Labs for Foundations of Applied Mathematics

Volume 2
Algorithm Design and Optimization

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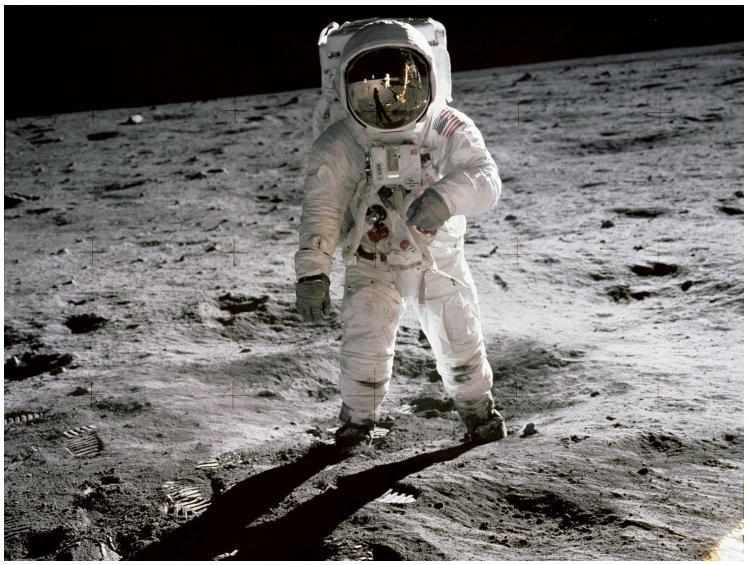

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Preface

This lab manual is designed to accompany the textbooks *Foundations of Applied Mathematics* by Humpherys and Jarvis.

Contents

Part I

Labs

1 Linked Lists

Lab Objective: *One of the fundamental problems in programming is knowing which data structures to use to optimize code. The type of data structure used determines how quickly data is accessed and modified, which affects the overall speed of a program. In this lab, we introduce a basic data structure called a linked list and create a class to implement it.*

A *linked list* is a data structure that chains data together. Every linked list needs a reference to the first item in the chain, called the `head`. A reference to the last item in the chain, called the `tail`, is also often included. Each item in the list stores a piece of data, plus at least one reference to another item in the list. The items in the list are called *nodes*.

Nodes

Think of data as several types of objects that need to be stored in a warehouse. A *node* is like a standard size box that can hold all the different types of objects. For example, suppose a particular warehouse stores lamps of various sizes. Rather than trying to carefully stack lamps of different shapes on top of each other, it is preferable to first put them in boxes of standard size. Then adding new boxes and retrieving stored ones becomes much easier. A *data structure* is like the warehouse, which specifies where and how the different boxes are stored.

A node class is usually simple. The data in the node is stored as an attribute. Other attributes may be added (or inherited) specific to a particular data structure.

Problem 1. Consider the following generic node class.

```
class Node:
    """A basic node class for storing data."""
    def __init__(self, data):
        """Store the data in the value attribute."""
        self.value = data
```

Modify the constructor so that it only accepts data of type `int`, `float`, or `str`. If another type of data is given, raise a `TypeError` with an appropriate error message. Modify the constructor docstring to document these restrictions.

The nodes of a *singly linked list* have a single reference to the next node in the list (see Figure 1.1), while the nodes of a *doubly linked list* have two references: one for the previous node, and one for the next node (see Figure 1.2). This allows for a doubly linked list to be traversed in both directions, whereas a singly linked list can only be traversed in one direction.

```
class LinkedListNode(Node):
    """A node class for doubly linked lists. Inherits from the Node class.
    Contains references to the next and previous nodes in the linked list.
    """
    def __init__(self, data):
        """Store the data in the value attribute and initialize
        attributes for the next and previous nodes in the list.
        """
        Node.__init__(self, data)       # Use inheritance to set self.value.
        self.next = None                # Reference to the next node.
        self.prev = None                # Reference to the previous node.
```

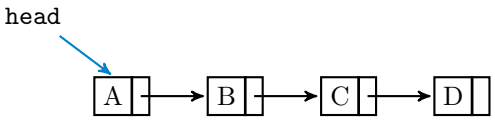


Figure 1.1: A singly linked list. Each node has a reference to the next node in the list. The head attribute is always assigned to the first node.

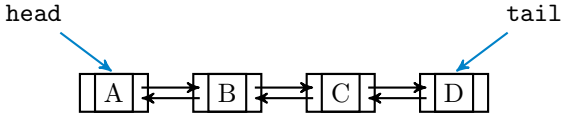


Figure 1.2: A doubly linked list. Each node has a reference to the node before it and a reference to the node after it. In addition to the head attribute, this list has a tail attribute that is always assigned to the last node.

The following `LinkedList` class chains `LinkedListNode` instances together by modifying each node's `next` and `prev` attributes. The list is empty initially, so the `head` and `tail` attributes are assigned the placeholder value `None` in the constructor. The `append()` method makes a new node and adds it to the very end of the list (see Figure 1.3). There are two cases for appending that must be considered separately in the implementation: either the list is empty, or the list is nonempty.

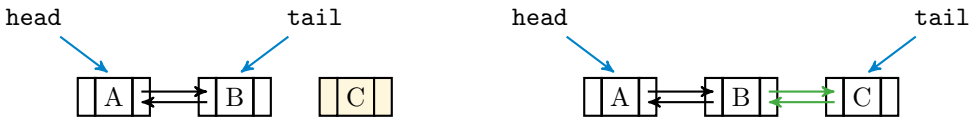


Figure 1.3: Appending a new node to the end of a nonempty doubly linked list. The green arrows are the new connections. Note that the `tail` attribute is reassigned from B to C.

```
class LinkedList:
    """Doubly linked list data structure class.

    Attributes:
        head (LinkedListNode): the first node in the list.
        tail (LinkedListNode): the last node in the list.
    """
    def __init__(self):
        """Initialize the head and tail attributes by setting
        them to None, since the list is empty initially.
        """
        self.head = None
        self.tail = None

    def append(self, data):
        """Append a new node containing the data to the end of the list."""
        # Create a new node to store the input data.
        new_node = LinkedListNode(data)
        if self.head is None:
            # If the list is empty, assign the head and tail attributes to
            # new_node, since it becomes the first and last node in the list.
            self.head = new_node
            self.tail = new_node
        else:
            # If the list is not empty, place new_node after the tail.
            self.tail.next = new_node               # tail --> new_node
            new_node.prev = self.tail               # tail <-- new_node
            # Now the last node in the list is new_node, so reassign the tail.
            self.tail = new_node
```

Achtung!

The `is` operator is **not** the same as the `==` operator. While `==` checks for numerical equality, `is` evaluates whether or not two objects are the same by checking their location in memory.

```
>>> 7 == 7.0            # True since the numerical values are the same.
True

# 7 is an int and 7.0 is a float, so they cannot be stored at the same
# location in memory. Therefore 7 "is not" 7.0.
>>> 7 is 7.0
False
```

For numerical comparisons, always use `==`. When comparing to built-in Python constants such as `None`, `True`, `False`, or `NotImplemented`, use `is` instead.

Locating Nodes

The `LinkedList` class only explicitly keeps track of the first and last nodes in the list via the `head` and `tail` attributes. To access any other node, use each successive node's `next` and `prev` attributes.

```
>>> my_list = LinkedList()
>>> for data in (2, 4, 6):
...     my_list.append(data)
...
# To access each value, use the head attribute of the LinkedList
# and the next and value attributes of each node in the list.
>>> my_list.head.value
2
>>> my_list.head.next.value                    # 2 --> 4
4
>>> my_list.head.next.next is my_list.tail     # 2 --> 4 --> 6
True
```

Problem 2. Add the following methods to the `LinkedList` class.

1. `find()`: Accept a piece of data and return the first node in the list containing that data (return the actual `LinkedListNode` object, not its `value`). If no such node exists, or if the list is empty, raise a `ValueError` with an appropriate error message.
   (Hint: if `n` is assigned to one of the nodes the list, what does `n = n.next` do?)

2. `get()`: Accept an integer i and return the ith node in the list. If i is negative or greater than or equal to the number of nodes in the list, raise an `IndexError`.
   (Hint: add an attribute that tracks the current size of the list. Update it every time a node is successfully added or removed, such as at the end of the `append()` method.)

Magic Methods

Endowing data structures with magic methods makes them much more intuitive to use. Consider, for example, how a Python list responds to built-in functions like `len()` and `print()`. At the bare minimum, the `LinkedList` class should have the same functionality.

Problem 3. Add the following magic methods to the `LinkedList` class.

1. Write the `__len__()` method so that the length of a `LinkedList` instance is equal to the number of nodes in the list.

2. Write the `__str__()` method so that when a `LinkedList` instance is printed, its output matches that of a Python list. Entries are separated by a comma and one space; strings are surrounded by single quotes, or by double quotes if the string itself has a single quote.
   (Hint: use `repr()` to deal with quotes easily.)

Removal

To delete a node, all references to the node must be removed. Python automatically deletes the object once there is no way for the user to access it. Naïvely, this might be done by finding the previous node to the one being removed, and setting its `next` attribute to `None`. However, there is a problem with this approach.

```
class LinkedList:
    # ...
    def remove(self, data):
        """Attempt to remove the first node containing the specified data.
        This method incorrectly removes additional nodes.
        """
        # Find the target node and sever the links pointing to it.
        target = self.find(data)
        target.prev.next = None                    # -/-> target
        target.next.prev = None                    # target <-/-
```

Removing all references to the target node deletes the node (see Figure 1.4). Unfortunately, the nodes before and after the target node are no longer linked.

```
>>> my_list = LinkedList()
>>> for i in range(10):
...     my_list.append(i)
...
>>> print(my_list)
[0, 1, 2, 3, 4, 5, 6, 7, 8, 9]

>>> my_list.remove(4)              # Removing a node improperly results in
>>> print(my_list)                 # the rest of the chain being lost.
[0, 1, 2, 3]                       # Should be [0, 1, 2, 3, 5, 6, 7, 8, 9].
```

Figure 1.4: Naïve removal for doubly linked Lists. Deleting all references pointing to C deletes the node, but it also separates nodes A and B from node D.

This can be remedied by pointing the previous node's `next` attribute to the node after the deleted node, and similarly changing that node's `prev` attribute. Then there will be no reference to the removed node and it will be deleted, but the chain will still be connected.

Figure 1.5: Correct removal for doubly linked Lists. To avoid gaps in the chain, nodes B and D must be linked together.

Problem 4. Modify the `remove()` method given above so that it correctly removes the first node in the list containing the specified data. Also account for the special cases of removing the first, last, or only node, in which `head` and/or `tail` must be reassigned. Raise a `ValueError` if there is no node in the list that contains the data.
(Hint: use the `find()` method from Problem 2 to locate the target node.)

ACHTUNG!

Python keeps track of the variables in use and automatically deletes a variable (freeing up the memory that stored the object) if there is no access to it. This feature is called *garbage collection*. In many other languages, leaving a reference to an object without explicitly deleting it can lead to a serious memory leak. See `https://docs.python.org/3/library/gc.html` for more information on Python's garbage collection system.

Insertion

The `append()` method can add new nodes to the end of the list, but not to the middle. To do this, get references to the nodes before and after where the new node should be, then adjust their `next` and `prev` attributes. Be careful not to disconnect the nodes in a way that accidentally deletes nodes like in Figure 1.4.

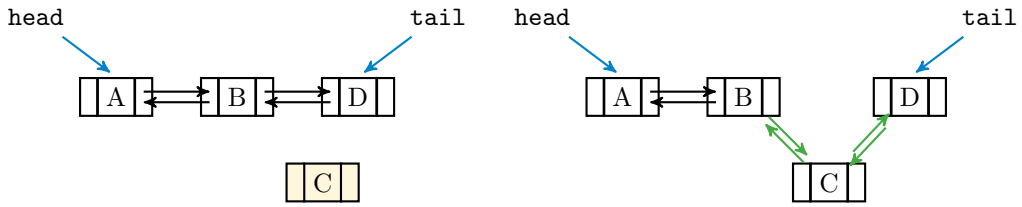


Figure 1.6: Insertion for doubly linked lists.

Problem 5. Add an `insert()` method to the `LinkedList` class that accepts an integer `index` and data to add to the list. Insert a new node containing the data immediately **before** the node in the list currently at position `index`. After the insertion, the new node should be at position `index`. For example, Figure 1.6 places a new node containing C at index 2. Carefully account for the special case of inserting before the first node, which requires `head` to be reassigned.
(Hint: except when inserting before the head, get references to the nodes that should be immediately before and after the new node following the insertion. Consider using the `get()` method from Problem 2 to locate one of these nodes.)

If `index` is equal to the number of nodes in the list, append the node to the end of the list by calling `append()`. If `index` is negative or strictly greater than the number of nodes in the list, raise an `IndexError`.

Note

The temporal complexity for inserting to the beginning or end of a linked list is $O(1)$, but inserting anywhere else is $O(n)$, where n is the number of nodes in the list. This is quite slow compared other data structures. In the next lab we turn our attention to *trees*, special kinds of linked lists that allow for much quicker sorting and data retrieval.

Restricted-Access Lists

It is sometimes wise to restrict the user's access to some of the data within a structure. In particular, because insertion, removal, and lookup are $O(n)$ for data in the middle of a linked list, cutting off access to the middle of the list forces the user to only use $O(1)$ operations at the front and end of the list. The three most common and basic restricted-access structures that implement this idea are *stacks*, *queues*, and *deques*. Each structure restricts the user's access differently, making them ideal for different situations.

- **Stack**: *Last In, First Out* (LIFO). Only the last item that was inserted can be accessed. A stack is like a pile of plates: the last plate put on the pile is (or should be) the first one to be taken off. Stacks usually have two main methods: `push()`, to insert new data, and `pop()`, to remove and return the last piece of data inserted.
- **Queue** (pronounced "cue"): *First In, First Out* (FIFO). New nodes are added to the end of the queue, but an existing node can only be removed or accessed if it is at the front of the queue. A queue is like a polite line at the bank: the person at the front of the line is served first, while newcomers add themselves to the back of the line. Queues also usually have a `push()` and a `pop()` method, but `push()` inserts data to the end of the queue while `pop()` removes and returns the data at the front of the queue. The `push()` and `pop()` operations are sometimes called `enqueue()` and `dequeue()`, respectively.
- **Deque** (pronounced "deck"): a double-ended queue. Data can be inserted or removed from either end, but data in the middle is inaccessible. A deque is like a deck of cards, where only the top and bottom cards are readily accessible. A deque has two methods for insertion and two for removal, usually called `append()`, `appendleft()`, `pop()`, and `popleft()`.

  A deque can act as a queue by using only `append()` and `popleft()` (or `appendleft()` and `pop()`), or as a stack by using only `append()` and `pop()` (or `appendleft()` and `popleft()`).

Problem 6. Write a `Deque` class that inherits from `LinkedList`.

1. Write the following methods. Since they all involve data at the endpoints, avoid iterating through the list so the resulting operations are $O(1)$.
   - `pop()`: Remove the last node in the list and return its data. Account for the special case of removing the only node in the list. Raise a `ValueError` if the list is empty.
   - `popleft()`: Remove the first node in the list and return its data. Raise a `ValueError` if the list is empty.
     (Hint: use inheritance and the `remove()` method of `LinkedList`.)

- `appendleft()`: Insert a new node at the beginning of the list.
  (Hint: use inheritance and the `insert()` method of `LinkedList`.)

Note that the `LinkedList` class already implements `append()`.

2. Override the `remove()` method with the following code.

```
def remove(*args, **kwargs):
    raise NotImplementedError("Use pop() or popleft() for removal")
```

This effectively disables `remove()` for the `Deque` class, preventing the user from removing a node from the middle of the list.

3. Disable `insert()` as well.

Note

The `*args` argument allows the `remove()` method to receive any number of positional arguments without raising a `TypeError`, and the `**kwargs` argument allows it to receive any number of keyword arguments. This is the most general form of a function signature.

Python lists have `append()` and `pop()` methods, so they can be used as stacks. However, data access and removal from the front is much slower than from the end, as Python lists are implemented as dynamic arrays and not linked lists.

The `collections` module in the standard library has a `deque` object that is implemented as a doubly linked list. This is an excellent object to use in practice instead of a Python list when speed is of the essence and data only needs to be accessed from the ends of the list. Both lists and deques are slow to modify elements in the middle, but lists can access middle elements quickly. Table 1.1 describes the complexity for common operations on lists v. deques in Python.

Operation	List Complexity	Deque Complexity
Append/Remove from the end	$O(1)$	$O(1)$
Append/Remove from the start	$O(n)$	$O(1)$
Insert/Delete in the middle	$O(n)$	$O(n)$
Access element at the start/end	$O(1)$	$O(1)$
Access element in the middle	$O(1)$	$O(n)$

Table 1.1: Complexity of operations on lists and deques.

Problem 7. Write a function that accepts the name of a file to be read and a file to write to. Read the first file, adding each line of text to a stack. After reading the entire file, pop each entry off of the stack one at a time, writing the result to the second file.

For example, if the file to be read has the following list of words on the left, the resulting file should have the list of words on the right.

```
My homework is too hard for me.          I am a mathematician.
I do not believe that                    Programming is hard, but
I can solve these problems.              I can solve these problems.
Programming is hard, but                 I do not believe that
I am a mathematician.                    My homework is too hard for me.
```

You may use a Python list, your `Deque` class, or `collections.deque` for the stack. Test your function on the file `english.txt`, which contains a list of over 58,000 English words in alphabetical order.

Additional Material

Possible Improvements to the LinkedList Class

The following are some ideas for expanding the functionality of the `LinkedList` class.

1. Add a keyword argument to the constructor so that if an iterable is provided, each element of the iterable is immediately added to the list. This makes it possible to cast an iterable as a `LinkedList` the same way that an iterable can be cast as one of Python's standard data structures.

```
>>> my_list = [1, 2, 3, 4, 5]
>>> my_linked_list = LinkedList(my_list)  # Cast my_list as a LinkedList.
>>> print(my_linked_list)
[1, 2, 3, 4, 5]
>>> type(my_linked_list)
LinkedList
```

2. Add the following methods.
   - `count()`: return the number of occurrences of a specified value.
   - `reverse()`: reverse the ordering of the nodes (in place).
   - `roll()`: shift the nodes a given number of steps to the right or left (in place).
   - `sort()`: sort the nodes by their data (in place).
3. Implement more magic methods.
   - `__add__()`: concatenate two lists.
   - `__getitem__()` and `__setitem__()`: enable standard bracket indexing. Try to allow for negative indexing as well.
   - `__iter__()`: support `for` loop iteration, the `iter()` built-in function, and the `in` statement.

Other Kinds of Linked Lists

The `LinkedList` class can also be used as the backbone for more specialized data structures.

1. A *sorted list* adds new nodes strategically so that the data is always kept in order. Therefore, a `SortedLinkedList` class should have an `add()` method that receives some `data` and inserts a new node containing `data` before the first node in the list that has a `value` that is greater or equal to `data` (thereby preserving the ordering). Other methods for adding nodes should be disabled. Note however, that a linked list is **not** an ideal implementation for a sorted list because each insertion is $O(n)$ (try sorting `english.txt`).
2. In a *circular linked list*, the "last" node connects back to the "first" node. Thus a reference to the tail is unnecessary. The `roll()` method mentioned above is used often so the `head` attribute is at an "active" part of the list where nodes are inserted, removed, or accessed often. This data structure can therefore decrease the average insertion or removal time for certain data sets.

2 Binary Search Trees

Lab Objective: *A tree is link-based data structure where each node may refer to more than one other node. This structure makes trees more useful and efficient than regular linked lists in many applications. Many trees are constructed recursively, so we begin with an overview of recursion. We then implement a recursively structured doubly linked binary search tree (BST). Finally, we compare the standard linked list, our BST, and an AVL tree to illustrate the relative strengths and weaknesses of each data structure.*

Recursion

A *recursive* function is one that calls itself. When the function is executed, it continues calling itself until reaching a *base case* where the value of the function is known. The function then exits without calling itself again, and each previous function call is resolved. The idea is to solve large problems by first solving smaller problems, then combining their results.

As a simple example, consider the function $f : \mathbb{N} \to \mathbb{N}$ that sums all positive integers from 1 to some integer n.

$$f(n) = \sum_{i=1}^{n} i = n + \sum_{i=1}^{n-1} i = n + f(n-1)$$

Since $f(n-1)$ appears in the formula for $f(n)$, f can be implemented recursively. Calculating $f(n)$ requires the value of $f(n-1)$, which requires $f(n-2)$, and so on. The base case is $f(1) = 1$, at which point the recursion halts and unwinds. For example, $f(4)$ is calculated as follows.

$$\begin{aligned} f(4) &= 4 + f(3) \\ &= 4 + (3 + f(2)) \\ &= 4 + (3 + (2 + f(1))) \\ &= 4 + (3 + (2 + 1)) \\ &= 4 + (3 + 3) \\ &= 4 + 6 \\ &= 10 \end{aligned}$$

The implementation accounts separately for the base case and the recursive case.

```
def recursive_sum(n):
    """Calculate the sum of all positive integers in [1, n] recursively."""
    if n <= 1:          # Base case: f(1) = 1.
        return 1
    else:               # Recursive case: f(n) = n + f(n-1).
        return n + recursive_sum(n-1)
```

Many problems that can be solved iteratively can also be solved with a recursive approach. Consider the function $g : \mathbb{N} \to \mathbb{N}$ that calculates the nth Fibonacci number.

$$g(n) = g(n-1) + g(n-2), \quad g(0) = 0, \quad g(1) = 1.$$

This function is doubly recursive since $g(n)$ calls itself twice, and there are two different base cases to deal with. On the other hand, $g(n)$ could be computed iteratively by calculating $g(0), g(1), \ldots, g(n)$ in that order. Compare the iterative and recursive implementations for g given below.

```
def iterative_fib(n):
    """Calculate the nth Fibonacci number iteratively."""
    if n <= 0:                  # Special case: g(0) = 0.
        return 0
    g0, g1 = 0, 1               # Initialize g(0) and g(1).
    for i in range(1, n):       # Calculate g(2), g(3), ..., g(n).
        g0, g1 = g1, g0 + g1
    return g1

def recursive_fib(n):
    """Calculate the nth Fibonacci number recursively."""
    if n <= 0:                  # Base case 1: g(0) = 0.
        return 0
    elif n == 1:                # Base case 2: g(1) = 1.
        return 1
    else:                       # Recursive case: g(n) = g(n-1) + g(n-2).
        return recursive_fib(n-1) + recursive_fib(n-2)
```

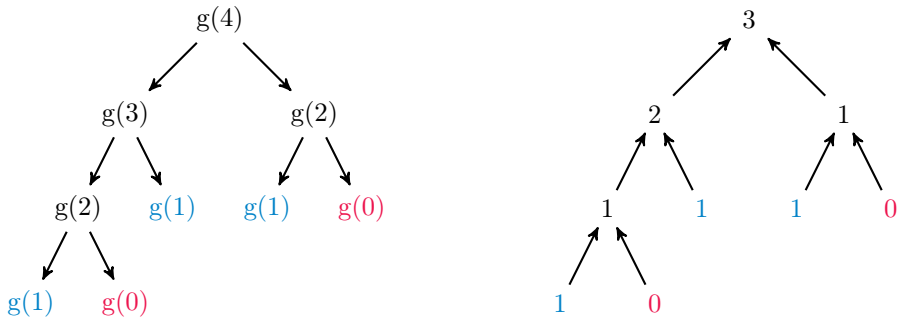


Figure 2.1: To calculate $g(n)$ recursively, call $g(n-1)$ and $g(n-2)$, down to the base cases $g(0)$ and $g(1)$. As the recursion unwinds, the values from the base cases are passed up to previous calls and combined, eventually giving the value for $g(n)$.

Problem 1. Consider the following class for singly linked lists.

```
class SinglyLinkedListNode:
    """A node with a value and a reference to the next node."""
    def __init__(self, data):
        self.value, self.next = data, None

class SinglyLinkedList:
    """A singly linked list with a head and a tail."""
    def __init__(self):
        self.head, self.tail = None, None

    def append(self, data):
        """Add a node containing the data to the end of the list."""
        n = SinglyLinkedListNode(data)
        if self.head is None:
            self.head, self.tail = n, n
        else:
            self.tail.next = n
            self.tail = n

    def iterative_find(self, data):
        """Search iteratively for a node containing the data."""
        current = self.head
        while current is not None:
            if current.value == data:
                return current
            current = current.next
        raise ValueError(str(data) + " is not in the list")
```

Write a method that does the same task as `iterative_find()`, but with the following recursive approach. Define a function within the method that checks a single node for the data. There are two base cases: if the node is `None`, meaning the data could not be found, raise a `ValueError`; if the node contains the data, return the node. Otherwise, call the function on the next node in the list. Start the recursion by calling this inner function on the head node.
(Hint: see `BST.find()` in the next section for a similar idea.)

Achtung!

It is usually **not** better to rewrite an iterative method recursively, partly because recursion results in an increased number of function calls. Each call requires a small amount of memory so the program remembers where to return to in the program. By default, Python raises a `RuntimeError` after 1000 calls to prevent a stack overflow. On the other hand, recursion lends itself well to some problems; in this lab, we use a recursive approach to construct a few data structures, but it is possible to implement the same structures with iterative strategies.

Binary Search Trees

Mathematically, a *tree* is a directed graph with no cycles. Trees can be implemented with link-based data structures that are similar to a linked list. The first node in a tree is called the *root*, like the `head` of a linked list. The root node points to other nodes, which are called its children. A node with no children is called a *leaf node*.

A *binary search tree* (BST) is a tree that allows each node to have up to two children, usually called `left` and `right`. The left child of a node contains a value that is less than its parent node's value; the right child's value is greater than its parent's value. This specific structure makes it easy to search a BST: while the computational complexity of finding a value in a linked list is $O(n)$ where n is the number of nodes, a well-built tree finds values in $O(\log n)$ time.

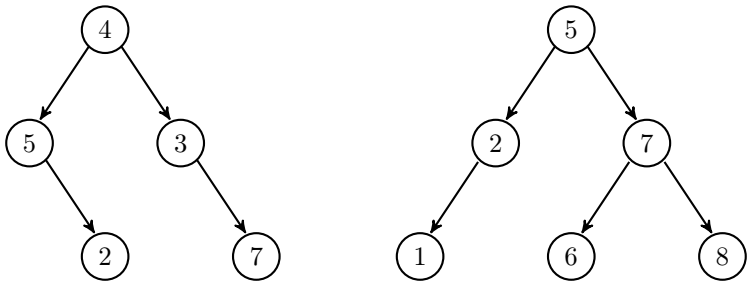


Figure 2.2: Both of these graphs are trees, but the tree on the left is not a binary search tree because 5 is to the left of 4. Swapping 5 and 3 in the graph on the left would result in a BST.

Binary search tree nodes have attributes that keep track of their value, their children, and (in doubly linked trees) their parent. The actual binary search tree has an attribute to keep track of its root node.

```
class BSTNode:
    """A node class for binary search trees. Contains a value, a
    reference to the parent node, and references to two child nodes.
    """
    def __init__(self, data):
        """Construct a new node and set the value attribute. The other
        attributes will be set when the node is added to a tree.
        """
        self.value = data
        self.prev = None        # A reference to this node's parent node.
        self.left = None        # self.left.value < self.value
        self.right = None       # self.value < self.right.value

class BST:
    """Binary search tree data structure class.
    The root attribute references the first node in the tree.
    """
    def __init__(self):
        """Initialize the root attribute."""
        self.root = None
```

> **Note**
>
> Conceptually, each node of a BST partitions the data of its subtree into two halves: the data that is less than the parent, and the data that is greater. We will extend this concept to higher dimensions in the next lab.

Locating Nodes

Finding a node in a binary search tree can be done recursively. Starting at the root, check if the target data matches the current node. If it does not, then if the data is less than the current node's value, search again on the left child; if the data is greater, search on the right child. Continue the process until the data is found or until hitting a dead end. This method illustrates the advantage of the binary structure—if a value is in a tree, then we know where it ought to be based on the other values in the tree.

```
class BST:
    # ...
    def find(self, data):
        """Return the node containing the data. If there is no such node
        in the tree, including if the tree is empty, raise a ValueError.
        """

        # Define a recursive function to traverse the tree.
        def _step(current):
            """Recursively step through the tree until the node containing
            the data is found. If there is no such node, raise a Value Error.
            """
            if current is None:                     # Base case 1: dead end.
                raise ValueError(str(data) + " is not in the tree.")
            if data == current.value:               # Base case 2: data found!
                return current
            if data < current.value:                # Recursively search left.
                return _step(current.left)
            else:                                   # Recursively search right.
                return _step(current.right)

        # Start the recursion on the root of the tree.
        return _step(self.root)
```

Insertion

New elements are always added to a BST as leaf nodes. To insert a new value, recursively step through the tree as if searching for the value until locating an empty slot. The node with the empty child slot becomes the parent of the new node; connect it to the new node by modifying the parent's `left` or `right` attribute (depending on which side the child should be on) and the child's `prev` attribute.

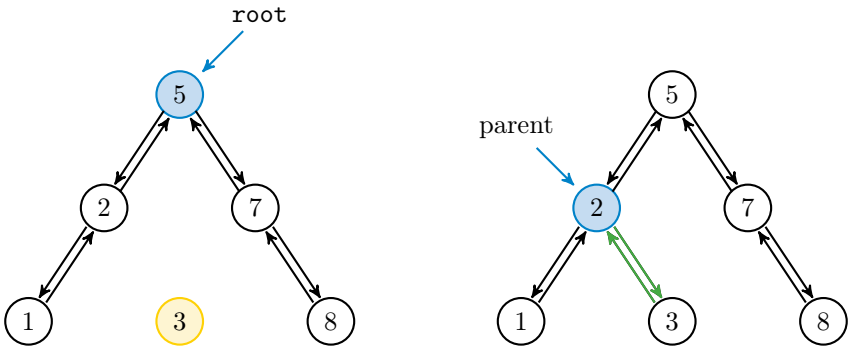


Figure 2.3: To insert 3 to the BST on the left, start at the root and recurse down the tree as if searching for 3: since $3 < 5$, step left to 2; since $2 < 3$, step right. However, 2 has no right child, so 2 becomes the parent of a new node containing 3.

Problem 2. Write an `insert()` method for the `BST` class that accepts some data.

1. If the tree is empty, assign the `root` attribute to a new `BSTNode` containing the data.
2. If the tree is nonempty, create a new `BSTNode` containing the data and find the existing node that should become its parent. Determine whether the new node will be the parent's `left` or `right` child, then double link the parent to the new node accordingly.
   (Hint: write a recursive function like `_step()` to find and link the parent).
3. Do not allow duplicates in the tree: if there is already a node in the tree containing the insertion data, raise a `ValueError`.

To test your method, use the `__str__()` and `draw()` methods provided in the Additional Materials section. Try constructing the binary search trees in Figures 2.2 and 2.3.

Removal

Node removal is much more delicate than node insertion. While insertion always creates a new leaf node, a remove command may target the root node, a leaf node, or anything in between. There are three main requirements for a successful removal.

1. The target node is no longer in the tree.
2. The former children of the removed node are still accessible from the root. In other words, if the target node has children, those children must be adopted by other nodes in the tree.
3. The tree still has an ordered binary structure.

When removing a node from a linked list, there are three possible cases that must each be accounted for separately: the target node is the head, the target node is the tail, or the target node is in the middle of the list. For BST node removal, we must similarly account separately for the removal of a leaf node, a node with one child, a node with two children, and the root node.

Removing a Leaf Node

Recall that Python's garbage collector automatically deletes objects that cannot be accessed by the user. If the node to be removed—called the *target node*—is a leaf node, then the only way to access it is via the target's parent. Locate the target with `find()`, get a reference to the parent node (using the `prev` attribute of the target), and set the parent's `right` or `left` attribute to `None`.

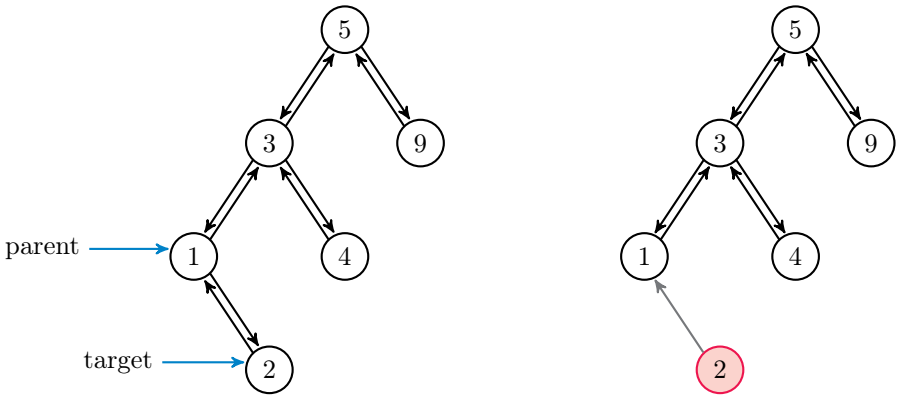


Figure 2.4: To remove 2, get a reference to its parent. Then set the parent's `right` attribute to `None`. Even though 2 still points to 1, 2 is deleted since nothing in the tree points to it.

Removing a Node with One Child

If the target node has one child, the child must be adopted by the target's parent in order to remain in the tree. That is, the parent's `left` or `right` attribute should be set to the child, and the child's `prev` attribute should be set to the parent. This requires checking which side of the target the child is on and which side of the parent the target is on.

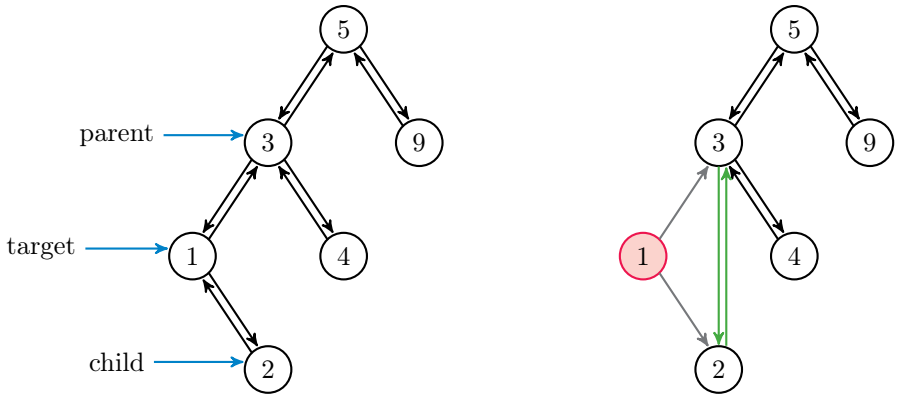


Figure 2.5: To remove 1, locate its parent (3) and its child (2). Set the parent's `left` attribute to the child and the child's `prev` attribute to the parent. Even though 1 still points to other nodes, it is deleted since nothing in the tree points to it.

Removing a Node with Two Children

Removing a node with two children requires a slightly different approach in order to preserve the ordering in the tree. The *immediate predecessor* of a node with value x is the node in the tree with the largest value that is still smaller than x. Replacing a target node with its immediate predecessor preserves the order of the tree because the predecessor's value is greater than the values in the target's left branch, but less than the values in the target's right branch. Note that because of how the predecessor is chosen, any immediate predecessor can only have at most one child.

To remove a target with two children, find its immediate predecessor by stepping to the left of the target (so that it's value is less than the target's value), and then to the right for as long as possible (so that it has the largest such value). Remove the predecessor, recording its value. Then overwrite the value of the target with the predecessor's value.

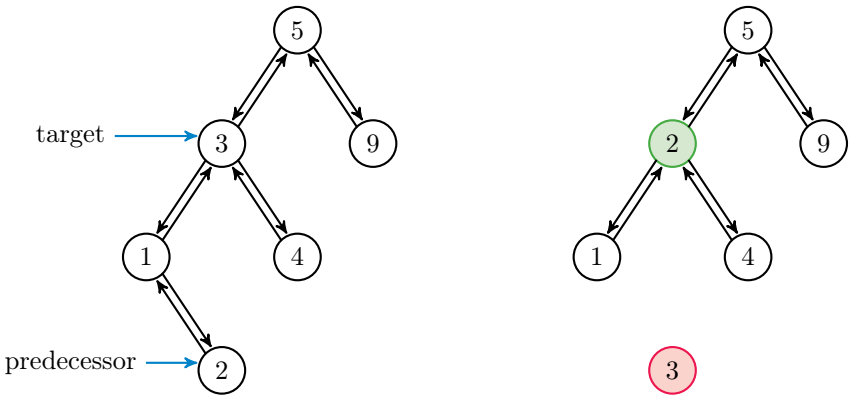


Figure 2.6: To remove 3, locate its immediate predecessor 2 by stepping left to 1, then right as far as possible. Since it is a leaf node, the predecessor can be deleted using the process in Figure 2.4. Delete the predecessor, and replace the value of the target with the predecessor's value. If the predecessor has a left child, it can be deleted with the procedure from Figure 2.5.

Removing the Root Node

If the target is the root node, the `root` attribute may need to be reassigned after the target is removed. This adds two extra cases to consider:

1. If the root has no children, meaning it is the only node in the tree, set the root to `None`.
2. If the root has one child, that child becomes the new root of the tree. The new root's `prev` attribute should be set to `None` so the garbage collector deletes the target.

When the targeted root has two children, the node stays where it is (only its value is changed), so `root` does not need to be reassigned.

Problem 3. Write a `remove()` method for the `BST` class that accepts some data. If the tree is empty, or if there is no node in the tree containing the data, raise a `ValueError`. Otherwise, remove the node containing the specified data using the strategies described in Figures 2.4–2.6. Test your solutions thoroughly.
(Hint: **Before coding anything**, outline the entire method with comments and `if-else` blocks. Consider using the following control flow to account for all possible cases.)

1. The target is a leaf node.
   (a) The target is the root.
   (b) The target is to the left of its parent.
   (c) The target is to the right of its parent.
2. The target has two children.
   (Hint: use `remove()` on the predecessor's value).
3. The target has one child.
   (Hint: start by getting a reference to the child.)
   (a) The target is the root.
   (b) The target is to the left of its parent.
   (c) The target is to the right of its parent.

AVL Trees

The advantage of a BST is that it organizes its data so that values can be located, inserted, or removed in $O(\log n)$ time. However, this efficiency is dependent on the *balance* of the tree. In a well-balanced tree, the number of descendants in the left and right subtrees of each node is about the same. An unbalanced tree has some branches with many more nodes than others. Finding a node at the end of a long branch is closer to $O(n)$ than $O(\log n)$. This is a common problem; inserting ordered data, for example, results in a "linear" tree, since new nodes always become the right child of the previously inserted node (see Figure 2.7). The resulting structure is essentially a linked list without a `tail` attribute.

An *Adelson-Velsky Landis tree* (AVL) is a BST that prevents any one branch from getting longer than the others by recursively "balancing" the branches as nodes are added or removed. Insertion and removal thus become more expensive, but the tree is guaranteed to retain its $O(\log n)$ search efficiency. The AVL's balancing algorithm is beyond the scope of this lab, but the Volume 2 text includes details and exercises on the algorithm.

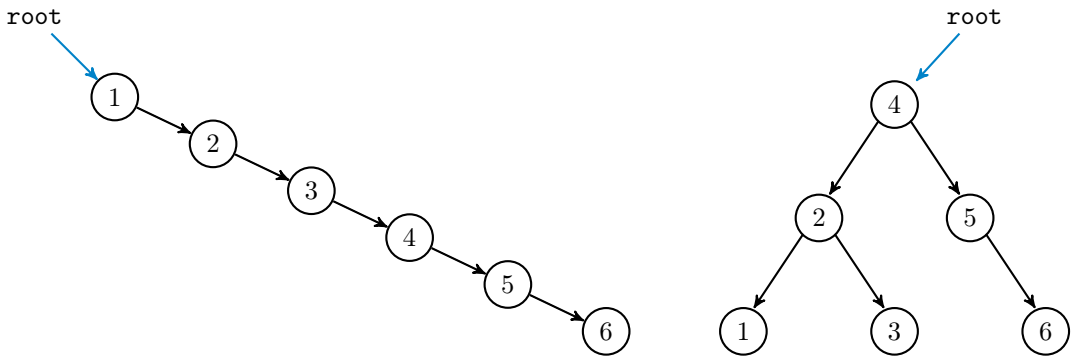


Figure 2.7: On the left, the unbalanced BST resulting from inserting 1, 2, 3, 4, 5, and 6, in that order. On the left, the balanced AVL tree that results from the same insertion. After each insertion, the AVL tree rebalances if necessary.

Problem 4. Write a function to compare the build and search times of the `SinglyLinkedList` from Problem 1, the `BST` from Problems 2 and 3, and the `AVL` provided in the Additional Materials section. Begin by reading the file `english.txt`, storing the contents of each line in a list. For $n = 2^3, 2^4, \dots, 2^{10}$, repeat the following experiment.

1. Get a subset of n **random** items from the data set.
   (Hint: use a function from the `random` or `np.random` modules.)
2. Time (separately) how long it takes to load a new `SinglyLinkedList`, a `BST`, and an `AVL` with the n items.
3. Choose 5 **random** items from the subset, and time how long it takes to find all 5 items in each data structure. Use the `find()` method for the trees, but to avoid exceeding the maximum recursion depth, use the provided `iterative_find()` method from Problem 1 to search the `SinglyLinkedList`.

Report your findings in a single figure with two subplots: one for build times, and one for search times. Use log scales where appropriate.

Additional Material

Possible Improvements to the BST Class

The following are a few ideas for expanding the functionality of the `BST` class.

1. Add a keyword argument to the constructor so that if an iterable is provided, each element of the iterable is immediately added to the tree. This makes it possible to cast other iterables as a `BST` the same way that an iterable can be cast as one of Python's standard data structures.

2. Add an attribute that keeps track of the number of items in the tree. Use this attribute to implement the `__len__()` magic method.

3. Add a method for translating the `BST` into a sorted Python list.
   (Hint: examine the provided `__str__()` method carefully.)

4. Add methods `min()` and `max()` that return the smallest or largest value in the tree, respectively. Consider adding `head` and `tail` attributes that point to the minimal and maximal elements; this would make inserting new minima and maxima $O(1)$.

Other Kinds of Binary Trees

In addition to the AVL tree, there are many other variations on the binary search tree, each with its own advantages and disadvantages. Consider writing classes for the following structures.

1. A *B-tree* is a tree whose nodes can contain more than one piece of data and point to more than one other node. See the Volume 2 text for details.

2. The nodes of a *red-black tree* are labeled either red or black. The tree satisfies the following rules to maintain a balanced structure.

   (a) Every leaf node is black.

   (b) Red nodes only have black children.

   (c) Every (directed) path from a node to any of its descendent leaf nodes contains the same number of black nodes.

   When a node is added that violates one of these constraints, the tree is rebalanced and recolored.

3. A *Splay Tree* includes an additional operation, called splaying, that makes a specified node the root of the tree. Splaying several nodes of interest makes them easier to access because they are placed close to the root.

4. A *heap* is similar to a BST but uses a different binary sorting rule: the value of every parent node is greater than each of the values of its children. This data structure is particularly useful for sorting algorithms; see the Volume 2 text for more details.

Additional Code: Tree Visualization

The following methods may be helpful for visualizing instances of the `BST` and `AVL` classes. Note that the `draw()` method uses NetworkX's `graphviz_layout`, which requires the `pygraphviz` module (install it with `pip install pygraphviz`).

```
import networkx as nx
from matplotlib import pyplot as plt
from networkx.drawing.nx_agraph import graphviz_layout

class BST:
    # ...
    def __str__(self):
        """String representation: a hierarchical view of the BST.

        Example:  (3)
                   / \     '[3]          The nodes of the BST are printed
                 (2) (5)    [2, 5]       by depth levels. Edges and empty
                 /   / \    [1, 4, 6]'   nodes are not printed.
               (1) (4) (6)
        """
        if self.root is None:
            return "[]"
        out, current_level = [], [self.root]
        while current_level:
            next_level, values = [], []
            for node in current_level:
                values.append(node.value)
                for child in [node.left, node.right]:
                    if child is not None:
                        next_level.append(child)
            out.append(values)
            current_level = next_level
        return "\n".join([str(x) for x in out])

    def draw(self):
        """Use NetworkX and Matplotlib to visualize the tree."""
        if self.root is None:
            return
        # Build the directed graph.
        G = nx.DiGraph()
        G.add_node(self.root.value)
        nodes = [self.root]
        while nodes:
            current = nodes.pop(0)
            for child in [current.left, current.right]:
                if child is not None:
                    G.add_edge(current.value, child.value)
                    nodes.append(child)
        # Plot the graph. This requires graphviz_layout (pygraphviz).
        nx.draw(G, pos=graphviz_layout(G, prog="dot"), arrows=True,
                with_labels=True, node_color="C1", font_size=8)
        plt.show()
```

Additional Code: AVL Tree

Use the following class for Problem 4. Note that it inherits from the `BST` class, so its functionality is dependent on the `insert()` method from Problem 2. Note that the `remove()` method is disabled, though it is possible for an AVL tree to rebalance itself after removing a node.

```
class AVL(BST):
    """Adelson-Velsky Landis binary search tree data structure class.
    Rebalances after insertion when needed.
    """
    def insert(self, data):
        """Insert a node containing the data into the tree, then rebalance."""
        BST.insert(self, data)      # Insert the data like usual.
        n = self.find(data)
        while n:                    # Rebalance from the bottom up.
            n = self._rebalance(n).prev

    def remove(*args, **kwargs):
        """Disable remove() to keep the tree in balance."""
        raise NotImplementedError("remove() is disabled for this class")

    def _rebalance(self,n):
        """Rebalance the subtree starting at the specified node."""
        balance = AVL._balance_factor(n)
        if balance == -2:                                   # Left heavy
            if AVL._height(n.left.left) > AVL._height(n.left.right):
                n = self._rotate_left_left(n)                   # Left Left
            else:
                n = self._rotate_left_right(n)                  # Left Right
        elif balance == 2:                                  # Right heavy
            if AVL._height(n.right.right) > AVL._height(n.right.left):
                n = self._rotate_right_right(n)                 # Right Right
            else:
                n = self._rotate_right_left(n)                  # Right Left
        return n

    @staticmethod
    def _height(current):
        """Calculate the height of a given node by descending recursively until
        there are no further child nodes. Return the number of children in the
        longest chain down.
        """
        if current is None:     # Base case: the end of a branch.
            return -1           # Otherwise, descend down both branches.
        return 1 + max(AVL._height(current.right), AVL._height(current.left))

    @staticmethod
    def _balance_factor(n):
        return AVL._height(n.right) - AVL._height(n.left)
```

```
    def _rotate_left_left(self, n):
        temp = n.left
        n.left = temp.right
        if temp.right:
            temp.right.prev = n
        temp.right = n
        temp.prev = n.prev
        n.prev = temp
        if temp.prev:
            if temp.prev.value > temp.value:
                temp.prev.left = temp
            else:
                temp.prev.right = temp
        if n is self.root:
            self.root = temp
        return temp

    def _rotate_right_right(self, n):
        temp = n.right
        n.right = temp.left
        if temp.left:
            temp.left.prev = n
        temp.left = n
        temp.prev = n.prev
        n.prev = temp
        if temp.prev:
            if temp.prev.value > temp.value:
                temp.prev.left = temp
            else:
                temp.prev.right = temp
        if n is self.root:
            self.root = temp
        return temp

    def _rotate_left_right(self, n):
        temp1 = n.left
        temp2 = temp1.right
        temp1.right = temp2.left
        if temp2.left:
            temp2.left.prev = temp1
        temp2.prev = n
        temp2.left = temp1
        temp1.prev = temp2
        n.left = temp2
        return self._rotate_left_left(n)

    def _rotate_right_left(self, n):
        temp1 = n.right
        temp2 = temp1.left
```

```
        temp1.left = temp2.right
        if temp2.right:
            temp2.right.prev = temp1
        temp2.prev = n
        temp2.right = temp1
        temp1.prev = temp2
        n.right = temp2
        return self._rotate_right_right(n)
```

3 Nearest Neighbor Search

Lab Objective: *The nearest neighbor problem is an optimization problem that arises in applications such as computer vision, internet marketing, and data compression. The problem can be solved efficiently with a k-d tree, a generalization of the binary search tree. In this lab we implement a k-d tree, use it to solve the nearest neighbor problem, then use that solution as the basis of an elementary machine learning algorithm.*

The Nearest Neighbor Problem

Let $X \subset \mathbb{R}^k$ be a collection of data, called the *training set*, and let $\mathbf{z} \in \mathbb{R}^k$, called the *target*. The *nearest neighbor search problem* is determining the point $\mathbf{x}^* \in X$ that is "closest" to $\mathbf{z}$.

For example, suppose you move into a new city with several post offices. Since your time is valuable, you wish to know which post office is closest to your home. The set X could be addresses or latitude and longitude data for each post office in the city; $\mathbf{z}$ would be the data that represents your new home. The task is to find the closest post office in $\mathbf{x} \in X$ to your home $\mathbf{z}$.

Metrics and Distance

Solving the nearest neighbor problem requires a definition for distance between $\mathbf{z}$ and elements of X. In $\mathbb{R}^k$, distance is typically defined by the *Euclidean metric*.

$$d(\mathbf{x}, \mathbf{z}) = \|\mathbf{x} - \mathbf{z}\| = \sqrt{\sum_{i=1}^{k} (x_i - z_i)^2} \tag{3.1}$$

Here $\|\cdot\|$ is the standard *Euclidean norm*, which computes vector length. In other words, $d(\mathbf{x}, \mathbf{z})$ is the length of the straight line from $\mathbf{x}$ to $\mathbf{z}$. With this notation, the nearest neighbor search problem can be written as follows.

$$\mathbf{x}^* = \operatorname*{argmin}_{\mathbf{x} \in X} d(\mathbf{x}, \mathbf{z}) \qquad d^* = \min_{\mathbf{x} \in X} d(\mathbf{x}, \mathbf{z}) \tag{3.2}$$

NumPy and SciPy implement the Euclidean norm (and other norms) in `linalg.norm()`. This function accepts vectors or matrices. Use the `axis` argument to compute the norm along the rows or columns of a matrix: `axis=0` computes the norm of each column, and `axis=1` computes the norm of each row (see the NumPy Visual Guide).

```
>>> import numpy as np
>>> from scipy import linalg as la

>>> x0 = np.array([1, 2, 3])
>>> x1 = np.array([6, 5, 4])

# Calculate the length of the vectors x0 and x1 using the Euclidean norm.
>>> la.norm(x0)
3.7416573867739413
>>> la.norm(x1)
8.7749643873921226

# Calculate the distance between x0 and x1 using the Euclidean metric.
>>> la.norm(x0 - x1)
5.9160797830996161

>>> A = np.array([[1, 2, 3],        # or A = np.vstack((x0,x1)).
...               [6, 5, 4]])
>>> la.norm(A, axis=0)              # Calculate the norm of each column of A.
array([ 6.08276253,  5.38516481,  5.        ])
>>> la.norm(A, axis=1)              # Calculate the norm of each row of A.
array([ 3.74165739,  8.77496439])   # This is ||x0|| and ||x1||.
```

Exhaustive Search

Consider again the post office example. One way to find out which post office is closest is to drive from home to each post office, measuring the distance travelled in each trip. That is, we solve (3.2) by computing $\|\mathbf{x} - \mathbf{z}\|$ for every point $\mathbf{x} \in X$. This strategy is called a *brute force* or *exhaustive search*.

Problem 1. Write a function that accepts a $m \times k$ NumPy array X (the training set) and a 1-dimensional NumPy array $\mathbf{z}$ with k entries (the target). Each of the m rows of X represents a point in $\mathbb{R}^k$ that is an element of the training set.

