable changes with each other variable at a point. Always a square matrix (rows = columns)

Example:

$$\frac{dA}{dt} = 3A - A^2 - AB$$

$$\frac{dB}{dt} = 2B - AB - 2B^2$$

$$y_1 = 3A - A^2 - AB$$

$$y_2 = 2B - AB - 2B^2$$

$$x_1 = A$$

$$x_2 = B$$

Calculating a Jacobian matrix

$$J = \begin{bmatrix} \dfrac{\partial y_1}{\partial x_1} & \dfrac{\partial y_1}{\partial x_2} \\ \dfrac{\partial y_2}{\partial x_1} & \dfrac{\partial y_2}{\partial x_2} \end{bmatrix}\Bigg|_{x_{1f},x_{2f}}$$

$$y_1 = 3A - A^2 - AB$$

$$y_2 = 2B - AB - 2B^2$$

$$x_1 = A$$

$$x_2 = B$$

{A=0,B=0}

$$J = \begin{bmatrix} \dfrac{\partial(3A - A^2 - AB)}{\partial A} & \dfrac{\partial(3A - A^2 - AB)}{\partial B} \\ \dfrac{\partial(2B - AB - 2B^2)}{\partial A} & \dfrac{\partial(2B - AB - 2B^2)}{\partial B} \end{bmatrix}\Bigg|_{A=0,B=0}$$

$$J = \begin{bmatrix} 3 - 2A - B & -A \\ -B & 2 - A - 4B \end{bmatrix}\Bigg|_{A=0,B=0} \Rightarrow J = \begin{bmatrix} 3 & 0 \\ 0 & 2 \end{bmatrix}$$

Calculating a Jacobian matrix

$$J = \left.\begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} \end{bmatrix}\right|_{x_{1f}, x_{2f}}$$

$$y_1 = 3A - A^2 - AB$$

$$y_2 = 2B - AB - 2B^2$$

$$x_1 = A$$

$$x_2 = B$$

{A=0,B=0}

Jacobian can also be solved analytically in Mathematica:

New mathematica function D[f(x,y,z}, z] = $\frac{\partial f(x,y,z)}{\partial z}$

Example:

D[A^2+BA+C+CA , A] --> 2A+B+C

Calculating a Jacobian matrix

```
e1 = 3 * A - A * A - A * B
e2 = 2 B - A * B - 2 * B ^ 2
```

$$3A - A^2 - AB$$

$$2B - AB - 2B^2$$

Original expressions

Solve for steady state

```
Solve[{e1 == 0, e2 == 0}, {A, B}]
```

$\{\{A \to 0, B \to 0\}, \{A \to 0, B \to 1\}, \{A \to 3, B \to 0\}, \{A \to 4, B \to -1\}\}$

```
Jac = {{D[e1, A], D[e1, B]}, {D[e2, A], D[e2, B]}};
```

$\{\{3 - 2A - B, -A\}, \{-B, 2 - A - 4B\}\}$

```
MatrixForm[Jac]
```

$$\begin{pmatrix} 3 - 2A - B & -A \\ -B & 2 - A - 4B \end{pmatrix}$$

Calculate Jacobian

Calculating a Jacobian matrix

```
Jac = {{D[e1, A], D[e1, B]}, {D[e2, A], D[e2, B]}}
{{3 - 2 A - B, -A}, {-B, 2 - A - 4 B}}

MatrixForm[Jac]
```

$$\begin{pmatrix} 3 - 2A - B & -A \\ -B & 2 - A - 4B \end{pmatrix}$$

Calculate Jacobian

```
a1 = Jac /. {A → 0, B → 0}
{{3, 0}, {0, 2}}
```

Substitute steady state values of A and B

$$J = \begin{bmatrix} 3 & 0 \\ 0 & 2 \end{bmatrix}$$

Note this is the same result we found by hand.

Linearization

1. Choose a relevant point to make your linear approximation.
2. Calculate the Jacobian matrix at that point
3. Solve to find the unknown constants

Nonlinear model

$$\frac{dA}{dt} = 3A - A^2 - AB$$

$$\frac{dB}{dt} = 2B - AB - 2B^2$$

$\Rightarrow$

Linear approximation

$$\begin{bmatrix} A' \\ B' \end{bmatrix} = \underbrace{\begin{bmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{bmatrix}}_{\textit{Jacobian}} \begin{bmatrix} A \\ B \end{bmatrix} + \underbrace{\begin{bmatrix} k_{13} \\ k_{23} \end{bmatrix}}_{??}$$

Nonlinear model

$$\frac{dA}{dt} = 3A - A^2 - AB$$

$$\frac{dB}{dt} = 2B - AB - 2B^2$$

$\Rightarrow$

Linear approximation

$$\begin{bmatrix} A' \\ B' \end{bmatrix} = \underbrace{\begin{bmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{bmatrix}}_{\text{Jacobian}} \begin{bmatrix} A \\ B \end{bmatrix} + \underbrace{\begin{bmatrix} k_{13} \\ k_{23} \end{bmatrix}}_{??}$$

