COT4501 Spring 2012
Homework V

This assignment has seven problems. The assignment is due in class on Thursday, March 29, 2012. There are seven regular problems and two computer problems (using MATLAB). For written problems, you need to show your work and it is insufficient to just give the results or answers. For the computer problems, turn in your results (e.g., graphs, plots, simple analysis and so on) and also a printout of your (MATLAB) code.

Problem 1 (15pts)

1. Suppose you are using an iterative method to solve a nonlinear equation $f(x) = 0$ for a root that is ill-conditioned, and you need to choose a convergence test. Would it be better to terminate the iteration when you find an iterate x_k for which $|f(x_k)|$ is mall, or when $|x_k - x_{k-1}|$ is small? Why?
   Solution: It will be better to to use $|x_k - x_{k-1}|$, since for ill-conditioned problem $||f(x)||$ could be small without x_k being near to the true solution (section 5.3 of book)

2. If the errors at successive iterations of an iterative method are as follows, how would you characterize the convergence rate?

   (a) $10^{-2}, 10^{-4}, 10^{-8}, 10^{-16}, ...,$
   (b) $10^{-2}, 10^{-4}, 10^{-6}, 10^{-8}, ...,$

   Solution:

   (a) $10^{-2}, 10^{-4}, 10^{-8}, 10^{-16}, ...,$ Quadratic
   (b) $10^{-2}, 10^{-4}, 10^{-6}, 10^{-8}, ...,$ Linear

3. Suppose you are using the bisection method to find a zero of a nonlinear function, starting with an initial bracketing interval $[a,\ b]$. Give a general expression for the number of iterations that will be required to achieve an error tolerance of tol for the length of the final bracketing interval.
   Solution:

   Let a and b be the two end points of the search interval. The initial interval length is $|x_1 - x_2| = |a - b|$. Since every time we decrease the length of the interval by half, we have, after n iterations, the search interval has length Nth iteration will us get us Then first $|x_n - x_{n+1}| = \frac{|a-b|}{2^n}$ Let ϵ be the tolerance tol. Then to achieve the given tolerance of ϵ, we need

   $$\frac{|a-b|}{2^n} < \epsilon \to \log_2 |a-b| - n < \log_2 \epsilon$$

   or

   $$n > \log_2 |a-b| - \log_2 \epsilon.$$

Problem 2 (15pts)

1. What is the convergence rate for Newton's method for finding the root $x = 2$ of each of the following equations?

   (a) $f(x) = (x - 1)(x - 2)^2 = 0$,

   (b) $f(x) = (x - 1)^2(x - 2) = 0$.

   Solution:

   (a) $f(x) = (x - 1)(x - 2)^2 = 0$, since the root has multiplicity of m=2, Newton's method is only linearly convergent with $C = 1 - (1/m)$

   (b) $f(x) = (x - 1)^2(x - 2) = 0$.: Newton's method will have quadratic convergence.

2. List one advantage and one disadvantage of the secant method compared with the bisection method for finding a simple zero of a single nonlinear equation.
   Solution: Secant method's convergence rate in general is superlinear whereas that of bisection method is linear. Unlike bisection method, secant method does not require that the root remain bracketed therefore might not always converge.

3. For solving a one-dimensional nonlinear equation, how many function or derivative evaluations are required per iteration of each of the following methods?

   (a) Newton's method,

   (b) Secant method.

Solution:

1. Newton's method: In every iteration, one function and derivative evaluation.
2. Secant method: In every iteration only one function evaluation.

Problem 3 (15pts) Consider the nonlinear equation

$$f(x) = x^2 - 2 = 0.$$

- With $x_0 = 1$ as a starting point, what is the value of x_1 if you use Newton's method for solving this problem?
- With $x_0 = 1$ and $x_1 = 2$ as starting points, what is the value of x_2 if you use the secant method for the same problem?

Solution:

- Derivative of $f(x)$ is $f'(x) = 2x$. Using Newton's method we will get $x_1 = 3/2$

- Secant method: $x_2 = 4/3$

Problem 4 (15pts)

1. Show that the iterative method

$$x_{k+1} = \frac{x_{k-1}f(x_k) - x_k f(x_{k-1})}{f(x_k) - f(x_{k-1})}$$

is mathematically equivalent to the secant method for solving a scalar nonlinear equation $f(x) = 0$.

