# 10.34: Numerical Methods Applied to Chemical Engineering

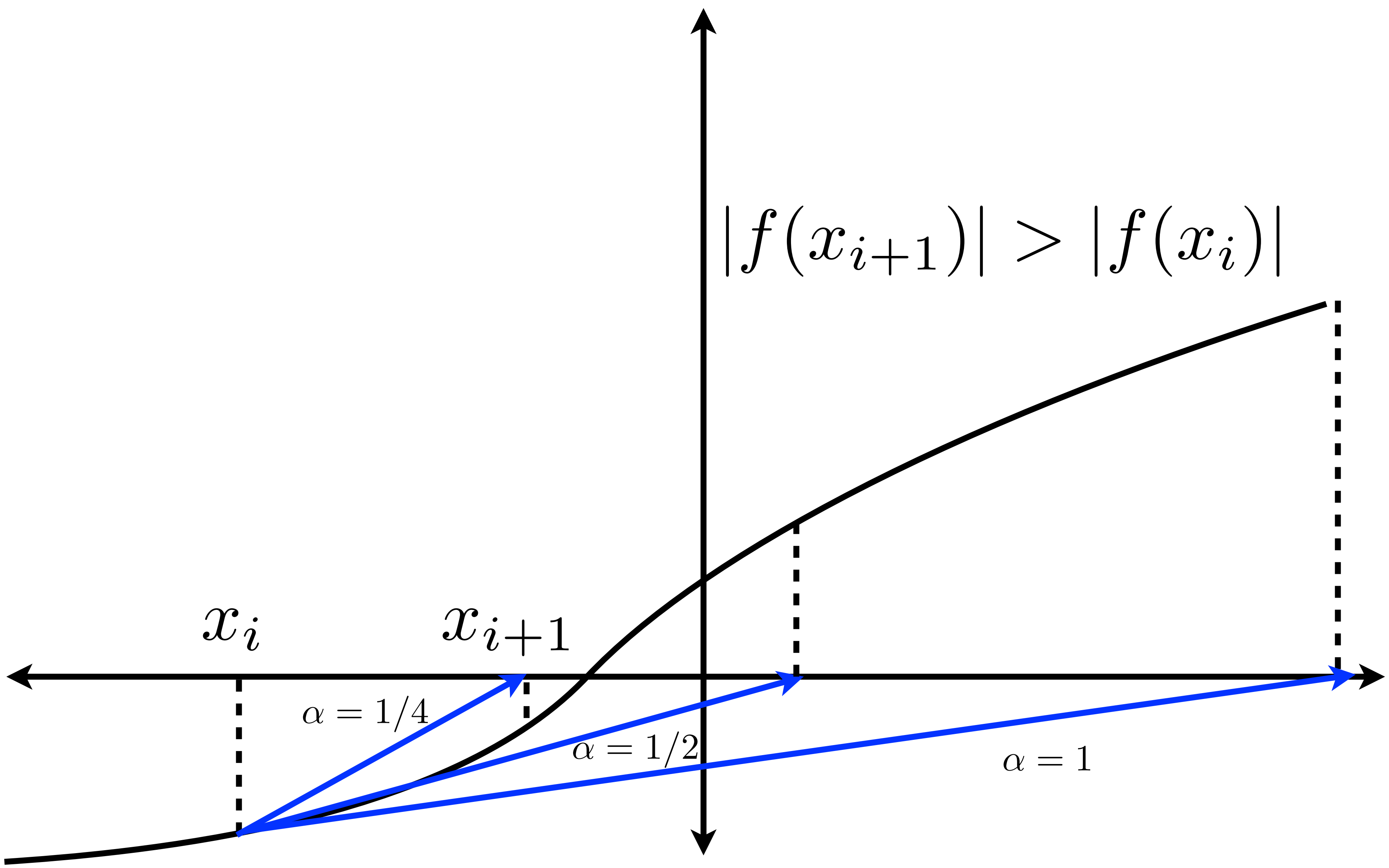
Lecture 9:
Homotopy and bifurcation

# Recap

- Quasi-Newton-Raphson methods

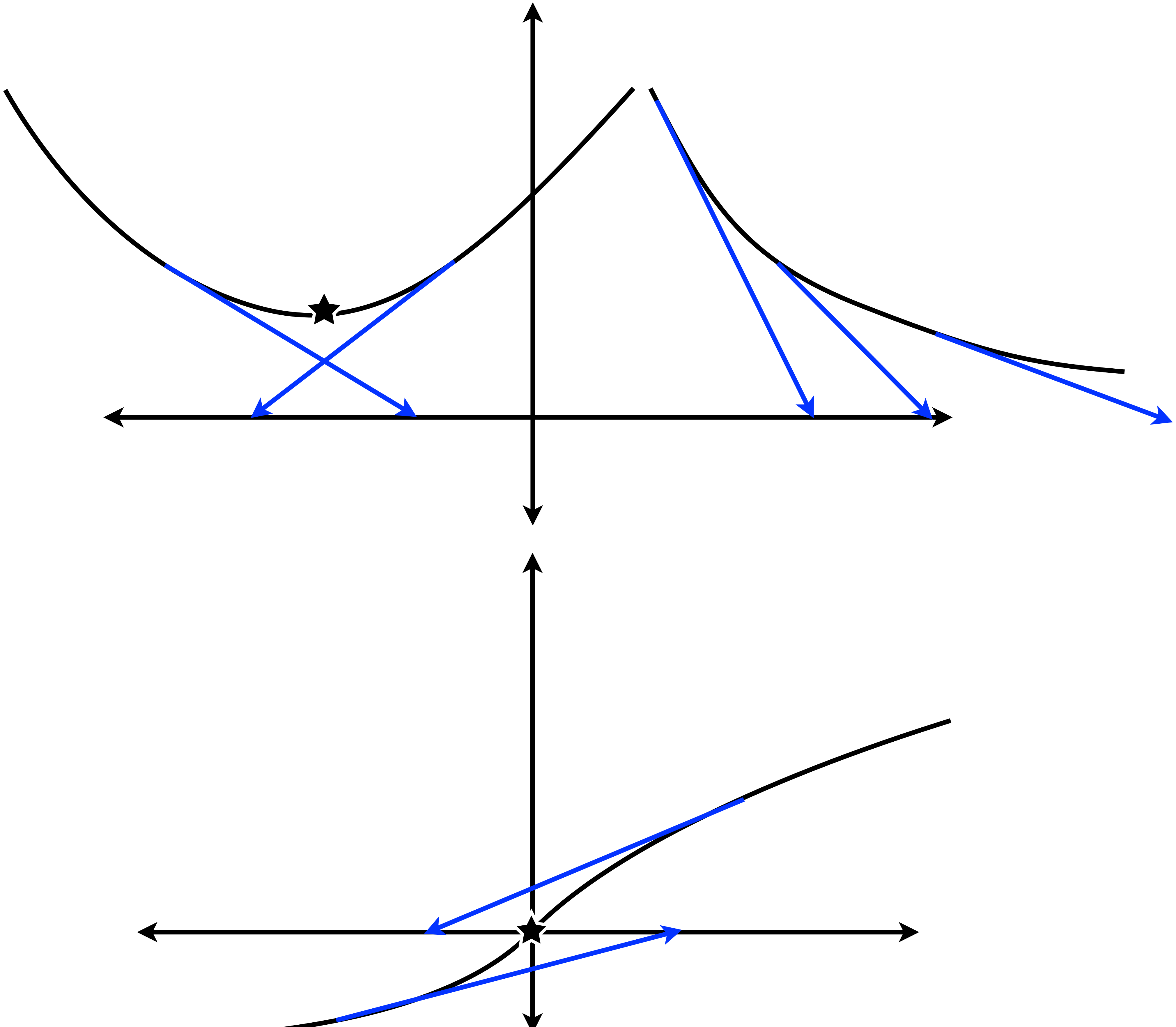
# Recap

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




backtracking line search

# Recap

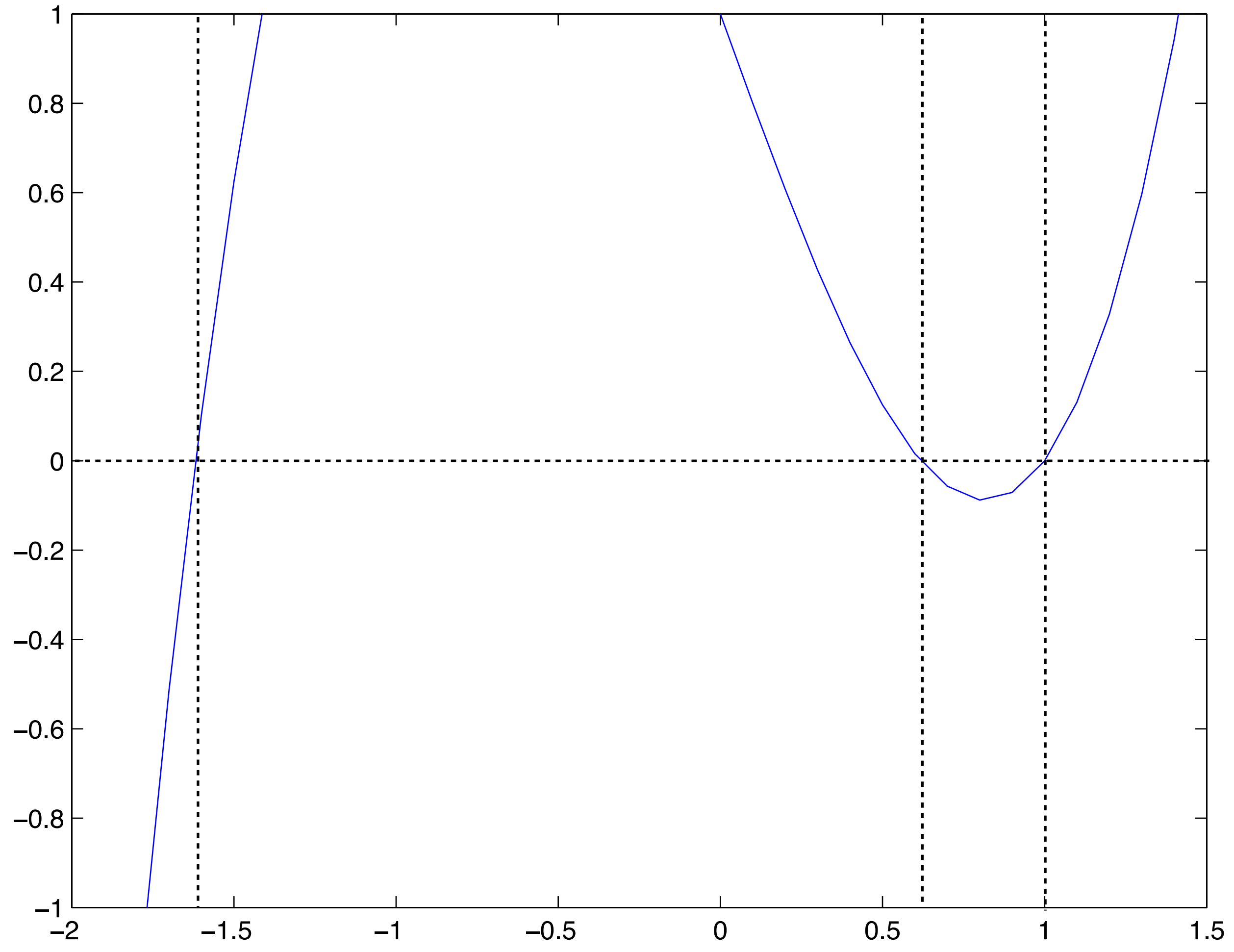


# Good Initial Guesses

- Solving nonlinear equations and optimization require good initial guesses
  - Where do these come from?
- Nonlinear equations can have multiple roots, optimization problems can have multiple minima.
  - How can we find them all?
- The concepts of continuation, homotopy and bifurcation are useful in this regard.

# Continuation

- Example:
  - Find the roots of: $f(x) = x^3 - 2x + 1$



