HWRS 561b
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HWRS 505: Vadose Zone Hydrology

Steady-state 1D unsat flow (Part 2)

Agenda:

Solution to nonlinear equations

Review

Acting like (nonlinear) **diffusion** for transporting water (i.e., θ_w or S_w)

- Steady-state unsaturated flow
  - Negative water pressure; flow driven by capillary pressure and gravity
  - Relative permeability is a nonlinear function of water saturation

Acting like (nonlinear) **advection** for transporting water (i.e., θ_w or S_w)

  - At heterogeneous interfaces, water saturation does not need to be continuous, but capillary pressure and water pressure have to be continuous.
  - Numerical solution of steady-state unsaturated flow.

Key idea: Divide the domain into many boxes and convert the **differential equation** to a system of (nonlinear) **algebraic equations**.

Technique: Use **finite difference** to approximate **derivatives**.

Note: There are other techniques available, but we will only discuss finite difference in this class. "*HWRS 504 Numerical Methods and Deep Learning for Environmental Modeling*" will cover other more advanced topics.

Solution to Nonlinear Equations

- Example: Determine $\sqrt[3]{25}$
  - ✓ First write the problem in a more easily-evaluated form:

If $x = \sqrt[3]{25}$, then $x^3 = 25$, or

$$F(x) = x^3 - 25$$

In general, we wish to find roots, or zeros, of the general nonlinear equation

$$F(x) = 0, \quad (\text{find } x)$$

For our example, $F(x) = x^3 - 25$

Solution to Nonlinear Equations

❑ Newton-Raphson method

✓ A systematic and very popular method based on truncated Taylor series.

Assume $F(x) \in C^2[a,b]$, and let the problem given by $F(x) = 0$. Let $x_0 \in [a,b]$.

Then:

$$F(x) = F(x_0) + (x - x_0)\frac{dF}{dx}\bigg|_{x_0} + \frac{(x - x_0)^2}{2}\frac{d^2F}{dx^2}\bigg|_{\xi} + \cdots = 0 \qquad \xi \in [x, x_0]$$

If the last term $O((\Delta x)^2)$ is neglected, then:

$$F(x_0) + (x - x_0)\frac{dF}{dx}\bigg|_{x_0} \approx 0$$

If this is set equal to zero, then an approximation to the true solution x may be solved for. Denote it by x_1, and set:

$F(x_0) + (x_1 - x_0)\frac{dF}{dx}\bigg|_{x_0} \approx 0 \Rightarrow x_1 = x_0 - \frac{F(x_0)}{\frac{dF}{dx}|_{x_0}}$, which is a better (updated) estimate of the root.

Then expand about x_1 to obtain: $x_2 = x_1 - \frac{F(x_1)}{\frac{dF}{dx}|_{x_1}}$

Solution to Nonlinear Equations

❑ Newton-Raphson method

- ✓ In general:

$$x_{n+1} = x_n - \frac{F(x_n)}{\frac{dF}{dx}\big|_{x_n}}$$

"Newton-Raphson" Approximation

- ✓ Criteria for stopping the iteration:

(a) $|x_{n+1} - x_n| < \epsilon$

(b) $\left|\frac{x_{n+1} - x_n}{x_{n+1}}\right| < \epsilon$ $(x_{n+1} \neq 0)$

(c) $|F(x_{n+1})| < \epsilon$

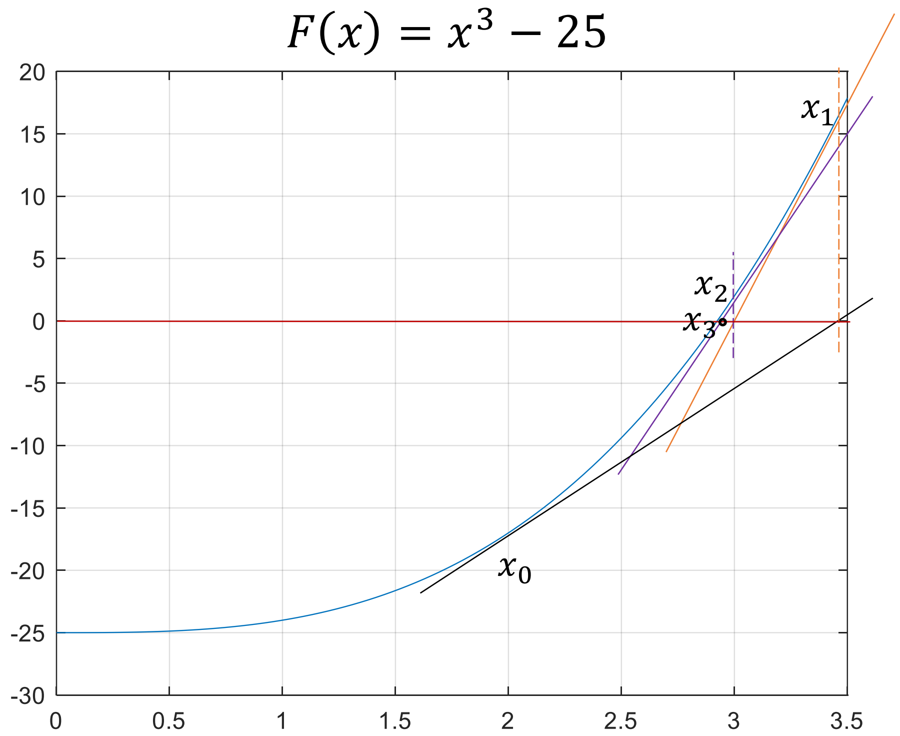
Solution to Nonlinear Equations

Newton-Raphson method: Examples

- Example 1a:

$$F(x) = x^3 - 25$$

$$\frac{dF}{dx} = 3x^2$$



Let $x_0 = 2$

$$x_1 = 2 - \frac{-17}{12} = 3.417$$

$$x_2 = 3.417 - 0.425 = 2.992$$

$$x_3 = 2.992 - 0.066 = 2.926$$

$$x_4 = 2.926 - 0.002 = 2.9240$$

$$x_5 = 2.9240 - 0.0000 = 2.9240$$ (correct to 4 figures, actually correct to ~7 figures)

So, in 4 iterations we arrive at a solution that is accurate to > 4 figures.

Solution to Nonlinear Equations

❑ Newton-Raphson method: Examples

✓ Example 1b:

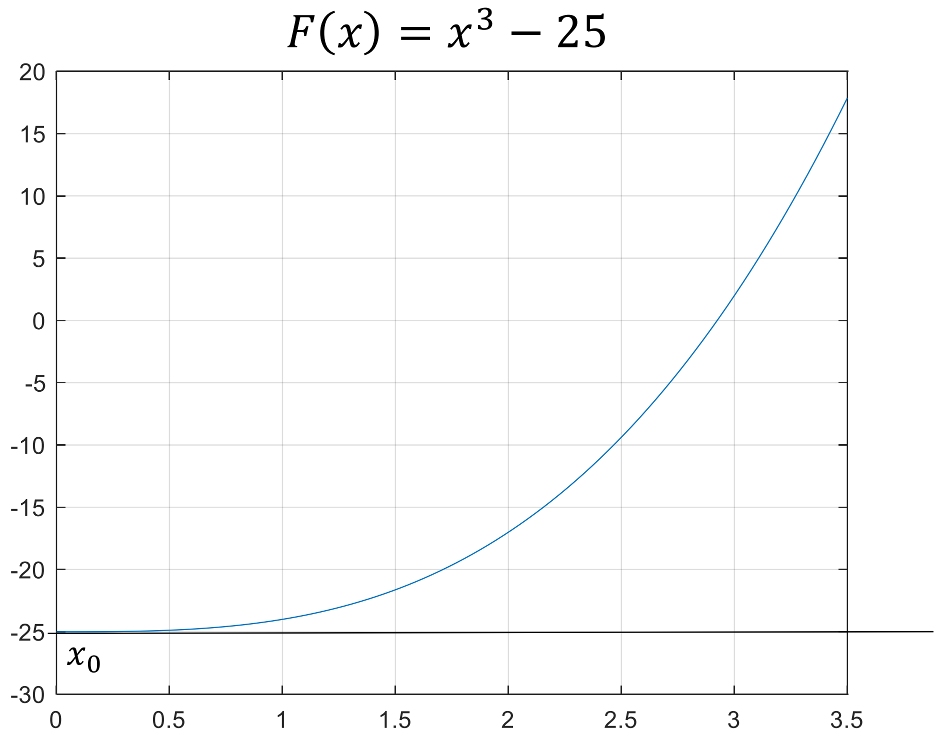
$$F(x) = x^3 - 25$$

$$\frac{dF}{dx} = 3x^2$$

Let $x_0 = 0$

$$\left.\begin{aligned} F(x_0) &= -25 \\ \left.\frac{dF}{dx}\right|_{x_0} &= 0 \end{aligned}\right\} \Rightarrow x_1 = 0 - \frac{-25}{0}$$

(Undefined!)



