HWRS 505: Vadose Zone Hydrology

Lecture 11

9/26/2023

Today:

Steady-state unsaturated flow and numerical solution

Review of Lecture 10

❖ Steady-state <u>unsaturated</u> flow

  ▪ Negative water pressure; flow driven by <u>capillary pressure</u> and <u>gravity</u>

  ▪ Relative permeability is a <u>nonlinear</u> function of water saturation

  ▪ 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.

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

<u>Technique</u>: 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 for Environmental Transport Problems*" will cover other more advanced topics.

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

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

$$\frac{\partial K_{unsat}}{\partial z}$$

$$= \frac{\partial K_{unsat}}{\partial S_w} \frac{\partial S_w}{\partial z}$$

wave elocity
(nonlinear function of S_w)

Steady-State Unsaturated Flow: Numerical Soln.

Slide from Lecture 10

$$\frac{\partial \theta_w}{\partial t}^{\,0} - \frac{\partial}{\partial z}\left(K \frac{\partial \psi_w}{\partial z}\right) - \frac{\partial K}{\partial z} = 0 \quad \xrightarrow{\text{Steady-state}} \quad \underbrace{\frac{d}{dz}\left(K \frac{d\psi_w}{dz}\right)}_{①} + \underbrace{\frac{dK}{dz}}_{②} = 0 \qquad (1)$$

z

z_N
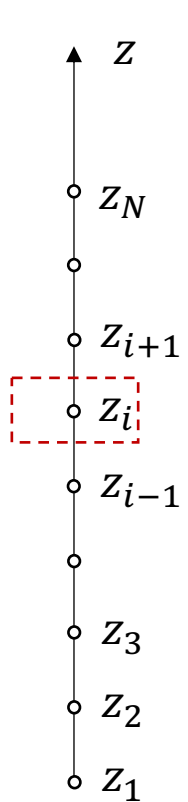
$① \quad \frac{d}{dz}\left(K \frac{d\psi_w}{dz}\right)\Big|_{z_i} \approx \frac{\left(K \frac{d\psi_w}{dz}\right)_{i+1/2} - \left(K \frac{d\psi_w}{dz}\right)_{i-1/2}}{\Delta z} \approx \frac{K_{i+1/2}\frac{\psi_{w,i+1} - \psi_{w,i}}{\Delta z} - K_{i-1/2}\frac{\psi_{w,i} - \psi_{w,i-1}}{\Delta z}}{\Delta z}$

z_{i+1}

$= \frac{K_{i+1/2}(\psi_{w,i+1} - \psi_{w,i}) - K_{i-1/2}(\psi_{w,i} - \psi_{w,i-1})}{\Delta z^2}$

$② \quad \frac{dK}{dz}\Big|_{z_i} \approx \frac{K_{i+1/2} - K_{i-1/2}}{\Delta z}$

z_i

z_{i-1}

$\Rightarrow \frac{K_{i+1/2}}{\Delta z^2}(\psi_{w,i+1} - \psi_{w,i}) - \frac{K_{i-1/2}}{\Delta z^2}(\psi_{w,i} - \psi_{w,i-1}) + K_{i+1/2}\frac{1}{\Delta z} - K_{i-1/2}\frac{1}{\Delta z} = 0$

z_3

z_2

$\Rightarrow \frac{K_{i+1/2}}{\Delta z^2}\psi_{w,i+1} - \left(\frac{K_{i+1/2}}{\Delta z^2} + \frac{K_{i-1/2}}{\Delta z^2}\right)\psi_{w,i} + \frac{K_{i-1/2}}{\Delta z^2}\psi_{w,i-1} + K_{i+1/2}\frac{1}{\Delta z} - K_{i-1/2}\frac{1}{\Delta z} = 0$

z_1

This is an algebraic equation with 3 unknowns. We can write such an algebraic equation for each node or box and we can get N algebraic equations for the N unknowns $(\psi_{w,1}, \psi_{w,2}, \dots, \psi_{w,N})$

Steady-State Unsaturated Flow: Numerical Soln.

