Introduction to Simulation - Lecture 9

Multidimensional Newton Methods

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Thanks to Deepak Ramaswamy, Jaime Peraire, Michal Rewienski, and Karen Veroy

Outline

- Quick Review of 1-D Newton
  - Convergence Testing
- Multidimensonal Newton Method
  - Basic Algorithm
  - Description of the Jacobian.
  - Equation formulation.
- Multidimensional Convergence Properties
  - Prove local convergence
  - Improving convergence

1-D Reminder

Newton Idea

Problem: Find x^* such that $f\left(x^*\right)=0$

Use a Taylor Series Expansion

$$\cancelto{0}{f\left(x^*\right)}=f\left(x\right)+\frac{\partial f\left(x\right)}{\partial x}\left(x^*-x\right)+\frac{\partial^2 f\left(\tilde{x}\right)}{\partial x^2}\left(x^*-x\right)^2$$

If x is close to the exact solution

$$\frac{\partial f\left(x\right)}{\partial x}\left(x^*-x\right)\approx -f\left(x\right)$$

1-D Reminder

Newton Algorithm

$x^0 =$ Initial Guess, $k = 0$

Repeat {

$$\frac{\partial f\left(x^k\right)}{\partial x}\left(x^{k+1} - x^k\right) = -f\left(x^k\right)$$

$$k = k + 1$$

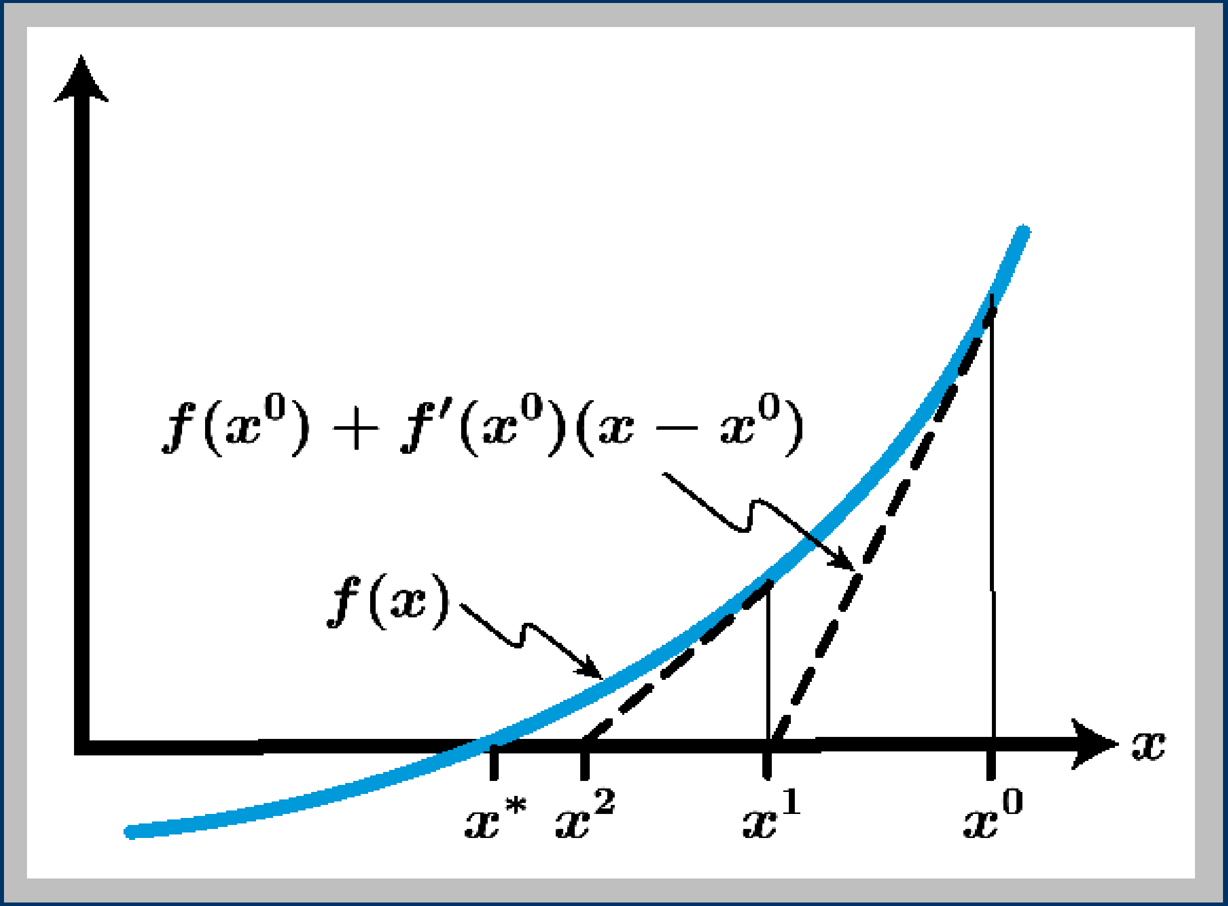
} Until ?

$\left\| x^{k+1} - x^k \right\| < threshold\,?$ $\quad \left\| f\left(x^{k+1}\right) \right\| < threshold\,?$