- Use slope of curve to project linearly to the F=0 axis
- Initial guess must be a "good" one

Note: When using the N-R method to solve PDEs, there is a natural "good" initial guess—solution from the previous time step.

Solution to Nonlinear Equations

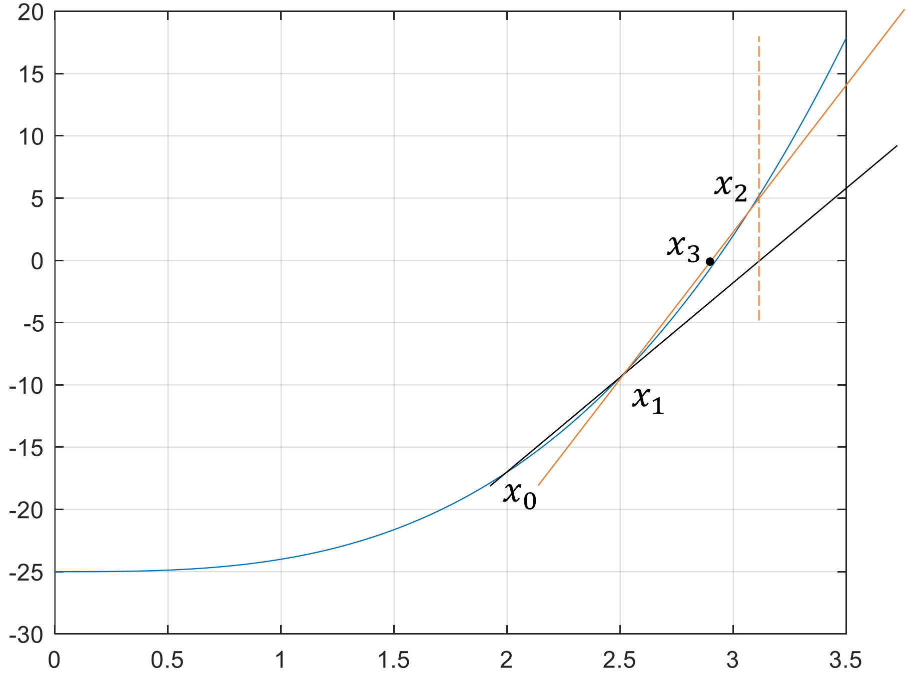
❑ An Variant of N-R: Secant Method

✓ Instead of evaluating $\frac{dF}{dx}|_{x_n}$, estimate this by FDA $\dfrac{F(x_n) - F(x_{n-1})}{x_n - x_{n-1}}$

$$\Rightarrow x_{n+1} = x_n - \frac{F(x_n)}{\left(\frac{F(x_n) - F(x_{n-1})}{x_n - x_{n-1}}\right)}$$

$$\Rightarrow x_{n+1} = x_n - \frac{F(x_n)(x_n - x_{n-1})}{F(x_n) - F(x_{n-1})}$$

$F(x) = x^3 - 25$



Solution to Nonlinear Equations

Systems of Nonlinear Equations

- Consider the general system of nonlinear equations:

$$F_1(x_1, x_2, \dots, x_N) = 0$$
$$F_2(x_1, x_2, \dots, x_N) = 0$$
$$\dots$$
$$F_N(x_1, x_2, \dots, x_N) = 0$$

How to solve?

Solution to Nonlinear Equations

❑ Systems of Nonlinear Equations

✓ Newton-Raphson

- Now we need a multidimensional Taylor series
- Choose point $\boldsymbol{x}^0 = (x_1^0, x_2^0, \dots, x_N^0)$

$$F_1(x_1, x_2, \dots, x_N) = F_1(\boldsymbol{x})$$

$$= F_1(\boldsymbol{x}_0) + (x_1 - x_1^0)\frac{\partial F_1}{\partial x_1}\bigg|_{\boldsymbol{x}^0} + (x_2 - x_2^0)\frac{\partial F_1}{\partial x_2}\bigg|_{\boldsymbol{x}^0} + \cdots + (x_N - x_N^0)\frac{\partial F_1}{\partial x_N}\bigg|_{\boldsymbol{x}^0} + O(\Delta x^2)$$

Similarly,

$$F_2(\boldsymbol{x}) = F_2(\boldsymbol{x}_0) + (x_1 - x_1^0)\frac{\partial F_2}{\partial x_1}\bigg|_{\boldsymbol{x}^0} + (x_2 - x_2^0)\frac{\partial F_2}{\partial x_2}\bigg|_{\boldsymbol{x}^0} + \cdots + (x_N - x_N^0)\frac{\partial F_2}{\partial x_N}\bigg|_{\boldsymbol{x}^0} + O(\Delta x^2)$$

