MA3232 Numerical Analysis

Week 2

To explain all nature is too difficult a task for any one man or even for any one age. `Tis much better to do a little with certainty, and leave the rest for others that come after you, than to explain all things.

--- Isaac Newton (1643-1727)

Isaac Newton was the great English mathematician of his generation. He laid the foundation for differential and integral calculus. His work on optics and gravitation make him the greatest scientist the world has known.

Go through Assignment 1. In Plot_1D_2D, add tic and toc in plot_fxy.m and plot_fxy_0.m to see why it is good to use vectors directly in MATLAB.

plot_fxy_0.m runs about 0.60 seconds

plot_fxy.m runs about 0.15 seconds

Example: Solve $f(x) = \exp(-x) - x = 0$

We have used dsolve and bisection method to solve it. Now we introduce another method.

Newton's method

Suppose $f(x)$ is differentiable. We start with a point x_0.

The goal of Newton's method is to find one root of $f(x) = 0$.

Taylor expansion of $f(x)$ around x_0:

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2}(x - x_0)^2 + \cdots$$

Near x_0, $f(x)$ is well approximated by $f(x_0) + f'(x_0)(x - x_0)$ (tangent line approximation or linear approximation)

Strategy:

Start with x_0

Instead of solving $f(x) = 0$, we solve $f(x_0) + f'(x_0)(x - x_0) = 0$.

Let x_1 be the solution of $f(x_0) + f'(x_0)(x - x_0) = 0$.

$$f(x_0) + f'(x_0)(x_1 - x_0) = 0$$

$$\Longrightarrow \quad x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

(Draw the graph of $f(x)$ and the tangent line at x_0)

Take x_1 as the new starting point and repeat the process.

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}$$

$$\vdots$$

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

If $|x_{n+1} - x_n| <$ tol, stop.

Matlab code (solving $\exp(-x) - x = 0$; note that $f(x) = e^{-x} - x,\ f'(x) = -e^{-x} - 1$)

```
clear;
x0 = 0;
err = 1.0;
tol = 1.0e–10;
n = 0;
while err  > tol,
    n = n+1;
    f0 = exp(–x0)–x0;
    fp0 = –exp(–x0)–1;
    x1 = x0–f0/fp0;
    err = abs(x1-x0);
    x0 = x1;
end
r = x0;
```

For this code, it takes $N = 5$ iterations to reach $\text{tol} = 10^{-10}$. You can also add "tic; toc" to see how long it takes to run the codes.

See NL_solvers/newton.m.

Question: If we want to solve $e^{-x} + x = 0$ with Newton's method, can we use $x_0 = 0$ as the initial value?

$$f(x) = e^{-x} + x, \quad f'(x) = -e^{-x} + 1, \ f'(x_0) = f'(0) = -e^0 + 1 = 0.$$

So we cannot use 0 as the initial guess.

See NL_solvers/newton_divg.m for an example where Newton's method diverges

vs NL_solvers/newton_convg.m for an example where Newton's method converges quadratically.

In order to write more user-friendly codes, one should use functions.

Explain Comp_curve/calc_data.m etc. and problem 1 of homework assignment 2.

Comparison of the bisection method and Newton's method

The bisection method:

has guaranteed convergence, converges slowly, cannot be extended to non-linear systems.

Newton's method:

may not converge, converges very fast if it converges, can be extended to non-linear systems, requires the calculation of $f'(x)$.

We have not analyzed the convergence of Newton's method yet.

Questions:

Q1: Does Newton's method converge?

Q2: If so, does it converge to a root of $f(x)=0$?

To answer these questions, we study a class of methods, called fixed point iterative methods.

Fixed point iterative methods (for solving $f(x)=0$)

The goal is to find one root of $f(x)=0$.

Strategy:

Start with x_0 (an initial approximation to a root of $f(x)=0$)

Use an iteration function $g(x)$ to improve the approximation

$$x_1 = g(x_0)$$

$$\vdots$$

$$x_{n+1} = g(x_n)$$

If $|x_{n+1} - x_n| <$ tol, stop.

This class of methods is called the fixed point iterative methods.

