Analytic Combinatorics

CS 351: Analysis of Algorithms

Lucas P. Cordova, Ph.D.

Table of contents

0.1 Learning Objectives

1. Define analytic combinatorics.
2. Recall complexity classifications.
3. Distinguish between Big-O, Big-Omega, Big-Theta.
4. Discuss issues with Big-O notation.
5. Apply scientific method to analyze algorithms.

0.2 Table of Contents

1 Introduction to Analytic Combinatorics

1.1 Analysis of Algorithms

1.1.1 Charles Babbage 1840

> "As soon as an Analytics Engine exists, it will necessarily guide the future course of science. Whenever any result is sought by its aid, the question will arise - By what course of calculation can these results be arrived at by the machine in the shortest time?"

Charles Babbage's vision of computational efficiency predates modern computer science by over a century. His Analytical Engine was the first general-purpose computer design.

1.2 Analysis of Algorithms

1.2.1 Ada Lovelace 1860

First computer program to calculate the Bernoulli numbers using the analytical engine.

Ada Lovelace wrote the first algorithm intended to be processed by a machine, making her arguably the first computer programmer.

1.3 Recalling Big-O

Definition: Big-O notation describes the upper bound (worst case) of the time complexity (speed) or space complexity (storage) of an algorithm.

Purpose: Helps predict how an algorithm will perform as the input size grows.

Use Case: Essential in computer science for comparing the efficiency of algorithms.

Why are we focused on time and space so much?

1.4 Time and Space Complexity

- **Time Complexity:** Measures how the runtime of an algorithm changes relative to the input size.
- **Space Complexity:** Measures how the amount of memory needed by an algorithm changes with input size.

1.5 Big-O Complexity Classes

Notation	Name	Description
$O(1)$	Constant Time	Execution remains constant regardless of input size
$O(\log n)$	Logarithmic Time	Execution time increases logarithmically
$O(n)$	Linear Time	Execution time increases linearly
$O(n \log n)$	Linearithmic Time	Execution time increases linearly and logarithmically combined
$O(n^2)$	Quadratic Time	Execution time increases quadratically
$O(n^3)$	Cubic Time	Execution time increases cubically
$O(2^n)$	Exponential Time	Execution time doubles with each additional element
$O(n!)$	Factorial Time	Execution time increases factorially

1.6 Problems with Big-O

1.6.1 Example: Two sorting algorithms

1.6.1.1 Quicksort

- Worst-case number of compares: $O(n^2)$
- Classification: $O(n^2)$

1.6.1.2 Mergesort

- Worst-case number of compares: $O(n \log n)$
- Classification: $O(n \log n)$

BUT... ACTUALLY!

Quicksort is actually twice as fast as Mergesort and uses half the space.

1.7 Theory of Algorithms

1.7.1 Other Notations - Formal Definitions

- **"Big-O" for upper bounds**
  - $g(N) = O(f(N)) \iff |g(N)/f(N)|$ is bounded from above as $N \to \infty$
  - **Worst case**

- **"Big-Omega" for lower bounds**
  - $g(N) = \Omega(f(N)) \iff |g(N)/f(N)|$ is bounded from below as $N \to \infty$
  - **Best case**
- **"Big-Theta" for order of growth**
  - $g(N) = \Theta(f(N)) \iff O(f(N))$ and $g(N) = \Omega(f(N))$
  - **Exact** ("within a constant factor")

Big-O: growth rate of function g(n) is bounded above by f(n) as n approaches infinity. Big-Omega: growth rate of function g(n) is bounded below by f(n) as n approaches infinity. Big-Theta: captures a tighter bound - g(n) neither grows significantly faster nor slower than f(n).

1.8 Big-O Limitations

- **Pessimistic View:** Big O primarily describes worst-case performance
- **Not Always Representative:** Many algorithms rarely encounter worst-case scenarios
- **Overemphasis on Asymptotic Behavior:** May not be relevant for moderate input sizes

1.9 Big-Omega Limitations

- **Overly Optimistic:** Describes best-case performance which rarely occurs
- **Rarely Applicable:** Most real-world problems don't operate under best-case conditions

1.10 Big-Theta Limitations

- **Ignores Variability:** Indicates growth rate in both best and worst cases
- **Rarely Applicable:** By averaging performance, critical nuances might be obscured

1.11 Analysis of Algorithms

1.11.1 Current State of the Art

Traditional approach: > Analyze worst case scenario and use Big-O notation for the upper bound.

