PHY407 – University of Toronto
Lecture 4: Solving linear and non-linear equations

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Supporting textbook chapters for week 4: 6.1, 6.2, 6.3

Lecture 4, topics: * Solving linear systems * Roots of nonlinear equations * Minima: golden ratio search

1 Solving linear systems

1.1 Gaussian elimination

- In linear algebra courses, you learn to solve linear systems of the form

$$Ax = v$$

  using Gaussian elimination.
- This works pretty well in many cases. Let's do an example based on Newman's `gausselim.py`, for

$$A = \begin{bmatrix} 6 & 5 \\ 4 & 2 \end{bmatrix}, \qquad v = \begin{pmatrix} 2 \\ 1 \end{pmatrix}$$

[4]:
```
import numpy as np
import gausselim_as_func as ge

A1 = np.array([[6, 5], [4, 3]], float)
V1 = np.array([2, 1], float)

ge.gausselim(A1, V1)
```

```
[-0.5  1. ]
```

Refresher on Gaussian elimination (how `gausselim` works): the previous equation was

$$6x + 5y = 2,$$

$$4x + 3y = 1$$

1. Divide 1st line by 1st (top-left) coefficient:

$$x + 5y/6 = 1/3,$$

$$4x + 3y = 1$$

2. $4 \times$ 1st eqn $-$ 2nd eqn $=$ new 2nd eqn:

$$x + 5y/6 = 1/3,$$

$$0x + y/3 = 1/3$$

   More eqns $\Rightarrow$ cancel all 1st coefficents of each line similarly.

3. (if more eqns: repeat from 2nd line to eliminate all 2nd coefficients below, and so on...)
4. (or 3.) Back-substitute: $y = 1 \Rightarrow x + 5/6 = 1/3 \Rightarrow x = -1/2$.

[5]:
```
# %load gausselim_as_func
from numpy import array, empty


def gausselim(A, v):

    N = len(v)

    # Gaussian elimination
    for m in range(N):

        # Divide by the diagonal element
        div = A[m, m]
        A[m, :] /= div
        v[m] /= div

        # Now subtract from the lower rows
        for i in range(m+1, N):
            mult = A[i, m]
            A[i, :] -= mult*A[m, :]
            v[i] -= mult*v[m]

    # Backsubstitution
    x = empty(N, float)
    for m in range(N-1, -1, -1):
        x[m] = v[m]
        for i in range(m+1, N):
            x[m] -= A[m, i]*x[i]

    print(x)
```

1.2 When Gaussian elimination breaks down

The example below is a valid system but the original code will "break".

$$A = \begin{bmatrix} 10^{-20} & 1 \\ 1 & 1 \end{bmatrix}, \qquad v = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

In theory, $x \approx \begin{pmatrix} -1 \\ 1 \end{pmatrix}$. But according to `gausselim`:

[6]:
```
A2 = np.array([[1e-20, 1], [1, 1]], float)  # I imported np earlier
V2 = np.array([1, 0], float)

ge.gausselim(A2, V2)
```

```
[0. 1.]
```

Don't divide by (close to) zero! * Had the top-left number actually been zero, Python would have thrown a `ZeroDivisionError`, * with $10^{-20} <$ machine precision, no tripwire from Python, but rounding errors.

[7]:
```
print("1/1e-20 =", 1/1e-20)  # possible because smaller than the biggest number␣
 ↪representable
print("1/0", 1/0.)  # that on the other hand is too obvious
```

```
1/1e-20 = 1e+20


        ---------------------------------------------------------------------------

        ZeroDivisionError                         Traceback (most recent call last)

        <ipython-input-7-3e9b82241f2b> in <module>
          1 print("1/1e-20 =", 1/1e-20)  # possible because smaller than the␣
 ↪biggest number representable
        ----> 2 print("1/0", 1/0.)  # that on the other hand is too obvious


        ZeroDivisionError: float division by zero
```

As of two years ago, the following gave the right answer, but it now gives the same, wrong result.

[13]:
```
np.linalg.solve(A2, V2)
```

[13]:
```
array([0., 1.])
```

SciPy does not do better, but at least it does so in a useful way.

