# 10.34: Numerical Methods Applied to Chemical Engineering

Lecture 7:
Solutions of nonlinear equations
Newton-Raphson method

# Recap

- Singular value decomposition
- Iterative solutions to linear equations

# Recap

- Iterative solutions to linear equations
    - Given: $\mathbf{x}_0$
    - Iterate on: $\mathbf{x}_{i+1} = \mathbf{C}\mathbf{x}_i + \mathbf{c}$
    - Until converged to solution of: $\mathbf{A}\mathbf{x} = \mathbf{b}$

- Assume the iterations converge. When should I stop?

# Systems of Nonlinear Eqns.

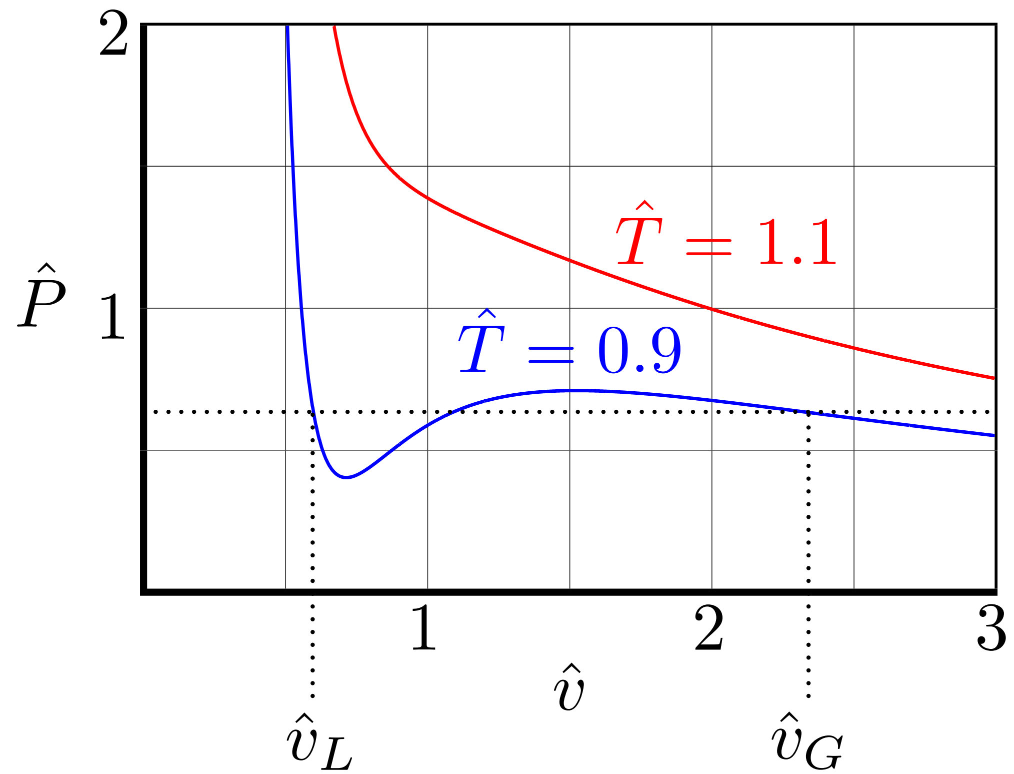
- Formally: $\mathbf{f}(\mathbf{x}) = 0$
  - where: $\mathbf{x} \in \mathbb{R}^N$
  - where: $\mathbf{f} : \mathbb{R}^N \to \mathbb{R}^N$
  - $\mathbf{x}$ are called the roots of $\mathbf{f}(\mathbf{x})$
  - linear equations are represented as $\mathbf{f}(\mathbf{x}) = \mathbf{A}\mathbf{x} - \mathbf{b}$
- Common chemical engineering examples include:
  - Equations of state
  - Energy balances
  - Mass balances with nonlinear reactions

# Systems of Nonlinear Eqns.

- Example: van der Waals equation of state

$$\left(\hat{P} + \frac{3}{\hat{v}^2}\right)\left(\hat{v} - \frac{1}{3}\right) = \frac{8}{3}\hat{T}$$

  - $\hat{P},\ \hat{T},\ \hat{v}$ are reduced pressure, temperature, and molar volume




- Given pressure and temperature, there are 1-3 molar volumes that satisfy the equation of state.

# Systems of Nonlinear Eqns.

- Example: van der Waals equation of state

$$\left(\hat{P} + \frac{3}{\hat{v}^2}\right)\left(\hat{v} - \frac{1}{3}\right) = \frac{8}{3}\hat{T}$$

  - Given pressure and temperature, 1, 2 or 3 solutions for molar volume possible.

$$f(\hat{v};\hat{P},\hat{T}) = \left(\hat{P} + \frac{3}{\hat{v}^2}\right)\left(\hat{v} - \frac{1}{3}\right) - \frac{8}{3}\hat{T} = 0$$

  - In general, nonlinear equations can have any number of solutions. It is impossible to predict beforehand.

  - For gas-liquid coexistence, can the pressure and temperature be specified independently?

# Systems of Nonlinear Eqns.

- Example: van der Waals equation of state
  - For gas-liquid coexistence, can the pressure and temperature be specified independently?
    - No!
    - Thermal equil. – same temperature in gas/liquid

$$\hat{T}_G = \hat{T}_L = \hat{T}$$

    - Mechanical equil. – same pressure in gas/liquid

$$\hat{P}_G = \hat{P}_L = \hat{P}_{\mathrm{sat}}$$

    - Chemical equil. – same chemical potential in gas/liquid

$$\int_{\hat{v}_G}^{\hat{v}_L} (\hat{P}(\hat{v}) - \hat{P}_{\mathrm{sat}})\, d\hat{v} = 0$$

# Systems of Nonlinear Eqns.

- Example: van der Waals equation of state
  - For gas-liquid coexistence, can the pressure and temperature be specified independently?
    - Given the temperature, there are 3 unknowns
      - The saturation pressure
      - The molar volumes of the gas and liquid
    - There are three nonlinear equations to solve:
      - Equation of state in gas/liquid
      - Maxwell equal area construction
  - Must solve: $\mathbf{f}(\hat{P}_{\rm sat}, \hat{v}_G, \hat{v}_L) = 0$