# Continuation

- Example:
  - Find the roots of: $f(x) = x^3 - 2x + 1$
    - Guess the roots based on a plot of the function
      - easy in 1-D, hard in many dimensions
    - Transform the problem from an easy to solve one to the problem we want to solve:
      - Let $f(x) = x^3 - 2\lambda x + 1$
      - Find roots as $\lambda$ grows from zero to one
      - When $\lambda = 0$, $x = -1$
      - Use solution for one value of $\lambda$ as guess for next

# Continuation

- Example:
  - Find the roots of: $f(x) = x^3 - 2x + 1$

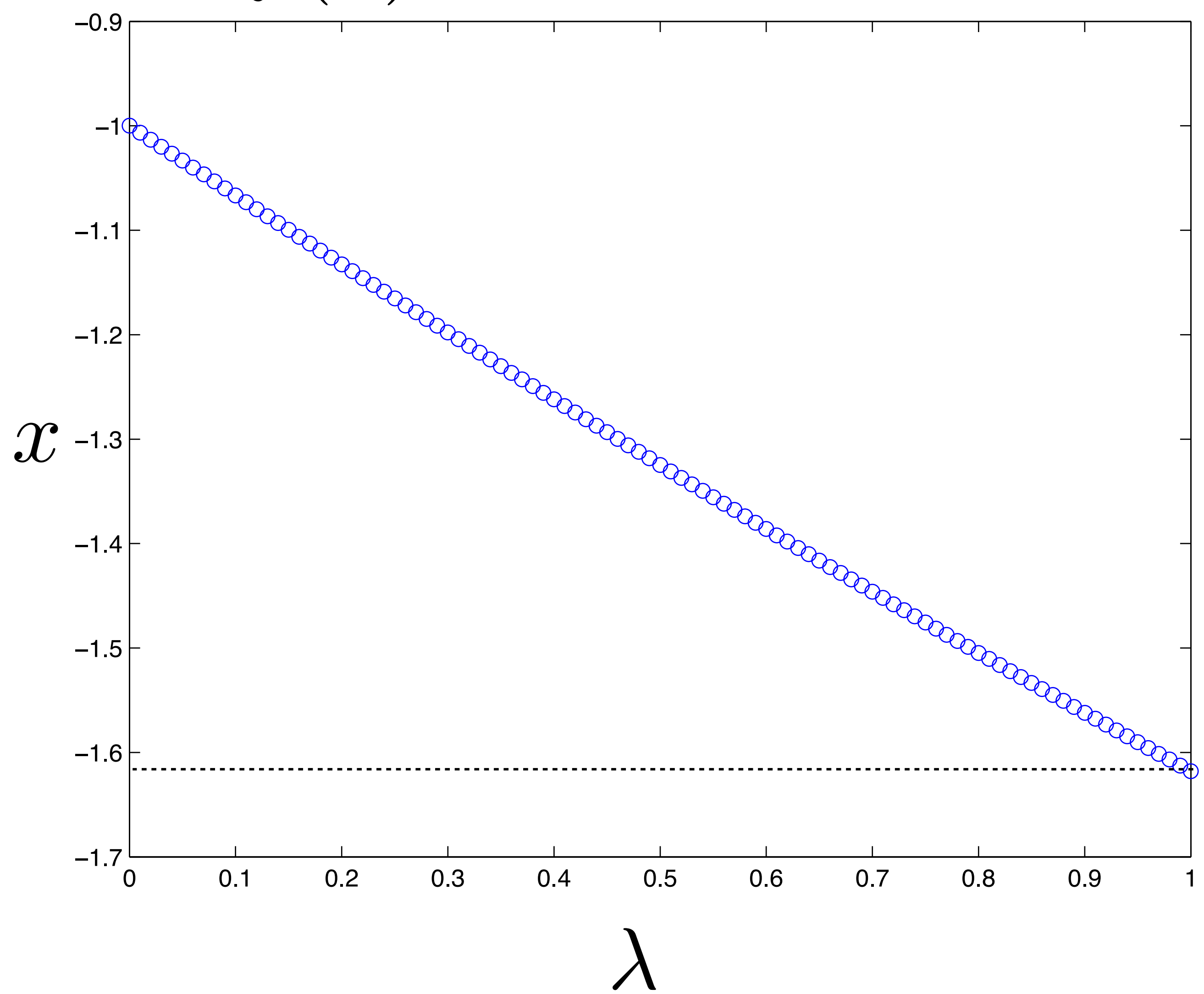
$$f(x) = x^3 - 2\lambda x + 1$$

```
lambda = [ 0:0.01:1 ];

xguess = -1;

for i = 1:length( lambda )

    f = @( x ) x .^ 3 - 2 * lambda( i ) * x + 1;

    x( i ) = fzero( @( x ) f( x ), xguess );

    xguess = x( i );

end;
```