1-D Reminder

Newton Algorithm

Algorithm Picture

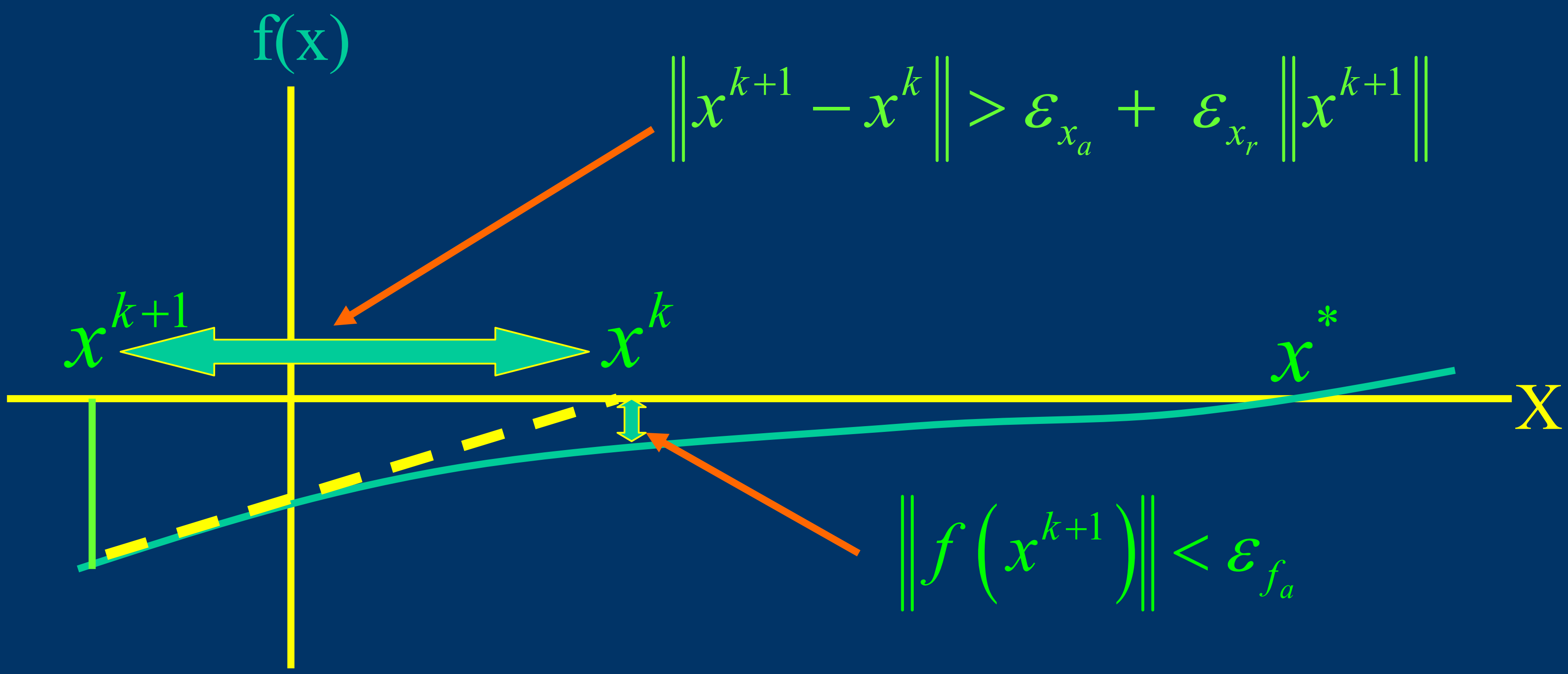


1-D Reminder

Newton Algorithm

Convergence Checks

Need a "delta-x" check to avoid false convergence

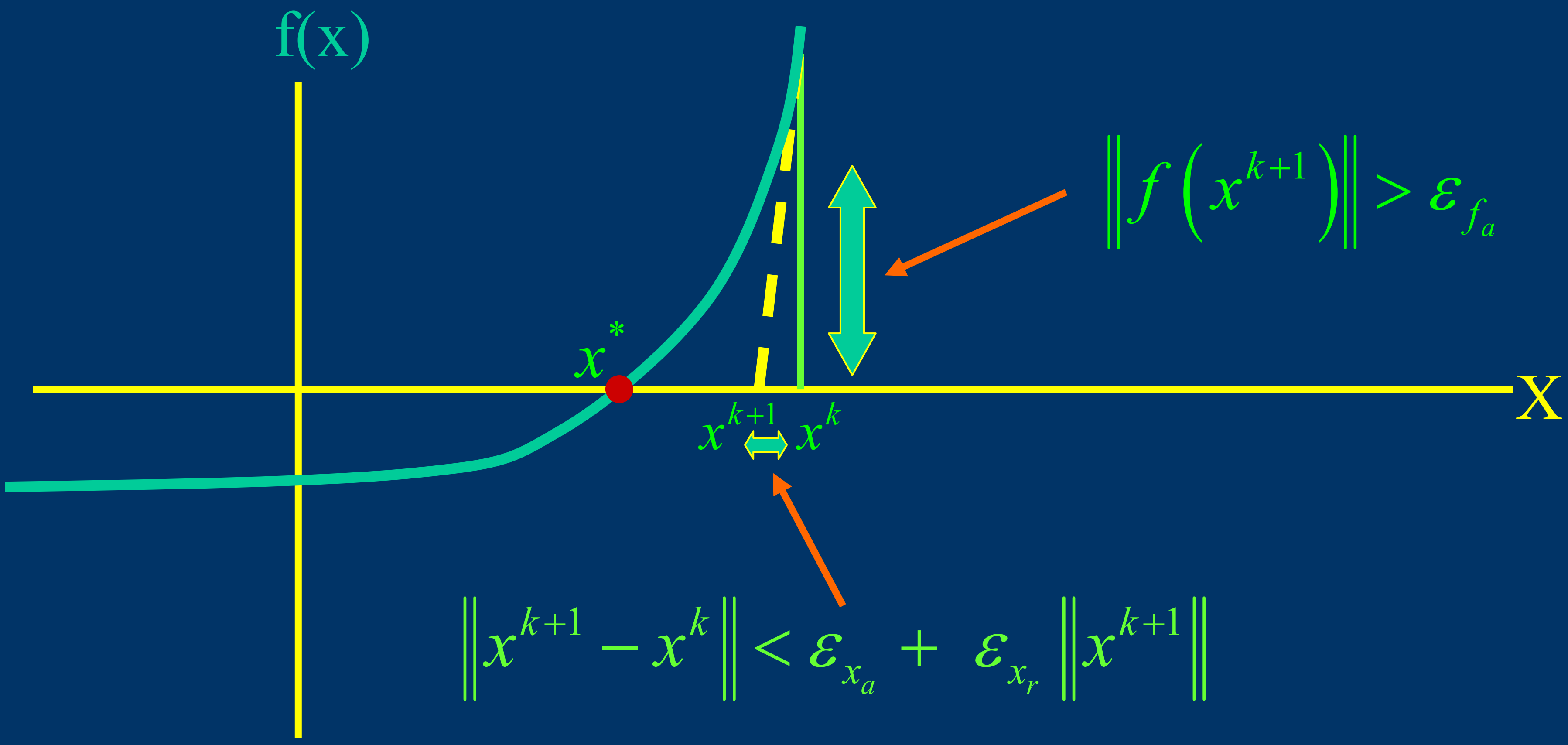


1-D Reminder

Newton Algorithm

Convergence Checks

Also need an "$f(x)$" check to avoid false convergence

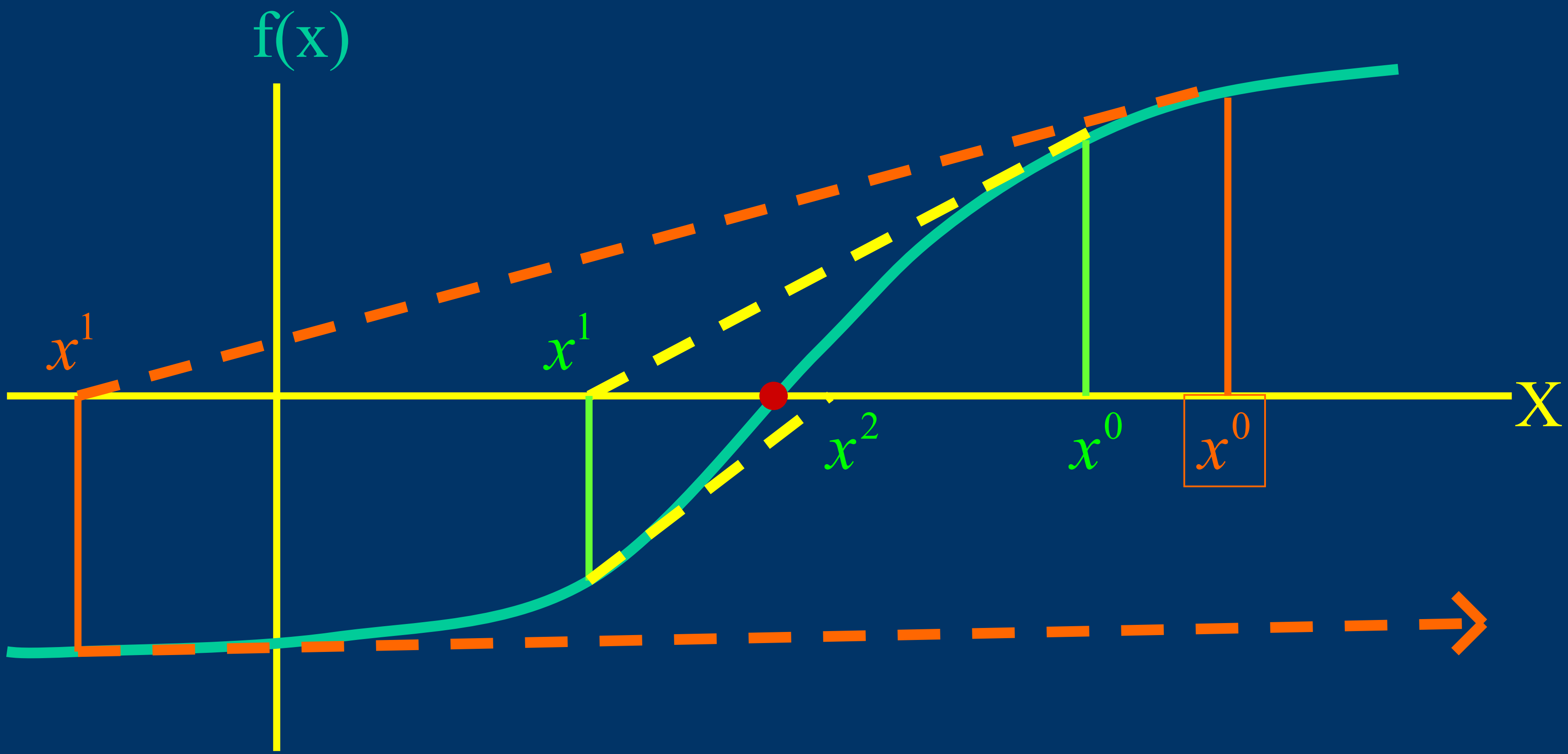


1-D Reminder

Newton Algorithm

Local Convergence

