06-262 Spring 2014: Newton's Method in MATLAB

From Pseudo-Code to Implementation in MATLAB

Introduction

- Newton's Method (also known as Newton-Raphson Method) is used to solve nonlinear (system) of equations, which can be represented as follows:

$$f(x) = 0$$

where $f(\cdot)$ is a general univariate nonlinear function and x is a (scalar) variable, and

$$\mathbf{F}(\mathbf{x}) = \mathbf{0}$$

where $\mathbf{F}(\cdot)$ is a <u>vector</u> of general <u>multivariate</u> nonlinear functions and $\mathbf{x}$ is a <u>vector</u> of variables

Examples

- **Single nonlinear equation**

$$\frac{1}{2}\frac{\epsilon^{3/2}}{(1-\epsilon)(1+\frac{1}{2}\epsilon)^{1/2}} - K_{eq} = 0$$

where ϵ is the (unknown) extent of reaction (variable to be solved for) and K_{eq} is a (known) equilibrium constant (a number)

- **System of nonlinear equations**

$$\mu_{\max}\left(1-\frac{C_p}{C_p^*}\right)^{0.52}\frac{C_c C_s}{K_s + C_s} - k_d C_c = 0$$

$$-Y_{s/c}\mu_{\max}\left(1-\frac{C_p}{C_p^*}\right)^{0.52}\frac{C_c C_s}{K_s + C_s} - m C_c = 0$$

$$Y_{p/c}\mu_{\max}\left(1-\frac{C_p}{C_p^*}\right)^{0.52}\frac{C_c C_s}{K_s + C_s} = 0$$

where $C_c,\ C_p,\ \text{and}\ C_s$ are unknowns and the other symbols are known

Newton's Method: Pseudo-Code

- Overview: http://en.wikipedia.org/wiki/Newton's_method
- Idea: given initial guess (crucial, as close to the solution as possible), iterate towards the solution of the nonlinear equation(s) using first-order derivative information (makes convergence fast). Method converges to <u>one</u> solution, but multiple solutions may exist that depend on the chosen initial guess.
- Pseudo-code for the univariate case:

Input: initial guess (x_0), maximum number of iterations (N), convergence criterion (tol)
Output: solution to nonlinear equation

$n \leftarrow 1$
while ($n \le N$)
    $f_{n-1} \leftarrow f(x_{n-1})$
    $f'_{n-1} \leftarrow f'(x_{n-1})$
    $x_n \leftarrow x_{n-1} - f_{n-1}/f'_{n-1}$
    if ($|f_{n-1}| \le tol$) ***then***
        break
    end
end

Newton's Method: MATLAB Code

Pseudo-Code

```
n ← 1
while (n ≤ N)
    f_{n−1} ← f(x_{n−1})
    f'_{n−1} ← f'(x_{n−1})
    x_n ← x_{n−1} − f_{n−1}/f'_{n−1}
    if (|f_{n−1}| ≤ tol) then
        break
    end
    n ← n + 1
end
```

MATLAB

```
n = 2;
while (n <= N + 1)
    fe = f(x(n - 1));
    fpe = fp(x(n - 1));
    x(n) = x(n - 1) - fe/fpe;
    if (abs(fe) <= tol)
        break;
    end
    n = n + 1;
end
```

- Note that arrays in MATLAB are one-based, thus `x(1)` ⇔ x_0
- Also note that the function (equation) and its first-order derivative must be provided
- You can use "anonymous functions" in MATLAB to avoid creating an M-file for each function

