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

Solving linear systems

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
$$A = \begin{bmatrix} 6 & 5 \\ 4 & 3 \end{bmatrix}, \qquad v = \begin{pmatrix} 2 \\ 1 \end{pmatrix}$$

Refresher on Gaussian elimination (how `gausselim` works): the equation we need to solve is
$$\begin{bmatrix} 6 & 5 \\ 4 & 3 \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \end{pmatrix}$$
and therefore
$$\begin{aligned} 6x_1 + 5x_2 &= 2, \\ 4x_1 + 3x_2 &= 1 \end{aligned}$$

1. Divide 1st line by 1st (top-left) coefficient:
$$\begin{aligned} x_1 + \frac{5}{6}x_2 &= \frac{1}{3}, \\ 4x_1 + 3x_2 &= 1 \end{aligned}$$

2. $4 \times$ 1st eqn $-$ 2nd eqn $=$ new 2nd eqn.:
$$\begin{aligned} x_1 + \frac{5}{6}x_2 &= \frac{1}{3}, \\ 0x_1 + \frac{1}{3}x_2 &= \frac{1}{3}, \end{aligned}$$
and $x_2 = 1$. 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: $x_2 = 1 \Rightarrow x_1 + 5/6 = 1/3 \Rightarrow x_1 = -1/2$.

In [5]:
```
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. ]
```

In [ ]:
```
# %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)
```

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` :

In [9]:
```
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.

In [10]:
```
print("1/1e-20 =", 1/1e-20)  # possible because smaller than the biggest number representable
```

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

In [11]:
```
print("1/0", 1/0.)  # that on the other hand is too obvious
```

```
---------------------------------------------------------------------------
ZeroDivisionError                         Traceback (most recent call last)
/var/folders/7y/707b3rbx7dv9jch1hz6swz1w0000gn/T/ipykernel_51741/1635138342.py in <module>
----> 1 print("1/0", 1/0.)  # that on the other hand is too obvious

ZeroDivisionError: float division by zero
```

In [12]:
```
# In a previous python version, the following gave the right answer...
# ... but it now gives the same, wrong result.
np.linalg.solve(A2, V2)
```

Out[12]:
```
array([0., 1.])
```

In [13]:
```
# SciPy does not give a better result ... but at least it gives a warning!
import scipy.linalg as la
la.solve(A2, V2)
```

```
/var/folders/7y/707b3rbx7dv9jch1hz6swz1w0000gn/T/ipykernel_51741/4139572006.py:2: LinAlgWarning: Ill-conditioned matrix
(rcond=1e-40): result may not be accurate.
  la.solve(A2, V2)
```

Out[13]:
```
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.

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 m^{th} element (absolute value)
    - Swap this row with the current m^{th} value
    - Proceed with Gaussian elimination

In [15]:
```
A3 = np.array([[1, 1], [1e-20, 1]], float)  # swapped rows
V3 = np.array([0, 1], float)  # need to swap this one too

ge.gausselim(A3, V3)
```

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

LU Decomposition

Motivation

Two pendulums, A and B, of identical masses m and lengths ℓ, coupled by spring of stiffness k.

Two pendulums, A and B, of identical masses m and lengths ℓ, coupled by spring of stiffness k.

Suppose each is driven differently:

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

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

- Can write these equations as $Ax = f$.
- A is always the same (depends on properties of pendulums and spring),
- but f_A, f_B, ω_1, ω_2 could change if the operator decides to change the driving.

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 that yields $U = L_n L_{n-1}\cdots L_0 A$, where U is upper triangular (i.e., result of Gaussian elimination):

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

(see Newman pp. 222-224 for a 4×4 example; easy but long)

The decomposition

$$\boxed{LU = A}$$

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

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 ⇒ back-substitution (pizza cake!)
- This method is used by `numpy.linalg.solve(A, f)`
- `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.

- Once you've done the LU decomposition of A, you don't need to do it again $\Rightarrow$ f can change over and over, $Ly = f$ is staightforward, and so is $Ux = y$.

Issues with LU Decomposition

LU Decomposition fails when A is close to singular, due to rounding error again.

For starters, take a matrix that is actually singular, e.g:

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

Depending on the RHS, we end up with either no solution, or one undetermined coefficient.

$A\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 3 \\ 5 \end{pmatrix}$ $\rightarrow$ can't have $x_1 + 2x_2 = 3$ and $= 5/2$ at the same time

$A\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 3 \\ 6 \end{pmatrix}$ $\rightarrow$ infinite number of solutions

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 δ is too small.