[15]:
```
import scipy.linalg as la
la.solve(A2, V2)
```

```
<ipython-input-15-cb28aa3d214d>:2: LinAlgWarning: Ill-conditioned matrix
(rcond=1e-40): result may not be accurate.
  la.solve(A2, V2)
```

[15]:
```
array([0., 1.])
```

Not the topic of this lecture, but always be careful of the evolution of the packages!

For this lab, it is possible that your results will differ, depending on the version of Python, NumPy, or both. Note that I cannot precisely know how, so, make sure your results make sense.

1.3 Partial pivoting:

- Eliminates the issue of dividing by zero if diagonal entries become zero (or very close to zero)

Algorithm outline: 1. At m^{th} row, check to see which of the rows below has the largest mth element (absolute value) * Swap this row with the current m^{th} value * Proceed with Gaussian elimination

[16]:
```
A3 = np.array([[1, 1], [1e-20, 1]], float)  # swapped rows
V3 = np.array([0,1], float)  # need to sap this one too

ge.gausselim(A3, V3)
```

```
[-1.  1.]
```

1.4 LU Decomposition

1.4.1 Motivation

Take two pendulums, A and B, of identical masses and lengths m and l, respectively, and coupled by spring of stiffness k. Suppose that each is driven differently, as in

$$m\ddot{x}_A + \frac{mg}{l}x_A + k(x_A - x_B) = f_A \cos(\omega_1 t),$$

$$m\ddot{x}_B + \frac{mg}{l}x_B - k(x_A - x_B) = f_B \cos(\omega_2 t),$$

- Can write these equations as $Ax = f$.
- A is always the same (depends on properties of pendulums and spring),
- but f could change.

The steps in the Gaussian elimination will always be the same: only need to do it once, then store.

Gaussian elimination on a matrix A can be written as a series of matrix multiplications $U = L_n L_{n-1} \cdots L_0 A$, where U is upper triangular (i.e., result of Gaussian elimination).

$$L^{-1} = L_n L_{n-1} \cdots L_0 \Rightarrow \; Ax = LUx = F$$

The decomposition

$$\boxed{LU = A}$$

is called the "LU decomposition" of the matrix A.

1.4.2 How to use LU in practice

- Suppose you know L, U from A.
- Then,
$$Ax = F \Leftrightarrow Ux = L^{-1}F.$$
- Break down into **two triangular-matrix problems,** $Ux = y$ **and** $Ly = f$.
- Triangular $\Rightarrow$ back-substitution (pizza cake!)
- This method is used by `numpy.linalg.solve`
- `scipy.linalg.lu_solve(scipy.linalg.lu_factor(A), f)` is equivalent to `numpy.linalg.solve(A, f)`, but intermediate steps give access to the decomposition and allow storage.

1.4.3 Issues with LU Decomposition

LU Decomposition fails when A is close to singular, duue to rounding error again. E.g.,

$$A = \begin{bmatrix} 1 & 2 \\ 2 & 4 \end{bmatrix}$$

is singular, we can't have

$$A \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 3 \\ 5 \end{bmatrix},$$

i.e., we can't have $x_1 + 2x_2 = 3$ and $5/2$ at the same time, or any other solution (even a compatible RHS leads to an undetermined coefficient).

So, LU won't find a solution when there is none: not really a drawback. But what about

$$A = \begin{bmatrix} 1 & 2 \\ 2 & 4+\delta \end{bmatrix},$$

with δ very small compared to other coefficients? Not singular, but LU won't work if smaller than machine precision.

