MAS212 Scientific Computing and Simulation

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Today's lecture

- **Solving linear systems $\mathbf{Ax} = \mathbf{b}$** using **Gauss-Jordan elimination**
- Numerical issues.
- **Well-conditioned** and **ill-conditioned** problems
- Example: Wilkinson's polynomial
- Matrices, norms and **condition number**
- Iterative methods:
  - Convergence and spectral radius
  - Solving matrix equations iteratively

Linear systems

- In numerical analysis, we frequently encounter problems of the form

$$\mathbf{Ax} = \mathbf{b}$$

  where **A** is an $N \times N$ matrix, **b** is vector of known values, and **x** is a vector of unknowns.

- For example, in fitting a linear model to a data set, we found **normal equations** of this form: $(\mathbf{X}^T\mathbf{X})\beta = (\mathbf{X}^T\mathbf{y})$.

- In this lecture we will examine:
  - A practical method to find numerical solutions to such equations;
  - A way to assess whether the system of equations is **ill-conditioned**, i.e., sensitive to small changes in **A** and **b**.

Gauss-Jordan elimination

- **Gauss-Jordan elimination** (cf. **Gaussian elimination**) is a robust method for solving a system of linear equations

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

  to find the solution $\mathbf{x}$ and the inverse matrix $\mathbf{A}^{-1}$.

- Here $\mathbf{A}$ is an $N \times N$ square matrix such that $\det \mathbf{A} \neq 0$.
- G-J elimination combines the following operations:
  - Interchanging any pair of **rows** of the system,
  - Multiplying all elements in a row by any scalar,
  - Combining rows in arbitrary linear combinations.

Gauss-Jordan elimination

Example

Apply Gauss-Jordan elimination to:

(i) find the unique solution $\mathbf{x}$ to $\mathbf{Ax} = \mathbf{b}$, where

$$\mathbf{A} = \begin{pmatrix} 0 & 2 & 1 \\ 2 & -1 & 1 \\ 1 & 3 & 2 \end{pmatrix}, \qquad \mathbf{b} = \begin{pmatrix} 7 \\ 3 \\ 13 \end{pmatrix},$$

(ii) find the inverse matrix $\mathbf{A}^{-1}$.

Gauss-Jordan elimination

- Form the augmented matrix:

$$\left(\begin{array}{ccc|ccc|c} 0 & 2 & 1 & 1 & 0 & 0 & 7 \\ 2 & -1 & 1 & 0 & 1 & 0 & 3 \\ 1 & 3 & 2 & 0 & 0 & 1 & 13 \end{array}\right)$$

- We want to eliminate coefficients in the **first column**. Swap the first two rows:

$$\left(\begin{array}{ccc|ccc|c} 2 & -1 & 1 & 0 & 1 & 0 & 3 \\ 0 & 2 & 1 & 1 & 0 & 0 & 7 \\ 1 & 3 & 2 & 0 & 0 & 1 & 13 \end{array}\right)$$

- Divide the first row by 2.

$$\left(\begin{array}{ccc|ccc|c} 1 & -1/2 & 1/2 & 0 & 1/2 & 0 & 3/2 \\ 0 & 2 & 1 & 1 & 0 & 0 & 7 \\ 1 & 3 & 2 & 0 & 0 & 1 & 13 \end{array}\right)$$

Gauss-Jordan elimination

- Subtract 1st row from 3rd row:

$$\left(\begin{array}{ccc|ccc|c} 1 & -1/2 & 1/2 & 0 & 1/2 & 0 & 3/2 \\ 0 & 2 & 1 & 1 & 0 & 0 & 7 \\ 0 & 7/2 & 3/2 & 0 & -1/2 & 1 & 23/2 \end{array}\right)$$

- Multiply 3rd row by 4:

$$\left(\begin{array}{ccc|ccc|c} 1 & -1/2 & 1/2 & 0 & 1/2 & 0 & 3/2 \\ 0 & 2 & 1 & 1 & 0 & 0 & 7 \\ 0 & 14 & 6 & 0 & -2 & 4 & 46 \end{array}\right)$$

- Subtract 7$\times$ 2nd row from the 3rd row. Divide 2nd row by 2.

$$\left(\begin{array}{ccc|ccc|c} 1 & -1/2 & 1/2 & 0 & 1/2 & 0 & 3/2 \\ 0 & 1 & 1/2 & 1/2 & 0 & 0 & 7/2 \\ 0 & 0 & -1 & -7 & -2 & 4 & -3 \end{array}\right)$$

Gauss-Jordan elimination

- Add $\frac{1}{2}\times$ 3rd row to the 2nd row. Add $\frac{1}{2}\times$ 3rd row to the 1st row. Multiply 3rd row by -1.