Solve (3.2) with an exhaustive search. Return the nearest neighbor $\mathbf{x}^*$ and its distance d^* from the target $\mathbf{z}$.
(Hint: use array broadcasting and the `axis` argument to avoid using a loop.)

The complexity of an exhaustive search for $X \subset \mathbb{R}^k$ with m points is $O(km)$, since (3.1) is $O(k)$ and there are m norms to compute. This method works, but it is only feasible for relatively small training sets. Solving the problem with greater efficiency requires the use of a specialized data structure.

K-D Trees

A *k-d tree* is a generalized binary search tree where each node in the tree contains k-dimensional data. Just as a BST makes searching easy in $\mathbb{R}$, a k-d tree provides a way to efficiently search $\mathbb{R}^k$.

A BST creates a partition of $\mathbb{R}$: if a node contains the value x, all of the nodes in its left subtree contain values that are less than x, and the nodes of its right subtree have values that are greater than x. Similarly, a k-d tree partitions $\mathbb{R}^k$. Each node is assigned a *pivot* value $i \in \{0, 1, \ldots, k-1\}$ corresponding to the depth of the node: the root has $i = 0$, its children have $i = 1$, their children have $i = 2$, and so on. If a node has $i = k - 1$, its children have $i = 0$, their children have $i = 1$, and so on. The tree is constructed such that for a node containing $\mathbf{x} = [x_0, x_1, \ldots, x_{k-1}]^T \in \mathbb{R}^k$, if a node in the left subtree contains $\mathbf{y}$, then $y_i < x_i$. Conversely, if a node in the right subtree contains $\mathbf{z}$, then $x_i \leq z_i$. See Figure 3.1 for an example where $k = 3$.

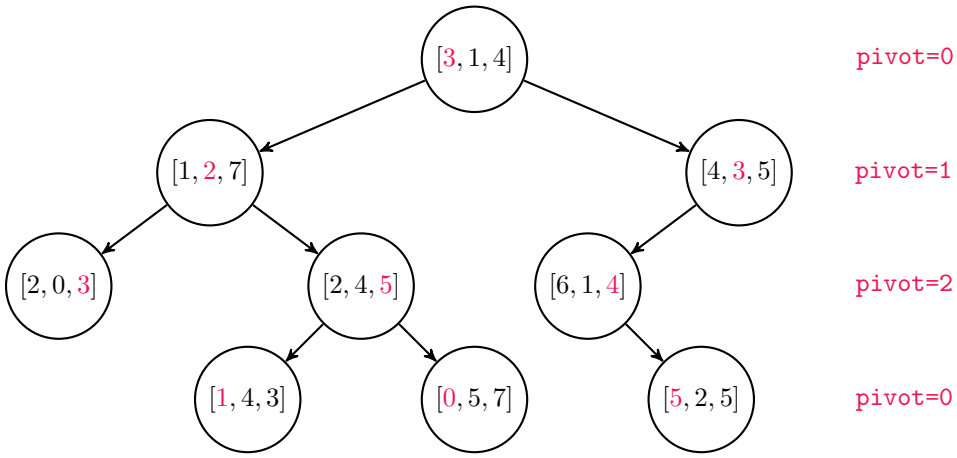


Figure 3.1: A k-d tree with $k = 3$. The root $[3, 1, 4]$ has an `pivot` of 0, so $[1, 2, 7]$ is to the left of the root because $1 < 3$, and $[4, 3, 5]$ is to the right since $3 \leq 4$. Similarly, the node $[2, 4, 5]$ has an `pivot` of 2, so $[1, 4, 3]$ is to its left since $4 < 5$ and $[0, 5, 7]$ is to its right because $5 \leq 7$. The nodes that are furthest from the root have an `pivot` of 0 because their parents have an `pivot` of $2 = k - 1$.

Problem 2. Write a `KDTNode` class whose constructor accepts a single parameter $\mathbf{x} \in \mathbb{R}^k$. If $\mathbf{x}$ is not a NumPy array (of type `np.ndarray`), raise a `TypeError`. Save $\mathbf{x}$ as an attribute called `value`, and initialize attributes `left`, `right`, and `pivot` as `None`. The `pivot` will be assigned when the node is inserted into the tree, and `left` and `right` will refer to child nodes.

Constructing the Tree

Locating Nodes

The `find()` methods for k-d trees and binary search trees are very similar. Both recursively compare the values of a target and nodes in the tree, but in a k-d tree, these values must be compared according to their `pivot` attribute. Every comparison in the recursive `_step()` function, implemented below, compares the data of `target` and `current` based on the `pivot` attribute of `current`. See Figure 3.2.

```
class KDT:
    """A k-dimensional tree for solving the nearest neighbor problem.

    Attributes:
        root (KDTNode): the root node of the tree. Like all other nodes in
```

```
            the tree, the root has a NumPy array of shape (k,) as its value.
        k (int): the dimension of the data in the tree.
    """
    def __init__(self):
        """Initialize the root and k attributes."""
        self.root = None
        self.k = None

    def find(self, data):
        """Return the node containing the data. If there is no such node in
        the tree, or if the tree is empty, raise a ValueError.
        """
        def _step(current):
            """Recursively step through the tree until finding the node
            containing the data. If there is no such node, raise a ValueError.
            """
            if current is None:                     # Base case 1: dead end.
                raise ValueError(str(data) + " is not in the tree")
            elif np.allclose(data, current.value):
                return current                      # Base case 2: data found!
            elif data[current.pivot] < current.value[current.pivot]:
                return _step(current.left)          # Recursively search left.
            else:
                return _step(current.right)         # Recursively search right.

        # Start the recursive search at the root of the tree.
        return _step(self.root)
```

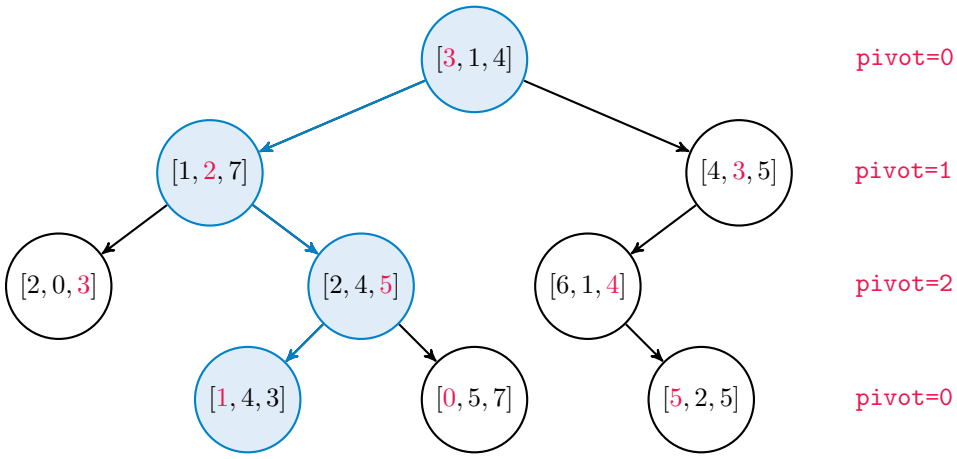
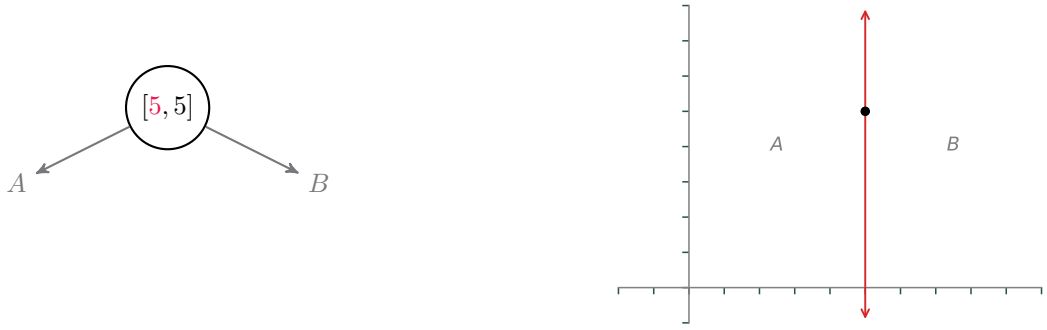
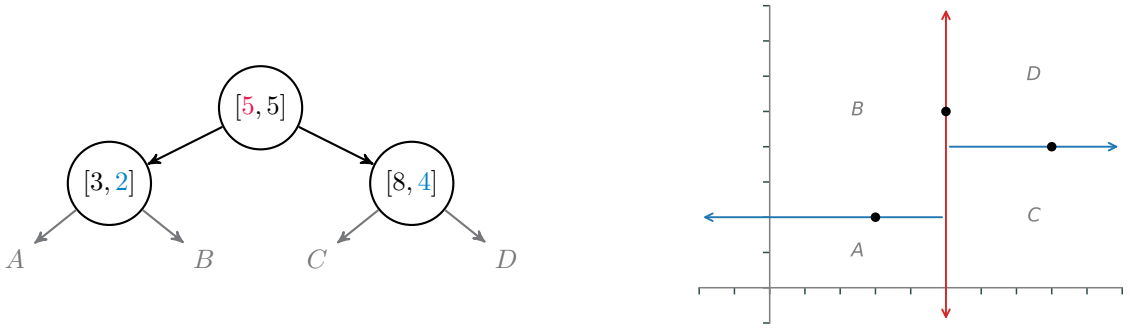


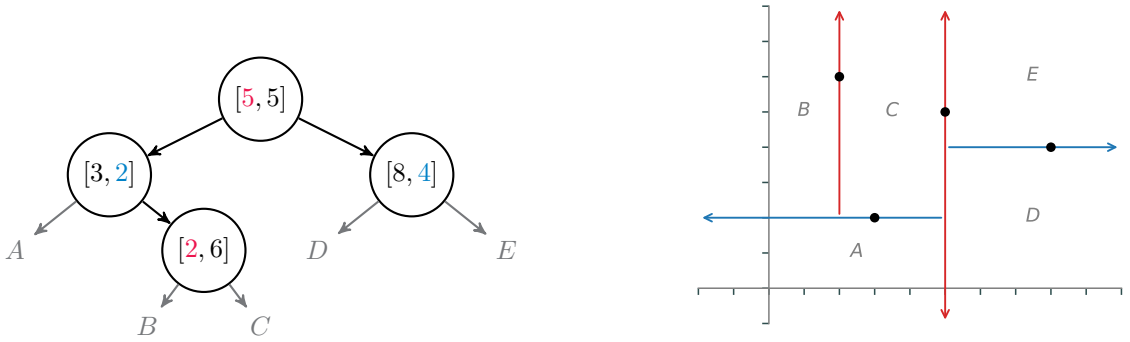
Figure 3.2: To locate the node containing $[1, 4, 3]$, start by comparing $[1, 4, 3]$ to the root $[3, 1, 4]$. The root has an `pivot` of 0, so compare the first component of the data to the first component of the root: since $1 < 3$, step left. Next, $[1, 4, 3]$ must be to the right of $[1, 2, 7]$ because $2 \leq 4$. Similarly, $[1, 4, 3]$ must be to the left of $[2, 4, 5]$ as $3 < 5$.



(a) Insert $[5, 5]$ as the root. The root always has an `pivot` of 0, so nodes to the left of the root contain points from $A = \{(x, y) \in \mathbb{R}^2 : x < 5\}$, and nodes on the right branch have points in $B = \{(x, y) \in \mathbb{R}^2 : 5 \leq x\}$.



(b) Insert $[3, 2]$, then $[8, 4]$. Since $3 < 5$, $[3, 2]$ becomes the left child of $[5, 5]$. Likewise, as $5 \leq 8$, $[8, 4]$ becomes the right child of $[5, 5]$. These new nodes have an `pivot` of 1, so they partition the space vertically: nodes to the right of $[3, 2]$ contain points from $B = \{(x, y) \in \mathbb{R}^2 : x < 5,\ 2 \leq y\}$; nodes to the left of $[8, 4]$ hold points from $C = \{(x, y) \in \mathbb{R}^2 : 5 \leq x,\ y < 8\}$.



(c) Insert $[2, 6]$. The `pivot` cycles back to 0 since $k = 2$, so nodes to the left of $[2, 6]$ have points that lie in $B = \{(x, y) \in \mathbb{R}^2 : x < 2,\ 2 \leq y\}$ and nodes to the right store points in $C = \{(x, y) \in \mathbb{R}^2 : 2 \leq x < 5,\ 2 \leq y\}$.

Figure 3.3: As a k-d tree is constructed (left), it creates a partition of $\mathbb{R}^k$ (right) by defining separating hyperplanes that pass through the points. The more points, the finer the partition.

Inserting Nodes

To add a new node to a k-d tree, determine which existing node should be the parent of the new node by recursively stepping down the tree as in the `find()` method. Next, assign the new node as the `left` or `right` child of the parent, and set its `pivot` based on its parent's `pivot`: if the parent's `pivot` is i, the new node's `pivot` should be $i+1$, or 0 if $i = k-1$.

Consider again the k-d tree in Figure 3.2. To insert $[2, 3, 4]$, search the tree for $[2, 3, 4]$ until hitting an empty slot. In this case, the search steps from the root down to $[1, 4, 3]$, which has an `pivot` of 0. Then since $1 \leq 2$, the new node should be to the right of $[1, 4, 3]$. However, $[1, 4, 3]$ has no right child, so it becomes the parent of $[2, 3, 4]$. The `pivot` of the new node should therefore be 1. See Figure 3.3 for another example.

Problem 3. Write an `insert()` method for the `KDT` class that accepts a point $\mathbf{x} \in \mathbb{R}^k$.

1. If the tree is empty, create a new `KDTNode` containing $\mathbf{x}$ and set its `pivot` to 0. Assign the `root` attribute to the new node and set the `k` attribute as the length of $\mathbf{x}$. Thereafter, raise a `ValueError` if data to be inserted is not in $\mathbb{R}^k$.
2. If the tree is nonempty, create a new `KDTNode` containing $\mathbf{x}$ and find the existing node that should become its parent. Determine whether the new node will be the parent's `left` or `right` child, then link the parent to the new node accordingly. Set the `pivot` of the new node based on its parent's `pivot`.
   (Hint: write a recursive function like `_step()` to find and link the parent.)
3. Do not allow duplicates in the tree: if there is already a node in the tree containing $\mathbf{x}$, raise a `ValueError`.

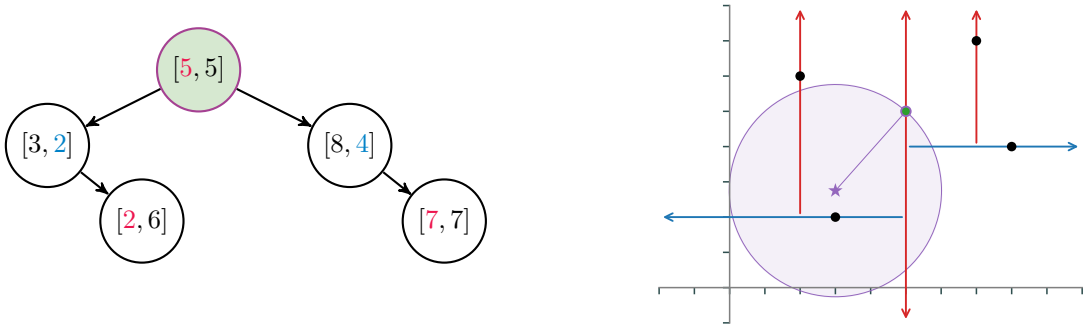
To test your method, use the `__str__()` method provided in the Additional Materials section. Try constructing the trees in Figures 3.1 and 3.3. Also check that the provided `find()` method works as expected.

Nearest Neighbor Search with K-D Trees

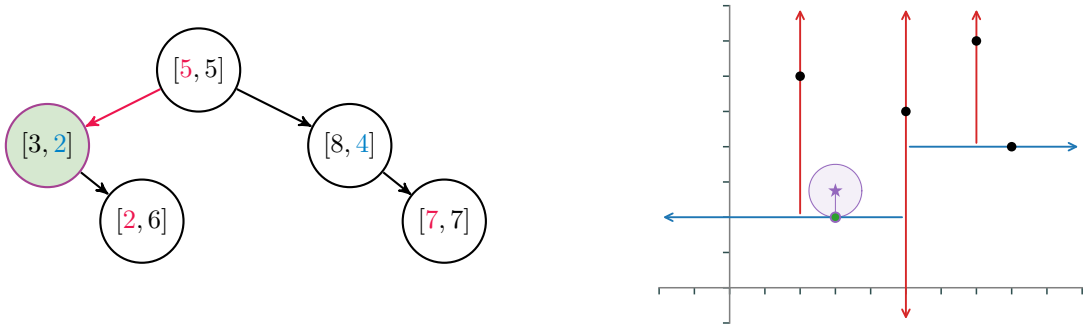
Given a target $\mathbf{z} \in \mathbb{R}^k$ and a k-d tree containing a set $X \subset \mathbb{R}^k$ of m points, the nearest neighbor problem can be solved by traversing the tree in a manner that is similar to the `find()` or `insert()` methods from the previous section. The advantage of this strategy over an exhaustive search is that not every $\mathbf{x} \in X$ has to be compared to $\mathbf{z}$ via (3.1); the tree structure makes it possible to rule out some elements of X without actually computing their distances to $\mathbf{z}$. The complexity is $O(k \log(m))$, a significant improvement over the $O(km)$ complexity of an exhaustive search.

To begin, set $\mathbf{x}^*$ as the value of the root and compute $d^* = d(\mathbf{x}^*, \mathbf{z})$. Starting at the root, step down through the tree as if searching for the target $\mathbf{z}$. At each step, determine if the value $\mathbf{x}$ of the current node is closer to $\mathbf{z}$ than $\mathbf{x}^*$. If it is, assign $\mathbf{x}^* = \mathbf{x}$ and recompute $d^* = d(\mathbf{x}^*, \mathbf{z})$. Continue this process until reaching a leaf node.

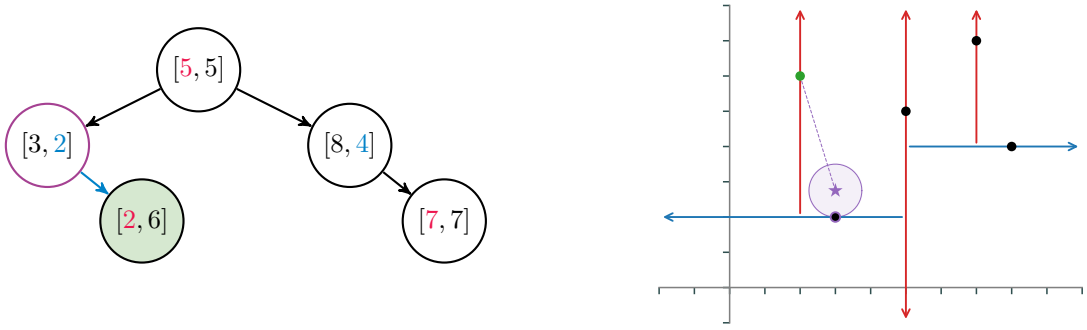
Next, backtrack along the search path and determine if the non-explored branch needs to be searched. To do this, check that the sphere of radius d^* centered at $\mathbf{z}$ does not intersect with the separating hyperplane defined by the current node. That is, if the separating hyperplane is further than d^* from $\mathbf{z}$, then no points on the other side of the hyperplane can possibly be the nearest neighbor. See Figure 3.4 for an example and Algorithm 3.1 for the details of the procedure.



(a) Start at the root, setting $\mathbf{x}^* = [5, 5]$. The sphere of radius $d^* = d(\mathbf{x}^*, \mathbf{z})$ centered at $\mathbf{z}$ intersects the hyperplane $x = 5$, so (at this point) it is possible that a nearer neighbor lies to the right of the root.



(b) If the target $\mathbf{z} = [3, 2.75]$ were in the tree, it would be to the left of the root, so step left and examine $\mathbf{x} = [3, 2]$. Since $d(\mathbf{x}, \mathbf{z}) < d(\mathbf{x}^*, \mathbf{z})$, reassign $\mathbf{x}^* = \mathbf{x}$ and recompute d^*. Now the sphere of radius d^* centered at $\mathbf{z}$ no longer intersects the root's hyperplane, so the nearest neighbor cannot be in the root's right subtree.



(c) Continuing the search, step right to check the point $\mathbf{x} = [2, 6]$. In this case $d(\mathbf{x}, \mathbf{z}) > d(\mathbf{x}^*, \mathbf{z})$, meaning $\mathbf{x}$ is **not** nearer to $\mathbf{z}$ than $\mathbf{x}^*$. Since $[2, 6]$ is a leaf node, retrace the search steps up the tree to check the non-searched branches. However, the sphere around $\mathbf{z}$ does not intersect any splitting hyperplanes defined by the tree, so $\mathbf{x}^*$ is guaranteed to be the nearest neighbor.

Figure 3.4: Nearest neighbor search of a k-d tree with $k = 2$. The target is $\mathbf{z} = [3, 2.75]$ and the nearest neighbor is $\mathbf{x}^* = [3, 2]$ with minimal distance $d^* = 0.75$. The tree structure allows the algorithm to eliminate $[8, 4]$ and $[7, 7]$ from consideration without computing their distance from $\mathbf{z}$.

Algorithm 3.1 k-d tree nearest neighbor search

```
1: procedure NEAREST NEIGHBOR SEARCH(z, root)
2:     procedure KDSEARCH(current, nearest, d*)
3:         if current is None then                          ▷ Base case: dead end.
4:             return nearest, d*
5:         x ← current.value
6:         i ← current.pivot
7:         if d(x, z) < d* then          ▷ Check if current is closer to z than nearest.
8:             nearest ← current
9:             d* ← d(x, z)
10:        if z_i < x_i then                                  ▷ Search to the left.
11:            nearest, d* ← KDSearch(current.left, nearest, d*)
12:            if z_i + d* ≥ x_i then                  ▷ Search to the right if needed.
13:                nearest, d* ← KDSearch(current.right, nearest, d*)
14:        else                                              ▷ Search to the right.
15:            nearest, d* ← KDSearch(current.right, nearest, d*)
16:            if z_i − d* ≤ x_i then                   ▷ Search to the left if needed.
17:                nearest, d* ← KDSearch(current.left, nearest, d*)
18:        return nearest, d*
19:    node, d* ← KDSearch(root, root, d(root.value, z))
20:    return node.value, d*
```

Problem 4. Write a method for the `KDT` class that accepts a target point $\mathbf{z} \in \mathbb{R}^k$. Use Algorithm 3.1 to solve (3.2). Return the nearest neighbor $\mathbf{x}^*$ (the actual NumPy array, not the `KDTNode`) and its distance d^* from $\mathbf{z}$.

Compare your method to the exhaustive search in Problem 1 and to SciPy's built-in `KDTree` class. This structure is essentially a heavily optimized version of the `KDT` class. To solve the nearest neighbor problem, initialize the tree with data, then "query" the tree with the target point. The `query()` method returns a tuple of the minimum distance and the index of the nearest neighbor in the data.

```
>>> from scipy.spatial import KDTree

# Initialize the tree with data (in this example, use random data).
>>> data = np.random.random((100,5))     # 100 5-dimensional points.
>>> target = np.random.random(5)
>>> tree = KDTree(data)

# Query the tree for the nearest neighbor and its distance from 'target'.
>>> min_distance, index = tree.query(target)
>>> print(min_distance)
0.24929868807
>>> tree.data[index]                          # Get the actual nearest neighbor.
array([ 0.26927057,  0.03160271,  0.46830759,  0.26766863,  0.63073275])
```

ACHTUNG!

There are a few caveats to using a k-d tree for the nearest neighbor search problem.

- Constructing the tree takes time. For small enough data sets, an exhaustive search may be faster than the combined time of constructing and searching a tree. On the other hand, once the tree is constructed, it can be used for multiple nearest-neighbor queries.
- In the worst case—when the tree is completely unbalanced—the search complexity is $O(km)$ instead of $O(k\log(m))$. Fortunately, there are algorithms for constructing the tree intelligently so that it is mostly balanced, and a random insertion order usually results in a somewhat balanced tree.

K-Nearest Neighbors

The nearest neighbor algorithm provides one way to solve a common machine learning problem. In *supervised learning*, a *training set* $X \subset D$ has a corresponding set of *labels* Y that specifies a category for each element of X. For instance, X could contain financial data on m individuals, and Y could be a set of m booleans indicating which individuals have filed for bankruptcy. Supervised learning algorithms use the training data to construct a function $f : D \to Y$ that maps points to their corresponding label. In other words, the algorithm "learns" enough about the relationship between X and Y to intelligently label arbitrary elements of D. In the bankruptcy example, a person could then use their own financial data to learn whether or not they look more like someone who files for bankruptcy or someone who does not.

A *k-nearest neighbors* classifier uses a simple strategy to label an arbitrary $\mathbf{z} \in D$: find the k elements of X that are nearest to $\mathbf{z}$ (usually in terms of the Euclidean metric) and choose the most common label from those k elements as the label of $\mathbf{z}$. That is, the points in the k labeled points that are most like $\mathbf{z}$ are allowed to "vote" on how $\mathbf{z}$ should be labeled. See Figure 3.5.

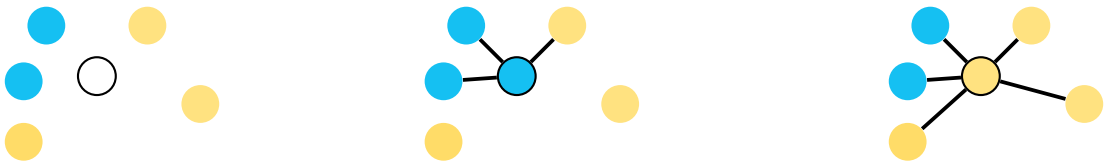


Figure 3.5: To classify the center node, determine its k-nearest neighbors and pick the most common label of the neighbors. If $k = 3$, the k nearest points are two blues and a yellow, so the center node is labeled blue. For $k = 5$, the k nearest points consists of two blues and three yellows, so the center node is labeled yellow.

ACHTUNG!

The k in k-d tree refers to the **dimension** of the data housed in the tree, but the k in k-nearest neighbors refers to the **number of neighbors** to use in the voting scheme. Unfortunately, both names are standard.

Problem 5. Write a `KNeighborsClassifier` class with the following methods.

1. The constructor should accept an integer `n_neighbors`, the number of neighbors to include in the vote (the k in k-nearest neighbors). Save this value as an attribute.

2. `fit()`: accept an $m \times k$ NumPy array X (the training set) and a 1-dimensional NumPy array `y` with m entries (the training labels). As in Problems 1 and 4, each of the m rows of X represents a point in $\mathbb{R}^k$. Here y_i is the label corresponding to row i of X.

   Load a SciPy `KDTree` with the data in X. Save the tree and the labels as attributes.

3. `predict()`: accept a 1-dimensional NumPy array `z` with k entries. Query the `KDTree` for the `n_neighbors` elements of X that are nearest to `z` and return the most common label of those neighbors. If there is a tie for the most common label (such as if $k = 2$ in Figure 3.5), choose the alphanumerically smallest label.
   (Hint: use `scipy.stats.mode()`. The default behavior splits ties correctly.)

   To get several nearest neighbors from the tree, specify `k` in `KDTree.query()`.

```
>>> data = np.random.random((100,5))     # 100 5-dimensional points.
>>> target = np.random.random(5)
>>> tree = KDTree(data)

# Query the tree for the 3 nearest neighbors.
>>> distances, indices = tree.query(target, k=3)
>>> print(indices)
[26 30 32]
```

NOTE

The format of the `KNeighborsClassifier` in Problem 5 conforms to the style of *scikit-learn* (`sklearn`), a large machine learning library in Python. In fact, scikit-learn has a class called `sklearn.neighbors.KNeighborsClassifier` that is a more robust version of the class from Problem 5. See `http://scikit-learn.org/stable/modules/neighbors.html` for more tools from scikit-learn for solving the nearest neighbor problem in the context of machine learning.

Handwriting Recognition

Computer vision is a challenging area of artificial intelligence that focuses on autonomously interpreting images. Perhaps the simplest computer vision problem is that of translating images into text. Roughly speaking, computers store grayscale images as $M \times N$ arrays of pixel brightness values: 0 corresponds to black, and 255 to white. Flattening out such an array yields a vector in $\mathbb{R}^{MN}$. Given some images of characters with labels (assigned by humans), a k-nearest neighbor classifier can intelligently decide what character the image represents.

Problem 6. The file `mnist_subset.npz` contains part of the MNIST dataset,[a] a collection of 28×28 images of handwritten digits and their labels. The data is split into four parts.

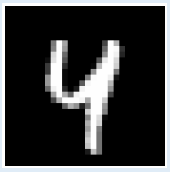
- `X_train`: A 3000×728 matrix, the training set. Each of the 3000 rows is a flattened 28×28 image to be used in training the classifier.
- `y_train`: A 1-dimensional NumPy array with 3000 entries. The entries are integers from 0 to 9, the labels corresponding to the images in `X_train`.
- `X_test`: A 500×728 matrix of 500 images to classify.
- `y_test`: A 1-dimensional NumPy array with 500 entries. These are the labels corresponding to `X_test`, the "right answers" that the classifier will try to guess.

The following code uses `np.load()` to extract the data.

```
>>> data = np.load("mnist_subset.npz")
>>> X_train = data["X_train"].astype(np.float)          # Training data
>>> y_train = data["y_train"]                           # Training labels
>>> X_test = data["X_test"].astype(np.float)            # Test data
>>> y_test = data["y_test"]                             # Test labels
```

To visualize one of the images, reshape it as a 28×28 array and use `plt.imshow()`.

```
>>> from matplotlib import pyplot as plt
>>> plt.imshow(X_test[0].reshape((28,28)), cmap="gray")
>>> plt.show()
```



Write a function than accepts an integer `n_neighbors`. Load a classifier from Problem 5 with the data `X_train` and the corresponding labels `y_train`. Use the classifier to predict the labels of each image in `X_test`. Return the classification accuracy, the percentage of predictions that match `y_test`. The accuracy should be at least 90% using 4 nearest neighbors.

[a] See `http://yann.lecun.com/exdb/mnist/`.

Note

The k-nearest neighbors algorithm is **not** the best machine learning algorithm for this problem, but it is a good starting point because of its simplicity. In fact, k-nearest neighbors is often used as a baseline to compare against more complicated machine learning techniques.

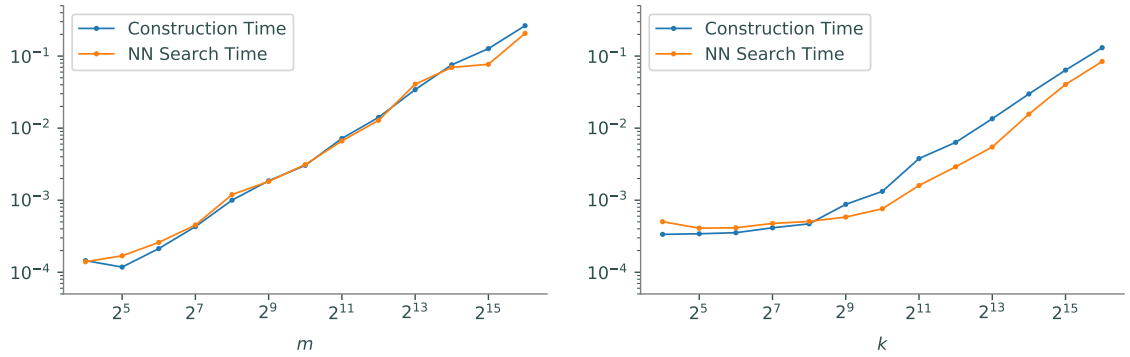
Additional Material

Ball Trees

The nearest neighbor problem can also be solved efficiently with a *ball tree*, another space-partitioning data structure. Instead of separating $\mathbb{R}^k$ by hyperplanes, a ball tree uses nested hyperspheres to split up the space. Since the partitioning scheme is different, a nearest neighbor search through a ball tree is more efficient than the k-d tree search for some data sets. See `https://en.wikipedia.org/wiki/Ball_tree` for more details.

The Curse of Dimensionality

The *curse of dimensionality* refers to a phenomena that occurs when dealing with high-dimensional data: the computational cost of an algorithm increases much more rapidly as the dimension increases than it does when the number of points increases. This problem occurs in many other areas involving multi-dimensional data, but it is quite apparent in a nearest neighbor search.



(a) Fixing k and increasing m leads to consistent growth in execution time.

(b) For fixed m, the times takes a sharp upturn around $k = 2^9$ relative to previous growth rates.

Figure 3.6: Construction and nearest neighbor search times for a k-d tree with a $m \times k$ training set.

See `https://en.wikipedia.org/wiki/Curse_of_dimensionality` for more examples. One way to avoid the curse of dimensionality is via *dimension reduction*, a process usually based on the singular value decomposition (SVD) that projects data into a lower-dimensional space.

Tiebreaker Strategies

As mentioned in Problem 5, the majority voting scheme in the k-nearest neighbor algorithm can often result in a tie. Breaking the tie intelligently is a science unto itself, but here are a few common strategies.

1. For binary classification (meaning there are only two labels), choose an odd k to avoid a tie in the first place.
2. Redo the search with $k - 1$ neighbors, repeating as needed until $k = 1$.
3. Choose the label that appears more frequently in the test set.
4. Choose randomly among the labels that are tied for most common.

Additional Code

The following code creates a string representation for the `KDT` class. Use this to test Problem 3.

```
class KDT:
    # ...
    def __str__(self):
        """String representation: a hierarchical list of nodes and their axes.

        Example:                            'KDT(k=2)
                    [5,5]                    [5 5]   pivot = 0
                    /   \                    [3 2]   pivot = 1
                [3,2]   [8,4]                [8 4]   pivot = 1
                    \       \                [2 6]   pivot = 0
                    [2,6]   [7,5]            [7 5]   pivot = 0'
        """
        if self.root is None:
            return "Empty KDT"
        nodes, strs = [self.root], []
        while nodes:
            current = nodes.pop(0)
            strs.append("{}\tpivot = {}".format(current.value, current.pivot))
            for child in [current.left, current.right]:
                if child:
                    nodes.append(child)
        return "KDT(k={})\n".format(self.k) + "\n".join(strs)
```

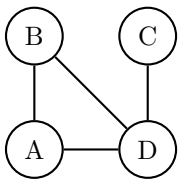
4 Breadth-first Search

Lab Objective: *Shortest path problems are an important part of graph theory and network analysis. Applications include finding the fastest way to drive between two points on the map, network routing, genealogy, automated circuit layout, and a variety of other problems. In this lab we learn to represent graphs as adjacency dictionaries, implement a shortest-path algorithm based on a breadth-first search, and use the NetworkX package to solve a shortest path problem on a large actor-movie network.*

Adjacency Dictionaries

Computers can represent mathematical graphs in various ways. Graphs with very specific structures are often stored with specialized data structures, such as binary search trees. More general graphs without structural constraints are usually represented with an *adjacency matrix*, where each row and column of the matrix corresponds to a node in the graph, and the entries indicate connections between nodes. Adjacency matrices are usually implemented in a sparse matrix format since only the entries corresponding to node connections are nonzero.

Another common graph data structure is an *adjacency dictionary*, a dictionary with a key for each node in the graph. The dictionary values list the nodes connected to the key node. Adjacency dictionaries automatically gain the advantages of a sparse matrix format since they only store the actual node connections. In Python, dictionaries are also much faster for lookup than matrices.



$$\begin{array}{c} \\ A \\ B \\ C \\ D \end{array} \begin{array}{c} \begin{array}{cccc} A & B & C & D \end{array} \\ \left[\begin{array}{cccc} 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{array}\right] \end{array}$$

$$\begin{aligned} &\{\text{A}: \{\text{B}, \text{D}\},\\ &\ \text{B}: \{\text{A}, \text{D}\},\\ &\ \text{C}: \{\text{D}\},\\ &\ \text{D}: \{\text{A}, \text{B}, \text{D}\}\} \end{aligned}$$

Figure 4.1: A simple unweighted graph (left), its adjacency matrix (middle), and its adjacency dictionary (right). The graph is undirected, so the adjacency matrix is symmetric. Note that the adjacency dictionary also encodes this behavior: since A and B are connected, B is in the set of values corresponding to the key A, and A is in the set of values corresponding to the key B.

Hash-based Data Structures

A Python `set` is an unordered data type with no repeated elements. The `set` class is implemented as a *hash table*, meaning it uses *hash values*—integers that uniquely identify an object—to organize its elements. Roughly speaking, in order to access, add, or remove and object x to a set, Python computes the hash value of x, and that value indicates where x is (or should be). In other words, there is only one place that x could be; if it isn't in that place, it isn't in the set. This implementation results in $O(1)$ lookup, insertion, and removal operations, an enormous improvement over the $O(n)$ search time for lists and the $O(\log n)$ search time for sorted structures. It is also why set elements are unique.

Method	Description
`add()`	Add an element to the set if not already in the set.
`remove()`	Remove the specified element from the set, raising an error if the element is not in the set.
`discard()`	Remove the specified element from the set without raising an error if the element is not in the set.
`pop()`	Remove and return an arbitrary set element.
`union()`	Return all elements that are in either set as a new set.
`intersection()`	Return all elements that are in both sets as a new set.
`update()`	Perform an in-place union of a set with others.

Table 4.1: Basic methods of the `set` class.

```
# Initialize a set. Note that repeats are not added.
>>> animals = {"cow", "cat", "dog", "mouse", "cow"}
>>> print(animals)
{'cow', 'dog', 'mouse', 'cat'}

>>> animals.add("horse")      # Add an object to the set.
>>> animals.remove("emu")     # Attempt to delete an object from the set,
KeyError: 'emu'               # resulting in an exception.

>>> animals.pop()             # Delete and return a random object from the set.
'dog'
>>> print(animals)
{'cat', 'mouse', 'cow', 'horse'}

# Add all of the elements of another set to this one.
>>> animals.update({"mouse", "velociraptor"})
>>> print(animals)
{'cat', 'mouse', 'velociraptor', 'cow', 'horse'}

# Intersect this set with another one.
>>> animals.intersection({"cat", "cow", "cheetah"})
{'cat', 'cow'}
```

Achtung!

Elements of a `set` and keys (but not values) of a `dict` must be *hashable*. Mutable objects—lists, sets and dictionaries—are not hashable, so they are not allowed as set elements or dictionary key values. This means that in order to represent a graph with an adjacency dictionary, each of the node labels should a string, a number, or some other hashable time.

Dictionaries are similar to sets, except that elements in a dictionary are key-value pairs. Keys in a dictionary must also be hashable, but values can be anything. Because, like sets, lookup in a dictionary is very fast, they can be very useful for storing the results of a computation, so that it need only be done once. The table below gives a quick review of dictionaries.

Method	Description
`keys()`	Return an iterator for the dictionary's keys.
`values()`	Return an iterator for the dictionary's values.
`items()`	Return an iterator for the dictionary's items (key-value pairs).
`pop()`	Remove and return a specified key from the dictionary.
`update()`	Add or overwrite key-value pairs with those from a new dictionary.

```
# Initialize a dictionary.
>>> classes = {"business": "A", "math": "A+", "visual arts": "B"}
>>> print(classes["math"])
A+

# Add a value indexed by 'science' and delete the 'business' keypair.
>>> classes["science"] = "A"
>>> classes.pop("business")  # Use pop() to remove.
A
>>> print(classes)
{'math': 'A+', 'visual arts': 'B', 'science': 'A'}

# Display the keys, values, and items.
>>> list(classes.keys())
['math', 'visual arts', 'science']
>>> classes.values()
dict_values(['A+', 'B', 'A'])
>>> for key, value in classes.items():
...   print(key, "=>", value)
...
math => A+
visual arts => B
science => A

# Add key-value pairs from another dictionary.
>>> classes.update({"cooking":"A+", "math": "C"})
>>> print(classes)
{'math': 'C', 'visual arts': 'B', 'science': 'A', 'cooking': 'A+'}
```

```
# Save time by pre-computing functions and storing results for quick lookup.
>>> f = lambda x: "My grade is " + x
>>> my_grades = {x:f(classes[x]) for x in ('math','science')}
>>> print(my_grades)
{'math': 'My grade is C', 'science': 'My grade is A'}
```

Figure 4.1 is an example of a simple graph. The following code defines its adjacency dictionary.

```
>>> adjacency_dictionary = {'A':{'B', 'D'},
                            'B':{'A', 'D'},
                            'C':{'D'},
                            'D':{'A', 'B', 'C'}}

# The nodes are stored as the dictionary keys.
>>> print(adjacency_dictionary.keys())
{'A', 'C', 'B', 'E', 'D'}

# The values are the nodes that the key is connected to.
>>> print(adjacency_dictionary['A'])
{'B', 'D'}            # A is connected to B and D.
```

Problem 1. Consider the following `Graph` class.

```
class Graph:
    """A graph object, stored as an adjacency dictionary. Each node in the
    graph is a key in the dictionary. The value of each key is a set of
    the corresponding node's neighbors.

    Attributes:
        d (dictionary): the adjacency dictionary of the graph.
    """
    def __init__(self, adjacency):
        """Store the adjacency dictionary as a class attribute"""
        self.d = adjacency

    def __str__(self):
        """String representation: a view of the adjacency dictionary."""
        return str(self.d)
```

Add the following methods to this class.

1. `add_node(self, n)`: Add a node `n` to the graph.
2. `add_edge(self, u, v)`: Add an edge from node `u` to node `v` in the graph. Make sure to add the nodes if they are not already in the graph.

3. `remove_node(self, n)`: Remove the node `n` from the graph. Make sure to remove all connections to `n` as well. Raise a `KeyError` if `n` is not in the graph.

4. `remove_edge(self, u, v)`: Remove the edge from node `u` to node `v` from the graph. Raise a `KeyError`: if `u` or `v` are not in the graph, or if there is no edge between `u` and `v`. (Hint: Dictionaries and sets already raise errors with certain inputs.)

Breadth-first Search

Many of the most common problems that arise in graph theory require finding the shortest path between two nodes in the graph. Doing so requires a way to strategically search the graph. Two common searches are depth-first search (DFS) and breadth-first search (BFS). The BFS strategy is typically better at finding shortest paths than the DFS strategy[1].

To traverse a graph with a BFS, choose a starting node. If the starting node is not the target node, explore each of the starting node's neighbors. If none of the neighbors are the target, explore each of the neighbors' neighbors. If none of those neighbors are the target, explore each of their neighbors. Continue the process until the target is found. Note that in this way, we explore the *breadth* of the tree before going deeper each time.

In order to avoid common pitfalls, use the following data structures to keep track of visited and current nodes, as well as those marked to be visited.

1. A list V - The nodes that have been visted (in the order that they were visited).

2. A queue Q - The order in which to visit nodes.

3. A set M (marked) - The nodes marked as visited, and marked for visitation.

Recall that a *queue* is a type of limited-access list. Data is inserted to the back of the queue, but removed from the front. At each level of the search, we add the neighbors of the current node to the back of Q if they aren't in M already. This dictates the order in which the nodes are visited. Note that Q enforces the 'breadth-first' nature of a BFS. Another data structure, or a different order on the nodes, would result in a different search.

By creating M, a set to contain all nodes that have already been visited, or that are marked to be visited, we avoid visiting these nodes again. Checking set membership is very fast, so this additional data structure has minimal impact on the program's speed (and is faster than checking the queue).

[1] `https://xkcd.com/761/`

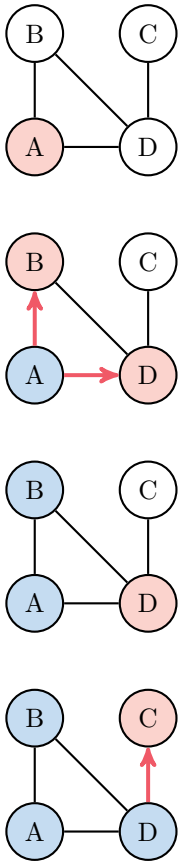


Figure 4.2: To start a breadth-first search from node A to node C, put A in the visit queue Q and mark it by adding it to the set M. Pop A off the queue and "visit" it by adding A to the visited list V and the neighboring nodes B and D to Q. Then visit B, but do not add anything to Q because all of the neighbors of B are already marked. Finally, visit D, at which point the target node C is located because it is adjacent to D. Visiting C is optional at this point.

Problem 2. Write a `traverse()` method for the `Graph` class that accepts a starting node and (optionally) a target node. Start from the specified node and proceed until the target is found. If no target is specified, proceed until all nodes in the graph have been visited. Return the list of visited nodes. If the starting node is not in the graph's adjacency dictionary, raise a `KeyError`.

Shortest Paths via BFS

In a BFS, as few neighborhoods are explored as possible before finding the target. At each neighborhood, the minimal path is marked from the source node, until the target node is encountered. Therefore, the path taken to get to the target must be the shortest path.

Examine again the graph in Figure 4.2. The shortest path from A to C starts at A, goes to D, and ends at C. During a BFS, D is visited because it is one of A's neighbors, and C is visited because it is one of D's neighbors. If we knew programmatically that A was the node that visited D, and that D was the node that visited C, we could retrace our steps to reconstruct the search path.

To implement this idea, initialize a dictionary before starting the BFS. When a node is added to the visit queue, add a key-value pair with the visiting node as the key, and the added node as the value. When the target node is found, step through the dictionary until arriving at the starting node, recording each step.

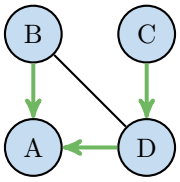


Figure 4.3: In the breadth-first search from Figure 4.2, nodes B and D were marked while visiting node A, and node C was marked while visiting node D (this is same as reversing the red arrows in Figure 4.2). Thus the "visit path" from C to A is C $\to$ D $\to$ A, so the shortest path from A to C is [A, D, C].

Problem 3. Add a method to the `Graph` class that accepts a start node and a target node. Begin at the specified starting node and proceed until the target is found. Return a list containing the node values in the shortest path from the start to the target (including the endpoints). If either of the inputs are not in the graph, raise a `KeyError`.

Shortest Paths via NetworkX

NetworkX is a Python package for creating, manipulating, and exploring large graphs. It contains a `Graph` object constructor as well as methods for adding nodes and edges to the graph. It also has methods for interpreting information about the graph and its structure from certain types of Python objects.

A node can be an int, a string, or a Python object, and an edge can be weighted or unweighted. There are several ways to add nodes and edges to the graph, some of which are listed below.

Method	Description
`add_node()`	Add a single node to the graph.
`add_nodes_from()`	Add a list of nodes to the graph.
`add_edge()`	Add an edge between two nodes.
`add_edges_from()`	Add a list of edges to the graph.

```
# Create a graph object using networkX using a known dictionary.
>>> import networkx as nx
>>> adjacency_dictionary = {'A':{'B', 'D'}, # The graph from earlier.
                            'B':{'A', 'D'},
                            'C':{'D'},
```

```
                              'D':{'A', 'B', 'C'}}
>>> nx_graph = nx.Graph(adjacency_dictionary)

# Access the nodes and edges.
>>> print(nx_graph.nodes())
['A', 'B', 'C', 'D']

>>> print(nx_graph.edges())
[('A', 'D'), ('A', 'B'), ('B', 'D'), ('C', 'D')]

>>> nx_graph.add_node('A')
>>> nx_graph.add_node('E')
>>> nx_graph.add_edge('A', 'F') # Node 'F' is added to the graph.
>>> nx_graph.add_edges_from([('A', 'E')])

# Access the nodes and edges.
>>> print(nx_graph.nodes())
['A', 'B', 'C', 'D', 'E', 'F']

>>> print(nx_graph.edges())
[('A', 'D'), ('A', 'B'), ('A', 'F'), ('A', 'E'), ('B', 'D'), ('C', 'D')]

# Small graphs can be visualized with nx.draw().
>>> from matplotlib import pyplot as plt
>>> nx.draw(nx_graph)
>>> plt.show()
```

The Kevin Bacon Problem

The 6 Degrees of Kevin Bacon is a vintage parlor game. The game is played by naming an actor, then trying to find a chain of actors that have worked with each other leading to Kevin Bacon. For example, Samuel L. Jackson was in the film *Captain America: The First Avenger* with Peter Stark, who was in *X-Men: First Class* with Kevin Bacon. Thus Samuel L. Jackson has a *Bacon number* of 2. Any actors who have been in a movie with Kevin Bacon have a Bacon number of 1.

Problem 4. Write a `MovieGraph` class to solve the Kevin Bacon problem.

The file `movieData.txt` contains data from about 13,000 movies. A single movie is listed on each line, followed by a sequence of actors that starred in it. The movie title and actors' names are separated by a `/` character. The actors are listed by last name first, followed by their first name.

Implement the constructor of `MovieGraph`. Accept a filename to read data from, and store the collection of values (the actors) as a class attribute, avoiding duplicates. Create a networkX `Graph` and store it as another class attribute. Note that in the graph, actors only have movies as neighbors, and movies only have actors as neighbors.
(Hint: recall the `split()` method for strings.)

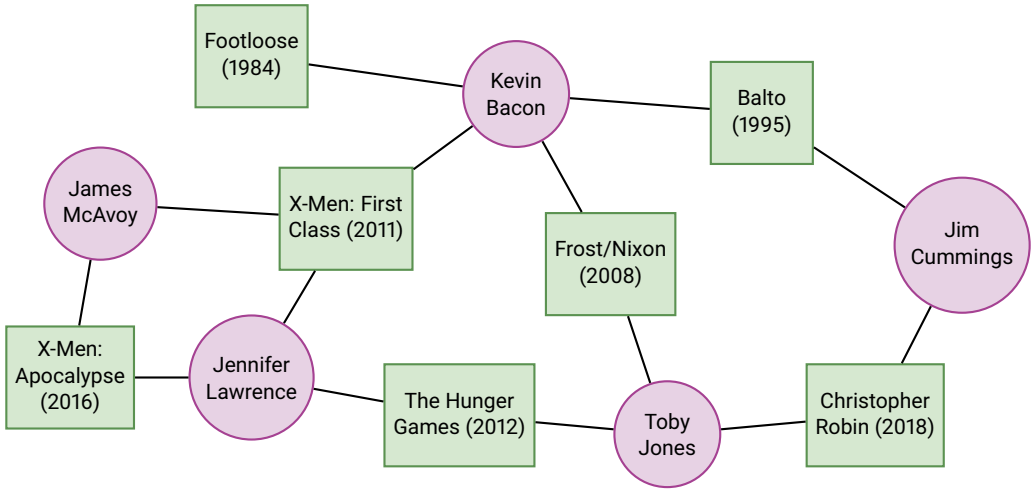


Figure 4.4: A **very** small subset of the data from `movieData.txt`. Each of the actors shown have a Bacon number of 1 because they have all been in a movie with Kevin Bacon. Every cast member of *The Hunger Games* has a Bacon number of at most 2 because of the paths through Jennifer Lawrence or Toby Jones.

Achtung!

Because of the size of the dataset, **do not** attempt to visualize the graph in Problem 4 with `nx.draw()`. The visualization tool in NetworkX is only effective on relatively small graphs. In fact, graph visualization in general remains a challenging and ongoing area of research.