Slide from Lecture 10

In matrix form:

$$\begin{pmatrix} 1 & 0 & 0 & & & & \\ \dfrac{K_{3/2}}{\Delta z^2} & -\dfrac{(K_{3/2}+K_{5/2})}{\Delta z^2} & \dfrac{K_{5/2}}{\Delta z^2} & & & & \\ & \dfrac{K_{5/2}}{\Delta z^2} & -\dfrac{(K_{5/2}+K_{7/2})}{\Delta z^2} & \dfrac{K_{7/2}}{\Delta z^2} & & & \\ & & \ddots & \ddots & \ddots & & \\ & & \dfrac{K_{i-1/2}}{\Delta z^2} & -\dfrac{(K_{i-1/2}+K_{i+1/2})}{\Delta z^2} & \dfrac{K_{i+1/2}}{\Delta z^2} & & \\ & & & \ddots & \ddots & \ddots & \\ & & & \dfrac{K_{n-1-1/2}}{\Delta z^2} & -\dfrac{(K_{n-1-1/2}+K_{n-1+1/2})}{\Delta z^2} & \dfrac{K_{n-1+1/2}}{\Delta z^2} \\ & & & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \psi_{w,1} \\ \psi_{w,2} \\ \psi_{w,3} \\ \vdots \\ \psi_{w,i} \\ \vdots \\ \psi_{w,n-1} \\ \psi_{w,n} \end{pmatrix} = \begin{pmatrix} B.C. \\ \dfrac{K_{3/2}-K_{5/2}}{\Delta z} \\ \dfrac{K_{5/2}-K_{7/2}}{\Delta z} \\ \vdots \\ \dfrac{K_{i-1/2}-K_{i+1/2}}{\Delta z} \\ \vdots \\ \dfrac{K_{n-1-1/2}-K_{n-1+1/2}}{\Delta z} \\ B.C. \end{pmatrix}$$

$$\Rightarrow \boldsymbol{F}(\boldsymbol{\psi}_w) \cdot \boldsymbol{\psi}_w = \boldsymbol{R}$$ How to solve this nonlinear system of algebraic equations?

=> Employ an iterative methods

Solution to Nonlinear Equations

❑ Example: Determine $\sqrt[3]{25}$

✓ First write the problem in a more easily-evaluated form:

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

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

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 <u>equal</u> to zero, then an approximation to the true solution x may be solved for.
Denote it by x_1, and set:

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

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

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

(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 $x_0 = 2$
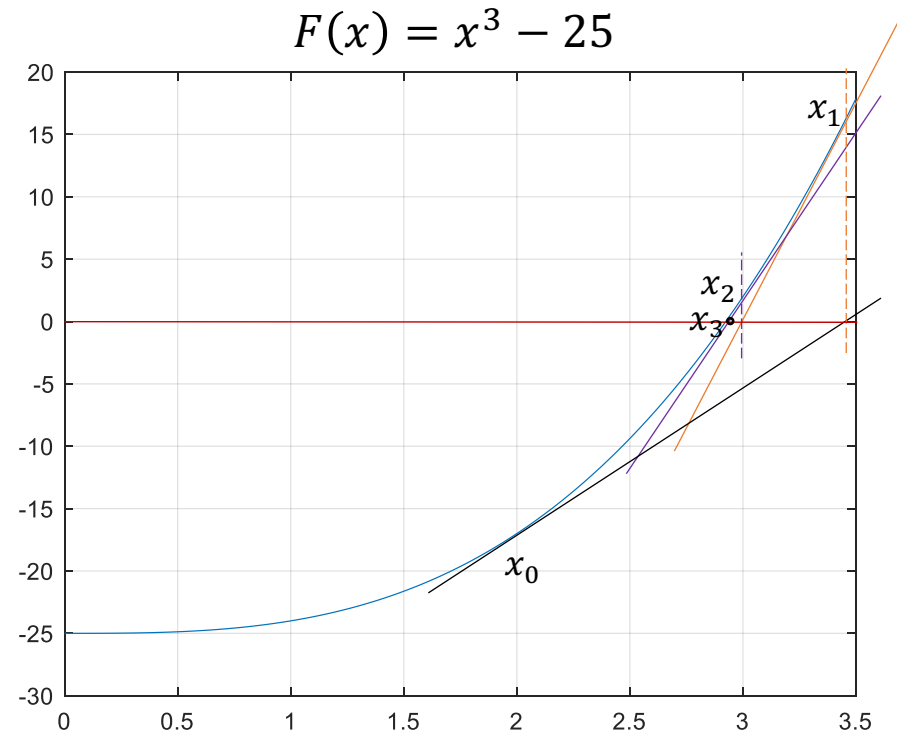
$$x_1 = 2 - \frac{-17}{12} = 3.417$$