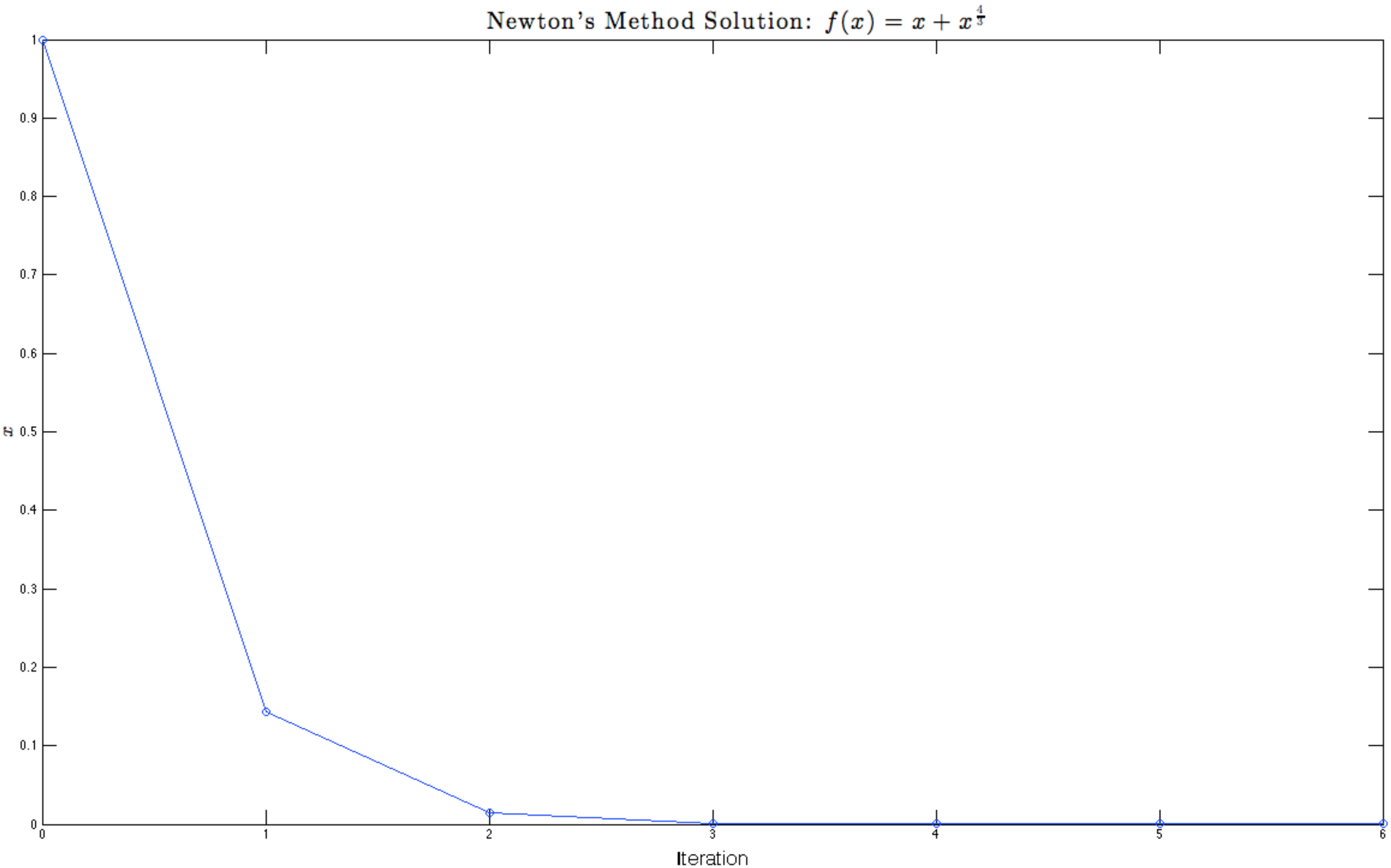
Numeric Example: MATLAB Script

```
f = @(x) x + x^(4/3); % Equation definition
fp = @(x) 1 + 4/3*x^(1/3); % First-order derivative of f
x0 = 1; % Initial guess
N = 10; % Maximum number of iterations
tol = 1E-6; % Convergence tolerance
x = zeros(N + 1,1); % Preallocate solution vector where row => iteration
x(1) = x0; % Set initial guess

% Newton's Method algorithm
n = 2;
nfinal = N + 1; % Store final iteration if tol is reached before N iterations
while (n <= N + 1)
    fe = f(x(n - 1));
    fpe = fp(x(n - 1));
    x(n) = x(n - 1) - fe/fpe;
    if (abs(fe) <= tol)
        nfinal = n; % Store final iteration
        break;
    end
    n = n + 1;
end

% Plot evolution of the solution
figure('Color','White')
plot(0:nfinal - 1,x(1:nfinal),'o-')
title('Newton''s Method Solution: $f(x) = x + x^{\frac{4}{3}}$','FontSize',
20,'Interpreter','latex')
xlabel('Iteration','FontSize',16)
ylabel('$x$','FontSize',16,'Interpreter','latex')
```

Numeric Example: Plot



MATLAB Builtin Functions

- For univariate nonlinear equations, you may use the function `fzero`
  - http://www.mathworks.com/help/matlab/ref/fzero.html

- For a system of nonlinear equations, you may use the function `fsolve`
  - http://www.mathworks.com/help/optim/ug/fsolve.html

- They are more robust and rigorous than the simple implementation shown in the previous slides