In [19]:
```
delta = 1e-16
A = np.array([[1, 2], [2, 4+delta]], float)
print(A)
v = np.array([3, 5], float)
np.linalg.solve(A, v)  # returns error if delta/4 < machine precision
```

```
[[1. 2.]
 [2. 4.]]

---------------------------------------------------------------------------
LinAlgError                               Traceback (most recent call last)
/var/folders/7y/707b3rbx7dv9jch1hz6swz1w0000gn/T/ipykernel_51741/3549545471.py in <module>
      3 print(A)
      4 v = np.array([3, 5], float)
----> 5 np.linalg.solve(A, v)  # returns error if delta/4 < machine precision

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

~/opt/anaconda3/lib/python3.8/site-packages/numpy/linalg/linalg.py in solve(a, b)
    391     signature = 'DD->D' if isComplexType(t) else 'dd->d'
    392     extobj = get_linalg_error_extobj(_raise_linalgerror_singular)
--> 393     r = gufunc(a, b, signature=signature, extobj=extobj)
    394
    395     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)
     86
     87 def _raise_linalgerror_singular(err, flag):
---> 88     raise LinAlgError("Singular matrix")
     89
     90 def _raise_linalgerror_nonposdef(err, flag):

LinAlgError: Singular matrix
```

QR decomposition for eigensystems

Looking for λ's and v's such that $Av = \lambda v$, with v eigenvector, λ eigenvalue

Or 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.

Don't get hung up on the details of the algorithm description below. Recall that it's iterative, and that it can break sometimes.

QR algorithm

- Gram-Schmidt on columns of A (Exercise 6.8) $\Rightarrow$ matrix of orthonormal basis of column vectors Q
- Denote QR decomposition of A as $A = QR$, where R is upper-triangular
- Q orthonormal $\Rightarrow$ $Q^TQ = I$ $\Rightarrow$ $R = Q^TA$.

Iterate:

- $A_1 = RQ = Q^T AQ$ ----------> Define A_1
- $A_1 = Q_1 R_1$ ----------> QR decomposition of A_1
- $A_2 = R_1 Q_1 = \underbrace{Q_1^T \underbrace{Q^T A Q}_{R} Q_1}_{R_1}$ --> Define A_2
- $A_2 = Q_2 R_2$ ----------> QR decomposition of A_2
- $A_3 = \ldots$ ... 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

$$A_k = \underbrace{(Q_k^T \cdots Q_1^T Q^T)}_{V^T \text{ (because } Q_i^T Q_i = I)} A \underbrace{(QQ_1 \cdots Q_k)}_{V}$$

$$\Rightarrow A_k = V^T AV \Rightarrow \boxed{AV = VA_k}.$$

- diagonal entries of A_k (off-diagonal entries are now tiny) are the eigenvalues: $\boxed{A_k = \Lambda}$.
- The eigenvectors are the columns of $\boxed{V = QQ_1 \cdots Q_k}$

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

In [20]:
```
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))
```

```
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]]
```

Be careful!

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

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

In [21]:
```
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('VL:\n', np.dot(V, L))
```

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

Result above should show that with A is not a symmetric matrix: $AV \neq \Lambda V$. There are less efficient algorithms that will work with non-symmetric A.

In [22]:
```
A = np.array([[2,3],[1,2]])
eig_vs, V = np.linalg.eig(A) # calculate eigenvalues & eigenvectors
L = np.diag(eig_vs)  # np.diag constructs a diagonal array

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

