Lecture 10, Sci. Comp. for DPhil Students

Nick Trefethen, Tuesday 14.11.19

Today

- III.1 Newton's method for a single equation
- III.2 Newton's method for a system of equations

Handouts

- Quiz 5
- m18_prettynewton.m
 m19_newtona.m, m19_newtonb.m, m19_newtonc.m
 m20_newtonsystem.m
 m21_newtonsystemChebfun2.m

Announcements

- Assignment 3 due on Tuesday
- Pass around Nocedal & Wright

We've finished with linear algebra and a Chebfun demo, and now for the final 3 lectures of this first term, we will talk about optimization. This subject keeps growing in importance.

III OPTIMIZATION

Optimization = minimization (& maximization) / zerofinding

... typically for functions of several variables

... often subject to equality or inequality constraints

Outstanding textbook: Nocedal & Wright, Numerical Optimization, 2nd ed., 2006 (see our Web page)

Our focus:

- continuous (not discrete)
- deterministic (not stochastic)
- medium scale, high-ish accuracy (not machine learning, data science)

III.1 Newton's method for a single equation

Given: function F(x), typically nonlinear. Goal: find a **zero** or **root** x^* of F, i.e., $F(x^*) = 0$. I presume you all know **Newton's method**:

	-
Given initial guess x	
0	
1	1
For $k = 0, 1, \ldots$	1
s = -F(x) / F'(x)	s stands for "step"
l k k k	1
1	1
x = x + s	1
k+1 k k	1
1	1

If F is twice differentiable and $F'(x^*) \neq 0$, then if x_0 is sufficiently close to x^* the convergence is **quadratic**—i.e., the number of correct digits asymptotically doubles at each step.

[m18_prettynewton.m]

[m19_newtona.m/m19_newtonb.m/m19_newtonc.m]

III.2 Newton's method for a system of equations

Consider now $F: \mathbb{R}^n \to \mathbb{R}^n$. Seek $x^* \in \mathbb{R}^n$ s.t. $F(x^*) = 0$. I.E., we have a system of n eqs in n unknowns:

$$F_1(x_1, \dots, x_n) = 0$$

$$\vdots$$

$$F_n(x_1, \dots, x_n) = 0$$

There's an exactly analogous Newton method. To state it we need to define the derivative of A. *Definition.* Given $F : \mathbb{R}^n \to \mathbb{R}^m$, the **derivative** of F at $x \in \mathbb{R}^n$ is the $m \times n$ **Jacobian matrix** defined by

$$[J(x)]_{ij} = [F'(x)]_{ij} = \frac{\partial F_i}{\partial x_j}(x)$$

Example. $F: \mathbb{R}^2 \to \mathbb{R}^3$.

$$F_1(x_1, x_2) = x_1^2$$
, $F_2(x_1, x_2) = x_1 + x_1 x_2$, $F_3(x_1, x_2) = x_1 \exp(x_2)$.

$$F'(x) = \begin{vmatrix} 2x & 0 & | \\ | & 1 & | \\ | & | \\ | & | \\ | & 1 + x & x & | \\ | & 2 & 1 & | \\ | & | \\ | & | \\ | exp(x) & x exp(x) | \\ | & 2 & 1 & 2 \end{vmatrix}$$

Motivation:

$$F(x + \Delta x) \approx F(x) + F'(x)\Delta x$$
 | | \ | n-vectors m-vectors

... with equality in limit $\Delta x \to 0$

Newton's method

_____ Given initial guess x 0 For k = 0, 1, ...Т Evaluate F(x) and F'(x)| (here n=m so F' is square) T k k 1 Solve F'(x) = -F(x) for $s \mid$ Ι kk k k | Ι 1 T x + s х k+1 k k 1 1 _____

Again, quadratic convergence under suitable hypotheses:

F twice differentiable, $F'(x^*)$ nonsingular, x_0 close enough to x^* .

In MATLAB: fzero for a scalar problem, fsolve for a system (in the Optimization Toolbox)

These do much more than just Newton's method: they are much more robust.

For an example, consider

$$F(x,y) = \begin{pmatrix} \sin(x+y) - e^{-x^2} \\ 3x - xy^2 - 1 \end{pmatrix}$$

with Jacobian

$$J(x,y) = \begin{pmatrix} \cos(x+y) + 2xe^{-x^2} & \cos(x+y) \\ 3 - y^2 & -2xy \end{pmatrix}$$

[m20_newtonsystem.m]

[m21_newtonsystemChebfun2.m]