# Systems of Nonlinear Eqns.

- Example: van der Waals equation of state
    - Must solve: $\mathbf{f}(\hat{P}_{\text{sat}}, \hat{v}_G, \hat{v}_L) = 0$

$$f_1(\hat{P}_{\text{sat}}, \hat{v}_G, \hat{v}_L) = \left(\hat{P}_{\text{sat}} + \frac{3}{\hat{v}_G^2}\right)\left(\hat{v}_G - \frac{1}{3}\right) - \frac{8}{3}\hat{T} = 0$$

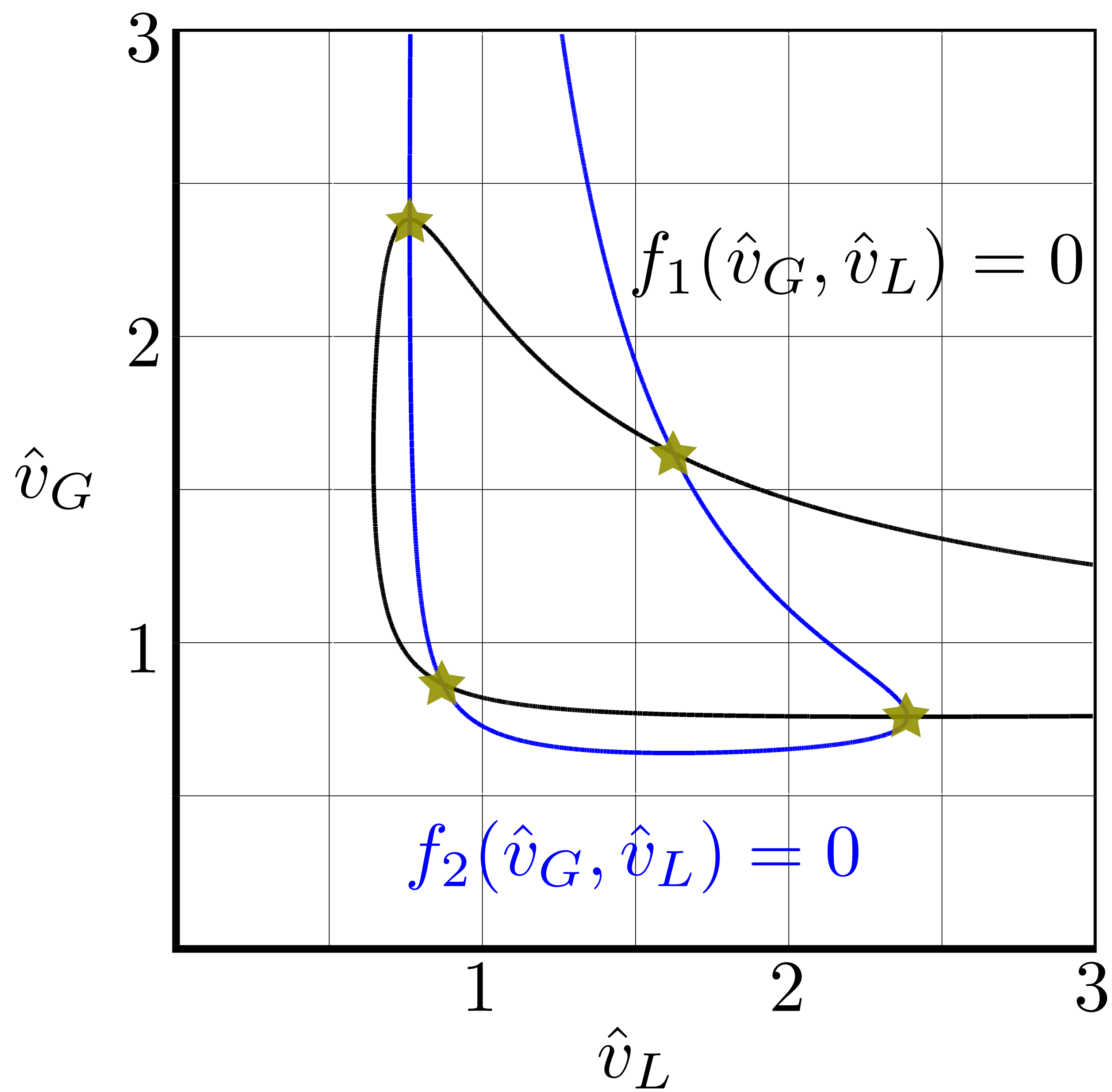
$$f_2(\hat{P}_{\text{sat}}, \hat{v}_G, \hat{v}_L) = \left(\hat{P}_{\text{sat}} + \frac{3}{\hat{v}_L^2}\right)\left(\hat{v}_L - \frac{1}{3}\right) - \frac{8}{3}\hat{T} = 0$$

$$f_3(\hat{P}_{\text{sat}}, \hat{v}_G, \hat{v}_L) = \int_{\hat{v}_G}^{\hat{v}_L} (\hat{P}(\hat{v}) - \hat{P}_{\text{sat}})\, d\hat{v} = 0$$

# Systems of Nonlinear Eqns.

- Example: van der Waals equation of state
  - Use $\hat{P}_{\text{sat}} = \frac{1}{\hat{v}_L - \hat{v}_G} \int_{\hat{v}_G}^{\hat{v}_L} \hat{P}(\hat{v}) d\hat{v}$ to eliminate $\hat{P}_{\text{sat}}$ from:

$$f_1(\hat{P}_{\text{sat}}, \hat{v}_G, \hat{v}_L), f_2(\hat{P}_{\text{sat}}, \hat{v}_G, \hat{v}_L),$$