```
AV:
 [[ 3.23205081 -0.23205081]
 [ 1.8660254   0.1339746 ]]
VL:
 [[ 3.23205081 -0.23205081]
 [ 1.8660254   0.1339746 ]]
```

Finding roots of nonlinear equations

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

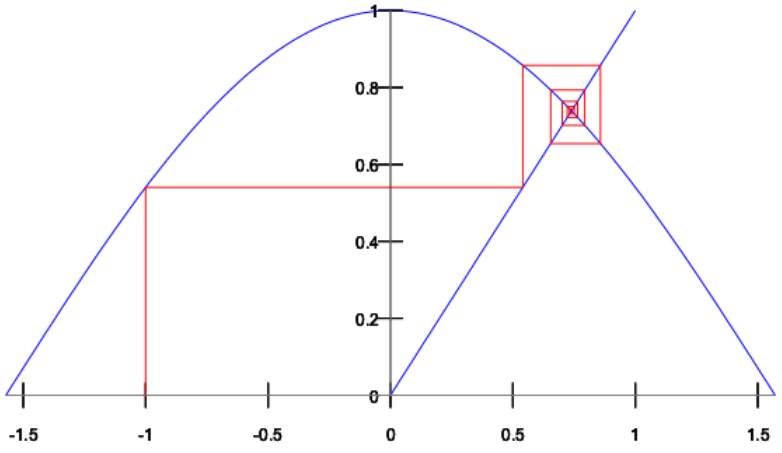
Let's review.

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

$$\begin{aligned} x_1 &= f(x_0) \\ x_2 &= f(x_1) \\ &\vdots \end{aligned}$$

- Caveat: Can only find *stable* fixed points

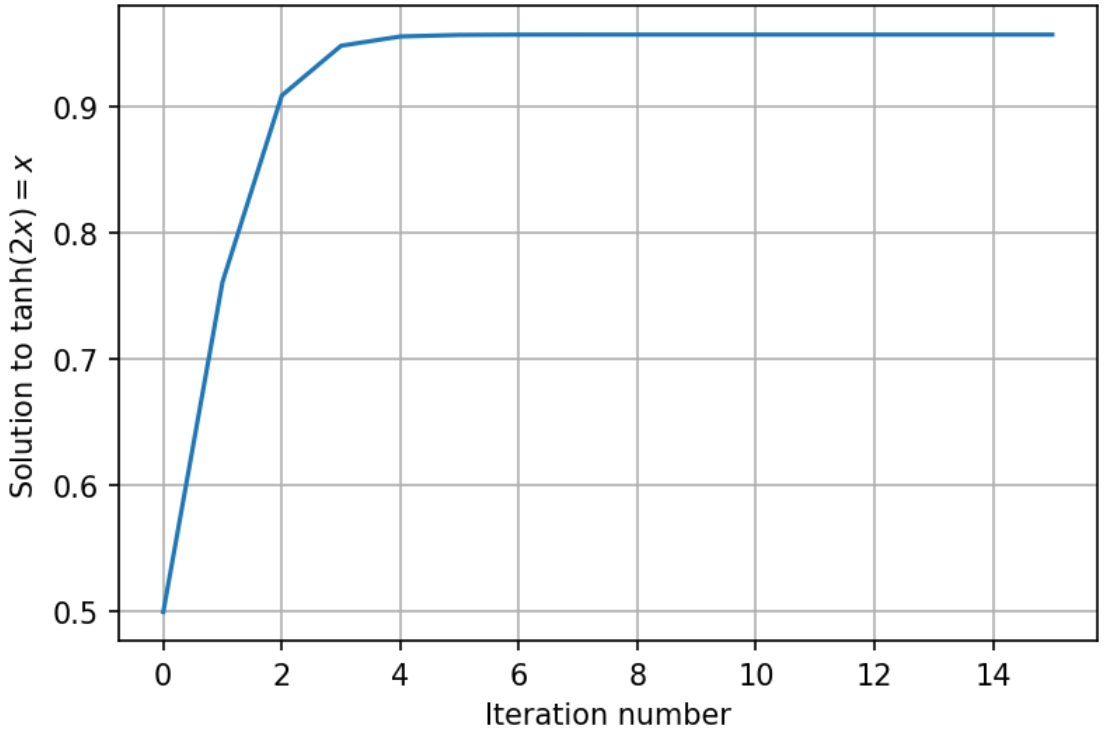


Let's do an example: find the (positive) solution to $\tanh(2x) = x$.

In [3]:
```
import numpy as np
def f(x):
    return np.tanh(2*x)

x = 0.5  # initial x guess
dx = 1  # initial distance (just needs to be big)
threshold = 1e-10  # convergence threshold
x_list = [x]  # will fill up with successive x's

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

```
0.9575040240732228
```

In [4]:
```
def print_sol():
    import matplotlib.pyplot as plt
    plt.figure(dpi=150)
    plt.plot(x_list)
    plt.xlabel("Iteration number")
    plt.ylabel(r"Solution to $\tanh(2x)=x$")
    plt.grid()

print_sol()
```