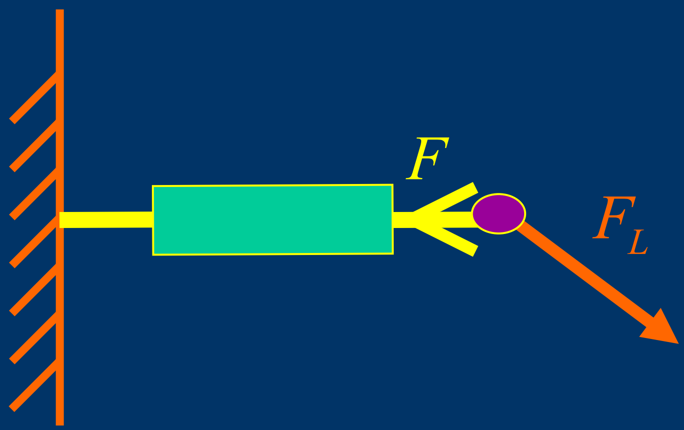
Convergence Depends on a Good Initial Guess



Multidimensional Newton Method

Example Problem

Strut and Joint



$$l = \sqrt{x^2 + y^2}$$

$$F = EA_c \frac{(l_o - l)}{l_o} = \varepsilon(l_o - l)$$

$$f_x = \frac{x}{l} F = \frac{x}{l} \varepsilon(l_o - l)$$

$$f_y = \frac{y}{l} F = \frac{y}{l} \varepsilon(l_o - l)$$

$$F(\vec{x}) = \begin{matrix} f_x + F_{L_x} = 0 \\ f_y + F_{L_y} = 0 \end{matrix}$$