NetworkX is equipped with a variety of methods to analyze graphs.

```
# Verify nx_graph has a path from 'C' to 'E'.
>>> nx.has_path(nx_graph, 'C', 'E')
True

# The shortest_path method is implemented with a
# bidirectional BFS (starting from both ends).
>>> nx.shortest_path(nx_graph, 'C', 'E')
['C', 'A', 'E']
```

Problem 5. Write a method for the `MovieGraph` class that accepts source and target values (actors' names). Set Kevin Bacon as the default target. Return a list with the shortest path from the source to the target, and the number of actors in the list. Note that this is different than the number of entries in the shortest path list, since movies do not contribute. If either input is not an actor's name, raise a `ValueError`.

```
>>> movie_graph = MovieGraph("movieData.txt")
```

```
>>> movie_graph.path_to_actor("Jackson, Samuel L.")
['Jackson, Samuel L.', 'Captain America: The First Avenger', 'Stark,
Peter', 'X-Men: First Class', 'Bacon, Kevin'], 2
```

Problem 6. Add a method to the `MovieGraph` class to calculate the average path length across all of the actors in the collection to the target (not including movies). Set Kevin Bacon as the default target. Use `plt.hist()` to plot the distribution of path lengths and return the average path length.
(Hint: The `path_to_actor()` method from Problem 5 is not the most efficient way of doing this. Also, consider how `bins` affects `plt.hist()`)

As an aside, the prolific Paul Erdős is considered the Kevin Bacon of the mathematical community. Someone with an "Erdős number" of 2 co-authored a paper with someone who co-authored a paper with Paul Erdős.

Additional Material

Depth-first Search

A *depth-first search* (DFS) takes the opposite approach of a breadth-first search. Instead of checking all neighbors of a single node before moving, on, it checks the first neighbor, then their first neighbor, then their first neighbor, and so on until reaching a leaf node. Then the algorithm back tracks to the previous node and checks its second neighbor. The DFS method was originally developed as a strategy for solving mazes. While a DFS is sometimes more useful than a BFS, a BFS is usually better[2] at finding the shortest path.

Consider adding a keyword argument to the `traverse()` method of the `Graph` class that specifies whether to use a BFS (the default) or a DFS. This can be done by changing a single line of the BFS code.

Improvements to the MovieGraph Class

Consider adding a `center_of_the_universe()` method in the `MovieGraph` class. This should plot the distribution of average numbers and return the 'center of the universe,' or the actor to whom all other actors are most closely connected. This can be found by returning the actor with the lowest average path length from all other actors.

More NetworkX

The following are interesting methods that may be of use in further graph analysis.

Function	Description
`adjacency_matrix()`	Returns the adjacency matrix as a SciPy sparse matrix.
`dijkstra_path()`	Returns the shortest path from a source to a target in a weighted graph.
`has_path()`	Returns `True` if the graph has a path from a source to a target.
`prim_mst()`	Returns a minimum spanning tree for a weighted graph.
`shortest_path()`	Returns the shortest path from a source to a target.

[2] `https://xkcd.com/761/`

5 Markov Chains

Lab Objective: *A Markov chain is a collection of states with specified probabilities for transitioning from one state to another. They are characterized by the fact that the future behavior of the system depends only on its current state. In this lab, we learn to construct, analyze, and interact with Markov chains, then apply a Markov chain to a natural language processing problem.*

State Space Models

Many systems can be described by a finite number of states. For example, a board game where players move around the board based on die rolls can be modeled by a Markov chain. Each space represents a state, and a player is said to be in a state if their piece is currently on the corresponding space. In this case, the probability of moving from one space to another only depends on the player's current location; where the player was on a previous turn does not affect their current turn.

Finite Markov chains have an associated *transition matrix* that stores the information about the transitions between the states in the chain. The (i, j)th entry of the matrix gives the probability of moving **from state j to state i**. Thus each of the columns of the transition matrix sum to 1.

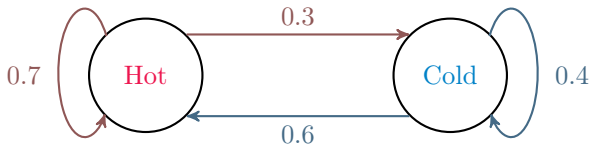
> **Note**
>
> A transition matrix where the columns sum to 1 is called *column stochastic* (or *left stochastic*). The rows of a *row stochastic* (or *right stochastic*) transition matrix each sum to 1 and the (i, j)th entry of the matrix is the probability of moving from state i to state j. Both representations are common, but in this lab we exclusively use column stochastic transition matrices for consistency.

Consider a very simple weather model where the probability of being hot or cold depends on the weather of the previous day. If the probability that tomorrow is hot given that today is hot is 0.7, and the probability that tomorrow is cold given that today is cold is 0.4, then by assigning hot to the 0th row and column, and cold to the 1^{st} row and column, this Markov chain has the following transition matrix.

$$\begin{array}{r} \\ \text{hot tomorrow} \\ \text{cold tomorrow} \end{array} \begin{array}{c} \begin{array}{cc} \text{hot today} & \text{cold today} \end{array} \\ \begin{bmatrix} 0.7 & 0.6 \\ 0.3 & 0.4 \end{bmatrix} \end{array}$$

The 0th column of the matrix says that if it is hot today, there is a 70% chance that tomorrow will be hot (0th row) and a 30% chance that tomorrow will be cold (1st row). The 1st column says if it is cold today, then there is a 60% chance of heat and a 40% chance of cold tomorrow.

Markov chains can be represented by a *state diagram*, a type of directed graph. The nodes in the graph are the states, and the edges indicate the state transition probabilities. The Markov chain described above has the following state diagram.



Problem 1. Transition matrices for Markov chains are efficiently stored as NumPy arrays. Write a function that accepts an integer n and returns the transition matrix for a random Markov chain with n states.
(Hint: use array broadcasting to avoid looping.)

Simulating State Transitions

A single draw from a *binomial distribution* with parameters n and p indicates the number of successes out of n independent experiments, each with probability p of success. The classic example is a series of coin flips, where p is the probability that the coin lands heads side up. NumPy's `random` module has an efficient tool, `binomial()`, for drawing from a binomial distribution.

```
>>> import numpy as np

# Draw from the binomial distribution with n = 1 and p = .5 (flip 1 coin).
>>> np.random.binomial(1, .5)
0                           # The coin flip resulted in tails.
```

Consider again the simple weather model and suppose that today is hot. The column that corresponds to "hot"in the transition matrix is $[0.7, 0.3]$. To determine whether tomorrow is hot or cold, draw from the binomial distribution with $n = 1$ and $p = 0.3$. If the draw is 1, which has 30% likelihood, then tomorrow is cold. If the draw is 0, which has 70% likelihood, then tomorrow is hot. The following function implements this idea.

```
def forecast():
    """Forecast tomorrow's weather given that today is hot."""
    transition = np.array([[0.7, 0.6], [0.3, 0.4]])
```

```
    # Sample from a binomial distribution to choose a new state.
    return np.binomial(1, transition[1, 0])
```

Problem 2. Modify `forecast()` so that it accepts an integer parameter `days` and runs a simulation of the weather for the number of days given. Return a list containing the day-by-day weather predictions (0 for hot, 1 for cold). Assume the first day is hot, but do not include the data from the first day in the list of predictions. The resulting list should therefore have `days` entries.

Larger Chains

The `forecast()` function makes one random draw from a binomial distribution to simulate a state change. Larger Markov chains require draws from a *multinomial distribution*, a multivariate generalization of the binomial distribution. A draw from a multinomial distribution parameters n and $(p_1,\ p_2,\ \ldots,\ p_k)$ indicates which of k outcomes occurs in n different experiments. In this case the classic example is a series of dice rolls, with 6 possible outcomes of equal probability.

```
>>> die_probabilities = np.array([1./6, 1./6, 1./6, 1./6, 1./6, 1./6])

# Draw from the multinomial distribution with n = 1 (roll a single die).
>>> np.random.multinomial(1, die_probabilities)
array([0, 0, 0, 1, 0, 0])     # The roll resulted in a 4.
```

Problem 3. Let the following matrix be the transition matrix for a Markov chain modeling weather with four states: hot, mild, cold, and freezing.

	hot	mild	cold	freezing
hot	0.5	0.3	0.1	0
mild	0.3	0.3	0.3	0.3
cold	0.2	0.3	0.4	0.5
freezing	0	0.1	0.2	0.2

Write a new function that accepts an integer parameter and runs the same kind of simulation as `forecast()`, but that uses this new four-state transition matrix. This time, assume that the first day is mild. Return a list containing the day-to-day results (0 for hot, 1 for mild, 2 for cold, and 3 for freezing).

General State Distributions

For a Markov chain with n states, the probability of being in each of the states can be encoded by a single $n \times 1$ vector $\mathbf{x}$, called a *state distribution vector*. The entries of $\mathbf{x}$ must be nonnegative and sum to 1. Then the ith entry x_i of $\mathbf{x}$ is the probability of being in state i. For example, the state distribution vector $\mathbf{x} = [0.8,\ 0.2]^\mathsf{T}$ corresponding to the 2-state weather model of Problem 2 indicates that there is a 80% chance that today is hot and a 20% chance that today is cold. On the other hand, the vector $\mathbf{x} = [0, 1]^\mathsf{T}$ implies that today is, with 100% certainty, cold.

If A is an $n \times n$ transition matrix for a Markov chain and $\mathbf{x}$ is a state distribution vector, then $A\mathbf{x}$ is also a state distribution vector. In fact, if $\mathbf{x}_k$ is the state distribution vector corresponding to a certain time k, then $\mathbf{x}_{k+1} = A\mathbf{x}_k$ contains the probabilities of being in each state after allowing the system to transition again. For the weather model, this means that if there is an 80% chance that it will be hot 5 days from now, written $\mathbf{x}_5 = [0.8,\ 0.2]^\mathsf{T}$, then since

$$\mathbf{x}_6 = A\mathbf{x}_5 = \begin{bmatrix} 0.7 & 0.6 \\ 0.3 & 0.4 \end{bmatrix} \begin{bmatrix} 0.8 \\ 0.2 \end{bmatrix} = \begin{bmatrix} 0.68 \\ 0.32 \end{bmatrix},$$

there is a 68% chance that 6 days from now will be a hot day.

Convergent Transition Matrices

Given an initial state distribution vector $\mathbf{x}_0$, defining $\mathbf{x}_{k+1} = A\mathbf{x}_k$ yields the following significant relation.

$$\mathbf{x}_k = A\mathbf{x}_{k-1} = A(A\mathbf{x}_{k-2}) = A(A(A\mathbf{x}_{x-3})) = \cdots = A^k\mathbf{x}_0$$

This indicates that the (i, j)th entry of A^k is the probability of transition from state j to state i in k steps. For the transition matrix of the 2-state weather model, something curious happens to A^k for even small values of k.

$$A = \begin{bmatrix} 0.7 & 0.6 \\ 0.3 & 0.4 \end{bmatrix} \quad A^2 = \begin{bmatrix} 0.67 & 0.66 \\ 0.33 & 0.34 \end{bmatrix} \quad A^3 = \begin{bmatrix} 0.667 & 0.666 \\ 0.333 & 0.334 \end{bmatrix}$$

As $k \to \infty$, the entries of A^k converge, written as follows.

$$\lim_{k\to\infty} A^k = \begin{bmatrix} 2/3 & 2/3 \\ 1/3 & 1/3 \end{bmatrix}. \tag{5.1}$$

In addition, for any initial state distribution vector $\mathbf{x}_0 = [a,\ b]^\mathsf{T}$, $a + b = 1$,

$$\lim_{k\to\infty} \mathbf{x}_k = \lim_{k\to\infty} A^k\mathbf{x}_0 = \begin{bmatrix} 2/3 & 2/3 \\ 1/3 & 1/3 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 2(a+b)/3 \\ (a+b)/3 \end{bmatrix} = \begin{bmatrix} 2/3 \\ 1/3 \end{bmatrix}.$$

Thus as $k \to \infty$, $\mathbf{x}_k \to \mathbf{x} = [2/3,\ 1/3]^\mathsf{T}$, regardless of the initial state distribution $\mathbf{x}_0$. So according to this model, no matter the weather today, the probability that it is hot a week from now is approximately 66.67%. In fact, approximately 2 out of 3 days in the year should be hot.

Steady State Distributions

The state distribution $\mathbf{x} = [2/3,\ 1/3]^\mathsf{T}$ has another important property.

$$A\mathbf{x} = \begin{bmatrix} 7/10 & 3/5 \\ 3/10 & 2/5 \end{bmatrix} \begin{bmatrix} 2/3 \\ 1/3 \end{bmatrix} = \begin{bmatrix} 14/30 + 3/15 \\ 6/30 + 2/15 \end{bmatrix} = \begin{bmatrix} 2/3 \\ 1/3 \end{bmatrix} = \mathbf{x}.$$

Any $\mathbf{x}$ satisfying $A\mathbf{x} = \mathbf{x}$ is called a *steady state distribution* or a *stable fixed point* of A. In other words, a steady state distribution is an eigenvector of A with corresponding eigenvalue $\lambda = 1$.

Every Markov chain has at least one steady state distribution. If some power A^k of A has all positive (nonzero) entries, then the steady state distribution is unique.[1] In this case, $\lim_{k\to\infty} A^k$ is the matrix whose columns are all equal to the unique steady state distribution, as in (5.1). Under these circumstances, the steady state distribution $\mathbf{x}$ can be found by iteratively calculating $\mathbf{x}_{k+1} = A\mathbf{x}_k$, as long as the initial vector $\mathbf{x}_0$ is a state distribution vector.

Achtung!

Though every Markov chain has at least one steady state distribution, the procedure described above fails if A^k fails to converge. Consider the following example.

$$A = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \quad A^k = \begin{cases} A & \text{if } k \text{ is odd} \\ I & \text{if } k \text{ is even} \end{cases}$$

In this case as $k \to \infty$, A^k oscillates between two different matrices.

Furthermore, the steady state distribution is not always unique; the transition matrix defined above, for example, has infinitely many.

Problem 4. Write a function that accepts an $n \times n$ transition matrix A, a convergence tolerance ε, and a maximum number of iterations N. Generate a random state distribution vector $\mathbf{x}_0$ and calculate $\mathbf{x}_{k+1} = A\mathbf{x}_k$ until $\|\mathbf{x}_{k-1} - \mathbf{x}_k\| < \varepsilon$. If k exceeds N, raise a `ValueError` to indicate that A^k does not converge. Return the approximate steady state distribution $\mathbf{x}$ of A.

To test your function, use Problem 1 to generate a random transition matrix A. Verify that $A\mathbf{x} = \mathbf{x}$ and that the columns of A^k approach $\mathbf{x}$ as $k \to \infty$. To compute A^k, use NumPy's (very efficient) algorithm for computing matrix powers.

```
>>> A = np.array([[.7, .6],[.3, .4]])
>>> np.linalg.matrix_power(A, 10)       # Compute A^10.
array([[ 0.66666667,  0.66666667],
       [ 0.33333333,  0.33333333]])
```

Finally, use your function to validate the results of Problems 2 and 3:

1. Calculate the steady state distributions corresponding to the transition matrices for each simulation.
2. Run each simulation for a large number of days and verify that the results match the steady state distribution (for example, check that approximately 2/3 of the days are hot for the smaller weather model).

[1] This is a consequence of the *Perron-Frobenius theorem*, which is presented in conjunction with spectral calculus in Volume I.

> **Note**
>
> Problem 4 is a special case of the *power method*, an algorithm for calculating an eigenvector of a matrix corresponding to the eigenvalue of largest magnitude. The general version of the power method, together with a discussion of its convergence conditions, is discussed in another lab.

Using Markov Chains to Simulate English

One of the original applications of Markov chains was to study natural languages. In the early 20th century, Markov used his chains to model how Russian switched from vowels to consonants. By mid-century, they had been used as an attempt to model English. It turns out that Markov chains are, by themselves, insufficient to model very good English. However, they can approach a fairly good model of bad English, with sometimes amusing results.

By nature, a Markov chain is only concerned with its current state. Thus a Markov chain simulating transitions between English words is completely unaware of context or even of previous words in a sentence. For example, a Markov chain's current state may be the word "continuous." Then the chain would say that the next word in the sentence is more likely to be "function" rather than "raccoon." However, without the context of the rest of the sentence, even two likely words stringed together may result in gibberish.

We restrict ourselves to a subproblem of modeling the English of a specific file. The transition probabilities of the resulting Markov chain reflect the sort of English that the source authors speak. Thus the Markov chain built from *The Complete Works of William Shakespeare* differs greatly from, say, the Markov chain built from a collection of academic journals. We call the source collection of works in the next problems the *training set*.

Making the Chain

With the weather models of the previous sections, we chose a fixed number of days to simulate. However, English sentences are of varying length, so we do not know beforehand how many words to choose (how many state transitions to make) before ending the sentence. To capture this feature, we include two extra states in our Markov model: a *start state* (\$tart) marking the beginning of a sentence, and a *stop state* (\$top) marking the end. Thus a training set with N unique words has an $(N+2) \times (N+2)$ transition matrix.

The start state only transitions to words that appear at the beginning of a sentence in the training set, and only words that appear at the end a sentence in the training set transition to the stop state. The stop state is called an *absorbing state* because once we reach it, we cannot transition back to another state.

After determining the states in the Markov chain, we need to determine the transition probabilities between the states and build the corresponding transition matrix. Consider the following small training set from Dr. Seuss as an example.

```
I am Sam Sam I am.
Do you like green eggs and ham?
I do not like them, Sam I am.
I do not like green eggs and ham.
```

If we include punctuation (so "ham?" and "ham." are counted as distinct words) and do not alter the capitalization (so "Do" and "do" are also different), there are 15 unique words in this training set:

I am Sam am. Do you like green
eggs and ham? do not them, ham.

With start and stop states, the transition matrix should be 17×17. Each state must be assigned a row and column index in the transition matrix. As easy way to do this is to assign the states an index based on the order that they appear in the training set. Thus our states and the corresponding indices will be as follows:

\$start	I	am	Sam	...	ham.	\$top
0	1	2	3	...	15	16

The start state should transition to the words "I" and "Do", and the words "am.", "ham?", and "ham." should each transition to the stop state. We first count the number of times that each state transitions to another state:

	\$start	I	am	Sam		ham.	\$top
\$start	0	0	0	0	...	0	0
I	3	0	0	2	...	0	0
am	0	1	0	0	...	0	0
Sam	0	0	1	1	...	0	0
	⋮	⋮	⋮	⋮	⋱	⋮	⋮
ham.	0	0	0	0	...	0	0
\$top	0	0	0	0	...	1	1

Now divide each column by its sum so that each column sums to 1.

	\$start	I	am	Sam		ham.	\$top
\$start	0	0	0	0	...	0	0
I	3/4	0	0	2/3	...	0	0
am	0	1/5	0	0	...	0	0
Sam	0	0	1	1/3	...	0	0
	⋮	⋮	⋮	⋮	⋱	⋮	⋮
ham.	0	0	0	0	...	0	0
\$top	0	0	0	0	...	1	1

The 3/4 indicates that 3 out of 4 times, the sentences in the training set start with the word "I". Similarly, the 2/3 and 1/3 tell us that "Sam" is followed by "I" twice and by "Sam" once in the training set. Note that "am" (without a period) always transitions to "Sam" and that "ham." (with a period) always transitions the stop state. Finally, to avoid a column of zeros, we place a 1 in the bottom right hand corner of the matrix (so the stop state always transitions to itself).

The entire procedure of creating the transition matrix for the Markov chain with words from a file as states is summarized below.

Algorithm 5.1 Convert a training set of sentences into a Markov chain.

```
procedure MakeTransitionMatrix
    Count the number of unique words in the training set.
    Initialize a square array of zeros of the appropriate size to be the transition
        matrix (remember to account for the start and stop states).
    Initialize a list of states, beginning with "$tart".
    for each sentence in the training set do
        Split the sentence into a list of words.
        Add each new word in the sentence to the list of states.
        Convert the list of words into a list of indices indicating which row and
            column of the transition matrix each word corresponds to.
        Add 1 to the entry of the transition matrix corresponding to
            transitioning from the start state to the first word of the sentence.
        for each consecutive pair (x, y) of words in the list of words do
            Add 1 to the entry of the transition matrix corresponding to
                transitioning from state x to state y.
        Add 1 to the entry of the transition matrix corresponding to
            transitioning from the last word of the sentence to the stop state.
    Make sure the stop state transitions to itself.
    Normalize each column by dividing by the column sums.
```

Problem 5. Write a class called `SentenceGenerator`. The constructor should accept a filename (the training set). Read the file and build a transition matrix from its contents as described in Algorithm 5.1.

You may assume that the file has one complete sentence written on each line, and your implementation may be either column- or row-stochastic.

Problem 6. Add a method to the `SentenceGenerator` class called `babble()`. Begin at the start state and use the strategy from Problem 3 to repeatedly transition through the object's Markov chain. Keep track of the path through the chain and the corresponding sequence of words. When the stop state is reached, stop transitioning to terminate the simulation. Return the resulting sentence as a single string.

For example, your `SentenceGenerator` class should be able to create random sentences that sound somewhat like Yoda speaking.

```
>>> yoda = SentenceGenerator("yoda.txt")
>>> for _ in range(3):
...     print(yoda.babble())
...
Impossible to my size, do not!
For eight hundred years old to enter the dark side of Congress there is.
But beware of the Wookiees, I have.
```

Additional Material

Large Training Sets

The approach in Problems 5 and 6 begins to fail as the training set grows larger. For example, a single Shakespearean play may not be large enough to cause memory problems, but *The Complete Works of William Shakespeare* certainly will.

To accommodate larger data sets, consider use a sparse matrix from `scipy.sparse` for the transition matrix instead of a regular NumPy array. Specifically, construct the transition matrix as a `lil_matrix` (which is easy to build incrementally), then convert it to the `csc_matrix` format (which supports fast column operations). Ensure that the process still works on small training sets, then proceed to larger training sets. How are the resulting sentences different if a very large training set is used instead of a small training set?

Variations on the English Model

Choosing a different state space for the English Markov model produces different results. Consider modifying your `SentenceGenerator` class so that it can determine the state space in a few different ways. The following ideas are just a few possibilities.

- Let each punctuation mark have its own state. In the example training set, instead of having two states for the words "ham?" and "ham.", there would be three states: "ham", "?", and ".", with "ham" transitioning to both punctuation states.
- Model paragraphs instead of sentences. Add a $tartParagraph state that always transitions to $tartSentence and a $topParagraph state that is sometimes transitioned to from $topSentence.
- Let the states be individual letters instead of individual words. Be sure to include a state for the spaces between words. We will explore this particular state space choice more in Volume III together with hidden Markov models.
- Construct the state space so that the next state depends on both the current and previous states. This kind of Markov chain is called a *Markov chain of order 2*. This way, every set of three consecutive words in a randomly generated sentence should be part of the training set, as opposed to only every consecutive pair of words coming from the set.
- Instead of generating random sentences from a single source, simulate a random conversation between n people. Construct a Markov chain M_i, for each person, $i = 1, \ldots, n$, then create a Markov chain C describing the conversation transitions from person to person; in other words, the states of C are the M_i. To create the conversation, generate a random sentence from the first person using M_1. Then use C to determine the next speaker, generate a random sentence using their Markov chain, and so on.

Natural Language Processing Tools

The Markov model of Problems 5 and 6 is a *natural language processing* application. Python's `nltk` module (natural language toolkit) has many tools for parsing and analyzing text for these kinds of problems. For example, `nltk.sent_tokenize()` reads a single string and splits it up into sentences.

```
>>> from nltk import sent_tokenize
>>> with open("yoda.txt", 'r') as yoda:
```

```
...     sentences = sent_tokenize(yoda.read())
...
>>> print(sentences)
['Away with your weapon!',
 'I mean you no harm.',
 'I am wondering - why are you here?',
 ...
```

The `nltk` module is **not** part of the Python standard library. For instructions on downloading, installing, and using `nltk`, visit `http://www.nltk.org/`.

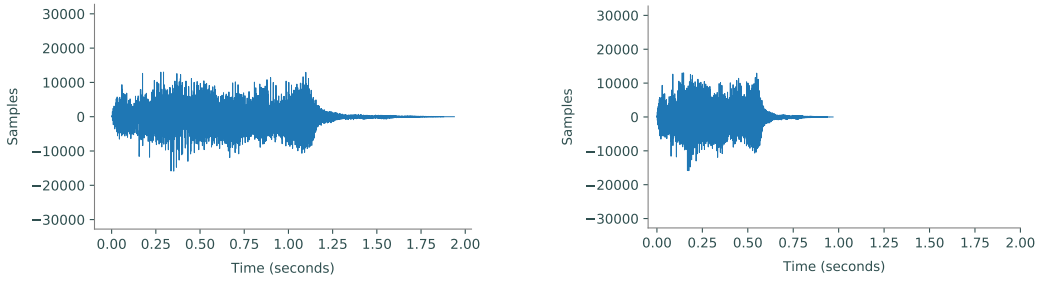
6 The Discrete Fourier Transform

Lab Objective: *The analysis of periodic functions has many applications in pure and applied mathematics, especially in settings dealing with sound waves. The Fourier transform provides a way to analyze such periodic functions. In this lab, we introduce how to work with digital audio signals in Python, implement the discrete Fourier transform, and use the Fourier transform to detect the frequencies present in a given sound wave. We strongly recommend completing the exercises in a Jupyter Notebook.*

Digital Audio Signals

Sound waves have two important characteristics: *frequency*, which determines the pitch of the sound, and *intensity* or *amplitude*, which determines the volume of the sound. Computers use *digital audio signals* to approximate sound waves. These signals have two key components: *sample rate*, which relates to the frequency of sound waves, and *samples*, which measure the amplitude of sound waves at a specific instant in time.

To see why the sample rate is necessary, consider an array with samples from a sound wave. The sound wave can be arbitrarily stretched or compressed to make a variety of sounds. If compressed, the sound becomes shorter and has a higher pitch. Similarly, the same set of samples with a lower sample rate becomes stretched and has a lower pitch.



(a) The plot of `tada.wav`.

(b) Compressed plot of `tada.wav`.

Figure 6.1: Plots of the same set of samples from a sound wave with varying sample rates. The plot on the left is the plot of the samples with the original sample rate. The sample rate of the plot on the right has been doubled, resulting in a compression of the actual sound when played back.

Given the rate at which a set of samples is taken, the wave can be reconstructed exactly as it was recorded. In most applications, this sample rate is measured in *Hertz* (Hz), the number of samples taken per second. The standard rate for high quality audio is 44100 equally spaced samples per second, or 44.1 kHz.

Wave File Format

One of the most common audio file formats across operating systems is the *wave* format, also called `wav` after its file extension. SciPy has built-in tools to read and create `wav` files. To read a `wav` file, use `scipy.io.wavfile.read()`. This function returns the signal's sample rate and its samples.

```
# Read from the sound file.
>>> from scipy.io import wavfile
>>> rate, samples = wavfile.read("tada.wav")
```

Sound waves can be visualized by plotting time against the amplitude of the sound, as in Figure 6.1. The amplitude of the sound at a given time is just the value of the sample at that time. Since the sample rate is given in samples per second, the length of the sound wave in seconds is found by dividing the number of samples by the sample rate:

$$\frac{\text{num samples}}{\text{sample rate}} = \frac{\text{num samples}}{\text{num samples/second}} = \text{second}. \tag{6.1}$$

Problem 1. Write a `SoundWave` class for storing digital audio signals.

1. The constructor should accept an integer sample rate and an array of samples. Store each input as an attribute.
2. Write a method that plots the stored sound wave. Use (6.1) to correctly label the x-axis in terms of seconds, and set the y-axis limits to $[-32768, 32767]$ (the reason for this is discussed in the next section).

Use SciPy to read `tada.wav`, then instantiate a corresponding `SoundWave` object and display its plot. Compare your plot to Figure 6.1a.

Scaling

To write to a `wav` file, use `scipy.io.wavfile.write()`. This function accepts the name of the file to write to, the sample rate, and the array of samples as parameters.

```
>>> import numpy as np

# Write a 2-second random sound wave sampled at a rate of 44100 Hz.
>>> samples = np.random.randint(-32768, 32767, 88200, dtype=np.int16)
>>> wavfile.write("white_noise.wav", 44100, samples)
```

For `scipy.io.wavfile.write()` to correctly create a `wav` file, the samples must be one of four numerical datatypes: 32-bit floating point (`np.float32`), 32-bit integers (`np.int32`), 16-bit integers (`np.int16`), or 8-bit unsigned integers (`np.uint8`). If samples of a different type are passed into the function, it may still write a file, but the sound will likely be distorted in some way. In this lab, we only work with 16-bit integer samples, unless otherwise specified.

A 16-bit integer is an integer between -32768 and 32767, inclusive. If the elements of an array of samples are not all within this range, the samples must be scaled before writing to a file: multiply the samples by 32767 (the largest number in the 16-bit range) and divide by the largest sample magnitude. This ensures the most accurate representation of the sound and sets it to full volume.

$$\texttt{np.int16}\left(\frac{\text{original samples} \times 32767}{\max(|\text{original samples}|)}\right) = \text{scaled samples} \tag{6.2}$$

Samples may sometimes contain complex values, especially after some processing. Make sure to scale and export only the real part (use the `real` attribute of the array).

Note

The IPython API includes a tool for embedding sounds in a Jupyter Notebook. The function `IPython.display.Audio()` accepts either a file name or a sample rate (`rate`) and an array of samples (`data`); calling the function generates an interactive music player in the Notebook.

```
In [1]: import IPython
        from scipy.io import wavfile

        # Embed tada.wav straight from the file.
        IPython.display.Audio(filename="tada.wav")

        # Alternatively, embed tada.wav using the raw data.
        # rate, samples = wavfile.read("tada.wav")
        # IPython.display.Audio(rate=rate, data=samples)
```

Out[1]: 

Achtung!

Turn the volume down before listening to any of the sounds in this lab.

Problem 2. Add a method to the `SoundWave` class that accepts a file name and a boolean `force`. Write to the specified file using the stored sample rate and the array of samples. If the array of samples does not have `np.int16` as its data type, or if `force` is `True`, scale the samples as in (6.2) before writing the file.

Use your method to create two new files that contains the same sound as `tada.wav`: one without scaling, and one with scaling (use `force=True`). Use `IPython.display.Audio()` to display `tada.wav` and the new files. All three files should sound identical, except the scaled file should be louder than the other two.

Generating Sounds

Sinusoidal waves correspond to pure frequencies, like a single note on the piano. Recall that the function $\sin(x)$ has a period of 2π. To create a specific tone for 1 second, we sample from the sinusoid with period 1,

$$f(x) = \sin(2\pi x k),$$

where k is the desired frequency. According to (6.1), generating a sound that lasts for s seconds at a sample rate r requires rs equally spaced samples in the interval $[0, s]$.

Problem 3. Write a function that accepts floats k and s. Create a `SoundWave` instance containing a tone with frequency k that lasts for s seconds. Use a sample rate of $r = 44100$.

The following table shows some frequencies that correspond to common notes. Octaves of these notes are obtained by doubling or halving these frequencies.

Note	Frequency (Hz)
A	440
B	493.88
C	523.25
D	587.33
E	659.25
F	698.46
G	783.99
A	880

Use your function to generate an A tone lasting for 2 seconds.

Problem 4. Digital audio signals can be combined by addition or concatenation. Adding samples overlays tones so they play simultaneously; concatenated samples plays one set of samples after the other with no overlap.

1. Implement the `__add__()` magic method for the `SoundWave` class so that if `A` and `B` are `SoundWave` instances, `A + B` creates a new `SoundWave` object whose samples are the element-wise sum of the samples from `A` and `B`. Raise a `ValueError` if the sample arrays from `A` and `B` are not the same length.

   Use your method to generate a three-second A minor chord (A, C, and E together).

2. Implement the `__rshift__()` magic method[a] for the `SoundWave` class so that if `A` and `B` are `SoundWave` instances, `A >> B` creates a new `SoundWave` object whose samples are the concatenation of the samples from `A`, then the samples from `B`. Raise a `ValueError` if the sample rates from the two objects are not equal.
   (Hint: `np.concatenate()`, `np.hstack()`, and/or `np.append()` may be useful.)

   Use your method to generate the arpeggio A → C → E, where each pitch lasts one second.

Consider using these two methods to produce elementary versions of some simple tunes.

[a]The `>>` operator is a *bitwise shift operator* and is usually reserved for operating on binary numbers.

The Discrete Fourier Transform

Under the right conditions, a continuous periodic function f with period T (meaning $f(t+T) = f(t)$ for all t) may be represented as a weighted sum of exponentials, i.e.,

$$f(x) = \sum_{k=-\infty}^{\infty} c_k e^{2\pi i k x/T}.$$

The constants c_k are called the *Fourier coefficients*.

The *discrete Fourier transform* (DFT) transforms a discrete array of samples to an array of corresponding Fourier coefficients. For an array of n samples $\mathbf{f} = \begin{bmatrix} f_0 & f_1 & \cdots & f_{n-1} \end{bmatrix}^\mathsf{T}$, the kth coefficient of the DFT of $\mathbf{f}$ is calculated as

$$c_k = \frac{1}{n} \sum_{\ell=0}^{n-1} \mathbf{f}_\ell e^{-2\pi i k \ell/n}, \tag{6.3}$$

where $i = \sqrt{-1}$ is the imaginary unit (`1j` in Python). Repeating this process for each k yields the DFT array of coefficients $\mathbf{c} = \begin{bmatrix} c_0 & c_1 & \cdots & c_{n-1} \end{bmatrix}^\mathsf{T}$. We write $F_n\mathbf{f} = \mathbf{c}$ to indicate that the DFT depends on the number of samples n.

Achtung!

There are several different conventions for defining the DFT. For example, instead of (6.3), `scipy.fftpack.fft()` uses the formula

$$\hat{c}_k = \sum_{\ell=0}^{n-1} \mathbf{f}_\ell e^{-2\pi i k \ell/n},$$

which is (6.3) without the factor of $1/n$ in front of the sum. Denoting this version of the DFT as $\hat{F}_n\mathbf{f} = \hat{\mathbf{c}}$, we have $nF_n = \hat{F}_n$ and $n\mathbf{c} = \hat{\mathbf{c}}$. The conversion is easy, but it is very important to be aware of which convention a particular implementation of the DFT uses.

Problem 5. Write a function that accepts an array $\mathbf{f}$ of samples. Use (6.3) to calculate the DFT of $\mathbf{f}$ (including the $1/n$ scaling in front of the sum).

Test your implementation on small, random arrays against `scipy.fftpack.fft()`, scaling your output $\mathbf{c}$ to match SciPy's output $\hat{\mathbf{c}}$. Once your function is working, try to optimize it so that each coefficient c_k is calculated in just one line of code, or—better yet—so that the entire array of coefficients is calculated in the one line.
(Hint: use array broadcasting to represent F_n as an $n \times n$ matrix.)

The Fast Fourier Transform

Calculating the DFT of a vector of n samples using only (6.3) is at least $O(n^2)$, which is incredibly slow for realistic sound waves. Fortunately, due to its inherent symmetry, the DFT can be implemented as a recursive algorithm by separating the computation into even and odd indices. This method of calculating the DFT is called the *fast Fourier transform* (FFT) and runs in $O(n \log n)$ time.

Algorithm 6.1 The fast Fourier transform for arrays with 2^a entries for some $a \in \mathbb{N}$.

```
1:  procedure SIMPLE_FFT(f, N)
2:      procedure SPLIT(g)
3:          n ← size(g)
4:          if n ≤ N then
5:              return nF_n g                ▷ Use the function from Problem 5 for small enough g.
6:          else
7:              even ← SPLIT(g_{::2})        ▷ Get the DFT of every other entry of g, starting from 0.
8:              odd ← SPLIT(g_{1::2})        ▷ Get the DFT of every other entry of g, starting from 1.
9:              z ← zeros(n)
10:             for k = 0, 1, ..., n − 1 do      ▷ Calculate the exponential parts of the sum.
11:                 z_k ← e^{−2πik/n}
12:             m ← n // 2                   ▷ Get the middle index for z (// is integer division).
13:             return [even + z_{:m} ⊙ odd, even + z_{m:} ⊙ odd]   ▷ Concatenate two arrays of length m.
14:     return SPLIT(f) / size(f)
```

Note that the base case in lines 4–5 of Algorithm 6.1 results from setting $n = 1$ in (6.3), yielding the single coefficient $c_0 = g_0$. The $\odot$ in line 13 indicates the component-wise product

$$\mathbf{f} \odot \mathbf{g} = \begin{bmatrix} f_0 g_0 & f_1 g_1 & \cdots & f_{n-1} g_{n-1} \end{bmatrix}^T,$$

which is also called the *Hadamard product* of $\mathbf{f}$ and $\mathbf{g}$.

This algorithm performs significantly better than the naïve implementation for (6.3), but the simple version described in Algorithm 6.1 only works if the number of original samples is exactly a power of 2. SciPy's FFT routines avoid this problem by padding the sample array with zeros until the size is a power of 2, then executing the remainder of the algorithm from there. Of course, SciPy also uses various other tricks to further speed up the computation.

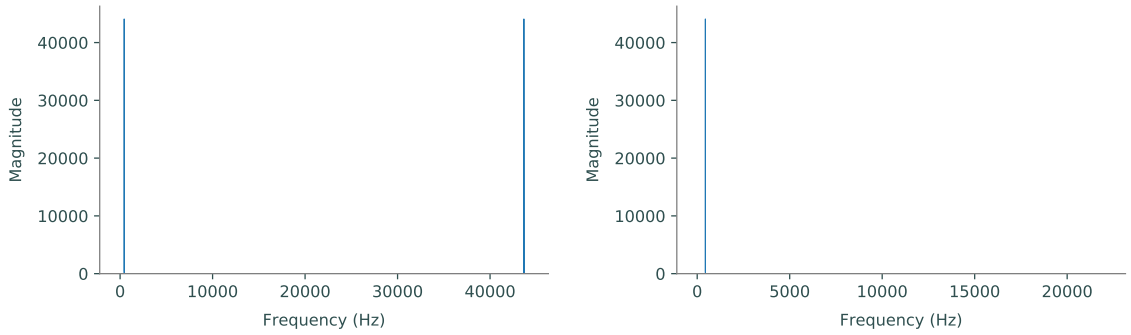
Problem 6. Write a function that accepts an array $\mathbf{f}$ of n samples where n is a power of 2. Use Algorithm 6.1 to calculate the DFT of $\mathbf{f}$.
(Hint: eliminate the loop in lines 10–11 with `np.arange()` and array broadcasting, and use `np.concatenate()` or `np.hstack()` for the concatenation in line 13.)

Test your implementation on random arrays against `scipy.fftpack.fft()`, scaling your output $\mathbf{c}$ to match SciPy's output $\hat{\mathbf{c}}$. Time your function from Problem 5, this function, and SciPy's function on an array with 8192 entries.
(Hint: Use `%time` in Jupyter Notebook to time a single line of code.)

Visualizing the DFT

The graph of the DFT of a sound wave is useful in a variety of applications. While the graph of the sound in the time domain gives information about the amplitude (volume) of a sound wave at a given time, the graph of the DFT shows which frequencies (pitches) are present in the sound wave. Plotting a sound's DFT is referred to as plotting in the *frequency domain*.

As a simple example, the single-tone notes generated by the function in Problem 3 contain only one frequency. For instance, Figure 6.2a graphs the DFT of an A tone. However, this plot shows two frequency spikes, despite there being only one frequency present in the actual sound. This is due to symmetries inherent to the DFT; for frequency detection, the second half of the plot can be ignored as in Figure 6.2b.



(a) The DFT of an A tone with symmetries.

(b) The DFT of an A tone without symmetries.

Figure 6.2: Plots of the DFT with and without symmetries. Notice that the x-axis of the symmetrical plot on the left goes up to 44100 (the sample rate of the sound wave) while the x-axis of the non-symmetric plot on the right goes up to only 22050 (half the sample rate). Also notice that the spikes occur at 440 Hz and 43660 Hz (which is $44100 - 440$).

The DFT of a more complicated sound wave has many frequencies, each of which corresponds to a different tone present in the sound wave. The magnitude of the coefficients indicates a frequency's influence in the sound wave; a greater magnitude means that the frequency is more influential.

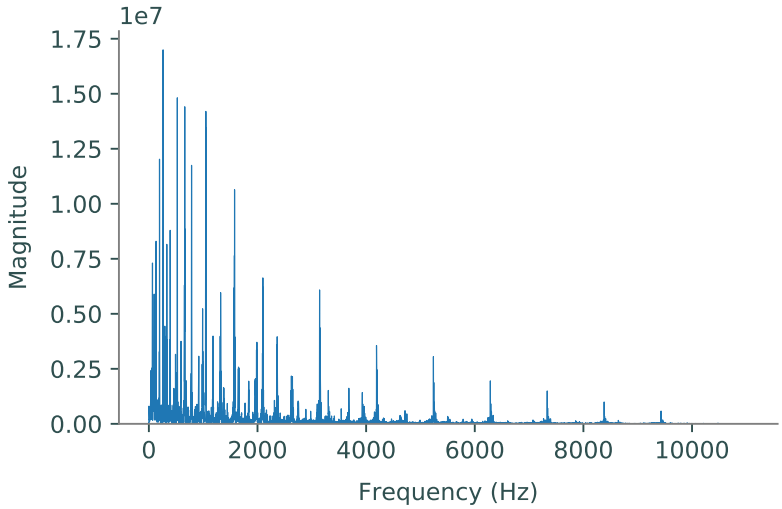


Figure 6.3: The discrete Fourier transform of `tada.wav`. Each spike in the graph corresponds to a frequency present in the sound wave. Since the sample rate of `tada.wav` is 22050 Hz, the plot of its DFT without symmetries only goes up to 11025 Hz, half of its sample rate.

Plotting Frequencies

Since the DFT represents the frequency domain, the x-axis of a plot of the DFT should be in terms of Hertz, which has units $1/s$. In other words, to plot the magnitudes of the Fourier coefficients against the correct frequencies, we must convert the frequency index k of each c_k to Hertz. This can be done by multiplying the index by the sample rate and dividing by the number of samples:

$$\frac{k}{\text{num samples}} \times \frac{\text{num samples}}{\text{second}} = \frac{k}{\text{second}}. \tag{6.4}$$

In other words, $kr/n = v$, where r is the sample rate, n is the number of samples, and v is the resulting frequency.

Problem 7. Modify your `SoundWave` plotting method from Problem 1 so that it accepts a boolean defaulting to `False`. If the boolean is `True`, take the DFT of the stored samples and plot—in a new subplot—the frequencies present on the x-axis and the magnitudes of those frequencies (use `np.abs()` to compute the magnitude) on the y-axis. Only display the first half of the plot (as in Figures 6.2b and 6.2b), and use (6.4) to adjust the x-axis so that it correctly shows the frequencies in Hertz. Use SciPy to calculate the DFT.

Display the DFT plots of the A tone and the A minor chord from Problem 4. Compare your results to Figures 6.2a and 6.4.

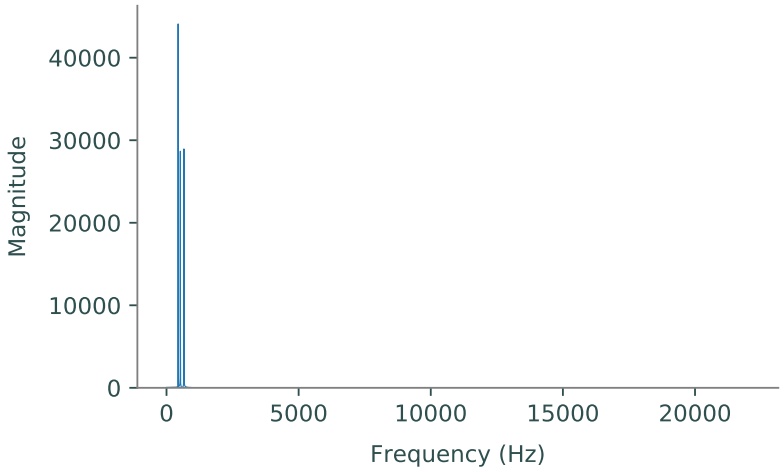


Figure 6.4: The DFT of the A minor chord.

If the frequencies present in a sound are already known before plotting its DFT, the plot may be interesting, but little new information is actually revealed. Thus, the main applications of the DFT involve sounds in which the frequencies present are unknown. One application in particular is sound filtering, which will be explored in greater detail in a subsequent lab. The first step in filtering a sound is determining the frequencies present in that sound by taking its DFT.

Consider the DFT of the A minor chord in Figure 6.4. This graph shows that there are three main frequencies present in the sound. To determine what those frequencies are, find which indices of the array of DFT coefficients have the three largest values, then scale these indices the same way as in (6.4) to translate the indices to frequencies in Hertz.

Problem 8. The file `mystery_chord.wav` contains an unknown chord. Use the DFT and the frequency table in Problem 3 to determine the individual notes that are present in the sound. (Hint: `np.argsort()` may be useful.)

7 Convolution and Filtering

Lab Objective: *The Fourier transform reveals information in the frequency domain about signals and images that might not be apparent in the usual time (sound) or spatial (image) domain. In this lab, we use the discrete Fourier transform to efficiently convolve sound signals and filter out some types of unwanted noise from both sounds and images. This lab is a continuation of the Discrete Fourier Transform lab and should be completed in the same Jupyter Notebook.*

Convolution

Mixing two sounds signals—a common procedure in signal processing and analysis—is usually done through a *discrete convolution*. Given two periodic sound sample vectors $\mathbf{f}$ and $\mathbf{g}$ of length n, the discrete convolution of $\mathbf{f}$ and $\mathbf{g}$ is a vector of length n where the kth component is given by

$$(\mathbf{f} * \mathbf{g})_k = \sum_{j=0}^{n-1} f_{k-j} g_j, \qquad k = 0, 1, 2, \ldots, n-1. \tag{7.1}$$

Since audio needs to be sampled frequently to create smooth playback, a recording of a song can contain tens of millions of samples; even a one-minute signal has $2,646,000$ samples if it is recorded at the standard rate of $44,100$ samples per second ($44,100$ Hz). The naïve method of using the sum in (7.1) n times is $O(n^2)$, which is often too computationally expensive for convolutions of this size.

Fortunately, the discrete Fourier transform (DFT) can be used compute convolutions efficiently. The *finite convolution theorem* states that the Fourier transform of a convolution is the element-wise product of Fourier transforms:

$$F_n(\mathbf{f} * \mathbf{g}) = n(F_n\mathbf{f}) \odot (F_n\mathbf{g}). \tag{7.2}$$

In other words, convolution in the time domain is equivalent to component-wise multiplication in the frequency domain. Here F_n is the DFT on $\mathbb{R}^n$, $*$ is discrete convolution, and $\odot$ is component-wise multiplication. Thus, the convolution of $\mathbf{f}$ and $\mathbf{g}$ can be computed by

$$\mathbf{f} * \mathbf{g} = nF_n^{-1}((F_n\mathbf{f}) \odot (F_n\mathbf{g})), \tag{7.3}$$

where F_n^{-1} is the *inverse discrete Fourier transform* (IDFT). The fast Fourier transform (FFT) puts the cost of (7.3) at $O(n \log n)$, a huge improvement over the naïve method.

Note

Although individual samples are real numbers, results of the IDFT may have small complex components due to rounding errors. These complex components can be safely discarded by taking only the real part of the output of the IDFT.

```
>>> import numpy
>>> from scipy.fftpack import fft, ifft # Fast DFT and IDFT functions.

>>> f = np.random.random(2048)
>>> f_dft_idft = ifft(fft(f)).real      # Keep only the real part.
>>> np.allclose(f, f_dft_idft)          # Check that IDFT(DFT(f)) = f.
True
```

Achtung!

SciPy uses a different convention to define the DFT and IDFT than this and the previous lab, resulting in a slightly different form of the convolution theorem. Writing SciPy's DFT as $\hat{F}_n$ and its IDFT as $\hat{F}_n^{-1}$, we have $\hat{F}_n = nF_n$, so (7.3) becomes

$$\mathbf{f} * \mathbf{g} = \hat{F}_n^{-1}((\hat{F}_n\mathbf{f}) \odot (\hat{F}_n\mathbf{g})), \tag{7.4}$$

without a factor of n. Use (7.4), not (7.3), when using `fft()` and `ifft()` from `scipy.fftpack`.

Circular Convolution

The definition (7.1) and the identity (7.3) require $\mathbf{f}$ and $\mathbf{g}$ to be periodic vectors. However, the convolution $\mathbf{f} * \mathbf{g}$ can always be computed by simply treating each vector as periodic. The convolution of two raw sample vectors is therefore called the *periodic* or *circular convolution*. This strategy mixes sounds from the end of each signal with sounds at the beginning of each signal.

Problem 1.

Implement the `__mul__()` magic method for the `SoundWave` class so that if `A` and `B` are `SoundWave` instances, `A * B` creates a new `SoundWave` object whose samples are the circular convolution of the samples from `A` and `B`. If the samples from `A` and `B` are not the same length, append zeros to the shorter array to make them the same length before convolving. Use `scipy.fftpack` and (7.4) to compute the convolution, and raise a `ValueError` if the sample rates from `A` and `B` are not equal.

A circular convolution creates an interesting effect on a signal when convolved with a segment of white noise: the sound loops seamlessly from the end back to the beginning. To see this, generate two seconds of white noise (at the same sample rate as `tada.wav`) with the following code.

```
>>> rate = 22050        # Create 2 seconds of white noise at a given rate.
>>> white_noise = np.random.randint(-32767, 32767, rate*2, dtype=np.int16)
```

Next, convolve `tada.wav` with the white noise. Finally, use the `>>` operator to append the convolution result to itself. This final signal sounds the same from beginning to end, even though it is the concatenation of two signals.

Linear Convolution

Although circular convolutions can give interesting results, most common sound mixtures do not combine sounds at the beginning of one signal with sounds at the end of another. Whereas circular convolution assumes that the samples represent a full period of a periodic function, *linear convolution* aims to combine non-periodic discrete signals in a way that prevents the beginnings and endings from interacting. Given two samples with lengths n and m, the simplest way to achieve this is to pad both samples with zeros so that they each have length $n+m-1$, compute the convolution of these larger arrays, and take the first $n+m-1$ entries of that convolution.

Problem 2.

Implement the `__pow__()` magic method for the `SoundWave` class so that if `A` and `B` are `SoundWave` instances, `A ** B` creates a new `SoundWave` object whose samples are the linear convolution of the samples from `A` and `B`. Raise a `ValueError` if the sample rates from `A` and `B` are not equal.

Because `scipy.fftpack` performs best when the length of the inputs is a power of 2, start by computing the smallest 2^a such that $2^a \geq n+m-1$, where $a \in \mathbb{N}$ and n and m are the number of samples from `A` and `B`, respectively. Append zeros to each sample so that they each have 2^a entries, then compute the convolution of these padded samples using (7.4). Use only the first $n+m-1$ entries of this convolution as the samples of the returned `SoundWave` object.

To test your method, read `CGC.wav` and `GCG.wav`. Time (separately) the convolution of these signals with `SoundWave.__pow__()` and with `scipy.signal.fftconvolve()`. Compare the results by listening to the original and convolved signals.

Problem 3. Clapping in a large room with an echo produces a sound that resonates in the room for up to several seconds. This echoing sound is referred to as the *impulse response* of the room, and is a way of approximating the acoustics of a room. When the sound of a single instrument in a carpeted room is convolved with the impulse response from a concert hall, the new signal sounds as if the instrument is being played in the concert hall.

The file `chopin.wav` contains a short clip of a piano being played in a room with little or no echo, and `balloon.wav` is a recording of a balloon being popped in a room with a substantial echo (the impulse). Use your method from Problem 2 or `scipy.signal.fftconvolve()` to compute the linear convolution of `chopin.wav` and `balloon.wav`.

Filtering Frequencies with the DFT

The DFT also provides a way to clean a signal by altering some of its frequencies. Consider `noisy1.wav`, a noisy recording of a short voice clip. The time-domain plot of the signal only shows that the signal has a lot of static. On the other hand, the signal's DFT suggests that the static may be the result of some concentrated noise between about 1250–2600 Hz. Removing these frequencies could result in a much cleaner signal.