Newton's method

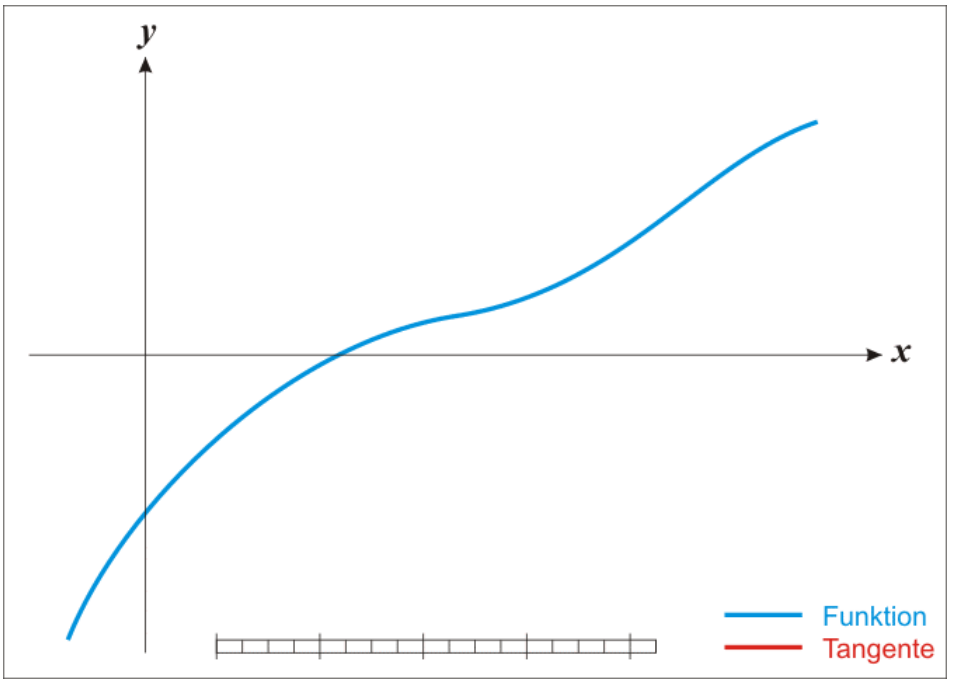
Solving for x in $f(x) = 0$

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 $f'(x)$ numerically - suggest using forward or backward difference, to avoid re-computing yet another $f(x_k)$



Pro:

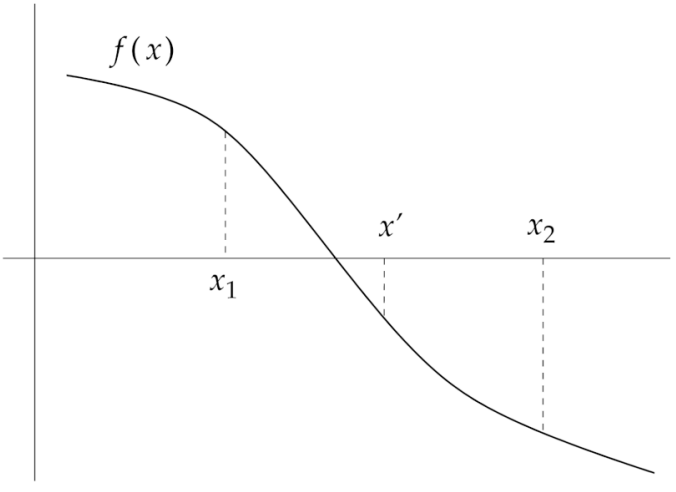
- Much faster than relaxation

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),
  - small f' gives x_{n+1} much farther away,
  - sometimes, it just does not converge. Period. (e.g., fractals)

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, $f(x_1) > 0$, $f(x') < 0$, so the next set of brackets is (x_1, x')



(Newman's fig. 6.3)

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 $f(x)$ reaches but does not cross 0 (think $f(x) = x^2$)
- Can't find even one root when there is an even number of roots.
- Large sample intervals can "miss" roots
- Slower than Newton

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	$\varepsilon = \Delta / 2^N$