# Continuation

- Example:
  - Find the roots of: $f(x) = x^3 - 2x + 1$

$$f(x) = x^3 - 2\lambda x + 1$$

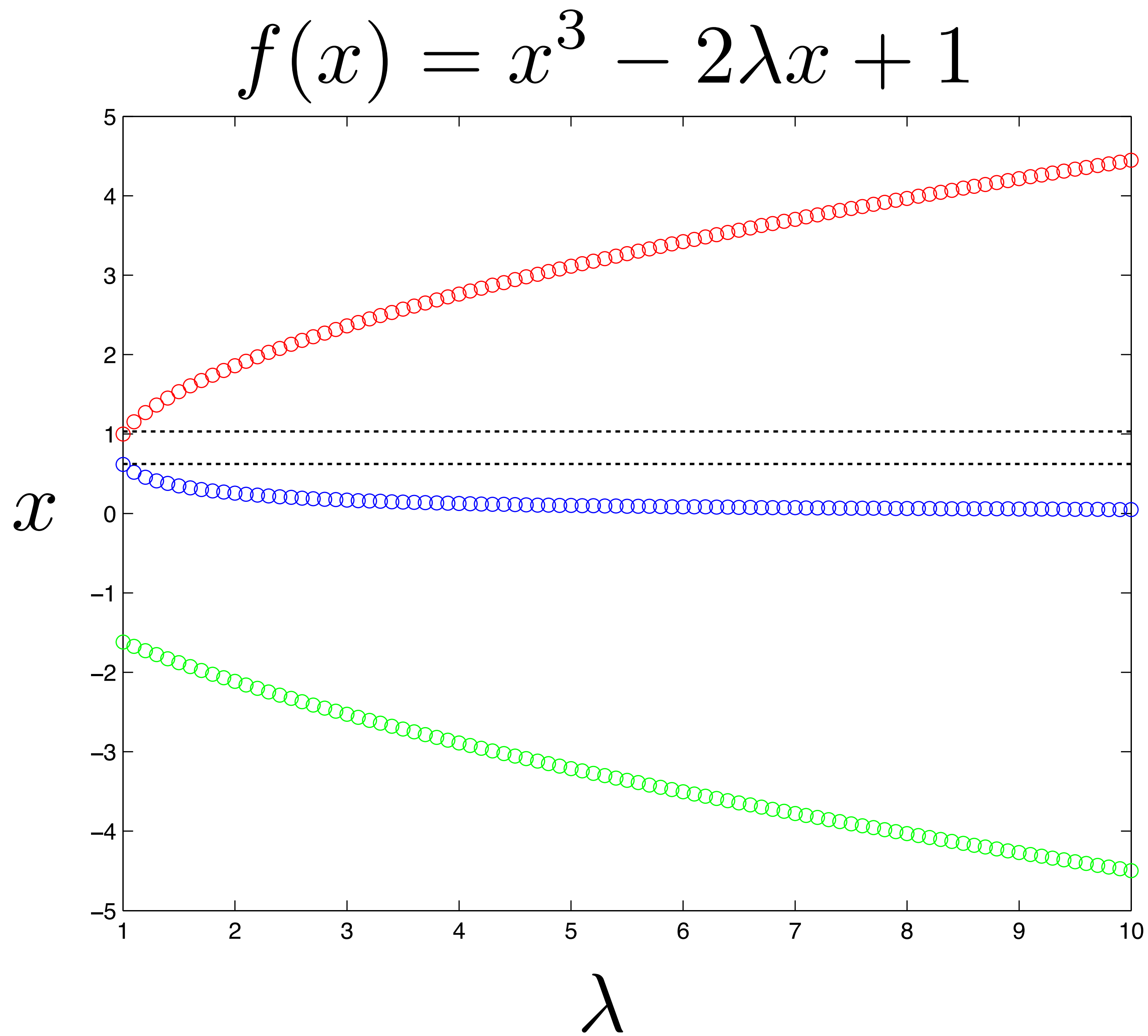


# Continuation

- Example:
  - Find the roots of: $f(x) = x^3 - 2x + 1$
    - Transform the problem from an easy to solve one to the problem we want to solve:
      - Let $f(x) = x^3 - 2\lambda x + 1$
      - When $\lambda$ is large $x \approx 1/(2\lambda), \pm\sqrt{2\lambda}$
      - Start with large $\lambda$ and trace back to $\lambda = 1$

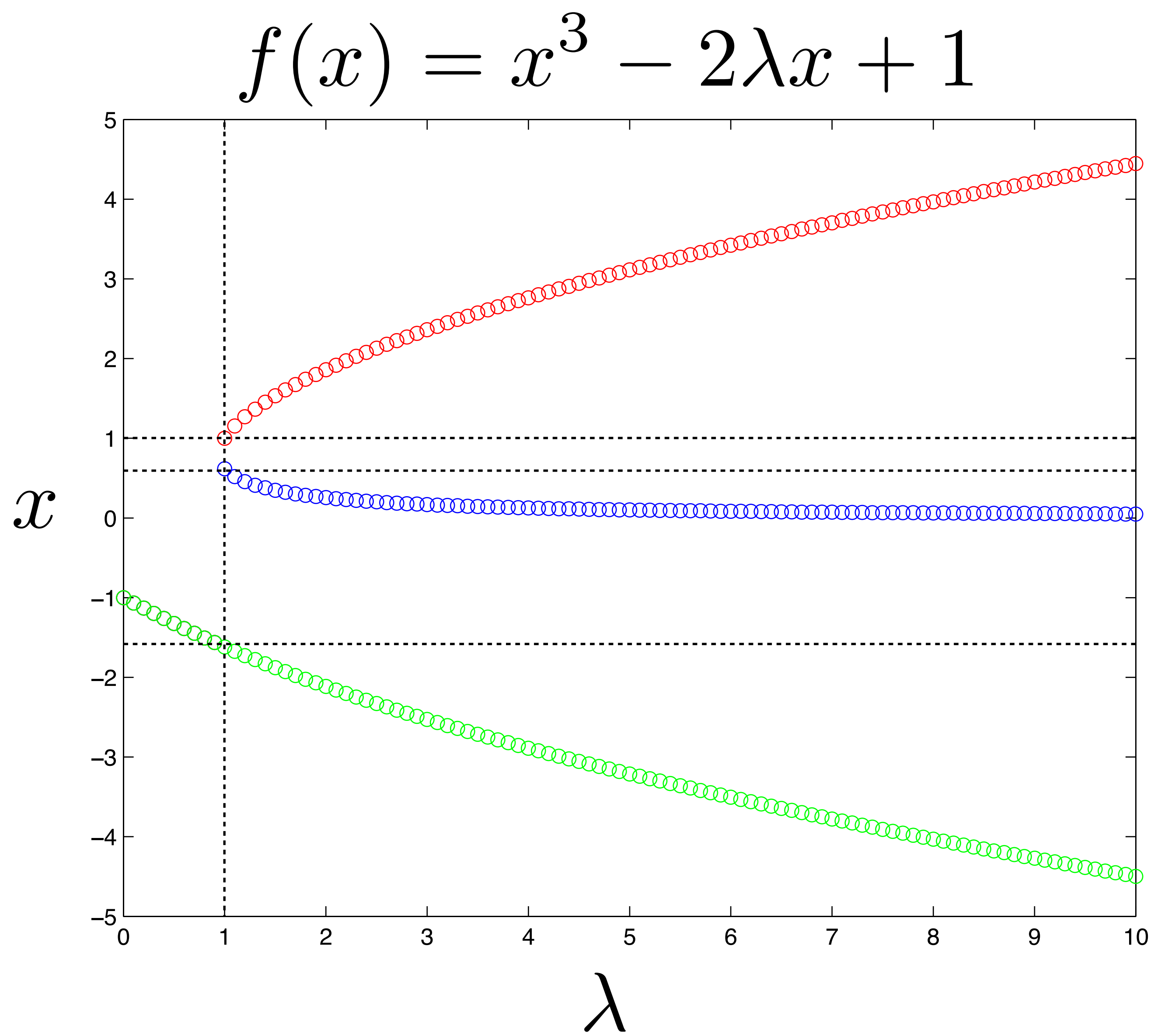
# Continuation

- Example:
  - Find the roots of: $f(x) = x^3 - 2x + 1$



# Continuation

- Example:
  - Find the roots of: $f(x) = x^3 - 2x + 1$



# Continuation

- Continuation can be used to generate a sequence of good initial guesses to different problems by varying a parameter by a small amount.
  - Examples:
    - fluid mechanics problems by varying the Reynolds number
    - mass transport problems by varying the Peclet number
    - multicomponent phase equilibria problems by varying temperature/pressure
    - reaction equilibrium problems by varying reaction rates

# Homotopy

- This transformation from one problem to another is termed homotopy.
- Generically, we seek the roots $\mathbf{x}^*(\lambda)$ of an equation:

$$\mathbf{h}(\mathbf{x};\lambda) = \lambda\mathbf{f}(\mathbf{x}) + (1-\lambda)\mathbf{g}(\mathbf{x})$$

  - When $\lambda = 0$, $\mathbf{h}(\mathbf{x};0) = \mathbf{g}(\mathbf{x})$
    - The roots $\mathbf{x}^*(0)$ are the roots of $\mathbf{g}(\mathbf{x})$
  - When $\lambda = 1$, $\mathbf{h}(\mathbf{x};1) = \mathbf{f}(\mathbf{x})$
    - The roots $\mathbf{x}^*(1)$ are the roots of $\mathbf{f}(\mathbf{x})$
  - There is a smooth transformation from $\mathbf{g}(\mathbf{x})$ to $\mathbf{f}(\mathbf{x})$
- $\lambda$ is varied in small increments from zero to one and the solution $\mathbf{x}^*(\lambda_i)$ is used as the initial guess for $\mathbf{x}^*(\lambda_{i+1})$