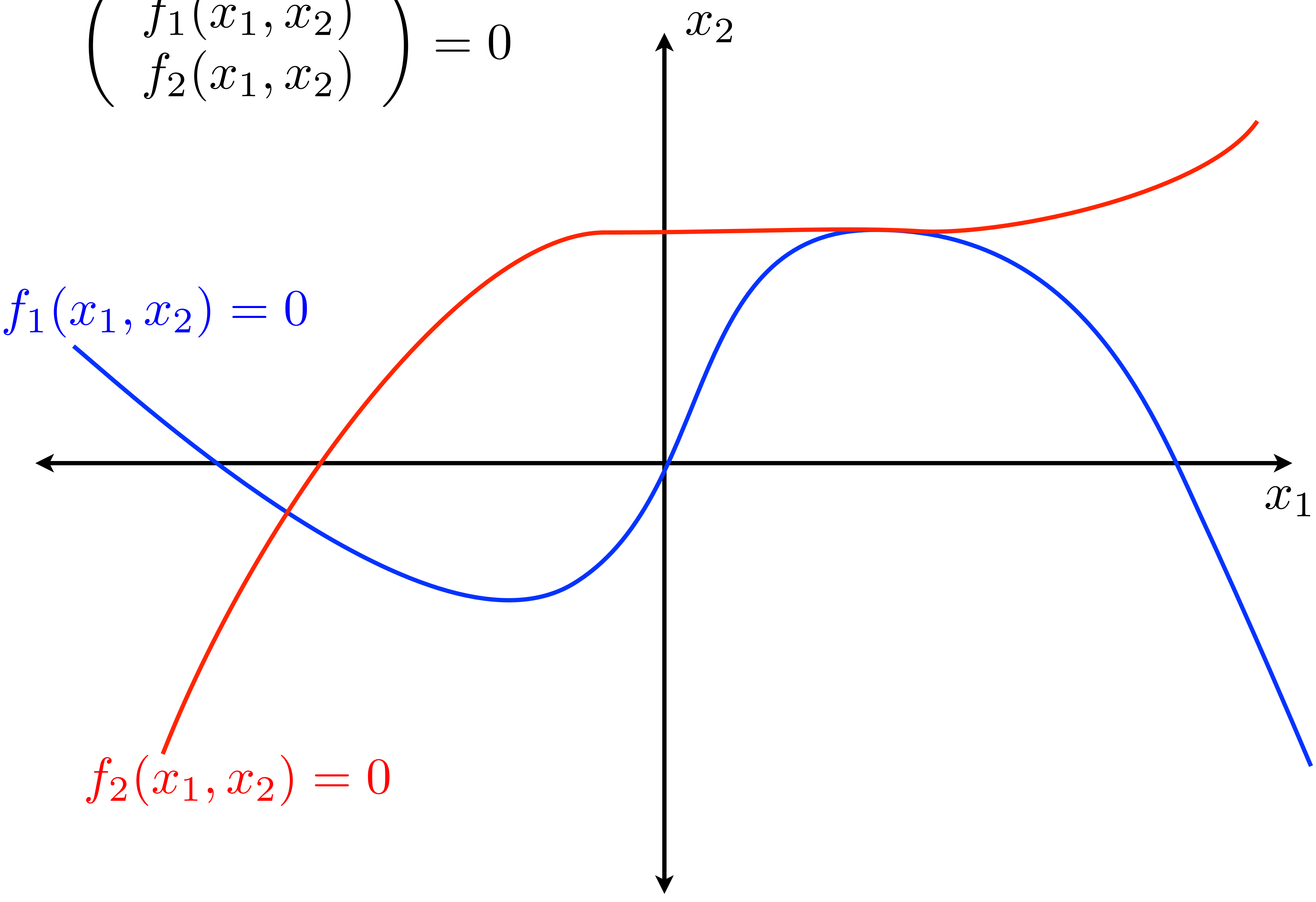
# Systems of Nonlinear Eqns.

- Given: $\mathbf{f} : \mathbb{R}^N \to \mathbb{R}^N$
- Find: $\mathbf{x}^* \in \mathbb{R}^N : \mathbf{f}(\mathbf{x}^*) = 0$
  - There could be no solutions
  - There could be $1 < n < \infty$ locally unique solutions
  - There could be $\infty$ solutions
- A solution, $\mathbf{x}^*$, is locally unique if there exists a ball of finite radius such that $\mathbf{x}^*$ is the only solution within the ball.
- Consider the simple function:

$$\begin{pmatrix} f_1(x_1, x_2) \\ f_2(x_1, x_2) \end{pmatrix} = 0$$

# Systems of Nonlinear Eqns.

$$\begin{pmatrix} f_1(x_1, x_2) \\ f_2(x_1, x_2) \end{pmatrix} = 0$$



# Systems of Nonlinear Eqns.

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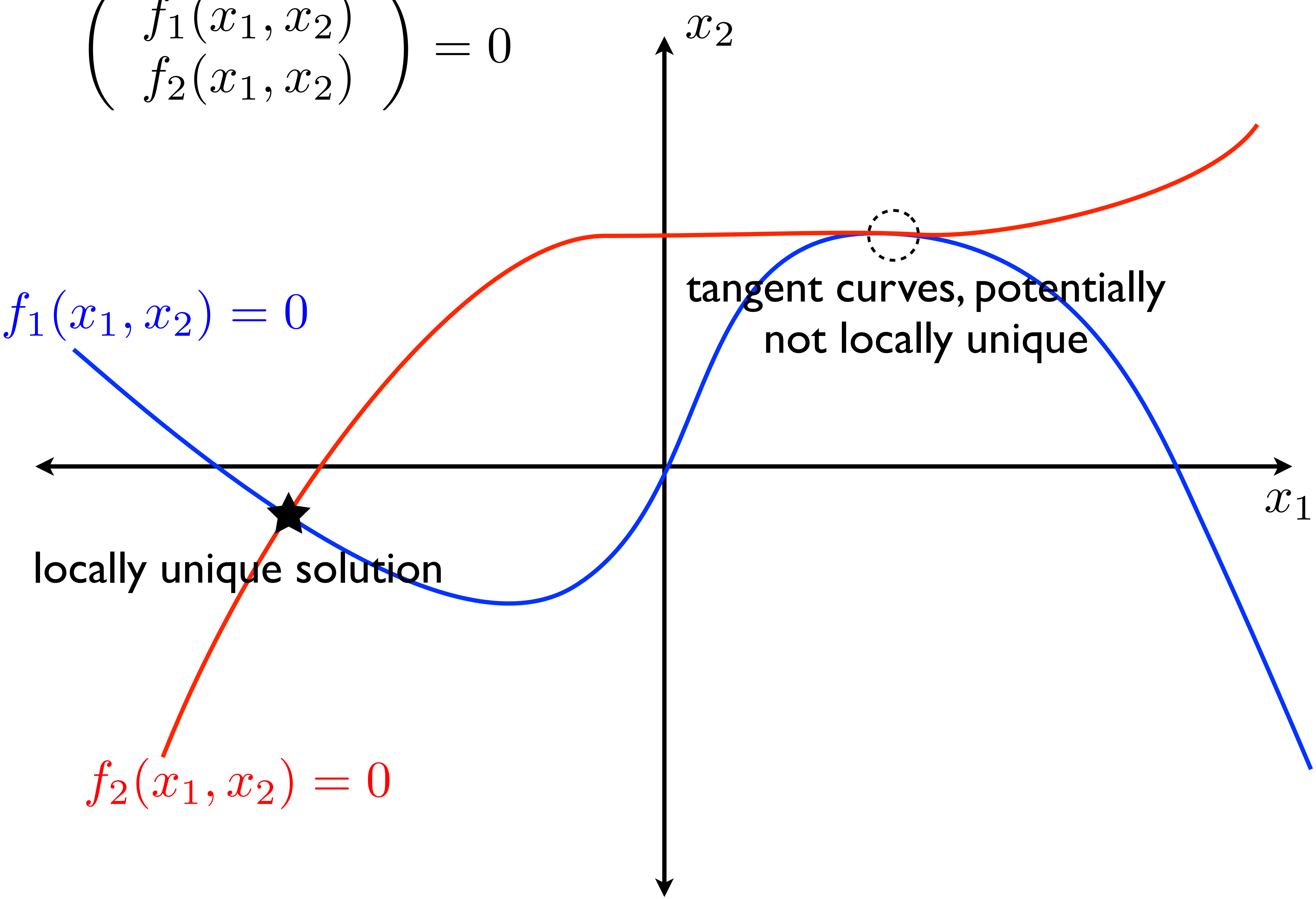