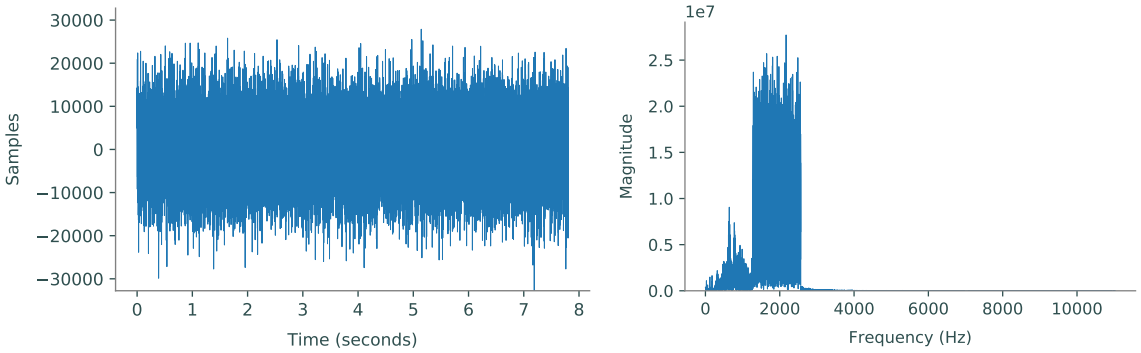


Figure 7.1: The time-domain plot (left) and DFT (right) of `noisy1.wav`.

To implement this idea, recall that the kth entry of the DFT array $\mathbf{c} = F_n\mathbf{f}$ corresponds to the frequency $v = kr/n$ in Hertz, where r is the sample rate and n is the number of samples. Hence, the DFT entry c_k corresponding to a given frequency v in Hertz has index $k = vn/r$, rounded to an integer if needed. In addition, since the DFT is symmetric, c_{n-k} also corresponds to this frequency. This suggests a strategy for filtering out an unwanted interval of frequencies $[v_{\text{low}}, v_{\text{high}}]$ from a signal:

1. Compute the integer indices k_{low} and k_{high} corresponding to v_{low} and v_{high}, respectively.
2. Set the entries of the signal's DFT from k_{low} to k_{high} and from $n - k_{\text{high}}$ to $n - k_{low}$ to zero, effectively removing those frequencies from the signal.
3. Take the IDFT of the modified DFT to obtain the cleaned signal.

Using this strategy to filter `noisy1.wav` results in a much cleaner signal. However, any "good" frequencies in the affected range are also removed, which may decrease the overall sound quality. The goal, then, is to remove only as many frequencies as necessary.

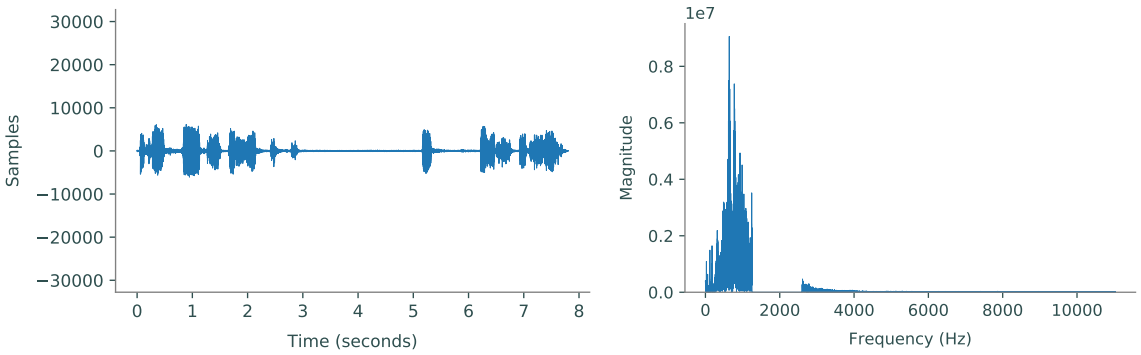


Figure 7.2: The time-domain plot (left) and DFT (right) of `noisy1.wav` after being cleaned.

Problem 4. Add a method to the `SoundWave` class that accepts two frequencies v_{low} and v_{high} in Hertz. Compute the DFT of the stored samples and zero out the frequencies in the range $[v_{\text{low}}, v_{\text{high}}]$ (remember to account for the symmetry DFT). Take the IDFT of the altered array and store it as the sample array.

Test your method by cleaning `noisy1.wav`, then clean `noisy2.wav`, which also has some artificial noise that obscures the intended sound.
(Hint: plot the DFT of `noisy2.wav` to determine which frequencies to eliminate.)

A digital audio signal made of a single sample vector with is called *monoaural* or *mono*. When several sample vectors with the same sample rate and number of samples are combined into a matrix, the overall signal is called *stereophonic* or *stereo*. This allows multiple speakers to each play one *channel*—one of the original sample vectors—simultaneously. "Stereo" usually means there are two channels, but there may be any number of channels (5.1 surround sound, for instance, has five).

Most stereo sounds are read as $n \times m$ matrices, where n is the number of samples and m is the number of channels (i.e., each column is a channel). However, some functions, including Jupyter's embedding tool `IPython.display.Audio()`, receive stereo signals as $m \times n$ matrices (each row is a channel). Be aware that both conventions are common.

Problem 5. During the 2010 World Cup in South Africa, large plastic horns called vuvuzelas were blown excessively throughout the games. Broadcasting organizations faced difficulties with their programs due to the incessant noise level. Eventually, audio filtering techniques were used to cancel out the sound of the vuvuzela, which has a frequency of around 200–500 Hz.

The file `vuvuzela.wav`[a] is a stereo sound with two channels. Use your function from Problem 4 to clean the sound clip by filtering out the vuvuzela frequencies in each channel. Recombine the two cleaned samples.

[a] See `https://www.youtube.com/watch?v=g_0NoBKWCT8`.

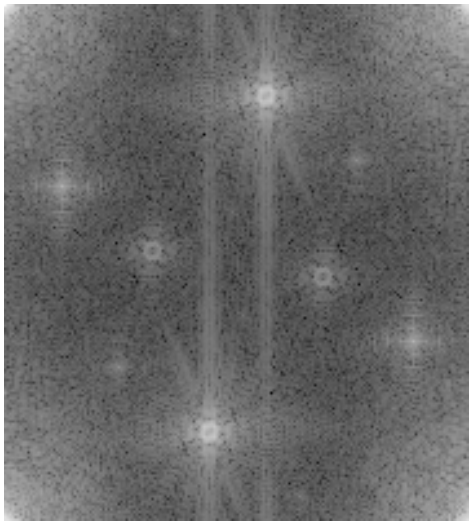
The Two-dimensional Discrete Fourier Transform

The DFT can be easily extended to any number of dimensions. Computationally, the problem reduces to performing the usual one-dimensional DFT iteratively along each of the dimensions. For example, to compute the two-dimensional DFT of an $m \times n$ matrix, calculate the usual DFT of each of the n columns, then take the DFT of each of the m rows of the resulting matrix. Calculating the two-dimensional IDFT is done in a similar fashion, but in reverse order: first calculate the IDFT of the rows, then the IDFT of the resulting columns.

```
>>> from scipy.fftpack import fft2, ifft2

>>> A = np.random.random((10,10))
>>> A_dft = fft2(A)                  # Calculate the 2d DFT of A.
>>> A_dft_ifft = ifft2(A_dft).real   # Calculate the 2d IDFT.
>>> np.allclose(A, A_dft_ifft)
True
```

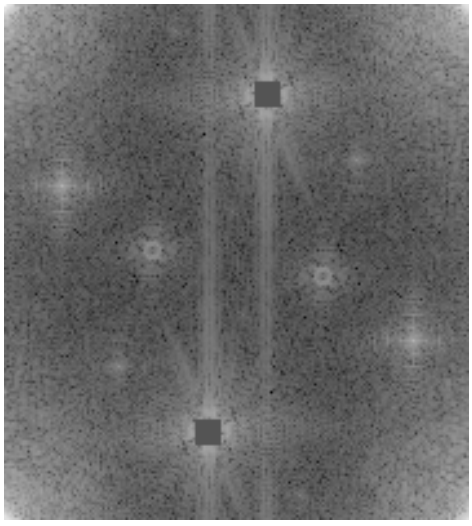
Just as the one-dimensional DFT can be used to remove noise in sounds, its two-dimensional counterpart can be used to remove "noise" in images. The procedure is similar to the filtering technique in Problems 4 and 5: take the two-dimensional DFT of the image matrix, modify certain entries of the DFT matrix to remove unwanted frequencies, then take the IDFT to get a cleaner version of the original image. This strategy makes the fairly strong assumption that the noise in the image is periodic and corresponds to certain frequencies. While this may seem like an unlikely scenario, it does actually occur in many digital images—for an example, try taking a picture of a computer screen with a digital camera.

(a) The original blurry image.



(b) The DFT of the original image.

(c) The improved image.



(d) The DFT of the improved image.

Figure 7.3: To remove noise from an image, take the DFT of the image and replace the abnormalities with values more consistent with the rest of the DFT. Notice that the new image is less noisy, but only slightly. This is because only some of the abnormalities in the DFT were changed; in order to further decrease the noise, we would need to further alter the DFT.

To begin cleaning an image with the DFT, take the two-dimensional DFT of the image matrix. Identify *spikes*—abnormally high frequency values that may be causing the noise—in the image DFT by plotting the log of the magnitudes of the Fourier coefficients. With `cmap="gray"`, spikes show up as bright spots. See Figures 7.3a–7.3b.

```
# Read the image.
>>> import imageio
>>> im = imageio.read("noisy_face.png")

# Plot the log magnitude of the image's DFT.
>>> im_dft = fft2(image)
>>> plt.imshow(np.log(np.abs(im_dft)), cmap="gray")
>>> plt.show()
```

Instead of setting spike frequencies to zero (as was the case for sounds), replace them with values that are similar to those around them. There are many ways to do this, but one convention is to simply "patch" each spike by setting portions of the DFT matrix to some set value, such as the mean of the DFT array. See Figure 7.3d.

Once the spikes have been covered, take the IDFT of the modified DFT to get a (hopefully cleaner) image. Notice that Figure 7.3c still has noise present, but it is a slight improvement over the original. However, it often suffices to remove some of the noise, even if it is not possible to remove it all with this method.

Problem 6. The file `license_plate.png` contains a noisy image of a license plate. The bottom right corner of the plate has is a sticker with information about the month and year that the vehicle registration was renewed. However, in its current state, the year is not clearly legible.

Use the two-dimensional DFT to clean up the image enough so that the year in the bottom right corner is legible. This may require a little trial and error.

8 Introduction to Wavelets

Lab Objective: *Wavelets are used to sparsely represent some types of information. This makes them useful in a variety of applications. We explore both the one- and two-dimensional discrete wavelet transforms using various types of wavelets. We then use a Python package called PyWavelets for further wavelet analysis including image cleaning and image compression.*

Wavelet Functions

Wavelets families are sets of orthogonal functions (wavelets) designed to decompose nonperiodic, piecewise continuous functions. These families have four types of wavelets: mother, daughter, father, and son functions. Father and son wavelets contain information related to the general movement of the function, while mother and daughter wavelets contain information related to the details of the function. The father and mother wavelets are the basis of a family of wavelets. Son and daughter wavelets are just scaled translates of the father and mother wavelets, respectively.

Haar Wavelets

The *Haar Wavelet* family is one of the most widely used wavelet families in wavelet analysis. This set includes the father, mother, son, and daughter wavelets defined below. The Haar father (scaling) function is given by

$$\varphi(x) = \begin{cases} 1 & \text{if } 0 \leq x < 1 \\ 0 & \text{otherwise.} \end{cases}$$

The Haar son wavelets are scaled and translated versions of the father wavelet:

$$\varphi_{jk}(x) = \varphi(2^j x - k) = \begin{cases} 1 & \text{if } \frac{k}{2^j} \leq x < \frac{k+1}{2^j} \\ 0 & \text{otherwise.} \end{cases}$$

The Haar mother wavelet function is defined as

$$\psi(x) = \begin{cases} 1 & \text{if } 0 \leq x < \frac{1}{2} \\ -1 & \text{if } \frac{1}{2} \leq x < 1 \\ 0 & \text{otherwise.} \end{cases}$$

The Haar daughter wavelets are scaled and translated versions of the mother wavelet

$$\psi_{jk} = \psi(2^j x - k)$$

Information (such as a mathematical function or image) can be stored and analyzed by considering its *wavelet decomposition*. A *wavelet decomposition* is a linear combination of wavelets. For example, a mathematical function f can be approximated as a combination of Haar son and daughter wavelets as follows:

$$f(x) = \sum_{k=-\infty}^{\infty} a_k \varphi_{m,k}(x) + \sum_{k=-\infty}^{\infty} b_{m,k}\psi_{m,k}(x) + \cdots + \sum_{k=-\infty}^{\infty} b_{n,k}\psi_{n,k}(x)$$

where $m < n$, and all but a finite number of the a_k and $b_{j,k}$ terms are nonzero. The a_k terms are often referred to as *approximation coefficients* while the $b_{j,k}$ terms are known as *detail coefficients*. The approximation coefficients typically capture the broader, more general features of a signal while the detail coefficients capture smaller details and noise.

A wavelet decomposition can be done with any family of wavelet functions. Depending on the properties of the wavelet and the function (or signal) f, f can be approximated to an arbitrary level of accuracy. Each arbitrary wavelet family has a mother wavelet ψ and a father wavelet φ which are the basis of the family. A countably infinite set of wavelet functions (daughter and son wavelets) can be generated using dilations and shifts of the first two functions where $m, k \in \mathbb{Z}$:

$$\psi_{m,k}(x) = \psi(2^m x - k)$$
$$\varphi_{m,k}(x) = \varphi(2^m x - k).$$

The Discrete Wavelet Transform

The mapping from a function to a sequence of wavelet coefficients is called the *discrete wavelet transform*. The discrete wavelet transform is analogous to the discrete Fourier transform. Now, instead of using trigonometric functions, different families of basis functions are used.

In the case of finitely-sampled signals and images, there exists an efficient algorithm for computing the wavelet coefficients. Most commonly used wavelets have associated high-pass and low-pass filters which are derived from the wavelet and scaling functions, respectively. When the low-pass filter is convolved with the sampled signal, low frequency (also known as approximation) information is extracted. This is similar to turning up the bass on a speaker, which extracts the low frequencies of a sound wave. This filter highlights the overall (slower-moving) pattern without paying too much attention to the high frequency details and extracts the approximation coefficients.

When the high-pass filter is convolved with the sampled signal, high frequency information (also known as detail) is extracted. This is similar to turning up the treble on a speaker, which extracts the high frequencies of a sound wave. This filter highlights the small changes found in the signal and extracts the detail coefficients.

The two primary operations of the algorithm are the discrete convolution and downsampling, denoted $*$ and DS, respectively. First, a signal is convolved with both filters. The resulting arrays will be twice the size of the original signal because the frequency of the sample will have changed by a factor of 2. To remove this redundant information, the resulting arrays are *downsampled*. Downsampling is the process of removing unimportant entries from an array. In the context of this lab, a *filter bank* is the combined process of convolving with a filter, and then downsampling. The result will be an array of approximation coefficients A and an array of detail coefficients D. This process can be repeated on the new approximation to obtain another layer of approximation and detail coefficients. See Figure 8.1.

A common lowpass filter is the averaging filter. Given an array $\mathbf{x}$, the averaging filter produces an array $\mathbf{y}$ where y_n is the average of x_n and x_{n-1}. In other words, the averaging filter convolves an array with the array $L = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \end{bmatrix}$. This filter preserves the main idea of the data. The corresponding highpass filter is the distance filter. Given an array $\mathbf{x}$, the distance filter produces an array $\mathbf{y}$ where y_n is the distance between x_n and x_{n-1}. In other words, the difference filter convolves an array with the array $H = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2} \end{bmatrix}$. This filter preserves the details of the data.

For the Haar Wavelet, we will use these lowpass and highpass filters. In order for this filters to have inverses, the filters must be normalized (for more on why this is, see Additional Materials). The resulting lowpass and highpass filters for the Haar Wavelets are the following:

$$L = \begin{bmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{bmatrix}$$
$$H = \begin{bmatrix} -\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{bmatrix}$$

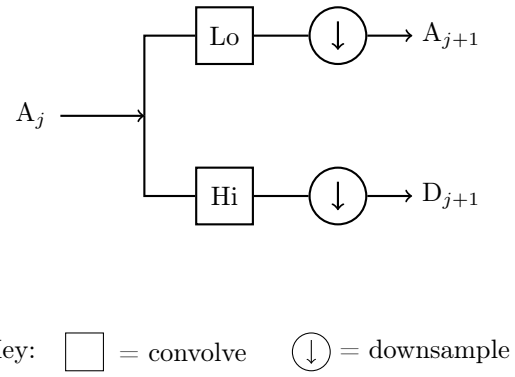


Figure 8.1: The one-dimensional discrete wavelet transform implemented as a filter bank.

As noted earlier, the key mathematical operations of the discrete wavelet transform are convolution and downsampling. Given a filter and a signal, the convolution can be obtained using `scipy.signal.fftconvolve()`.

```
>>> from scipy.signal import fftconvolve
>>> # Initialize a filter.
>>> L = np.ones(2)/np.sqrt(2)
>>> # Initialize a signal X.
>>> X = np.sin(np.linspace(0,2*np.pi,16))
>>> # Convolve X with L.
>>> fftconvolve(X, L)
[ -1.84945741e-16   2.87606238e-01   8.13088984e-01   1.19798126e+00
   1.37573169e+00   1.31560561e+00   1.02799937e+00   5.62642704e-01
   7.87132986e-16  -5.62642704e-01  -1.02799937e+00  -1.31560561e+00
  -1.37573169e+00  -1.19798126e+00  -8.13088984e-01  -2.87606238e-01
  -1.84945741e-16]
```

The convolution operation alone gives redundant information, so it is downsampled to keep only what is needed. The array will be downsampled by a factor of 2, which means keeping only every other entry:

```
>>> # Downsample an array X.
>>> sampled = X[1::2] # Keeps odd entries
```

Both the approximation and detail coefficients are computed in this manner. The approximation uses the low-pass filter while the detail uses the high-pass filter. Implementation of a filter bank is found in Algorithm 8.1.

Algorithm 8.1 The one-dimensional discrete wavelet transform. X is the signal to be transformed, L is the low-pass filter, H is the high-pass filter and n is the number of filter bank iterations.

1: **procedure** DWT(X, L, H, n)
2: $A_0 \leftarrow X$ ▷ Initialization.
3: **for** $i = 0 \dots n-1$ **do**
4: $D_{i+1} \leftarrow DS(A_i * H)$ ▷ High-pass filter and downsample.
5: $A_{i+1} \leftarrow DS(A_i * L)$ ▷ Low-pass filter and downsample.
6: **return** $A_n, D_n, D_{n-1}, \dots, D_1$.

Problem 1. Write a function that calculates the discrete wavelet transform using Algorithm 8.1. The function should return a list of one-dimensional NumPy arrays in the following form: $[A_n, D_n, \dots, D_1]$.

Test your function by calculating the Haar wavelet coefficients of a noisy sine signal with $n = 4$:

```
domain = np.linspace(0, 4*np.pi, 1024)
noise =  np.random.randn(1024)*.1
noisysin = np.sin(domain) + noise
coeffs = dwt(noisysin, L, H, 4)
```

Plot the original signal with the approximation and detail coefficients and verify that they match the plots in Figure 8.2.
(Hint: Use array broadcasting)

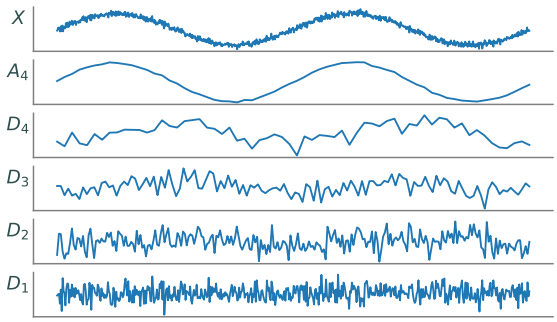


Figure 8.2: A level four wavelet decomposition of a signal. The top panel is the original signal, the next panel down is the approximation, and the remaining panels are the detail coefficients. Notice how the approximation resembles a smoothed version of the original signal, while the details capture the high-frequency oscillations and noise.

Inverse Discrete Wavelet Transform

The process of the discrete wavelet transform is reversible. Using modified filters, a set of detail coefficients and a set of approximation coefficients can be manipulated and added together to recreate a signal. The Haar wavelet filters for the inverse transformation are found by reversing the operations for each filter. The original lowpass filter found the average of elements, so the inverse filter will find the distance. The original highpass filter found the distance of elements, so the inverse filter will find the average. The Haar inverse filters are given below:

$$L^{-1} = \begin{bmatrix} \frac{\sqrt{2}}{2} & -\frac{\sqrt{2}}{2} \end{bmatrix}$$
$$H^{-1} = \begin{bmatrix} \frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} \end{bmatrix}$$

The first row refers to the inverse high-pass filter and the second row refers to the inverse low-pass filter.

Suppose the wavelet coefficients A_n and D_n have been computed. A_{n-1} can be recreated by tracing the schematic in Figure 8.1 backwards: A_n and D_n are first upsampled, and then are convolved with the inverse low-pass and high-pass filters, respectively. In the case of the Haar wavelet, *upsampling* involves doubling the length of an array by inserting a 0 at every other position. To complete the operation, the new arrays are convolved and added together to obtain A_{n-1}.

```
>>> # Upsample the coefficient arrays A and D.
>>> up_A = np.zeros(2*A.size)
>>> up_A[::2] = A
>>> up_D = np.zeros(2*D.size)
>>> up_D[::2] = D
>>> # Convolve and add, discarding the last entry.
>>> A = fftconvolve(up_A, L)[:-1] + fftconvolve(up_D, H)[:-1]
```

This process is continued with the newly obtained approximation coefficients and with the next detail coefficients until the original signal is recovered.

Problem 2. Write a function that performs the inverse wavelet transform. The function should accept a list of arrays (of the same form as the output of Problem 1), a reverse low-pass filter, and a reverse high-pass filter. The function should return a single array, which represents the recovered signal.

Note that the input list of arrays has length $n+1$ (consisting of A_n together with $D_n, D_{n-1}, \dots, D_1$), so your code should perform the process given above n times.

To test your function, first perform the inverse transform on the noisy sine wave that you created in the first problem. Then, compare the original signal with the signal recovered by your inverse wavelet transform function using `np.allclose()`.

ACHTUNG!

Although Algorithm 8.1 and the preceding discussion apply in the general case, the code implementations apply only to the Haar wavelet. Because of the nature of the discrete convolution, when convolving with longer filters, the signal to be transformed needs to undergo a different type of lengthening in order to avoid information loss during the convolution. As such, the functions written in Problems 1 and 2 will only work correctly with the Haar filters and would require modifications to be compatible with more wavelets.

The Two-dimensional Wavelet Transform

The generalization of the wavelet transform to two dimensions is similar to one dimensional transforms. Again, the two primary operations used are convolution and downsampling. The main difference in the two-dimensional case is the number of convolutions and downsamples per iteration. First, the convolution and downsampling are performed along the rows of an array. This results in two new arrays, as in the one dimensional case. Then, convolution and downsampling are performed along the columns of the two new arrays. This results in four final arrays that make up the new approximation and detail coefficients. See Figure 8.3.

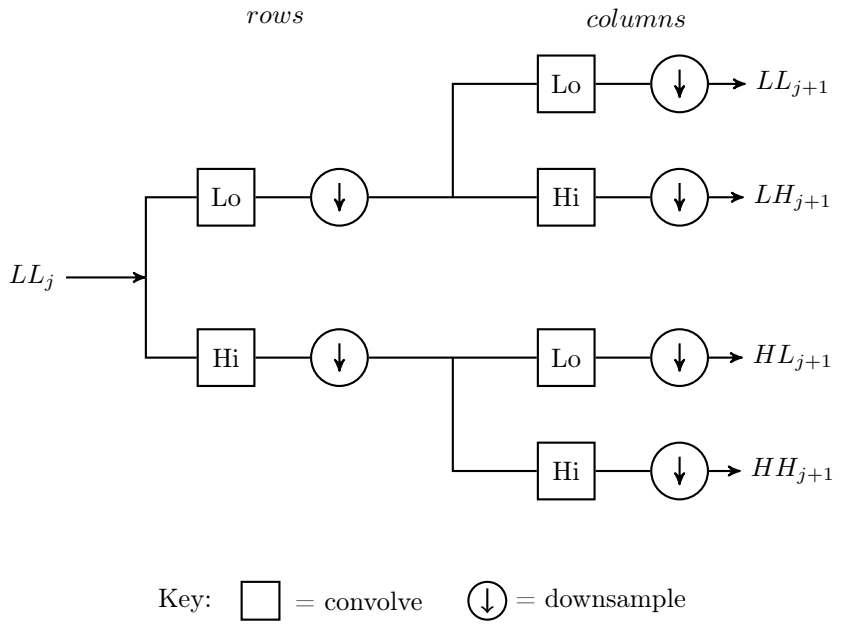


Figure 8.3: The two-dimensional discrete wavelet transform implemented as a filter bank.

When implemented as an iterative filter bank, each pass through the filter bank yields one set of approximation coefficients plus three sets of detail coefficients, rather than just one. More specifically, if the two-dimensional array X is the input to the filter bank, the arrays LL, LH, HL, and HH are obtained. LL is a smoothed approximation of X (similar to A_n in the one-dimensional case), and the other three arrays contain detail coefficients that capture high-frequency oscillations in vertical, horizontal, and diagonal directions. The arrays LL, LH, HL, and HH are known as *subbands*. Any or all of the subbands can be fed into a filter bank to further decompose the signal into different subbands. This decomposition can be represented by a partition of a rectangle, called a *subband pattern*. The subband pattern for one pass of the filter bank is shown in Figure 8.4, with an example of an image decomposition given in Figure 8.5.

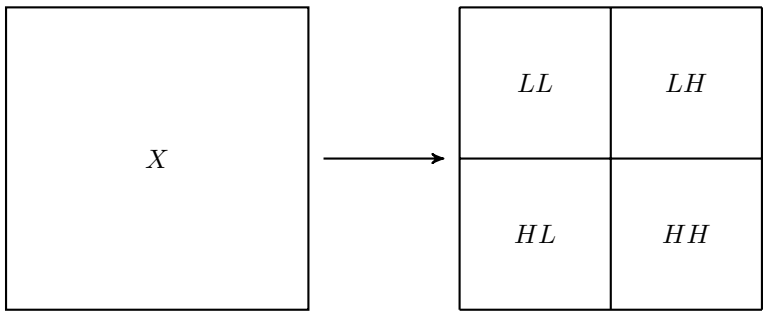


Figure 8.4: The subband pattern for one step in the 2-dimensional wavelet transform.

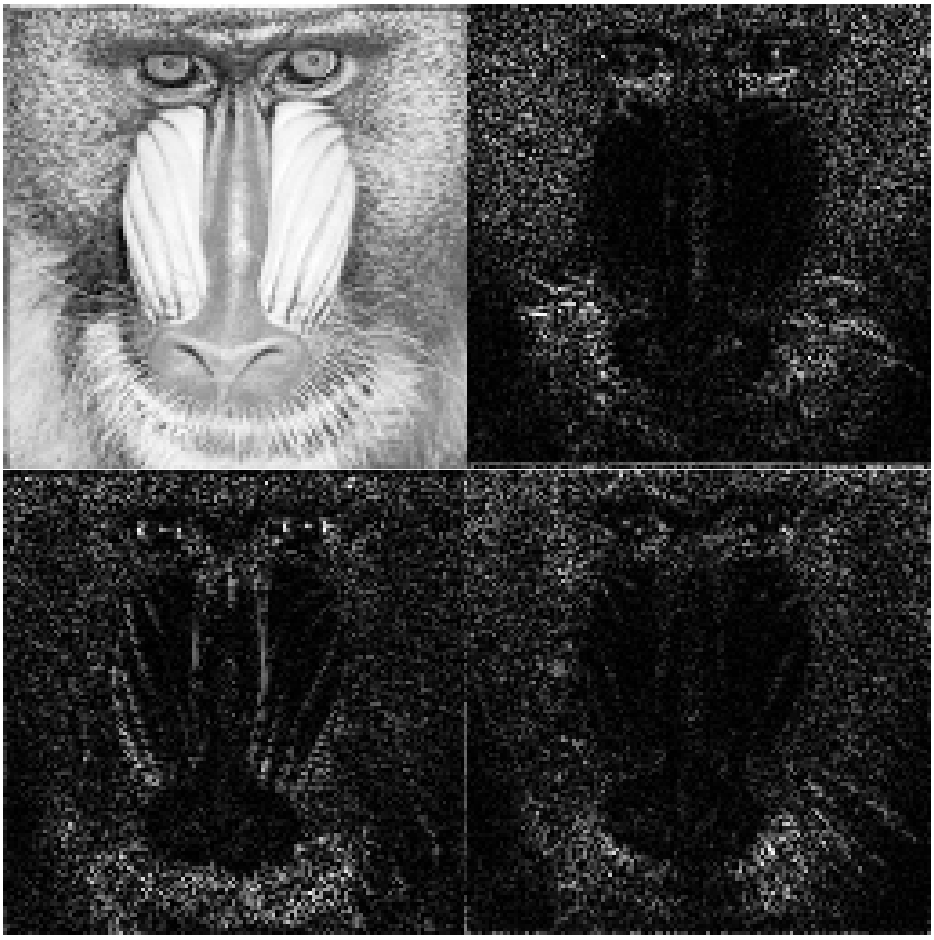


Figure 8.5: Subbands for the mandrill image after one pass through the filter bank. Note how the upper left subband (LL) is an approximation of the original Mandrill image, while the other three subbands highlight the stark vertical, horizontal, and diagonal changes in the image.
Original image source: `http://sipi.usc.edu/database/`.

The wavelet coefficients obtained from a two-dimensional wavelet transform are used to analyze and manipulate images at differing levels of resolution. Images are often sparsely represented by wavelets; that is, most of the image information is captured by a small subset of the wavelet coefficients. This is the key fact for wavelet-based image compression and will be discussed in further detail later in the lab.

The PyWavelets Module

PyWavelets is a Python package designed for wavelet analysis. Although it has many other uses, in this lab it will primarily be used for image manipulation. PyWavelets can be installed using the following command:

```
$ pip install PyWavelets
```

PyWavelets provides a simple way to calculate the subbands resulting from one pass through the filter bank. The following code demonstrates how to find the approximation and detail subbands of an image.

```
>>> from imageio import imread
>>> import pywt                                # The PyWavelets package.
# The True parameter produces a grayscale image.
>>> mandrill = imread('mandrill1.png', True)
# Use the Daubechies 4 wavelet with periodic extension.
>>> lw = pywt.dwt2(mandrill, 'db4', mode='per')
```

The function `pywt.dwt2()` calculates the subbands resulting from one pass through the filter bank. The `mode` keyword argument sets the extension mode, which determines the type of padding used in the convolution operation. For the problems in this lab, always use `mode='per'`, which is the periodic extension. The second positional argument specifies the type of wavelet to be used in the transform. The function `dwt2()` returns a list. The first entry of the list is the LL, or approximation, subband. The second entry of the list is a tuple containing the remaining subbands, LH, HL, and HH (in that order). As noted, the second positional argument is a string that gives the name of the wavelet to be used. PyWavelets supports a number of different wavelets which are divided into different classes known as families. The supported families and their wavelet instances can be listed by executing the following code:

```
>>> # List the available wavelet families.
>>> print(pywt.families())
['haar', 'db', 'sym', 'coif', 'bior', 'rbio', 'dmey', 'gaus', 'mexh', 'morl', '↩
    cgau', 'shan', 'fbsp', 'cmor']
>>> # List the available wavelets in a given family.
>>> print(pywt.wavelist('coif'))
['coif1', 'coif2', 'coif3', 'coif4', 'coif5', 'coif6', 'coif7', 'coif8', 'coif9↩
    ', 'coif10', 'coif11', 'coif12', 'coif13', 'coif14', 'coif15', 'coif16', '↩
    coif17']
```

Different wavelets have different properties; the most suitable wavelet is dependent on the specific application. For example, the morlet wavelet is closely related to human hearing and vision. Note that not all of these families work with the function `pywt.dwt2()`, because they are continuous wavelets. Choosing which wavelet is used is partially based on the properties of a wavelet, but since many wavelets share desirable properties, the best wavelet for a particular application is often not known until some type of testing is done.

Problem 3. Explore the two-dimensional wavelet transform by completing the following:

1. Save a picture of a raccoon with the following code

   ```
   >>> from scipy.misc import face
   >>> racoon = face(True)
   ```

2. Plot the subbands of raccoon as described above (using the Daubechies 4 wavelet with periodic extension). Compare this with the subbands of the mandrill image shown in Figure 8.5.

3. Compare the subband patterns of the haar, symlet, and coiflet wavelets by plotting the LH subband pattern using the picture of the raccoon. The haar subband should have more detail than the symlet subband, and the symlet subband should have more detail than the coiflet wavelet.

The function `pywt.wavedec2()` is similar to `pywt.dwt2()`, but it also includes a keyword argument, `level`, which specifies the number of times to pass an image through the filter bank. It will return a list of subbands, the first of which is the final approximation subband, while the remaining elements are tuples which contain sets of detail subbands (LH, HL, and HH). If `level` is not specified, the number of passes through the filter bank will be determined at runtime. The function `pywt.waverec2()` accepts a list of subband patterns (like the output of `pywt.wavedec2()` or `pywt.dwt2()`), a name string denoting the wavelet, and a keyword argument `mode` for the extension mode. It returns a reconstructed image using the reverse filter bank. When using this function, be sure that the wavelet and mode match the deconstruction parameters. PyWavelets has many other useful functions including `dwt()`, `idwt()` and `idwt2()` which can be explored further in the documentation for PyWavelets, `http://pywavelets.readthedocs.io/en/latest/contents.html`.

Applications

Noise Reduction

Noise in an image is defined as unwanted visual artifacts that obscure the true image. Images acquire noise from a variety of sources, including cameras, data transfer, and image processing algorithms. This section will focus on reducing a particular type of noise in images called *Gaussian white noise*.

Gaussian white noise causes every pixel in an image to be perturbed by a small amount. Many types of noise, including Gaussian white noise, are very high-frequency. Since many images are relatively sparse in high-frequency domains, noise in an image can be safely removed from the high frequency subbands while minimally distorting the true image. A basic, but effective, approach to reducing Gaussian white noise in an image is thresholding. Thresholding can be done in two ways, referred to as hard and soft thresholding.

Given a positive threshold value τ, hard thresholding sets every wavelet coefficient whose magnitude is less than τ to zero, while leaving the remaining coefficients untouched. Soft thresholding also zeros out all coefficients of magnitude less than τ, but in addition maps the remaining positive coefficients β to $\beta - \tau$ and the remaining negative coefficients α to $\alpha + \tau$.

Once the coefficients have been thresholded, the inverse wavelet transform is used to recover the denoised image. The threshold value is generally a function of the variance of the noise, and in real situations, is not known. In fact, noise variance estimation in images is a research area in its own right, but that goes beyond the scope of this lab.

Problem 4. Write two functions that accept a list of wavelet coefficients in the usual form, as well as a threshold value. Each function returns the thresholded wavelet coefficients (also in the usual form). The first function should implement hard thresholding and the second should implement soft thresholding. While writing these two functions, remember that only the detail coefficients are thresholded, so the first entry of the input coefficient list should remain unchanged.

To test your functions, perform hard and soft thresholding on `noisy_darkhair.png` and plot the resulting images together. When testing your function, use the Daubechies 4 wavelet and four sets of detail coefficients (`level=4` when using `wavedec2()`). For soft thresholding use $\tau = 20$, and for hard thresholding use $\tau = 40$.

Image Compression

Transform methods based on Fourier and wavelet analysis play an important role in image compression; for example, the popular JPEG image compression standard is based on the discrete cosine transform. The JPEG2000 compression standard and the FBI Fingerprint Image database, along with other systems, take the wavelet approach.

The general framework for compression is as follows. First, the image to be compressed undergoes some form of preprocessing, depending on the particular application. Next, the discrete wavelet transform is used to calculate the wavelet coefficients, and these are then *quantized*, i.e. mapped to a set of discrete values (for example, rounded to the nearest integer). The quantized coefficients are then passed through an entropy encoder (such as Huffman Encoding), which reduces the number of bits required to store the coefficients. What remains is a compact stream of bits that can be saved or transmitted much more efficiently than the original image. The steps above are nearly all invertible (the only exception being quantization), allowing the original image to be almost perfectly reconstructed from the compressed bitstream. See Figure 8.6.

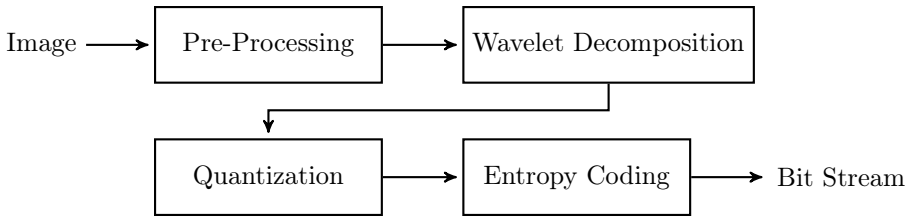
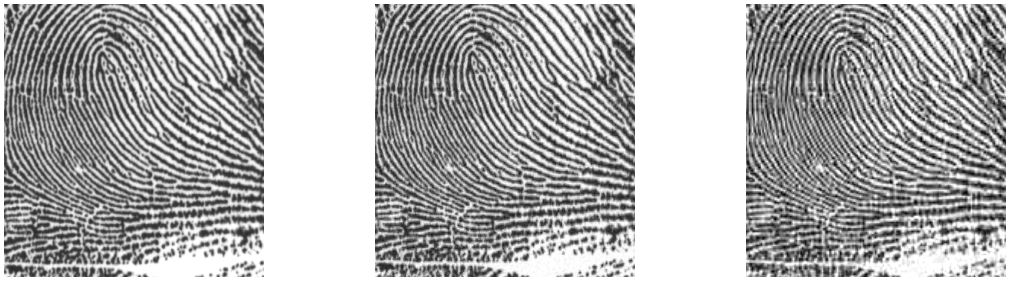


Figure 8.6: Wavelet Image Compression Schematic

WSQ: The FBI Fingerprint Image Compression Algorithm

The Wavelet Scalar Quantization (WSQ) algorithm is among the first successful wavelet-based image compression algorithms. It solves the problem of storing millions of fingerprint scans efficiently while meeting the law enforcement requirements for high image quality. This algorithm is capable of achieving compression ratios in excess of 10-to-1 while retaining excellent image quality; see Figure 8.7. This section of the lab steps through a simplified version of this algorithm by writing a Python class that performs both the compression and decompression. Differences between this simplified algorithm and the complete algorithm are found in the Additional Material section at the end of this lab. Also included in Additional Materials is a more thorough explanation of all the methods in the WSQ class.



(a) Uncompressed (b) 12:1 compressed (c) 26:1 compressed

Figure 8.7: Fingerprint scan at different levels of compression.
Original image source: `http://www.nist.gov/itl/iad/ig/wsq.cfm`.

WSQ: Preprocessing

Preprocessing in this algorithm ensures that roughly half of the new pixel values are negative, while the other half are positive, and all fall in the range $[-128, 128]$. The input to the algorithm is a matrix of nonnegative 8-bit integer values giving the grayscale pixel values for the fingerprint image. The image is processed by the following formula:

$$M' = \frac{M - m}{s},$$

where M is the original image matrix, M' is the processed image, m is the mean pixel value, and $s = \max\{\max(M) - m, m - \min(M)\}/128$ (here $\max(M)$ and $\min(M)$ refer to the maximum and minimum pixel values in the matrix).

Problem 5. Implement the preprocessing step as well as its inverse by implementing the class methods `pre_process()` and `post_process()`. Each method accepts a NumPy array (the image) and returns the processed image as a NumPy array. In the `pre_process()` method, calculate the values of m and s given above and store them in the class attributes `_m` and `_s`.

WSQ: Calculating the Wavelet Coefficients

The next step in the compression algorithm is decomposing the image into subbands of wavelet coefficients. In this implementation of the WSQ algorithm, the image is decomposed into five sets of detail coefficients (`level=5`) and one approximation subband, as shown in Figure 8.8. Each of these subbands should be placed into a list in the same ordering as in Figure 8.8 (another way to consider this ordering is the approximation subband followed by each level of detail coefficients $[LL_5, LH_5, HL_5, HH_5, LH_4, HL_4, \ldots, HH_1]$).

Problem 6. Implement the class method `decompose()`. This function should accept an image to decompose and should return a list of ordered subbands. Use the function `pywt.wavedec2()` with the `'coif1'` wavelet to obtain the subbands. These subbands should then be ordered in a single list as described above.

Implement the inverse of the decomposition by writing the class method `recreate()`. This function should accept a list of 16 subbands (ordered like the output of `decompose()`) and should return a reconstructed image. Use `pywt.waverec2()` to reconstruct an image from the subbands. Note that you will need to adjust the accepted list in order to adhere to the required input for `waverec2()`.

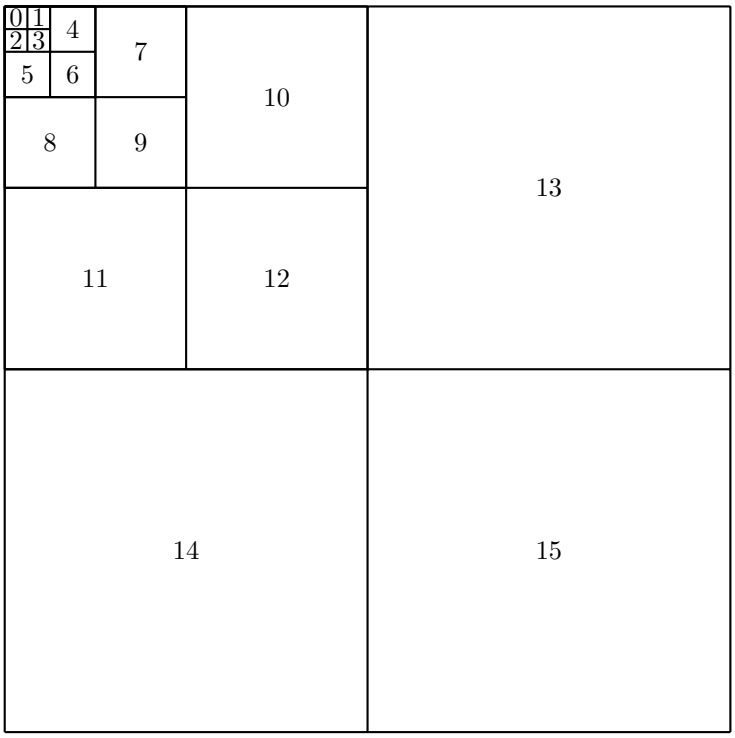


Figure 8.8: Subband Pattern for simplified WSQ algorithm.

WSQ: Quantization

Quantization is the process of mapping each wavelet coefficient to an integer value and is the main source of compression in the algorithm. By mapping the wavelet coefficients to a relatively small set of integer values, the complexity of the data is reduced, which allows for efficient encoding of the information in a bit string. Further, a large portion of the wavelet coefficients will be mapped to 0 and discarded completely. The fact that fingerprint images tend to be very nearly sparse in the wavelet domain means that little information is lost during quantization. Care must be taken, however, to perform this quantization in a manner that achieves good compression without discarding so much information that the image cannot be accurately reconstructed.

Given a wavelet coefficient a in subband k, the corresponding quantized coefficient p is given by

$$p = \begin{cases} \left\lfloor \frac{a - Z_k/2}{Q_k} \right\rfloor + 1, & a > Z_k/2 \\ 0, & -Z_k/2 \leq a \leq Z_k/2 \\ \left\lceil \frac{a + Z_k/2}{Q_k} \right\rceil - 1, & a < -Z_k/2. \end{cases}$$

The values Z_k and Q_k are dependent on the subband, and determine how much compression is achieved. If $Q_k = 0$, all coefficients are mapped to 0.

Selecting appropriate values for these parameters is a tricky problem in itself, and relies on heuristics based on the statistical properties of the wavelet coefficients. Therefore, the methods that calculate these values have already been initialized.

Quantization is not a perfectly invertible process. Once the wavelet coefficients have been quantized, some information is permanently lost. However, wavelet coefficients $\hat{a}_k$ in subband k can be roughly reconstructed from the quantized coefficients p using the following formula. This process is called *dequantization*.

$$\hat{a}_k = \begin{cases} (p - C)Q_k + Z_k/2, & p > 0 \\ 0, & p = 0 \\ (p + C)Q_k - Z_k/2, & p < 0 \end{cases}$$

Note the inclusion of a new dequantization parameter C. Again, if $Q_k = 0$, $\hat{a}_k = 0$ should be returned.

Problem 7. Implement the quantization step by writing the `quantize()` method of your class. This method should accept a NumPy array of coefficients and the quantization parameters Q_k and Z_k. The function should return a NumPy array of the quantized coefficients.

Also implement the `dequantize()` method of your class using the formula given above. This function should accept the same parameters as `quantize()` as well as a parameter C which defaults to .44. The function should return a NumPy array of dequantized coefficients.

Masking and array slicing will help keep your code short and fast when implementing both of these methods. Remember the case for $Q_k = 0$. Test your functions by comparing the output of your functions to a hand calculation on a small matrix.

WSQ: The Rest

The remainder of the compression and decompression methods have already been implemented in the WSQ class. The following discussion explains the basics of what happens in those methods. Once all of the subbands have been quantized, they are divided into three groups. The first group contains the smallest ten subbands (positions zero through nine), while the next two groups contain the three subbands of next largest size (positions ten through twelve and thirteen through fifteen, respectively). All of the subbands of each group are then flattened and concatenated with the other subbands in the group. These three arrays of values are then mapped to Huffman indices. Since the wavelet coefficients for fingerprint images are typically very sparse, special indices are assigned to lists of sequential zeros of varying lengths. This allows large chunks of information to be stored as a single index, greatly aiding in compression. The Huffman indices are then assigned a bit string representation through a Huffman map. Python does not natively include all of the tools necessary to work with bit strings, but the Python package bitstring does have these capabilities. Download bitstring using the following command:

```
$ pip install bitstring
```

Import the package with the following line of code:

```
>>> import bitstring as bs
```

WSQ: Calculating the Compression Ratio

The methods of compression and decompression are now fully implemented. The final task is to verify how much compression has taken place. The compression ratio is the ratio of the number of bits in the original image to the number of bits in the encoding. Assuming that each pixel of the input image is an 8-bit integer, the number of bits in the image is just eight times the number of pixels (the number of pixels in the original source image is stored in the class attribute `_pixels`). The number of bits in the encoding can be calculated by adding up the lengths of each of the three bit strings stored in the class attribute `_bitstrings`.

Problem 8. Implement the method `get_ratio()` by calculating the ratio of compression. The function should not accept any parameters and should return the compression ratio.

Your compression algorithm is now complete! You can test your class with the following code:

```
# Try out different values of r between .1 to .9.
r = .5
finger = imread('uncompressed_finger.png', True)
wsq = WSQ()
wsq.compress(finger, r)
print(wsq.get_ratio())
new_finger = wsq.decompress()
plt.subplot(211)
plt.imshow(finger, cmap=plt.cm.Greys_r)
plt.subplot(212)
plt.imshow(np.abs(new_finger), cmap=plt.cm.Greys_r)
plt.show()
```

Additional Material

Haar Wavelet Transform

The Haar Wavelet is a general matrix transform used to convolve Haar Wavelets. It is found by combining the convolution matrices for a lowpass and highpass filter such that one is directly on top of the other. The lowpass filter is taking the average of every two elements in an array and the highpass filter is taking the difference of every two elements in an array. Redundant information given in the new matrix is then removed via downsampling. However, in order for the transform matrix to have the property $A^T = A^{-1}$, the columns of the matrix must be normalized. Thus, each column is normalized (and subsequently the filters) and the resulting matrix is the Haar Wavelet Transform.

For more on the Haar Wavelet Transform, see *Discrete Wavelet Transformations: An Elementary Approach with Applications* by Patrick J. Van Fleet.

WSQ Algorithm

The official standard for the WSQ algorithm is slightly different from the version implemented in this lab. One of the largest differences is the subband pattern that is used in the official algorithm; this pattern is demonstrated in Figure 8.9. The pattern used may seem complicated and somewhat arbitrary, but it is used because of the relatively good empirical results when used in compression. This pattern can be obtained by performing a single pass of the 2-dimensional filter bank on the image then passing each of the resulting subbands through the filter bank resulting in 16 total subbands. This same process is then repeated with the LL, LH and HL subbands of the original approximation subband creating 46 additional subbands. Finally, the subband corresponding to the top left of Figure 8.9 should be passed through the 2-dimensional filter bank a single time.

As in the implementation given above, the subbands of the official algorithm are divided into three groups. The subbands 0 through 18 are grouped together, as are 19 through 51 and 52 through 63. The official algorithm also uses a wavelet specialized for image compression that is not included in the PyWavelets distribution. There are also some slight modifications made to the implementation of the discrete wavelet transform that do not drastically affect performace.

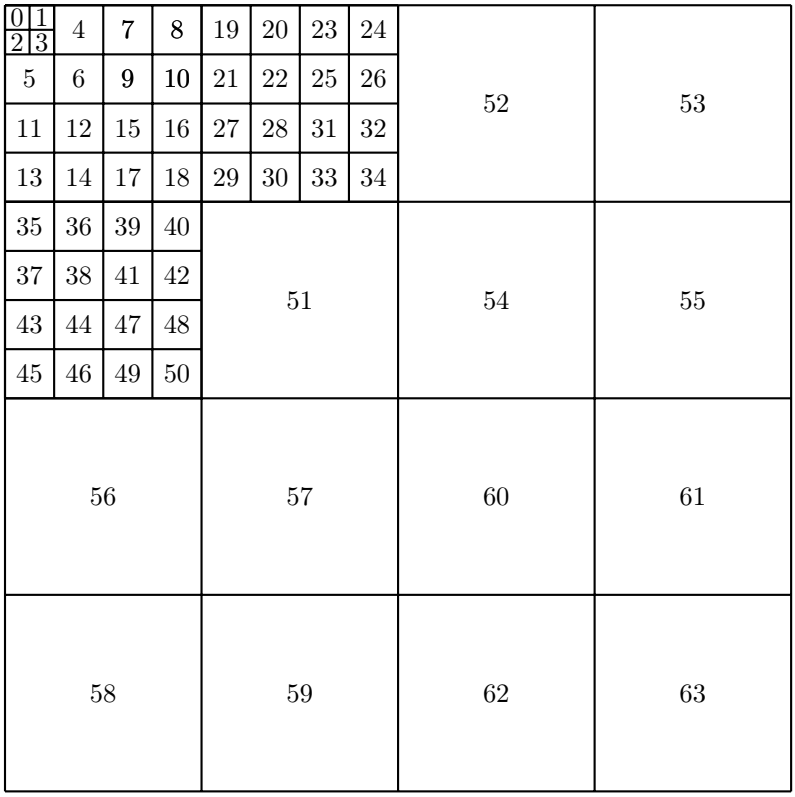


Figure 8.9: True subband pattern for WSQ algorithm.