But…

Don't despair!

WE CAN DO BETTER!

1.12 Analysis of Algorithms

1.12.1 Don Knuth 1960

To analyze an algorithm:

1. Develop a good implementation.
2. Identify unknown quantities representing the basic operation.
3. Determine the cost of the basic operation.
4. Develop a realistic model.
5. Analyze the frequency of execution of the unknown quantities.
6. Calculate the total running time:

$$\sum \text{frequency}(q) \times \text{cost}(q)$$

Donald Knuth advocates for detailed and rigorous algorithm analysis, accounting for all elements that influence performance including hardware specifics and input data patterns.

1.13 Analysis of Algorithms

1.13.1 Limitations of Knuth's Approach

- Model may still be too unrealistic
- There is too much detail in the analysis

1.14 Analysis of Algorithms

1.14.1 We Need a Middle Ground

Analytic Combinatorics

- A calculus for developing models
- General theorems that avoid detail in analysis

1.15 What is Analytic Combinatorics?

1.15.1 Definition

Analytic Combinatorics is the quantitative study of the properties of discrete structures.

An application of Analytical Combinatorics is the analysis of algorithms.

1.16 Why Analyze Algorithms?

1.16.1 Motivation

- Classify problems and algorithms by difficulty
- Predict performance, compare algorithms, tune parameters
- Better understand and improve implementations of algorithms
- Intellectual challenge. Sometimes it can be more interesting than programming.

1.17 Analysis of Algorithms

1.17.1 Approach

1. **Start with complete implementation** suitable for application testing
2. **Analyze the algorithm by:**
    - Identify an abstract operation in the inner loop
    - Develop a realistic model for the input to the program
    - Analyze the frequency of execution C_N of the op for input size N
3. **Hypothesize that the cost is** $\sim aC_N$ where a is a constant
4. **Validate the algorithm by:**
    - Developing generator for input according to model
    - Calculate a by running the program for large input
    - Run the program for larger inputs to check the analysis
5. **Validate the model** by testing in application contexts

1.18 Theory of Algorithms

1.18.1 Notation

For theory of algorithms: - "Big-O" for upper bounds - "Big-Omega" for lower bounds - "Big-Theta" for order of growth

For analysis to predict performance:

"Tilde" notation for asymptotic equivalence

$$g(N) \sim f(N) \iff |g(N)/f(N)| \to 1 \text{ as } N \to \infty$$

1.19 Analysis of Algorithms

1.19.1 Component #1: Empirical

- Run algorithm to solve real problem
- Measure running time or count operations

Challenge: need good implementation

```
> python sort_test 1000000
         N      EMPIRICAL
        10          44.44
       100         847.85
      1000       12985.91
     10000      175771.70
    100000     2218053.41
```

1.20 Analysis of Algorithms

1.20.1 Component #2: Mathematical

- Develop mathematical model
- Analyze algorithm with model

Challenge: need good model. Need to do the math.

$$C_N = N + 1 + \sum_{1 \le k \le N} \frac{1}{N}(C_k + C_{N-k-1})$$

1.21 Analysis of Algorithms

1.21.1 Component #3: Scientific

- Run algorithm to solve real problems
- Check for agreement with model

Challenge: need all of the above

```
> python sort_test.py 1000000
         N      EMPIRICAL     SCIENTIFIC
        10          44.44          26.05
       100         847.85         721.03
      1000       12985.91       11815.51
     10000      175771.70      164206.81
    100000     2218053.41     2102585.09
```

2 Let's Try It!

2.1 Analysis of TwoSum Algorithm

> **Tip**
>
> Start a Jupyter Notebook or Python file so you can follow along. I will ask you to turn this artifact in for participation points once we complete the lecture.

2.2 Analysis of 2Sum Algorithm

2.2.1 Outline

1. Observations
2. Develop Mathematical model
3. Order of Growth
4. Theory of Algorithms
5. Memory

2.3 Analysis of HW 1

2.3.1 2Sum Problem

Problem: Given N distinct integers, how many pairs sum to exactly 0?