Approach:

1) solve both models at the point A=0, B=0

$$\frac{dA}{dt} = 3(0) - (0)^2 - 0 * 0 = 0$$

$$\frac{dB}{dt} = 2 * 0 - 0 * 0 - 2(0)^2 = 0$$

$$\begin{bmatrix} A' \\ B' \end{bmatrix} = \begin{bmatrix} 3 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \end{bmatrix} + \begin{bmatrix} k_{13} \\ k_{23} \end{bmatrix}$$

2) Force derivatives of the linear and nonlinear model to agree by setting unknown constants

$k_{13} = 0 \quad k_{23} = 0$

Nonlinear model

$$\frac{dA}{dt} = 3A - A^2 - AB$$

$$\frac{dB}{dt} = 2B - AB - 2B^2$$

$\Rightarrow$

Linear approximation

$$\begin{bmatrix} A' \\ B' \end{bmatrix} = \underbrace{\begin{bmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{bmatrix}}_{\text{Jacobian}} \begin{bmatrix} A \\ B \end{bmatrix} + \underbrace{\begin{bmatrix} k_{13} \\ k_{23} \end{bmatrix}}_{??}$$

Therefore the full linear approximation at A=0, B=0 is:

$$\begin{bmatrix} A' \\ B' \end{bmatrix} = \begin{bmatrix} 3 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Or in a different format

$$\frac{dA}{dt} = 3A$$

$$\frac{dB}{dt} = 2B$$

Nonlinear model

$$\frac{dA}{dt} = 3A - A^2 - AB$$

$$\frac{dB}{dt} = 2B - AB - 2B^2$$

Linear approximation

$$\begin{bmatrix} A' \\ B' \end{bmatrix} = \underbrace{\begin{bmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{bmatrix}}_{\textit{Jacobian}} \begin{bmatrix} A \\ B \end{bmatrix} + \underbrace{\begin{bmatrix} k_{13} \\ k_{23} \end{bmatrix}}_{??}$$

Note: the unknown constants are not always 0. E.g. linear approximation at steady state A=0, B=1

$$\underbrace{\frac{dA}{dt} = 3(0) - (0)^2 - 0*1 = 0 \qquad \frac{dB}{dt} = 2*1 - 0*1 - 2(1)^2 = 0}_{\textit{By definition will always be zero for a fixed point.}}$$

$$\begin{bmatrix} A' \\ B' \end{bmatrix} = \underbrace{\begin{bmatrix} 2 & 0 \\ -1 & -2 \end{bmatrix}}_{\substack{\textit{Jacobian} \\ \textit{At A=0, B=1}}} \begin{bmatrix} 0 \\ 1 \end{bmatrix} + \begin{bmatrix} k_{13} \\ k_{23} \end{bmatrix}$$

<u>Linear algebra aside</u>: How to solve this?

$$\begin{bmatrix} A' \\ B' \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ -1 & -2 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} + \begin{bmatrix} k_{13} \\ k_{23} \end{bmatrix}$$

1) Convert to a more familiar algebraic expression using matrix multiplication

$$\frac{dA}{dt} = 2*0 + 0*1 + k_{13}$$

$$\frac{dB}{dt} = -1*0 - 2*1 + k_{23}$$

$\Rightarrow$ *Substitute in derivatives from nonlinear expression*

$$0 = 2*0 + 0*1 + k_{13}$$

$$0 = -1*0 - 2*1 + k_{23}$$

2) Solve

$k_{13}=0$, $k_{23}=2$

Nonlinear model

$$\frac{dA}{dt} = 3A - A^2 - AB$$

$$\frac{dB}{dt} = 2B - AB - 2B^2$$

$\Rightarrow$

Linear approximation

$$\begin{bmatrix} A' \\ B' \end{bmatrix} = \underbrace{\begin{bmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{bmatrix}}_{\text{Jacobian}} \begin{bmatrix} A \\ B \end{bmatrix} + \underbrace{\begin{bmatrix} k_{13} \\ k_{23} \end{bmatrix}}_{??}$$

Therefore the full linear approximation at A=0, B=1 is:

$$\begin{bmatrix} A' \\ B' \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ -1 & -2 \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} + \begin{bmatrix} 0 \\ 2 \end{bmatrix}$$

Or in a different format

$$\frac{dA}{dt} = 2A$$

$$\frac{dB}{dt} = -A - 2B + 2$$

Take Home Messages

- Nonlinear models are more realistic but harder to manipulate
- Any nonlinear model can be approximated as a linear one at a point
- The linear approximation is exactly correct at the point, but less accurate away from the point.