9 Polynomial Interpolation

Lab Objective: *Learn and compare three methods of polynomial interpolation: standard Lagrange interpolation, Barycentric Lagrange interpolation and Chebyshev interpolation. Explore Runge's phenomenon and how the choice of interpolating points affect the results. Use polynomial interpolation to study air polution by approximating graphs of particulates in air.*

Polynomial Interpolation

Polynomial interpolation is the method of finding a polynomial that matches a function at specific points in its range. More precisely, if $f(x)$ is a function on the interval $[a, b]$ and $p(x)$ is a polynomial then $p(x)$ interpolates the function $f(x)$ at the points $x_0, x_1, \dots, x_n$ if $p(x_j) = f(x_j)$ for all $j = 0, 1, \dots, n$. In this lab most of the discussion is focused on using interpolation as a means of approximating functions or data, however, polynomial interpolation is useful in a much wider array of applications.

Given a function $f(x)$ and a set of unique points $\{x\}_{i=0}^{n}$, it can be shown that there exists a unique interpolating polynomial $p(x)$. That is, there is one and only one polynomial of degree n that interpolates $f(x)$ through those points. This uniqueness property is why, for the remainder of this lab, an interpolating polynomial is referred to as *the* interpolating polynomial. One approach to finding the unique interpolating polynomial of degree n is Lagrange interpolation.

Lagrange interpolation

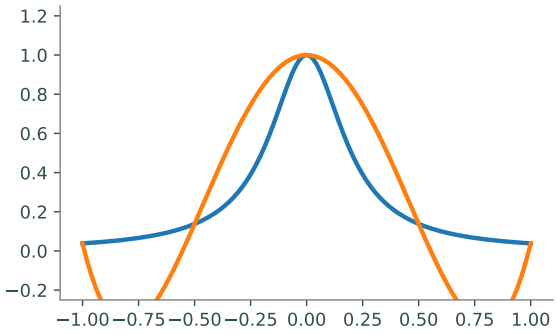
Given a set $\{x_i\}_{i=1}^{n}$ of n points to interpolate, a family of n basis functions with the following property, is constructed:

$$L_j(x_i) = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases}.$$

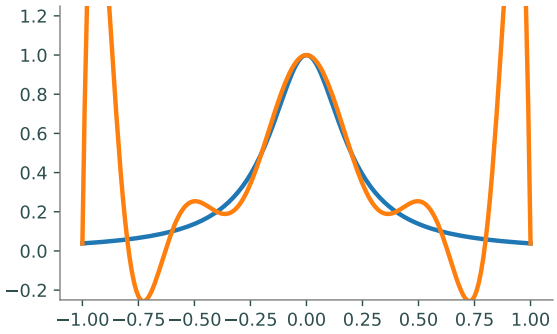
Once each of the n polynomials in this family of basis functions is known, they can be combined with the y-values $y_i = f(x_i)$ of the function to be interpolated in the following manner:

$$p(x) = \sum_{j=1}^{n} y_j L_j(x) \tag{9.1}$$

This will create the unique interpolating polynomial.



(a) Interpolation using 5 equally spaced points.



(b) Interpolation using 11 equally spaced points.

Figure 9.1: Interpolations of Runge's function $f(x) = \frac{1}{1+25x^2}$ with equally spaced interpolating points.

The Lagrange form of this family of basis functions is

$$L_j(x) = \frac{\prod_{k=1, k\neq j}^{n} (x - x_k)}{\prod_{k=1, k\neq j}^{n} (x_j - x_k)} \tag{9.2}$$

Each of these Lagrange basis functions is of degree $n-1$ and has the necessary properties as given above. *Lagrange interpolation* consists of computing the Lagrange basis functions then combining them with the y-values.

Since polynomials are typically represented in their expanded form with coefficients on each of the terms, it may seem like the best option when working with polynomials would be to use Sympy, or NumPy's `poly1d` class to compute the coefficients of the interpolating polynomial individually. This is rarely the best approach, however, since expanding out the large polynomials that are required can quickly lead to instability (especially when using large numbers of interpolating points). Instead, it is usually best just to leave the polynomials in unexpanded form (which is still a polynomial, just not a pretty-looking one), and compute values of the polynomial directly from this unexpanded form.

```
# Evaluate the polynomial (x-2)(x+1) at 10 points without expanding the ↩
    expression.
>>> pts = np.arange(10)
>>> (pts - 2) * (pts + 1)
array([ 2,  0,  0,  2,  6, 12, 20, 30, 42, 56])
```

In the given example, there would have been no instability if the expression had actually been expanded but in the case of a large polynomial, stability issues can dominate the computation. Although the coefficients of the interpolating polynomials will not be explicitly computed in this lab, polynomials are still being used, albeit in a different form.

Problem 1. Write a function that uses the Lagrange method to find an interpolating polynomial for a set of data points and evaluates the calculated polynomial at specified values. This function should accept two NumPy arrays which contain the x and y values of the interpolation points as well as a NumPy array of values (of length m) at which the interpolating polynomial will be evaluated. Your function should return a NumPy array of the evaluated points. The following steps will help in writing your function:

1. Compute the denominator of each L_j (as in Equation 9.2) .
2. Using the previous step, evaluate each L_j at all points in the compuational domain (this will give you m values for each of the n L_j functions).
3. Combine all of these values as in Equation 9.1, this will give you the final array of length m.

Note that steps one and two can be done in the same loop. You may find the function `np.delete()` to be useful while writing this method.

You can test your function by plotting Runge's function $f(x) = \frac{1}{1+25x^2}$ and your interpolating polynomial on the same plot for different values of n equally spaced interpolating values then comparing your plot to the plots given in Figure 9.1.

The Lagrange form of polynomial interpolation is useful in some theoretical contexts and is easier to understand than other methods, however, it has some serious drawbacks that prevent it from being a useful method of interpolation. First, Lagrange interpolation is $O(n^2)$ where other interpolation methods are $O(n^2)$ (or faster) at startup but only $O(n)$ at run-time, Second, Lagrange interpolation is an unstable algorithm which causes it to return innacurate answers when larger numbers of interpolating points are used. Thus, while useful in some situations, Lagrange interpolation is not desirable in most instances.

Barycentric Lagrange interpolation

Barycentric Lagrange interpolation is simple variant of Lagrange interpolation that performs much better than plain Lagrange interpolation. It is essentially just a rearrangement of the order of operations in Lagrange multiplication which results in vastly improved perfomance, both in speed and stability.

Barycentric Lagrange interpolation relies on the observation that each basis function L_j can be rewritten as

$$L_j(x) = \frac{w(x)}{(x - x_j)} w_j$$

where

$$w(x) = \prod_{j=1}^{n} (x - x_j)$$

and

$$w_j = \frac{1}{\prod_{k=1, k\neq j}^{n} (x_j - x_k)}.$$

The w_j's are known as the *barycentric weights*.

Using the previous equations, the interpolating polynomial can be rewritten

$$p(x) = w(x) \sum_{j=1}^{n} \frac{w_j y_j}{x - x_j}$$

which is the *first barycentric form*. The computation of $w(x)$ can be avoided by first noting that

$$1 = w(x) \sum_{j=1}^{n} \frac{w_j}{x - x_j}$$

which allows the interpolating polynomial to be rewriten as

$$p(x) = \frac{\sum_{j=1}^{n} \frac{w_j y_j}{x - x_j}}{\sum_{j=1}^{n} \frac{w_j}{x - x_j}}$$

This form of the Lagrange interpolant is known as the *second barycentric form* which is the form used in Barycentric Lagrange interpolation. So far, the changes made to Lagrange interpolation have resulted in an algorithm that is $O(n)$ once the barycentric weights (w_j) are known. The following adjustments will improve the algorithm so that it is numerically stable and later discussions will allow for the quick addition of new interpolating points after startup.

The second barycentric form makes it clear that any factors that are common to the w_k can be ignored (since they will show up in both the numerator and denominator). This allows for an important improvement to the formula that will prevent overflow error in the arithmetic. When computing the barycentric weights, each element of the product $\prod_{k=1,k\neq j}^{n}(x_j - x_k)$ should be multiplied by C^{-1}, where $4C$ is the width of the interval being interpolated (C is known as the *capacity* of the interval). In effect, this scales each barycentric weight by C^{1-n} which helps to prevent overflow during computation. Thus, the new barycentric weights are given by

$$w_j = \frac{1}{\prod_{k=1,k\neq j}^{n} [(x_j - x_k)C]}.$$

Once again, this change is possible since the extra factor C^{1-n} is cancelled out in the final product. This process is summed up in the following code:

```
# Given a NumPy array xint of interpolating x-values, calculate the weights.
>>> n = len(xint)                   # Number of interpolating points.
>>> w = np.ones(n)                  # Array for storing barycentric weights.
# Calculate the capacity of the interval.
>>> C = (np.max(xint) - np.min(xint)) / 4

>>> shuffle = np.random.permutation(n-1)
>>> for j in range(n):
>>>     temp = (xint[j] - np.delete(xint, j)) / C
>>>     temp = temp[shuffle]         # Randomize order of product.
>>>     w[j] /= np.product(temp)
```

The order of `temp` was randomized so that the arithmetic does not overflow due to poor ordering (if standard ordering is used, overflow errors can be encountered since all of the points of similar magnitude are multiplied together at once). When these two fixes are combined, the Barycentric Algorithm becomes numerically stable.

Problem 2. Create a class that performs Barycentric Lagrange interpolation. The constructor of your class should accept two NumPy arrays which contain the x and y values of the interpolation points. Store these arrays as attributes. In the constructor, compute the corresponding barycentric weights and store the resulting array as a class attribute. Be sure that the relative ordering of the arrays remains unchanged.

Implement the `__call__()` method so that it accepts a NumPy array of values at which to evaluate the interpolating polynomial and returns an array of the evaluated points. Your class can be tested in the same way as the Lagrange function written in Problem 1

ACHTUNG!

As currently explained and implemented, the Barycentric class from Problem 2 will fail when a point to be evaluated exactly matches one of the x-values of the interpolating points. This happens because a divide by zero error is encountered in the final step of the algorithm. The fix for this, although not required here, is quite easy: keep track of any problem points and replace the final computed value with the corresponding y-value (since this is a point that is exactly interpolated). If you do not implement this fix, just be sure not to pass in any points that exactly match your interpolating values.

Another advantage of the barycentric method is that it allows for the addition of new interpolating points in $O(n)$ time. Given a set of existing barycentric weights $\{w_j\}_{j=1}^n$ and a new interpolating point x_i, the new barycentric weight is given by

$$w_i = \frac{1}{\prod_{k=1}^{n}(x_i - x_k)}.$$

In addition to calculating the new barycentric weight, all existing weights should be updated as follows $w_j = \frac{w_j}{x_j - x_i}$.

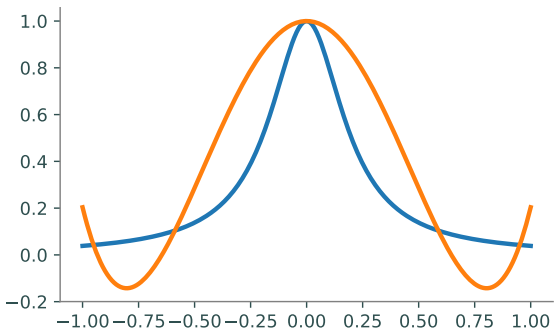
Problem 3. Include a method in the class written in Problem 2 that allows for the addition of new interpolating points by updating the barycentric weights. Your function should accept two NumPy arrays which contain the x and y values of the new interpolation points. Update and store the old weights then extend the class attribute arrays that store the weights, and the x and y values of the interpolation points with the new data. When updating all class attributes, make sure to maintain the same relative order.

The implementation outlined here calls for the y-values of the interpolating points to be known during startup, however, these values are not needed until run-time This allows the y-values to be changed without having to recompute the barycentric weights. This is an additional advantage of Barycentric Lagrange interpolation.

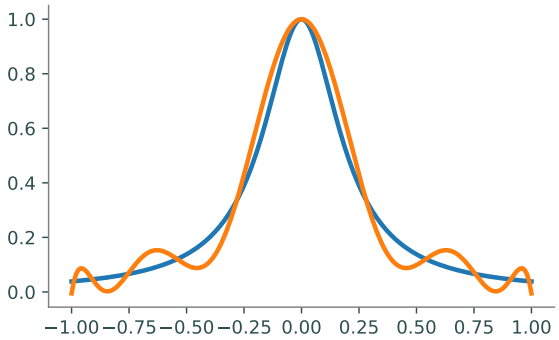
Scipy's Barycentric Lagrange class

Scipy includes a Barycentric interpolator class. This class includes the same functionality as the class described in Problems 2 and 3 in addition to the ability to update the y-values of the interpolation points. The following code will produce a figure similar to Figure 9.1b.

```
>>> from scipy.interpolate import BarycentricInterpolator

>>> f = lambda x: 1/(1+25 * x**2)   # Function to be interpolated.
# Obtain the Chebyshev extremal points on [-1,1].
>>> n = 11
>>> pts = np.linspace(-1, 1, n)
>>> domain = np.linspace(-1, 1, 200)

>>> poly = BarycentricInterpolator(pts[:-1])
>>> poly.add_xi(pts[-1])          # Oops, forgot one of the points.
>>> poly.set_yi(f(pts))           # Set the y values.

>>> plt.plot(domain, f(domain))
>>> plt.plot(domain, poly.eval(domain))
```



(a) Polynomial using 5 Chebyshev roots.



(b) Polynomial using 11 Chebyshev roots.

Figure 9.2: Example of overcoming Runge's phenomenon by using Chebyshev nodes for interpolating values. Plots made using Runge's function $f(x) = \frac{1}{1+25x^2}$. Compare with Figure 9.1

Chebyshev Interpolation

Chebyshev Nodes

As has been mentioned previously, the Barycentric version of Lagrange interpolation is a stable process that does not accumulate large errors, even with extreme inputs. However, polynomial interpolation itself is, in general, an ill-conditioned problem. Thus, even small changes in the interpolating values can give drastically different interpolating polynomials. In fact, poorly chosen interpolating points can result in a very bad approximation of a function. As more points are added, this approximation can worsen. This increase in error is called *Runge's phenomenon*.

The set of equally spaced points is an example of a set of points that may seem like a reasonable choice for interpolation but in reality produce very poor results. Figure 9.1 gives an example of this using Runge's function. As the number of interpolating points increases, the quality of the approximation deteriorates, especially near the endpoints.

Although polynomial interpolation has a great deal of potential error, a good set of interpolating points can result in fast convergence to the original function as the number of interpolating points is increased. One such set of points is the Chebyshev extremal points which are related to the Chebyshev polynomials (to be discussed shortly). The $n+1$ Chebyshev extremal points on the interval $[a,b]$ are given by the formula $y_j = \frac{1}{2}(a+b+(b-a)\cos(\frac{j\pi}{n}))$ for $j = 0, 1, \ldots, n$. These points are shown in Figure 9.3. One important feature of these points is that they are clustered near the endpoints of the interval, this is key to preventing Runge's phenomenon.

Problem 4. Write a function that defines a domain $\mathbf{x}$ of 400 equally spaced points on the interval $[-1,1]$. For $n = 2^2, 2^3, \ldots, 2^8$, repeat the following experiment.

1. Interpolate Runge's function $f(x) = 1/(1+25x^2)$ with n equally spaced points over $[-1,1]$ using SciPy's `BarycentricInterpolator` class, resulting in an approximating function $\tilde{f}$. Compute the absolute error $\|f(\mathbf{x}) - \tilde{f}(\mathbf{x})\|_\infty$ of the approximation using `la.norm()` with `ord=np.inf`.
2. Interpolate Runge's function with $n+1$ Chebyshev extremal points, also via SciPy, and compute the absolute error.

Plot the errors of each method against the number of interpolating points n in a log-log plot.

To verify that your figure make sense, try plotting the interpolating polynomials with the original function for a few of the larger values of n.

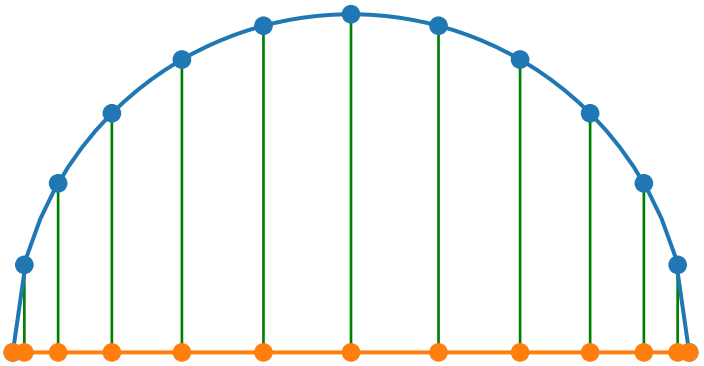


Figure 9.3: The Chebyshev extremal points. The n points where the Chebyshev polynomial of degree n reaches its local extrema. These points are also the projection onto the x-axis of n equally spaced points around the unit circle.

Chebyshev Polynomials

The Chebyshev roots and Chebyshev extremal points are closely related to a set of polynomials known as the Chebyshev polynomials. The first two Chebyshev polynomials are defined as $T_0(x) = 1$ and $T_1(x) = x$. The remaining polynomials are defined by the recursive algorithm $T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$. The Chebyshev polynomials form a complete basis for the polynomials in $\mathbb{R}$ which means that for any polynomial $p(x)$, there exists a set of unique coefficients $\{a_k\}_{k=0}^n$ such that

$$p(x) = \sum_{k=0}^{n} a_k T_k.$$

Finding the Chebyshev representation of an interpolating polynomial is a slow process (dominated by matrix multiplication or solving a linear system), but when the interpolating values are the Chebyshev extrema, there exists a fast algorithm for computing the Chebyshev coefficients of the interpolating polynomial. This algorithm is based on the Fast Fourier transform which has temporal complexity $O(n \log n)$. Given the $n+1$ Chebyshev extremal points $y_j = \cos(\frac{j\pi}{n})$ for $j = 0, 1, \ldots, n$ and a function f, the unique n-degree interpolating polynomial $p(x)$ is given by

$$p(x) = \sum_{k=0}^{n} a_k T_k$$

where

$$a_k = \gamma_k \Re \left[DFT(f(y_0), f(y_1), \ldots, f(y_{2n-1})) \right]_k .$$

Note that although this formulation includes y_j for $j > n$, there are really only $n+1$ distinct values being used since $y_{n-k} = y_{n+k}$. Also, $\Re$ denotes the real part of the Fourier transform and γ_k is defined as

$$\gamma_k = \begin{cases} 1 & k \in \{0, n\} \\ 2 & \text{otherwise.} \end{cases}$$

Problem 5. Write a function that accepts a function f and an integer n. Compute the $n+1$ Chebyshev coefficients for the degree n interpolating polynomial of f using the Fourier transform (`np.real()` and `np.fft.fft()` will be helpful). When using NumPy's `fft()` function, multiply every entry of the resulting array by the scaling factor $\frac{1}{2n}$ to match the derivation given above.

Validate your function with `np.polynomial.chebyshev.poly2cheb()`. The results should be exact for polynomials.

```
# Define f(x) = -3 + 2x^2 - x^3 + x^4 by its (ascending) coefficients.
>>> f = lambda x: -3 + 2*x**2 - x**3 + x**4
>>> pcoeffs = [-3, 0, 2, -1, 1]
>>> ccoeffs = np.polynomial.chebyshev.poly2cheb(pcoeffs)

# The following callable objects are equivalent to f().
>>> fpoly = np.polynomial.Polynomial(pcoeffs)
>>> fcheb = np.polynomial.Chebyshev(ccoeffs)
```

Lagrange vs. Chebyshev

As was previously stated, Barycentric Lagrange interpolation is $O(n^2)$ at startup and $O(n)$ at runtime while Chebyshev interpolation is $O(n \log n)$. This improved speed is one of the greatest advantages of Chebyshev interpolation. Chebyshev interpolation is also more accurate than Barycentric interpolation, even when using the same points. Despite these significant advantages in accuracy and temporal complexity, Barycentric Lagrange interpolation has one very important advantage over Chebyshev interpolation: Barycentric interpolation can be used on any set of interpolating points while Chebyshev is restricted to the Chebyshev nodes. In general, because of their better accuracy, the Chebyshev nodes are more desirable for interpolation, but there are situations when the Chebyshev nodes are not available or when specific points are needed in an interpolation. In these cases, Chebyshev interpolation is not possible and Barycentric Lagrange interpolation must be used.

Utah Air Quality

The Utah Department of Environmental Quality has air quality stations throughout the state of Utah that measure the concentration of particles found in the air. One particulate of particular interest is $PM_{2.5}$ which is a set of extremely fine particles known to cause tissue damage to the lungs. The file `airdata.npy` has the hourly concentration of $PM_{2.5}$ in micrograms per cubic meter for a particular measuring station in Salt Lake County for the year 2016. The given data presents a fairly smooth function which can be reasonably approximated by an interpolating polynomial. Although Chebyshev interpolation would be preferable (because of its superior speed and accuracy), it is not possible in this case because the data is not continous and the information at the Chebyshev nodes is not known. In order to get the best possible interpolation, it is still preferable to use points close to the Chebyshev extrema with Barycentric interpolation. The following code will take the $n+1$ Chebyshev extrema and find the closest match in the non-continuous data found in the variable `data` then calculate the barycentric weights.

```
>>> fx = lambda a, b, n: .5*(a+b + (b-a) * np.cos(np.arange(n+1) * np.pi / n))
>>> a, b = 0, 366 - 1/24
>>> domain = np.linspace(0, b, 8784)
>>> points = fx(a, b, n)
>>> temp = np.abs(points - domain.reshape(8784, 1))
>>> temp2 = np.argmin(temp, axis=0)

>>> poly = barycentric(domain[temp2], data[temp2])
```

Problem 6. Write a function that interpolates the given data along the whole interval at the closest approximations to the $n+1$ Chebyshev extremal nodes. The function should accept n, perform the Barycentric interpolation then plot the original data and the approximating polynomial on the same domain on two separate subplots. Your interpolating polynomial should give a fairly good approximation starting at around 50 points. Note that beyond about 200 points, the given code will break down since it will attempt to return multiple of the same points causing a divide by 0 error. If you did not perform the fix suggested in the `ACHTUNG` box, make sure not to pass in any points that exactly match the interpolating values.

Additional Material

The *Clenshaw Algorithm* is a fast algorithm commonly used to evaluate a polynomial given its representation in Chebyshev coefficients. This algorithm is based on the recursive relation between Chebyshev polynomials and is the algorithm used by NumPy's `polynomial.chebyshev` module.

Algorithm 9.1 Accepts an array x of points at which to evaluate the polynomial and an array $a = [a_0, a_1, \ldots, a_{n-1}]$ of Chebyshev coefficients.

```
1: procedure ClenshawRecursion(x, a)
2:     u_{n+1} ← 0
3:     u_n ← 0
4:     k ← n − 1
5:     while k ≥ 1 do
6:         u_k ← 2x u_{k+1} − u_{k+2} + a_k
7:         k ← k − 1
8:     return a_0 + x u_1 − u_2
```

10 Gaussian Quadrature

Lab Objective: *Learn the basics of Gaussian quadrature and its application to numerical integration. Build a class to perform numerical integration using Legendre and Chebyshev polynomials. Compare the accuracy and speed of both types of Gaussian quadrature with the built-in Scipy package. Perform multivariate Gaussian quadrature.*

Legendre and Chebyshev Gaussian Quadrature

It can be shown that for any class of orthogonal polynomials $p \in \mathbb{R}[x; 2n+1]$ with corresponding weight function $w(x)$, there exists a set of points $\{x_i\}_{i=0}^n$ and weights $\{w_i\}_{i=0}^n$ such that

$$\int_a^b p(x)w(x)dx = \sum_{i=0}^{n} p(x_i)w_i.$$

Since this relationship is exact, a good approximation for the integral

$$\int_a^b f(x)w(x)dx$$

can be expected as long as the function $f(x)$ can be reasonably interpolated by a polynomial at the points x_i for $i = 0, 1, \dots, n$. In fact, it can be shown that if $f(x)$ is $2n+1$ times differentiable, the error of the approximation will decrease as n increases.

Gaussian quadrature can be performed using any basis of orthonormal polynomials, but the most commonly used are the Legendre polynomials and the Chebyshev polynomials. Their weight functions are $w_l(x) = 1$ and $w_c(x) = \frac{1}{\sqrt{1-x^2}}$, respectively, both defined on the open interval $(-1, 1)$.

Problem 1. Define a class for performing Gaussian quadrature. The constructor should accept an integer n denoting the number of points and weights to use (this will be explained later) and a label indicating which class of polynomials to use. If the label is not either `"legendre"` or `"chebyshev"`, raise a `ValueError`; otherwise, store it as an attribute.

The weight function $w(x)$ will show up later in the denominator of certain computations. Define the reciprocal function $w(x)^{-1} = 1/w(x)$ as a `lambda` function and save it as an attribute.

Calculating Points and Weights

All sets of orthogonal polynomials $\{u_k\}_{k=0}^n$ satisfy the three-term recurrence relation

$$u_0 = 1, \qquad u_1 = x - \alpha_1, \qquad u_{k+1} = (x - \alpha_k)u_k - \beta_k u_{k-1}$$

for some coefficients $\{\alpha_k\}_{k=1}^n$ and $\{\beta_k\}_{k=1}^n$. For the Legendre polynomials, they are given by

$$\alpha_k = 0, \qquad \beta_k = \frac{k^2}{4k^2 - 1},$$

and for the Chebyshev polynomials, they are

$$\alpha_k = 0, \qquad \beta_k = \begin{cases} \frac{1}{2} & \text{if } k = 1 \\ \frac{1}{4} & \text{otherwise.} \end{cases}$$

Given these values, the corresponding *Jacobi matrix* is defined as follows.

$$J = \begin{bmatrix} \alpha_1 & \sqrt{\beta_1} & 0 & \dots & 0 \\ \sqrt{\beta_1} & \alpha_2 & \sqrt{\beta_2} & \dots & 0 \\ 0 & \sqrt{\beta_2} & \alpha_3 & \ddots & 0 \\ \vdots & & \ddots & \ddots & \vdots \\ 0 & \dots & & & \sqrt{\beta_{n-1}} \\ 0 & \dots & & \sqrt{\beta_{n-1}} & \alpha_n \end{bmatrix}$$

According to the *Golub-Welsch algorithm*,[1] the n eigenvalues of J are the points x_i to use in Gaussian quadrature, and the corresponding weights are given by $w_i = \mu_w(\mathbb{R})v_{i,0}^2$ where $v_{i,0}$ is the first entry of the ith eigenvector and $\mu_w(\mathbb{R}) = \int_{-\infty}^{\infty} w(x)dx$ is the *measure* of the weight function. Since the weight functions for Legendre and Chebyshev polynomials have compact support on the interval $(-1, 1)$, their measures are given as follows.

$$\mu_{w_l}(\mathbb{R}) = \int_{-\infty}^{\infty} w_l(x)dx = \int_{-1}^{1} 1dx = 2 \qquad \mu_{w_c}(\mathbb{R}) = \int_{-\infty}^{\infty} w_c(x)dx = \int_{-1}^{1} \frac{1}{\sqrt{1-x^2}}dx = \pi$$

Problem 2. Write a method for your class from Problem 1 that accepts an integer n. Construct the $n \times n$ Jacobi matrix J for the polynomial family indicated in the constructor. Use SciPy to compute the eigenvalues and eigenvectors of J, then compute the points $\{x_i\}_{i=1}^n$ and weights $\{w_i\}_{i=1}^n$ for the quadrature. Return both the array of points and the array weights.

Test your method by checking your points and weights against the following values using the Legendre polynomials with $n = 5$.

x_i	$-\frac{1}{3}\sqrt{5+2\sqrt{\frac{10}{7}}}$	$-\frac{1}{3}\sqrt{5-2\sqrt{\frac{10}{7}}}$	0	$\frac{1}{3}\sqrt{5-2\sqrt{\frac{10}{7}}}$	$\frac{1}{3}\sqrt{5+2\sqrt{\frac{10}{7}}}$
w_i	$\frac{322-13\sqrt{70}}{900}$	$\frac{322+13\sqrt{70}}{900}$	$\frac{128}{225}$	$\frac{322+13\sqrt{70}}{900}$	$\frac{322-13\sqrt{70}}{900}$

[1] See `http://gubner.ece.wisc.edu/gaussquad.pdf` for a complete treatment of the Golub-Welsch algorithm, including the computation of the recurrence relation coefficients for arbitrary orthogonal polynomials.

Finally, modify the constructor of your class so that it calls your new function and stores the resulting points and weights as attributes.

Integrating with Given Weights and Points

Now that the points and weights have been obtained, they can be used to approximate the integrals of different functions. For a given function $f(x)$ with points x_i and weights w_i,

$$\int_{-1}^{1} f(x)w(x)dx \approx \sum_{i=1}^{n} f(x_i)w_i.$$

There are two problems with the preceding formula. First, the weight function is part of the integral being approximated, and second, the points obtained are only found on the interval $(-1, 1)$ (in the case of the Legendre and Chebyshev polynomials). To solve the first problem, define a new function $g(x) = f(x)/w(x)$ so that

$$\int_{-1}^{1} f(x)dx = \int_{-1}^{1} g(x)w(x)dx \approx \sum_{i=1}^{n} g(x_i)w_i. \tag{10.1}$$

The integral of $f(x)$ on $[-1, 1]$ can thus be approximated with the inner product $\mathbf{w}^\mathsf{T} g(\mathbf{x})$, where $g(\mathbf{x}) = [g(x_1), \dots, g(x_n)]^\mathsf{T}$ and $\mathbf{w} = [w_1, \dots, w_n]^\mathsf{T}$.

Problem 3. Write a method for your class that accepts a callable function f. Use (10.1) and the stored points and weights to approximate of the integral of f on the interval $[-1, 1]$. (Hint: Use $w(x)^{-1}$ from Problem 1 to compute $g(x)$ without division.)

Test your method with examples that are easy to compute by hand and by comparing your results to `scipy.integrate.quad()`.

```
>>> import numpy as np
>>> from scipy.integrate import quad

# Integrate f(x) = 1 / sqrt(1 - x**2) from -1 to 1.
>>> f = lambda x: 1 / np.sqrt(1 - x**2)
>>> quad(f, -1, 1)[0]
3.141592653589591
```

Note

Since the points and weights for Gaussian quadrature do not depend on f, they only need to be computed once and can then be reused to approximate the integral of any function. The class structure in Problems 1–4 takes advantage of this fact, but `scipy.integrate.quad()` does not. If a larger n is needed for higher accuracy, however, the computations must be repeated to get a new set of points and weights.

Shifting the Interval of Integration

Since the weight functions for the Legendre and Chebyshev polynomials have compact support on the interval $(-1, 1)$, all of the quadrature points are found on that interval as well. To integrate a function on an arbitrary interval $[a, b]$ requires a change of variables. Let

$$u = \frac{2x - b - a}{b - a}$$

so that $u = -1$ when $x = a$ and $u = 1$ when $x = b$. Then

$$x = \frac{b-a}{2}u + \frac{a+b}{2} \qquad \text{and} \qquad dx = \frac{b-a}{2}du,$$

so the transformed integral is given by

$$\int_a^b f(x)dx = \frac{b-a}{2}\int_{-1}^{1} f\left(\frac{b-a}{2}u + \frac{a+b}{2}\right)du.$$

By defining a new function $h(x)$ as

$$h(x) = f\left(\frac{(b-a)}{2}x + \frac{(a+b)}{2}\right),$$

the integral of f can be approximated by integrating h over $[-1, 1]$ with (10.1). This results in the final quadrature formula

$$\int_a^b f(x)dx = \frac{b-a}{2}\int_{-1}^{1} h(x)dx = \frac{b-a}{2}\int_{-1}^{1} g(x)w(x)dx \approx \frac{b-a}{2}\sum_{i=1}^{n} g(x_i)w_i, \tag{10.2}$$

where now $g(x) = h(x)/w(x)$.

Problem 4. Write a method for your class that accepts a callable function f and bounds of integration a and b. Use (10.2) to approximate the integral of f from a to b.
(Hint: Define $h(x)$ and use your method from Problem 3.)

Problem 5. The *standard normal distribution* has the following probability density function.

$$f(x) = \frac{1}{\sqrt{2\pi}}e^{-x^2/2}$$

This function has no symbolic antiderivative, so it can only be integrated numerically. The following code gives an "exact" value of the integral of $f(x)$ from $-\infty$ to a specified value.

```
>>> from scipy.stats import norm

>>> norm.cdf(1)                    # Integrate f from -infty to 1.
0.84134474606854293
>>> norm.cdf(1) - norm.cdf(-1)     # Integrate f from -1 to 1.
0.68268949213708585
```

Write a function that uses `scipy.stats` to calculate the "exact" value

$$F = \int_{-3}^{2} f(x)dx.$$

Then repeat the following experiment for $n = 5, 10, 15, \ldots, 50$.

1. Use your class from Problems 1–4 with the Legendre polynomials to approximate F using n points and weights. Calculate and record the error of the approximation.
2. Use your class with the Chebyshev polynomials to approximate F using n points and weights. Calculate and record the error of the approximation.

Plot the errors against the number of points and weights n, using a log scale for the y-axis. Finally, plot a horizontal line showing the error of `scipy.integrate.quad()` (which doesn't depend on n).

Multivariate Quadrature

The extension of Gaussian quadrature to higher dimensions is fairly straightforward. The same set of points $\{z_i\}_{i=1}^n$ and weights $\{w_i\}_{i=1}^n$ can be used in each direction, so the only difference from 1-D quadrature is how the function is shifted and scaled. To begin, let $h : \mathbb{R}^2 \to \mathbb{R}$ and define $g : \mathbb{R}^2 \to \mathbb{R}$ by $g(x, y) = h(x, y)/(w(x)w(y))$ so that

$$\int_{-1}^{1}\int_{-1}^{1} h(x, y)dx\, dy. = \int_{-1}^{1}\int_{-1}^{1} g(x, y)w(x)w(y)dx\, dy \approx \sum_{i=1}^{n}\sum_{j=1}^{n} w_i w_j g(z_i, z_j). \tag{10.3}$$

To integrate $f : \mathbb{R}^2 \to \mathbb{R}$ over an arbitrary box $[a_1, b_1] \times [a_2, b_2]$, set

$$h(x, y) = f\left(\frac{b_1 - a_1}{2}x + \frac{a_1 + b_1}{2},\ \frac{b_2 - a_2}{2}y + \frac{a_2 + b_2}{2}\right)$$

so that

$$\int_{a_2}^{b_2}\int_{a_1}^{b_1} f(x)dx\, dy = \frac{(b_1 - a_1)(b_2 - a_2)}{4}\int_{-1}^{1}\int_{-1}^{1} h(x, y)dx\, dy. \tag{10.4}$$

Combining (10.3) and (10.4) gives the final 2-D Gaussian quadrature formula. Compare it to (10.2).

$$\int_{a_2}^{b_2}\int_{a_1}^{b_1} f(x)dx\, dy \approx \frac{(b_1 - a_1)(b_2 - a_2)}{4}\sum_{i=1}^{n}\sum_{j=1}^{n} w_i w_j g(z_i, z_j) \tag{10.5}$$

Problem 6. Write a method for your class that accepts a function $f : \mathbb{R}^2 \to \mathbb{R}$ (which actually accepts two separate arguments, not one array with two elements) and bounds of integration a_1, a_2, b_1, and b_2. Use (10.5) to compute the double integral

$$\int_{a_2}^{b_2}\int_{a_1}^{b_1} f(x)dx\, dy.$$

Validate your method by comparing it `scipy.integrate.nquad()`. Note carefully that this function has slightly different syntax for the bounds of integration.

```
>>> from scipy.integrate import nquad

# Integrate f(x,y) = sin(x) + cos(y) over [-10,10] in x and [-1,1] in y.
>>> f = lambda x, y: np.sin(x) + np.cos(y)
>>> nquad(f, [[-10, 10], [-1, 1]])[0]
33.658839392315855
```

Note

Although Gaussian quadrature can obtain reasonable approximations in lower dimensions, it quickly becomes intractable in higher dimensions due to the curse of dimensionality. In other words, the number of points and weights required to obtain a good approximation becomes so large that Gaussian quadrature become computationally infeasible. For this reason, high-dimensional integrals are often computed via *Monte Carlo methods*, numerical integration techniques based on random sampling. However, quadrature methods are generally significantly more accurate in lower dimensions than Monte Carlo methods.

11 One-dimensional Optimization

Lab Objective: *Most mathematical optimization problems involve estimating the minimizer(s) of a scalar-valued function. Many algorithms for optimizing functions with a high-dimensional domain depend on routines for optimizing functions of a single variable. There are many techniques for optimization in one dimension, each with varying degrees of precision and speed. In this lab, we implement the golden section search method, Newton's method, and the secant method, then apply them to the backtracking problem.*

Golden Section Search

A function $f : [a, b] \to \mathbb{R}$ satisfies the *unimodal property* if it has exactly one local minimum and is monotonic on either side of the minimizer. In other words, f decreases from a to its minimizer x^*, then increases up to b (see Figure 11.1). The *golden section search* method optimizes a unimodal function f by iteratively defining smaller and smaller intervals containing the unique minimizer x^*. This approach is especially useful if the function's derivative does not exist, is unknown, or is very costly to compute.

By definition, the minimizer x^* of f must lie in the interval $[a, b]$. To shrink the interval around x^*, we test the following strategically chosen points.

$$\tilde{a} = b - \frac{b-a}{\varphi} \qquad \tilde{b} = a + \frac{b-a}{\varphi}$$

Here $\varphi = \frac{1+\sqrt{5}}{2}$ is the *golden ratio*. At each step of the search, $[a, b]$ is refined to either $[a, \tilde{b}]$ or $[\tilde{a}, b]$, called the *golden sections*, depending on the following criteria.

If $f(\tilde{a}) < f(\tilde{b})$, then since f is unimodal, it must be increasing in a neighborhood of $\tilde{b}$. The unimodal property also guarantees that f must be increasing on $[\tilde{b}, b]$ as well, so $x^* \in [a, \tilde{b}]$ and we set $b = \tilde{b}$. By similar reasoning, if $f(\tilde{a}) > f(\tilde{b})$, then $x^* \in [\tilde{a}, b]$ and we set $a = \tilde{a}$. If, however, $f(\tilde{a}) = f(\tilde{b})$, then the unimodality of f does not guarantee anything about where the minimizer lies. Assuming either $x^* \in [a, \tilde{b}]$ or $x^* \in [\tilde{a}, b]$ allows the iteration to continue, but the method is no longer guaranteed to converge to the local minimum.

At each iteration, the length of the search interval is divided by φ. The method therefore converges linearly, which is somewhat slow. However, the idea is simple and each step is computationally inexpensive.

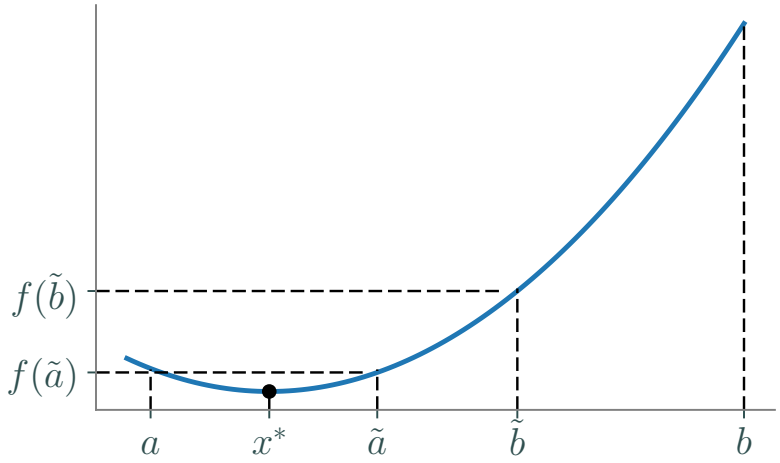


Figure 11.1: The unimodal $f : [a, b] \to \mathbb{R}$ can be minimized with a golden section search. For the first iteration, $f(\tilde{a}) < f(\tilde{b})$, so $x^* \in [a, \tilde{b}]$. New values of $\tilde{a}$ and $\tilde{b}$ are then calculated from this new, smaller interval.

Algorithm 11.1 The Golden Section Search

```
procedure GOLDEN_SECTION(f, a, b, tol, maxiter)
    x_0 ← (a + b)/2                ▷ Set the initial minimizer approximation as the interval midpoint.
    φ = (1 + √5)/2
    for i = 1, 2, ..., maxiter do          ▷ Iterate only maxiter times at most.
        c ← (b − a)/φ
        ã ← b − c
        b̃ ← a + c
        if f(ã) ≤ f(b̃) then                ▷ Get new boundaries for the search interval.
            b ← b̃
        else
            a ← ã
        x_1 ← (a + b)/2            ▷ Set the minimizer approximation as the interval midpoint.
        if |x_0 − x_1| < tol then
            break                  ▷ Stop iterating if the approximation stops changing enough.
        x_0 ← x_1
    return x_1
```

Problem 1. Write a function that accepts a function $f : \mathbb{R} \to \mathbb{R}$, interval limits a and b, a stopping tolerance `tol`, and a maximum number of iterations `maxiter`. Use Algorithm 11.1 to implement the golden section search. Return the approximate minimizer x^*, whether or not the algorithm converged (`true` or `false`), and the number of iterations computed.

Test your function by minimizing $f(x) = e^x - 4x$ on the interval $[0, 3]$, then plotting the function and the computed minimizer together. Also compare your results to SciPy's golden section search, `scipy.optimize.golden()`.

```
>>> from scipy import optimize as opt
>>> import numpy as np

>>> f = lambda x : np.exp(x) - 4*x
>>> opt.golden(f, brack=(0,3), tol=.001)
1.3862578679031485              # ln(4) is the minimizer.
```

Newton's Method

Newton's method is an important root-finding algorithm that can also be used for optimization. Given $f : \mathbb{R} \to \mathbb{R}$ and a good initial guess x_0, the sequence $(x_k)_{k=1}^{\infty}$ generated by the recursive rule

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$$

converges to a point $\bar{x}$ satisfying $f(\bar{x}) = 0$. The first-order necessary conditions from elementary calculus state that if f is differentiable, then its derivative evaluates to zero at each of its local minima and maxima. Therefore using Newton's method to find the zeros of f' is a way to identify potential minima or maxima of f. Specifically, starting with an initial guess x_0, set

$$x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)} \tag{11.1}$$

and iterate until $|x_k - x_{k-1}|$ is satisfactorily small. Note that this procedure does not use the actual function f at all, but it requires many evaluations of its first and second derivatives. As a result, Newton's method converges in few iterations, but it can be computationally expensive.

Each step of (11.1) can be thought of approximating the objective function f by a quadratic function q and finding its unique extrema. That is, we first approximate f with its second-degree Taylor polynomial centered at x_k.

$$q(x) = f(x_k) + f'(x_k)(x - x_k) + \frac{1}{2}f''(x_k)(x - x_k)^2$$

This quadratic function satisfies $q(x_k) = f(x_k)$ and matches f fairly well close to x_k. Thus the optimizer of q is a reasonable guess for an optimizer of f. To compute that optimizer, solve $q'(x) = 0$.

$$0 = q'(x) = f'(x_k) + f''(x_k)(x - x_k) \qquad \Longrightarrow \qquad x = x_k - \frac{f'(x_k)}{f''(x_k)}$$

This agrees with (11.1) using x_{k+1} for x. See Figure 11.2.

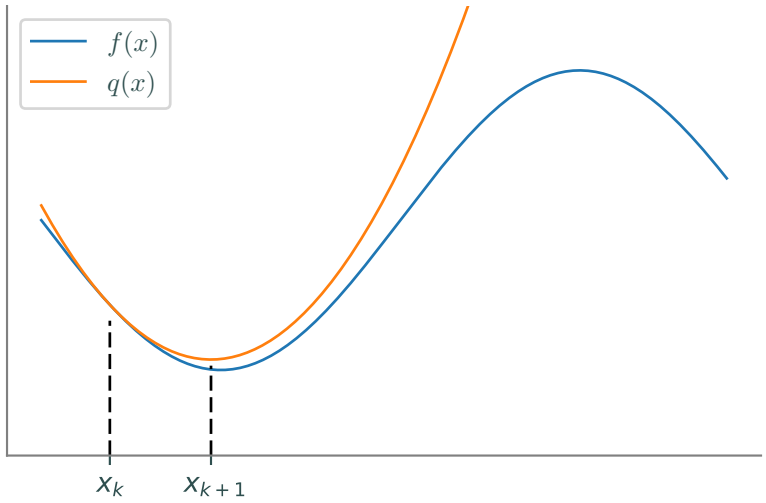


Figure 11.2: A quadratic approximation of f at x_k. The minimizer x_{k+1} of q is close to the minimizer of f.

Newton's method for optimization works well to locate minima when $f''(x) > 0$ on the entire domain. However, it may fail to converge to a minimizer if $f''(x) \leq 0$ for some portion of the domain. If f is not unimodal, the initial guess x_0 must be sufficiently close to a local minimizer x^* in order to converge.

Problem 2. Let $f : \mathbb{R} \to \mathbb{R}$. Write a function that accepts f', f'', a starting point x_0, a stopping tolerance `tol`, and a maximum number of iterations `maxiter`. Implement Newton's method using (11.1) to locate a local optimizer. Return the approximate optimizer, whether or not the algorithm converged, and the number of iterations computed.

Test your function by minimizing $f(x) = x^2 + \sin(5x)$ with an initial guess of $x_0 = 0$. Compare your results to `scipy.optimize.newton()`, which implements the root-finding version of Newton's method.

```
>>> df = lambda x : 2*x + 5*np.cos(5*x)
>>> d2f = lambda x : 2 - 25*np.sin(5*x)
>>> opt.newton(df, x0=0, fprime=d2f, tol=1e-10, maxiter=500)
-1.4473142236328096
```

Note that other initial guesses can yield different minima for this function.

The Secant Method

The second derivative of an objective function is not always known or may be prohibitively expensive to evaluate. The *secant method* solves this problem by numerically approximating the second derivative with a difference quotient.

$$f''(x) \approx \frac{f'(x+h) - f'(x)}{h}$$

Selecting $x = x_k$ and $h = x_{k-1} - x_k$ gives the following approximation.

$$f''(x_k) \approx \frac{f'(x_k + x_{k-1} - x_k) - f'(x_k)}{x_{k-1} - x_k} = \frac{f(x_k) - f'(x_{k-1})}{x_k - x_{k-1}} \tag{11.2}$$

Inserting (11.2) into (11.1) results in the complete secant method formula.

$$x_{k+1} = x_k - \frac{x_k - x_{k-1}}{f'(x_k) - f'(x_{k-1})} f'(x_k) = \frac{x_{k-1} f'(x_k) - x_k f'(x_{k-1})}{f'(x_k) - f'(x_{k-1})} \tag{11.3}$$

Notice that this recurrence relation requires two previous points (both x_k and x_{k-1}) to calculate the next estimate. This method converges superlinearly—slower than Newton's method, but faster than the golden section search—with convergence criteria similar to Newton's method.

Problem 3. Write a function that accepts a first derivative f', starting points x_0 and x_1, a stopping tolerance `tol`, and a maximum of iterations `maxiter`. Use (11.3) to implement the Secant method. Try to make as few computations as possible by only computing $f'(x_k)$ once for each k. Return the minimizer approximation, whether or not the algorithm converged, and the number of iterations computed.

Test your code with the function $f(x) = x^2 + \sin(x) + \sin(10x)$ and with initial guesses of $x_0 = 0$ and $x_1 = -1$. Plot your answer with the graph of the function. Also compare your results to `scipy.optimize.newton()`; without providing the `fprime` argument, this function uses the secant method. However, it still only takes in one initial condition, so it may converge to a different local minimum than your function.

```
>>> df = lambda x: 2*x + np.cos(x) + 10*np.cos(10*x)
>>> opt.newton(df, x0=0, tol=1e-10, maxiter=500)
-3.2149595174761636
```

Descent Methods

Consider now a function $f : \mathbb{R}^n \to \mathbb{R}$. *Descent methods*, also called *line search methods*, are optimization algorithms that create a convergent sequence $(x_k)_{k=1}^{\infty}$ by the following rule.

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{p}_k \tag{11.4}$$

Here $\alpha_k \in \mathbb{R}$ is called the *step size* and $\mathbf{p}_k \in \mathbb{R}^n$ is called the *search direction*. The choice of $\mathbf{p}_k$ is usually what distinguishes an algorithm; in the one-dimensional case ($n = 1$), $p_k = f'(x_k)/f''(x_k)$ results in Newton's method, and using the approximation in (11.2) results in the secant method.

To be effective, a descent method must also use a good step size α_k. If α_k is too large, the method may repeatedly overstep the minimum; if α_k is too small, the method may converge extremely slowly. See Figure 11.3.

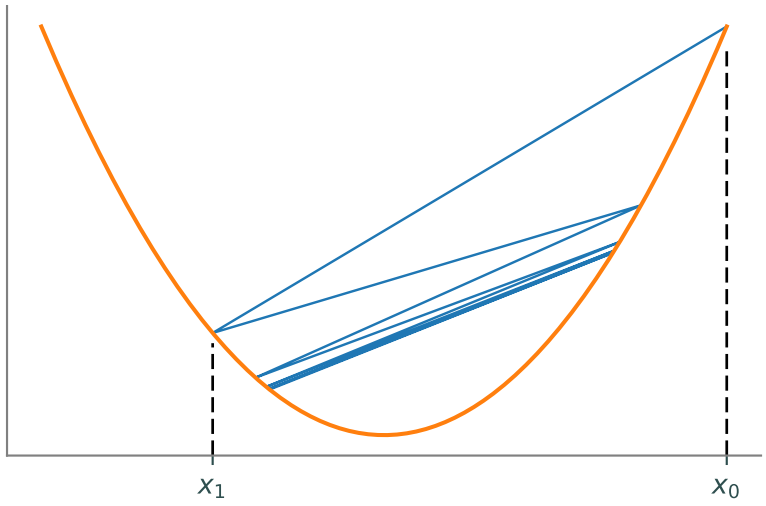


Figure 11.3: If the step size α_k is too large, a descent method may repeatedly overstep the minimizer.

Given a search direction $\mathbf{p}_k$, the best step size α_k minimizes the function $\phi_k(\alpha) = f(\mathbf{x}_k + \alpha\mathbf{p}_k)$. Since f is scalar-valued, $\phi_k : \mathbb{R} \to \mathbb{R}$, so any of the optimization methods discussed previously can be used to minimize ϕ_k. However, computing the best α_k at every iteration is not always practical. Instead, some methods use a cheap routine to compute a step size that may not be optimal, but which is good enough. The most common approach is to find an α_k that satisfies the *Wolfe conditions*:

$$f(\mathbf{x}_k + \alpha_k\mathbf{p}_k) \leq f(\mathbf{x}_k) + c_1\alpha_k Df(\mathbf{x}_k)^\mathsf{T}\mathbf{p}_k \tag{11.5}$$

$$-Df(\mathbf{x}_k + \alpha_k\mathbf{p}_k)^\mathsf{T}\mathbf{p}_k \leq -c_2 Df(\mathbf{x}_k)^\mathsf{T}\mathbf{p}_k \tag{11.6}$$

where $0 < c1 < c2 < 1$ (for the best results, choose $c1 << c2$). The condition (11.5) is also called the *Armijo rule* and ensures that the step decreases f. However, this condition is not enough on its own. By Taylor's theorem,

$$f(\mathbf{x}_k + \alpha_k\mathbf{p}_k) = f(\mathbf{x}_k) + \alpha_k Df(\mathbf{x}_k)^\mathsf{T}\mathbf{p}_k + \mathcal{O}(\alpha_k^2).$$

Thus, a very small α_k will always satisfy (11.5) since $Df(\mathbf{x}_k)^\mathsf{T}\mathbf{p}_k < 0$ (as $\mathbf{p}_k$ is a descent direction). The condition (11.6), called the *curvature condition*, ensures that the α_k is large enough for the algorithm to make significant progress.