[17]:
```
A = np.array([[1, 2], [2, 4+1e-16]], float)
v = np.array([3, 6], float)
np.linalg.solve(A, v)  # returns error
```

```
---------------------------------------------------------------------------

LinAlgError                               Traceback (most recent call last)

<ipython-input-17-67414738b59d> in <module>
  1 A = np.array([[1, 2], [2, 4+1e-16]], float)
```

```
      2 v = np.array([3, 6], float)
----> 3 np.linalg.solve(A, v)  # returns error


<__array_function__ internals> in solve(*args, **kwargs)


~/opt/anaconda3/lib/python3.8/site-packages/numpy/linalg/linalg.py in␣
↪solve(a, b)
    397     signature = 'DD->D' if isComplexType(t) else 'dd->d'
    398     extobj = get_linalg_error_extobj(_raise_linalgerror_singular)
--> 399     r = gufunc(a, b, signature=signature, extobj=extobj)
    400
    401     return wrap(r.astype(result_t, copy=False))


~/opt/anaconda3/lib/python3.8/site-packages/numpy/linalg/linalg.py in␣
↪_raise_linalgerror_singular(err, flag)
     95
     96 def _raise_linalgerror_singular(err, flag):
---> 97     raise LinAlgError("Singular matrix")
     98
     99 def _raise_linalgerror_nonposdef(err, flag):


LinAlgError: Singular matrix
```

1.5 QR decomposition

For eigensystems: i.e., looking for λ's and v's such that

$Av = \lambda v$, with * v: eigenvector * λ eivengalue

or looking for Λ and V such that $AV = V\Lambda$, with * V: orthonormal matrix of eigenvectors * Λ: diagonal matrix of eigenvalues

If A is square and either symmetric-real or Hermitian (complex), we can solve this problem with a QR decomposition.

1.5.1 QR algorithm

- Use Gram-Schmidt orthogonalization on columns of $A \Rightarrow$ matrix of orthonormal basis of column vectors Q.
- Denote QR decomposition of A as $A = QR$, where R is upper-triangular (assume we know how to decompose)
- Q orthonormal $\Rightarrow\ Q^TQ = I\ \Rightarrow\ R = Q^TA$.

Iterate: * $A_1 = RQ = Q^TAQ$ ————-> Define A_1 * $A_1 = Q_1R_1$ ————————> QR decomposition of A_1 * $A_2 = R_1Q_1 = Q_1^TQ^TAQQ_1$ —> Define A_2 * $A_2 = Q_2R_2$ ————————> QR

decomposition of $A_2 * A_3 = \ldots$

$\ldots$ and so on, until obtaining an A_k such that all off-diagnonal terms are small enough.

- Eventually, "it can be proven" that this iteration converges to a (near-)diagonal output $A_k = (Q_k^T \cdots Q_1^T Q^T) A (Q Q_1 \cdots Q_k)$
- diagonal entries of A_k (there are no non-diagonal entries) are the eigenvalues. Let $A_k = \Lambda$.
- The eigenvectors are the columns of $V = Q Q_1 \cdots Q_k$

$$\Rightarrow \; A_k = \Lambda = V^T A V \; \Rightarrow \; \boxed{V\Lambda = AV}$$

`numpy.linalg` implements the QR algorithm in the `numpy.linalg.eigh` function

[27]:
```
A = np.array([[2,1],[1,2]]) # imported numpy as np earlier

print('A:\n', A)

eig_vs, V = np.linalg.eigh(A) # calculate eigenvalues & eigenvectors
L = np.diag(eig_vs)  # np.diag constructs a diagonal array

print('\neigenvalues: ', eig_vs)
print('eigenvectors:\n', V)

# we expect that AV = VD
print('\nAV\n:', np.dot(A, V))
print('VL:\n', np.dot(V, L)) # np.diag constructs a diagonal array
```

```
A:
 [[2 1]
 [1 2]]

eigenvalues:  [1. 3.]
eigenvectors:
 [[-0.70710678  0.70710678]
 [ 0.70710678  0.70710678]]

AV
: [[-0.70710678  2.12132034]
 [ 0.70710678  2.12132034]]
VL:
 [[-0.70710678  2.12132034]
 [ 0.70710678  2.12132034]]
```

1.5.2 Be careful!

- `eigh` takes only Hermitian or real symmetric matrices as input
- What happens if we try a different (non-symmetric) matrix?

$$A = \begin{bmatrix} 2 & 3 \\ 1 & 2 \end{bmatrix}$$

[28]:
```
A = np.array([[2,3],[1,2]])
eig_vs, V = np.linalg.eigh(A) # calculate eigenvalues & eigenvectors
L = np.diag(eig_vs)  # np.diag constructs a diagonal array

print('AV:\n', np.dot(A, V))
print('VD:\n', np.dot(V, L))
```

```
AV:
 [[0.70710678 3.53553391]
 [0.70710678 2.12132034]]
VD:
 [[-0.70710678  2.12132034]
 [ 0.70710678  2.12132034]]
```

With non-symmetric matrix: $AV \neq \Lambda V$.

