Lecture7

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Newton method

- Solve $x^2 - 1 = 0$.
  - Its solution is $x = \pm 1$, of course.
  - First, assume a temporal solution, x_0.
  - Then, define how far we are from the real solution.
$$r(x_0) = x_0^2 - 1$$
  - For the exact solutions, it becomes zero.
  - We hope that the next solution, $x + \delta x$, becomes the exact solution.
$$(x_0 + \delta x)^2 - 1 = 0$$
  - Simple manipulation yields
$$2x_0 \delta x + (\delta x)^2 = -(x_0^2 - 1)$$
  - We can calculate δx with the first-order approximation.

An example

- Start from $x_0 = 2$.
  - Remember that $2x_0\delta x + (\delta x)^2 \approx 2x_0\delta x = -(x_0^2 - 1)$
  - Therefore, $\delta x = -\frac{3}{4}$
  - Then, we set $x_1 = x_0 + \delta x = \frac{5}{4}$, which is already much closer to 1.
  - Once again, $2x_1\delta x = -(x_1^2 - 1)$ and $\delta x = -\frac{9}{40}$
  - Now, we have $x_2 = x_1 + \delta x = \frac{41}{40}$
- Start from $x_0 = -2$. Is your solution approaching to 1?

Coupled nonlinear equations

- Consider a set of coupled nonlinear equations.
  - Three variables, ϕ_1, ϕ_2, and ϕ_3.
  - Three equations read

$$
\begin{aligned}
F_1(\phi_1, \phi_2, \phi_3) &= \phi_2 - 2\phi_1 - e^{\phi_1} = 0 \\
F_2(\phi_1, \phi_2, \phi_3) &= \phi_3 - 2\phi_2 + \phi_1 - e^{\phi_2} = 0 \\
F_3(\phi_1, \phi_2, \phi_3) &= -2\phi_3 + \phi_2 - e^{\phi_3} + 4 = 0
\end{aligned}
$$

  - How can we find the solution by using a numerical means?

Newton-Raphson method (1)

- What is our goal?
  - To find a set of ϕ_1, ϕ_2, and ϕ_3, which satisfies

$$\begin{bmatrix} F_1(\phi_1, \phi_2, \phi_3) \\ F_2(\phi_1, \phi_2, \phi_3) \\ F_3(\phi_1, \phi_2, \phi_3) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

  - Of course, we don't know the solution.
  - We can make a guess, $\phi^0 = [\phi_1^0 \quad \phi_2^0 \quad \phi_3^0]^T$.

$$r = \begin{bmatrix} F_1(\phi_1^0, \phi_2^0, \phi_3^0) \\ F_2(\phi_1^0, \phi_2^0, \phi_3^0) \\ F_3(\phi_1^0, \phi_2^0, \phi_3^0) \end{bmatrix} \neq \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

  - By correcting our guess, we want to make r small.

Newton-Raphson method (2)

- Update vector, $\delta\phi = [\delta\phi_1 \quad \delta\phi_2 \quad \delta\phi_3]^T$
  - We hope that $\phi^0 + \delta\phi$ is the real solution.

$$\begin{bmatrix} F_1(\phi_1^0 + \delta\phi_1, \phi_2^0 + \delta\phi_2, \phi_3^0 + \delta\phi_3) \\ F_2(\phi_1^0 + \delta\phi_1, \phi_2^0 + \delta\phi_2, \phi_3^0 + \delta\phi_3) \\ F_3(\phi_1^0 + \delta\phi_1, \phi_2^0 + \delta\phi_2, \phi_3^0 + \delta\phi_3) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

  - By using the linearization, we can have the following equation:

$$\begin{bmatrix} F_1(\phi_1^0, \phi_2^0, \phi_3^0) \\ F_2(\phi_1^0, \phi_2^0, \phi_3^0) \\ F_3(\phi_1^0, \phi_2^0, \phi_3^0) \end{bmatrix} + \begin{bmatrix} \partial F_1/\partial\phi_1 & \partial F_1/\partial\phi_2 & \partial F_1/\partial\phi_3 \\ \partial F_2/\partial\phi_1 & \partial F_2/\partial\phi_2 & \partial F_2/\partial\phi_3 \\ \partial F_3/\partial\phi_1 & \partial F_3/\partial\phi_2 & \partial F_3/\partial\phi_3 \end{bmatrix} \begin{bmatrix} \delta\phi_1 \\ \delta\phi_2 \\ \delta\phi_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

Newton-Raphson method (3)

- Introducing Jacobian matrix, J, and residue vector, r
  - In terms of these quantities, the update vector, $\delta\phi$, is written as:

$$J\delta\phi = -r$$

  - Once after $\delta\phi$ is calculated, the improved solution vector, ϕ^1, is constructed:

$$\phi^1 = \phi^0 + \delta\phi$$

  - In every Newton-Raphson step, r and $\delta\phi$ are monitored. When these vectors approach to the null vector, we have a better solution.

