HWRS 505: Vadose Zone Hydrology

Lecture 11

10/1/2024

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.

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)

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

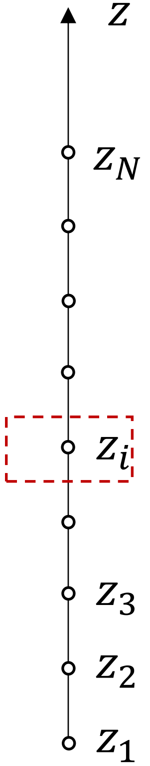
<u>Technique</u>: Use **finite difference** to approximate **derivatives**.

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.

Steady-State Unsaturated Flow: Numerical Soln.

Slide from Lecture 10

$$\cancelto{0}{\frac{\partial \theta_w}{\partial t}} - \frac{\partial}{\partial z}\left(K\frac{\partial \psi_w}{\partial z}\right) - \frac{\partial K}{\partial z} = 0 \quad \xrightarrow{\text{Steady-state}} \quad \frac{\mathrm{d}}{\mathrm{d}z}\left(K\frac{\mathrm{d}\psi_w}{\mathrm{d}z}\right) + \frac{\mathrm{d}K}{\mathrm{d}z} = 0 \qquad (1)$$



1

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

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

2

$$\left.\frac{\mathrm{d}K}{\mathrm{d}z}\right|_{z_i} \approx \frac{K_{i+1/2} - K_{i-1/2}}{\Delta z}$$

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

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

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:

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

$\Rightarrow \boldsymbol{F}(\boldsymbol{\psi}_w) \cdot \boldsymbol{\psi}_w = \boldsymbol{R}$ 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:

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

$F(x_0) + (x_1 - x_0)\frac{dF}{dx}\Big|_{x_0} \approx 0 \Rightarrow\ x_1 = x_0 - \frac{F(x_0)}{\frac{dF}{dx}|_{x_0}}$, 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 $x_0 = 2$

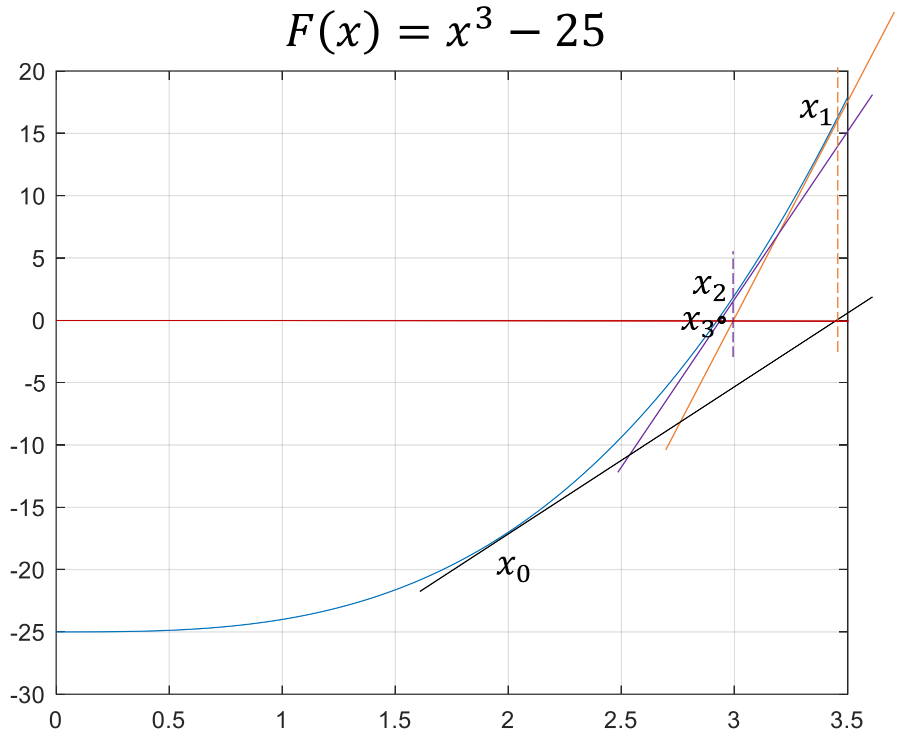
$$x_1 = 2 - \frac{-17}{12} = 3.417$$

$$x_2 = 3.417 - 0.425 = 2.992$$

$$x_3 = 2.992 - 0.066 = 2.926$$

$$x_4 = 2.926 - 0.002 = 2.9240$$

$$x_5 = 2.9240 - 0.0000 = 2.9240$$ (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:

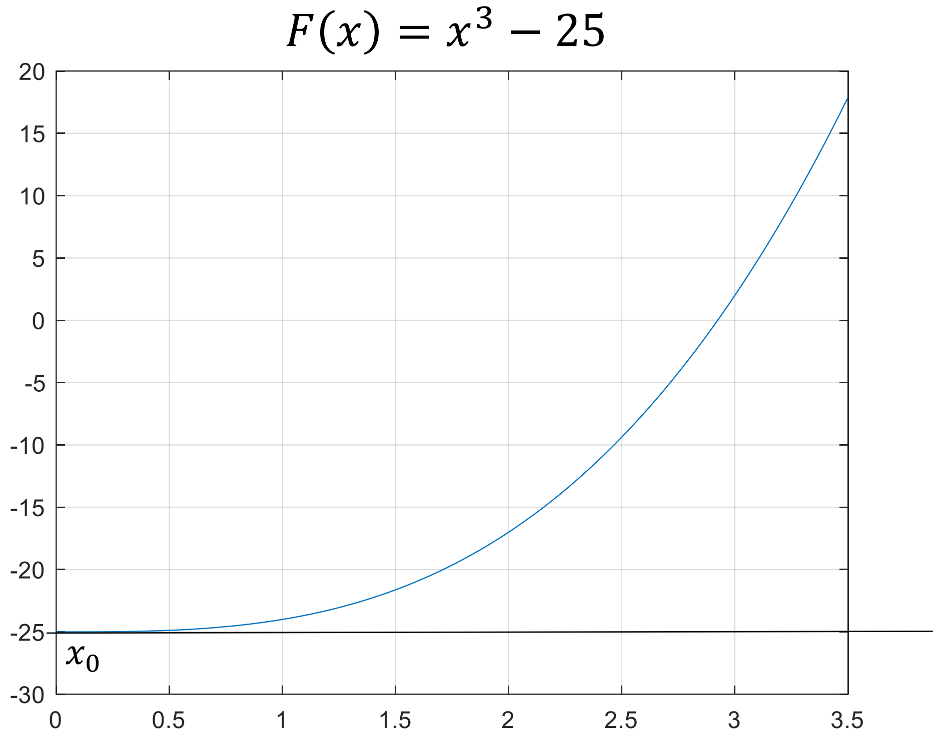
$$F(x) = x^3 - 25$$

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

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

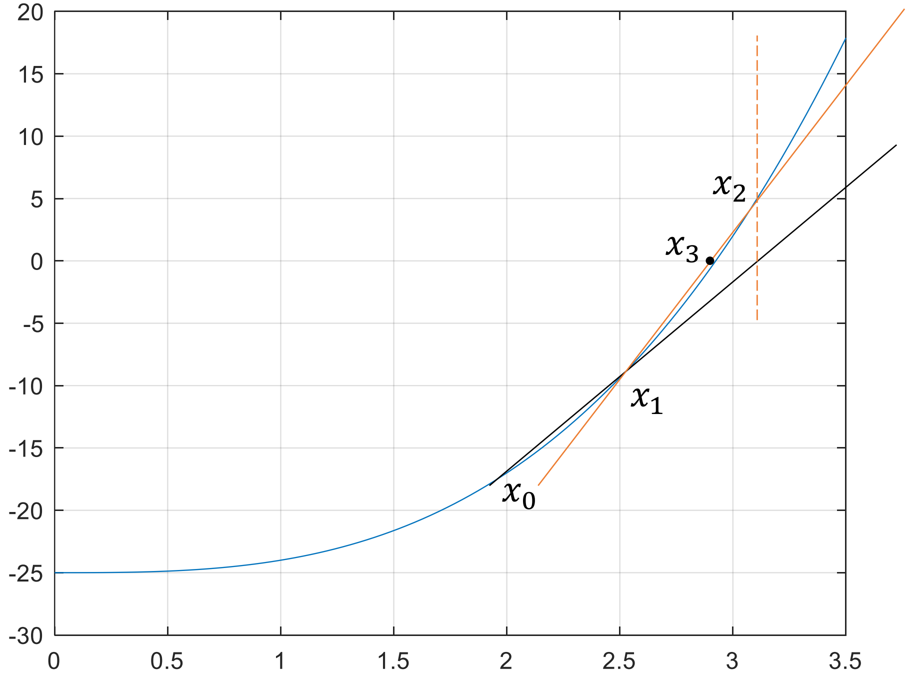
❑ An Variant of N-R: Secant Method

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

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

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

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



Solution to Nonlinear Equations

❑ Systems of Nonlinear Equations

- ✓ Consider the general system of nonlinear equations:

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

$$\dots$$

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

<u>How to solve?</u>

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