Here $g(x)$ is called the iteration function.

Even though the choice of $g(x)$ is not unique, it has to satisfy certain conditions.

Consistency

First, we study Question #2. Suppose $\lim_{n\to\infty} x_n = x^*$.

$$x_{n+1} = g(x_n) \Rightarrow \lim_{n\to\infty} x_{n+1} = \lim_{n\to\infty} g(x_n) \overset{\text{assume g is continuous}}{=} g\left(\lim_{n\to\infty} x_n\right)$$

==> $\quad x^* = g(x^*)$

Definition:

If $x^* = g(x^*)$, then x^* is called a fixed point of $g(x)$.

We want to make sure that if x_n converges, it converges to a root of $f(x) = 0$.

Consistency condition:

We require that all fixed points of $g(x)$ be roots of $f(x) = 0$.

That is, $x^* = g(x^*)$ implies $f(x^*) = 0$.

Example: Newton's method satisfies the consistency condition.

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

We write it in the form of fixed point iterative methods

$$x_{n+1} = g(x_n), \qquad g(x) = x - \frac{f(x)}{f'(x)}$$

Let us check the consistency condition. Let x^* be a fixed point of $g(x)$.

$$x^* = g(x^*)$$

==> $\quad x^* = x^* - \dfrac{f(x^*)}{f'(x^*)}$

==> $\quad \dfrac{f(x^*)}{f'(x^*)} = 0$

==> $\quad f(x^*) = 0$

Other examples of fixed point iterative methods:

Example: Design an iterative method for solving $\sin(x+2) - 2x = 0$.

$$\sin(x+2) - 2x = 0$$

==> $x = \frac{\sin(x+2)}{2}$

We can try $x_{n+1} = \frac{\sin(x_n + 2)}{2}$.

That is, $x_{n+1} = g(x_n)$, $g(x) = \frac{\sin(x+2)}{2}$

Example: Design an iterative method for solving $x^2 - 2x + 0.75 = 0$.

$x^2 - 2x + 0.75 = 0$

==> $x = \frac{x^2 + 0.75}{2}$

We can try $x_{n+1} = \frac{x_n^2 + 0.75}{2}$.

That is, $x_{n+1} = g(x_n)$, $g(x) = \frac{x^2 + 0.75}{2}$.

See NL_solvers/iter_divg.m.

If $x_0 < 1.5$, $x_n \to 0.5$;

If $x_0 > 1.5$, x_n diverges.

Example: Design an iterative method for solving $e^{-x} - x = 0$.

$x = e^{-x} = g(x)$

$\Rightarrow x_{n+1} = g(x_n) = \exp(-x_n)$

The method converges linearly.

See NL_solvers/iter_convg.m.

Convergence

Now, we study Question #1: "Under what condition does the iteration $x_{n+1} = g(x_n)$ converge?"

Let x^* be a fixed point of $g(x)$ (also a root of $f(x) = 0$). We have

$x_{n+1} = g(x_n)$

$x^* = g(x^*)$

==> $x_{n+1} - x^* = g(x_n) - g(x^*)$

Recall the mean value theorem

If $g(x)$ is differentiable in $[a, b]$, then there exists $c \in [a, b]$ such that

$$g(b) - g(a) = g'(c)(b-a)$$

Applying the mean value theorem, we get

$$x_{n+1} - x^* = g(x_n) - g(x^*) = g'(\tilde{x}_n)(x_n - x^*),$$ where $\tilde{x}_n$ is between x_n and x^*

==> $|x_{n+1} - x^*| = |g'(\tilde{x}_n)||x_n - x^*|$

We discuss 3 cases.

<u>Case #1:</u> Suppose $|g'(x)| \le q < 1$ for all values of *x*.

==> $|x_{n+1} - x^*| \le q|x_n - x^*|$

==> $|x_n - x^*| \le q|x_{n-1} - x^*| \le q^2|x_{n-2} - x^*| \le \cdots$

==> $|x_n - x^*| \le q^n|x_0 - x^*|$

==> $|x_n - x^*| \to 0$ as $n \to \infty$

Therefore, $\lim_{n\to\infty} x_n = x^*$ for all values of x_0

<u>Conclusion for case #1:</u> Suppose $|g'(x)| \le q < 1$ for all values of *x*. Then the iteration $x_{n+1} = g(x_n)$ converges to x^* for all values of x_0.