$$\left(\begin{array}{ccc|ccc|c} 1 & -1/2 & 0 & -7/2 & -1/2 & 2 & 0 \\ 0 & 1 & 0 & -3 & -1 & 2 & 2 \\ 0 & 0 & 1 & 7 & 2 & -4 & 3 \end{array}\right)$$

- Add $1/2$ of 2nd row to the 1st row:

$$\left(\begin{array}{ccc|ccc|c} 1 & 0 & 0 & -5 & -1 & 3 & 1 \\ 0 & 1 & 0 & -3 & -1 & 2 & 2 \\ 0 & 0 & 1 & 7 & 2 & -4 & 3 \end{array}\right)$$

- The middle values give the inverse matrix $\mathbf{A}^{-1}$.
- The red values are the solution to $\mathbf{Ax} = \mathbf{b}$:

$$x = 1, \quad y = 2, \quad z = 3.$$

Row operations are straightforward in Python:

```
import numpy as np
def swaprows(M, i, j):
    M[i-1,:], M[j-1,:] = M[j-1,:].copy(), M[i-1,:].copy()

aug = np.matrix("0,2,1,1,0,0,7; 2,-1,1,0,1,0,3; 1,3,2,0,0,1,13")
M = np.array(aug, dtype=np.float64)
swaprows(M,1,2)
M[0,:] = M[0,:] / 2.0
M[2,:] = M[2,:] - M[0,:]
M[2,:] = M[2,:]*4
M[2,:] = M[2,:] - 7*M[1,:]
M[1,:] = M[1,:]/2
M[1,:] = M[1,:] + M[2,:]/2
M[0,:] = M[0,:] + M[2,:]/2
M[2,:] = M[2,:]*(-1)
M[0,:] = M[0,:] + M[1,:]/2
print(M[:,-1])
print(M[:,3:6])
```

Gauss-Jordan elimination

Gauss-Jordan method with partial pivoting: pseudo-code

1. Construct the augmented matrix. Set row number $i = 1$.
2. Find the row $j \geq i$ with the largest absolute value in column i. This is the **pivot row**. Swap rows i and j so that the pivot row becomes row i.
3. Divide the pivot row by a_{ii} so that the new element in row i, column i becomes 1.
4. Eliminate the entries in column i and rows $j > i$ using linear combinations of the pivot row i.
5. Increment the row number i by 1 and repeat, until the system is in **upper diagonal form**.
6. Use the last row $i = N$ to eliminate all entries in the last column for all rows $j < N$.
7. Use the second-to-last row to eliminate the second-to-last column entries
8. Continue in this way until the left-hand part of the augmented matrix is the identity matrix.
9. Read off the inverse matrix $\mathbf{A}^{-1}$ and the solution $\mathbf{x}$.

Numerical issues

- The linear system $\mathbf{Ax} = \mathbf{b}$ is **singular** if $\det \mathbf{A} = 0$.
  In this case there may be no solutions, or infinitely many.
- If $\det \mathbf{A} \neq 0$ then a unique solution exists, in principle.
- In practice, at least two things can go wrong:
  1. Some of the equations are so close to linearly dependent that roundoff error render them linearly dependent at some point in the solution process.
  2. If N is large, the accumulated roundoff errors in the process can swamp the true solution.
- The Gauss-Jordan method is reasonably stable, and reasonable efficient, **provided that pivoting is used**.

Conditioning

- Suppose we have some **problem** with parameters λ_i ...
- ... and a **solution** represented by functions $f_k(\lambda_i)$.
- We say that the problem is:
  - **well-conditioned** if small changes in λ_i produce small changes in f_k.
  - **ill-conditioned** if small changes in λ_i produce some **large** or **non-smooth** changes in f_k.
- The **condition number** C is an attempt to quantify the sensitivity of the solution to changes in the parameters.
- As small changes in parameters can be produced by numerical errors (e.g. round-off error), numerical solutions of ill-conditioned problems are **unreliable**.