# Systems of Nonlinear Eqns.

- Inverse function theorem:
  - If $\mathbf{f}(\mathbf{x}^*) = 0$ and $\det \mathbf{J}(\mathbf{x}^*) \neq 0$,
  - then $\mathbf{x}^*$ is a locally unique solution,
  - where the Jacobian is:

$$\mathbf{J}(\mathbf{x}) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_N}{\partial x_1} & \frac{\partial f_N}{\partial x_2} & \cdots & \frac{\partial f_N}{\partial x_N} \end{pmatrix}$$

- The Jacobian describes the rate of change of a vector function with respect to all of its independent variables.
- If $\det \mathbf{J}(\mathbf{x}^*) = 0$, solution may/may not be locally unique
- Most numerical methods can only find one locally unique solution at a time.

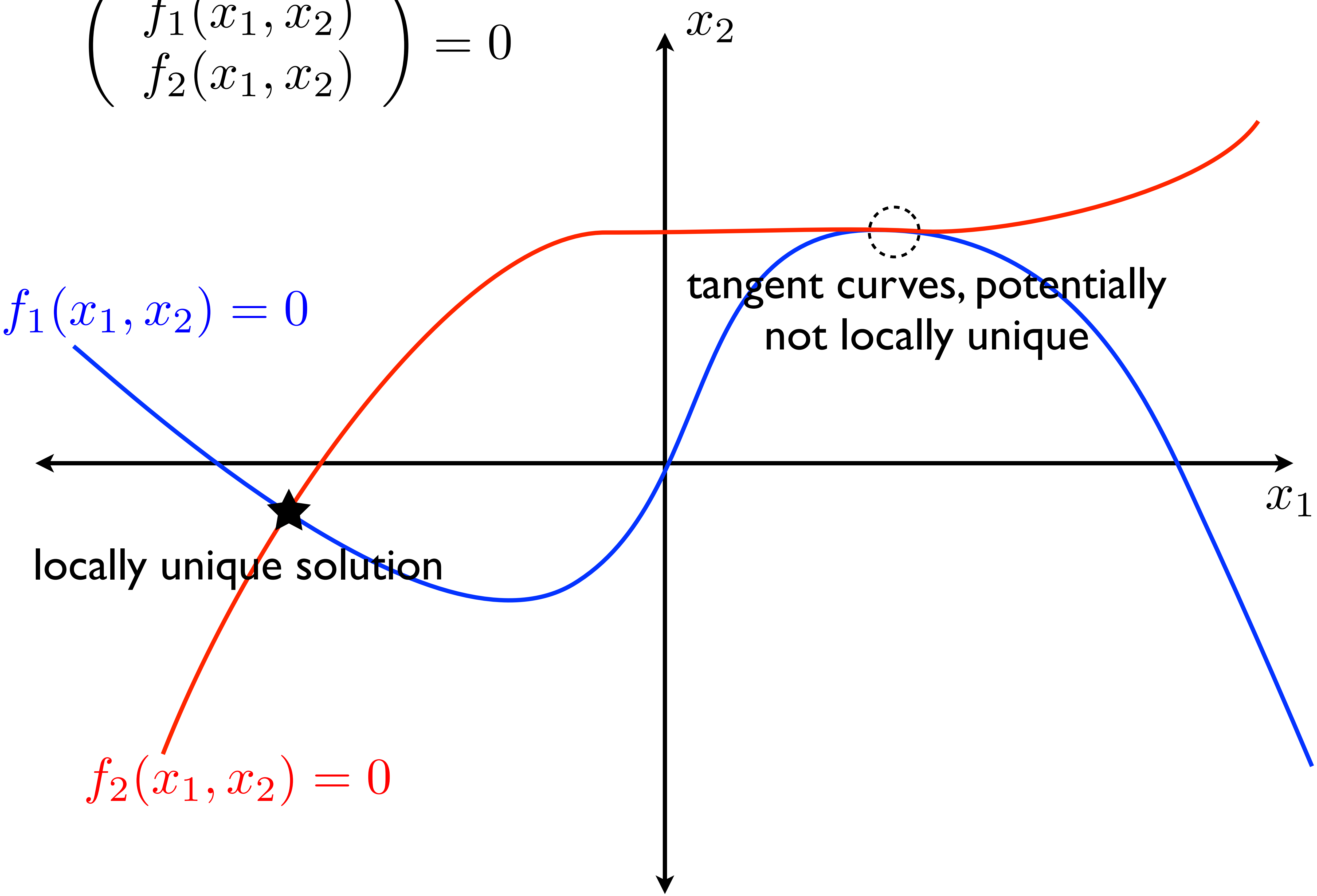
# Systems of Nonlinear Eqns.