$$x_2 = 3.417 - 0.425 = 2.992$$

$$x_3 = 2.992 - 0.066 = 2.926$$

$$x_4 = 2.926 - 0.002 = 2.9240$$

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

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

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

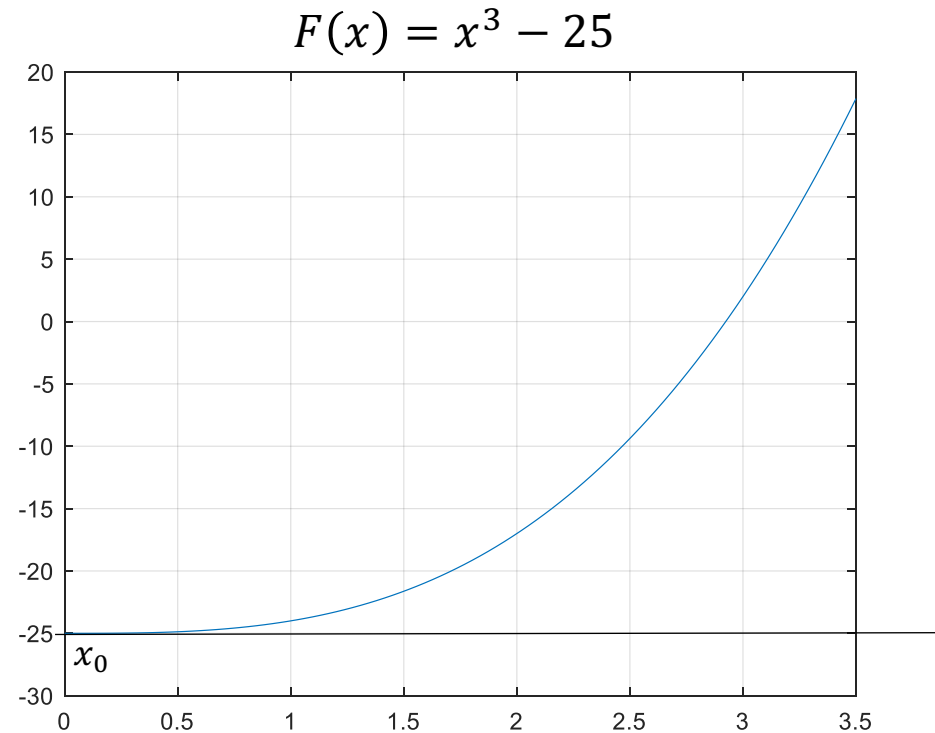# Solution to Nonlinear Equations

❑ Newton-Raphson method: Examples

✓ Example 1b:

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

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

Let $x_0 = 0$

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

(Undefined!)