OR

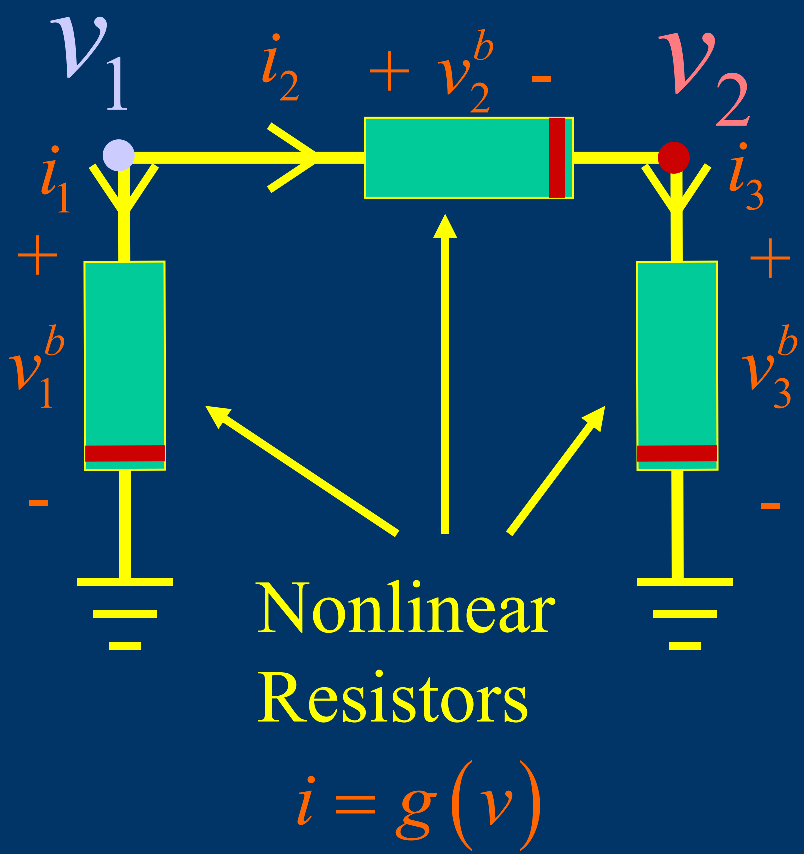
$$\frac{x}{l} \varepsilon(l_o - l) + F_{L_x} = 0$$

$$\frac{y}{l} \varepsilon(l_o - l) + F_{L_y} = 0$$

Multidimensional Newton Method

Example Problem

Nonlinear Resistors



Nodal Analysis

At Node 1: $i_1 + i_2 = 0$

$$\Rightarrow g(v_1) + g(v_1 - v_2) = 0$$

At Node 2: $i_3 - i_2 = 0$

$$\Rightarrow g(v_3) - g(v_1 - v_2) = 0$$

Two coupled nonlinear equations in two unknowns

Multidimensional Newton Method

General Setting

Problem: Find x^* such that $F\left(x^*\right) = 0$

$x^* \in \mathbb{R}^N$ and $F : \mathbb{R}^N \rightarrow \mathbb{R}^N$

Use a Taylor Series Expansion

$$\underbrace{\cancel{F\left(x^*\right)}}_{}^{0} = F(x) + \underbrace{J_F(x)}_{Jacobian\ Matrix} \left(x^* - x\right) + H.O.T.$$

If x is close to the exact solution

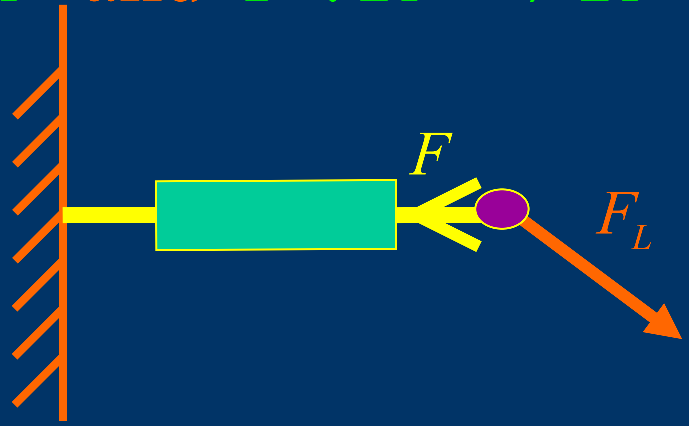
$$J_F(x)\left(x^* - x\right) \approx -F(x)$$

Multidimensional Newton Method

Nodal Analysis

Strut and Joint

$x^* \in \mathbb{R}^2$ and $F : \mathbb{R}^2 \to \mathbb{R}^2$



$$\frac{x}{l}\varepsilon(l_o - l) + F_{L_x} = 0$$

$$\frac{y}{l}\varepsilon(l_o - l) + F_{L_y} = 0$$

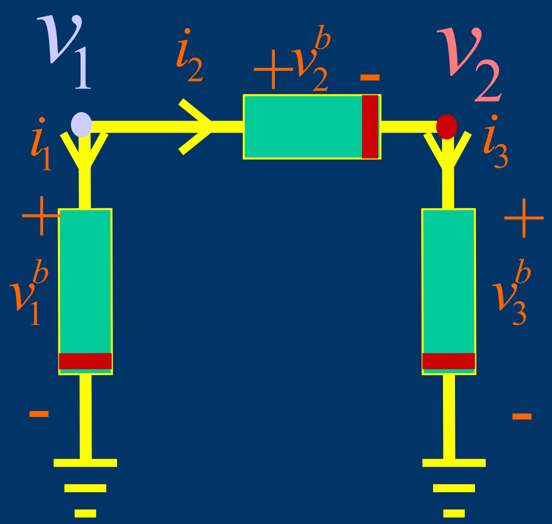
$$J_F(\vec{x}) = \begin{bmatrix} ? & ? \\ ? & ? \end{bmatrix}$$

Multidimensional Newton Method

Nodal Analysis

Nonlinear Resistor

$$x^* \in \mathbb{R}^2 \text{ and } F : \mathbb{R}^2 \rightarrow \mathbb{R}^2$$



At Node 1: $i_1 + i_2 = 0$

$$\Rightarrow F_1(\vec{v}) = g(v_1) + g(v_1 - v_2) = 0$$

At Node 2: $i_3 - i_2 = 0$

$$\Rightarrow F_2(\vec{v}) = g(v_3) - g(v_1 - v_2) = 0$$

$$J_F(\vec{x}) = \begin{bmatrix} ? & ? \\ ? & ? \end{bmatrix}$$

Multidimensional Newton Method

Jacobian Matrix

$$J_F(x)\Delta x \approx F(x+\Delta x) - F(x)$$

$$J_F(x)\Delta x \equiv \begin{bmatrix} \dfrac{\partial F_1(x)}{\partial x_1} & \cdots & \dfrac{\partial F_1(x)}{\partial x_N} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial F_N(x)}{\partial x_1} & \cdots & \dfrac{\partial F_N(x)}{\partial x_N} \end{bmatrix} \begin{bmatrix} \Delta x_1 \\ \vdots \\ \Delta x_N \end{bmatrix}$$