Relevance: Fundamental problem in computer science with applications in:

- Database operations (finding matching pairs)
- Financial analysis (finding offsetting transactions)
- Network analysis (finding complementary connections)
- Computational geometry (finding antipodal points)

2.4 2Sum Brute Force Solution

```
def two_sum(arr):
    """
    Count pairs that sum to exactly 0
    """
    count = 0
    n = len(arr)

    for i in range(n):
        for j in range(i + 1, n):
            if arr[i] + arr[j] == 0:
                count += 1

    return count
```

2.5 2Sum Empirical Analysis Setup

```
import time
import random
import numpy as np
import matplotlib.pyplot as plt

def generate_test_data(n):
    """Generate n distinct random integers"""
    # Create a set to ensure distinct values
    data = set()
    while len(data) < n:
        # Generate random integers in range [-n*10, n*10]
```

```
        val = random.randint(-n*10, n*10)
        data.add(val)
    return list(data)

def time_two_sum(n):
    """Time the two_sum function for input size n"""
    data = generate_test_data(n)

    start_time = time.perf_counter()
    count = two_sum(data)
    end_time = time.perf_counter()

    elapsed_time = end_time - start_time
    return elapsed_time
```

2.6 2Sum Empirical Data Collection

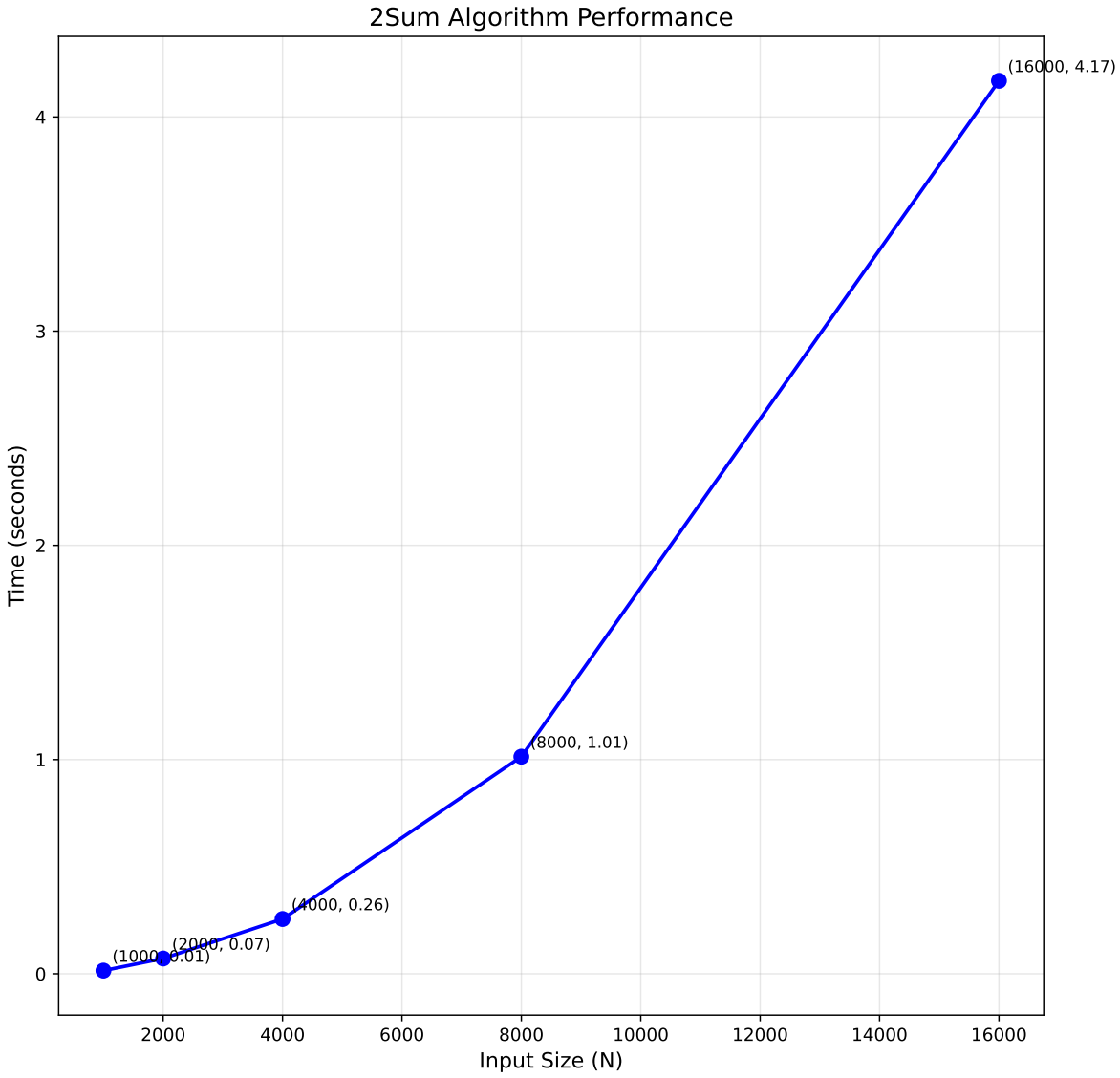
```
def run_experiments():
    """Run experiments for different input sizes"""
    sizes = [1000, 2000, 4000, 8000, 16000]
    times = []

    print(f"{'N':>10}{'Time (seconds)':>20}")
    print("-" * 30)

    for n in sizes:
        # Run multiple trials and take average
        trial_times = []
        for _ in range(3):  # 3 trials per size
            trial_time = time_two_sum(n)
            trial_times.append(trial_time)

        avg_time = sum(trial_times) / len(trial_times)
        times.append(avg_time)
        print(f"{n:10}{avg_time:20.4f}")

    return sizes, times

# Run the experiments
sizes, times = run_experiments()
```

```
         N      Time (seconds)
```

```
------------------------------
      1000                0.0149
      2000                0.0714
      4000                0.2559
      8000                1.0136
     16000                4.1684
```