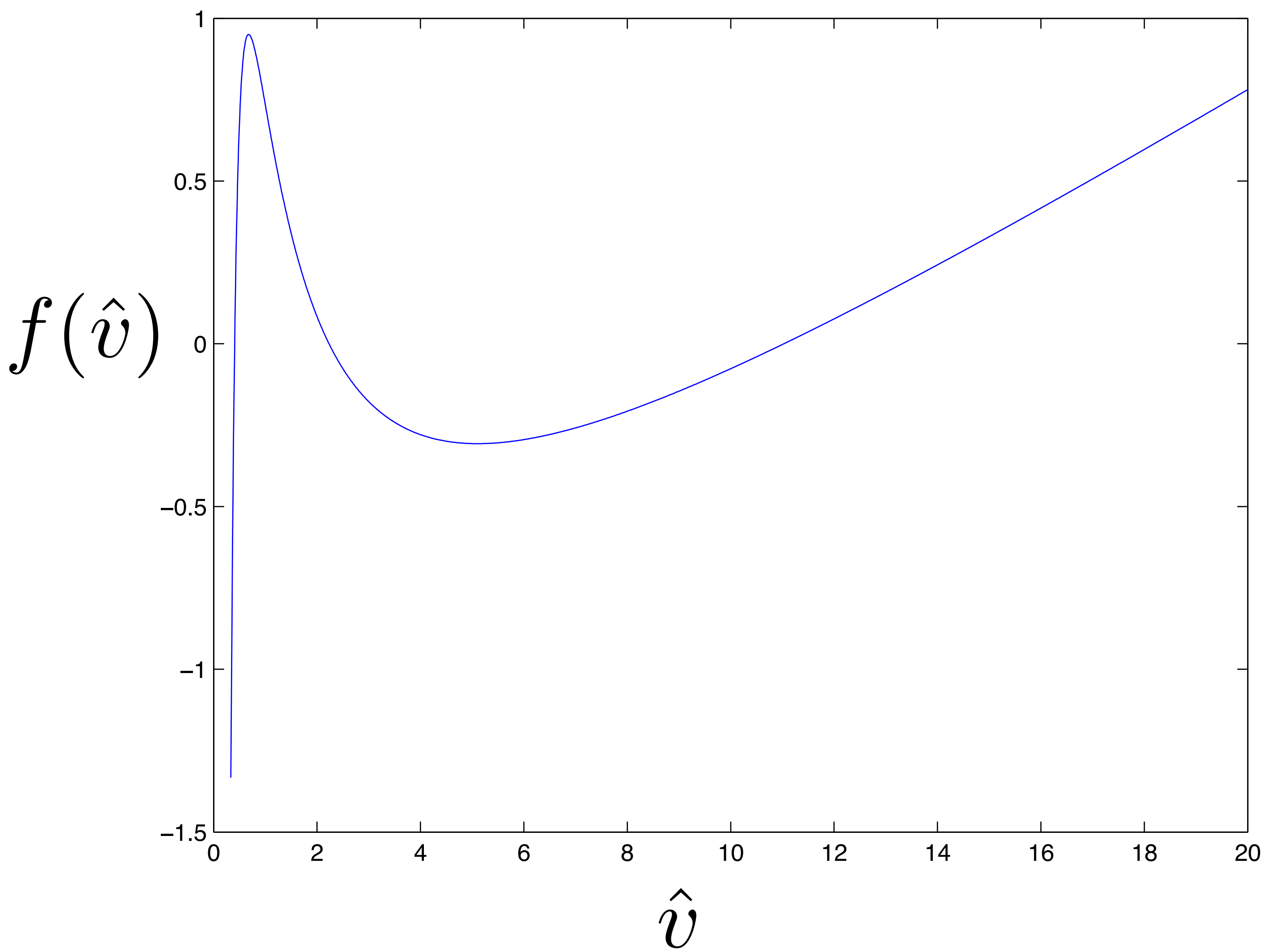
# Homotopy

- For small changes in the homotopy parameter, the previous solution will be a good initial guess.
- Newton-Raphson like methods can be expected to converge quickly.
- In practice, the function $\mathbf{f}(\mathbf{x})$ is associated with the problem of interest, but the function $\mathbf{g}(\mathbf{x})$ is arbitrary.
  - It may be difficult to find a good function $\mathbf{g}(\mathbf{x})$
  - Physically based homotopies are usually preferable.

# Homotopy

- Example:
  - Find roots of the van der Waals equation of state given: $\hat{P} = 0.1, \hat{T} = 0.5$

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



# Homotopy

- Example:
  - Find roots of the van der Waals equation of state given: $\hat{P} = 0.1, \hat{T} = 0.5$

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

  - Create the homotopy:

$$h(\hat{v}) = \lambda f(\hat{v}) + (1-\lambda) g(\hat{v})$$

    - with the ideal gas function:

$$g(\hat{v}) = \hat{P}\hat{v} - \frac{8}{3}\hat{T}$$

  - $\lambda = 0$, ideal gas; $\lambda = 1$, van der Waals

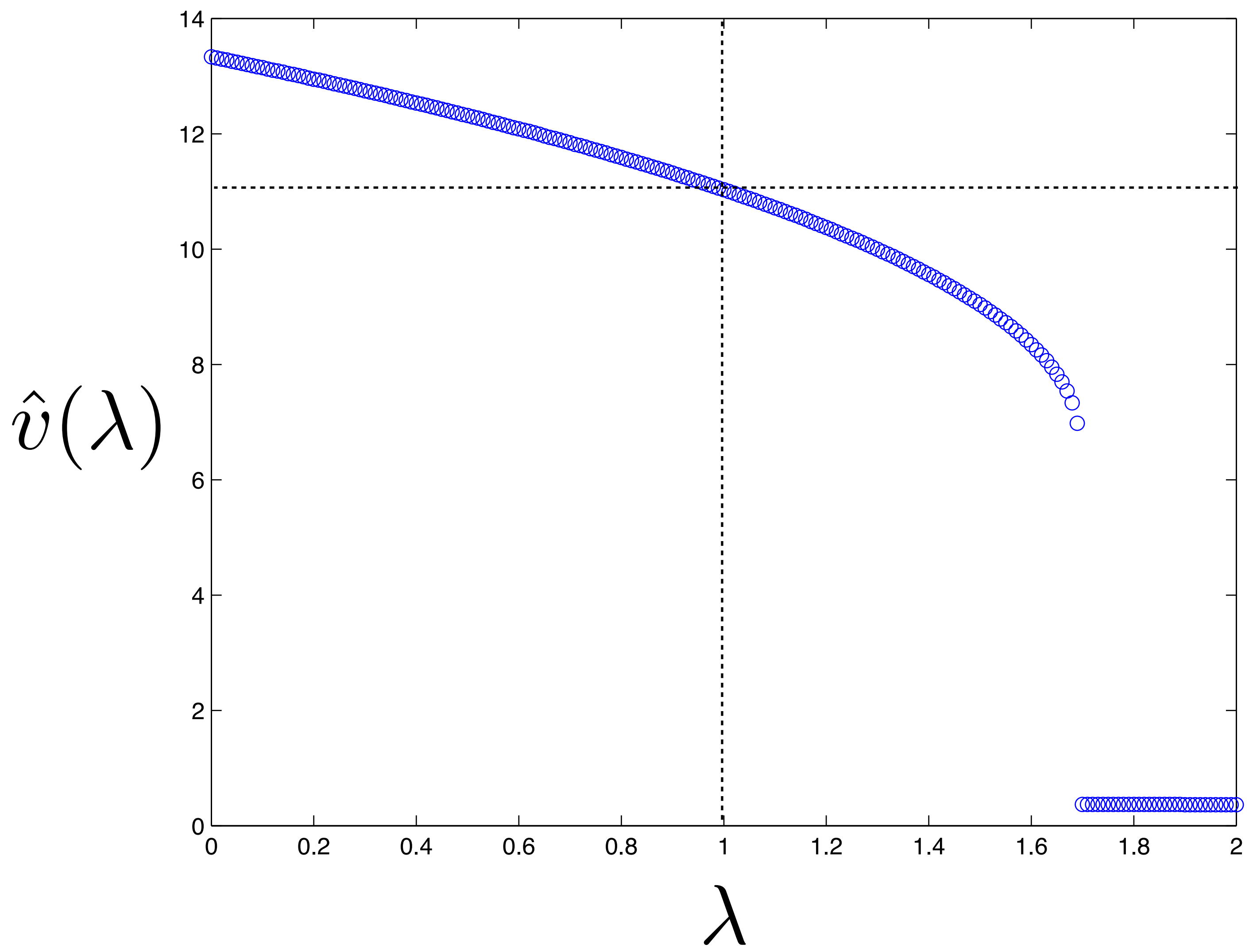
# Homotopy

- Example:
  - Find roots of the van der Waals equation of state given: $\hat{P} = 0.1, \hat{T} = 0.5$

```
T = 0.5;
P = 0.1;

vguess = 8 / 3 * T / P;

f = @( v ) ( P + 3 ./ v .^ 2 ) .* ( v - 1/ 3 ) - 8 / 3 * T;
g = @( v ) P .* v - 8 / 3 * T;
h = @( v, l ) l * f( v ) + ( 1 - l ) * g( v );

lambda = [ 0:0.01:1 ];

for i = 1:length( lambda )

    v( i ) = fzero( @( v ) h( v, lambda( i ) ), vguess );
    vguess = v( i );

end;
```

# Homotopy

- Example:
  - Find roots of the van der Waals equation of state given: $\hat{P} = 0.1, \hat{T} = 0.5$



# Homotopy

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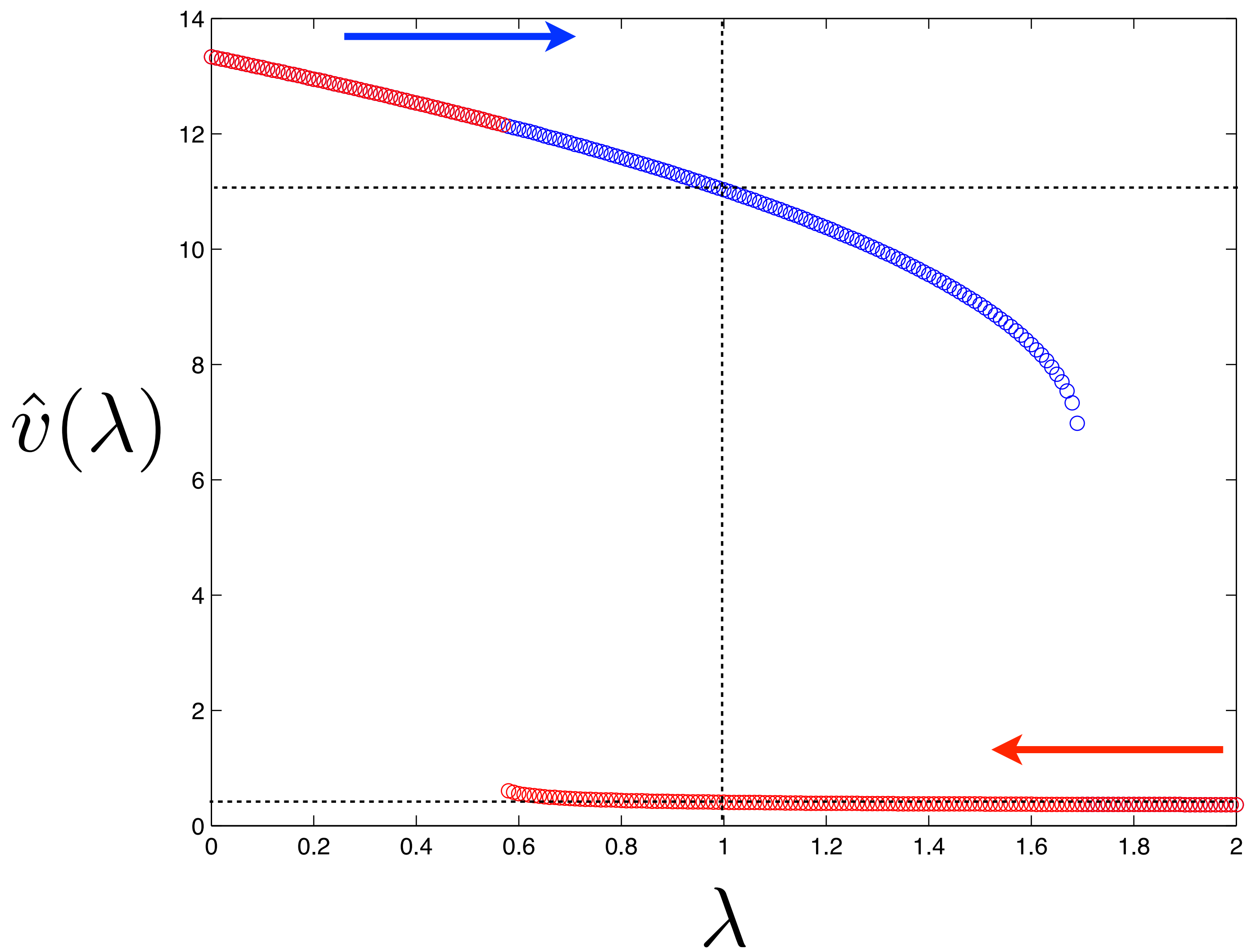