Example: Wilkinson's polynomial

- Consider the polynomial

$$P_n(x) = (x-1)(x-2)\dots(x-n) = \prod_{k=1}^{n}(x-k)$$

- The equation $P_n(x) = 0$ has **roots** $x = 1, 2, \dots, n$.
- Now consider a **slightly-perturbed** polynomial, for example,

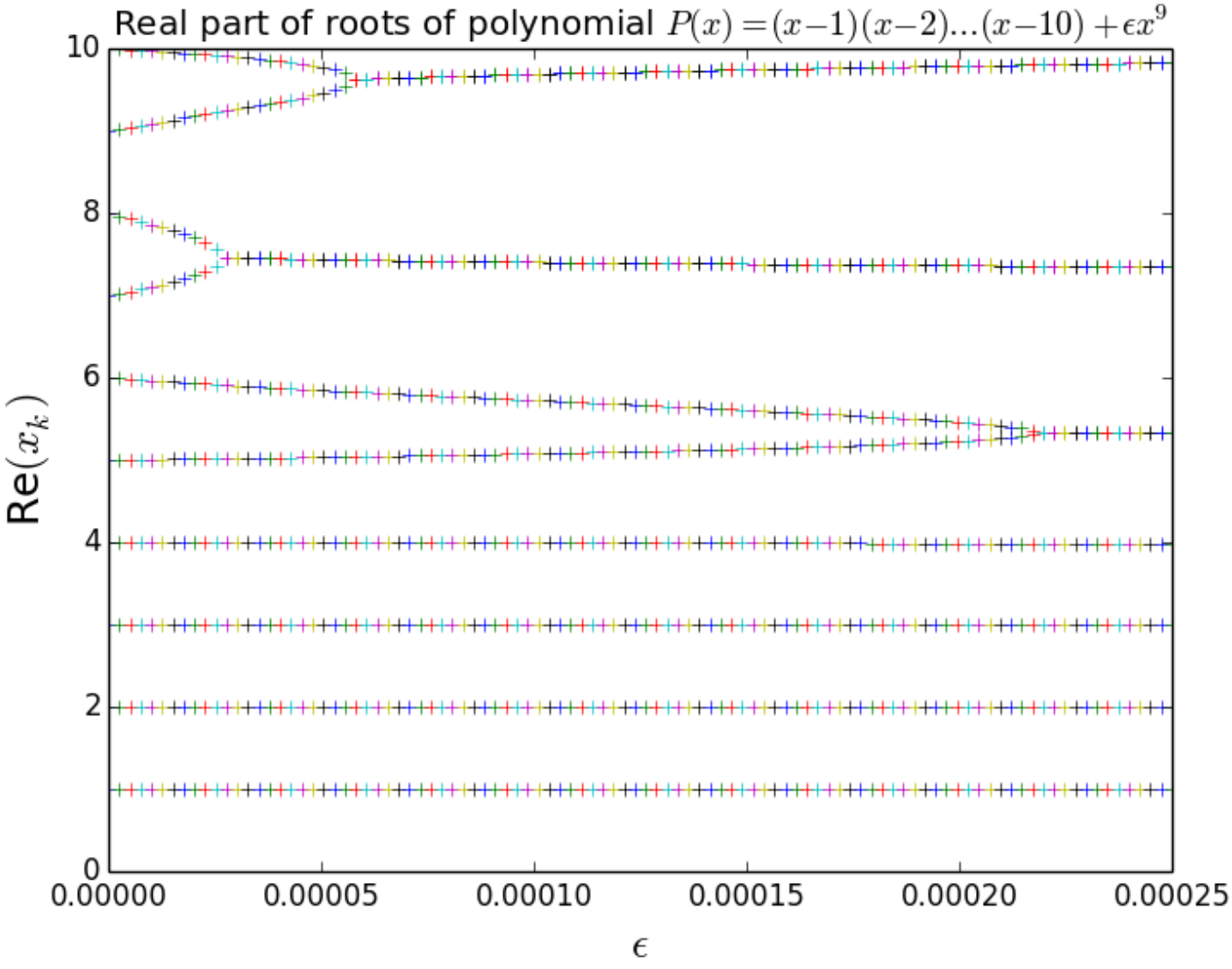
$$\tilde{P}_n(x) = P_n(x) + \epsilon x^{n-1}, \qquad \epsilon \ll 1.$$

- How do the roots of $\tilde{P}_n(x)$ differ from the roots of $P_n(x)$?
- Let us investigate by plotting the roots x_k as a function of ϵ, for the cases $n = 10$ and $n = 15$.