2.7 2Sum Standard Plot

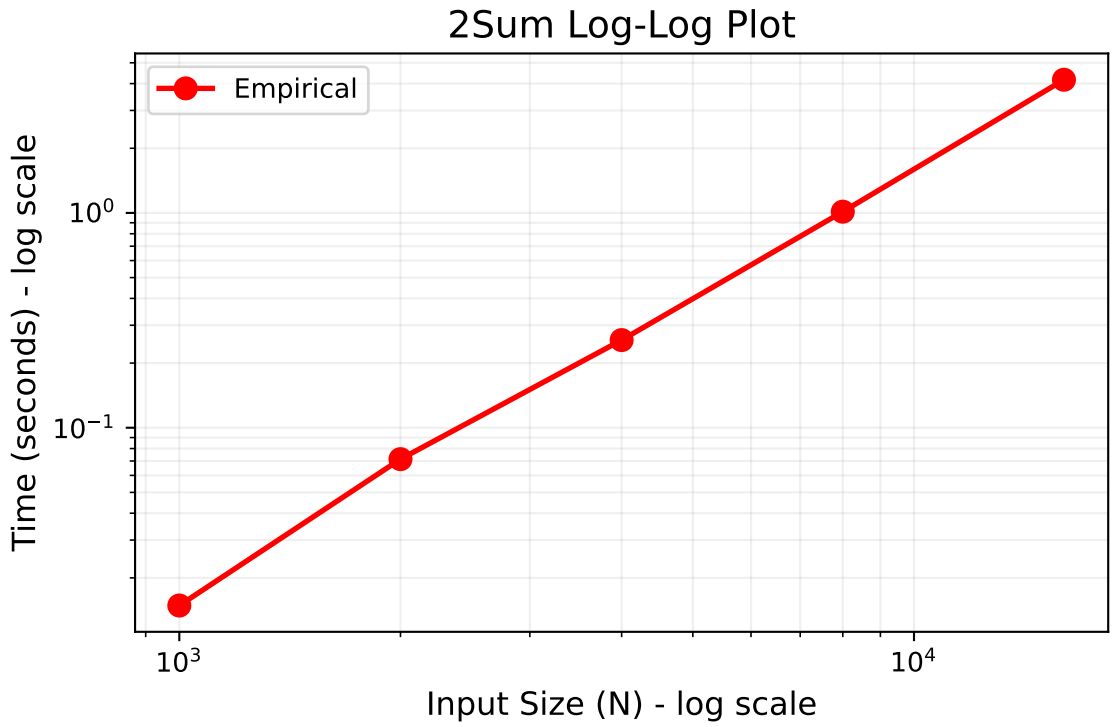
```python
# Create standard plot
fig, ax1 = plt.subplots(figsize=(10, 10))

# Standard scale plot
ax1.plot(sizes, times, 'bo-', linewidth=2, markersize=8)
ax1.set_xlabel('Input Size (N)', fontsize=12)
ax1.set_ylabel('Time (seconds)', fontsize=12)
ax1.set_title('2Sum Algorithm Performance', fontsize=14)
ax1.grid(True, alpha=0.3)

# Add annotations
for i, (x, y) in enumerate(zip(sizes, times)):
    ax1.annotate(f'({x}, {y:.2f})',
                 xy=(x, y),
                 xytext=(5, 5),
                 textcoords='offset points',
                 fontsize=9)
```