Multidimensional Newton Method

Jacobian Matrix

Singular Case

Suppose $J_F(x)$ is singular?

$$J_F(x)\Delta x = \begin{bmatrix} \frac{\partial F_1(x)}{\partial x_1} & \cdots & \frac{\partial F_1(x)}{\partial x_N} \\ \vdots & \ddots & \vdots \\ \frac{\partial F_N(x)}{\partial x_1} & \cdots & \frac{\partial F_N(x)}{\partial x_N} \end{bmatrix} \begin{bmatrix} \Delta x_1 \\ \vdots \\ \Delta x_N \end{bmatrix} = 0$$

What does it mean?

Multidimensional Newton Method

Newton Algorithm

$x^0 =$ Initial Guess, $k = 0$

Repeat {

Compute $F\left(x^k\right), J_F\left(x^k\right)$

Solve $J_F\left(x^k\right)\left(x^{k+1} - x^k\right) = -F\left(x^k\right)$ for x^{k+1}

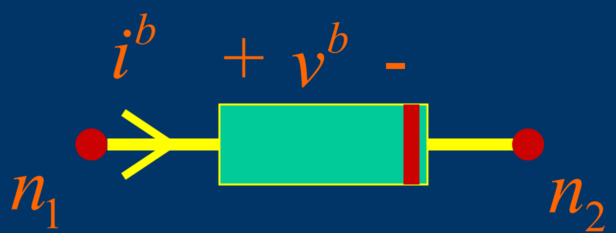
$k = k + 1$

} Until $\left\|x^{k+1} - x^k\right\|$, $\left\|f\left(x^{k+1}\right)\right\|$ small enough

Multidimensional Newton Method

Computing the Jacobian and the Function

Consider the contribution of one nonlinear resistor
Connected between nodes n_1 and n_2



$$i^b = g\left(v^b\right)$$

Summing currents at Node n_1: $F_{n_1}(v) = g\left(v_{n_1} - v_{n_2}\right) + \dots$

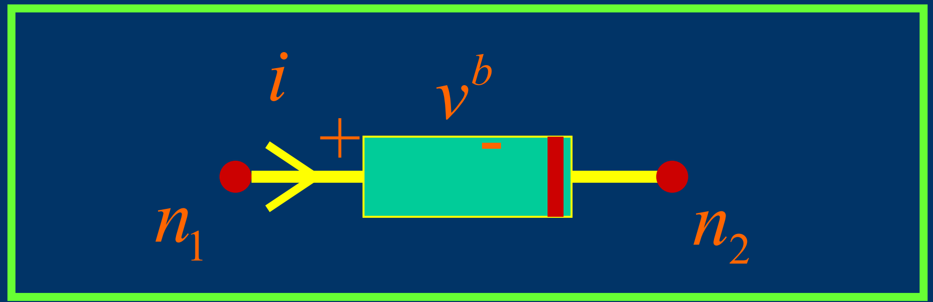
Summing currents at Node n_2: $F_{n_2}(v) = -g\left(v_{n_1} - v_{n_2}\right) + \dots$

Differenting at Node n_1: $\dfrac{\partial F_{n_1}(v)}{\partial v_{n_1}} = \underbrace{\dfrac{\partial g\left(v_{n_1} - v_{n_2}\right)}{\partial v_{n_1}}}_{\frac{\partial g}{\partial v}} + \dots$ $\quad \dfrac{\partial F_{n_1}(v)}{\partial v_{n_2}} = \underbrace{\dfrac{\partial g\left(v_{n_1} - v_{n_2}\right)}{\partial v_{n_2}}}_{-\frac{\partial g}{\partial v}} + \dots$

Multidimensional Newton Method

Computing the Jacobian and the Function

Stamping a Resistor



$$\underbrace{\begin{array}{c} \\ n_1 \\ \\ n_2 \\ \\ \end{array}\begin{array}{c}\begin{array}{ccccc} & n_1 & & n_2 & \end{array}\\ \begin{bmatrix} \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \frac{\partial g\left(v_{n_1}-v_{n_2}\right)}{\partial v} & \vdots & -\frac{\partial g\left(v_{n_1}-v_{n_2}\right)}{\partial v} & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & -\frac{\partial g\left(v_{n_1}-v_{n_2}\right)}{\partial v} & \vdots & \frac{\partial g\left(v_{n_1}-v_{n_2}\right)}{\partial v} & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}\end{array}}_{J_F(v)} \qquad \underbrace{\begin{bmatrix} \vdots \\ g\left(v_{n_1}-v_{n_2}\right) \\ \vdots \\ -g\left(v_{n_1}-v_{n_2}\right) \\ \vdots \end{bmatrix}}_{F(v)}\begin{array}{c} \\ n_1 \\ \\ n_2 \\ \\ \end{array}$$