It is possible to find an α_k that satisfies the Wolfe conditions, but that is far from the minimizer of $\phi_k(\alpha)$. The *strong Wolfe conditions* modify (11.6) to ensure that α_k is near the minimizer.

$$|Df(\mathbf{x}_k + \alpha_k\mathbf{p}_k)^\mathsf{T}\mathbf{p}_k| \leq c_2|Df(\mathbf{x}_k)^\mathsf{T}\mathbf{p}_k|$$

The *Armijo–Goldstein conditions* provide another alternative to (11.6):

$$f(\mathbf{x}_k) + (1-c)\alpha_k Df(\mathbf{x}_k)^\mathsf{T}\mathbf{p}_k \leq f(\mathbf{x}_k + \alpha_k\mathbf{p}_k) \leq f(\mathbf{x}_k) + c\alpha_k Df(\mathbf{x}_k)^\mathsf{T}\mathbf{p}_k,$$

where $0 < c < 1$. These conditions are very similar to the Wolfe conditions (the right inequality is (11.5)), but they do not require the calculation of the directional derivative $Df(\mathbf{x}_k + \alpha_k\mathbf{p}_k)^\mathsf{T}\mathbf{p}_k$.

Backtracking

A *backtracking line search* is a simple strategy for choosing an acceptable step size α_k: start with an fairly large initial step size α, then repeatedly scale it down by a factor ρ until the desired conditions are satisfied. The following algorithm only requires α to satisfy (11.5). This is usually sufficient, but if it finds α's that are too small, the algorithm can be modified to satisfy (11.6) or one of its variants.

Algorithm 11.2 Backtracking using the Armijo Rule

procedure BACKTRACKING(f, Df, $\mathbf{x}_k$, $\mathbf{p}_k$, α, ρ, c)
    `Dfp` $\leftarrow Df(\mathbf{x}_k)^T\mathbf{p}_k$ ▷ Compute these values only once.
    `fx` $\leftarrow f(\mathbf{x}_k)$
    while $\big(f(\mathbf{x}_k + \alpha\mathbf{p}_k) >$ `fx` $+ c\alpha$`Dfp`$\big)$ **do**
        $\alpha \leftarrow \rho\alpha$
    return α

Problem 4. Write a function that accepts a function $f : \mathbb{R}^n \to \mathbb{R}$, its derivative $Df : \mathbb{R}^n \to \mathbb{R}^n$, an approximate minimizer $\mathbf{x}_k$, a search direction $\mathbf{p}_k$, an initial step length α, and parameters ρ and c. Implement the backtracking method of Algorithm 11.2. Return the computed step size.

The functions f and Df should both accept 1-D NumPy arrays of length n. For example, if $f(x, y, z) = x^2 + y^2 + z^2$, then f and Df could be defined as follows.

```
>>> f = lambda x: x[0]**2 + x[1]**2 + x[2]**2
>>> Df = lambda x: np.array([2*x[0], 2*x[1], 2*x[2]])
```

SciPy's `scipy.optimize.linesearch.scalar_search_armijo()` finds an acceptable step size using the Armijo rule. It may not give the exact answer as your implementation since it decreases α differently, but the answers should be similar.

```
>>> from scipy.optimize import linesearch
>>> from autograd import numpy as anp
>>> from autograd import grad

# Get a step size for f(x,y,z) = x^2 + y^2 + z^2.
>>> f = lambda x: x[0]**2 + x[1]**2 + x[2]**2
>>> x = anp.array([150., .03, 40.])          # Current minimizer guesss.
>>> p = anp.array([-.5, -100., -4.5])        # Current search direction.
>>> phi = lambda alpha: f(x + alpha*p)       # Define phi(alpha).
>>> dphi = grad(phi)
>>> alpha, _ = linesearch.scalar_search_armijo(phi, phi(0.), dphi(0.))
```

12 Newton and Quasi-Newton Methods

Lab Objective: *Newton's method is the basis of several iterative methods for optimization. Though it converges quickly, it is often very computationally expensive. Variants on Newton's method, including BFGS, remedy the problem somewhat by numerically approximating Hessian matrices. In this lab we implement Newton's method, BFGS, and the Gauss-Newton method for nonlinear least squares problems.*

Newton's Method

For $g : \mathbb{R} \to \mathbb{R}$, Newton's method finds a root $\bar{x}$ of the equation $g(x) = 0$ with the following rule.

$$x_{k+1} = x_k - \frac{g(x_k)}{g'(x_k)} \tag{12.1}$$

Let $f : \mathbb{R} \to \mathbb{R}$. Substituting $g = f'$ into (12.1) yields an iterative method for locating a critical point x^* of f satisfying $f'(x^*) = 0$.

$$x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)} \tag{12.2}$$

This technique generalizes to higher dimensions. For $g : \mathbb{R}^n \to \mathbb{R}^n$, the following iterative technique finds $\bar{\mathbf{x}}$ such that $g(\bar{\mathbf{x}}) = \mathbf{0}$.

$$\mathbf{x}_{k+1} = \mathbf{x}_k - Dg(\mathbf{x}_k)^{-1} g(\mathbf{x}_k) \tag{12.3}$$

Now let $f : \mathbb{R}^n \to \mathbb{R}$. To calculate an optimal value $\mathbf{x}^*$ of f satisfying $Df(\mathbf{x}^*) = \mathbf{0}$, plug $g = Df$ into (12.3) to get the following equation.

$$\mathbf{x}_{k+1} = \mathbf{x}_k - D^2 f(\mathbf{x}_k)^{-1} Df(\mathbf{x}_k)^\mathsf{T} \tag{12.4}$$

Here the first derivative $Df : \mathbb{R}^n \to \mathbb{R}^n$ evaluates to the row vector $Df(\mathbf{x}) = [D_1 f(\mathbf{x}) \ \dots \ D_n f(\mathbf{x})]$, and the second derivative $D^2 f : \mathbb{R}^n \to \mathbb{R}^{n \times n}$ evaluates to the $n \times n$ *Hessian* matrix

$$D^2 f(\mathbf{x}) = \begin{bmatrix} D_1 D_1 f(\mathbf{x}) & \dots & D_n D_1 f(\mathbf{x}) \\ D_1 D_2 f(\mathbf{x}) & \dots & D_n D_2 f(\mathbf{x}) \\ \vdots & & \vdots \\ D_1 D_n f(\mathbf{x}) & \dots & D_n D_n f(\mathbf{x}) \end{bmatrix} = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_1 \partial x_n} & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_n} \end{bmatrix}.$$

Problem 1. Write a function that accepts functions $Df : \mathbb{R}^n \to \mathbb{R}^n$ and $D^2f : \mathbb{R}^n \to \mathbb{R}^{n\times n}$, a starting point $\mathbf{x}_0 \in \mathbb{R}^n$, a stopping tolerance `tol` defaulting to $1e^{-5}$, and an integer `maxiter` defaulting to 20 . Use Newton's method in (12.4) to optimize f. Return the final estimate $\mathbf{x}_k$, whether or not the method converged (`True` or `False`), and the number of iterations computed.

Your implementation should include the following items.

- Iterate until either $\|Df(\mathbf{x}_k)\|_\infty <$ `tol` or $k >$ `maxiter`. The criteria $\|\mathbf{x}_k - \mathbf{x}_{k-1}\| <$ `tol` is also common, but making sure Df is near zero works better in many circumstances.
- Instead of inverting $D^2f(\mathbf{x}_k)$ at each step, solve the equation $D^2f(\mathbf{x}_k)\mathbf{z}_k = Df(\mathbf{x}_k)^\mathsf{T}$ and compute $\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{z}_k$. In other words, use `la.solve()` instead of `la.inv()`.
- Avoid recomputing values by only computing $Df(\mathbf{x}_k)$ and $D^2f(\mathbf{x}_k)$ once for each k.

The *Rosenbrock function* is a common test function for optimization methods.

$$f(x, y) = 100(y - x^2)^2 + (1 - x)^2$$

The minimizer is $\mathbf{x}^* = (1, 1)$ with minimum value $f(1, 1) = 0$. Test your function by minimizing the Rosenbrock function using an initial guess $\mathbf{x}_0 = (-2, 2)$. The function and its derivatives are implemented as `rosen()`, `rosen_der()`, and `rosen_hess()` in `scipy.optimize`. Compare your results to `scipy.optimize.fmin_bfgs()`.

```
>>> from scipy import optimize as opt

>>> f = opt.rosen                    # The Rosenbrock function.
>>> df = opt.rosen_der               # The first derivative.
>>> d2f = opt.rosen_hess             # The second derivative (Hessian).
>>> opt.fmin_bfgs(f=f, x0=[-2,2], fprime=df, maxiter=50)
Optimization terminated successfully.
         Current function value: 0.000000
         Iterations: 35
         Function evaluations: 42
         Gradient evaluations: 42
array([ 1.00000021,  1.00000045])
```

BFGS

Newton's method enjoys quadratic convergence when the initial guess is good enough. However, computing and inverting the Hessian matrix at each step of (12.4) is often prohibitively expensive. The idea behind *quasi-Newton methods* is to numerically approximate the inverse of the Hessian at each step. These methods sacrifice some convergence properties in exchange for becoming less computationally expensive. They also make it possible to optimize functions where D^2f is unknown.

Broyden's method is a high-dimensional generalization of the secant method. Just as the secant method approximates the second derivative of f in (12.2) by using the first derivative at nearby points, Broyden's method uses the first derivative to update an approximated Hessian matrix.

$$\mathbf{x}_{k+1} = \mathbf{x}_k - A_k^{-1} Df(\mathbf{x}_k)^\mathsf{T}, \qquad A_{k+1} = A_k + \frac{\mathbf{y}_k - A_k\mathbf{s}_k}{\|\mathbf{s}_k\|^2}\mathbf{s}_k^\mathsf{T}, \tag{12.5}$$

where $\mathbf{s}_k = \mathbf{x}_{k+1} - \mathbf{x}_k$ and $\mathbf{y}_k = Df(\mathbf{x}_{k+1})^\mathsf{T} - Df(\mathbf{x}_k)^\mathsf{T}$.

Though this method no longer explicitly calculates the Hessian $D^2 f(\mathbf{x}_k)$, it still involves a matrix inversion. The *Sherman-Morrison-Woodbury* formula translates the update rule for A_k in (12.5) into the following update rule for A_k^{-1}.

$$A_{k+1}^{-1} = A_k^{-1} + \frac{\mathbf{s}_k - A_k^{-1}\mathbf{y}_k}{\mathbf{s}_k^\mathsf{T} A_k^{-1}\mathbf{y}_k}(\mathbf{s}_k^\mathsf{T} A_k^{-1})$$

Unfortunately, even if $D^2 f(\mathbf{x}_k)$ is positive definite (which is desirable for minimization), the first-order approximation A_k is not guaranteed to be positive definite, so Broyden's method is unreliable. The *Broyden-Fletcher-Goldfarb-Shanno* (BFGS) method remedies this problem by using the following positive definite second-order approximation for the Hessian.

$$A_{k+1} = A_k + \frac{\mathbf{y}_k\mathbf{y}_k^\mathsf{T}}{\mathbf{y}_k^\mathsf{T}\mathbf{s}_k} - \frac{A_k\mathbf{s}_k\mathbf{s}_k^\mathsf{T}A_k}{\mathbf{s}_k^\mathsf{T}A_k\mathbf{s}_k}$$

The Sherman-Morrison-Woodbury formula can also be applied in this situation to yield a computationally efficient form of BFGS.

$$\mathbf{x}_{k+1} = \mathbf{x}_k - A_k^{-1} Df(\mathbf{x}_k)^\mathsf{T} \tag{12.6}$$

$$A_{k+1}^{-1} = A_k^{-1} + \frac{(\mathbf{s}_k^\mathsf{T}\mathbf{y}_k + \mathbf{y}_k^\mathsf{T}A_k^{-1}\mathbf{y}_k)\mathbf{s}_k\mathbf{s}_k^\mathsf{T}}{(\mathbf{s}_k^\mathsf{T}\mathbf{y}_k)^2} - \frac{A_k^{-1}\mathbf{y}_k\mathbf{s}_k^\mathsf{T} + \mathbf{s}_k\mathbf{y}_k^\mathsf{T}A_k^{-1}}{\mathbf{s}_k^\mathsf{T}\mathbf{y}_k} \tag{12.7}$$

Here $\mathbf{s}_k = \mathbf{x}_{k+1} - \mathbf{x}_k$ and $\mathbf{y}_k = Df(\mathbf{x}_{k+1})^\mathsf{T} - Df(\mathbf{x}_k)^\mathsf{T}$ as before.

Problem 2. Write a function that accepts a function $Df : \mathbb{R}^n \to \mathbb{R}^n$, a starting point $\mathbf{x}_0 \in \mathbb{R}^n$, a stopping tolerance `tol` defaulting to $1e^{-5}$, and an integer `maxiter` defaulting to 80. Use BFGS as given in (12.6) and (12.7) to optimize f, with $A_0^{-1} = I$ (the $n \times n$ identity matrix) as the initial approximation to the inverse of the Hessian. Return the final estimate $\mathbf{x}_k$, whether or not the method converged, and the number of iterations computed.

This method is a little tricky and can have issues if $\mathbf{x}_0$ is chosen poorly. Consider the following as you implement your function.

- Use the same stopping criteria as in Problem 1, iterating until either $\|Df(\mathbf{x}_k)\|_\infty <$ `tol` or $k >$ `maxiter`. The usual criteria $\|\mathbf{x}_k - \mathbf{x}_{k-1}\| <$ `tol` is **not** a good choice for BFGS.
- Avoid recomputing values by only calculating each $Df(\mathbf{x}_k)$, $\mathbf{s}_k$, $\mathbf{y}_k$, and $\mathbf{s}_k^\mathsf{T}\mathbf{y}_k$ once.
- Note that $\mathbf{s}_k\mathbf{s}_k^\mathsf{T}$, $\mathbf{y}_k\mathbf{s}_k^\mathsf{T}$, and $\mathbf{s}_k\mathbf{y}_k^\mathsf{T}$ are all *outer products* that result in $n \times n$ matrices. Use `np.outer()` instead of `np.dot()` or the `@` operator for these computations. Carefully identify which parts of (12.7) are scalars and which parts are matrices.
- If $(\mathbf{s}_k^\mathsf{T}\mathbf{y}_k)^2 = 0$, terminate the iteration early to avoid dividing by zero.

Test your function on the Rosenbrock function as in Problem 1.

Note

The formula in (12.7) is not the only way to approximate the inverse Hessian. For example, the *Davidon-Fletcher-Powell* (DFP) method uses the following updating scheme.

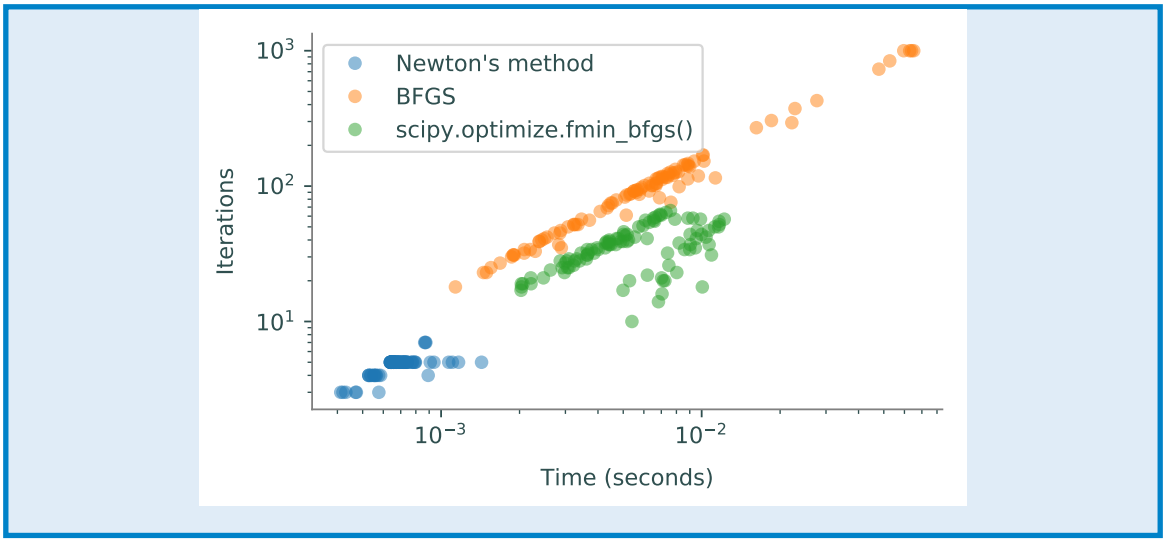
$$A_{k+1}^{-1} = A_k^{-1} + \frac{\mathbf{s}_k\mathbf{s}_k^\mathsf{T}}{\mathbf{s}_k^\mathsf{T}\mathbf{y}_k} - \frac{A_k^{-1}\mathbf{y}_k\mathbf{y}_k^\mathsf{T}A_k^{-1}}{\mathbf{y}_k^\mathsf{T}A_k^{-1}\mathbf{y}_k}$$

This approximation works well for many problems, but BFGS is considered to be the superior method in general.

Problem 3. Write a function that accepts an integer N and performs the following N times.

1. Sample a random initial guess $\mathbf{x}_0$ from the 2-D uniform distribution over $[-3, 3] \times [-3, 3]$. (Hint: Use `np.random.uniform()` or `np.random.random()`.)
2. Time (separately) your implementation of Newton's method from Problem 1, your BFGS routine from Problem 2, and `scipy.optimize.bfgs_fmin()` for minimizing the Rosenbrock function with an initial guess of $\mathbf{x}_0$.
3. Record the number of iterations from each method. For `scipy.optimize.fmin_bfgs()`, set `disp=False` to suppress printing the convergence message and `retall=True` to get the list of $\mathbf{x}_k$ at each iteration (to count the number of iterations).

Plot the computation times versus the number of iterations with a log-log scale, using different colors for each method. For $N = 100$, your plot should resemble the following figure. Note that Newton's method consistently converges much faster than BFGS. In addition, SciPy's BFGS algorithm will likely converge faster than your BFGS implementation because it employs a line search to choose an intelligent step size at each iteration.



The Gauss-Newton Method

Non-linear Least Squares Problems

Least Squares problems aim to fit a line (or model parameters) to a given set of data points. These problems arise in many scientific fields, including economics, physics, and statistics and represent unconstrained optimization problems that minimize an objective function of the form

$$f(\mathbf{x}) = \frac{1}{2}\sum_{j=1}^{m} r_j^2(\mathbf{x}),$$

where each $r_i : \mathbb{R}^n \to \mathbb{R}$ is smooth and $m \geq n$. This case of least squares problems can be solved with a Newton-like method.

Specifically, with data points $(t_1, y_1), (t_2, y_2), \ldots, (t_m, y_m)$, where $t_i, y_i \in \mathbb{R}$ for $i = 1, \ldots, m$. Let $\phi(\mathbf{x}, \mathbf{t})$ be a possible model for this data set, where $\mathbf{x}$ is a vector of parameters of the model, and $\mathbf{t} \in \mathbb{R}^n$. The error at the i-th data point, called the *residual*, is the value

$$r_i(\mathbf{x}) := \phi(x_i, t_i) - y_i.$$

Summing the squares of these errors gives the following non-linear least squares objective function.

$$f(\mathbf{x}) = \frac{1}{2}\sum_{j=1}^{m} r_j^2(\mathbf{x}).$$

The first and second derivatives of this function can then be expressed as

$$Df(\mathbf{x}) = J(\mathbf{x})^{\mathsf{T}} r(\mathbf{x}),$$

$$D^2 f(\mathbf{x}) = J(\mathbf{x})^{\mathsf{T}} J(\mathbf{x}) + \sum_{j=1}^{m} r_j(\mathbf{x}) D^2 r_j(\mathbf{x}).$$

with $\mathbf{r}(\mathbf{x}) = [r_1(\mathbf{x}), r_2(\mathbf{x}), \ldots, r_m(\mathbf{x})]^{\mathsf{T}}$ and

$$J(\mathbf{x}) = \begin{bmatrix} \frac{Dr_1(\mathbf{x})}{Dr_2(\mathbf{x})} \\ \hline \vdots \\ \hline Dr_m(\mathbf{x}) \end{bmatrix} \in \mathbb{R}^{m \times n}.$$

The second term in the formula for $D^2 f$ involves second derivatives and can be problematic to compute. In practice, the second term in the formula for $D^2 f$ is small, either because the residuals themselves are small, or because they are nearly affine in a neighborhood of the solution. The simplest method for solving the nonlinear least squares problem, known as the *Gauss-Newton Method*, exploits this observation, simply ignoring the second term and making the approximation

$$D^2 f(\mathbf{x}) \approx J(\mathbf{x})^\mathsf{T} J(\mathbf{x}).$$

The method then proceeds in a manner similar to Newton's method. Thus, at each iteration, we find $\mathbf{x}_{k+1}$ as follows:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - (J(\mathbf{x}_k)^\mathsf{T} J(\mathbf{x}_k))^{-1} J(\mathbf{x}_k)^\mathsf{T} \mathbf{r}(\mathbf{x}_k). \tag{12.8}$$

As an example, suppose we have data points generated from the function $y = 3\sin(x/2)$ and slightly perturbed by Gaussian noise. To fit the data to a model $\phi(\mathbf{x}, t_i) = \phi(x_0, x_1, t_i) = x_0 \sin(x_1 t_i)$, we must select values for $\mathbf{x} = [x_0, x_1]^\mathsf{T}$ (since we know how the data was generated, we expect to find that $x_0 \approx 3$ and $x_1 \approx 1/2$). Begin by writing functions for the proposed model, the residual vector, and the Jacobian of the residuals.

```
>>> import numpy as np
>>> from matplotlib import pyplot as plt

# Generate random data for t = 0, 1, ..., 10.
>>> T = np.arange(10)
>>> y = 3*np.sin(0.5*T)+ 0.5*np.random.randn(10)    # Perturbed data.

# Define the model function and the residual (based on the data).
>>> model = lambda x, t: x[0]*np.sin(x[1]*t)        # phi(x,t)
>>> residual = lambda x: model(x, T) - y            # r(x) = phi(x,t) - y

# Define the Jacobian of the residual function, computed by hand.
>>> jac = lambda x: np.column_stack((np.sin(x[1]*t), x[0]*t*np.cos(x[1]*t)))
```

By inspecting the data, an initial guess for the parameters could be $x_0 = (2.5, 0.6)$. A function implementing Gauss Newton can then be used to find the least squares solution.

```
>>> x0 = np.array([2.5,.6])
>>> x, conv, niters = gauss_newton(jac, residual, x0, tol=1e-3, maxiter=10)

# Plot the fitted model with the observed data and the data-generating curve.
>>> dom = np.linspace(0, 10, 200)
>>> plt.plot(T, y, '*')                          # Observed data.
>>> plt.plot(dom, 3*np.sin(.5*dom), '--')        # Data-generating curve.
>>> plt.plot(dom, model(x, dom))                 # Fitted model.
>>> plt.show()
```

Problem 4. Write a function that accepts a function for the proposed model $\phi(\mathbf{x})$, the model derivative $D\phi(\mathbf{x})$, a function that returns the residual vector $r(\mathbf{x})$, a callable function that returns the Jacobian of the residual $Dr(\mathbf{x}) = J(\mathbf{x})$, a starting point $\mathbf{x}_0$, a stopping tolerance `tol` defaulting to $1e^{-5}$, and a max number of iterations `maxiter` defaulting to 10. This method should implement the Gauss-Newton Method and return a list containing: the minimizing x value, the number of iterations performed, and if the method converged as a boolean.

Test your function by using the Jacobian function, residual function, and starting point given in the example above. Compare your results to `scipy.optimize.leastsq()`.

```
>>> minx = opt.leastsq(func=residual, x0=np.array([2.5,.6]), Dfun=jac)
```

Problem 5. The file `population.npy` contains census data from the United States every ten years since 1790 for 16 decades. The first column ($\mathbf{t}$) gives the number of decades since 1790 in the decade $(0, 1, \ldots)$ and the second column ($\mathbf{y}$) gives the population count in millions of people.

By plotting the data, and with a little knowledge about population growth, it is reasonable to hypothesize an *exponential model* for the population:

$$\phi(x_1, x_2, x_3, t) = x_1 \exp(x_2(t + x_3)).$$

Use the initial guess $(1.5, .4, 2.5)$ for the parameters (x_1, x_2, x_3) and your Gauss Newton function or `scipy.optimize.leastsq()` to fit this model. Plot the resulting curve along with the actual data points.

Unfortunately, the exponential model isn't a very good fit for the data because the population grows exponentially for only the first 8 or so decades.[a] Instead, consider the following *logistic model*.

$$\phi(x_1, x_2, x_3, t) = \frac{x_1}{1 + \exp(-x_2(t + x_3))}.$$

A reasonable initial guess for the parameters (x_1, x_2, x_3) is $(150, .4, -15)$. Write functions for the model and the corresponding residual vector, then fit the model. Plot the data against the fitted curve (in the same plot as before). It should be a much better fit than the exponential curve.

[a] Fitting an exponential model to only the first 8 data points results in a good model for those points (but not for later data).

13 Gradient Descent Methods

Lab Objective: *Iterative optimization methods choose a search direction and a step size at each iteration. One simple choice for the search direction is the negative gradient, resulting in the method of steepest descent. While theoretically foundational, in practice this method is often slow to converge. An alternative method, the conjugate gradient algorithm, uses a similar idea that results in much faster convergence in some situations. In this lab we implement a method of steepest descent and two conjugate gradient methods, then apply them to regression problems.*

The Method of Steepest Descent

Let $f : \mathbb{R}^n \to \mathbb{R}$ with first derivative $Df : \mathbb{R}^n \to \mathbb{R}^n$. The following iterative technique is a common template for methods that aim to compute a local minimizer $\mathbf{x}^*$ of f.

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{p}_k \tag{13.1}$$

Here $\mathbf{x}_k$ is the kth approximation to $\mathbf{x}^*$, α_k is the *step size*, and $\mathbf{p}_k$ is the *search direction*. Newton's method and its relatives follow this pattern, but they require the calculation (or approximation) of the inverse Hessian matrix $Df^2(\mathbf{x}_k)^{-1}$ at each step. The following idea is a simpler and less computationally intensive approach than Newton and quasi-Newton methods.

The derivative $Df(\mathbf{x})^\mathsf{T}$ (often called the *gradient* of f at $\mathbf{x}$, sometimes notated $\nabla f(\mathbf{x})$) is a vector that points in the direction of greatest **increase** of f at $\mathbf{x}$. It follows that the negative derivative $-Df(\mathbf{x})^\mathsf{T}$ points in the direction of steepest **decrease** at $\mathbf{x}$. The *method of steepest descent* chooses the search direction $\mathbf{p}_k = -Df(\mathbf{x}_k)^\mathsf{T}$ at each step of (13.1), resulting in the following algorithm.

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k Df(\mathbf{x}_k)^\mathsf{T} \tag{13.2}$$

Setting $\alpha_k = 1$ for each k is often sufficient for Newton and quasi-Newton methods. However, a constant choice for the step size in (13.2) can result in oscillating approximations or even cause the sequence $(\mathbf{x}_k)_{k=1}^\infty$ to travel away from the minimizer $\mathbf{x}^*$. To avoid this problem, the step size α_k can be chosen in a few ways.

- Start with $\alpha_k = 1$, then set $\alpha_k = \frac{\alpha_k}{2}$ until $f(\mathbf{x}_k - \alpha_k Df(\mathbf{x}_k)^\mathsf{T}) < f(\mathbf{x}_k)$, terminating the iteration if α_k gets too small. This guarantees that the method actually descends at each step and that α_k satisfies the Armijo rule, without endangering convergence.

- At each step, solve the following one-dimensional optimization problem.

$$\alpha_k = \underset{\alpha}{\operatorname{argmin}}\ f(\mathbf{x}_k - \alpha Df(\mathbf{x}_k)^\mathsf{T})$$

  Using this choice is called *exact steepest descent*. This option is more expensive per iteration than the above strategy, but it results in fewer iterations before convergence.

Problem 1. Write a function that accepts an objective function $f : \mathbb{R}^n \to \mathbb{R}$, its derivative $Df : \mathbb{R}^n \to \mathbb{R}^n$, an initial guess $\mathbf{x}_0 \in \mathbb{R}^n$, a convergence tolerance `tol` defaulting to $1e^{-5}$, and a maximum number of iterations `maxiter` defaulting to 100. Implement the exact method of steepest descent, using a one-dimensional optimization method to choose the step size (use `opt.minimize_scalar()` or your own 1-D minimizer). Iterate until $\|Df(\mathbf{x}_k)\|_\infty <$ `tol` or $k >$ `maxiter`. Return the approximate minimizer $\mathbf{x}^*$, whether or not the algorithm converged (`True` or `False`), and the number of iterations computed.

Test your function on $f(x, y, z) = x^4 + y^4 + z^4$ (easy) and the Rosenbrock function (hard). It should take many iterations to minimize the Rosenbrock function, but it should converge eventually with a large enough choice of `maxiter`.

The Conjugate Gradient Method

Unfortunately, the method of steepest descent can be very inefficient for certain problems. Depending on the nature of the objective function, the sequence of points can zig-zag back and forth or get stuck on flat areas without making significant progress toward the true minimizer.

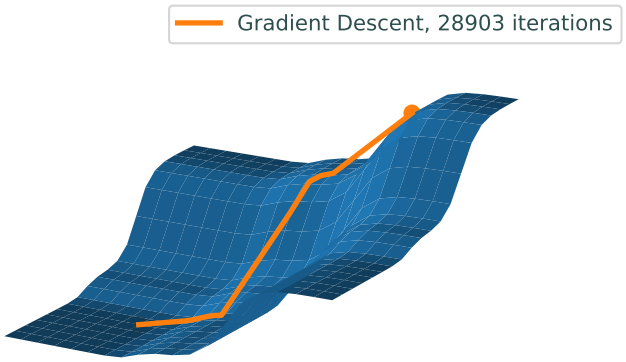


Figure 13.1: On this surface, gradient descent takes an extreme number of iterations to converge to the minimum because it gets stuck in the flat basins of the surface.

Unlike the method of steepest descent, the *conjugate gradient algorithm* chooses a search direction that is guaranteed to be a descent direction, though not the direction of greatest descent. These directions are using a generalized form of orthogonality called *conjugacy*.

Let Q be a square, positive definite matrix. A set of vectors $\{\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_m\}$ is called *Q-conjugate* if each distinct pair of vectors $\mathbf{x}_i, \mathbf{x}_j$ satisfy $\mathbf{x}_i^\mathsf{T} Q \mathbf{x}_j = 0$. A Q-conjugate set of vectors is linearly independent and can form a basis that diagonalizes the matrix Q. This guarantees that an iterative method to solve $Q\mathbf{x} = \mathbf{b}$ only require as many steps as there are basis vectors.

Solve a positive definite system $Q\mathbf{x} = \mathbf{b}$ is valuable in and of itself for certain problems, but it is also equivalent to minimizing certain functions. Specifically, consider the quadratic function

$$f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^\mathsf{T} Q \mathbf{x} - \mathbf{b}^\mathsf{T}\mathbf{x} + c.$$

Because $Df(\mathbf{x})^\mathsf{T} = Q\mathbf{x} - \mathbf{b}$, minimizing f is the same as solving the equation

$$\mathbf{0} = Df(\mathbf{x})^\mathsf{T} = Q\mathbf{x} - \mathbf{b} \quad \Rightarrow \quad Q\mathbf{x} = \mathbf{b},$$

which is the original linear system. Note that the constant c does not affect the minimizer, since if $\mathbf{x}^*$ minimizes $f(\mathbf{x})$ it also minimizes $f(\mathbf{x}) + c$.

Using the conjugate directions guarantees an iterative method to converge on the minimizer because each iteration minimizes the objective function over a subspace of dimension equal to the iteration number. Thus, after n steps, where n is the number of conjugate basis vectors, the algorithm has found a minimizer over the entire space. In certain situations, this has a great advantage over gradient descent, which can bounce back and forth. This comparison is illustrated in Figure 13.2. Additionally, because the method utilizes a basis of conjugate vectors, the previous search direction can be used to find a conjugate projection onto the next subspace, saving computational time.

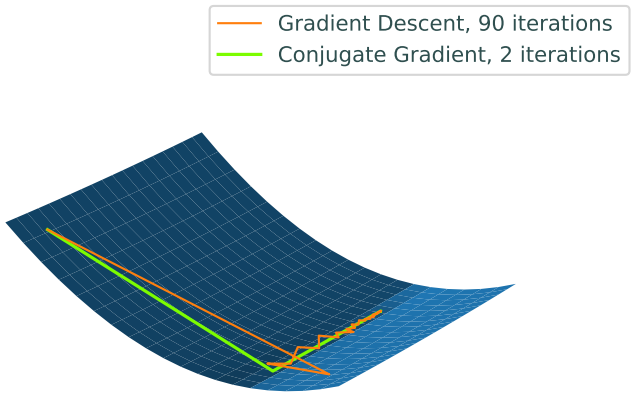


Figure 13.2: Paths traced by Gradient Descent (orange) and Conjugate Gradient (red) on a quadratic surface. Notice the zig-zagging nature of the Gradient Descent path, as opposed to the Conjugate Gradient path, which finds the minimizer in 2 steps.

Algorithm 13.1

procedure CONJUGATE GRADIENT($\mathbf{x}_0$, Q, $\mathbf{b}$, `tol`)
  $\mathbf{r}_0 \leftarrow Q\mathbf{x}_0 - \mathbf{b}$
  $\mathbf{d}_0 \leftarrow -\mathbf{r}_0$
  $k \leftarrow 0$
  while $\|\mathbf{r}_k\| \geq$ `tol`, $k \leq n$ **do**
    $\alpha_k \leftarrow \mathbf{r}_k^\mathsf{T}\mathbf{r}_k / \mathbf{d}_k^\mathsf{T} Q \mathbf{d}_k$
    $\mathbf{x}_{k+1} \leftarrow \mathbf{x}_k + \alpha_k \mathbf{d}_k$
    $\mathbf{r}_{k+1} \leftarrow \mathbf{r}_k + \alpha_k Q \mathbf{d}_k$
    $\beta_{k+1} \leftarrow \mathbf{r}_{k+1}^\mathsf{T}\mathbf{r}_{k+1} / \mathbf{r}_k^\mathsf{T}\mathbf{r}_k$
    $\mathbf{d}_{k+1} \leftarrow -\mathbf{r}_{k+1} + \beta_{k+1}\mathbf{d}_k$
    $k \leftarrow k + 1$.
  return $\mathbf{x}_k$

The points $\mathbf{x}_k$ are the successive approximations to the minimizer, the vectors $\mathbf{d}_k$ are the conjugate descent directions, and the vectors $\mathbf{r}_k$ (which actually correspond to the steepest descent directions) are used in determining the conjugate directions. The constants α_k and β_k are used, respectively, in the line search, and in ensuring the Q-conjugacy of the descent directions.

Problem 2. Write a function that accepts an $n \times n$ positive definite matrix Q, a vector $\mathbf{b} \in \mathbb{R}^n$, an initial guess $\mathbf{x}_0 \in \mathbb{R}^n$, and a stopping tolerance. Use Algorithm 13.1 to solve the system $Q\mathbf{x} = \mathbf{b}$. Continue the algorithm until $\|\mathbf{r}_k\|$ is less than the tolerance, iterating no more than n times. Return the solution $\mathbf{x}$, whether or not the algorithm converged in n iterations or less, and the number of iterations computed.

Test your function on the simple system

$$Q = \begin{bmatrix} 2 & 0 \\ 0 & 4 \end{bmatrix}, \qquad \mathbf{b} = \begin{bmatrix} 1 \\ 8 \end{bmatrix},$$

which has solution $\mathbf{x}^* = \left[\frac{1}{2}, 2\right]^\mathsf{T}$. This is equivalent to minimizing the quadratic function $f(x, y) = x^2 + 2y^2 - x - 8y$; check that your function from Problem 1 gets the same solution.

More generally, you can generate a random positive definite matrix Q for testing by setting setting $Q = A^\mathsf{T}A$ for any A of full rank.

```
>>> import numpy as np
>>> from scipy import linalg as la

# Generate Q, b, and the initial guess x0.
>>> n = 10
>>> A = np.random.random((n,n))
>>> Q = A.T @ A
>>> b, x0 = np.random.random((2,n))

>>> x = la.solve(Q, b)      # Use your function here.
>>> np.allclose(Q @ x, b)
True
```

Non-linear Conjugate Gradient

The algorithm presented above is only valid for certain linear systems and quadratic functions, but the basic strategy may be adapted to minimize more general convex or non-linear functions. Though the non-linear version does not have guaranteed convergence as the linear formulation does, it can still converge in less iterations than the method of steepest descent. Modifying the algorithm for more general functions requires new formulas for α_k, $\mathbf{r}_k$, and β_k.

- The scalar α_k is simply the result of performing a line-search in the given direction $\mathbf{d}_k$ and is thus defined $\alpha_k = \underset{\alpha}{\text{argmin}}\ f(\mathbf{x}_k + \alpha \mathbf{d}_k)$.
- The vector $\mathbf{r}_k$ in the original algorithm was really just the gradient of the objective function, so now define $\mathbf{r}_k = Df(\mathbf{x}_k)^\mathsf{T}$.
- The constants β_k can be defined in various ways, and the most correct choice depends on the nature of the objective function. A well-known formula, attributed to Fletcher and Reeves, is $\beta_k = Df(\mathbf{x}_k)Df(\mathbf{x}_k)^\mathsf{T} / Df(\mathbf{x}_{k-1})Df(\mathbf{x}_{k-1})^\mathsf{T}$.

Algorithm 13.2

procedure NON-LINEAR CONJUGATE GRADIENT(f, Df, $\mathbf{x}_0$, `tol`, `maxiter`)
  $\mathbf{r}_0 \leftarrow -Df(\mathbf{x}_0)^\mathsf{T}$
  $\mathbf{d}_0 \leftarrow \mathbf{r}_0$
  $\alpha_0 \leftarrow \underset{\alpha}{\text{argmin}} f(\mathbf{x}_0 + \alpha \mathbf{d}_0)$
  $\mathbf{x}_1 \leftarrow \mathbf{x}_0 + \alpha_0 \mathbf{d}_0$
  $k \leftarrow 1$
  while $\|\mathbf{r}_k\| \geq$ `tol`, $k <$ `maxiter` **do**
    $\mathbf{r}_k \leftarrow -Df(\mathbf{x}_k)^\mathsf{T}$
    $\beta_k = \mathbf{r}_k^\mathsf{T}\mathbf{r}_k / \mathbf{r}_{k-1}^\mathsf{T}\mathbf{r}_{k-1}$
    $\mathbf{d}_k \leftarrow \mathbf{r}_k + \beta_n \mathbf{d}_{k-1}$.
    $\alpha_k \leftarrow \underset{\alpha}{\text{argmin}}\ f(\mathbf{x}_k + \alpha \mathbf{d}_k(\mathbf{x}_k))$.
    $\mathbf{x}_{k+1} \leftarrow \mathbf{x}_k + \alpha_k \mathbf{d}_k$.
    $k \leftarrow k + 1$.

Problem 3. Write a function that accepts a convex objective function f, its derivative Df, an initial guess $\mathbf{x}_0$, a convergence tolerance defaultin to $1e^{-5}$, and a maximum number of iterations defaultin to 100. Use Algorithm 13.2 to compute the minimizer $\mathbf{x}^*$ of f. Return the approximate minimizer, whether or not the algorithm converged, and the number of iterations computed.

Compare your function to SciPy's `opt.fmin_cg()`.

```
>>> opt.fmin_cg(opt.rosen, np.array([10, 10]), fprime=opt.rosen_der)
Optimization terminated successfully.
         Current function value: 0.000000
         Iterations: 44
         Function evaluations: 102  # Much faster than steepest descent!
         Gradient evaluations: 102
```

```
array([ 1.00000007,  1.00000015])
```

Regression Problems

A major use of the conjugate gradient method is solving linear least squares problems. Recall that a least squares problem can be formulated as an optimization problem:

$$\mathbf{x}^* = \min_{\mathbf{x}} \|A\mathbf{x} - \ \mathbf{b}\|_2,$$

where A is an $m \times n$ matrix with full column rank, $\mathbf{x} \in \mathbb{R}^n$, and $\mathbf{b} \in \mathbb{R}^m$. The solution can be calculated analytically, and is given by

$$\mathbf{x}^* = (A^\mathsf{T}A)^{-1}A^\mathsf{T}\mathbf{b}.$$

In other words, the minimizer solves the linear system

$$A^\mathsf{T}A\mathbf{x} = A^\mathsf{T}\mathbf{b}. \tag{13.3}$$

Since A has full column rank, it is invertible, $A^\mathsf{T}A$ is positive definite, and for any non-zero vector $\mathbf{z}$, $A\mathbf{z} \neq 0$. Therefore, $\mathbf{z}^\mathsf{T}A^\mathsf{T}A\mathbf{z} = \|A\mathbf{z}\|^2 > 0$. As $A^\mathsf{T}A$ is positive definite, conjugate gradient can be used to solve Equation 13.3.

Linear least squares is the mathematical underpinning of *linear regression*. Linear regression involves a set of real-valued data points $\{y_1, \dots, y_m\}$, where each y_i is paired with a corresponding set of predictor variables $\{x_{i,1}, x_{i,2}, \dots, x_{i,n}\}$ with $n < m$. The linear regression model posits that

$$y_i = \beta_0 + \beta_1 x_{i,1} + \beta_2 x_{i,2} + \cdots + \beta_n x_{i,n} + \varepsilon_i$$

for $i = 1, 2, \dots, m$. The real numbers $\beta_0, \dots, \beta_n$ are known as the parameters of the model, and the ε_i are independent, normally-distributed error terms. The goal of linear regression is to calculate the parameters that best fit the data. This can be accomplished by posing the problem in terms of linear least squares. Define

$$\mathbf{b} = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}, \quad A = \begin{bmatrix} 1 & x_{1,1} & x_{1,2} & \cdots & x_{1,n} \\ 1 & x_{2,1} & x_{2,2} & \cdots & x_{2,n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{m,1} & x_{m,2} & \cdots & x_{m,n} \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_n \end{bmatrix}.$$

The solution $\mathbf{x}^* = [\beta_0^*, \beta_1^*, \dots, \beta_n^*]^\mathsf{T}$ to the system $A^\mathsf{T}A\mathbf{x} = A^\mathsf{T}\mathbf{b}$ gives the parameters that best fit the data. These values can be understood as defining the hyperplane that best fits the data.

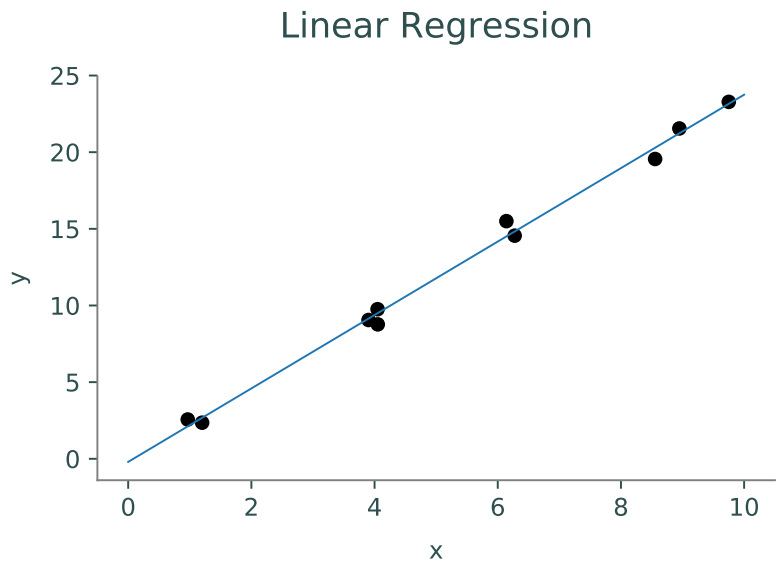


Figure 13.3: Solving the linear regression problem results in a best-fit hyperplane.

Problem 4. Using your function from Problem 2, solve the linear regression problem specified by the data contained in the file[a] `linregression.txt`. This is a whitespace-delimited text file formatted so that the i-th row consists of $y_i, x_{i,1}, \ldots, x_{i,n}$. Use `np.loadtxt()` to load in the data and return the solution to the normal equations.

[a]Source: Statistical Reference Datasets website at `http://www.itl.nist.gov/div898/strd/lls/data/LINKS/v-Longley.shtml`.

Logistic Regression

Logistic regression is another important technique in statistical analysis and machine learning that builds off of the concepts of linear regression. As in linear regression, there is a set of predictor variables $\{x_{i,1}, x_{i,2}, \ldots, x_{i,n}\}_{i=1}^m$ with corresponding outcome variables $\{y_i\}_{i=1}^m$. In logistic regression, the outcome variables y_i are binary and can be modeled by a *sigmoidal* relationship. The value of the predicted y_i can be thought of as the probability that $y_i = 1$. In mathematical terms,

$$\mathbb{P}(y_i = 1 \,|\, x_{i,1}, \ldots, x_{i,n}) = p_i,$$

where

$$p_i = \frac{1}{1 + \exp(-(\beta_0 + \beta_1 x_{i,1} + \cdots + \beta_n x_{i,n}))}.$$

The parameters of the model are the real numbers $\beta_0, \beta_1, \ldots, \beta_n$. Note that $p_i \in (0, 1)$ regardless of the values of the predictor variables and parameters.

The probability of observing the outcome variables y_i under this model, assuming they are independent, is given by the *likelihood function* $\mathcal{L} : \mathbb{R}^{n+1} \to \mathbb{R}$

$$\mathcal{L}(\beta_0, \ldots, \beta_n) = \prod_{i=1}^m p_i^{y_i} (1 - p_i)^{1 - y_i}.$$

The goal of logistic regression is to find the parameters $\beta_0, \dots, \beta_k$ that maximize this likelihood function. Thus, the problem can be written as:

$$\max_{(\beta_0,\dots,\beta_n)} \mathcal{L}(\beta_0, \dots, \beta_n).$$

Maximizing this function is often a numerically unstable calculation. Thus, to make the objective function more suitable, the logarithm of the objective function may be maximized because the logarithmic function is strictly monotone increasing. Taking the log and turning the problem into a minimization problem, the final problem is formulated as:

$$\min_{(\beta_0,\dots,\beta_n)} -\log \mathcal{L}(\beta_0, \dots, \beta_n).$$

A few lines of calculation reveal that this objective function can also be rewritten as

$$\begin{aligned} -\log \mathcal{L}(\beta_0, \dots, \beta_n) = &\sum_{i=1}^{m} \log(1 + \exp(-(\beta_0 + \beta_1 x_{i,1} + \cdots + \beta_n x_{i,n})))+ \\ &\sum_{i=1}^{m} (1 - y_i)(\beta_0 + \beta_1 x_{i,1} + \cdots + \beta_n x_{i,n}). \end{aligned}$$

The values for the parameters $\{\beta_i\}_{i=1}^n$ that we obtain are known as the *maximum likelihood estimate* (MLE). To find the MLE, conjugate gradient can be used to minimize the objective function.

For a one-dimensional binary logistic regression problem, we have predictor data $\{x_i\}_{i=1}^m$ with labels $\{y_i\}_{i=1}^m$ where each $y_i \in \{0, 1\}$. The negative log likelihood then becomes the following.

$$-\log \mathcal{L}(\beta_0, \beta_1) = \sum_{i=1}^{m} \log(1 + e^{-(\beta_0+\beta_1 x_i)}) + (1 - y_i)(\beta_0 + \beta_1 x_i) \tag{13.4}$$

Problem 5. Write a class for doing binary logistic regression in one dimension that implement the following methods.

1. `fit()`: accept an array $\mathbf{x} \in \mathbb{R}^n$ of data, an array $\mathbf{y} \in \mathbb{R}^n$ of labels (0s and 1s), and an initial guess $\boldsymbol{\beta}_0 \in \mathbb{R}^2$. Define the negative log likelihood function as given in (13.4), then minimize it (with respect to $\boldsymbol{\beta}$) with your function from Problem 3 or `opt.fmin_cg()`. Store the resulting parameters β_0 and β_1 as attributes.

2. `predict()`: accept a float $x \in \mathbb{R}$ and calculate

$$\sigma(x) = \frac{1}{1 + \exp(-(\beta_0 + \beta_1 x))},$$

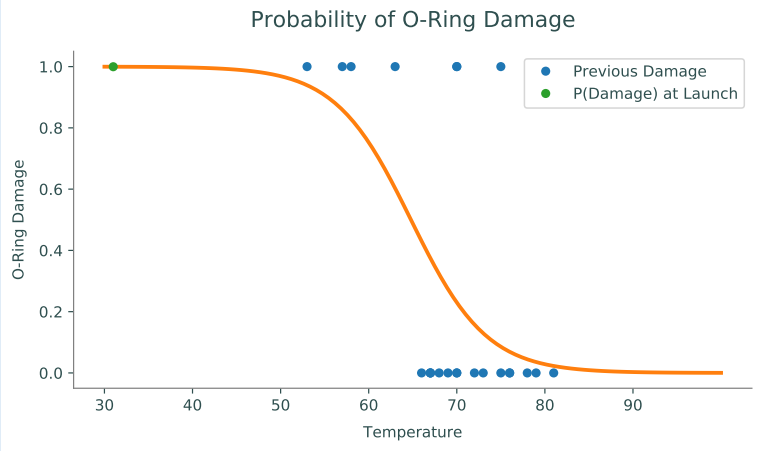
where β_0 and β_1 are the optimal values calculated in `fit()`. The value $\sigma(x)$ is the probability that the observation x should be assigned the label $y = 1$.

This class does not need an explicit constructor. You may assume that `predict()` will be called after `fit()`.

Problem 6. On January 28, 1986, less than two minutes into the Challenger space shuttle's 10th mission, there was a large explosion that originated from the spacecraft, killing all seven crew members and destroying the shuttle. The investigation that followed concluded that the malfunction was caused by damage to O-rings that are used as seals for parts of the rocket engines. There were 24 space shuttle missions before this disaster, some of which had noted some O-ring damage. Given the data, could this disaster have been predicted?

The file `challenger.npy` contains data for 23 missions (during one of the 24 missions, the engine was lost at sea). The first column ($\mathbf{x}$) contains the ambient temperature, in Fahrenheit, of the shuttle launch. The second column ($\mathbf{y}$) contains a binary indicator of the presence of O-ring damage (1 if O-ring damage was present, 0 otherwise).

Instantiate your class from Problem 5 and fit it to the data, using an initial guess of $\boldsymbol{\beta}_0 = [20, -1]^\mathsf{T}$. Plot the resulting curve $\sigma(x)$ for $x \in [30, 100]$, along with the raw data. Return the predicted probability (according to this model) of O-ring damage on the day the shuttle was launched, given that it was 31°F.



14 CVXOPT

Lab Objective: *CVXOPT is a package of Python functions and classes designed for the purpose of convex optimization. In this lab we use these tools for linear and quadratic programming. We will solve various optimization problems using CVXOPT and optimize allocating land using linear programming.*

Linear Programs

A *linear program* is a linear constrained optimization problem. Such a problem can be stated in several different forms, one of which is

$$\begin{aligned} \text{minimize} \quad & \mathbf{c}^\mathsf{T}\mathbf{x} \\ \text{subject to} \quad & G\mathbf{x} \preceq \mathbf{h} \\ & A\mathbf{x} = \mathbf{b}. \end{aligned}$$

The symbol $\preceq$ denotes that the components of $G\mathbf{x}$ are less than the components of $\mathbf{h}$. In other words, if $\mathbf{x} \preceq \mathbf{y}$, then $x_i < y_i$ for all $x_i \in \mathbf{x}$ and $y_i \in \mathbf{y}$.