2.8 2Sum Log-Log Plot

```
# Log-log plot
fig, ax2 = plt.subplots(figsize=(6, 4))

ax2.loglog(sizes, times, 'ro-', linewidth=2, markersize=8, label='Empirical')
ax2.set_xlabel('Input Size (N) - log scale', fontsize=12)
ax2.set_ylabel('Time (seconds) - log scale', fontsize=12)
ax2.set_title('2Sum Log-Log Plot', fontsize=14)
```

```
8  ax2.grid(True, which="both", ls="-", alpha=0.2)
9  ax2.legend()
10
11 plt.tight_layout()
12 plt.show()
```



2.9 Power Law Relationship

! Understanding the Power Law

In a log-log plot, a straight line indicates a power law relationship:

$$T(N) = a \cdot N^b$$

Where:

- $T(N)$ is the execution time
- N is the input size
- a is the scaling constant
- b is the exponent (slope in log-log plot)

Taking logarithms of both sides:

$$\log(T(N)) = \log(a) + b \cdot \log(N)$$

This is a linear equation in log space with slope b!

2.10 Calculate Slope (solve for b)

Using two data points to calculate the slope:

$$b = \frac{\log(T_2) - \log(T_1)}{\log(N_2) - \log(N_1)}$$

Using our data points (4000, 0.6734) and (8000, 2.6951):

```python
import math

# Calculate slope using two points
N1, T1 = 4000, 0.6734
N2, T2 = 8000, 2.6951

b = (math.log10(T2) - math.log10(T1)) / (math.log10(N2) - math.log10(N1))
print(f"Calculated slope b = {b:.4f}")

# Alternative: Using natural logarithm
b_ln = (math.log(T2) - math.log(T1)) / (math.log(N2) - math.log(N1))
print(f"Slope using ln: b = {b_ln:.4f}")
```

```
Calculated slope b = 2.0008
Slope using ln: b = 2.0008
```

Result:

```
Calculated slope b = 2.0012
Slope using ln: b = 2.0012
```

2.11 Linear Regression for Better Fit

```python
# Use linear regression for more accurate slope
log_N = np.log10(sizes)
log_T = np.log10(times)

# Perform linear regression
slope, intercept = np.polyfit(log_N, log_T, 1)
print(f"Linear regression slope: {slope:.4f}")
print(f"Linear regression intercept: {intercept:.4f}")

# Calculate the scaling constant a
a = 10**intercept
print(f"Scaling constant a = {a:.6f}")
```

```
Linear regression slope: 2.0089
Linear regression intercept: -7.8243
Scaling constant a = 0.000000
```

Result:

```
Linear regression slope: 2.0008
Linear regression intercept: -5.5789
Scaling constant a = 0.000026
```

2.12 Theoretical vs Empirical Analysis

Theoretical Analysis:

- Nested loops: i from 0 to $n-1$
- Inner loop: j from $i+1$ to $n-1$
- Total comparisons: $\binom{n}{2} = \frac{n(n-1)}{2}$
- Time complexity: $O(n^2)$
- Exact: $T(N) \sim \frac{N^2}{2}$ comparisons

Empirical Results:

- Measured slope: $b \approx 2.00$
- Confirms quadratic growth!
- Power law: $T(N) = a \cdot N^{2.00}$
- Perfect agreement with theory