Multidimensional Newton Method

More Complete Newton Algorithm

$x^0 =$ Initial Guess, $k = 0$

Repeat {

Compute $F\left(x^k\right), J_F\left(x^k\right)$

Zero $\mathrm{J_F}$ and F

for each element

Compute element currents and derivatives

Sum currents to F, sum derivatives to J_F

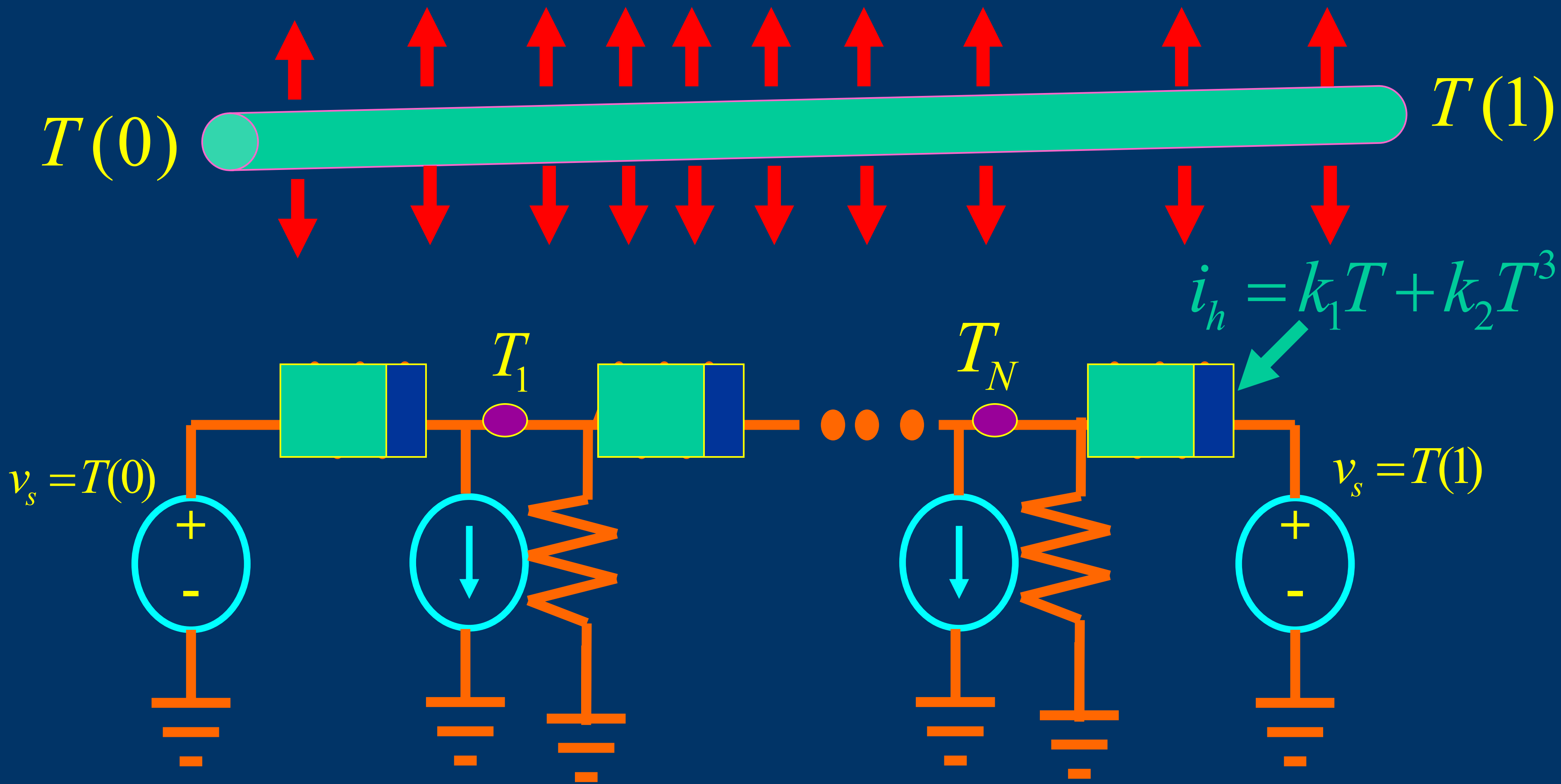
Solve $J_F\left(x^k\right)\left(x^{k+1} - x^k\right) = -F\left(x^k\right)$ for x^{k+1}

$k = k + 1$

} Until $\left\|x^{k+1} - x^k\right\|, \left\|f\left(x^{k+1}\right)\right\|$ small enough

Multidimensional Newton's Method

Example: Heat Flow in leaky bar



What is the Jacobian?

Main Theorem

If

$a)\ \left\|J_F^{-1}\left(x^k\right)\right\| \le \beta$ (Inverse is bounded)

$b)\ \left\|J_F\left(x\right) - J_F\left(y\right)\right\| \le \ell \left\|x - y\right\|$ (Derivative is Lipschitz Cont)

Then Newton's method converges given a sufficiently close initial guess

Multidimensional Newton Method

Multidimensional Convergence Theorem

Key Lemma

If $\left\| J_F(x) - J_F(y) \right\| \leq \ell \left\| x - y \right\|$ (Derivative is Lipschitz Cont)

Then $\left\| F(x) - F(y) - J_F(y)(x-y) \right\| \leq \frac{\ell}{2} \left\| x - y \right\|^2$

There is no multidimensional mean value theorem.

Multidimensional Newton Method

Multidimensional Convergence Theorem

Theorem Proof

By definition of the Newton Iteration and the assumed bound on the inverse of the Jacobian

$$\left\| x^{k+1} - x^k \right\| = \left\| J_F^{-1}\left(x^k\right) F\left(x^k\right) \right\| \leq \beta \left\| F\left(x^k\right) \right\|$$

Again applying the Newton iteration definition

$$\left\| x^{k+1} - x^k \right\| \leq \beta \left\| F\left(x^k\right) - \underbrace{F\left(x^{k-1}\right) - J_F\left(x^{k-1}\right)\left(x^k - x^{k-1}\right)}_{0} \right\|$$

Finally using the Lemma

$$\left\| x^{k+1} - x^k \right\| \leq \frac{\beta \ell}{2} \left\| x^k - x^{k-1} \right\|^2$$