*Frustrating points: * How to QR-decompose? * Proof of convergence? * Where in the proof is it necessary that A be symmetric?*

2 Finding roots of nonlinear equations

Newman discusses several methods of this: Relaxation, Newton's method, bisection...

Let's review.

2.1 Relaxation

- Solving for x in an equation $x = f(x)$
- Guess an initial value x_0 and iterate until the function converges to a fixed point

$$x_1 = f(x_0)$$
$$x_2 = f(x_1)$$
$$\vdots$$

- Caveat: Can only find *stable* fixed points

[12]:
```
a = 0.5

dx = 1

threshold = 1e-10

def f(x):
    return np.tanh(2*x)
```

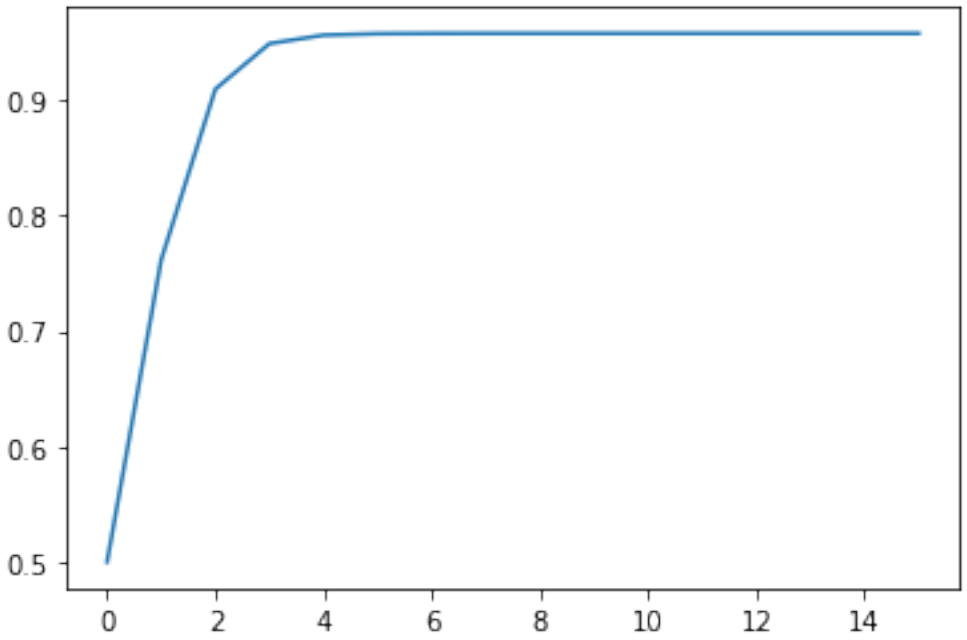
```
a_list = [a]
print(a_list)

while dx > threshold:
    a_list.append(f(a_list[-1]))
    dx = np.abs(a_list[-1]-a_list[-2])

import matplotlib.pyplot as plt

plt.plot(a_list)
print(a_list[-1])
```

```
[0.5]
0.9575040240732228
```