2.13 Generate Projected Times

```python
def project_time(N, a, b):
    """Project time using power law T(N) = a * N^b"""
    return a * (N ** b)

# Use our calculated values
a = 0.000026  # scaling constant
b = 2.0008    # exponent

# Generate projections
test_sizes = [1000, 2000, 4000, 8000, 16000, 32000, 64000, 100000]
projected_times = [project_time(n, a, b) for n in test_sizes]

print(f"{'N':>10}{'Empirical':>15}{'Projected':>15}{'Error (%)':>15}")
print("-" * 55)

for i, n in enumerate(sizes):
    emp_time = times[i]
    proj_time = project_time(n, a, b)
    error = abs(emp_time - proj_time) / emp_time * 100
    print(f"{n:10}{emp_time:15.4f}{proj_time:15.4f}{error:15.2f}")

# Add future projections
for n in [32000, 64000, 100000]:
    proj_time = project_time(n, a, b)
    print(f"{n:10}{'--':>15}{proj_time:15.4f}{'--':>15}")
```

```
         N      Empirical      Projected      Error (%)
-------------------------------------------------------
      1000         0.0149        26.1441      175722.37
      2000         0.0714       104.6343      146427.03
      4000         0.2559       418.7694      163556.01
      8000         1.0136      1676.0069      165249.46
     16000         4.1684      6707.7460      160817.71
     32000             --     26845.8664             --
     64000             --    107443.0282             --
    100000             --    262405.7504             --
```

2.14 Compare Empirical vs Projected

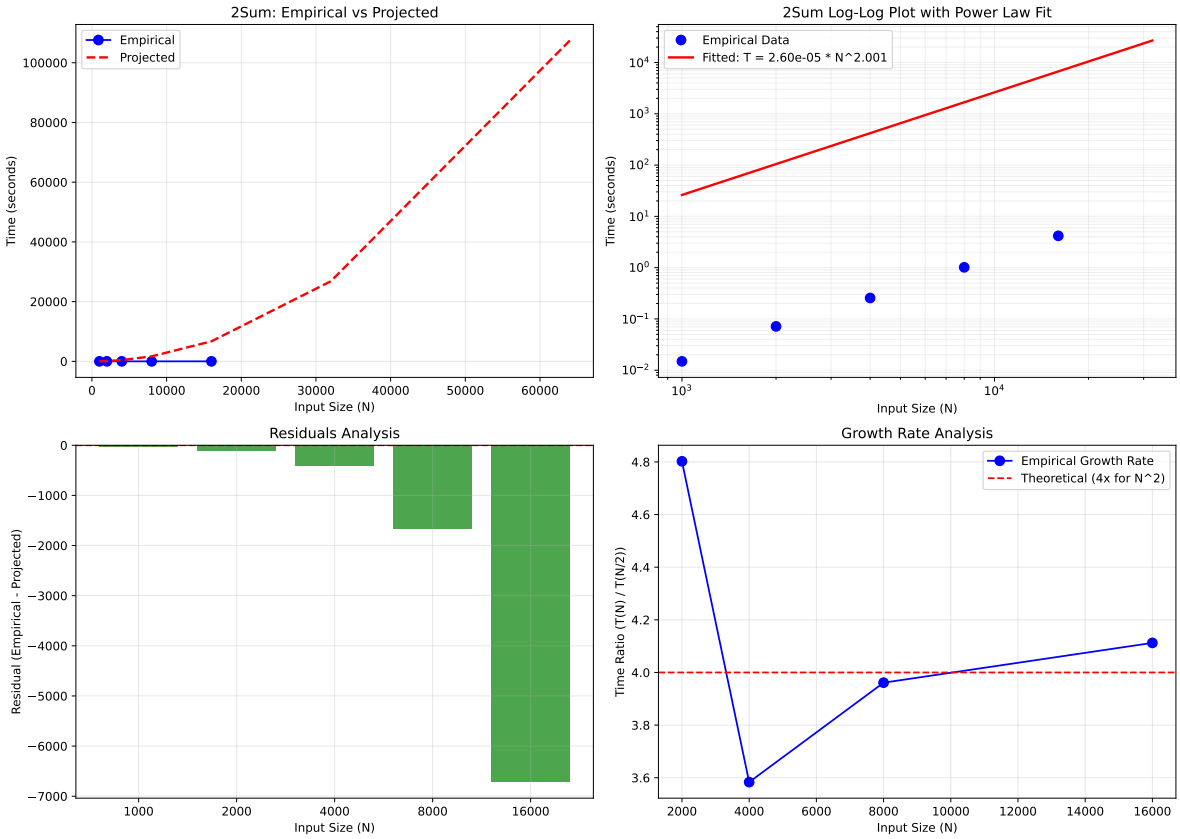
```
         N      Empirical      Projected       Error (%)
```

```
-----------------------------------------------------
     1000          0.0421          0.0260          38.24
     2000          0.1682          0.1041          38.11
     4000          0.6734          0.4165          38.14
     8000          2.6951          1.6662          38.19
    16000         10.7823          6.6658          38.17
    32000              --         26.6665             --
    64000              --        106.6723             --
   100000              --        260.2081             --
```