Example: Wilkinson's polynomial

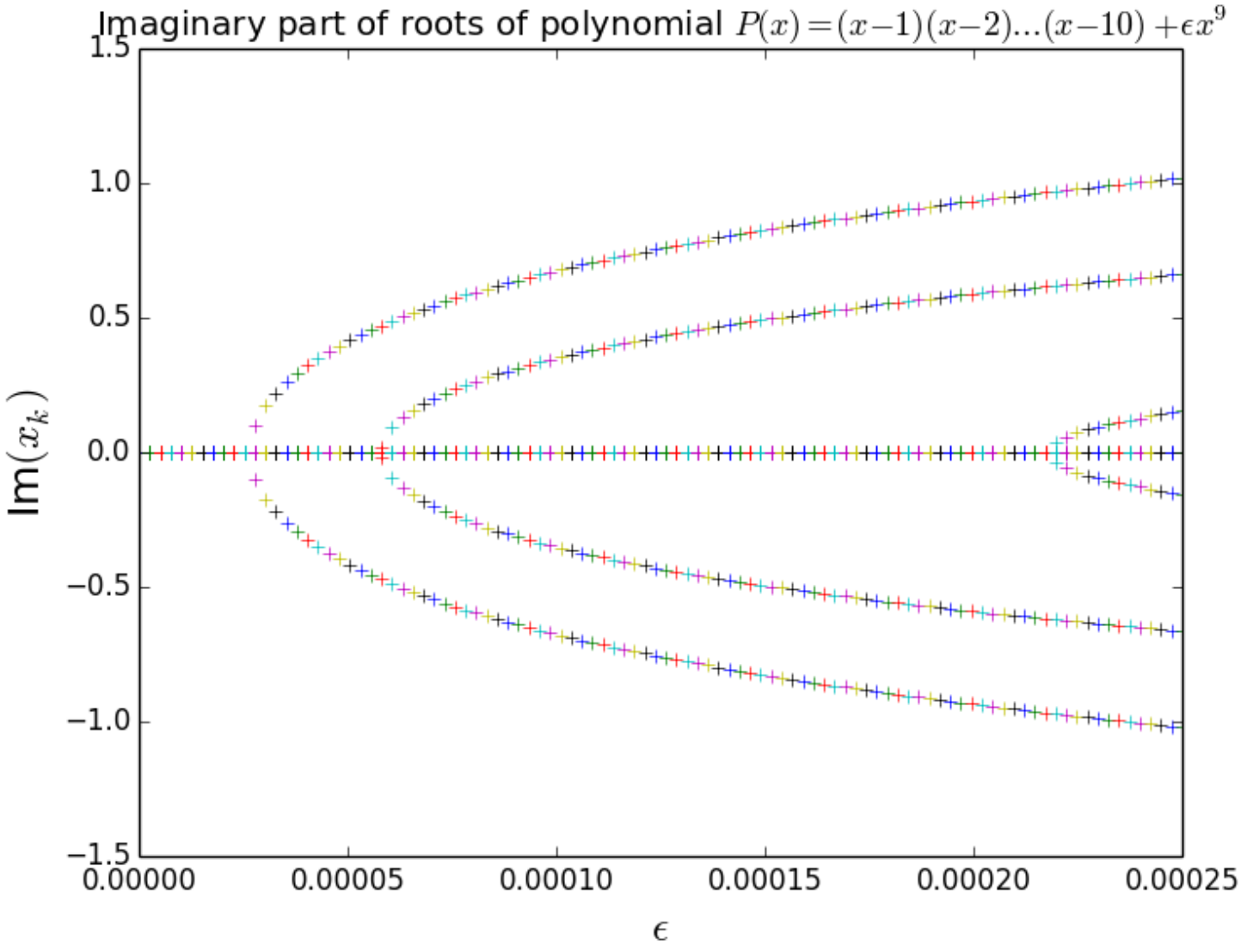
```
import numpy as np
import matplotlib.pyplot as plt
n = 10
# Coefficients of Wilkinson's polynomial for n=10
a = np.array([1,-55,1320,-18150,157773,-902055,3416930,
          -8409500,12753576,-10628640,3628800], dtype=np.float64)
print "The unperturbed roots are : ", np.roots(a)
b = np.copy(a)  # for the modified coefficients
eps = np.linspace(0.0, 2.5e-4, 100)
for ep in eps:
    b[1] = M[1] + ep  # make a small change to x^{n-1} coefficient
    roots = np.roots(b) # find the roots of the modified polynomial
    plt.plot(ep*np.ones(n), roots.real, '+')
plt.show()
```