2.2 Newton's method

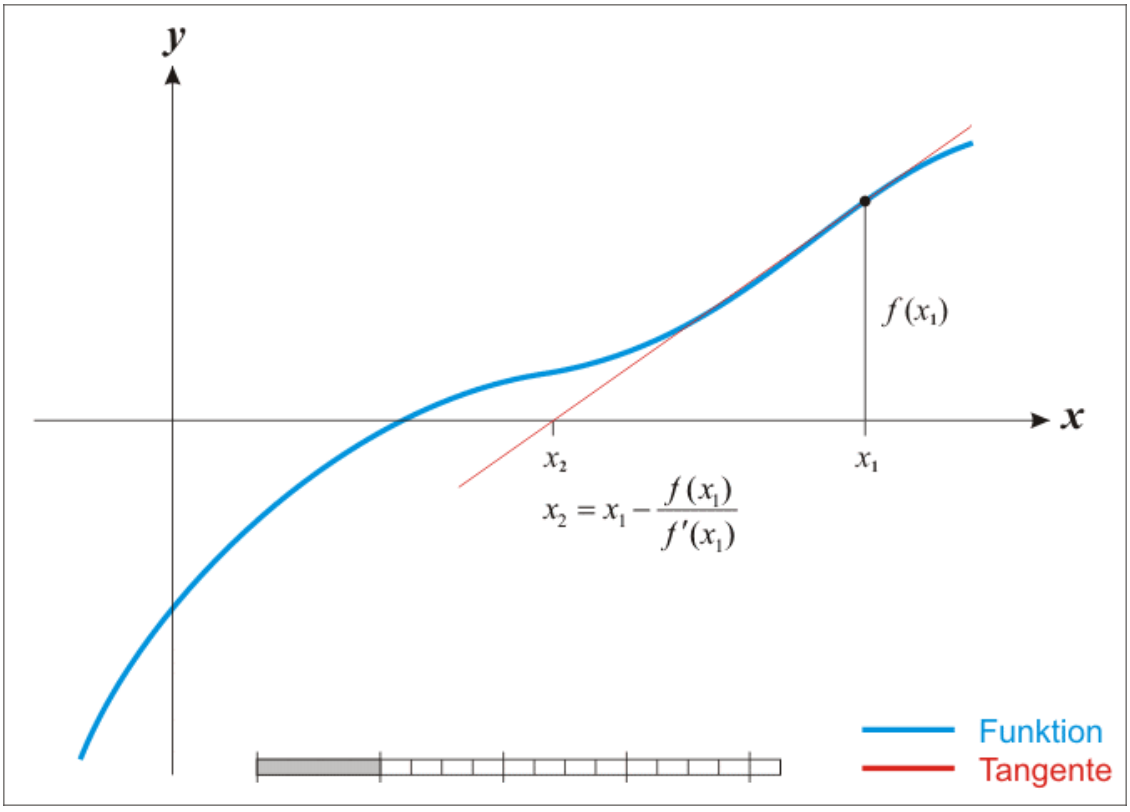
Solving for x in $f(x) = 0$

1. Start with some value x_1, calculate tangent $f'(x_1)$
2. Travel along tangent line to intersection with x-axis at x_2
3. Repeat (calculate tangent $f'(x_2)$, etc.)

Mathematically:

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

Secant method: If analytic form of f is unknown, calculate $f'(x)$ using numerical difference (usually forward or backward, to avoid re-computing yet another $f(x_k)$).



Pro: * Much faster than relaxation

Cons: * Need to know f' (although this issue is addressed by the secant method) * Doesn't always converge * need to have good initial guess (like relaxation), * may follow slope in wrong direction, * small f' gives x_{n+1} much farther away, * sometimes, it just does not converge. Period. (e.g., fractals)

2.3 Bisection (or Binary Search)

- Bracket a single root on either side of the zero of the function (x_1, x_2)
- Use midpoint x' as subsequent bracket
- Choose brackets depending on the sign of the value at the midpoint;
  - For this example, $f(x') < 0$, so the next set of brackets is (x_1, x')

Pro: * Incredibly easy to remember, therefore to implement * When there's a root, there's a way (no worries about converging towards at least *a* root)

Cons: * Only works with a single bracketed root * Can't find "double roots" where $f(x)$ does not cross 0 (think $f(x) = x^2$) * Large sample intervals can "miss" roots * Slower than Newton