Multidimensional Newton Method

Multidimensional Convergence Theorem

Theorem Proof Continued

Reorganizing the equation

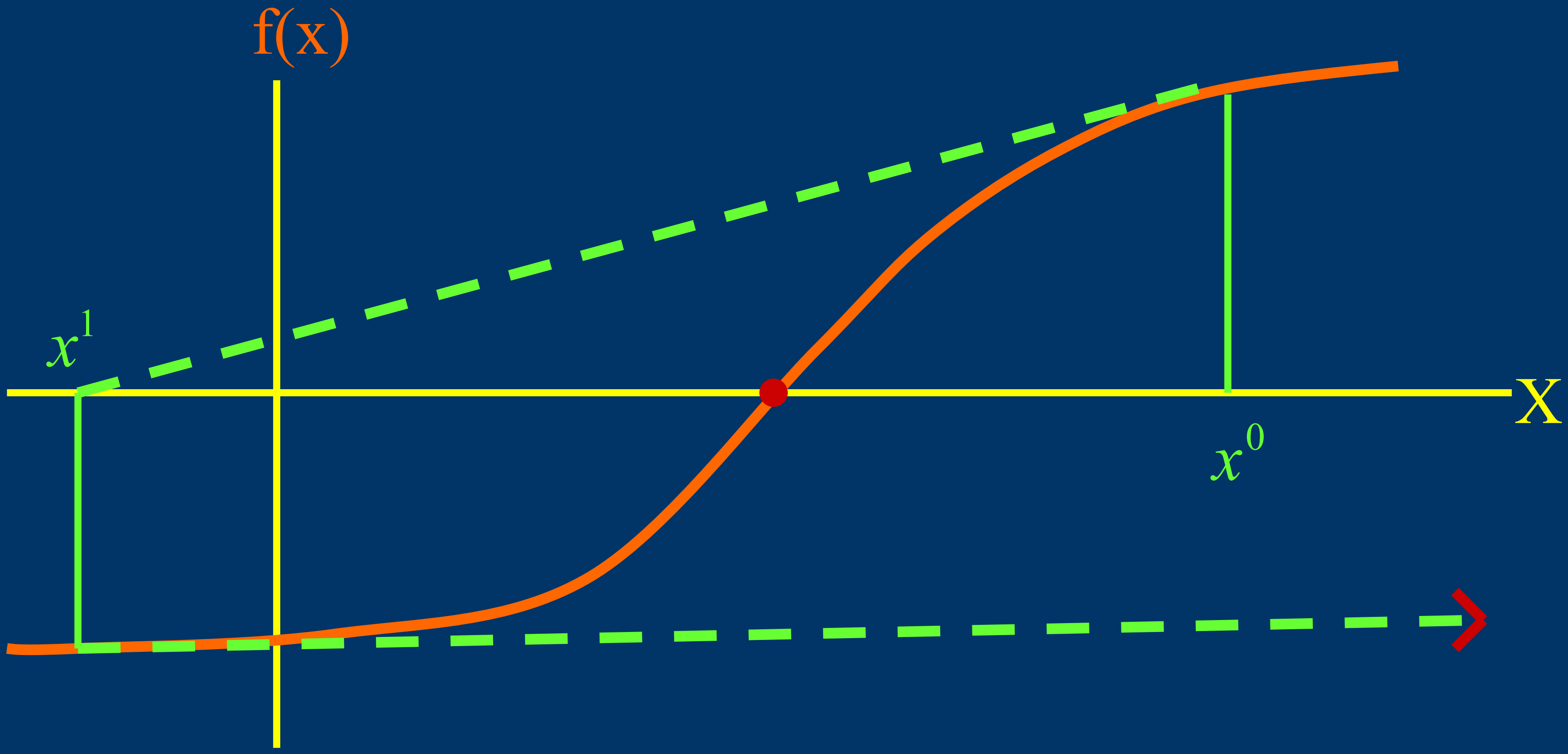
$$\left\| x^{k+1} - x^{k} \right\| \le \left(\frac{\beta \ell}{2} \left\| x^{k} - x^{k-1} \right\| \right) \left\| x^{k} - x^{k-1} \right\|$$

If $\left(\frac{\beta \ell}{2} \left\| x^{1} - x^{0} \right\| \right) \le \gamma < 1$

$$\left\| x^{k+1} - x^{k} \right\| \le \gamma^{k} \Rightarrow \sum_{k=0}^{\infty} \left(x^{k+1} - x^{k} \right) + x^{0} \text{ converges}$$

Non-converging Case

1-D Picture



Must Somehow Limit the changes in X

Newton Algorithm for Solving $F(x) = 0$

$x^0 =$ Initial Guess, $k = 0$

Repeat {

Compute $F(x^k), J_F(x^k)$

Solve $J_F(x^k)\Delta x^{k+1} = -F(x^k)$ for Δx^{k+1}

$x^{k+1} = x^k + \text{limited}(\Delta x^{k+1})$

$k = k + 1$

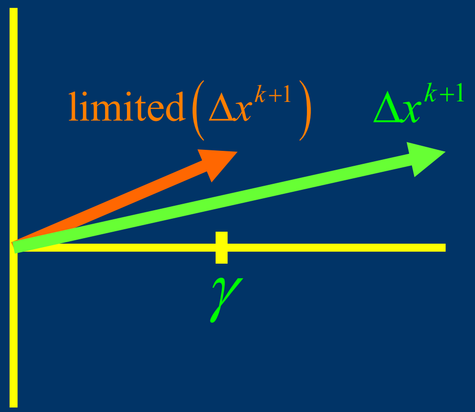
} Until $\|\Delta x^{k+1}\|, \|F(x^{k+1})\|$ small enough

Newton Method with Limiting

Limiting Methods

- Direction Corrupting

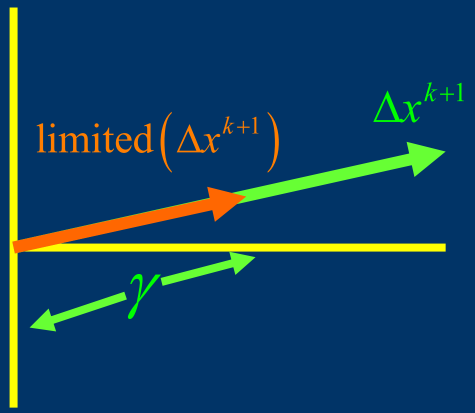
$$\text{limited}\left(\Delta x^{k+1}\right)_i = \begin{cases} \Delta x_i^{k+1} \text{ if } \left|\Delta x_i^{k+1}\right| < \gamma \\ \gamma\, sign\left(\Delta x_i^{k+1}\right) \text{ otherwise} \end{cases}$$



- NonCorrupting

$$\text{limited}\left(\Delta x^{k+1}\right) = \alpha \Delta x^{k+1}$$

$$\alpha = \min\left\{1, \frac{\gamma}{\left\|\Delta x^{k+1}\right\|}\right\}$$



Heuristics, No Guarantee of Global Convergence

Newton Method with Limiting

Damped Newton Scheme

General Damping Scheme

Solve $J_F\left(x^k\right)\Delta x^{k+1} = -F\left(x^k\right)$ for Δx^{k+1}

$$x^{k+1} = x^k + \alpha^k \Delta x^{k+1}$$

Key Idea: Line Search

Pick α^k to minimize $\left\|F\left(x^k + \alpha^k \Delta x^{k+1}\right)\right\|_2^2$

$$\left\|F\left(x^k + \alpha^k \Delta x^{k+1}\right)\right\|_2^2 \equiv F\left(x^k + \alpha^k \Delta x^{k+1}\right)^T F\left(x^k + \alpha^k \Delta x^{k+1}\right)$$