Example: Wilkinson's polynomial



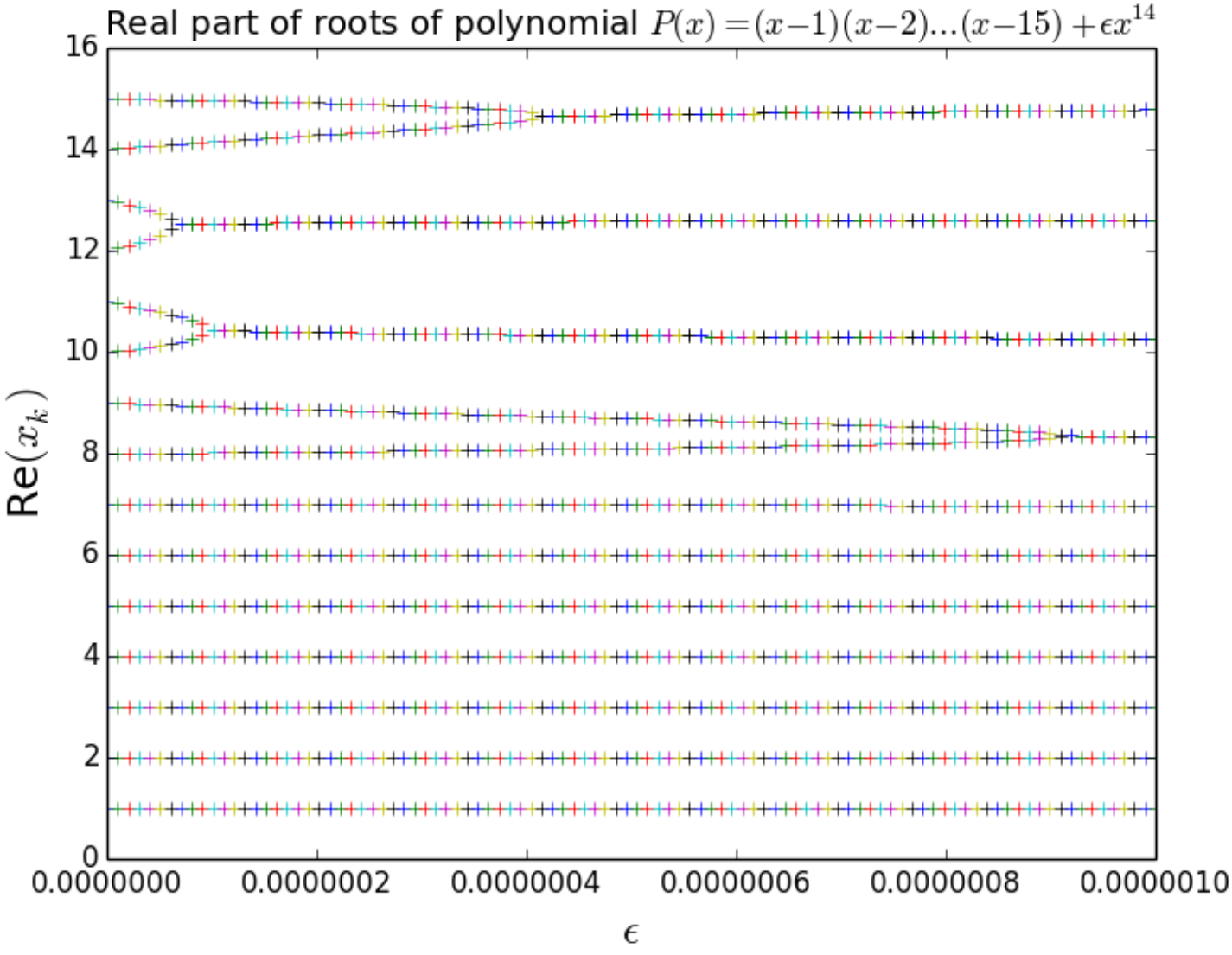
$n = 10$, real part of root

Example: Wilkinson's polynomial



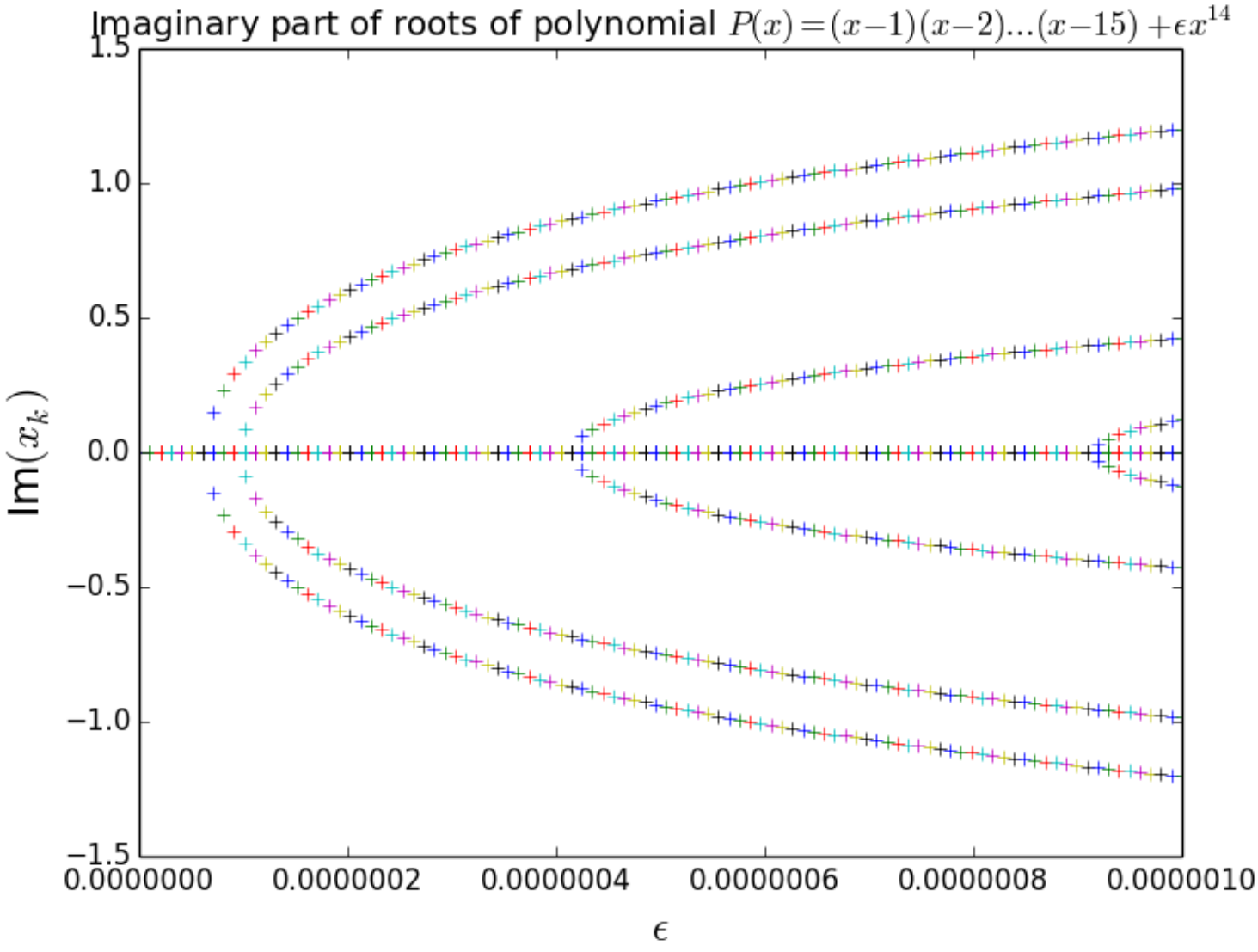
$n = 10$, imaginary part of root

Example: Wilkinson's polynomial



$n = 15$, real part of root

Example: Wilkinson's polynomial



$n = 15$, imaginary part of root

Roots of Wilkinson's polynomial

- For $n = 15$ case, the first merger of roots occurs around $\epsilon \sim 10^{-7}$
- For $n = 20$ case, a tiny change $\epsilon \sim 10^{-10}$ has a large effect on at least one pair of roots.
- As n increases, the roots become **extremely sensitive** to the polynomial coefficients
  $\Rightarrow$ problem is **ill-conditioned**.
- Wilkinson used this polynomial to illustrate the **ubiquity** of ill-conditioned problems, and later commented on the impact of the discovery:

In *The Perfidious Polynomial* (1984)

"Speaking for myself I regard it as the most traumatic experience in my career as a numerical analyst."

A cautionary tale

- Suppose we wished to find the **eigenvalues** λ of a large $n \times n$ matrix A.
- The eigenvalues are the roots of the **characteristic polynomial** $p(x)$ defined by

$$p(x) = \det(A - xI)$$

- As Wilkinson's example shows, large-n polynomials can be **ill-conditioned**, even when the roots are not close together (i.e. even when eigenvalue problem is well-conditioned).

Matrix equations

- In numerical analysis, we frequently encounter problems of the form

$$\mathbf{Ax} = \mathbf{b}$$

  where **A** is an $n \times n$ matrix, **b** is vector of known values, and **x** is a vector of unknowns.

- For example, in fitting a linear model to a data set, we found **normal equations** of this form: $(\mathbf{X}^T\mathbf{X})\beta = (\mathbf{X}^T\mathbf{y})$.

- We would like to be able to test, in practical cases, whether the system of equations is **ill-conditioned**.

- Even better, we would like to calculate a **condition number** C : the **'worst case' ratio** of the relative change in output to the relative change in input.

Example:

$$\begin{pmatrix} 1 & 2 \\ 2 & 3.999 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 4 \\ 7.999 \end{pmatrix}$$

Is this system well-conditioned?