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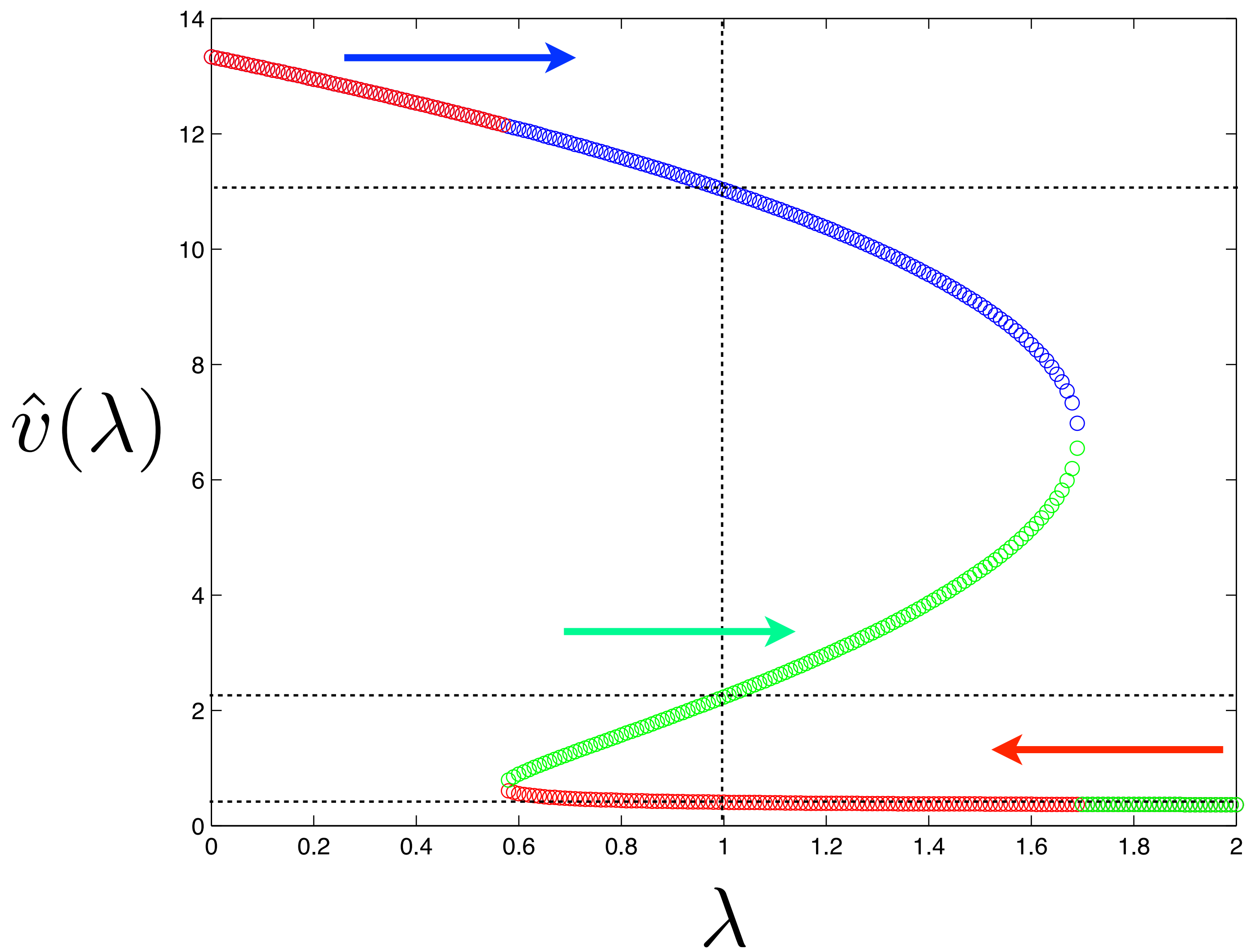

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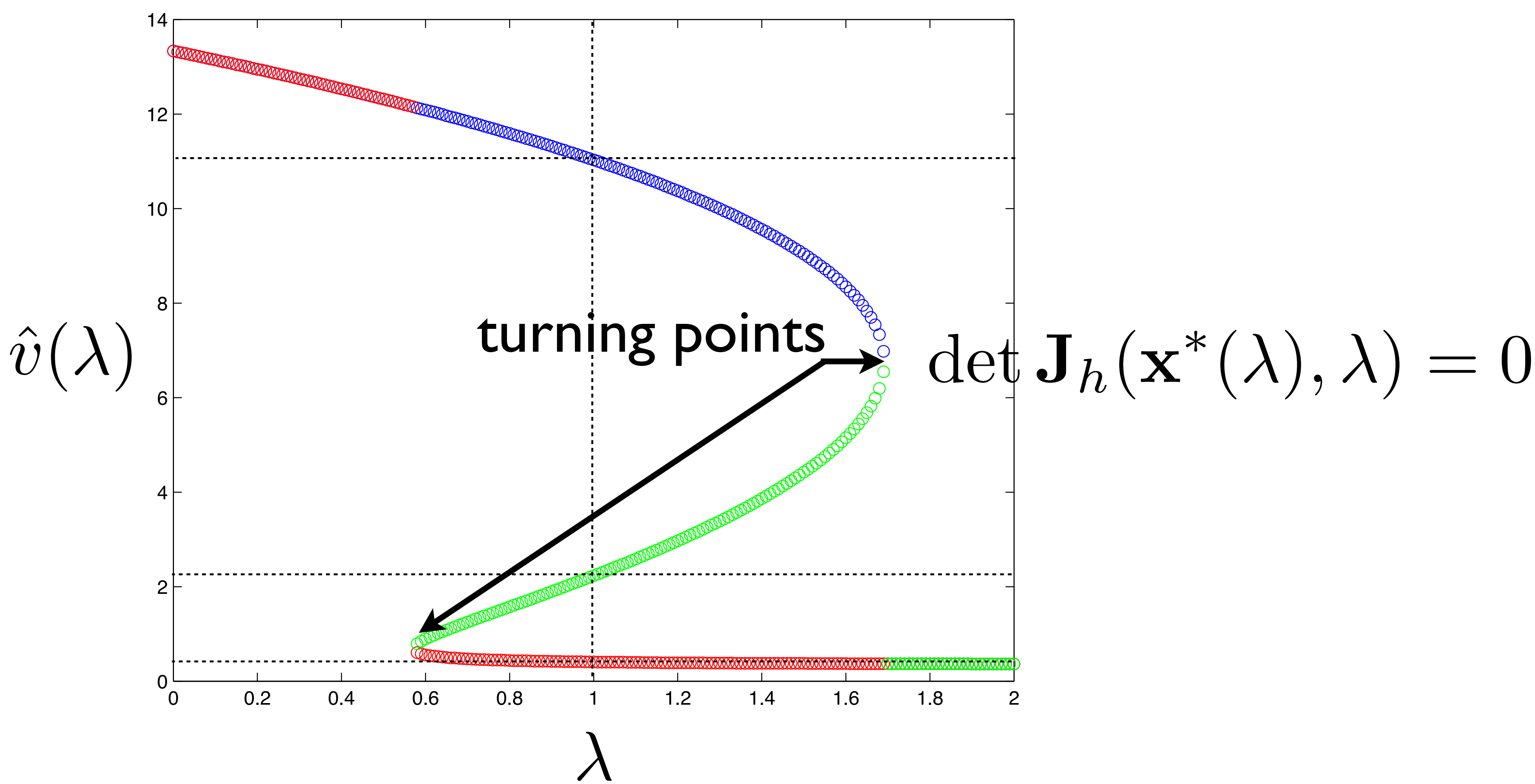
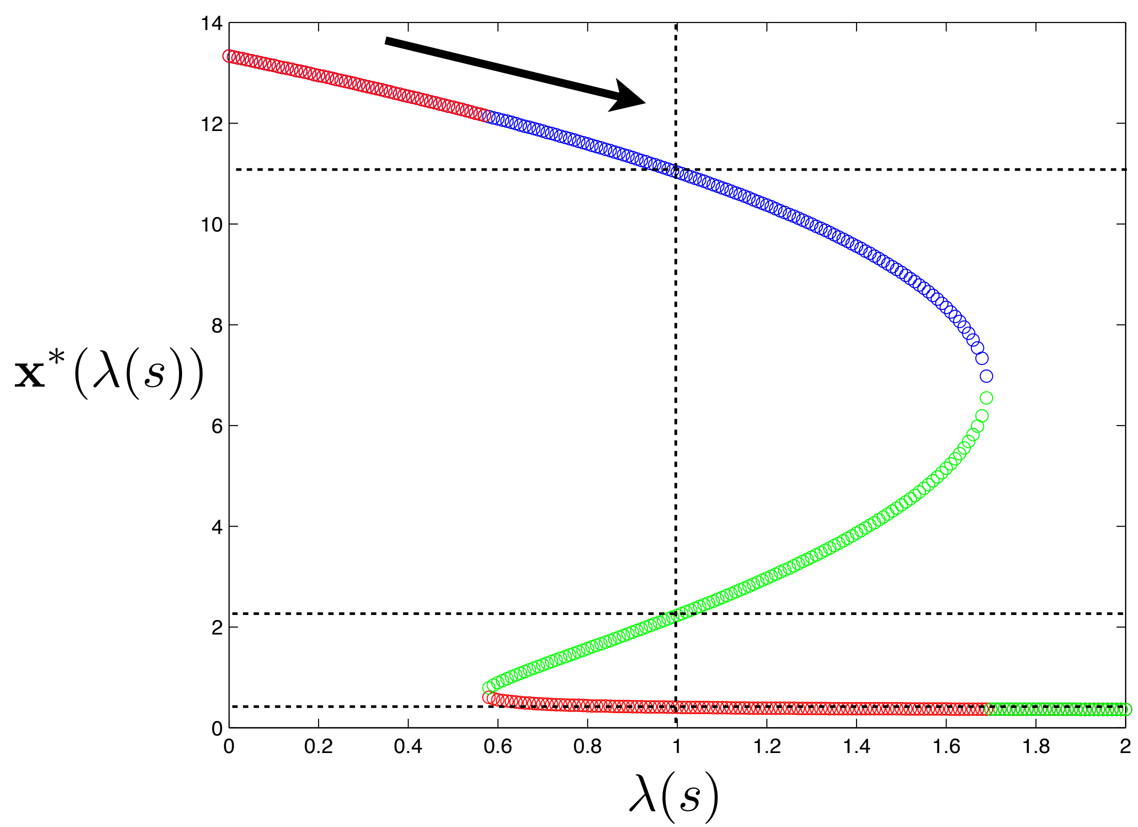