Jacobian matrix

- Key step
  - For the k-th step with a solution vector of ϕ^k, the Jacobam matrix of our example reads

$$J = \begin{bmatrix} -2 - \exp \phi_1^k & 1 & 0 \\ 1 & -2 - \exp \phi_2^k & 1 \\ 0 & 1 & -2 - \exp \phi_3^k \end{bmatrix}$$

MATLAB example (1)

- Step-by-step procedure
  - First, set up the solution vector, `phi`.

```
phi = [1; 2; 3;];
```

  - Using the solution vector, construct the Jacobain matrix, `Jaco`, and the residue vector, `res`.

```
Jaco(1,: ) = [-2-exp(phi(1)) 1 0];
Jaco(2,: ) = [1 -2-exp(phi(2)) 1];
Jaco(3,: ) = [0 1 -2-exp(phi(3))];
res(1,1) = [phi(2)-2*phi(1)-exp(phi(1))];
res(2,1) = [phi(3)-2*phi(2)+phi(1)-exp(phi(2))];
res(3,1) = [4-2*phi(3)+phi(2)-exp(phi(3))];
```

MATLAB example (2)

- Step-by-step procedure (continued)
  - Calculate the update vector, `update`.

```
update = Jaco \ (-res);
```

  - The solution is now updated.

```
phi = phi + update;
```

  - You can repeat it!

MATLAB example (3)

- Full code
  - Repeat ten times and plot the solution.

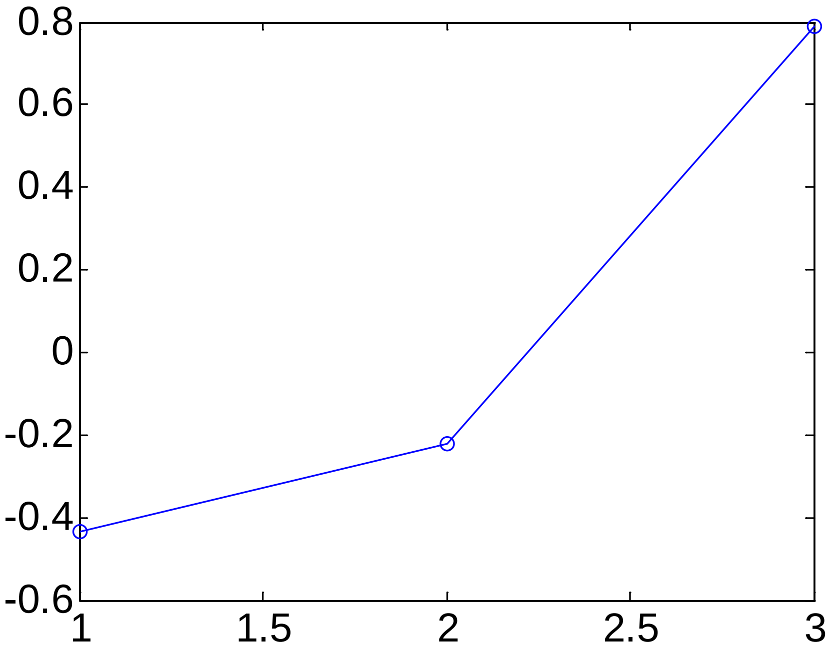
```
phi = [1; 2; 3;];
for newton=1:10
   Jaco(1,: ) = [-2-exp(phi(1)) 1 0];
   Jaco(2,: ) = [1 -2-exp(phi(2)) 1];
   Jaco(3,: ) = [0 1 -2-exp(phi(3))];
   res(1,1) = [phi(2)-2*phi(1)-exp(phi(1))];
   res(2,1) = [phi(3)-2*phi(2)+phi(1)-exp(phi(2))];
   res(3,1) = [4-2*phi(3)+phi(2)-exp(phi(3))];
   update = Jaco \ (-res);
   phi = phi + update;
end
plot(phi)
```

MATLAB example (4)

- Solution vector after ten steps

```
phi =

   -0.4352
   -0.2233
    0.7884
```



Homework#5

- Due: AM08:00, October 8
- Problem#1
  - Calculate the electrostatic potential, ϕ, by using the Newton method.

$$N^{+} + n_{int} e^{-\frac{\phi}{V_T}} - n_{int} e^{\frac{\phi}{V_T}} = 0$$

  Assume the room temperature. The intrinsic carrier density, n_{int}, of silicon at 300 K is 10^{10} cm^{-3}. Test your code for positive/negative values of N^{+}. Its absolute value varies from 10^{10} cm^{-3} to 10^{18} cm^{-3}.

  - Of course, it has also an analytic solution related to the arcsinh function. Compare your numerical results with the analytic solution.