Chap. 6

Solution of Linear and Nonlinear Equations

Soon-Hyung Yook

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The Relaxation Method (RM) I

A single variable equation

$$x = f(x)$$

- Iterate the "Equation"
  1. guess the initial value of x_0
  2. plug it into $f(x)$ and set $x_1 = f(x_0)$.
  3. set $x_0 = x_1$ and repeat the procedures (1) and (2) until x_1 converges to a certain value.

Example

$$x = 2 - e^{-x}$$

The Relaxation Method (RM) II

```
from math import exp

def f(x):
  y=2-exp(-x)
  return y

x=1.0
for i in range(10):
  x=f(x)
  print(x)
```

The Relaxation Method (RM) III

Problems:

- There can be more than one solution.
  - The value of solution found by the relaxation method depends on the initial value of x.
  - So if you have some approximate idea of the position of the solution you'er looking for, you should choose a value near it for your starting point.
- However, there are some solutions to some equations that you cannot find by this method no matter what starting value you choose.

example:

$$x = e^{1-x^2} \tag{1}$$

Known solution: $x = 1$ but the relaxation method fails to find it!
Trick: rearrange the equation as

$$x = \sqrt{1 - \ln x}$$

Mathematical Background for Relaxation Method I

Assume we have an equation

$$x = f(x), \tag{2}$$

that has a solution at $x = x^*$ (true solution).

- Let us consider the behavior of the relaxation method when x_0 is close to x^*.
- Performing a Taylor expansion, the value x_1 after an iteration of the method is given by the value x_0 (previous one) by

$$x_1 = f(x_0) = f(x^*) + (x_0 - x^*)f'(x^*) + \cdots \tag{3}$$

- $x^* = f(x^*)$ because x^* is the solution of Eq. (2). Thus,

$$x_1 - x^* \simeq (x_0 - x^*)f'(x^*) \tag{4}$$

- Eq. (4) means that the distance $x_0 - x^*$ to the true solution of the equation gets multiplied on each iteration of the method by a factor $f'(x^*)$.
- The relaxation method will converge if an only if $|f'(x^*)| < 1$.

Mathematical Background for Relaxation Method II

For Eq. (1) in which $x^* = 1$:

$$|f'(x^*)| = \left| \left[-2xe^{1-x^2} \right]_{x=1} \right| = 2 > 1 \qquad (5)$$

Thus the relaxation method does not converge.

Tricks for $|f'(x^*)| < 1$

- Rearrange the function $x = f(x)$ by inverting the function f to get $x = f^{-1}(x)$.
- Now, if the derivative of f^{-1} is less than one at x^*, then the relaxation method will work.
- Derivative of f^{-1}.
  - Let $u = f^{-1}(x)$.
  - The derivative we want is du/dx.
  - $dx = \frac{f(u)}{du} du$
  - when $x = x^*$, $x^* = f^{-1}(x^*) = u(x^*)$.
  - Thus,

$$\frac{du}{dx} = \frac{1}{\left.\frac{df(u)}{du}\right|_{u=x^*}} = \frac{1}{f'(x^*)} \qquad (6)$$

  - Thus, if $|f'(x^*)| > 1$, then $\left|(f^{-1})'(x^*)\right| < 1$

RM: Error Estimation

- Let $x^* = x_0 - \epsilon_0$ and $x^* = x_1 - \epsilon_1$.
- ϵ_0 and ϵ_1 are the errors.
- From Eq. (4) when x is close to x^*:

$$\epsilon_1 = \epsilon_0 f'(x^*) \tag{7}$$

- Then

$$x^* = x_0 + \epsilon_0 = x_0 + \frac{\epsilon_1}{f'(x^*)} \tag{8}$$

- using $x^* = x_1 + \epsilon_1$,

$$\epsilon_1 = \frac{x_0 - x_1}{1 - 1/f'(x^*)} \simeq \frac{x_0 - x_1}{1 - 1/f'(x_0)} \tag{9}$$

Example: Ferromagnetism I

Mean-Field Theory

Find the nonzero solution for

$$m = \tanh \frac{Cm}{T}, \tag{10}$$

where we set $C = 1$ for simplicity and $T \in (0, 2.0]$ with accuracy $\pm 10^{-6}$.