# Arclength Continuation

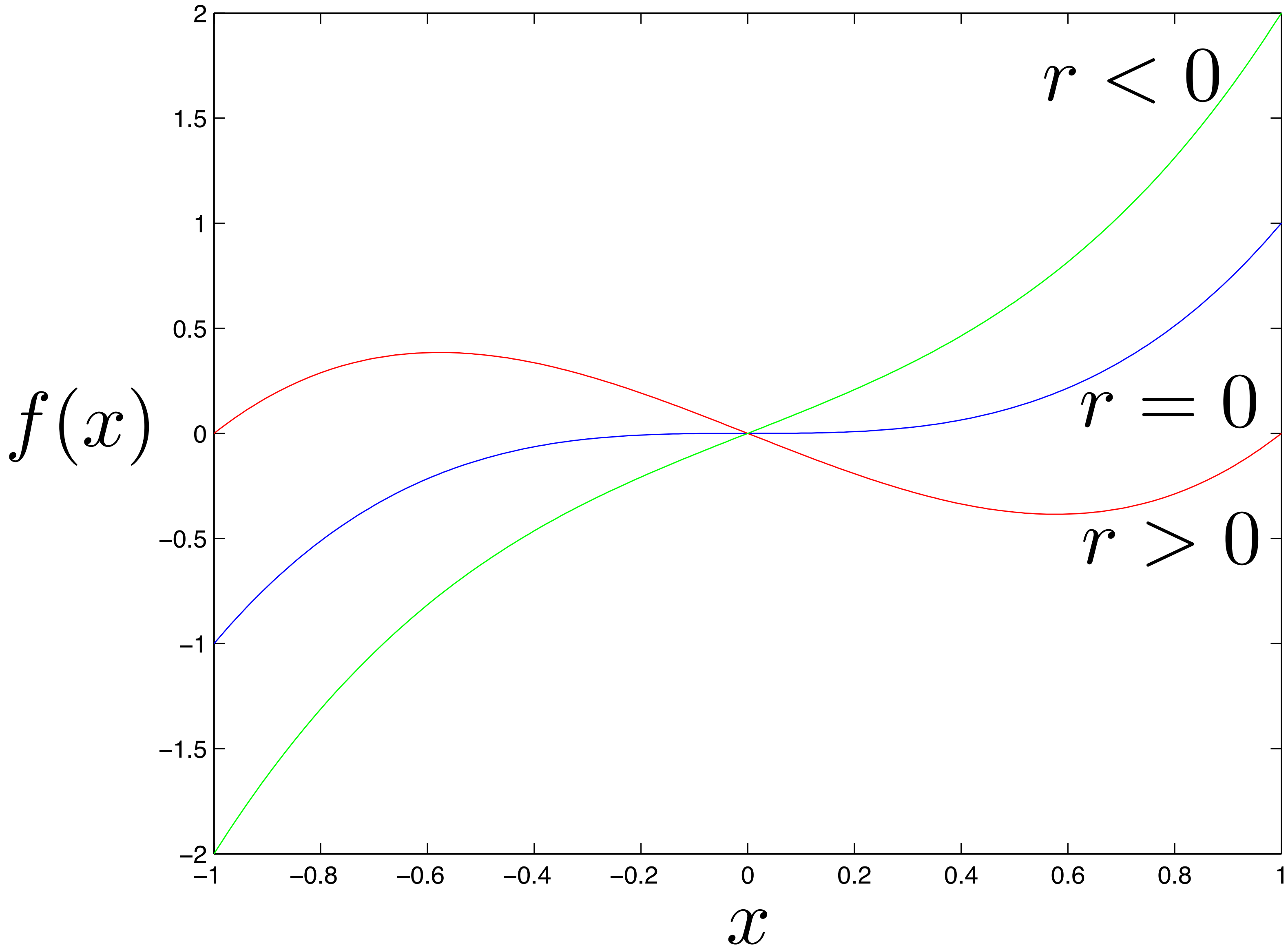
- Parameterize the roots and homotopy parameter in terms of the distance travelled along the solution curve:
  - $\mathbf{x}^*(\lambda(s)), \lambda(s)$
- Determine how to change homotopy parameter from arclength constraint:

$$\|\frac{d}{ds}\mathbf{x}^*(\lambda(s))\|_2^2 + \left(\frac{d}{ds}\lambda(s)\right)^2 = 1$$