Note: This case uses the global property of $g'(x)$ (i.e. $|g'(x)| \le q < 1$ for all values of *x*) to derive property of convergence.

<u>Definition:</u>

$g(x)$ is called a contraction mapping if it satisfies that $|g'(x)| \le q < 1$ for all values of *x*.

<u>Theorem:</u>

If $g(x)$ is a contraction mapping, then it has one and only one fixed point.

<u>Example:</u> Use the iteration $x_{n+1} = \dfrac{\sin(x_n + 2)}{2}$ to solve $\sin(x+2) - 2x = 0$.

$$x_{n+1} = g(x_n), \qquad g(x) = \frac{\sin(x+2)}{2}$$

==> $g'(x) = \dfrac{\cos(x+2)}{2}$

==> $|g'(x)| = \left|\dfrac{\cos(x+2)}{2}\right| \le \dfrac{1}{2} < 1$ for all values of *x*.

==> $\lim_{n\to\infty} x_n = x^*$ for all values of x_0

<u>Example:</u> Use the iteration $x_{n+1} = g(x_n) = e^{-x_n}$ to solve $e^{-x} - x = 0 \Leftrightarrow x = e^{-x}$.

$g(x) = e^{-x} \Rightarrow g'(x) = -e^{-x} \Rightarrow |g'(x)| = |e^{-x}|$

If $x \geq 0$, $|g'(x)| \leq 1$

So we cannot apply the conclusion in case 1.

Now we use the local property of $g'(x)$ at the fixed point to get convergence property. We will skip the proof and give the conclusion directly.

<u>Case #2:</u> Suppose $|g'(x^*)| < 1$ at a fixed point x^*.

Let $q = |g'(x^*)| + \varepsilon < 1$.

There exists $\delta > 0$ such that $|g'(x)| \leq q < 1$ for $|x - x^*| \leq \delta$.

If $|x_0 - x^*| \leq \delta$, then $|\tilde{x}_0 - x^*| \leq \delta$

==> $|x_1 - x^*| = |g'(\tilde{x}_0)||x_0 - x^*| \leq q|x_0 - x^*|$

Noticing that $|x_1 - x^*| \leq \delta$, we obtain

$$|x_2 - x^*| = |g'(\tilde{x}_1)||x_1 - x^*| \leq q|x_1 - x^*| \leq q^2|x_0 - x^*|$$

$$\vdots$$

==> $|x_n - x^*| \leq q^n |x_0 - x^*|$

==> $|x_n - x^*| \to 0$ as $n \to \infty$

Therefore, $\lim_{n\to\infty} x_n = x^*$ if $|x_0 - x^*| \leq \delta$

<u>Conclusion for case #2:</u> Suppose $|g'(x^*)| < 1$ at a fixed point x^*. Then the iteration $x_{n+1} = g(x_n)$ converges to x^* if x_0 is sufficiently close to x^*.

<u>Case #3:</u> Suppose $|g'(x^*)| > 1$ at a fixed point x^*.

Let $q = |g'(x^*)| - \varepsilon > 1$.

There exists $\delta > 0$ such that $|g'(x)| \geq q > 1$ for $|x - x^*| \leq \delta$.

If $|x_0 - x^*| \leq \delta$, then $|\tilde{x}_0 - x^*| \leq \delta$

==> $|x_1 - x^*| = |g'(\tilde{x}_0)||x_0 - x^*| \geq q|x_0 - x^*| > |x_0 - x^*|$

It is clear that the sequence $\{x_n\}$ will be pushed away from x^*.

Therefore, the iteration $x_{n+1} = g(x_n)$ does not converge to x^*.

Conclusion for case #3: Suppose $\left|g'(x^*)\right| > 1$ at a fixed point x^*. Then the iteration $x_{n+1} = g(x_n)$ does not converge to x^* (it may diverge or it may converge to a different fixed point).