- Example:
  - Compute the Jacobian of:

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

# Systems of Nonlinear Eqns.

$$\begin{pmatrix} f_1(x_1, x_2) \\ f_2(x_1, x_2) \end{pmatrix} = 0$$



# Systems of Nonlinear Eqns.

- Inverse function theorem:
  - Consider a linear equation: $\mathbf{f}(\mathbf{x}) = \mathbf{A}\mathbf{x} - \mathbf{b}$
  - The Jacobian of the function is:

    $$\mathbf{J}(\mathbf{x}) = \mathbf{A}$$

  - The equation: $\mathbf{f}(\mathbf{x}) = 0$, has a locally unique solution when $\det \mathbf{J}(\mathbf{x}) = \det \mathbf{A} \neq 0$
  - There is a locally unique solution when $\mathbf{A}$ is invertible
- The inverse function theorem is just a generalization of what we learned in our study of linear algebra.
- In fact, in a neighborhood close to a root of $\mathbf{f}(\mathbf{x})$, we can often treat the function as linear!

# Linearization

- Linearizing 1-D nonlinear functions:
  - $f(x + \Delta x) = f(x) + f'(x)\Delta x + O(\Delta x^2)$
  - typically valid as $\Delta x \to 0$
- Linearizing generalized nonlinear functions:
  - $\mathbf{f}(\mathbf{x} + \Delta \mathbf{x}) = \mathbf{f}(\mathbf{x}) + \mathbf{J}(\mathbf{x})\Delta \mathbf{x} + O(\|\Delta \mathbf{x}\|_2^2)$
  - typically valid as $\|\Delta \mathbf{x}\|_2 \to 0$
- Part of a Taylor expansion for each component of $\mathbf{f}(\mathbf{x})$:

$$f_i(\mathbf{x} + \Delta \mathbf{x}) = f_i(\mathbf{x}) + \sum_{j=1}^{N} \frac{\partial f_i(\mathbf{x})}{\partial x_j} \Delta x_j$$

$$+ \frac{1}{2} \sum_{j=1}^{N} \sum_{k=1}^{N} \frac{\partial^2 f_i(\mathbf{x})}{\partial x_j \partial x_k} \Delta x_j \Delta x_k + \ldots$$

# Iterative Solutions to NLEs

- Nonlinear equations, $\mathbf{f}(\mathbf{x}^*) = 0$, are solved iteratively
- The algorithmic map: $\mathbf{x}_{i+1} = \mathbf{g}(\mathbf{x}_i)$ , is designed so that:
  - $\mathbf{x}^* = \mathbf{g}(\mathbf{x}^*)$
  - equivalently, $\mathbf{x}^*$ is a fixed point of the map, $\mathbf{g}(\mathbf{x})$
- Iterations stop when the map is sufficiently converged.
- Two common criterion for stopping are:
  - Function norm criterion:

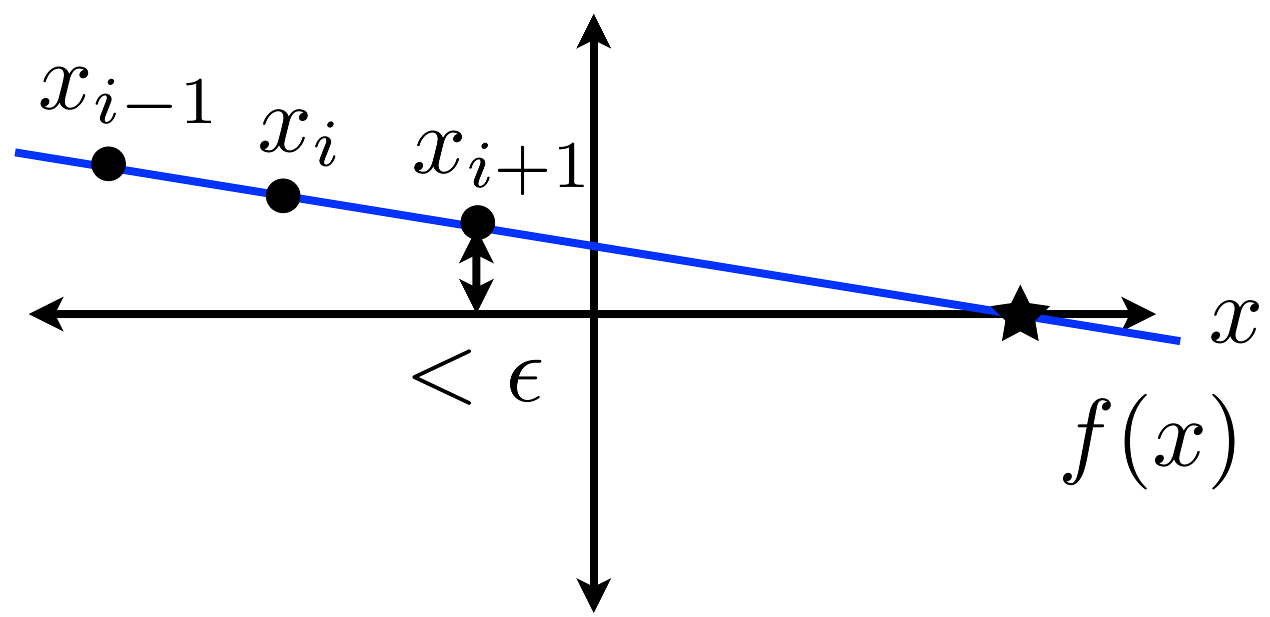
    $$\|\mathbf{f}(\mathbf{x}_{i+1})\|_p \leq \epsilon$$

  - Step norm criterion:

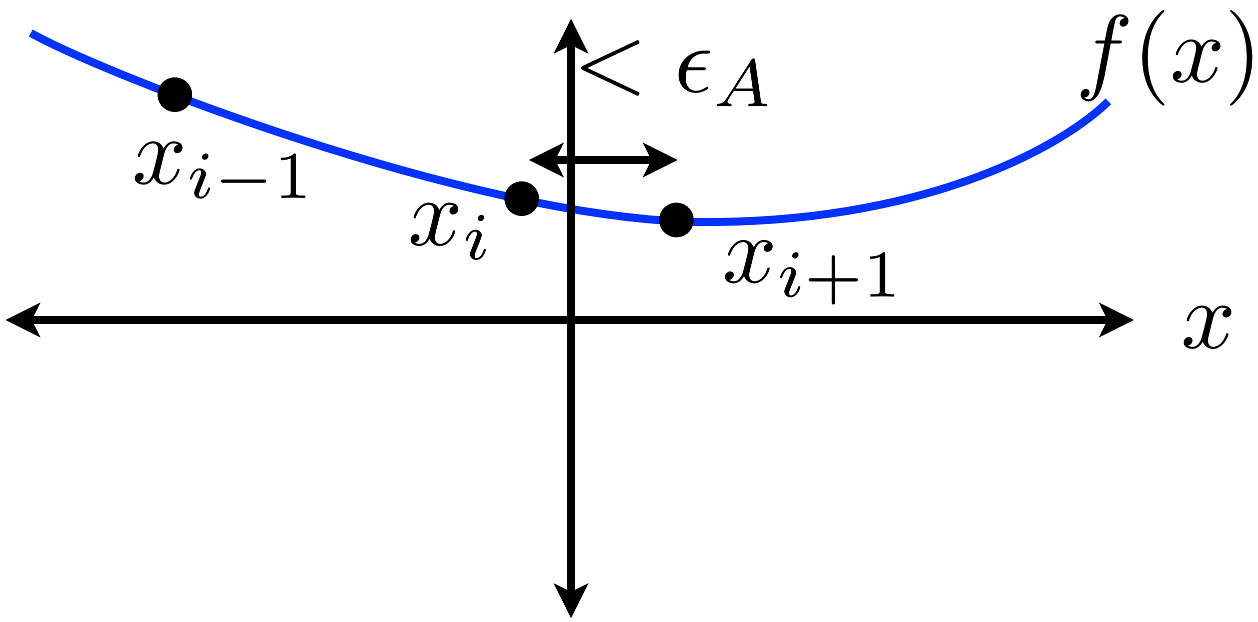
    $$\|\mathbf{x}_{i+1} - \mathbf{x}_i\|_p \leq \epsilon_R \|\mathbf{x}_{i+1}\|_p + \epsilon_A$$

# Iterative Solutions to NLEs

- Failure of function norm criterion:




- Failure of step norm criterion:



# Convergence Rate

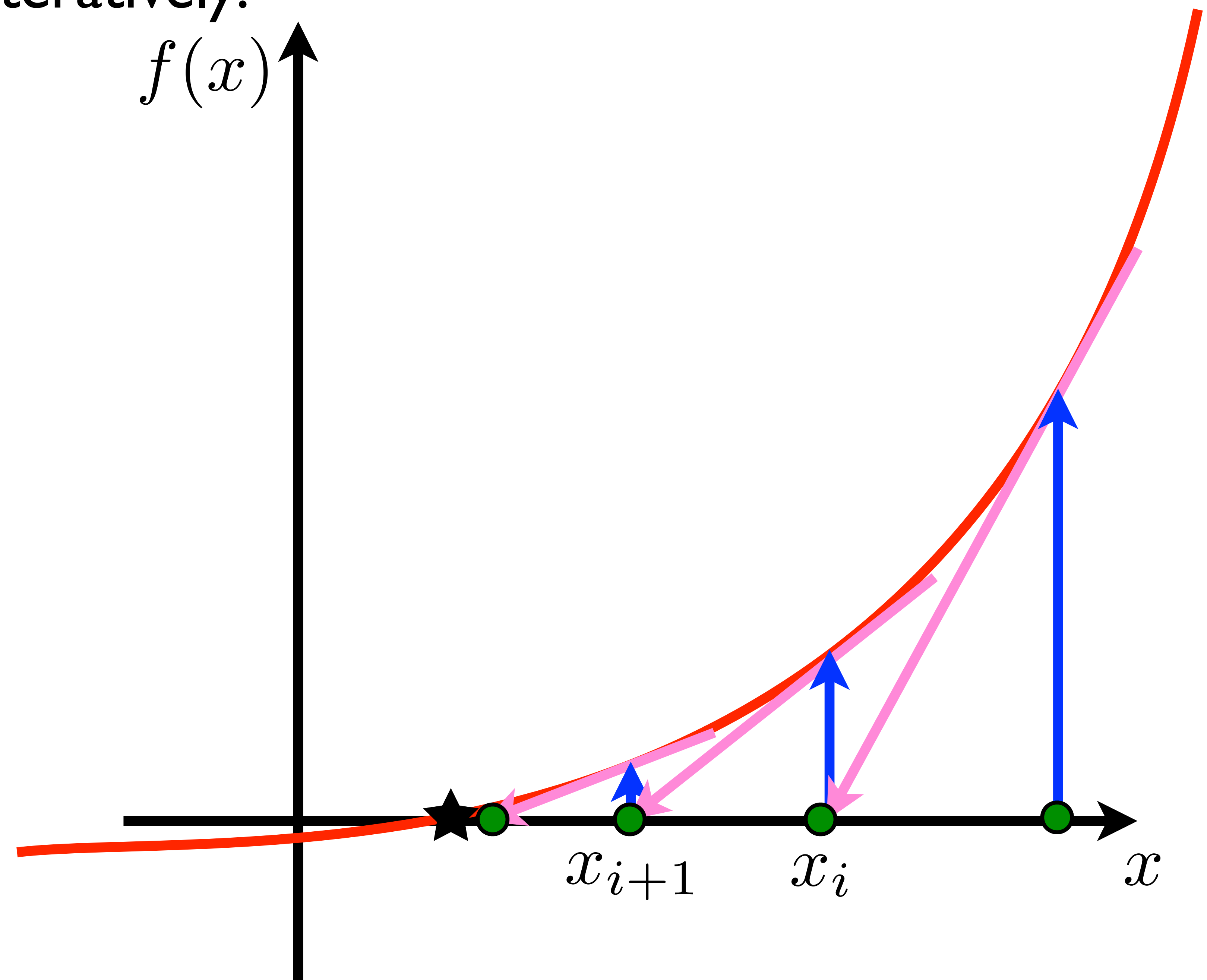
- The rate of convergence is addressed by examining:

$$\lim_{k\to\infty} \frac{\|\mathbf{x}_{i+1} - \mathbf{x}^*\|_p}{\|\mathbf{x}_i - \mathbf{x}^*\|_p^q} = C$$