…

$$F_i(\boldsymbol{x}) = F_i(\boldsymbol{x}_0) + \sum_{j=1}^{N}(x_j - x_j^0)\frac{\partial F_i}{\partial x_j}\bigg|_{\boldsymbol{x}^0} + O(\Delta x^2)$$

…

Solution to Nonlinear Equations

❑ Systems of Nonlinear Equations

✓ Newton-Raphson

- Now we have a set of algebraic equations:

$$(x_1 - x_1^0)\frac{\partial F_1}{\partial x_1}\bigg|_{\boldsymbol{x}^0} + (x_2 - x_2^0)\frac{\partial F_1}{\partial x_2}\bigg|_{\boldsymbol{x}^0} + \cdots + (x_N - x_N^0)\frac{\partial F_1}{\partial x_N}\bigg|_{\boldsymbol{x}^0} + O(\Delta x^2) = F_1(\boldsymbol{x}) - F_1(\boldsymbol{x}^0)$$
$$= 0 - F_1(\boldsymbol{x}^0)$$
$$= -F_1(\boldsymbol{x}^0)$$

…

$$(x_1 - x_1^0)\frac{\partial F_i}{\partial x_1}\bigg|_{\boldsymbol{x}^0} + (x_2 - x_2^0)\frac{\partial F_i}{\partial x_2}\bigg|_{\boldsymbol{x}^0} + \cdots + (x_N - x_N^0)\frac{\partial F_i}{\partial x_N}\bigg|_{\boldsymbol{x}^0} + O(\Delta x^2) = -F_i(\boldsymbol{x}^0)$$

…

If we neglect the $O(\Delta x^2)$ terms and replace $\boldsymbol{x}$ on LHS by approximating value $\boldsymbol{x}^1$, then this is a system of linear algebraic equation for the variables $\left(x_j^1 - x_j^0\right), j = 1, 2, \dots, N$. That is,

Solution to Nonlinear Equations

❑ Systems of Nonlinear Equations

- ✓ Newton-Raphson

$$\begin{bmatrix} \left.\frac{\partial F_1}{\partial x_1}\right|_{\boldsymbol{x}^0} & \left.\frac{\partial F_1}{\partial x_2}\right|_{\boldsymbol{x}^0} & \cdots & \left.\frac{\partial F_1}{\partial x_N}\right|_{\boldsymbol{x}^0} \\ \left.\frac{\partial F_2}{\partial x_1}\right|_{\boldsymbol{x}^0} & \left.\frac{\partial F_2}{\partial x_2}\right|_{\boldsymbol{x}^0} & \cdots & \left.\frac{\partial F_2}{\partial x_N}\right|_{\boldsymbol{x}^0} \\ \cdots & \cdots & \cdots & \cdots \\ \left.\frac{\partial F_N}{\partial x_1}\right|_{\boldsymbol{x}^0} & \left.\frac{\partial F_N}{\partial x_2}\right|_{\boldsymbol{x}^0} & \cdots & \left.\frac{\partial F_N}{\partial x_N}\right|_{\boldsymbol{x}^0} \end{bmatrix} \begin{bmatrix} (x_1^1 - x_1^0) \\ (x_2^1 - x_2^0) \\ \cdots \\ (x_N^1 - x_N^0) \end{bmatrix} = \begin{bmatrix} -F_1(\boldsymbol{x}^0) \\ -F_2(\boldsymbol{x}^0) \\ \cdots \\ -F_N(\boldsymbol{x}^0) \end{bmatrix}$$

<u>OR</u>

$$\boldsymbol{J}^0 \cdot \delta \boldsymbol{x}^1 = -\boldsymbol{F}^0$$

The matrix $\boldsymbol{J}$ is often referred to as the <u>Jacobian matrix</u>.

Solution to Nonlinear Equations

❑ Systems of Nonlinear Equations

✓ Newton-Raphson

- The general iteration is then of the form:

$$\boldsymbol{J}^n \cdot \delta \boldsymbol{x}^{n+1} = -\boldsymbol{F}^n$$

- This is of the form:

$$\boldsymbol{J}^n \cdot (\boldsymbol{x}^{n+1} - \boldsymbol{x}^n) = -\boldsymbol{F}^n$$

$$\boldsymbol{x}^{n+1} = \boldsymbol{x}^n - (\boldsymbol{J}^n)^{-1} \cdot \boldsymbol{F}^n$$

- Can also define “quasi-Newton” methods (such as the secant method) by approximating the derivatives in $\boldsymbol{J}$ using FDA