2. When implemented in finite-precision floating-point arithmetic, what advantages or disadvantages does the formula given in **Part 1** have compared with the usual formula for the secant method

$$x_{k+1} = x_k - \frac{f(x_k)(x_k - x_{k-1})}{f(x_k) - f(x_{k-1})} \; ?$$

Soulution:

1. :

$$x_{k+1} = \frac{x_{k-1}f(x_k) - x_k f(x_{k-1})}{f(x_k) - f(x_{k-1})}$$

$$x_{k+1} = x_k - \frac{f(x_k)(x_k - x_{k-1})}{f(x_k) - f(x_{k-1})} - x_k + \frac{f(x_k)(x_k - x_{k-1})}{f(x_k) - f(x_{k-1})} + \frac{x_{k-1}f(x_k) - x_k f(x_{k-1})}{f(x_k) - f(x_{k-1})}$$

$$x_{k+1} = x_k - \frac{f(x_k)(x_k - x_{k-1})}{f(x_k) - f(x_{k-1})} - x_k + \frac{x_k f(x_k) - x_k f(x_{k-1})}{f(x_k) - f(x_{k-1})}$$

$$x_{k+1} = x_k - \frac{f(x_k)(x_k - x_{k-1})}{f(x_k) - f(x_{k-1})} - x_k + \frac{x_k(f(x_k) - f(x_{k-1}))}{f(x_k) - f(x_{k-1})}$$

$$x_{k+1} = x_k - \frac{f(x_k)(x_k - x_{k-1})}{f(x_k) - f(x_{k-1})}$$

2. The formula in part (a) gives the new iterate as a quotient of two differences, each of which is between two quantities that are nearly equal, and hence may suffer substantial cancellation. The standard formula gives the new iterate as a small perturbation to the previous iterate, and only the perturbation computation suffers from potential cancellation

Problem 5 (15pts) Suppose we wish to develop an iterative method to compute the square root of a given positive number y, i.e., to solve the nonlinear equation $f(x) = x^2 - y = 0$ given the value of y. Each of the functions g_1 and g_2 listed below gives a fixed-point problem that is equivalent to the equation $f(x) = 0$. For each of these functions, determine whether the corresponding fixed-point iteration scheme $x_{k+1} = g_i(x_k)$ is locally convergent to $\sqrt{y}$ if $y = 3$. Explain your reasoning in each case.

1. $g_1(x) = y + x - x^2$,
2. $g_2(x) = 1 + x - \frac{x^2}{y}$,
3. What is the fixed-point iteration function given by Newton's method for this particular problem?

Solution:

1. $g_1'(x) = 1 - 2x$ which gives $|g_1'(\sqrt{3})| = |1 - 2\sqrt{3}| > 1$. Hence iterative scheme is not convergent.
2. $g_2'(x) = 1 - 2x/y$ which gives $|g_2'(\sqrt{3})| = |1 - 2\sqrt{3}/3| < 1$. Hence iterative scheme is locally convergent.

Problem 6 (10pts) Express the Newton iteration for solving each of the following systems of nonlinear equations.

1. $$\begin{aligned} x_1^2 + x_2^2 &= 1, \\ x_1^2 - x_2 &= 0. \end{aligned}$$

2. $$\begin{aligned} x_1 + x_2 - 2x_1x_2 &= 0, \\ x_1^2 + x_2^2 - 2x_1 + 2x_2 &= -1. \end{aligned}$$

Solution:

1. Solve for the s_k
$$J_f(x_k)s_k = \begin{bmatrix} 2x_1 & 2x_2 \\ 2x_1 & -1 \end{bmatrix} \begin{bmatrix} s_1 \\ s2 \end{bmatrix} = -\begin{bmatrix} x_1^2 + x_2^2 - 1 \\ x_1^2 - x_2 \end{bmatrix}$$
2. Solve for the s_k
$$J_f(x_k)s_k = \begin{bmatrix} 1 - 2x_1 & 1 - 2x_2 \\ 2x_1 - 2 & 2x_2 + 2 \end{bmatrix} \begin{bmatrix} s_1 \\ s2 \end{bmatrix} = -\begin{bmatrix} x_1 + x_2 - 2x_1x_2 \\ x_1^2 + x_2^2 - 2x_1 + 2x_2 + 1 \end{bmatrix}$$

Problem 7 (15pts) Newton's method for solving a scalar nonlinear equation $f(x) = 0$ requires computation of the derivative of f at each iteration. Suppose that we instead replace the true derivative with a constant value d, that is, we use the iteration scheme

$$x_{k+1} = x_k - \frac{f(x_k)}{d}.$$

1. Under what condition on the value of d will this scheme be locally convergent?

2. What will be the convergence rate, in general?

3. Is there any value of d that would still yield quadratic convergence?

Solution:

1. $g(x^*) = x^* - f(x^*)/d$. For convergence we need to find derivative $g'(x^*) = 1 - f'(x^*)/d$. For local convergence the condition is

$$\begin{aligned} |1 - f'(x^*)/d| &< 1 \\ \implies -1 < 1 - f'(x^*)/d &< 1 \\ \implies 0 < f'(x^*)/d &< -2 \end{aligned}$$

2. In general, the convergence rate will be linear with the constant $C = |1 - f'(x^*)/d|$

3. For the quadratic convergence we need $1 - f'(x^*)/d = 0$ which implies $d = f'(x^*)$

Computer Problem 1 (15pts) For the equation

$$f(x) = x^2 - 3x + 2 = 0,$$

each of the following functions yields an equivalent fixed-point problem:

$$\begin{aligned} g_1(x) &= (x^2 + 2)/3, \\ g_2(x) &= \sqrt{3x - 2}, \\ g_3(x) &= 3 - \frac{2}{x}, \\ g_4(x) &= \frac{x^2 - 2}{2x - 3}. \end{aligned}$$

- Analyze the convergence properties of each of the corresponding fixed-point iteration schemes for the root $x = 2$ by considering $|g_i'(2)|$.