Method Performs a one-dimensional search in Newton Direction

Newton Method with Limiting

Damped Newton

Convergence Theorem

If

$a)\ \left\| J_F^{-1}\left(x^k\right) \right\| \le \beta \quad \left(\text{Inverse is bounded}\right)$

$b)\ \left\| J_F\left(x\right) - J_F\left(y\right) \right\| \le \ell \left\| x - y \right\| \quad \left(\text{Derivative is Lipschitz Cont}\right)$

Then

There exists a set of α^k's $\in \left(0,1\right]$ such that

$$\left\| F\left(x^{k+1}\right) \right\| = \left\| F\left(x^k + \alpha^k \Delta x^{k+1}\right) \right\| < \gamma \left\| F\left(x^k\right) \right\| \text{ with } \gamma < 1$$

Every Step reduces F-- Global Convergence!

Newton Method with Limiting

Damped Newton

Nested Iteration

$x^0 =$ Initial Guess, $k = 0$

Repeat {

Compute $F\left(x^k\right), J_F\left(x^k\right)$

Solve $J_F\left(x^k\right)\Delta x^{k+1} = -F\left(x^k\right)$ for Δx^{k+1}

Find $\alpha^k \in (0,1]$ such that $\left\| F\left(x^k + \alpha^k \Delta x^{k+1}\right)\right\|$ is minimized

$x^{k+1} = x^k + \alpha^k \Delta x^{k+1}$

$k = k+1$

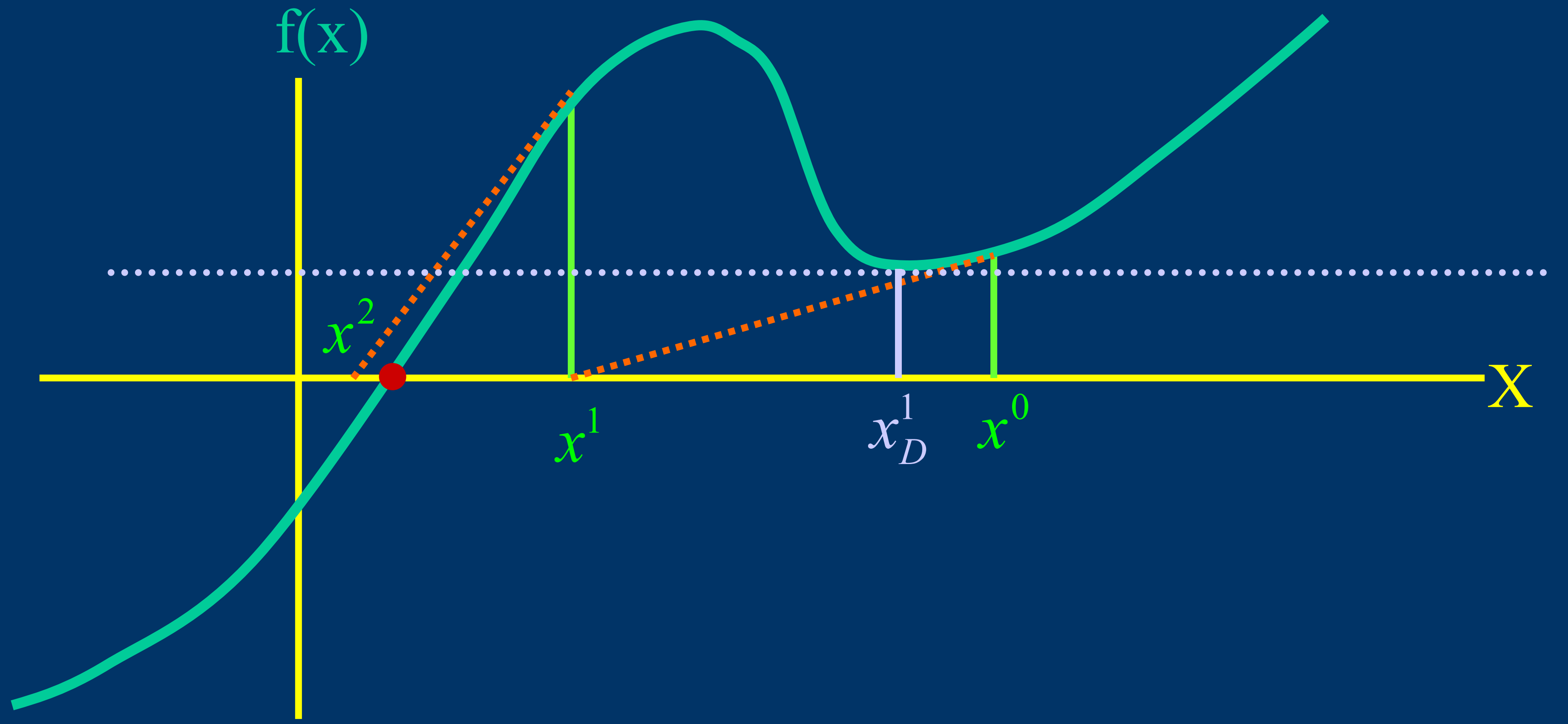
} Until $\left\|\Delta x^{k+1}\right\|$, $\left\| F\left(x^{k+1}\right)\right\|$ small enough

How can one find the damping coefficients?

Newton Method with Limiting

Damped Newton

Singular Jacobian Problem



Damped Newton Methods "push" iterates to local minimums
Finds the points where Jacobian is Singular

Summary

- Quick Review of 1-D Newton
  - Convergence Testing
- Multidimensonal Newton Method
  - Basic Algorithm
  - Description of the Jacobian.
  - Jacobian Construction.
  - Local Convergence Theorem
- Damped Newton Method
  - Nested Algorithm with line search
  - Global convergence **IF** Jacobian nonsingular