Define vector $\mathbf{s} \succeq \mathbf{0}$ such that the constraint $G\mathbf{x} + \mathbf{s} = \mathbf{h}$. This vector is known as a *slack variable*. Since $\mathbf{s} \succeq \mathbf{0}$, the constraint $G\mathbf{x} + \mathbf{s} = \mathbf{h}$ is equivalent to $G\mathbf{x} \preceq \mathbf{h}$.

With a slack variable, a new form of the linear program is found:

$$\begin{aligned} \text{minimize} \quad & \mathbf{c}^\mathsf{T}\mathbf{x} \\ \text{subject to} \quad & G\mathbf{x} + \mathbf{s} = \mathbf{h} \\ & A\mathbf{x} = \mathbf{b} \\ & \mathbf{s} \succeq \mathbf{0}. \end{aligned}$$

This is the formulation used by CVXOPT. In this formulation, we require that the matrix A has full row rank, and that the block matrix $[G \quad A]^\mathsf{T}$ has full column rank.

Consider the following example:

$$\begin{aligned} \text{minimize} \quad & -4x_1 - 5x_2 \\ \text{subject to} \quad & x_1 + 2x_2 \leq 3 \\ & 2x_1 + x_2 = 3 \\ & x_1, x_2 \geq 0 \end{aligned}$$

Recall that all inequalities must be less than or equal to, such that $G\mathbf{x} \preceq \mathbf{h}$. Because the final two constraints are $x_1, x_2 \geq 0$, they need to be adjusted to be $\leq$ constraints. This is easily done by multiplying by -1, resulting in the constraints $-x_1, -x_2 \leq 0$. If we define

$$G = \begin{bmatrix} 1 & 2 \\ -1 & 0 \\ 0 & -1 \end{bmatrix}, \qquad \mathbf{h} = \begin{bmatrix} 3 \\ 0 \\ 0 \end{bmatrix}, \qquad A = \begin{bmatrix} 2 & 1 \end{bmatrix}, \quad \text{and} \qquad \mathbf{b} = \begin{bmatrix} 3 \end{bmatrix}$$

then we can express the constraints compactly as

$$\begin{aligned} G\mathbf{x} &\preceq \mathbf{h}, \\ A\mathbf{x} &= \mathbf{b}, \end{aligned} \qquad \text{where} \qquad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}.$$

By adding a slack variable $\mathbf{s}$, we can write our constraints as

$$G\mathbf{x} + \mathbf{s} = \mathbf{h},$$

which matches the form discussed above.

To solve the problem using CVXOPT, initialize the arrays $\mathbf{c}$, G, $\mathbf{h}$, A, and $\mathbf{b}$ and pass them to the appropriate function. CVXOPT uses its own data type for an array or matrix. While similar to the NumPy array, it does have a few differences, especially when it comes to initialization. Below, we initialize CVXOPT matrices for $\mathbf{c}$, G, $\mathbf{h}$, A, and $\mathbf{b}$. We then use the CVXOPT function for linear programming `solvers.lp()`, which accepts $\mathbf{c}$, G, $\mathbf{h}$, A, and $\mathbf{b}$ as arguments.

```
>>> from cvxopt import matrix, solvers

>>> c = matrix([-4., -5.])
>>> G = matrix([[1., -1., 0.],[2., 0., -1.]])
>>> h = matrix([ 3., 0., 0.])
>>> A = matrix([[2.],[1.]])
>>> b = matrix([3.])

>>> sol = solvers.lp(c, G, h, A, b)
     pcost       dcost       gap    pres   dres   k/t
 0: -8.5714e+00 -1.4143e+01  4e+00  0e+00  3e-01  1e+00
 1: -8.9385e+00 -9.2036e+00  2e-01  3e-16  1e-02  3e-02
 2: -8.9994e+00 -9.0021e+00  2e-03  3e-16  1e-04  3e-04
 3: -9.0000e+00 -9.0000e+00  2e-05  1e-16  1e-06  3e-06
 4: -9.0000e+00 -9.0000e+00  2e-07  1e-16  1e-08  3e-08
Optimal solution found.
>>> print(sol['x'])
[ 1.00e+00]
[ 1.00e+00]
>>> print(sol['primal objective'])
-8.999999939019435
>>> print(type(sol['x']))
<class 'cvxopt.base.matrix'>
```

Achtung!

CVXOPT matrices only accept floats. Other data types will raise a `TypeError`.

Additionally, CVXOPT matrices are initialized column-wise rather than row-wise (as in the case of NumPy). Alternatively, we can initialize the arrays first in NumPy (a process with which you should be familiar), and then simply convert them to the CVXOPT matrix data type.

```
>>> import numpy as np

>>> c = np.array([-4., -5.])
>>> G = np.array([[1., 2.],[-1., 0.],[0., -1]])
>>> h = np.array([3., 0., 0.])
>>> A = np.array([[2., 1.]])
>>> b = np.array([3.])

# Convert the arrays to the CVXOPT matrix type.
>>> c = matrix(c)
>>> G = matrix(G)
>>> h = matrix(h)
>>> A = matrix(A)
>>> b = matrix(b)
```

In this lab, we will initialize non-trivial matrices first as NumPy arrays for consistency.

Note

Although it is often helpful to see the progress of each iteration of the algorithm, you may suppress this output by first running,

```
solvers.options['show_progress'] = False
```

The function `solvers.lp()` returns a dictionary containing useful information. For now, we will only focus on the value of `x` and the primal objective value (i.e. the minimum value achieved by the objective function).

Achtung!

Note that the minimizer `x` returned by the `solvers.lp()` function is a `cvxopt.base.matrix` object. `np.ravel()` is a NumPy function that takes an object and returns its values as a flattened NumPy array. Use `np.ravel()` to return all minimizers in this lab as flattened NumPy arrays.

Problem 1. Solve the following convex optimization problem:

$$\begin{aligned} \text{minimize} \quad & 2x_1 + x_2 + 3x_3 \\ \text{subject to} \quad & x_1 + 2x_2 \geq 3 \\ & 2x_1 + 10x_2 + 3x_3 \geq 10 \\ & x_1 \geq 0 \\ & x_2 \geq 0 \\ & x_3 \geq 0 \end{aligned}$$

Return the minimizer $\mathbf{x}$ and the primal objective value.
(Hint: make the necessary adjustments so that all inequality constraints are $\leq$ rather than $\geq$).

l_1 Norm

The l_1 norm is defined

$$||\mathbf{x}||_1 = \sum_{i=1}^{n} |x_i|.$$

A l_1 minimization problem is minimizing a vector's l_1 norm, while fitting certain constraints. It can be written in the following form:

$$\begin{aligned} \text{minimize} \quad & \|\mathbf{x}\|_1 \\ \text{subject to} \quad & A\mathbf{x} = \mathbf{b}. \end{aligned}$$

This problem can be converted into a linear program by introducing an additional vector $\mathbf{u}$ of length n. Define $\mathbf{u}$ such that $|x_i| \leq |u_i|$. Thus, $-u_i - x_i \leq 0$ and $-u_i + x_i \leq 0$. These two inequalities can be added to the linear system as constraints. Additionally, this means that $||\mathbf{x}||_1 \leq ||\mathbf{u}||_1$. So minimizing $||\mathbf{u}||_1$ subject to the given constraints will in turn minimize $||\mathbf{x}||_1$. This can be written as follows:

$$\begin{aligned} \text{minimize} \quad & \begin{bmatrix} \mathbf{1}^\top & \mathbf{0}^\top \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{x} \end{bmatrix} \\ \text{subject to} \quad & \begin{bmatrix} -I & I \\ -I & -I \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{x} \end{bmatrix} \preceq \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \\ & \begin{bmatrix} \mathbf{0} & A \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{x} \end{bmatrix} = \mathbf{b}. \end{aligned}$$

Solving this gives values for the optimal $\mathbf{u}$ and the optimal $\mathbf{x}$, but we only care about the optimal $\mathbf{x}$.

Problem 2. Write a function called `l1Min()` that accepts a matrix A and vector $\mathbf{b}$ as NumPy arrays and solves the l_1 minimization problem. Return the minimizer $\mathbf{x}$ and the primal objective value. Remember to first discard the unnecessary u values from the minimizer.

To test your function consider the matrix A and vector $\mathbf{b}$ below.

$$A = \begin{bmatrix} 1 & 2 & 1 & 1 \\ 0 & 3 & -2 & -1 \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} 7 \\ 4 \end{bmatrix}$$

The linear system $A\mathbf{x} = \mathbf{b}$ has infinitely many solutions. Use `l1Min()` to verify that the solution which minimizes $||\mathbf{x}||_1$ is approximately $\mathbf{x} = [1.41, 2.40, 2.40, 0.79]^T$ and the minimum objective value is approximately 7.

The Transportation Problem

Consider the following transportation problem: A piano company needs to transport thirteen pianos from their three supply centers (denoted by 1, 2, 3) to two demand centers (4, 5). Transporting a piano from a supply center to a demand center incurs a cost, listed in Table 14.3. The company wants to minimize shipping costs for the pianos while meeting the demand.

Supply Center	Number of pianos available
1	7
2	2
3	4

Table 14.1: Number of pianos available at each supply center

Demand Center	Number of pianos needed
4	5
5	8

Table 14.2: Number of pianos needed at each demand center

Supply Center	Demand Center	Cost of transportation	Number of pianos
1	4	4	p_1
1	5	7	p_2
2	4	6	p_3
2	5	8	p_4
3	4	8	p_5
3	5	9	p_6

Table 14.3: Cost of transporting one piano from a supply center to a demand center

A system of constraints is defined for the variables p_1, p_2, p_3, p_4, p_5, and p_6, First, there cannot be a negative number of pianos so the variables must be nonnegative. Next, the Tables 14.1 and 14.2 define the following three supply constraints and two demand constraints:

$$\begin{aligned} p_1 + p_2 &= 7 \\ p_3 + p_4 &= 2 \\ p_5 + p_6 &= 4 \\ p_1 + p_3 + p_5 &= 5 \\ p_2 + p_4 + p_6 &= 8 \end{aligned}$$

The objective function is the number of pianos shipped from each location multiplied by the respective cost (found in Table 14.3):

$$4p_1 + 7p_2 + 6p_3 + 8p_4 + 8p_5 + 9p_6.$$

Note

Since our answers must be integers, in general this problem turns out to be an NP-hard problem. There is a whole field devoted to dealing with integer constraints, called *integer linear programming*, which is beyond the scope of this lab. Fortunately, we can treat this particular problem as a standard linear program and still obtain integer solutions.

Recall the variables are nonnegative, so $p_1, p_2, p_3, p_4, p_5, p_6 \geq 0$. Thus, G and $\mathbf{h}$ constrain the variables to be non-negative. Because CVXOPT uses the format $G\mathbf{x} \preceq \mathbf{h}$, we see that this inequality must be multiplied by -1. So, G must be a 6×6 identity matrix multiplied by -1, and

$\mathbf{h}$ is a column vector of zeros. Since the supply and demand constraints are equality constraints, they are A and $\mathbf{b}$. Initialize these arrays and solve the linear program by entering the code below.

```
>>> c = matrix(np.array([4., 7., 6., 8., 8., 9.]))
>>> G = matrix(-1*np.eye(6))
>>> h = matrix(np.zeros(6))
>>> A = matrix(np.array([[1.,1.,0.,0.,0.,0.],
                         [0.,0.,1.,1.,0.,0.],
                         [0.,0.,0.,0.,1.,1.],
                         [1.,0.,1.,0.,1.,0.],
                         [0.,1.,0.,1.,0.,1.]]))
>>> b = matrix(np.array([7., 2., 4., 5., 8.]))
>>> sol = solvers.lp(c, G, h, A, b)
     pcost       dcost       gap    pres   dres   k/t
 0:  8.9500e+01  8.9500e+01  2e+01  2e-16  2e-01  1e+00
 1:  8.7023e+01  8.7044e+01  3e+00  1e-15  3e-02  2e-01
Terminated (singular KKT matrix).
>>> print(sol['x'])
[ 4.31e+00]
[ 2.69e+00]
[ 3.56e-01]
[ 1.64e+00]
[ 3.34e-01]
[ 3.67e+00]
>>> print(sol['primal objective'])
87.023
```

Notice that some problems occurred. First, CVXOPT alerted us to the fact that the algorithm terminated prematurely (due to a singular matrix). Second, the minimizer and solution obtained do not consist of integer entries.

So what went wrong? Recall that the matrix A is required to have full row rank, but we can easily see that the rows of A are linearly dependent. We rectify this by converting the last row of the equality constraints into two *inequality* constraints, so that the remaining equality constraints define a new matrix A with linearly independent rows.

This is done as follows:

Suppose we have the equality constraint

$$x_1 + 2x_2 - 3x_3 = 4.$$

This is equivalent to the pair of inequality constraints

$$\begin{aligned} x_1 + 2x_2 - 3x_3 &\leq 4, \\ x_1 + 2x_2 - 3x_3 &\geq 4. \end{aligned}$$

The linear program requires only $\leq$ constraints, so we obtain the pair of constraints

$$\begin{aligned} x_1 + 2x_2 - 3x_3 &\leq 4, \\ -x_1 - 2x_2 + 3x_3 &\leq -4. \end{aligned}$$

Apply this process to the last equality constraint of the transportation problem. Then define a new matrix G with several additional rows (to account for the new inequality constraints), a new vector $\mathbf{h}$ with more entries, a smaller matrix A, and a smaller vector $\mathbf{b}$.

Problem 3. Solve the transportation problem by converting the last equality constraint into an inequality constraint. Return the minimizer $\mathbf{x}$ and the primal objective value.

Quadratic Programming

Quadratic programming is similar to linear programming, but the objective function is quadratic rather than linear. The constraints, if there are any, are still of the same form. Thus, $G, \mathbf{h}, A$, and $\mathbf{b}$ are optional. The formulation that we will use is

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2}\mathbf{x}^\mathsf{T} Q \mathbf{x} + \mathbf{r}^\mathsf{T}\mathbf{x} \\ \text{subject to} \quad & G\mathbf{x} \preceq \mathbf{h} \\ & A\mathbf{x} = \mathbf{b}, \end{aligned}$$

where Q is a positive semidefinite symmetric matrix. In this formulation, we require again that A has full row rank, and that the block matrix $[Q \quad G \quad A]^\mathsf{T}$ has full column rank.

As an example, consider the quadratic function

$$f(x_1, x_2) = 2x_1^2 + 2x_1x_2 + x_2^2 + x_1 - x_2.$$

There are no constraints, so we only need to initialize the matrix Q and the vector $\mathbf{r}$. To find these, we first rewrite our function to match the formulation given above. If we let

$$Q = \begin{bmatrix} a & b \\ b & c \end{bmatrix}, \qquad \mathbf{r} = \begin{bmatrix} d \\ e \end{bmatrix}, \qquad \text{and} \qquad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix},$$

then

$$\begin{aligned} \frac{1}{2}\mathbf{x}^\mathsf{T} Q \mathbf{x} + \mathbf{r}^\mathsf{T}\mathbf{x} &= \frac{1}{2}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}^\mathsf{T} \begin{bmatrix} a & b \\ b & c \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} d \\ e \end{bmatrix}^\mathsf{T} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \\ &= \frac{1}{2}ax_1^2 + bx_1x_2 + \frac{1}{2}cx_2^2 + dx_1 + ex_2 \end{aligned}$$

Thus, we see that the proper values to initialize our matrix Q and vector $\mathbf{r}$ are:

$$\begin{aligned} a &= 4 & d &= 1 \\ b &= 2 & e &= -1 \\ c &= 2 \end{aligned}$$

Now that we have the matrix Q and vector $\mathbf{r}$, we are ready to use the CVXOPT function for quadratic programming `solvers.qp()`.

```
>>> Q = matrix(np.array([[4., 2.], [2., 2.]]))
>>> r = matrix([1., -1.])
>>> sol=solvers.qp(Q, r)
>>> print(sol['x'])
[-1.00e+00]
[ 1.50e+00]
>>> print sol['primal objective']
-1.25
```

Problem 4. Find the minimizer and minimum of

$$g(x_1, x_2, x_3) = \frac{3}{2}x_1^2 + 2x_1x_2 + x_1x_3 + 2x_2^2 + 2x_2x_3 + \frac{3}{2}x_3^2 + 3x_1 + x_3$$

(Hint: Write the function g to match the formulation given above before coding.)

Problem 5. The l_2 minimization problem is to

$$\begin{array}{ll} \text{minimize} & \|\mathbf{x}\|_2 \\ \text{subject to} & A\mathbf{x} = \mathbf{b}. \end{array}$$

This problem is equivalent to a quadratic program, since $\|\mathbf{x}\|_2 = \mathbf{x}^\mathsf{T}\mathbf{x}$. Write a function that accepts a matrix A and vector $\mathbf{b}$ and solves the l_2 minimization problem. Return the minimizer $\mathbf{x}$ and the primal objective value.

To test your function, use the matrix A and vector $\mathbf{b}$ from Problem 2. The minimizer is approximately $\mathbf{x} = [1.55, 2.36, 2.36, 0.73]^T$ and the minimum primal objective value is approximately 14.09.

Allocation Models

Allocation models lead to simple linear programs. An allocation model seeks to allocate a valuable resource among competing needs. Consider the following example taken from "Optimization in Operations Research" by Ronald L. Rardin.

The U.S. Forest service has used an allocation model to deal with the task of managing national forests. The model begins by dividing the land into a set of analysis areas. Several land management policies (also called prescriptions) are then proposed and evaluated for each area. An *allocation* is how much land (in acreage) in each unique analysis area will be assigned to each of the possible prescriptions. We seek to find the best possible allocation, subject to forest-wide restrictions on land use.

The file `ForestData.npy` contains data for a fictional national forest (you can also find the data in Table 14.4). There are 7 areas of analysis and 3 prescriptions for each of them.

Column 1: i, area of analysis

Column 2: s_i, size of the analysis area (in thousands of acres)

Column 3: j, prescription number

Column 4: $p_{i,j}$, net present value (NPV) per acre in area i under prescription j

Column 5: $t_{i,j}$, protected timber yield per acre in area i under prescription j

Column 6: $g_{i,j}$, protected animal grazing capability per acre for area i under prescription j

Column 7: $w_{i,j}$, wilderness index rating (0 to 100) for area i under prescription j

Forest Data

Analysis Area i	Acres (1000)'s s_i	Prescription j	NPV (per acre) $p_{i,j}$	Timber (per acre) $t_{i,j}$	Grazing (per acre) $g_{i,j}$	Wilderness Index $w_{i,j}$
1	75	1	503	310	0.01	40
		2	140	50	0.04	80
		3	203	0	0	95
2	90	1	675	198	0.03	55
		2	100	46	0.06	60
		3	45	0	0	65
3	140	1	630	210	0.04	45
		2	105	57	0.07	55
		3	40	0	0	60
4	60	1	330	112	0.01	30
		2	40	30	0.02	35
		3	295	0	0	90
5	212	1	105	40	0.05	60
		2	460	32	0.08	60
		3	120	0	0	70
6	98	1	490	105	0.02	35
		2	55	25	0.03	50
		3	180	0	0	75
7	113	1	705	213	0.02	40
		2	60	40	0.04	45
		3	400	0	0	95

Table 14.4

Let $x_{i,j}$ be the amount of land in area i allocated to prescription j. Under this notation, an allocation is a one-dimensional vector consisting of the $x_{i,j}$'s. For this particular example, there are 7 acres, with 3 prescriptions each. So the allocation vector is a one-dimensional vector with 21 entries. Our goal is to find the allocation vector that maximizes net present value, while producing at least 40 million board-feet of timber, at least 5 thousand units of grazing capability, and keeping the average wilderness index at least 70. The allocation vector is also constrained to be nonnegative, and all of the land must be allocated precisely.

Since acres are in thousands, divide the constraints of timber and animal grazing by 1000 in the problem setup, and compensate for this after obtaining a solution.

The problem can be written as follows:

$$\begin{aligned}
\text{maximize } & \sum_{i=1}^{7}\sum_{j=1}^{3} p_{i,j}x_{i,j} \\
\text{subject to } & \sum_{j=1}^{3} x_{i,j} = s_i \text{ for } i = 1,..,7 \\
& \sum_{i=1}^{7}\sum_{j=1}^{3} t_{i,j}x_{i,j} \geq 40,000 \\
& \sum_{i=1}^{7}\sum_{j=1}^{3} g_{i,j}x_{i,j} \geq 5 \\
& \frac{1}{788}\sum_{i=1}^{7}\sum_{j=1}^{3} w_{i,j}x_{i,j} \geq 70 \\
& x_{i,j} \geq 0 \text{ for } i = 1,...,7 \text{ and } j = 1,2,3
\end{aligned}$$

Problem 6. Solve the allocation problem above. Return the minimizing allocation vector of $x_{i,j}$'s and the maximum total net present value. Remember to consider the following:

1. The allocation vector should be a (21,1) NumPy array.
2. Recall that the constraints of timber and animal grazing were divided by 1000. To compensate, the maximum total net value will be equal to the primal objective of the appropriately minimized linear function multiplied by -1000.

You can learn more about CVXOPT at `http://cvxopt.org/index.html`.

15 Interior Point 1: Linear Programs

Lab Objective: *For decades after its invention, the Simplex algorithm was the only competitive method for linear programming. The past 30 years, however, have seen the discovery and widespread adoption of a new family of algorithms that rival–and in some cases outperform–the Simplex algorithm, collectively called* Interior Point methods. *One of the major shortcomings of the Simplex algorithm is that the number of steps required to solve the problem can grow exponentially with the size of the linear system. Thus, for certain large linear programs, the Simplex algorithm is simply not viable. Interior Point methods offer an alternative approach and enjoy much better theoretical convergence properties. In this lab we implement an Interior Point method for linear programs, and in the next lab we will turn to the problem of solving quadratic programs.*

Introduction

Recall that a linear program is a constrained optimization problem with a linear objective function and linear constraints. The linear constraints define a set of allowable points called the *feasible region*, the boundary of which forms a geometric object known as a *polytope*. The theory of convex optimization ensures that the optimal point for the objective function can be found among the vertices of the feasible polytope. The Simplex Method tests a sequence of such vertices until it finds the optimal point. Provided the linear program is neither unbounded nor infeasible, the algorithm is certain to produce the correct answer after a finite number of steps, but it does not guarantee an efficient path along the polytope toward the minimizer. Interior point methods do away with the feasible polytope and instead generate a sequence of points that cut through the interior (or exterior) of the feasible region and converge iteratively to the optimal point. Although it is computationally more expensive to compute such interior points, each step results in significant progress toward the minimizer. See Figure 15.1. In general, the Simplex Method requires many more iterations (though each iteration is less expensive computationally).

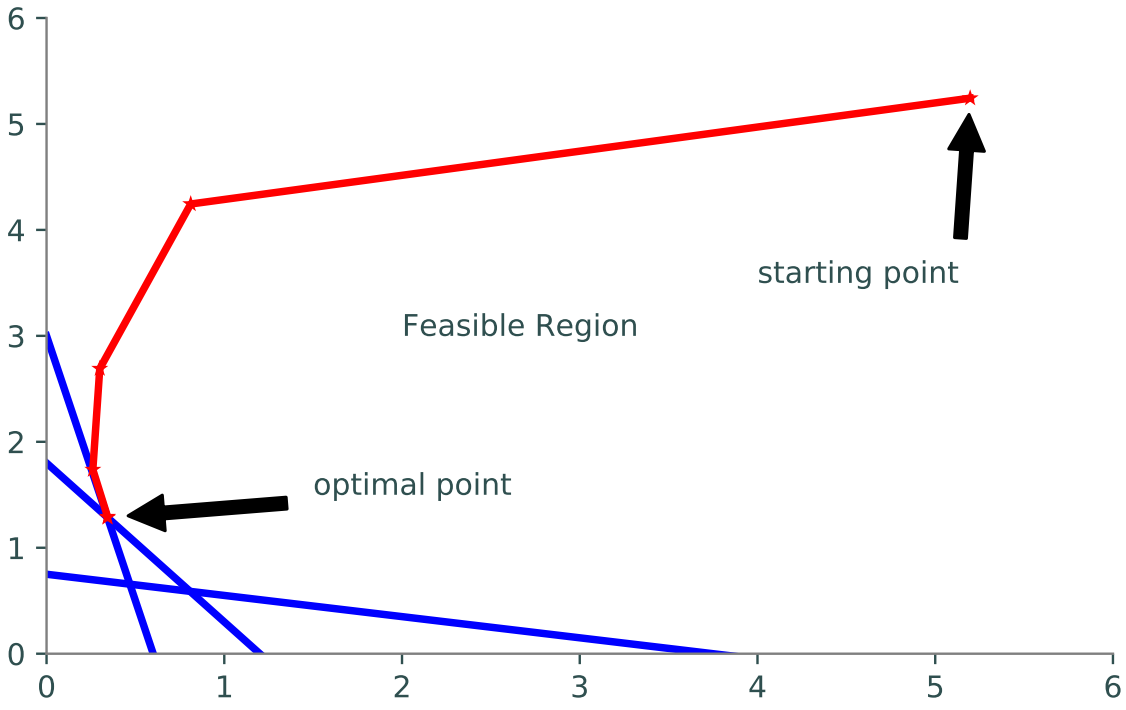


Figure 15.1: A path traced by an Interior Point algorithm.

Primal-Dual Interior Point Methods

Some of the most popular and successful types of Interior Point methods are known as Primal-Dual Interior Point methods. Consider the following linear program:

$$\begin{aligned} \text{minimize} \quad & \mathbf{c}^\mathsf{T}\mathbf{x} \\ \text{subject to} \quad & A\mathbf{x} = \mathbf{b} \\ & \mathbf{x} \succeq \mathbf{0}. \end{aligned}$$

Here, $\mathbf{x}, \mathbf{c} \in \mathbb{R}^n$, $\mathbf{b} \in \mathbb{R}^m$, and A is an $m \times n$ matrix with full row rank. This is the *primal* problem, and its *dual* takes the form:

$$\begin{aligned} \text{maximize} \quad & \mathbf{b}^\mathsf{T}\boldsymbol{\lambda} \\ \text{subject to} \quad & A^\mathsf{T}\boldsymbol{\lambda} + \boldsymbol{\mu} = \mathbf{c} \\ & \boldsymbol{\mu}, \boldsymbol{\lambda} \succeq \mathbf{0}, \end{aligned}$$

where $\boldsymbol{\lambda} \in \mathbb{R}^m$ and $\boldsymbol{\mu} \in \mathbb{R}^n$.

KKT Conditions

The theory of convex optimization gives us necessary and sufficient conditions for the solutions to the primal and dual problems via the Karush-Kuhn-Tucker (KKT) conditions. The Lagrangian for the primal problem is as follows:

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = \mathbf{c}^\mathsf{T}\mathbf{x} + \boldsymbol{\lambda}^\mathsf{T}(\mathbf{b} - A\mathbf{x}) - \boldsymbol{\mu}^\mathsf{T}\mathbf{x}$$

The KKT conditions are

$$\begin{aligned} A^\mathsf{T}\boldsymbol{\lambda} + \boldsymbol{\mu} &= \mathbf{c} \\ A\mathbf{x} &= \mathbf{b} \\ x_i\mu_i &= 0, \quad i = 1, 2, \ldots, n, \\ \mathbf{x}, \boldsymbol{\mu} &\succeq 0. \end{aligned}$$

It is convenient to write these conditions in a more compact manner, by defining an almost-linear function F and setting it equal to zero:

$$F(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) := \begin{bmatrix} A^\mathsf{T}\boldsymbol{\lambda} + \boldsymbol{\mu} - \mathbf{c} \\ A\mathbf{x} - \mathbf{b} \\ M\mathbf{x} \end{bmatrix} = \mathbf{0}, \quad (\mathbf{x}, \boldsymbol{\mu} \succeq \mathbf{0}),$$

where $M = \text{diag}(\mu_1, \mu_2, \ldots, \mu_n)$. Note that the first row of F is the KKT condition for dual feasibility, the second row of F is the KKT condition for the primal problem, and the last row of F accounts for complementary slackness.

Problem 1. Define a function `interiorPoint()` that will be used to solve the complete interior point problem. This function should accept A, $\mathbf{b}$, and $\mathbf{c}$ as parameters, along with the keyword arguments `niter=20` and `tol=1e-16`. The keyword arguments will be used in a later problem.

For this problem, within the `interiorPoint()` function, write a function for the vector-valued function F described above. This function should accept $\mathbf{x}$, $\boldsymbol{\lambda}$, and $\boldsymbol{\mu}$ as parameters and return a 1-dimensional NumPy array with $2n + m$ entries.

Search Direction

A Primal-Dual Interior Point method is a line search method that starts with an initial guess $(\mathbf{x}_0^\mathsf{T}, \boldsymbol{\lambda}_0^\mathsf{T}, \boldsymbol{\mu}_0^\mathsf{T})$ and produces a sequence of points that converge to $(\mathbf{x}^{*\mathsf{T}}, \boldsymbol{\lambda}^{*\mathsf{T}}, \boldsymbol{\mu}^{*\mathsf{T}})$, the solution to the KKT equations and hence the solution to the original linear program. The constraints on the problem make finding a search direction and step length a little more complicated than for the unconstrained line search we have studied previously.

In the spirit of Newton's Method, we can form a linear approximation of the system $F(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = \mathbf{0}$ centered around our current point $(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu})$, and calculate the direction $(\triangle\mathbf{x}^\mathsf{T}, \triangle\boldsymbol{\lambda}^\mathsf{T}, \triangle\boldsymbol{\mu}^\mathsf{T})$ in which to step to set the linear approximation equal to $\mathbf{0}$. This equates to solving the linear system:

$$DF(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) \begin{bmatrix} \triangle\mathbf{x} \\ \triangle\boldsymbol{\lambda} \\ \triangle\boldsymbol{\mu} \end{bmatrix} = -F(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) \tag{15.1}$$

Here $DF(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu})$ denotes the total derivative matrix of F. We can calculate this matrix block-wise by obtaining the partial derivatives of each block entry of $F(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu})$ with respect to $\mathbf{x}$, $\boldsymbol{\lambda}$, and $\boldsymbol{\mu}$, respectively. We thus obtain:

$$DF(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = \begin{bmatrix} 0 & A^\mathsf{T} & I \\ A & 0 & 0 \\ M & 0 & X \end{bmatrix}$$

where $X = \text{diag}(x_1, x_2, \dots, x_n)$.

Unfortunately, solving Equation 15.1 often leads to a search direction that is too greedy. Even small steps in this direction may lead the iteration out of the feasible region by violating one of the constraints. To remedy this, we define the *duality measure* ν[1] of the problem:

$$\nu = \frac{\mathbf{x}^\mathsf{T}\boldsymbol{\mu}}{n}$$

The idea is to use Newton's method to identify a direction that strictly decreases ν. Thus instead of solving Equation 15.1, we solve:

$$DF(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) \begin{bmatrix} \triangle\mathbf{x} \\ \triangle\boldsymbol{\lambda} \\ \triangle\boldsymbol{\mu} \end{bmatrix} = -F(\mathbf{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) + \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \\ \sigma\nu\mathbf{e} \end{bmatrix} \tag{15.2}$$

where $\mathbf{e} = (1, 1, \dots, 1)^\mathsf{T}$ and $\sigma \in [0, 1)$ is called the *centering parameter*. The closer σ is to 0, the more similar the resulting direction will be to the plain Newton direction. The closer σ is to 1, the more the direction points inward to the interior of the of the feasible region.

Problem 2. Within `interiorPoint()`, write a subroutine to compute the search direction $(\triangle\mathbf{x}^\mathsf{T}, \triangle\boldsymbol{\lambda}^\mathsf{T}, \triangle\boldsymbol{\mu}^\mathsf{T})$ by solving Equation 15.2. Use $\sigma = \frac{1}{10}$ for the centering parameter.

Note that only the last block row of DF will need to be changed at each iteration (since M and X depend on $\boldsymbol{\mu}$ and $\mathbf{x}$, respectively). Consider using the functions `lu_factor()` and `lu_solve()` from the `scipy.linalg` module to solving the system of equations efficiently.

Step Length

Now that we have our search direction, it remains to choose our step length. We wish to step nearly as far as possible without violating the problem's constraints, thus remaining in the interior of the feasible region. First, we calculate the maximum allowable step lengths for $\mathbf{x}$ and $\boldsymbol{\mu}$, respectively:

$$\alpha_{\max} = \min\{1, \min\{-\mu_i/\triangle\mu_i \mid \triangle\mu_i < 0\}\}$$
$$\delta_{\max} = \min\{1, \min\{-x_i/\triangle x_i \mid \triangle x_i < 0\}\}$$

Next, we back off from these maximum step lengths slightly:

$$\alpha = \min(1, 0.95\alpha_{\max})$$
$$\delta = \min(1, 0.95\delta_{\max}).$$

These are our final step lengths. Thus, the next point in the iteration is given by:

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \delta\triangle\mathbf{x}_k$$
$$(\boldsymbol{\lambda}_{k+1}, \boldsymbol{\mu}_{k+1}) = (\boldsymbol{\lambda}_k, \boldsymbol{\mu}_k) + \alpha(\triangle\boldsymbol{\lambda}_k, \triangle\boldsymbol{\mu}_k).$$

[1] ν is the Greek letter for n, pronounced "nu."

Problem 3. Within `interiorPoint()`, write a subroutine to compute the step size after the search direction has been computed. Avoid using loops when computing $\alpha_{\max}$ and $\beta_{\max}$ (use masking and NumPy functions instead).

Initial Point

Finally, the choice of initial point $(\mathbf{x}_0, \boldsymbol{\lambda}_0, \boldsymbol{\mu}_0)$ is an important, nontrivial one. A naïvely or randomly chosen initial point may cause the algorithm to fail to converge. The following function will calculate an appropriate initial point.

```
def starting_point(A, b, c):
    """Calculate an initial guess to the solution of the linear program
    min c\trp  x, Ax = b, x>=0.
    Reference: Nocedal and Wright, p. 410.
    """
    # Calculate x, lam, mu of minimal norm satisfying both
    # the primal and dual constraints.
    B = la.inv(A @ A.T))
    x = A.T @ B @ b
    lam = B @ A @ c
    mu = c - (A.T @ lam)

    # Perturb x and s so they are nonnegative.
    dx = max((-3./2)*x.min(), 0)
    dmu = max((-3./2)*mu.min(), 0)
    x += dx*np.ones_like(x)
    mu += dmu*np.ones_like(mu)

    # Perturb x and mu so they are not too small and not too dissimilar.
    dx = .5*(x*mu).sum()/mu.sum()
    dmu = .5*(x*mu).sum()/x.sum()
    x += dx*np.ones_like(x)
    mu += dmu*np.ones_like(mu)

    return x, lam, mu
```

Problem 4. Complete the implementation of `interiorPoint()`.

Use the function `starting_point()` provided above to select an initial point, then run the iteration `niter` times, or until the duality measure is less than `tol`. Return the optimal point $\mathbf{x}^*$ and the optimal value $\mathbf{c}^T\mathbf{x}^*$.

The duality measure ν tells us in some sense how close our current point is to the minimizer. The closer ν is to 0, the closer we are to the optimal point. Thus, by printing the value of ν at each iteration, you can track how your algorithm is progressing and detect when you have converged.

To test your implementation, use the following code to generate a random linear program, along with the optimal solution.

```
    """Generate a linear program min c\trp  x s.t. Ax = b, x>=0.
    First generate m feasible constraints, then add
    slack variables to convert it into the above form.
    Inputs:
        m (int >= n): number of desired constraints.
        n (int): dimension of space in which to optimize.
    Outputs:
        A ((m,n+m) ndarray): Constraint matrix.
        b ((m,) ndarray): Constraint vector.
        c ((n+m,), ndarray): Objective function with m trailing 0s.
        x ((n,) ndarray): The first 'n' terms of the solution to the LP.
    """
    A = np.random.random((m,n))*20 - 10
    A[A[:,-1]<0] *= -1
    x = np.random.random(n)*10
    b = np.zeros(m)
    b[:n] = A[:n,:] @ x
    b[n:] = A[n:,:] @ x + np.random.random(m-n)*10
    c = np.zeros(n+m)
    c[:n] = A[:n,:].sum(axis=0)/n
    A = np.hstack((A, np.eye(m)))
    return A, b, -c, x
```

```
>>> m, n = 7, 5
>>> A, b, c, x = randomLP(m, n)
>>> point, value = interiorPoint(A, b, c)
>>> np.allclose(x, point[:n])
True
```

Least Absolute Deviations (LAD)

We now return to the familiar problem of fitting a line (or hyperplane) to a set of data. We have previously approached this problem by minimizing the sum of the squares of the errors between the data points and the line, an approach known as *least squares*. The least squares solution can be obtained analytically when fitting a linear function, or through a number of optimization methods (such as Conjugate Gradient) when fitting a nonlinear function.

The method of *least absolute deviations* (LAD) also seeks to find a best fit line to a set of data, but the error between the data and the line is measured differently. In particular, suppose we have a set of data points $(y_1, \mathbf{x}_1), (y_2, \mathbf{x}_2), \dots, (y_m, \mathbf{x}_m)$, where $y_i \in \mathbb{R}$, $\mathbf{x}_i \in \mathbb{R}^n$ for $i = 1, 2, \dots, m$. Here, the $\mathbf{x}_i$ vectors are the *explanatory variables* and the y_i values are the *response variables*, and we assume the following linear model:

$$y_i = \boldsymbol{\beta}^\mathsf{T}\mathbf{x}_i + b, \qquad i = 1, 2, \dots, m,$$

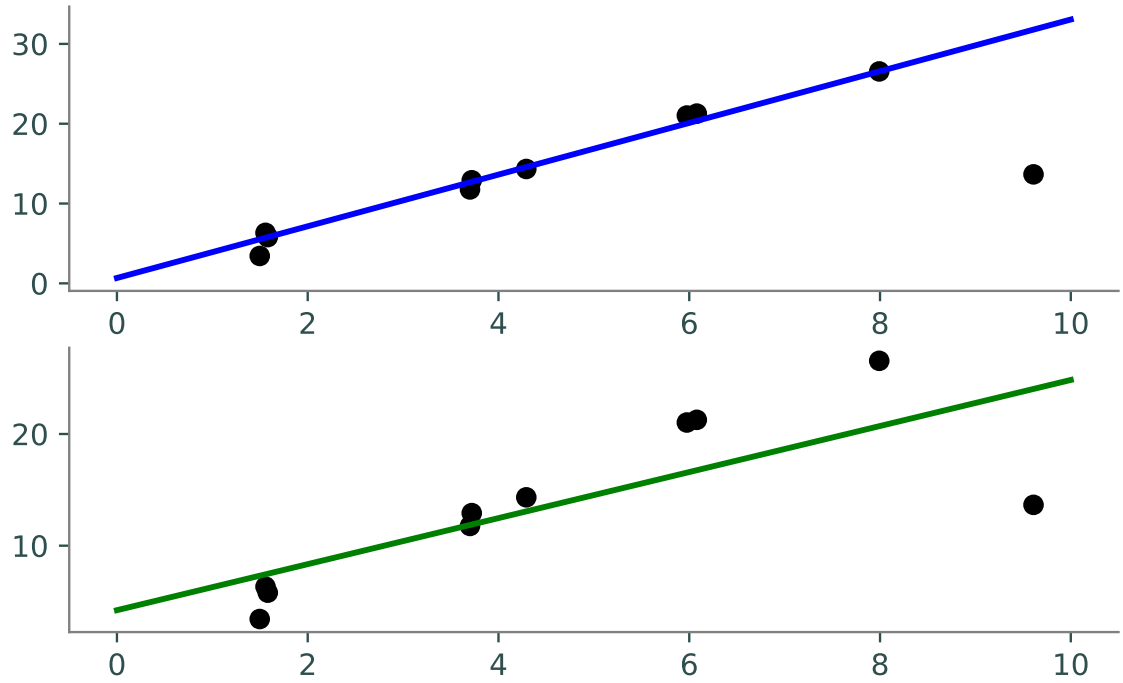


Figure 15.2: Fitted lines produced by least absolute deviations (top) and least squares (bottom). The presence of an outlier accounts for the stark difference between the two lines.

where $\boldsymbol{\beta} \in \mathbb{R}^n$ and $b \in \mathbb{R}$. The error between the data and the proposed linear model is given by

$$\sum_{i=1}^{n} |\boldsymbol{\beta}^{\mathsf{T}} \mathbf{x}_i + b - y_i|,$$

and we seek to choose the parameters $\boldsymbol{\beta}, b$ so as to minimize this error.

Advantages of LAD

The most prominent difference between this approach and least squares is how they respond to outliers in the data. Least absolute deviations is robust in the presence of outliers, meaning that one (or a few) errant data points won't severely affect the fitted line. Indeed, in most cases, the best fit line is guaranteed to pass through at least two of the data points. This is a desirable property when the outliers may be ignored (perhaps because they are due to measurement error or corrupted data). Least squares, on the other hand, is much more sensitive to outliers, and so is the better choice when outliers cannot be dismissed. See Figure 15.2.

While least absolute deviations is robust with respect to outliers, small horizontal perturbations of the data points can lead to very different fitted lines. Hence, the least absolute deviations solution is less stable than the least squares solution. In some cases there are even infinitely many lines that minimize the least absolute deviations error term. However, one can expect a unique solution in most cases.

The least absolute deviations solution arises naturally when we assume that the residual terms $\boldsymbol{\beta}^\mathsf{T}\mathbf{x}_i+b-y_i$ have a particular statistical distribution (the Laplace distribution). Ultimately, however, the choice between least absolute deviations and least squares depends on the nature of the data at hand, as well as your own good judgment.

LAD as a Linear Program

We can formulate the least absolute deviations problem as a linear program, and then solve it using our interior point method. For $i = 1, 2, \ldots, m$ we introduce the artificial variable u_i to take the place of the error term $|\boldsymbol{\beta}^\mathsf{T}\mathbf{x}_i + b - y_i|$, and we require this variable to satisfy $u_i \geq |\boldsymbol{\beta}^\mathsf{T}\mathbf{x}_i + b - y_i|$. This constraint is not yet linear, but we can split it into an equivalent set of two linear constraints:

$$\begin{aligned} u_i &\geq \boldsymbol{\beta}^\mathsf{T}\mathbf{x}_i + b - y_i, \\ u_i &\geq y_i - \boldsymbol{\beta}^\mathsf{T}\mathbf{x}_i - b. \end{aligned}$$

The u_i are implicitly constrained to be nonnegative.

Our linear program can now be stated as follows:

$$\begin{aligned} \text{minimize} \quad & \sum_{i=1}^{m} u_i \\ \text{subject to} \quad & u_i \geq \boldsymbol{\beta}^\mathsf{T}\mathbf{x}_i + b - y_i, \\ & u_i \geq y_i - \boldsymbol{\beta}^\mathsf{T}\mathbf{x}_i - b. \end{aligned}$$

Now for each inequality constraint, we bring all variables $(u_i, \boldsymbol{\beta}, b)$ to the left hand side and introduce a nonnegative slack variable to transform the constraint into an equality:

$$\begin{aligned} u_i - \boldsymbol{\beta}^\mathsf{T}\mathbf{x}_i - b - s_{2i-1} &= -y_i, \\ u_i + \boldsymbol{\beta}^\mathsf{T}\mathbf{x}_i + b - s_{2i} &= y_i, \\ s_{2i-1}, s_{2i} &\geq 0. \end{aligned}$$

Notice that the variables $\boldsymbol{\beta}, b$ are not assumed to be nonnegative, but in our interior point method, all variables are assumed to be nonnegative. We can fix this situation by writing these variables as the difference of nonnegative variables:

$$\begin{aligned} \boldsymbol{\beta} &= \boldsymbol{\beta}_1 - \boldsymbol{\beta}_2, \\ b &= b_1 - b_2, \\ \boldsymbol{\beta}_1, \boldsymbol{\beta}_2 &\succeq \mathbf{0}; b_1, b_2 \geq 0. \end{aligned}$$

Substituting these values into our constraints, we have the following system of constraints:

$$\begin{aligned} u_i - \boldsymbol{\beta}_1^\mathsf{T}\mathbf{x}_i + \boldsymbol{\beta}_2^\mathsf{T}\mathbf{x}_i - b_1 + b_2 - s_{2i-1} &= -y_i, \\ u_i + \boldsymbol{\beta}_1^\mathsf{T}\mathbf{x}_i - \boldsymbol{\beta}_2^\mathsf{T}\mathbf{x}_i + b_1 - b_2 - s_{2i} &= y_i, \\ \boldsymbol{\beta}_1, \boldsymbol{\beta}_2 &\succeq \mathbf{0}; u_i, b_1, b_2, s_{2i-1}, s_{2i} \geq 0. \end{aligned}$$

Writing $\mathbf{y} = (-y_1, y_1, -y_2, y_2, \ldots, -y_m, y_m)^\mathsf{T}$ and $\boldsymbol{\beta}_i = (\beta_{i,1}, \ldots, \beta_{i,n})^\mathsf{T}$ for $i = \{1, 2\}$, we can aggregate all of our variables into one vector as follows:

$$\mathbf{v} = (u_1, \ldots, u_m, \beta_{1,1}, \ldots, \beta_{1,n}, \beta_{2,1}, \ldots, \beta_{2,n}, b_1, b_2, s_1, \ldots, s_{2m})^\mathsf{T}.$$

Defining $\mathbf{c} = (1, 1, \ldots, 1, 0, \ldots, 0)^\mathsf{T}$ (where only the first m entries are equal to 1), we can write our objective function as

$$\sum_{i=1}^{m} u_i = \mathbf{c}^\mathsf{T}\mathbf{v}.$$

Hence, the final form of our linear program is:

$$\begin{aligned} \text{minimize} \quad & \mathbf{c}^\mathsf{T}\mathbf{v} \\ \text{subject to} \quad & A\mathbf{v} = \mathbf{y}, \\ & \mathbf{v} \succeq \mathbf{0}, \end{aligned}$$

where A is a matrix containing the coefficients of the constraints. Our constraints are now equalities, and the variables are all nonnegative, so we are ready to use our interior point method to obtain the solution.

LAD Example

Consider the following example. We start with an array `data`, each row of which consists of the values $y_i, x_{i,1}, \ldots, x_{i,n}$, where $\mathbf{x}_i = (x_{i,1}, x_{i,2}, \ldots, x_{i,n})^\mathsf{T}$. We will have $3m + 2(n + 1)$ variables in our linear program. Below, we initialize the vectors $\mathbf{c}$ and $\mathbf{y}$.

```
>>> m = data.shape[0]
>>> n = data.shape[1] - 1
>>> c = np.zeros(3*m + 2*(n + 1))
>>> c[:m] = 1
>>> y = np.empty(2*m)
>>> y[::2] = -data[:, 0]
>>> y[1::2] = data[:, 0]
>>> x = data[:, 1:]
```

The hardest part is initializing the constraint matrix correctly. It has $2m$ rows and $3m+2(n+1)$ columns. Try writing out the constraint matrix by hand for small m, n, and make sure you understand why the code below is correct.

```
>>> A = np.ones((2*m, 3*m + 2*(n + 1)))
>>> A[::2, :m] = np.eye(m)
>>> A[1::2, :m] = np.eye(m)
>>> A[::2, m:m+n] = -x
>>> A[1::2, m:m+n] = x
>>> A[::2, m+n:m+2*n] = x
>>> A[1::2, m+n:m+2*n] = -x
>>> A[::2, m+2*n] = -1
>>> A[1::2, m+2*n+1] = -1
>>> A[:, m+2*n+2:] = -np.eye(2*m, 2*m)
```

Now we can calculate the solution by calling our interior point function.

```
>>> sol = interiorPoint(A, y, c, niter=10)[0]
```

The variable `sol`, however, holds the value for the vector

$$\mathbf{v} = (u_1, \dots, u_m, \beta_{1,1}, \dots, \beta_{1,n}, \beta_{2,1}, \dots, \beta_{2,n}, b_1, b_2, s_1, \dots, s_{2m+1})^\mathsf{T}.$$

We extract values of $\boldsymbol{\beta} = \boldsymbol{\beta}_1 - \boldsymbol{\beta}_2$ and $b = b_1 - b_2$ with the following code:

```
>>> beta = sol[m:m+n] - sol[m+n:m+2*n]
>>> b = sol[m+2*n] - sol[m+2*n+1]
```

Problem 5. The file `simdata.txt` contains two columns of data. The first gives the values of the response variables (y_i), and the second column gives the values of the explanatory variables ($\mathbf{x}_i$). Find the least absolute deviations line for this data set, and plot it together with the data. Plot the least squares solution as well to compare the results.

```
>>> from scipy.stats import linregress
>>> slope, intercept = linregress(data[:,1], data[:,0])[:2]
>>> domain = np.linspace(0,10,200)
>>> plt.plot(domain, domain*slope + intercept)
```

16 Interior Point 2: Quadratic Programs

Lab Objective: *Interior point methods originated as an alternative to the Simplex method for solving linear optimization problems. However, they can also be adapted to treat convex optimization problems in general. In this lab, we implement a primal-dual Interior Point method for convex quadratic constrained optimization and explore applications in elastic membrane theory and finance.*

Quadratic Optimization Problems

A *quadratic constrained optimization problem* differs from a linear constrained optimization problem only in that the objective function is quadratic rather than linear. We can pose such a problem as follows:

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2}\mathbf{x}^\mathsf{T} Q\mathbf{x} + \mathbf{c}^\mathsf{T}\mathbf{x} \\ \text{subject to} \quad & A\mathbf{x} \succeq \mathbf{b}, \\ & G\mathbf{x} = \mathbf{h}. \end{aligned}$$

We will restrict our attention to quadratic programs involving positive semidefinite quadratic terms (in general, indefinite quadratic objective functions admit many local minima, complicating matters considerably). Such problems are called *convex*, since the objective function is convex. To simplify the exposition, we will also only allow inequality constraints (generalizing to include equality constraints is not difficult). Thus, we have the problem

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2}\mathbf{x}^\mathsf{T} Q\mathbf{x} + \mathbf{c}^\mathsf{T}\mathbf{x} \\ \text{subject to} \quad & A\mathbf{x} \succeq \mathbf{b} \end{aligned}$$

where Q is an $n \times n$ positive semidefinite matrix, $\mathbf{x}, \mathbf{c} \in \mathbb{R}^n$, A is an $m \times n$ matrix, and $\mathbf{b} \in \mathbb{R}^m$.

The Lagrangian function for this problem is:

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\mu}) = \frac{1}{2}\mathbf{x}^\mathsf{T} Q\mathbf{x} + \mathbf{c}^\mathsf{T}\mathbf{x} - \boldsymbol{\mu}^\mathsf{T}(A\mathbf{x} - \mathbf{b}), \tag{16.1}$$

where $\boldsymbol{\mu} \in \mathbb{R}^m$ is the (as of yet unknown) Lagrange multiplier.