Error Estimation:

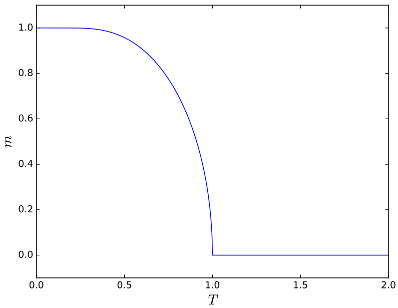
$$\epsilon_1 = \frac{m_0 - m_1}{1 - T \cosh^2(m_0/T)} \tag{11}$$

Example: Ferromagnetism II

```
from math import tanh, cosh
from numpy import linspace
from pylab import plot, show, ylim, xlabel, ylabel

#Constants
Tmax=2.0
points=1000
accuracy=1e-6

#set up lists for plotting
y=[]
temp=linspace(0.01,Tmax,points)

# Loop for temperature
for T in temp:
  m0=1.0
  error=1.0

  #Loop for solving Equation
  while error>accuracy:
    m1=tanh(m0/T)
    error=abs((m0-m1)/(1-T*cosh(m0/T)**2))
    m0=m1

  y.append(m1)
```

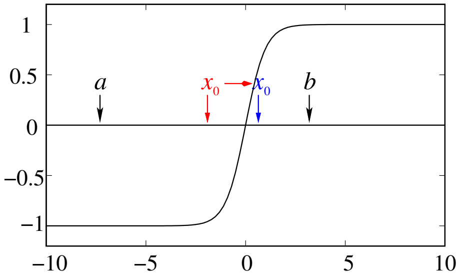
Example: Ferromagnetism III

```
# Plot the graph
plot(temp,y)
ylim(-0.1,1.1)
xlabel("$T$",fontsize=18)
ylabel("$m$",fontsize=18)
show()
```



Binary Search–Bisection Method:

- The simplest and the most intuitive method.
- Find roots of equation $f(x) = 0$.
- Assume that we know the root x_r is in the interval $[a, b]$.



Algorithm

1. set $x_0 = \frac{a+b}{2}$
2. If $f(a)f(x_0) < 0$ then let $b = x_0$
3. else set $a = x_0$.
4. repeat 1-3 until $|a - b| \leq \delta$.
5. if $|a - b| \leq \delta$ then set $x^* = (a + b)/2$.

δ is a tolerance.

Bisection–Example I

Ferromagnetism again:

```
from math import tanh,cosh
from numpy import linspace
from pylab import plot,show,ylim,xlabel,ylabel

def f(x):
  y=x-tanh(x/T)
  return y

#Constants
Tmax=2.0
points=1000
accuracy=1e-6

#set up lists for plotting
y=[]
temp=linspace(0.01,Tmax,points)

# Loop for temperature
for T in temp:
  a=1.1
  b=-0.001
  error=1.0

  #Loop for solving Equation
```

Bisection–Example II

```
  while error>accuracy:
    x0=(a+b)/2.0
    if f(a)*f(x0)<0:
      b=x0
    else:
      a=x0
    error=abs(a-b)

  y.append((a+b)/2.0)

# Plot the graph
plot(temp,y)
ylim(-0.1,1.1)
xlabel("$T$",fontsize=18)
ylabel("$m$",fontsize=18)
show()
```

Bisection–Homeworks

Homework I

Let $f(x) = e^x \ln x - x^2$ and find the root of an equation $f(x) = 0$ using bisection method. Hint: $x = 1 \to f(1) = -1$ and $x = 2 \to f(2) = 2$ so let $a = 1$ and $b = 2$.

Homework II

Find the solution of the equation

$$f(x) = x^5 - 3x^4 - 5x^3 + x^2 + x + 3 = 0$$

in the interval $x \in [-2, 4]$ using bisection method.

Newton-Raphson Method

Assume a smooth function around its root.

$$f(x_r) = 0, \qquad x_r = \text{root}$$

Use Taylor expansion around x_r.

$$f(x) = f(x_r) + (x_r - x)f'(x_r) + \cdots = 0 \tag{12}$$

Idea: Let x_k be a trial value for the root of $f(x) = 0$ (i.e., x_r) at k-th step and approximate x_r at $(k+1)$-th step based on x_k.
From Eq. (12)

$$f(x_{k+1}) \simeq f(x_k) + (x_{k+1} - x_k)f'(x_k) \simeq 0 \tag{13}$$

$$x_{k+1} = x_k - \frac{f_k}{f'_k} = x_k + \Delta x_k \tag{14}$$

Here $f_k = f(x_k)$ and Δx_k is a kind of a correction.

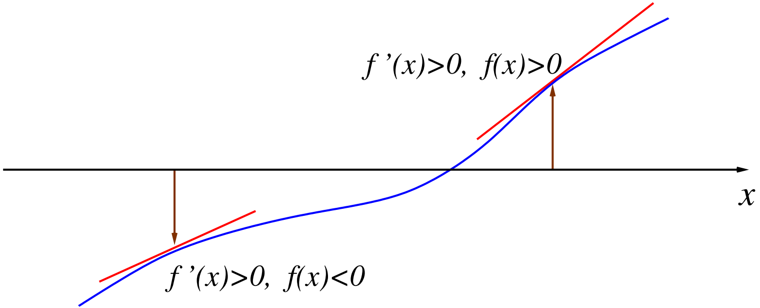
Newton-Raphson Method (NRM)

Newton-Raphson Method

- Iteration:

$$x_{k+1} = x_k - \frac{f_k}{f'_k} = x_k + \Delta x_k$$

- $\Delta x = -\frac{f(x_k)}{f'(x_k)}$



NRM–Example I

Ex.6.4: Inverse Hyperbolic Tangent

Use NRM to calculate the inverse hyperbolic tangent of a number u.