2.3.1 Convergence characteristics

Method	Convergence Test	Formula
Relaxation	Taylor expansion, assuming proximity to root	$\varepsilon = \frac{x - x'}{1 - 1/f'(x)}$
Newton	Taylor expansion about solution of f(x)=0. Very fast convergence.	$\varepsilon = x - x'$ $\varepsilon = O\left(\varepsilon_0^{2^N}\right)$
Binary search	Error decreases by a factor of two each iteration	$\varepsilon = \Delta / 2^N$

|
Method |Convergence test |Formula |
—————	—————————	—————————
Relaxation	Taylor expansion, assuming proximity to root	$\epsilon = \frac{x-x'}{1-1/f'(x)}$
Newton	Taylor expansion about solution of $f(x) = 0$. Very fast convergence.	$\epsilon = x - x' = O(\epsilon_0^{2^N})$
Binary search	Error decreases by a factor of 2 with each iteration	$\epsilon = \frac{\Delta}{2^N}$

2.4 Finding minima/maxima

- Many ways to do this
- This week's example: Golden Ratio search

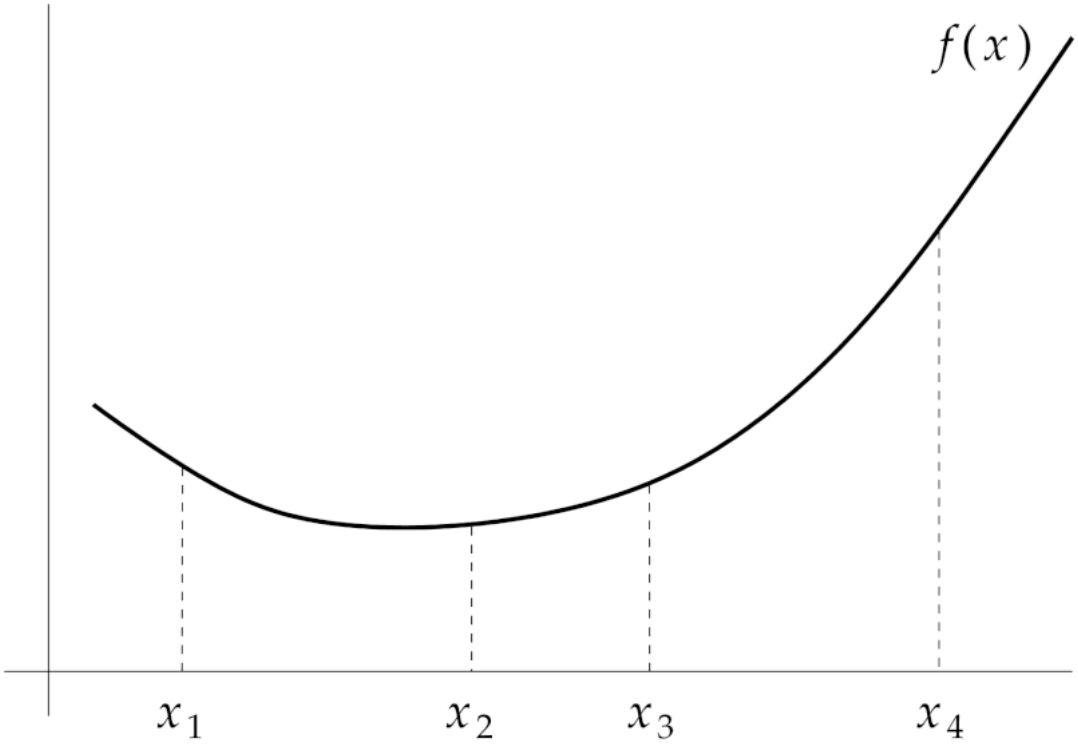
2.5 Golden ratio search

Similar to binary search: find minimum by shrinking intervals

1. Start with 2 points a, b bracketing the interval
2. Choose 2 points x_1, x_2 inside the interval

- Check which of $f(x_1)$ and $f(x_2)$ is lower to determine new brackets

Use the golden ratio to determine the most optimal placement of the internal points x_1, x_2



2.6 Golden ratio search: intuition

[Will expand]

- Interior points x_1, x_2 are symmetric about the midpoint of the interval
- With each iteration, we want the new interior points to have the same ratio to the edges

$$\frac{b-a}{x_2-a} = \frac{b'-a'}{x_2'-a'} \qquad \frac{A+B}{A}$$
$$= \frac{x_2-a}{x_1-a} \qquad \frac{A}{B}$$