- The solution is $x = 2$, $y = 1$.
- Now change the RHS slightly, to $\begin{pmatrix} 4.001 \\ 7.998 \end{pmatrix}$, and recalculate.
- The new solution is $x = -3.999$, $y = 4$
- A small change in b produced a **large** change in the solution $\Rightarrow$ **ill-conditioned** system.
- How could we see this **without** computing the solutions?

```python
import numpy as np
A = np.matrix("1 2 ; 2 3.999")
b = np.matrix("4 ; 7.999")
db = np.matrix("0.001 ; -0.001")  # a small perturbation
sol0 = np.linalg.solve(A,b)
sol1 = np.linalg.solve(A,b+db)
print("Original solution:\n", sol0)
print("Perturbed solution:\n", sol1)
```

```
Original solution:
 [[ 2.]
 [ 1.]]
Perturbed solution:
 [[-3.999]
 [ 4.   ]]
```

- How could we see this **without** finding the solutions?

Definition :

- The **row sum norm** of an $m \times n$ matrix A is defined as

$$\|A\| = \max_{1 \le i \le m} \sum_{j=1}^{n} \left|a_{ij}\right|$$

  where a_{ij} is the element in the ith row and jth column of A.

- i.e. for each row, compute the sum of the absolute values of its elements; then take the maximum of these sums; this is the row-sum norm.

- Suppose we introduce some small change Δb in b, which produces a change Δx in the solution x, i.e.,

$$\begin{aligned} Ax &= b, \quad \text{and} \\ A(x + \Delta x) &= b + \Delta b \\ \Rightarrow \quad A\,\Delta x &= \Delta b \\ \Rightarrow \quad \Delta x &= A^{-1}\Delta b \end{aligned}$$

- We make use of an inequality for the row-sum norm, which holds that for any matrix or vector B, C:

$$\|BC\| \leq \|B\|\,\|C\|$$

- For example,

$$\begin{aligned} \|b\| &= \|A\,x\| \\ \Rightarrow \quad \|b\| &\leq \|A\|\,\|x\| \end{aligned}$$

- Similarly,

$$||\Delta x|| \leq ||A^{-1}||\,||\Delta b||$$

- Thus,

$$||b||\,||\Delta x|| \leq ||A||\,||A^{-1}||\,||x||\,||\Delta b||$$

and so

$$\Rightarrow \quad \frac{||\Delta x||}{||x||} \leq C\,\frac{||\Delta b||}{||b||}$$

where $C \equiv ||A||\,||A^{-1}||$.

Definition :

The **condition number** for a matrix A is defined as

$$C = \|A\| \left\|A^{-1}\right\|$$

- We have shown that

$$\frac{\|\Delta x\|}{\|x\|} \leq C \frac{\|\Delta b\|}{\|b\|}$$

- A matrix equation $Ax = b$ is said to be **ill-conditioned** if

$$C \gtrsim 10^n$$

where n is the number of equations.

Example:

Find the condition number of the matrix

$$A = \begin{pmatrix} 1 & 2 \\ 2 & 3.999 \end{pmatrix}$$

Solution :

- Determinant: $\det A = 3.999 - 4 = -0.001$
- Matrix inverse:

$$A^{-1} = \frac{1}{\det A}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix} = -1000 \times \begin{pmatrix} 3.999 & -2 \\ -2 & 1 \end{pmatrix}$$

- Row-sum norms:

$$\begin{aligned} \|A\| &= \max(1+2, 2+3.999) = 5.999 \\ \|A^{-1}\| &= 1000 \times \max(3.999+2, 2+1) = 5999 \end{aligned}$$

- Condition number:

$$\Rightarrow \quad C = \|A\|\,\|A^{-1}\| = 35988$$

- $C \approx 3.6 \times 10^4 > 10^2 \quad \Rightarrow \quad Ax = b$ is **ill-conditioned**.

```
def norm(A):
    """Returns the row sum norm of A."""
    rowsums = [abs(M[k,:]).sum() for k in range(A.shape[0])]
    return max(rowsums)

def cond(A):
    """Returns the condition number of A"""
    return norm(A)*norm(np.linalg.inv(A))

def wellcond(A):
    condA = cond(A)
    w = "well" if (condA < 10**(A.shape[0])) else "ill"
    print("A is " + w + "-conditioned:  C = %e" % condA)
```

```
>>> wellcond(A)
A is ill-conditioned: C = 3.598800e+04
```