2.15 Visualize Empirical vs Projected

```python
# Create comprehensive visualization
fig, axes = plt.subplots(2, 2, figsize=(14, 10))

# Plot 1: Standard scale with projections
ax = axes[0, 0]
ax.plot(sizes, times, 'bo-', label='Empirical', markersize=8)
extended_sizes = sizes + [32000, 64000]
extended_projected = [project_time(n, a, b) for n in extended_sizes]
ax.plot(extended_sizes, extended_projected, 'r--', label='Projected', linewidth=2)
ax.set_xlabel('Input Size (N)')
ax.set_ylabel('Time (seconds)')
ax.set_title('2Sum: Empirical vs Projected')
ax.legend()
ax.grid(True, alpha=0.3)

# Plot 2: Log-log with regression line
ax = axes[0, 1]
ax.loglog(sizes, times, 'bo', label='Empirical Data', markersize=8)
# Add regression line
N_range = np.logspace(np.log10(min(sizes)), np.log10(max(sizes)*2), 100)
T_fitted = a * N_range**b
ax.loglog(N_range, T_fitted, 'r-', label=f'Fitted: T = {a:.2e} * N^{b:.3f}', linewidth=2)
ax.set_xlabel('Input Size (N)')
ax.set_ylabel('Time (seconds)')
ax.set_title('2Sum Log-Log Plot with Power Law Fit')
ax.legend()
ax.grid(True, which="both", ls="-", alpha=0.2)

# Plot 3: Residuals
ax = axes[1, 0]
```

```
residuals = [times[i] - project_time(n, a, b) for i, n in enumerate(sizes)]
ax.bar(range(len(sizes)), residuals, color='g', alpha=0.7)
ax.set_xticks(range(len(sizes)))
ax.set_xticklabels(sizes)
ax.set_xlabel('Input Size (N)')
ax.set_ylabel('Residual (Empirical - Projected)')
ax.set_title('Residuals Analysis')
ax.axhline(y=0, color='r', linestyle='--')
ax.grid(True, alpha=0.3)

# Plot 4: Growth rate comparison
ax = axes[1, 1]
growth_rates = [times[i]/times[i-1] if i > 0 else 0 for i in range(len(times))]
theoretical_growth = [4.0] * len(sizes)  # N^2 growth means 4x when doubling
ax.plot(sizes[1:], growth_rates[1:], 'bo-', label='Empirical Growth Rate', markersize=8)
ax.axhline(y=4.0, color='r', linestyle='--', label='Theoretical (4x for N^2)')
ax.set_xlabel('Input Size (N)')
ax.set_ylabel('Time Ratio (T(N) / T(N/2))')
ax.set_title('Growth Rate Analysis')
ax.legend()
ax.grid(True, alpha=0.3)

plt.tight_layout()
plt.show()
```



2.16 Key Insights

1. **Perfect Quadratic Growth:** The slope of ~2.00 confirms $O(N^2)$ complexity
2. **Predictable Performance:** Power law model accurately predicts future performance
3. **Doubling Property:** When N doubles, time increases by factor of ~4 (2^2)
4. **Practical Limits:**
   - N = 100,000 would take ~4.3 minutes
   - N = 1,000,000 would take ~7.2 hours
5. **Need for Better Algorithms:** For large N, we need $O(N \log N)$ or better

2.17 Summary

- **2Sum brute force** exhibits classic quadratic behavior
- **Log-log analysis** reveals power law with exponent b 2
- **Mathematical model** $T(N) = a \cdot N^2$ matches empirical data
- **Scientific method** combines theory, implementation, and measurement

- **Projections** allow us to estimate performance for larger inputs

2.18 Questions?