Course of Numerical Methods for Engineering
Lab 3

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MOX - Politecnico di Milano

PHYS-ENG, A.Y. 2020-21

28-29/09/2020

Topics of this session:

- **Methods for nonlinear equations**
- **Minimization methods**

Numerical solution of nonlinear equations

We want to find a numerical approximation of the solutions $\xi \in \mathbb{R}$ of a nonlinear equation $f(\xi) = 0$, with $f : I = (a, b) \in \mathbb{R} \to \mathbb{R}$.

The MATLAB/Octave command `x=fsolve(fun,x0,options)`

- **Requires the optimization toolbox, if not installed can be installed in MATLAB via installer or Home→Add-ons→Get Add-ons)**
- **Can be used to find the zeros of** `fun` **using various algorithms and an initial guess $x0$ (see help and doc pages for** `fsolve` **and** `optimoptions`**)**

Iterative methods and residual

We consider **iterative** **methods, i.e. we want to generate a sequence of values** $x^{(k)}$ **such that:**

$$\lim_{k\to\infty} x^{(k)} = \xi$$

Let $f \in \mathcal{C}^0[a, b]$**, and let** $x^{(k)} \in [a, b]$ **an approximation of the solution of** $f(x) = 0$ **computed by an iterative method. The quantity** $|f(x^{(k)})|$ **is called the** **residual** **of the iterative method at iteration** k**.**

Newton's method

Let $f \in \mathcal{C}^1[a,b]$ and let $x^{(0)} \in [a,b]$. Newton's method for the solution of $f(x) = 0$ is defined by the recursive sequence

$$x^{(k+1)} = x^{(k)} + \delta x^{(k)}, \quad \delta x^{(k)} = -\frac{f(x^{(k)})}{f'(x^{(k)})} \quad k \geq 1$$

Stopping criterion based on:

- **Error:** $\delta x^{(k)} < \varepsilon_{tol}$, $\dfrac{\delta x^{(k)}}{x^{(k)}} < \varepsilon_{tol}$
- **Residual:** $|f(x^{(k)})| < \varepsilon_{tol}$

Chord, secant, and modified Newton methods

Let $f \in \mathcal{C}^1[a,b]$ and let $x^{(0)} \in [a,b]$, $\epsilon, k > 0$.

The chord method has:

$$\delta x^{(k)} = -(b-a)\frac{f(x^{(k)})}{f(x^{(k)}) - f(x^{(k-1)})}$$

The secant method has ($k \geq 2$, $x^{(1)}$ given):

$$\delta x^{(k)} = -(x^{(k)} - x^{(k-1)})\frac{f(x^{(k)})}{f(x^{(k)}) - f(x^{(k-1)})}$$

The Modified Newton method has:

$$\delta x^{(k)} = -\epsilon\frac{f(x^{(k)})}{f(x^{(k)}+\epsilon) - f(x^{(k)})}$$

Exercise 1

Consider the nonlinear equation $f(x) = x^2 - x + 1 - e^{-x} = 0$ **for** $x \in [-2, 1]$.

a) **Plot the function** $f(x)$ **on the given interval and graphically identify possible initial guesses for the solutions of the equation;**

b) **Use these guesses to compute approximations of all the solutions, using the MATLAB function** `fsolve` **with an absolute error tolerance** 10^{-10} **and tolerance on the residual** 10^{-12}**;**

c) **Write a MATLAB function implementing the Newton method (compute the derivative analytically and define it as a function handle) and compute again the approximations of all the solutions with absolute error tolerance** 10^{-10}**.**

Exercise 2

Consider the nonlinear equations

$$f(x) = x^4 - x^3 - 7x^2 + x + 6 = 0 \qquad g(x) = x^4 - 3x^3 - 3x^2 + 11x - 6 = 0$$

for $x \in [-3, 4]$.

a) **Plot the function $f(x)$ on the given interval and graphically identify initial guesses for the solutions of the equation;**

b) **Use these guesses to compute approximations of all the solutions, using the Newton method with absolute error tolerance 10^{-10};**

c) **Compare the convergence behaviour observed for all the solutions of the two equations;**

d) **Compare the results with those obtained using the MATLAB function `fsolve` with the same initial guesses and absolute error tolerance.**

Minimization problems

If ξ is such that $f(\xi) = 0$, then ξ is a minimum point of $\phi(x) = |f(x)|^2 \Longrightarrow$ methods used to find minima of ϕ can be used to find solutions of $f(x) = 0$.

Let $x^{(0)}$ an initial approximation for the minimum of ϕ.
The steepest descent method is defined by

$$x^{(k+1)} = x^{(k)} - \gamma_k \phi'(x^{(k)}) \qquad \gamma_k, k \geq 0$$

In the modified steepest descent method, $\gamma_k = \gamma/2^m$, with $\gamma \in \mathbb{R}$, and $m \in \mathbb{Z}$ the smallest integer such that

$$\phi\left(x^{(k)} - \frac{\gamma}{2^m}\phi'(x^{(k)})\right) - \phi(x^{(k)}) \leq -\frac{1}{2}\frac{\gamma}{2^m}|\phi'(x^{(k)})|^2$$

Exercise 3

Reformulate Exercises 1 and 2 as the minimization of $\phi(x) = f(x)^2$ and compute the solutions using:

1. **The steepest descent method with a fixed step length $\gamma_k = \gamma$ (experiment with several γ values);**
2. **The modified steepest descent method.**

Use the same initial guesses of Exercises 1 an 2, relative error tolerance 10^{-8} (use absolute error tolerance for zero roots). Check that the method converges monotonically to the local minima of $\phi(x)$.

Exercise 4

Write MATLAB functions implementing the chord, secant, and modified Newton (experiment with several ϵ values) methods and apply them to solve the problems in Exercises 1 and 2.

Exercise 5

Consider the function $\phi(x) = [1 - \exp(-x^2)] \sin(3x)$ **on the interval** $x \in [-3, 3]$.

a) **Plot the function** $\phi(x)$ **on the given interval and graphically identify initial guesses for computation of its local minima.**

b) **Compute the local minima using the modified gradient method using an absolute error tolerance** 10^{-9}.