Finding minima/maxima

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

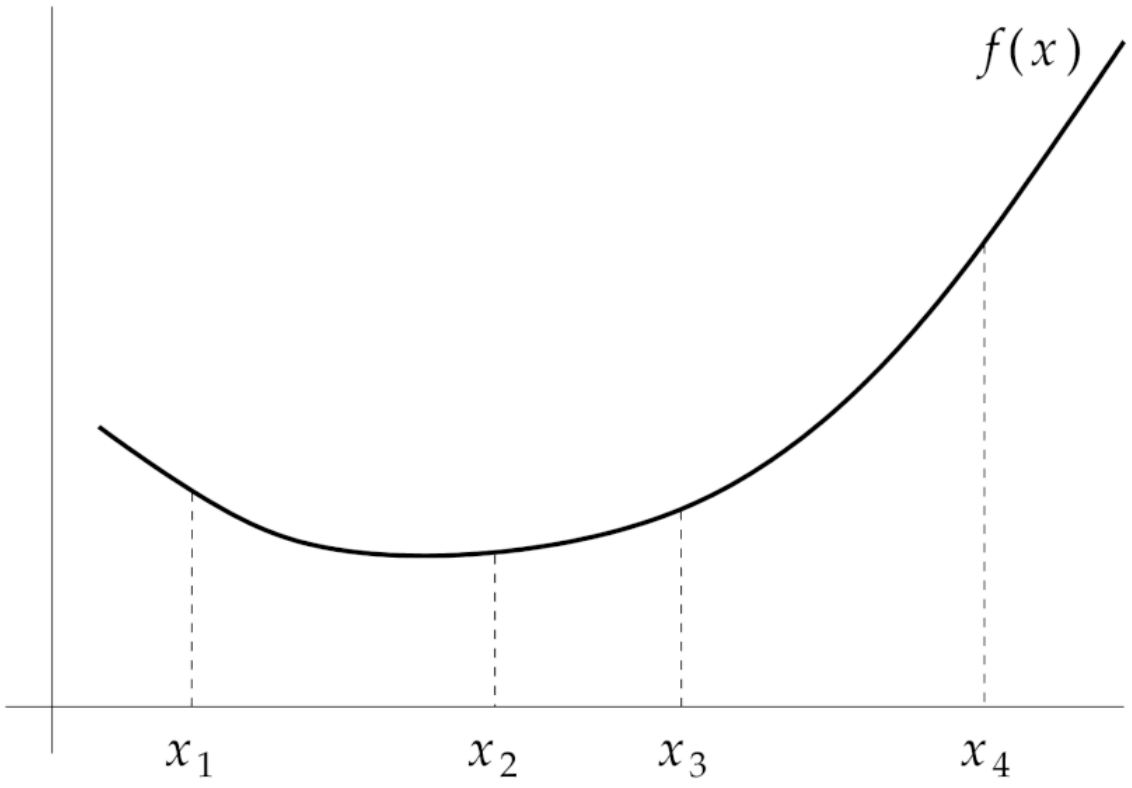
Golden ratio search

Similar to binary search: find minimum by shrinking intervals

1. Start with 2 points x_1, x_4 bracketing the interval
2. Choose 2 points x_2, x_3 inside the interval

- Check which of $f(x_2)$ and $f(x_3)$ is lower to determine new brackets
  - In this example: $f(x_2) < f(x_3) \Rightarrow$ new interval is $[x_1, x_3]$

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



Golden ratio search: intuition

- Interior points x_2, x_3 must be symmetric about the midpoint of the interval (why favour one side vs. the other?)
- If you place interior points close (distance ϵ) to the centre of interval:
  - you'll divide your search interval by ≈ 2 (very good), but
  - next step will be difficult: new "interior" point will be bar from new centre, next step will only divide the search interval by $\approx 1 - \epsilon$ (very bad)
- If you place interior points close to edges creates the opposite: first step very bad, next step very good
- **Solution**: find sweet spot(s) to make sure the search interval is divided by same ratio each time.
- See pp. 281-282 of textbook for explanation of why this ratio needs to be

$$z = \frac{1+\sqrt{5}}{2} \approx 1.618$$

the *Golden Ratio*. I.e., $x_4 - x_1 = (x_3 - x_1)z = (x_4 - x_2)z$.

Summary

Finding solutions of linear systems $Ax = v$

- Gaussian elimination if you know the 1st coefficient will always be OK
- Partial pivot to be safe: re-order equations such that biggest first coefficient shows up first
- LU decomposition is strictly the same as Partial pivot, but storing L and U saves times when A stays the same but v changes often

Finding eigenvalues/eigenvectors

- Matrix is real symmetric or Hermitian: QR algorithm is iterative (can take time to converge) but efficient.
- Otherwise: SciPy will find them for you if patient.

Finding roots of nonlinear equations

$$f(x) = 0 \quad \text{or} \quad f(x) - x = 0$$

- Relaxation for $f(x) = x$ is easy but works only for stable fixed points
- Newton's method is super fast but you need a good initial guess and confidence that a root exists
- Binary search is easy, converges slowly, has a lot of caveat (double roots, need a good initial bracket...)

Finding minima/maxima: Golden ratio search, slow and suffers from same limitations as binary search, but works.