Note: If $\left|g'(x^*)\right| = 1$ at a fixed point x^*, then we cannot draw any conclusion on convergence.

Example: Use the iteration $x_{n+1} = \dfrac{x_n^{\,2} + 0.75}{2}$ to solve $x^2 - 2x + 0.75 = 0$.

$$x_{n+1} = g(x_n), \qquad g(x) = \frac{x^2 + 0.75}{2}$$

$g(x)$ has two fixed points: $r_1 = 0.5$, $r_2 = 1.5$.

$$g'(x) = x$$

At $r_1 = 0.5$, $\left|g'(r_1)\right| = \left|r_1\right| = 0.5 < 1$

==> $\lim\limits_{n\to\infty} x_n = r_1$ if x_0 is sufficiently close to r_1.

At $r_2 = 1.5$, $\left|g'(r_2)\right| = \left|r_2\right| = 1.5 > 1$

==> The iteration $x_{n+1} = g(x_n)$ does not converge to r_2.

Numerical experiments show that

For $x_0 > 1.5$, the iteration $x_{n+1} = g(x_n)$ diverges to ∞.

For $x_0 < 1.5$, the iteration $x_{n+1} = g(x_n)$ converges to r_1.

See NL_solvers/iter_divg.m.

Go through the two MATLAB codes NL_solvers/iter_divg.m and iter_convg.m.

Now we consider the convergence of Newton's method.

Example: Convergence of Newton's method

$$x_{n+1} = g(x_n), \qquad g(x) = x - \frac{f(x)}{f'(x)}$$

$$g'(x) = 1 - \frac{f'(x)f'(x) - f(x)f''(x)}{\left(f'(x)\right)^2} = \frac{f(x)f''(x)}{\left(f'(x)\right)^2}$$

Apparently we cannot apply case 1 since we don't have a global property of $g'(x)$.

So we look at the local property of $g'(x)$ at a fixed point.

Let x^* be a fixed point of $g(x)$ (also a root of $f(x)=0$).

If $f'(x^*)\neq 0$, then $g'(x^*)=0 \Rightarrow |g'(x^*)|<1$ This is case 2..

If $f'(x^*)=0$, then $g'(x)=\frac{0}{0}$ type and to estimate its value we will try to avoid the calculation of $f''(x)$. We take the following approach.

First, we can use the Taylor expansion to find $g'(x^*)$.

$$f(x)= f(x^*)+ f'(x^*)(x-x^*)+\frac{f''(x^*)}{2!}(x-x^*)^2+\cdots$$

$$=\frac{f^{(p)}(x^*)}{p!}(x-x^*)^p+\cdots \qquad \text{for some } p\geq 2$$

$$\Longrightarrow \quad f'(x)=\frac{f^{(p)}(x^*)}{(p-1)!}(x-x^*)^{p-1}+\cdots$$

$$\Longrightarrow \quad \frac{f(x)}{f'(x)}=\frac{1}{p}(x-x^*)+\cdots$$

$$\Rightarrow g(x)=x-\frac{f(x)}{f'(x)}=x-\frac{1}{p}(x-x^*)+\cdots$$

$$=(x-x^*)+x^*-\frac{1}{p}(x-x^*)+\cdots$$

$$=x^*+\left(1-\frac{1}{p}\right)(x-x^*)+\cdots$$

$$\overset{x^* \text{ is a fixed point of } g(x)}{=} g(x^*)+\left(1-\frac{1}{p}\right)(x-x^*)+\cdots$$

Compare the expansion above with the Taylor expansion of $g(x)$

$$g(x)=g(x^*)+g'(x^*)(x-x^*)+\cdots$$

we obtain $g'(x^*)=1-\frac{1}{p}$

Therefore, for Newton's method we have $|g'(x^*)|<1$ since $g'(x^*)=1-\frac{1}{p}$ and $p\geq 2$.

⇨ Newton's method converges if x_0 is sufficiently close to x^*.

Talk about Assignment 2 problem 1. Pay attention to the use of "function" in MATLAB. The function fp.m uses the analytical form of $f'(x)$ (which is problem-dependent) whereas the function fp_2.m uses the numerical differentiation (which is problem-independent).