  - when the limit exists and is not zero:
    - $q = 1, C < 1$, convergence is linear
      - If $C = 10^{-1}$ each iteration is 1 digit more accurate than the previous
    - $q > 1$, convergence is super-linear
    - $q = 2$, convergence is quadratic
      - The number of accurate digits doubles with each iteration.
- Jacobi and Gauss-Seidel showed linear convergence rates

# Newton-Raphson Method

- Utilize linear approximations of the function to find a root iteratively:




$$f(x_{i+1}) \approx 0 = f(x_i) + f'(x_i)(x_{i+1} - x_i)$$

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

# Newton-Raphson Method

- When the iterate is sufficiently close to the root, convergence is guaranteed (local convergence)!
- Extending this idea to systems nonlinear equations is easy:
  - Approximate the function as linear:

$$\mathbf{f}(\mathbf{x}_{i+1}) \approx 0 = \mathbf{f}(\mathbf{x}_i) + \mathbf{J}(\mathbf{x}_i)(\mathbf{x}_{i+1} - \mathbf{x}_i)$$

$$\mathbf{f}(\mathbf{x}_{i+1}) \approx 0 = \mathbf{f}(\mathbf{x}_i) + \mathbf{J}(\mathbf{x}_i)\mathbf{d}_i$$

  - Solve for the displacement:

$$\mathbf{J}(\mathbf{x}_i)\mathbf{d}_i = -\mathbf{f}(\mathbf{x}_i) \Rightarrow \mathbf{d}_i = -[\mathbf{J}(\mathbf{x}_i)]^{-1}\mathbf{f}(\mathbf{x}_i)$$

  - Update the iterate:

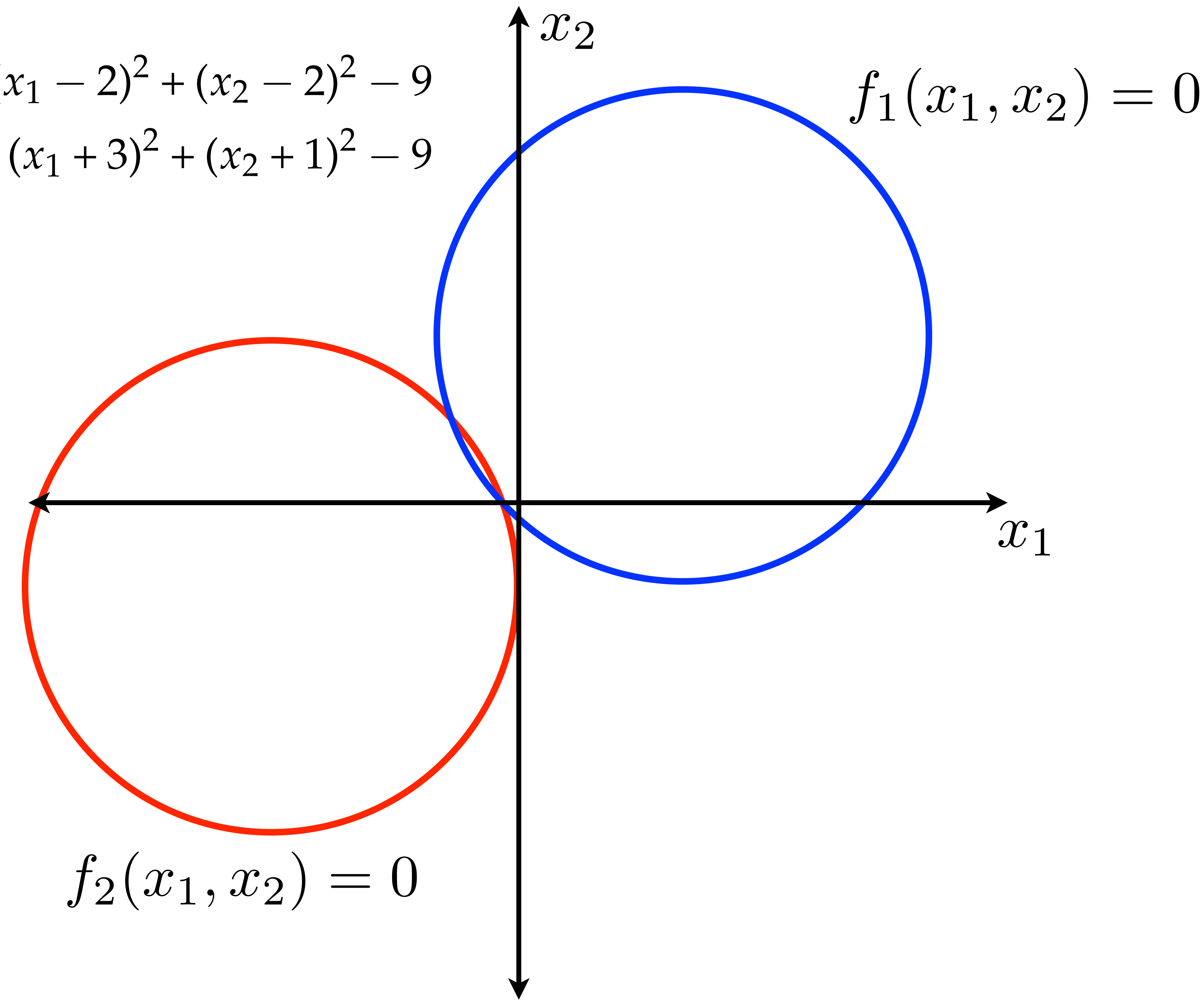
$$\mathbf{x}_{i+1} = \mathbf{x}_i + \mathbf{d}_i$$

$$\mathbf{x}_{i+1} = \mathbf{x}_i - [\mathbf{J}(\mathbf{x}_i)]^{-1}\mathbf{f}(\mathbf{x}_i)$$