# Bifurcation

- Example:
  - Find the real roots of $f(x) = x^3 - rx$



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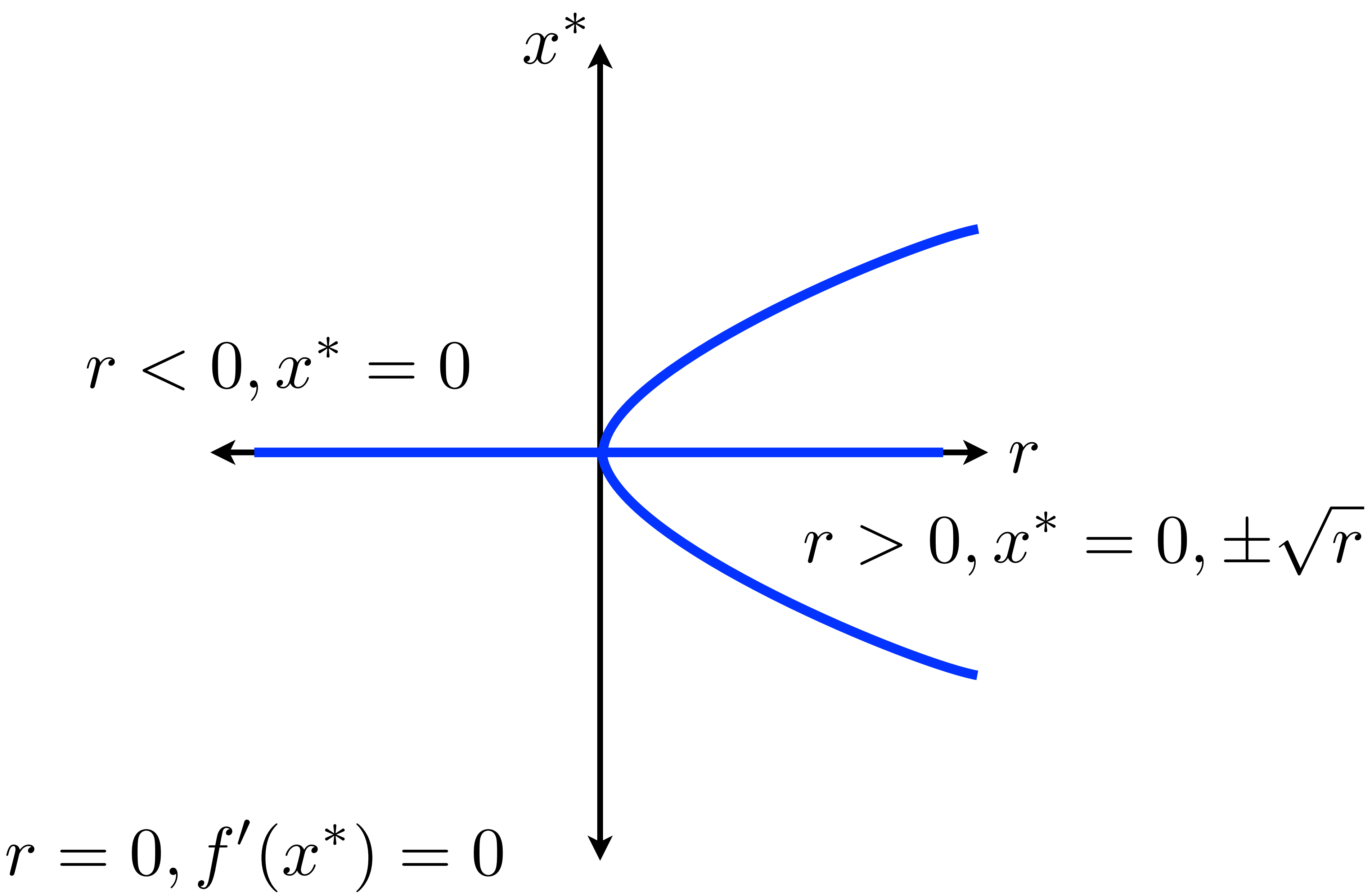
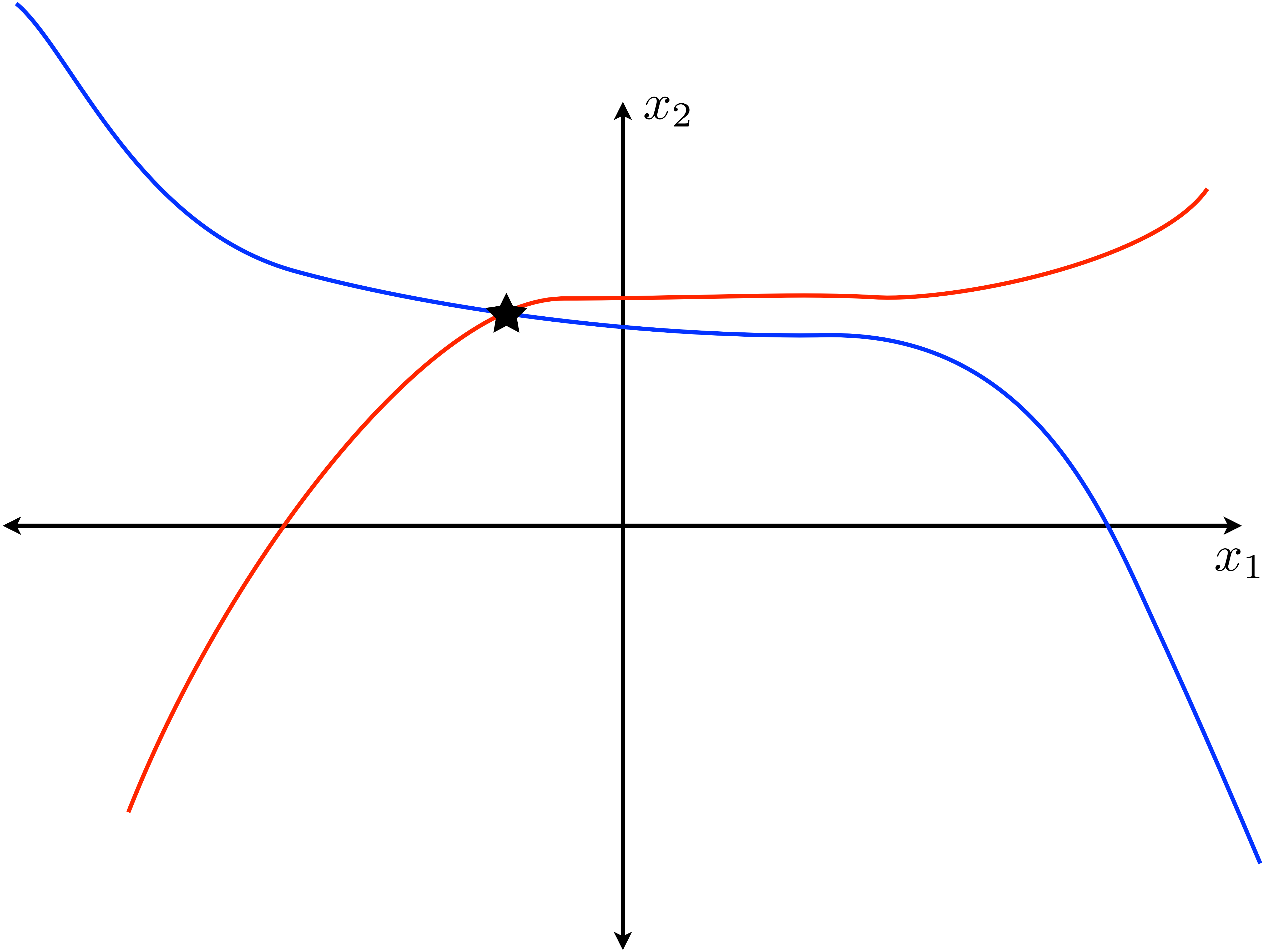


# Bifurcation

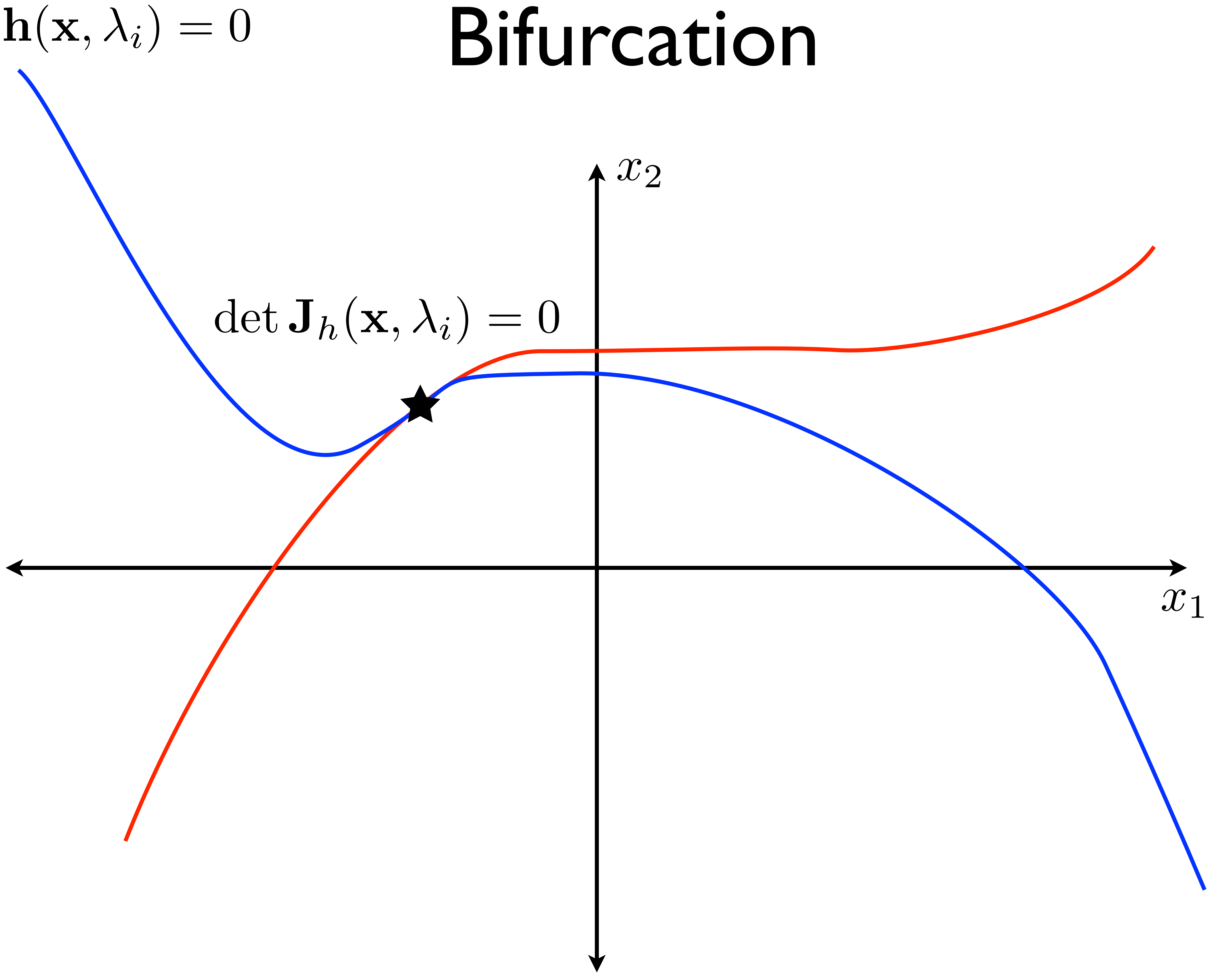
- Occasionally, a problem will switch from having 1 solution to having many solutions as a parameter is varied.
- We have seen how this occurs discontinuously with turning points.
- When additional solutions appear continuously, it is termed bifurcation.
- Bifurcations in a homotopy enable finding of multiple solutions to the same nonlinear equation
- Finding bifurcation (and turning) points can be of great physical interest.
- Like turning points, the Jacobian is singular at a bifurcation point: $\det \mathbf{J}(\mathbf{x}^*) = 0$