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

- 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.
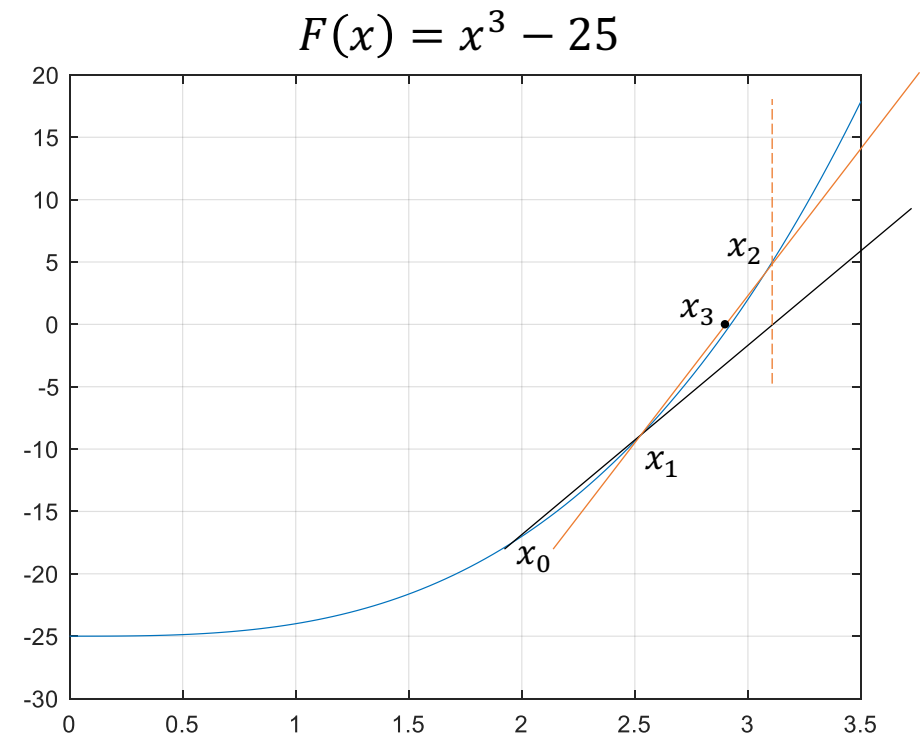
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Solution to Nonlinear Equations

❑ **An Variant of N-R: Secant Method**

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

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

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

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

Solution to Nonlinear Equations

❑ Systems of Nonlinear Equations

✓ Consider the general system of nonlinear equations:

$$F_1(x_1, x_2, \ldots, x_N) = 0$$

$$F_2(x_1, x_2, \ldots, x_N) = 0$$

$$\ldots$$

$$F_N(x_1, x_2, \ldots, x_N) = 0$$

How to solve?

Solution to Nonlinear Equations

❑ Systems of Nonlinear Equations

✓ Newton-Raphson

- Now we need a multidimensional Taylor series

- Choose point $\boldsymbol{x}^0 = (x_1^0, x_2^0, \ldots, x_N^0)$

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

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

Similarly,

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

…

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

…

Solution to Nonlinear Equations

❑ Systems of Nonlinear Equations

✓ Newton-Raphson

- Now we have a set of algebraic equations:

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

...

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

...

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

Solution to Nonlinear Equations

❑ Systems of Nonlinear Equations

✓ Newton-Raphson

$$\begin{bmatrix} \left.\dfrac{\partial F_1}{\partial x_1}\right|_{x^0} & \left.\dfrac{\partial F_1}{\partial x_2}\right|_{x^0} & \cdots & \left.\dfrac{\partial F_1}{\partial x_N}\right|_{x^0} \\[2mm] \left.\dfrac{\partial F_2}{\partial x_1}\right|_{x^0} & \left.\dfrac{\partial F_2}{\partial x_2}\right|_{x^0} & \cdots & \left.\dfrac{\partial F_2}{\partial x_N}\right|_{x^0} \\[1mm] \cdots & \cdots & \cdots & \cdots \\[1mm] \left.\dfrac{\partial F_N}{\partial x_1}\right|_{x^0} & \left.\dfrac{\partial F_N}{\partial x_2}\right|_{x^0} & \cdots & \left.\dfrac{\partial F_N}{\partial x_N}\right|_{x^0} \end{bmatrix} \begin{bmatrix} (x_1^1 - x_1^0) \\[2mm] (x_2^1 - x_2^0) \\[2mm] \cdots \\[2mm] (x_N^1 - x_N^0) \end{bmatrix} = \begin{bmatrix} -F_1(\boldsymbol{x}^0) \\[2mm] -F_2(\boldsymbol{x}^0) \\[2mm] \cdots \\[2mm] -F_N(\boldsymbol{x}^0) \end{bmatrix}$$

<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