- Confirm your analysis by implementing each of the schemes and verifying its convergence (or lack thereof) and approximate convergence rate.

Solution:

$|g_1'(x)| = |2x|/3 = 4/3 > 1$ which implies divergences
$|g_2'(x)| = |\frac{3}{2\sqrt{3x-2}}| = 3/4 < 1$ which implies linear convergence with constant 0.75
$|g_3'(x)| = |2/x^2| = 1/2 < 1$ which implies linear convergence with constant 0.5
$|g_4'(x)| = |\frac{-2(x^2-2)}{(2x-3)^2} + \frac{2x}{2x-3}| = 0$ which implies quadratic convergence

```
function cp05_02 % fixed-point iteration
fs = {'(x^2+2)/3' 'sqrt(3*x-2)' '3-2/x' '(x^2-2)/(2*x-3)'};
tol = eps; maxits = 10; x_true = 2; disp('(b)');
for i=1:4
fprintf('g_%g(x) = %s\n', i, fs{i}); g = inline(fs{i},'x');
disp([' k x err ',...
' ratio']);
k = 0; x = 2.5; err = abs(x-x_true);
fprintf('%3d %20.12e %20.12e\n', k, x, err);
while err > tol & k < maxits
k = k+1; x = g(x); err_new = abs(x-x_true);
ratio = err_new/err; err = err_new;
fprintf('%3d %20.12e %20.12e %20.12e\n', k, x, err, ratio);
end; disp(' ');
end
```

Computer Problem 2 (25pts)

1. According to quantum mechanics, the ground state of a particle in a spherical well is determined by the system of nonlinear equations

$$\frac{x}{\tan(x)} = -y,$$
$$x^2 + y^2 = s^2,$$

where s depends on the mass and radius of the particle and the strength of the potential. in appropriate units, $s = 3.5$. Use any method of your choice to solve this nonlinear system.

2. The first excited state of the particle is determined by the nonlinear system

$$\frac{1}{x\tan(x)} - \frac{1}{x^2} = \frac{1}{y} + \frac{1}{y^2},$$
$$x^2 + y^2 = s^2.$$

Again, use any method of your choice to solve this nonlinear system.

Solution:

```
function cp05_20 % ground and excited states in spherical well
global s; s = 3.5;
disp('(a)'); x = fsolve(@fa, [1; 2], optimset('Display','off'))
disp('(b)'); x = fsolve(@fb, [2; 1], optimset('Display','off'))
fT(1, 2);
fT2(2, 1);
end
function [y] = fa(x); global s;
y = [x(1)/tan(x(1))+x(2); x(1)^2+x(2)^2-s^2];
end
function [y] = fb(x); global s;
y = [1/(x(1)*tan(x(1)))-1/(x(1)^2)-1/x(2)-1/(x(2)^2); ...
    x(1)^2+x(2)^2-s^2];
end
function fT2(x,y)
X = [x; y];
for k=1:100
    J = fnJ2(X(1), X(2));
    %det(J)
    vMat = fn2(X(1), X(2), 3.5);
    dX = -pinv(J'*J)*J'*vMat;
    vMat'*vMat
    X  = X+1*dX;
end


X
end
function fT(x,y)
X = [x; y];
for k=1:1000
    J = fnJac(X(1), X(2));
    vMat = fn(X(1), X(2), 3.5);
    dX = -pinv(J'*J)*J'*vMat;
    X  = X+0.1*dX;
end

```

```
X

end

function vMat = fn(x,y,s)
vMat = [x/tan(x)+y; x^2+y^2-s^2];
end
function J = fnJac(x1,x2)
%J = [1+y*(sec(x)^2) x+tan(x); 2*x 2*y];
J = [ 1/tan(x1) - (x1*(tan(x1)^2 + 1))/tan(x1)^2,     1;...
      2*x1, 2*x2];

end
function vMat = fn2(x1,x2,s)
vMat = [1/(x1*tan(x1))-1/(x1^2)-1/x2-1/(x2^2); x1^2+x2^2-s^2];
end

function J = fnJ2(x1,x2)
J = [ 2/x1^3-1/(x1^2*tan(x1))-(tan(x1)^2 + 1)/(x1*tan(x1)^2), ... 1/x2^2+2/x2^3;...
     2*x1,             2*x2];
end
```