# Bifurcation

$\mathbf{h}(\mathbf{x}, \lambda_{i-1}) = 0$

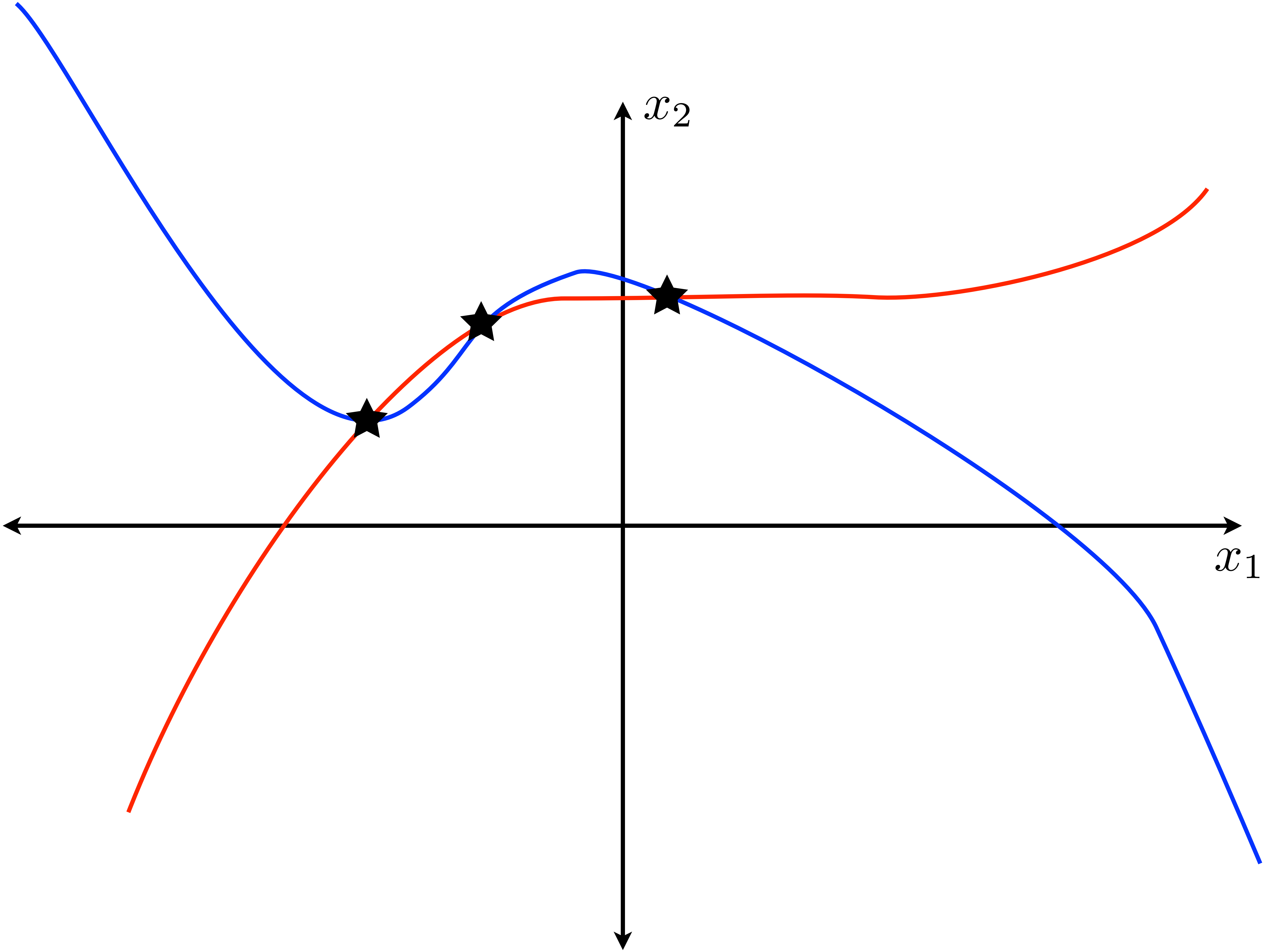


# Bifurcation



# Bifurcation

$\mathbf{h}(\mathbf{x}, \lambda_{i+1}) = 0$



# Bifurcation

- In practice, it is hard to hit the bifurcation point exactly while stepping with the homotopy parameter.
  - The bifurcation is detected by checking the sign of the determinant of the Jacobian.
  - If $\det \mathbf{J}_h(\mathbf{x}, \lambda) = 0$ at the bifurcation, then it changed from positive to negative (or negative to positive) as the homotopy parameter changed.
- We can find the bifurcation point exactly by solving an augmented system of nonlinear equations:

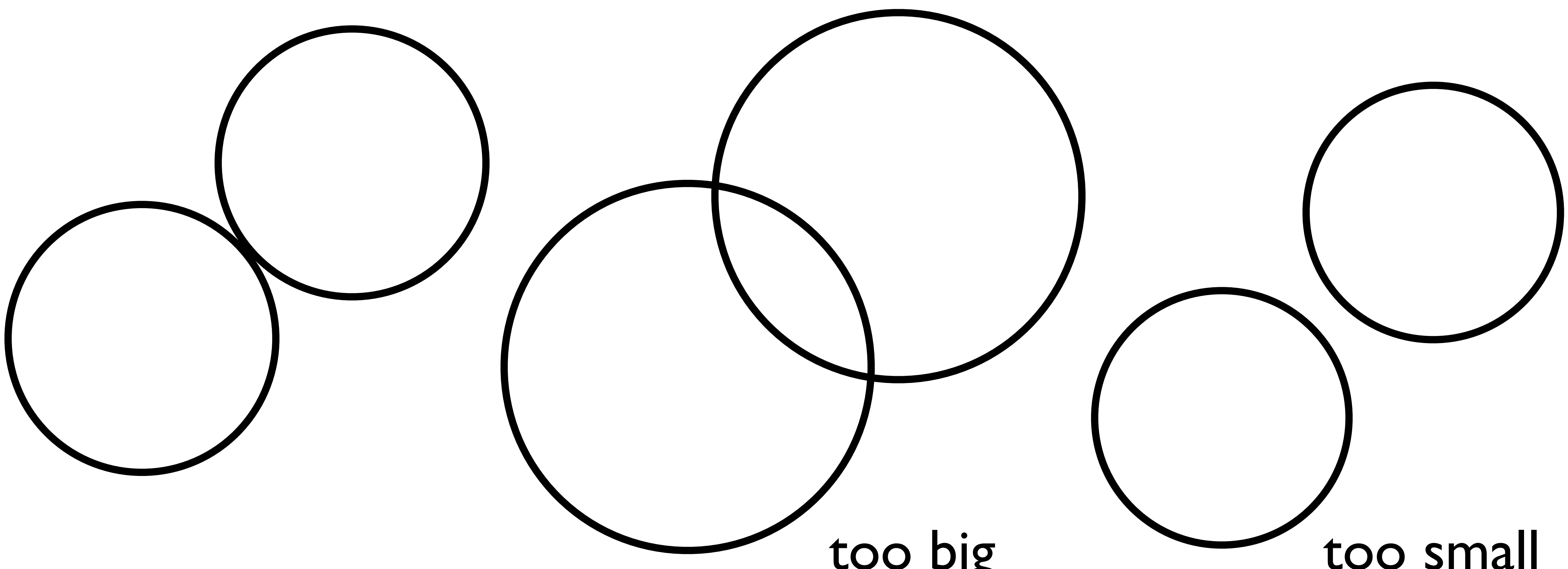
$$\begin{pmatrix} \mathbf{h}(\mathbf{x}; \lambda) \\ \det \mathbf{J}_h(\mathbf{x}, \lambda) \end{pmatrix} = 0$$

  - which finds the value of $\mathbf{x}$ and $\lambda$ at the bifurcation

# Bifurcation

- Example:
  - Find the radius where two circles just touch:

$$\mathbf{f}(\mathbf{x}) = \begin{pmatrix} (x_1+3)^2 + (x_2+1)^2 - R^2 \\ (x_1-2)^2 + (x_2-2)^2 - R^2 \end{pmatrix}$$



# Bifurcation

- Example:
  - Find the radius where two circles just touch:

$$\mathbf{f}(\mathbf{x}) = \begin{pmatrix} (x_1+3)^2 + (x_2+1)^2 - R^2 \\ (x_1-2)^2 + (x_2-2)^2 - R^2 \end{pmatrix}$$

  - This is a bifurcation point (from 0 to 2 solutions)

$$\begin{aligned} \mathbf{f}(\mathbf{x}) &= 0 \\ \det \mathbf{J}(\mathbf{x}) &= 0 \end{aligned}$$

  - Find this point by solving the augmented equations

$$\begin{pmatrix} \mathbf{f}(\mathbf{x}) \\ \det \mathbf{J}(\mathbf{x}) \end{pmatrix} = 0 \qquad \text{for} \qquad \mathbf{y} = \begin{pmatrix} \mathbf{x} \\ R \end{pmatrix}$$

# Bifurcation

- Example:
  - Find this point by solving the augmented equations:

$$\begin{pmatrix} \mathbf{f}(\mathbf{x}) \\ \det \mathbf{J}(\mathbf{x}) \end{pmatrix} = 0 \qquad \text{for} \qquad \mathbf{y} = \begin{pmatrix} \mathbf{x} \\ R \end{pmatrix}$$

  - Newton-Raphson iteration:

$$\mathbf{y}_{i+1} = \mathbf{y}_i + \Delta \mathbf{y}_i$$

$$\left.\begin{pmatrix} \mathbf{J}(\mathbf{x}) & \frac{\partial}{\partial R}\mathbf{f}(\mathbf{x}) \\ \nabla \det \mathbf{J}(\mathbf{x}) & \frac{\partial}{\partial R} \det \mathbf{J}(\mathbf{x}) \end{pmatrix}\right|_{\mathbf{y}_i} \Delta \mathbf{y}_i = - \left.\begin{pmatrix} \mathbf{f}(\mathbf{x}) \\ \det \mathbf{J}(\mathbf{x}) \end{pmatrix}\right|_{\mathbf{y}_i}$$