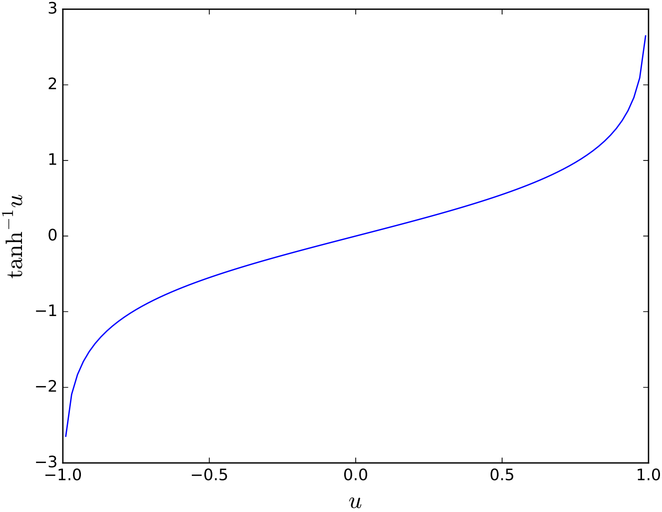
- By definition, $\tanh^{-1} u$ is the number x such that $u = \tanh x$.
- Thus, the problem is to find a root of an equation $\tanh x - u = 0$ for a given u.
- $\frac{d(\tanh x)}{dx} = \frac{1}{\cosh^2 x}$
- Therefore, from Eq. (14) one has to iteratively calculate

$$x_{k+1} = x_k - (\tanh x_k - u) \cosh^2 x_k \tag{15}$$

NRM–Example II

```
from math import tanh, cosh
from numpy import linspace
from pylab import plot, show, xlabel, ylabel

accuracy=1e-12

def arctanh(u):
  x=0.0
  delta=1.0
  while abs(delta)>accuracy:
    delta=(tanh(x)-u)*cosh(x)**2
    x-=delta
  return x

upoints=linspace(-0.99,0.99,100)
xpoints=[]

for u in upoints:
  xpoints.append(arctanh(u))
plot(upoints, xpoints)
ylabel(r"$\tanh^{-1} u$", fontsize=18)
xlabel("$u$", fontsize=18)
show()
```

NRM–Example III



NRM–Homeworks

Homework I

Let $f(x) = e^x \ln x - x^2$ and find the root of an equation $f(x) = 0$ using NRM.
Hint: $x = 1 \rightarrow f(1) = -1$ and $x = 2 \rightarrow f(2) = 2$ so let $a = 1$ and $b = 2$.

Homework II

Find the solution of the equation

$$f(x) = x^5 - 3x^4 - 5x^3 + x^2 + x + 3 = 0$$

in the interval $x \in [-2, 4]$ using NRM.

Secant Method (SM)

- More generalized version of Newton-Raphson method.
- Important: This will be also used in shooting method to find a solution of differential equation with given boundary condition.
- If $f(x)$ has an implicit dependence on x.
    - Or if $f(x)$ is give by the numerical data (numbers).
    - Thus it is difficult to find out the derivative, $f'(x)$.

$\Rightarrow$ use the two points definition of $f'(x)$

From Eq. (14)

$$x_{k+1} \simeq x_k - (x_k - x_{k-1})\frac{f_k}{f_k - f_{k-1}} = x_i + \Delta x_i$$

Example: Inverse hyperbolic tangent I

```
from math import tanh,cosh
from numpy import linspace
from pylab import plot,show,xlabel,ylabel

accuracy=1e-12
def f(x,u):
  y=tanh(x)-u
  return y

def arctanh(u):
  x1=0.0
  x2=0.1
  delta=1.0
  while abs(delta)>accuracy:
    delta=f(x2,u)*(x2-x1)/(f(x2,u)-f(x1,u))
    x=x2-delta
    x1,x2=x2,x
  return x

upoints=linspace(-0.99,0.99,100)
xpoints=[]

for u in upoints:
  xpoints.append(arctanh(u))
plot(upoints,xpoints)
```

Example: Inverse hyperbolic tangent II

```
ylabel(r"$\tanh^{-1} u$",fontsize=18)
xlabel("$u$",fontsize=18)
show()
```

SM–Homeworks

Homework I

Let $f(x) = e^x \ln x - x^2$ and find the root of an equation $f(x) = 0$ using SM.
Hint: $x = 1 \to f(1) = -1$ and $x = 2 \to f(2) = 2$ so let $a = 1$ and $b = 2$.

Homework II

Find the solution of the equation

$$f(x) = x^5 - 3x^4 - 5x^3 + x^2 + x + 3 = 0$$

in the interval $x \in [-2, 4]$ using SM.