Iterative improvement

$$\boxed{\mathbf{A}\mathbf{x} = \mathbf{b}}$$

- Suppose $\mathbf{A} = \mathbf{A}_0 + \Delta\mathbf{A}$ where $\mathbf{A}_0$ is some matrix whose inverse is **known**, $\mathbf{B}_0 \equiv \mathbf{A}_0^{-1}$.
- Suppose we wanted to solve **iteratively**, i.e. **without** finding the inverse directly, or applying Gaussian elimination.
- Then, starting with an initial guess $\mathbf{x}_0$, we may try an iterative approach:

$$\begin{aligned} \mathbf{A}_0\mathbf{x} &= \mathbf{b} - \Delta\mathbf{A}\,\mathbf{x} \\ \Rightarrow \quad \mathbf{x}_{k+1} &= \mathbf{B}_0\left(\mathbf{b} - \Delta\mathbf{A}\,\mathbf{x}_k\right) \\ &= \mathbf{R}\mathbf{x}_k + \mathbf{c} \end{aligned}$$

where $\mathbf{R} \equiv -\mathbf{B}_0\Delta\mathbf{A}$ is the **residual matrix** and $c = \mathbf{B}_0\mathbf{b}$.

Iterative improvement

$$\boxed{\mathbf{x}_{k+1} = \mathbf{R}\mathbf{x}_k + \mathbf{c}}$$

- When do iterative methods of this type **converge**?
- Repeated application leads to

$$\mathbf{x}_n = \mathbf{R}^n\mathbf{x}_0 + \left(\mathbf{I} + \mathbf{R} + \mathbf{R}^2 + \ldots + \mathbf{R}^{n-1}\right)\mathbf{c}$$

- For convergence, we require $\mathbf{R}^n \to 0$ as $n \to \infty$.

Spectral radius and convergence

Definition :

The **spectral radius** $\rho(\mathbf{R})$ of an $n \times n$ matrix $\mathbf{R}$ is given by the maximum magnitude of its eigenvalues λ_i :

$$\rho(\mathbf{R}) = \max_{i=1\ldots n} |\lambda_i| .$$

Theorem :

- $\lim_{k\to\infty} \mathbf{R}^k = 0$ **if and only if** $\rho(\mathbf{R}) < 1$

- Thus an iterative method can be used iff $\mathbf{R}$ is **'small enough'** that all of its eigenvalues have a magnitude of less than unity.
- Iterative methods are used (e.g.) to efficiently solve the linear equations arising in *implicit methods*.

Example:

Let

$$\mathbf{A} = \begin{pmatrix} 1.1 & 0.2 \\ -0.3 & 1.9 \end{pmatrix}, \quad \mathbf{x} = \begin{pmatrix} x \\ y \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

Solve the matrix equation $\mathbf{Ax} = \mathbf{b}$ iteratively with

$$\mathbf{A}_0 = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$$

Example

- Let $\mathbf{B}_0 = \mathbf{A}_0^{-1}$

$$\begin{aligned} (\mathbf{A}_0 + \Delta\mathbf{A})\mathbf{x} &= \mathbf{b} \\ \Rightarrow \quad (\mathbf{I} + \mathbf{B}_0\Delta\mathbf{A})\,\mathbf{x} &= \mathbf{B}_0\mathbf{b} \\ \Rightarrow \quad \mathbf{x} &= -(\mathbf{B}_0\Delta\mathbf{A})\mathbf{x} + \mathbf{B}_0\mathbf{b} \end{aligned}$$

- Turn into an iterative equation:

$$\mathbf{x}_{n+1} = \mathbf{R}\mathbf{x}_n + \mathbf{c}$$

  where $\mathbf{R} = -\mathbf{B}_0\Delta\mathbf{A}$ and $\mathbf{c} = \mathbf{B}_0\mathbf{b}$

- In this case, $\mathbf{A}_0 = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix} \quad \Rightarrow \quad \mathbf{B}_0 = \begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$ and $\Delta\mathbf{A} = \begin{pmatrix} 0.1 & 0.2 \\ -0.3 & -0.1 \end{pmatrix}$.

Example

```
B0 = np.matrix("1 0 ; 0 0.5")
dA = np.matrix("0.1 0.2 ; -0.3 -0.1")
b = np.matrix("1; 2")
R = -np.dot(B0, dA)
c = np.dot(B0, b)
x0 = np.matrix("0 ; 1")
for k in range(13):
    print(k, x0.transpose())
    x0 = R*x0 + c
```

Example

```
 0 [[0 1]]
1 [[ 0.8   1.05]]
2 [[ 0.71    1.1725]]
3 [[ 0.6945    1.165125]]
4 [[ 0.697525    1.16243125]]
5 [[ 0.69776125  1.16275031]]
6 [[ 0.69767381  1.1628017 ]]
7 [[ 0.69767228  1.16279116]]
8 [[ 0.69767454  1.1627904 ]]
9 [[ 0.69767447  1.1627907 ]]
10 [[ 0.69767441  1.1627907 ]]
11 [[ 0.69767442  1.1627907 ]]
12 [[ 0.69767442  1.1627907 ]]
```