# Newton-Raphson Method

- Example: the intersection of circles

$$0 = f_1(x_1, x_2) = (x_1 - 2)^2 + (x_2 - 2)^2 - 9$$
$$0 = f_2(x_1, x_2) = (x_1 + 3)^2 + (x_2 + 1)^2 - 9$$



# Newton-Raphson Method

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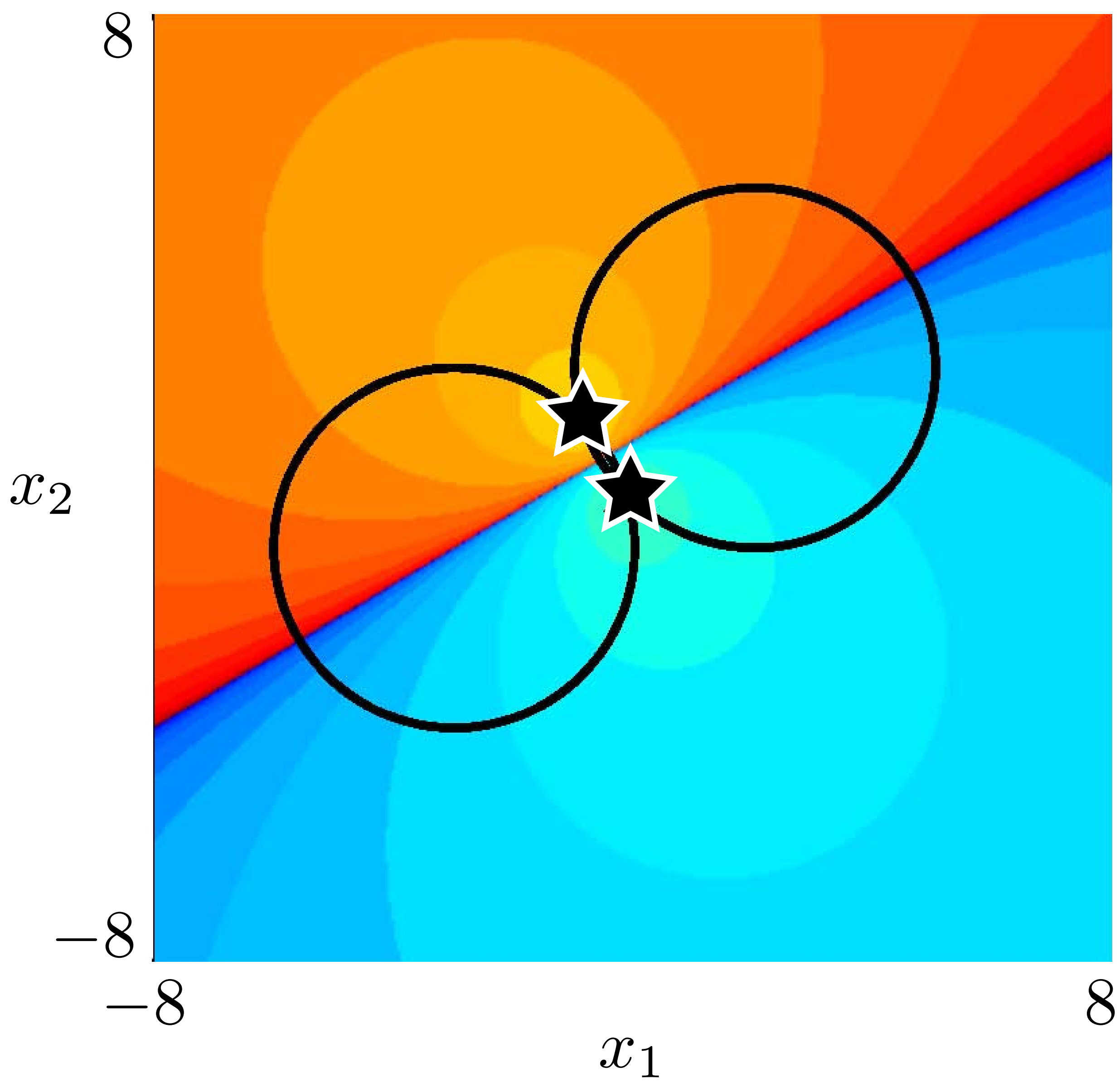
$$0 = f_1(x_1, x_2) = (x_1 - 2)^2 + (x_2 - 2)^2 - 9$$
$$0 = f_2(x_1, x_2) = (x_1 + 3)^2 + (x_2 + 1)^2 - 9$$

$$\boldsymbol{J}(\boldsymbol{x}) = \left( \qquad \qquad \qquad \right)$$

| $k$ | $\boldsymbol{x}^{(k)}$ | $\boldsymbol{f}(\boldsymbol{x}^{(k)})$ | $\lVert\boldsymbol{x}^{(k)} - \boldsymbol{x}^{(k-1)}\rVert_2$ | $\lVert\boldsymbol{f}(\boldsymbol{x}^{(k)})\rVert_2$ |
|---|---|---|---|---|
| 0 | $(-1.00, 3.00)$ | $(1.00, 11.0)$ | | 11.1 |
| 1 | $(-1.25, 1.75)$ | $(1.63, 1.63)$ | 0.556 | 2.30 |
| 2 | $(-0.963, 1.27)$ | $(0.310, 0.310)$ | 0.173 | 0.439 |
| 3 | $(-0.875, 1.124)$ | $(0.030, 0.030)$ | 0.020 | 0.042 |
| 4 | $(-0.864, 1.101)$ | $(0.004, 0.004)$ | 0.003 | 0.006 |

# Newton-Raphson Method

- Example: the intersection of circles




$$\det\left(\boldsymbol{J}(\boldsymbol{x})\right) = 4(x_1 - 2)(x_2 + 1) - 4(x_2 - 2)(x_1 + 3)$$

- Notice that convergence is slowest near where $\det \mathbf{J}(\mathbf{x}) = 0$

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Fall 2015