We also introduce a nonnegative slack vector $\mathbf{y} \in \mathbb{R}^m$ to change the inequality

$$A\mathbf{x} - \mathbf{b} \succeq \mathbf{0}$$

into the equality

$$A\mathbf{x} - \mathbf{b} - \mathbf{y} = \mathbf{0} \qquad \Longrightarrow \qquad \mathbf{y} = A\mathbf{x} - \mathbf{b} \tag{16.2}$$

Equations 16.1 and 16.2, together with complementary slackness, gives us our complete set of KKT conditions:

$$\begin{aligned} Q\mathbf{x} - A^\mathsf{T}\boldsymbol{\mu} + \mathbf{c} &= \mathbf{0}, \\ A\mathbf{x} - \mathbf{y} - \mathbf{b} &= \mathbf{0}, \\ y_i\mu_i &= 0, \qquad i = 1, 2, \ldots, m, \\ \mathbf{y}, \boldsymbol{\mu} &\succeq \mathbf{0}. \end{aligned}$$

Quadratic Interior Point Method

The Interior Point method we describe here is an adaptation of the method we used with linear programming. Define $Y = \operatorname{diag}(y_1, y_2, \ldots, y_m)$, $M = \operatorname{diag}(\mu_1, \mu_2, \ldots, \mu_m)$, and let $\mathbf{e} \in \mathbb{R}^m$ be a vector of all ones. Then the roots of the function

$$F(\mathbf{x}, \mathbf{y}, \boldsymbol{\mu}) = \begin{bmatrix} Q\mathbf{x} - A^\mathsf{T}\boldsymbol{\mu} + c \\ A\mathbf{x} - \mathbf{y} - \mathbf{b} \\ YM\mathbf{e} \end{bmatrix} = \mathbf{0}, \qquad (\mathbf{y}, \boldsymbol{\mu}) \succeq \mathbf{0}$$

satisfy the KKT conditions. The derivative matrix of this function is given by

$$DF(\mathbf{x}, \mathbf{y}, \boldsymbol{\mu}) = \begin{bmatrix} Q & 0 & -A^\mathsf{T} \\ A & -I & 0 \\ 0 & M & Y \end{bmatrix},$$

and the duality measure ν for this problem is

$$\nu = \frac{\mathbf{y}^\mathsf{T}\boldsymbol{\mu}}{m}.$$

Search Direction

We calculate the search direction for this algorithm the same way that we did in the linear programming case. That is, we solve the system:

$$DF(\mathbf{x}, \mathbf{y}, \boldsymbol{\mu}) \begin{bmatrix} \triangle\mathbf{x} \\ \triangle\mathbf{y} \\ \triangle\boldsymbol{\mu} \end{bmatrix} = -F(\mathbf{x}, \mathbf{y}, \boldsymbol{\mu}) + \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \\ \sigma\nu\mathbf{e} \end{bmatrix}, \tag{16.3}$$

where $\sigma \in [0, 1)$ is the centering parameter.

Problem 1. Copy your `interiorPoint()` function from the previous lab into your solutions file for this lab, renaming it `qInteriorPoint()`. This new function should accept the arrays $Q, \mathbf{c}, A$, and $\mathbf{b}$, a tuple of arrays `guess` giving initial estimates for $\mathbf{x}, \mathbf{y}$, and $\boldsymbol{\mu}$ (this will be explained later), along with the keyword arguments `niter=20` and `tol=1e-16`.

Modify your code to match the F and DF described above, and calculate the search direction $(\triangle\mathbf{x}^\mathsf{T}, \triangle\mathbf{y}^\mathsf{T}, \triangle\boldsymbol{\mu}^\mathsf{T})$ by solving Equation 16.3. Use $\sigma = \frac{1}{10}$ for the centering parameter.

Hint: What are the dimensions of F and DF?

Step Length

Now that we have our search direction, we select a step length. We want to step nearly as far as possible without violating the nonnegativity constraints. We back off slightly from the maximum allowed step length, however, because an overly greedy step at one iteration may prevent a decent step at the next iteration. Thus, we choose our step size

$$\alpha = \max\{a \in (0, 1] \mid \tau(\mathbf{y}, \boldsymbol{\mu}) + a(\triangle\mathbf{y}, \triangle\boldsymbol{\mu}) \succeq \mathbf{0}\},$$

where $\tau \in (0, 1)$ controls how much we back off from the maximal step length. For now, choose $\tau = 0.95$. In general, τ can be made to approach 1 at each successive iteration, and this may speed up convergence in some cases.

This is equivalent to the method of choosing a step direction used in the previous lab. In this case, however, we will use a single step length for all three of the parameters.

$$\begin{aligned}\beta_{\max} &= \min\{1, \min\{-\mu_i/\triangle\mu_i \mid \triangle\mu_i < 0\}\} \\ \delta_{\max} &= \min\{1, \min\{-y_i/\triangle y_i \mid \triangle y_i < 0\}\}\end{aligned}$$

Since $\boldsymbol{\mu}, \mathbf{y} \geq \mathbf{0}$. If all of the entries of $\triangle\mu$ are positive, we let $\beta_{\max} = 1$, and likewise for $\delta_{\max}$. Next, we back off from these maximum step lengths slightly:

$$\begin{aligned}\beta &= \min(1, \tau\beta_{\max}) \\ \delta &= \min(1, \tau\delta_{\max}) \\ \alpha &= \min(\beta, \delta)\end{aligned}$$

This α is our final step length. Thus, the next point in the iteration is given by:

$$(\mathbf{x}_{k+1}, \mathbf{y}_{k+1}, \boldsymbol{\mu}_{k+1}) = (\mathbf{x}_k, \mathbf{y}_k, \boldsymbol{\mu}_k) + \alpha(\triangle\mathbf{x}_k, \triangle\mathbf{y}_k, \triangle\boldsymbol{\mu}_k).$$

This completes one iteration of the algorithm.

Initial Point

As usual, the starting point $(\mathbf{x}_0, \mathbf{y}_0, \boldsymbol{\mu}_0)$ has an important effect on the convergence of the algorithm. The code listed below will calculate an appropriate starting point:

```
def startingPoint(G, c, A, b, guess):
    """
    Obtain an appropriate initial point for solving the QP
```

```
    .5 x\trp  Gx + x\trp  c s.t. Ax >= b.
    Parameters:
        G -- symmetric positive semidefinite matrix shape (n,n)
        c -- array of length n
        A -- constraint matrix shape (m,n)
        b -- array of length m
        guess -- a tuple of arrays (x, y, l) of lengths n, m, and m, resp.
    Returns:
        a tuple of arrays (x0, y0, l0) of lengths n, m, and m, resp.
    """
    m,n = A.shape
    x0, y0, l0 = guess

    # initialize linear system
    N = np.zeros((n+m+m, n+m+m))
    N[:n,:n] = G
    N[:n, n+m:] = -A.T
    N[n:n+m, :n] = A
    N[n:n+m, n:n+m] = -np.eye(m)
    N[n+m:, n:n+m] = np.diag(l0)
    N[n+m:, n+m:] = np.diag(y0)
    rhs = np.empty(n+m+m)
    rhs[:n] = -(G.dot(x0) - A.T.dot(l0)+c)
    rhs[n:n+m] = -(A.dot(x0) - y0 - b)
    rhs[n+m:] = -(y0*l0)

    sol = la.solve(N, rhs)
    dx = sol[:n]
    dy = sol[n:n+m]
    dl = sol[n+m:]

    y0 = np.maximum(1, np.abs(y0 + dy))
    l0 = np.maximum(1, np.abs(l0+dl))

    return x0, y0, l0
```

Notice that we still need to provide a tuple of arrays `guess` as an argument. Do your best to provide a reasonable guess for the array $\mathbf{x}$, and we suggest setting $\mathbf{y}$ and $\boldsymbol{\mu}$ equal to arrays of ones. We summarize the entire algorithm below.

---

procedure INTERIOR POINT METHOD FOR QP
  Choose initial point $(\mathbf{x}_0, \mathbf{y}_0, \boldsymbol{\mu}_0)$.
  while $k <$ `niters` and $\nu <$ `tol`: **do**
    Calculate the duality measure ν.
    Solve 16.3 for the search direction $(\triangle\mathbf{x}_k, \triangle\mathbf{y}_k, \triangle\boldsymbol{\mu}_k)$.
    Calculate the step length α.
    $(\mathbf{x}_{k+1}, \mathbf{y}_{k+1}, \boldsymbol{\mu}_{k+1}) = (\mathbf{x}_k, \mathbf{y}_k, \boldsymbol{\mu}_k) + \alpha(\triangle\mathbf{x}_k, \triangle\mathbf{y}_k, \triangle\boldsymbol{\mu}_k)$.

Problem 2. Complete the implementation of `qInteriorPoint()`. Return the optimal point $\mathbf{x}$ as well as the final objective function value. You may want to print out the duality measure ν to check the progress of the iteration.

Test your algorithm on the simple problem

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2}x_1^2 + x_2^2 - x_1x_2 - 2x_1 - 6x_2 \\ \text{subject to} \quad & -x_1 - x_2 \geq -2, \\ & x_1 - 2x_2 \geq -2, \\ & -2x_1 - x_2 \geq -3, \\ & x_1, x_2 \geq 0. \end{aligned}$$

In this case, we have for the objective function matrix Q and vector $\mathbf{c}$,

$$Q = \begin{bmatrix} 1 & -1 \\ -1 & 2 \end{bmatrix}, \qquad \mathbf{c} = \begin{bmatrix} -2 \\ -6 \end{bmatrix}.$$

The constraint matrix A and vector $\mathbf{b}$ are given by:

$$A = \begin{bmatrix} -1 & -1 \\ 1 & -2 \\ -2 & -1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}, \qquad \mathbf{b} = \begin{bmatrix} -2 \\ -2 \\ -3 \\ 0 \\ 0 \end{bmatrix}.$$

Use $\mathbf{x} = [.5, .5]$ as the initial guess. The correct minimizer is $\left[\frac{2}{3}, \frac{4}{3}\right]$.

NOTE

The Interior Point methods presented in this and the preceding labs are only special cases of the more general Interior Point algorithm. The general version can be used to solve many convex optimization problems, provided that one can derive the corresponding KKT conditions and duality measure ν.

Application: Optimal Elastic Membranes

The properties of elastic membranes (stretchy materials like a thin rubber sheet) are of interest in certain fields of mathematics and various sciences. A mathematical model for such materials can be used by biologists to study interfaces in cellular regions in an organism, or by engineers to design tensile structures. Often we can describe configurations of elastic membranes as a solution to an optimization problem. As a simple example, we will find the shape of a large circus tent by solving a quadratic constrained optimization problem using our Interior Point method.

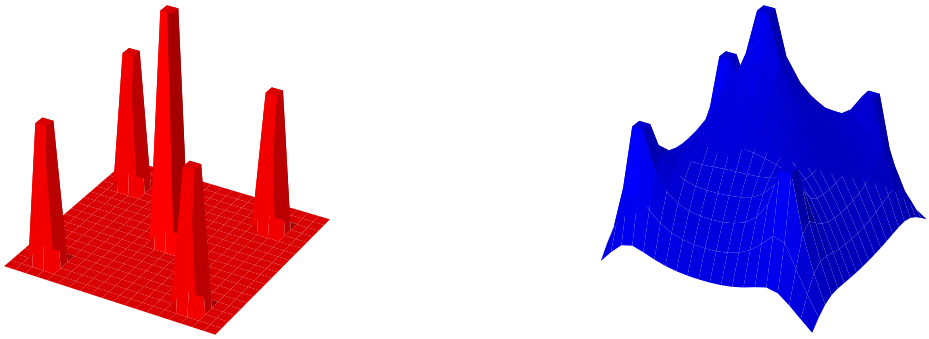


Figure 16.1: Tent pole configuration (left) and optimal elastic tent (right).

Imagine a large circus tent held up by a few poles. We can model the tent by a square two-dimensional grid, where each grid point has an associated number that gives the height of the tent at that point. At each grid point containing a tent pole, the tent height is constrained to be at least as large as the height of the tent pole. At all other grid points, the tent height is simply constrained to be greater than zero (ground height). In Python, we can store a two-dimensional grid of values as a simple two-dimensional array. We can then flatten this array to give a one-dimensional vector representation of the grid. If we let $\mathbf{x}$ be a one-dimensional array giving the tent height at each grid point, and L be the one-dimensional array giving the underlying tent pole structure (consisting mainly of zeros, except at the grid points that contain a tent pole), we have the linear constraints:

$$\mathbf{x} \succeq L.$$

The theory of elastic membranes claims that such materials tend to naturally minimize a quantity known as the *Dirichlet energy*. This quantity can be expressed as a quadratic function of the membrane. Then since we have modeled our tent with a discrete grid of values, this energy function has the form

$$\frac{1}{2}\mathbf{x}^\mathsf{T} H\mathbf{x} + \mathbf{c}^\mathsf{T}\mathbf{x},$$

where H is a particular positive semidefinite matrix closely related to Laplace's Equation, $\mathbf{c}$ is a vector whose entries are all equal to $-(n-1)^{-2}$, and n is the side length of the grid. Our circus tent is therefore given by the solution to the quadratic constrained optimization problem:

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2}\mathbf{x}^\mathsf{T} H\mathbf{x} + \mathbf{c}^\mathsf{T}\mathbf{x} \\ \text{subject to} \quad & \mathbf{x} \succeq L. \end{aligned}$$

See Figure 16.1 for an example of a tent pole configuration and the corresponding tent.

We provide the following function for producing the Dirichlet energy matrix H.

```
from scipy.sparse import spdiags
def laplacian(n):
    """Construct the discrete Dirichlet energy matrix H for an n x n grid."""
    data = -1*np.ones((5, n**2))
    data[2,:] = 4
    data[1, n-1::n] = 0
    data[3, ::n] = 0
    diags = np.array([-n, -1, 0, 1, n])
    return spdiags(data, diags, n**2, n**2).toarray()
```

Now we initialize the tent pole configuration for a grid of side length n, as well as initial guesses for $\mathbf{x}$, $\mathbf{y}$, and $\boldsymbol{\mu}$.

```
# Create the tent pole configuration.
>>> L = np.zeros((n,n))
>>> L[n//2-1:n//2+1,n//2-1:n//2+1] = .5
>>> m = [n//6-1, n//6, int(5*(n/6.))-1, int(5*(n/6.))]
>>> mask1, mask2 = np.meshgrid(m, m)
>>> L[mask1, mask2] = .3
>>> L = L.ravel()

# Set initial guesses.
>>> x = np.ones((n,n)).ravel()
>>> y = np.ones(n**2)
>>> mu = np.ones(n**2)
```

We leave it to you to initialize the vector $\mathbf{c}$, the constraint matrix A, and to initialize the matrix H with the `laplacian()` function. We can solve and plot the tent with the following code:

```
>>> from matplotlib import pyplot as plt
>>> from mpl_toolkits.mplot3d import axes3d

# Calculate the solution.
>>> z = qInteriorPoint(H, c, A, L, (x,y,mu))[0].reshape((n,n))

# Plot the solution.
>>> domain = np.arange(n)
>>> X, Y = np.meshgrid(domain, domain)
>>> fig = plt.figure()
>>> ax1 = fig.add_subplot(111, projection='3d')
>>> ax1.plot_surface(X, Y, z,  rstride=1, cstride=1, color='r')
>>> plt.show()
```

Problem 3. Solve the circus tent problem with the tent pole configuration given above, for grid side length $n = 15$. Plot your solution.

Application: Markowitz Portfolio Optimization

Suppose you have a certain amount of money saved up, with no intention of consuming it any time soon. What will you do with this money? If you hide it somewhere in your living quarters or on your person, it will lose value over time due to inflation, not to mention you run the risk of burglary or accidental loss. A safer choice might be to put the money into a bank account. That way, there is less risk of losing the money, plus you may even add to your savings through interest payments from the bank. You could also consider purchasing bonds from the government or stocks from various companies, which come with their own sets of risks and returns. Given all of these possibilities, how can you invest your money in such a way that maximizes the return (i.e. the wealth that you gain over the course of the investment) while still exercising caution and avoiding excessive risk? Economist and Nobel laureate Harry Markowitz developed the mathematical underpinnings of and answer to this question in his work on modern portfolio theory.

A *portfolio* is a set of investments over a period of time. Each investment is characterized by a financial asset (such as a stock or bond) together with the proportion of wealth allocated to the asset. An asset is a random variable, and can be described as a sequence of values over time. The variance or spread of these values is associated with the risk of the asset, and the percent change of the values over each time period is related to the return of the asset. For our purposes, we will assume that each asset has a positive risk, i.e. there are no *riskless* assets available.

Stated more precisely, our portfolio consists of n risky assets together with an allocation vector $\mathbf{x} = (x_1, \dots, x_n)^\mathsf{T}$, where x_i indicates the proportion of wealth we invest in asset i. By definition, the vector $\mathbf{x}$ must satisfy

$$\sum_{i=1}^{n} x_i = 1.$$

Suppose the ith asset has an expected rate of return μ_i and a standard deviation σ_i. The total return on our portfolio, i.e. the expected percent change in our invested wealth over the investment period, is given by

$$\sum_{i=1}^{n} \mu_i x_i.$$

We define the risk of this portfolio in terms of the covariance matrix Q of the n assets:

$$\sqrt{\mathbf{x}^\mathsf{T} Q \mathbf{x}}.$$

The covariance matrix Q is always positive semidefinite, and captures the variance and correlations of the assets.

Given that we want our portfolio to have a prescribed return R, there are in general many possible allocation vectors $\mathbf{x}$ that make this possible. It would be wise to choose the vector minimizing the risk. We can state this as a quadratic program:

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2}\mathbf{x}^\mathsf{T} Q \mathbf{x} \\ \text{subject to} \quad & \sum_{i=1}^{n} x_i = 1 \\ & \sum_{i=1}^{n} \mu_i x_i = R. \end{aligned}$$

Note that we have slightly altered our objective function for convenience, as minimizing $\frac{1}{2}\mathbf{x}^\mathsf{T}Q\mathbf{x}$ is equivalent to minimizing $\sqrt{\mathbf{x}^\mathsf{T}Q\mathbf{x}}$. The solution to this problem will give the portfolio with least risk having a return R. Because the components of $\mathbf{x}$ are not constrained to be nonnegative, the solution may have some negative entries. This indicates short selling those particular assets. If we want to disallow short selling, we simply include nonnegativity constraints, stated in the following problem:

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2}\mathbf{x}^\mathsf{T}Q\mathbf{x} \\ \text{subject to} \quad & \sum_{i=1}^{n} x_i = 1 \\ & \sum_{i=1}^{n} \mu_i x_i = R \\ & \mathbf{x} \succeq \mathbf{0}. \end{aligned}$$

Each return value R can be paired with its corresponding minimal risk σ. If we plot these risk-return pairs on the risk-return plane, we obtain a hyperbola. In general, the risk-return pair of any portfolio, optimal or not, will be found in the region bounded on the left by the hyperbola. The positively-sloped portion of the hyperbola is known as the *efficient frontier*, since the points there correspond to optimal portfolios. Portfolios with risk-return pairs that lie to the right of the efficient frontier are inefficient portfolios, since we could either increase the return while keeping the risk constant, or we could decrease the risk while keeping the return constant. See Figure 16.2.

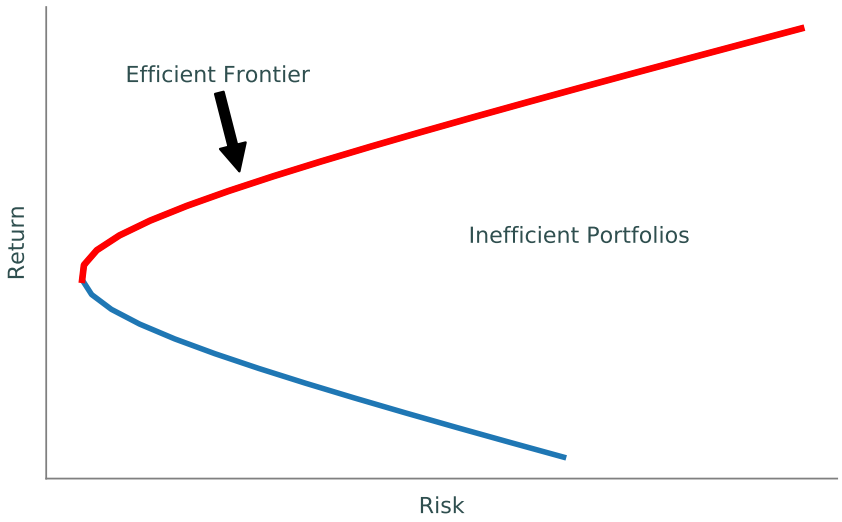


Figure 16.2: Efficient frontier on the risk-return plane.

One difficulty of this model is that the risk and return of each asset is in general unknown. After all, no one can predict the stock market with complete certainty. There are various ways of estimating these values given past stock prices, and we take a very straightforward approach. Suppose for each asset we have k previous return values of the asset. That is, for asset i, we have the data vector

$$y^i = [y_1^i, \ \ldots, \ y_k^i]^\mathsf{T}.$$

We estimate the expected rate of return for asset i by simply taking the average of $y_1, \dots, y_k$, and we estimate the variance of asset i by taking the variance of the data. We can estimate the covariance matrix for all assets by taking the covariance matrix of the vectors $y^1, \dots, y^n$. In this way, we obtain estimated values for Q and each μ_i.

Problem 4. The text file `portfolio.txt` contains historical stock data for several assets (U.S. bonds, gold, S&P 500, etc). In particular, the first column gives the years corresponding to the data, and the remaining eight columns give the historical returns of eight assets over the course of these years. Use this data to estimate the covariance matrix Q as well as the expected rates of return μ_i for each asset. Assuming that we want to guarantee an expected return of $R = 1.13$ for our portfolio, find the optimal portfolio both with and without short selling.

Since the problem contains both equality and inequality constraints, use the QP solver in CVXOPT rather than your `qInteriorPoint()` function.

Hint: Use `numpy.cov()` to compute Q.

17 Dynamic Programming

Lab Objective: *Sequential decision making problems are a class of problems in which the current choice depends on future choices. They are a subset of Markov decision processes, an important class of problems with applications in business, robotics, and economics. Dynamic programming is a method of solving these problems that optimizes the solution by breaking the problem down into steps and optimizing the decision at each time period. In this lab, we use dynamic programming to solve two classic dynamic optimization problems.*

The Marriage Problem

Many dynamic optimization problems can be classified as *optimal stopping* problems, where the goal is to determine at what time to take an action to maximize the expected reward. For example, when hiring a secretary, how many people should you interview before hiring the current interviewer? Or how many people should you date before you get married? These problems try to determine at what person t to stop in order to maximize the chance of getting the best candidate.

For instance, let N be the number of people you could date. After dating each person, you can either marry them or move on; you can't resume a relationship once it ends. In addition, you can rank your current relationship to all of the previous options, but not to future ones. The goal is to find the policy that maximizes the probability of choosing the best marriage partner. That policy may not always choose the best candidate, but it should get an almost-best candidate most of the time.

Let $V(t-1)$ be the probability that we choose the best partner when we have passed over the first $t-1$ candidates with an optimal policy. By Bellman's optimality equations,

$$V(t-1) = \frac{t-1}{t}V(t) + \frac{1}{t}\max\left\{\frac{t}{N}, V(t)\right\} = \max\left\{\frac{t-1}{t}V(t) + \frac{1}{N}, V(t)\right\}. \tag{17.1}$$

That is, $V(t-1)$ is split into two possibilities. When candidate t is not the best so far, we use the left-hand side of the last equation, $\frac{t-1}{t}V(t)+\frac{1}{N}$. Unless this is the last candidate, we don't want to choose them because we've seen someone better. When candidate t is the best so far, we use the right-hand side, $V(t)$. We can either choose this candidate, in which case they turn out to be the best match with probability $\frac{t}{N}$, or move on. Notice that (17.1) implies that $V(t-1) \geq V(t)$ for all $t \leq N$. Hence, the probability of selecting the best match $V(t)$ is non-increasing. Conversely, the probability that if candidate t is the best so far, then they are also the best overall, $\frac{t}{N}$, is strictly increasing. Therefore, there is some t_0, called the *optimal stopping point*, such that $V(t) \leq \frac{t}{N}$ for all $t \geq t_0$. After t_0 relationships, we choose the next partner who is better than all of the previous ones. We can write (17.1) as

$$V(t-1) = \begin{cases} V(t_0) & t < t_0, \\ \frac{t-1}{t}V(t)+\frac{1}{N} & t \geq t_0. \end{cases}$$

The goal of an optimal stopping problem is to find t_0, which we can do by backwards induction on the second piece of $V(t-1)$. We start at the final candidate, who always has probability 0 of being the best overall if they are not the best so far, and work our way backwards, computing the expected value $V(t)$, for $t = N, N-1, \ldots, 1$. Notice that the first candidate is always the best so far, so the probability that they are the best overall is just 1 divided by the number of candidates, $V(1) = \frac{1}{N}$.

If $N = 4$, we have

$$\begin{aligned} V(4) &= 0, \\ V(3) &= \frac{3}{4}V(4) + \frac{1}{4} = .25, \\ V(2) &= \frac{2}{3}V(3) + \frac{1}{4} = .4166, \\ V(1) &= \frac{1}{4} \qquad\qquad = .25. \end{aligned}$$

In this case, the maximum expected value is .4166 and the stopping point is 2. Sometimes it is also useful to look at the optimal stopping percentage of people to date before stopping, which in this case is $2/4 = .5$.

Problem 1. Write a function that accepts a number of candidates N. Calculate the expected values of choosing candidate t when they are not the best candidate so far for $t = 0, 1, \ldots, N-1$. Return the highest expected value $V(t_0)$ and its index t_0.
(Hint: Since Python starts indices at 0, in code the first candidate is $t = 0$.)

Check your answer for $N = 4$ with the example detailed above.

Problem 2. Write a function that takes in an integer M and runs your function from Problem 1 for each $N = 3, 4, \ldots, M$. Graph the percentage of candidates (t_0/N) to interview and the maximum probability $V(t_0)$ against N. Return the optimal stopping percentage for N.

Run your function with $M = 1000$. What values do $V(t_0)$ and t_0 converge to as $N \to \infty$?

Both the stopping time and the probability of choosing the best person converge to $\frac{1}{e} \approx .36788$. Then to maximize the chance of having the best marriage, you should date at least $\frac{N}{e}$ people before choosing the next best person. This famous problem is also known as the *secretary problem*, the *sultan's dowry problem*, and the *best choice problem*. For more information, see `https://en.wikipedia.org/wiki/Secretary_problem`.

The Cake Eating Problem

Imagine you are given a cake. How do you eat it to maximize your enjoyment? Some people may prefer to eat all of their cake at once and not save any for later. Others may prefer to eat a little bit at a time. If we are to consume a cake of size W over $T+1$ time periods, then our consumption at each step is represented as a vector

$$\begin{bmatrix} c_0 & c_1 & \cdots & c_T \end{bmatrix}^\mathsf{T},$$

where

$$\sum_{i=0}^{T} c_i = W.$$

This vector is called a *policy vector* and describes how much cake is eaten at each time period. The enjoyment of eating a slice of cake is represented by a utility function. For some amount of consumption $c_0 \in [0, W]$, the utility gained is given by $u(c_0)$.

For this lab, we assume the utility function satisfies $u(0) = 0$, that $W = 1$, and that W is cut into N equally-sized pieces so that each c_i must be of the form $\frac{i}{N}$ for some integer $0 \leq i \leq N$.

Discount Factors

A person or firm typically has a time preference for saving or consuming. For example, a dollar today can be invested and yield interest, whereas a dollar received next year does not include the accrued interest. Since cake gets stale as it gets older, we assume that cake in the present yields more utility than cake in the future. We can model this by multiplying future utility by a discount factor $\beta \in (0, 1)$. For example, if we were to consume c_0 cake at time 0 and c_1 cake at time 1, with $c_0 = c_1$ then the utility gained at time 0 is larger than the utility at time 1:

$$u(c_0) > \beta u(c_1).$$

The total utility for eating the cake is

$$\sum_{t=0}^{T} \beta^t u(c_t).$$

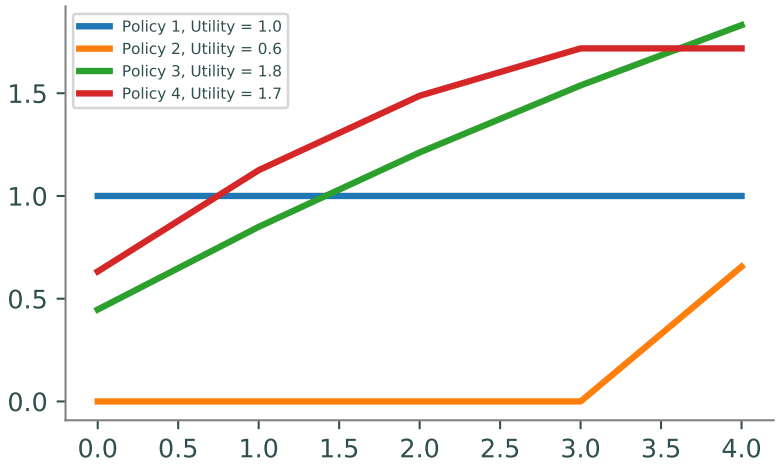


Figure 17.1: Plots for various policies with $u(x) = \sqrt{x}$ and $\beta = 0.9$. Policy 1 eats all of the cake in the first step while policy 2 eats all of the cake in the last step. Their difference in utility demonstrate the effect of the discount factor on waiting to eat. Policy 3 eats the same amount of cake at each step, while policy 4 begins by eating .4 of the cake, then .3, .2, and .1.

The Value Function

The cake eating problem is an optimization problem where we maximize utility.

$$\begin{aligned} &\max_{c_t} \sum_{t=0}^{T} \beta^t u(c_t) \\ \text{subject to } &\sum_{t=0}^{T} c_t = W \\ &c_t \geq 0. \end{aligned} \tag{17.2}$$

One way to solve it is with the value function. The value function $V(a, b, W)$ gives the utility gained from following an optimal policy from time a to time b.

$$\begin{aligned} V(a, b, W) = &\max_{c_t} \sum_{t=a}^{b} \beta^t u(c_t) \\ \text{subject to } &\sum_{t=a}^{b} c_t = W \\ &c_t \geq 0. \end{aligned}$$

$V(0, T, W)$ gives how much utility we gain in T days and is the same as Equation 17.2. $V(a, b, \frac{W}{2})$ gives how much utility we will gain by proceeding optimally from $t = a$ if half of a cake of size W was eaten before time $t = a$.

Let W_t represent the total amount of cake left at time t. Observe that $W_{t+1} \leq W_t$ for all t, because our problem does not allow for the creation of more cake. Notice that $V(t+1, T, W_{t+1})$ can be represented by $\beta V(t, T-1, W_{t+1})$, which is the value of eating W_{t+1} cake later. Then we can express the value function as the sum of the utility of eating $W_t - W_{t+1}$ cake now and W_{t+1} cake later.

$$V(t, T, W_t) = \max_{W_{t+1}} \left(u(W_t - W_{t+1}) + \beta V(t, T-1, W_{t+1})\right) \tag{17.3}$$

where $u(W_t - W_{t+1})$ is the value gained from eating $W_t - W_{t+1}$ cake at time t.

Let $\mathbf{w} = \begin{bmatrix} 0 & \frac{1}{N} & \cdots & \frac{N-1}{N} & 1 \end{bmatrix}^\mathsf{T}$. We define the *consumption matrix* C by $C_{ij} = u(w_i - w_j)$. Note that C is an $(N+1) \times (N+1)$ lower triangular matrix since we assume $j \leq i$; we can't consume more cake than we have. The consumption matrix will help solve the value function by calculating all possible value of $u(W_t - W_{t+1})$ at once. At each time t, W_t can only have $N+1$ values, which will be represented as $w_i = \frac{i}{N}$, which is i pieces of cake remaining. For example, if $N = 4$, then $w = [0, .25, .5, .75, 1]^\mathsf{T}$, and $w_3 = 0.75$ represents having three pieces of cake left. In this case, we get the following consumption matrix. Notice that $C_{20} = u(w_2 - w_0) = u(.5 - 0)$ and $C_{52} = u(w_5 - w_2) = u(1 - .25) = u(.75)$.

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ u(0.25) & 0 & 0 & 0 & 0 \\ u(0.5) & u(0.25) & 0 & 0 & 0 \\ u(0.75) & u(0.5) & u(0.25) & 0 & 0 \\ u(1) & u(0.75) & u(0.5) & u(0.25) & 0 \end{bmatrix}.$$

Problem 3. Write a function that accepts the number of equal sized pieces that divides the cake N and a utility function $u(x)$. Assume $W = 1$, and create a partition vector whose entries correspond to possible amounts of cake. Return the consumption matrix.

Solving the Optimization Problem

As mentioned above, $V(t, T-1, W_{t+1})$ in 17.3 is a new value function problem with $a = t, b = T-1$, and $W = W_{t+1}$, making 17.3 a recursion formula. By using the optimal value of the value function in the future, $V(t, T-1, W_{t+1})$, we can determine the optimal value for the present, $V(t, T, W_t)$. $V(t, T, W_t)$ can be solved by trying each possible W_{t+1} and choosing the one that gives the highest utility.

The $(N+1) \times (T+1)$ matrix A that solves the value function is called the *value function matrix*. A_{ij} is the value of having w_i cake at time j. $A_{0j} = 0$ because there is never any value in having w_0 cake, $u(w_0) = u(0) = 0$.

Initially we do not know how much cake to eat at $t = 0$: should we eat one piece of cake (w_1), or perhaps all of the cake (w_N)? It may not be obvious which option is best and that option may change depending on the discount factor β.

Instead of asking how much cake to eat at some time t, we ask how valuable w_i cake is at time t. We start at the last time period. Since there is no value in having any cake left over when time runs out, the decision at time T is obvious: eat the rest of the cake. The amount of utility gained from having w_i cake at time T is given by $u(w_i)$. So $A_{iT} = u(w_i)$. Written in the form of (17.3),

$$A_{iT} = V(0, 0, w_i) = \max_{w_j} \left(u(w_i - w_j) + \beta V(0, -1, w_j)\right) = u(w_i). \tag{17.4}$$

This happens because $V(0, -1, w_j) = 0$. As mentioned, there is no value in saving cake so this equation is maximized when $w_j = 0$. All possible values of w_i are calculated so that the value of having w_i cake at time T is known.

Achtung!

Given a time interval from $t = 0$ to $t = T$ the utility of waiting until time T to eat w_i cake is actually $\beta^T u(W_i)$. However, through backwards induction, the problem is solved backwards by beginning with $t = T$ as an isolated state and calculating its value. This is why the value function above is $V(0, 0, W_i)$ and not $V(T, T, W_i)$.

For example, the following matrix results with $T = 3$, $N = 4$, and $\beta = 0.9$.

$$\begin{bmatrix} 0 & 0 & 0 & u(0) \\ 0 & 0 & 0 & u(0.25) \\ 0 & 0 & 0 & u(0.5) \\ 0 & 0 & 0 & u(0.75) \\ 0 & 0 & 0 & u(1) \end{bmatrix}.$$

Problem 4. Write a function that accepts a stopping time T, a number of equal sized pieces that divides the cake N, a discount factor β, and a utility function $u(x)$. Return the value function matrix for $t = T$ (the matrix should have zeros everywhere except the last column). Return a matrix of zeros for the policy matrix.

Next, we use the fact that $A_{jT} = V(0, 0, w_j)$ to evaluate the $T-1$ column of the value function matrix, $A_{i(T-1)}$, by modifying (17.4) as follows,

$$A_{i(T-1)} (= V(0, 1, w_i) = \max_{w_j} \left(u(w_i - w_j) + \beta V(0, 0, w_j)\right) = \max_{w_j} \left(u(w_i - w_j) + \beta A_{jT}\right). \tag{17.5}$$

Remember that there is a limited set of possibilities for w_j, and we only need to consider options such that $w_j \leq w_i$. Instead of doing these one by one for each w_i, we can compute the options for each w_i simultaneously by creating a matrix. This information is stored in an $(N + 1) \times (N + 1)$ matrix known as the *current value matrix*, or CV^t, where the (ij)th entry is the value of eating $w_i - w_j$ pieces of cake at time t and saving j pieces of cake until the next period. For $t = T - 1$,

$$CV_{ij}^{T-1} = u(w_i - w_j) + \beta A_{jT}. \tag{17.6}$$

The largest entry in the ith row of CV^{T-1} is the optimal value that the value function can attain at $T-1$, given that we start with w_i cake. The maximal values of each row of CV^{T-1} become the column of the value function matrix, A, at time $T - 1$. We then compute CV^{T-2} using $A_{j(T-1)}$ and iterate backwards to fill in the rest of A.

ACHTUNG!

The notation CV^t does not mean raising the matrix to the tth power; rather, it indicates what time period we are in. All of the CV^t could be grouped together into a three-dimensional matrix, CV, that has dimensions $(N+1) \times (N+1) \times (T+1)$. Although this is possible, we will not use CV in this lab, and will instead only consider CV^t for any given time t.

The following matrix is CV^2 where $T = 3$, $\beta = .9$, $N = 4$, and $u(x) = \sqrt{x}$. The maximum value of each row, circled in red, is used in the 3^{rd} column of A. Remember that A's column index begins at 0, so the 3^{rd} column represents $j = 2$.

$$CV^2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0.5 & 0.45 & 0 & 0 & 0 \\ 0.707 & 0.95 & 0.636 & 0 & 0 \\ 0.866 & 1.157 & 1.136 & 0.779 & 0 \\ 1 & 1.316 & 1.343 & 1.279 & 0.9 \end{bmatrix}$$

Now that the column of A corresponding to $t = T-1$ has been calculated, we repeat the process for $T-2$ and so on until we have calculated each column of A. In summary, at each time step t, find CV^t and then set A_{it} as the maximum value of the ith row of CV^t. Generalizing (17.5) and (17.6) shows

$$CV_{ij}^t = u(w_i - w_j) + \beta A_{j(t+1)}. \qquad A_{it} = \max_j \left(CV_{ij}^t\right). \tag{17.7}$$

The full value function matrix corresponding to the example is below.

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0.5 & 0.5 & 0.5 & 0.5 \\ 0.95 & 0.95 & 0.95 & 0.707 \\ 1.355 & 1.355 & 1.157 & 0.866 \\ 1.7195 & 1.562 & 1.343 & 1 \end{bmatrix}.$$

Figure 17.2: The value function matrix where $T = 3$, $\beta = .9$, $N = 4$, and $u(x) = \sqrt{x}$. The bottom left entry indicates the highest utility that can be achieved is 1.7195.

Problem 5. Complete your function from Problem 4 so it returns the entire value function matrix. Starting from the next to last column, iterate backwards by

- calculating the current value matrix for time t using (17.7),
- finding the largest value in each row of the current value matrix, and

- filling in the corresponding column of A with these values.

Solving for the Optimal Policy

With the value function matrix constructed, the optimization problem is solved in some sense. The value function matrix contains the maximum possible utility to be gained. However, it is not immediately apparent what policy should be followed by only inspecting the value function matrix A. The $(N+1) \times (T+1)$ policy matrix, P, is used to find the optimal policy. The (ij)th entry of the policy matrix indicates how much cake to eat at time j if we have i pieces of cake. Like A and CV, i and j begin at 0.

The last column of P is calculated similarly to last column of A. $P_{iT} = w_i$, because at time T we know that the remainder of the cake should be eaten. Recall that the column of A corresponding to t was calculated by the maximum values of CV^t. The column of P for time t is calculated by taking $w_i - w_j$, where j is the smallest index corresponding to the maximum value of CV^t,

$$P_{it} = w_i - w_j.$$

$$\text{where } j = \{\, min\{j\} \mid CV^t_{ij} \geq CV^t_{ik} \,\forall\, k \in [0, 1, \ldots, N] \,\}$$

Recall CV^2 in our example with $T = 3$, $\beta = .9$, $N = 4$, and $u(x) = \sqrt{x}$ above.

$$CV^2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0.5 & 0.45 & 0 & 0 & 0 \\ 0.707 & 0.95 & 0.636 & 0 & 0 \\ 0.866 & 1.157 & 1.136 & 0.779 & 0 \\ 1 & 1.316 & 1.343 & 1.279 & 0.9 \end{bmatrix}$$

To calculate P_{12}, we look at the second row ($i = 1$) in CV^2. The maximum, .5, occurs at CV^2_{10}, so $j = 0$ and $P_{12} = w_1 - w_0 = .25 - 0$. Similarly, $P_{42} = w_4 - w_2 = 1 - .5 = .5$. Observe that the jth index corresponds to the red ovals. Continuing in this manner,

$$P = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0.25 & 0.25 & 0.25 & 0.25 \\ 0.25 & 0.25 & 0.25 & 0.5 \\ 0.25 & 0.25 & 0.5 & 0.75 \\ 0.25 & 0.5 & 0.5 & 1. \end{bmatrix}$$

The optimal policy is found by starting at the (ij)th entry where i is the number of slices of cake available at the jth time interval. At each time intervals, eat as much cake as the (ij)th entry indicates, as traced out by the red arrows. So when $N = 4$ and $j = 0$, we eat $A_{40} = .25$ cake. Then at the next time interval, $j = 1$, $N = 3$ so we eat $A_{31} = .25$ of the cake. The blue arrows trace out the policy that would occur if we only had 2 time intervals instead of 4. In this case, we need to start at $j = 2$ so that the last time interval $T = 3$ corresponds to the second time interval, when $j = 3$. What would be the optimal policy if we had 3 time intervals?

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 \\ \sqrt{0.25} & \sqrt{0.25} & \sqrt{0.25} & \sqrt{0.25} \\ \sqrt{0.25}+\beta\sqrt{0.25} & \sqrt{0.25}+\beta\sqrt{0.25} & \sqrt{0.25}+\beta\sqrt{0.25} & \sqrt{0.5} \\ \sqrt{0.25}+\beta\sqrt{0.25}+\beta^2\sqrt{0.25} & \sqrt{0.25}+\beta\sqrt{0.25}+\beta^2\sqrt{0.25} & \sqrt{0.5}+\beta\sqrt{0.25} & \sqrt{0.75} \\ \sqrt{0.25}+\beta\sqrt{0.25}+\beta^2\sqrt{0.25}+\beta^3\sqrt{0.25} & \sqrt{0.5}+\beta\sqrt{0.25}+\beta^2\sqrt{0.25} & \sqrt{0.5}+\beta\sqrt{0.5} & \sqrt{1} \end{bmatrix}$$

The non-simplified version of Figure 17.2. Notice that the value of A_{ij} is equal to following optimal path if you start at P_{ij}. A_{40} has the same values traced by the red arrows in P above and A_{42} has the same values traced by the blue arrows.

Problem 6. Modify your function from Problem 4 to determine the policy matrix. Initialize the matrix as zeros and fill it in starting from the last column at the same time that you calculate the value function matrix.
(Hint: You may find `np.argmax()` useful.)

Problem 7. The (ij)th entry of the policy matrix tells us how much cake to eat at time j if we start with i pieces. Use this information to write a function `find_policy()` that will find the optimal policy for the stopping time T, a cake of size 1 split into N pieces, a discount factor β, and the utility function u.

18 Policy Function Iteration

Lab Objective: *Iterative methods can be powerful ways to solve dynamic optimization problems without computing the exact solution. Often we can iterate very quickly to the true solution, or at least within some ε error of the solution. These methods are significantly faster than computing the exact solution using dynamic programming. We demonstrate two iterative methods, value iteration (VI) and policy iteration (PI), and use them to solve a deterministic Markov decision process.*

Dynamic Optimization

Many dynamic optimization problem take the form of a *Markov decision process.* They are formulated as follows.

$\mathbb{T}$ is a set of discrete time periods. In this lab, $\mathbb{T} = 0, 1, \dots, T$. S is the set of possible states. The set of allowable actions for each state s is A_s. $s_{t+1} = g(s_t, a_t)$ is a transition function that describes how the state changes, based on the previous state and action. The reward $u_t(s, a)$ is the reward for taking action a while in state s at time t. If the Markov process is stochastic, $p_t(s, a)$ is probability of taking action a at time t while in state s. A deterministic Markov process has $p_t(s, a) = 1\ \forall s, a$. The time discount factor $\beta \in [0, 1]$ determines how much less a reward is worth in the future. Then the dynamic optimization problem is

$$\max_a \sum_{t=0}^{T} \beta^t u(s_t, a_t)$$
$$\text{subject to } s_{t+1} = g(s_t, a_t)\ \forall t.$$

The cake eating problem described in the previous lab follows this format where S consists of the possible amounts of remaining cake ($\frac{i}{W}$), c_t is the amount of cake we can eat, and the amount of cake remaining $s_{t+1} = g(s_t, a_t)$ is $w_t - c_t$, the amount of cake we have, w_i, minus the cake we eat, c_t.

Moving on a Grid

Now consider an $N \times N$ grid. Assume that a robot moves around the grid, one space at a time, until it reaches the lower right hand corner and stops. Each square is a state, $S = \{0, 1, \dots, N^2 - 1\}$, and the set of actions is $\{Left, Down, Right, Up\}$. For this lab, $Left = 0$, $Down = 1$, $Right = 2$, and $Up = 3$.

Achtung!

It is important to remember that the actions do not correspond to the states the robot is in after the action. When the robot is in state 0 and takes action 1, he is then in state 2.

A_s is the set of actions that keep the robot on the grid. If the robot is in the top left hand corner, the only allowed actions are *Down* and *Right* so $A_0 = \{1, 2\}$. The transition function $g(s_t, a_t) = s_{t+1}$ can be explicitly defined for each s, a where s_{t_1} is the new state after moving. For this lab, we define a dictionary P to represent the decision process. P[state][action]=[(prob, nextstate, reward, is_terminal),...] This dictionary contains all of the information about the states, actions, probabilities, and rewards. The final entry in the tuple, is_terminal, indicates if the new state is a stopping point.

Let $N = 2$ and label the squares as displayed below. In this example, we define the reward to be -1 if the robot moves into 2, -1 if the robot moves into 0 from 1, and 1 when it reaches the end, 3. This simplifies to $u_t(s, a) = u(a)$ except when moving into state 0. Similarly, $p_t(s, a) = p(a) = 1$.

0	1
2	3

All of this information is encapsulated in P. We define $P[state][action]$ for all states and actions, even if they are not possible. This simplifies coding the algorithm but is not necessary.

```
P[0][0] = [(0, 0, 0, False)]    P[2][0] = [(0, 2, -1, False)]
P[0][1] = [(1, 2, -1, False)]   P[2][1] = [(0, 2, -1, False)]
P[0][2] = [(1, 1, 0, False)]    P[2][2] = [(1, 3, 1, True)]
P[0][3] = [(0, 0, 0, False)]    P[2][3] = [(1, 0, 0, False)]
P[1][0] = [(1, 0, -1, False)]   P[3][0] = [(0, 0, 0, True)]
P[1][1] = [(1, 3, 1, True)]     P[3][1] = [(0, 0, 0, True)]
P[1][2] = [(0, 0, 0, False)]    P[3][2] = [(0, 0, 0, True)]
P[1][3] = [(0, 0, 0, False)]    P[3][3] = [(0, 0, 1, True)]
```

We define the *value function* $V(s)$ to be the maximum possible reward of starting in state s. Then using Bellman's optimality equation,

$$V(s) = \max_{a \in A_s} \{\Sigma[p(a) * (u(a) + \beta V(a))]\}. \tag{18.1}$$

The summation occurs when $p(s, a) < 1$ so $P[s][a]$ consists of more than one tuple. For example, if the robot is in the top left corner and moves right, we could have that the probability the robot actually moves right is .5. In this case, $P[0][2] = [(.5, 1, 0, False), (.5, 2, -1, False)]$. This will occur later in the lab. We also observe that in this scenario, $V(a)$ is $V(s')$ where s' is the state after taking action a in state s.

Value Iteration

In the previous lab, we used dynamic programming to solve for the value function. This was a recursive method where we calculated all possible values for each state and time period. *Value iteration* is another algorithm that solves the value function by taking an initial value function and calculating a new value function iteratively. Since we are not calculating all possible values, it is typically faster than dynamic programming.

Convergence of Value Iteration

A function f that is a contraction mapping has a *fixed point* p such that $f(p) = p$. Blackwell's contraction theorem can be used to show that Bellman's equation is a "fixed point" (it actually acts more like a fixed function in this case) for an operator $T : L^\infty(X; \mathbb{R}) \to L^\infty(X; \mathbb{R})$ where $L^\infty(X; \mathbb{R})$ is the set of all bounded functions:

$$[T(f)](s) = \max_{a \in A_s} \{\Sigma[p(a) * (u(a) + \beta f(a))]\} \tag{18.2}$$

It can be shown that **??** is the fixed "point" of our operator T. A result of contraction mappings is that there exists a unique solution to 18.2.

$$V_{k+1}(s_i) = [T(V_k)](s_i) = \max_{a \in A_s} \{\Sigma[p(a) * (u(a) + \beta V_k(a))]\} \tag{18.3}$$

where an initial guess for $V_0(s)$ is used. As $k \to \infty$, it is guaranteed that $(V_k(s)) \to V^*(s)$. Because of the contraction mapping, if $V_{k+1}(s) = V_k(s)\ \forall\, s$, we have found the true value function, $V^*(s)$. Using this information, we define the value iteration algorithm to find V^*:

Algorithm 18.1 Value Function Iteration

```
procedure VALUE ITERATION FUNCTION(P, S, A, β, ε, maxiter)
    V_0 ← [V_0(s_0), V_0(s_1), ..., V_0(s_N)]        ▷ Common choice is V_0(s_i) = u(s_i)
    for i = 1, 2, ..., maxiter do                    ▷ Iterate only maxiter times at most.
        for s ∈ S do
            V_{k+1}(s) = max_{a∈A_s} {Σ[p(a) * (u(a) + β * V_k(a))]}
        if ||V_{k+1} − V_k|| < ε then
            break                                    ▷ Stop iterating if the approximation stops changing enough.
    return V_k
```

Let $V_0 = [0, 0, 0, 0]$ and $\beta = 1$. We calculate $V_1(s)$ from the example above.

$$\begin{aligned}
V_1(0) &= \max_{a \in A_0} \{\Sigma[p(a) * (u(a) + V_0(a))]\} \\
&= \max\{p(1) * (u(1) + V_0(1)), p(2) * (u(2) + V_0(2)))\} \\
&= \max\{1(-1 + 0), 1(0 + 0)\} \\
&= \max\{-1, 0\} \\
&= 0 \\
V_1(1) &= \max\{p(0) * (u(0) + V_0(0)), p(2) * (u(2) + V_0(2))\} \\
&= \max\{1(0 + 0), 1(1 + 0)\} \\
&= 1
\end{aligned}$$

Calculating $V_1(2)$ and $V_1(3)$ gives $V_1 = [0, 1, 1, 0]$. Repeating the process, $V_2 = [1, 1, 1, 0]$, which is the solution. It means that maximum reward the robot can achieve by starting on square i is $V_2[i]$.

Most iterative algorithms have a `maxiter` parameter that will terminate the algorithm after `maxiter` iterations regardless of whether or not it has converged. This is because even though we have guaranteed convergence, we might have a convergence rate that is too slow to be useful. However, generally this algorithm will converge much faster than computing the true value function using dynamic programming.

Problem 1. Write a function called `value_iteration()` that will accept a dictionary P representing the decision process, the number of states, the number of actions, a discount factor $\beta \in (0, 1)$, defaulting to 1, the tolerance amount ε defaulting to $1e^{-}8$, and the maximum number of iterations `maxiter` defaulting to 3000. Perform value iteration until $\|V_{k+1} - V_k\| < \varepsilon$ or $k >$ `max_iter`. Return the final vector representing V^* and the number of iterations. Test your code on the example given above.

Calculating the Policy

While knowing the maximum expected value is helpful, it is usually more important to know the policy that generates the most value. Value Iteration tells the robot what reward he can expect, but not how to get it. The policy vector, $\mathbf{c}$, is found by using the policy function: $\pi : \mathbb{R} \to \mathbb{R}$. $\pi(s)$ is the action we should take while in state s to maximize reward. We can modify the Bellman equation using $V^*(s)$ to find π:

$$\pi(s) = \text{argmax}_{a \in A_s}\{\Sigma[p(a) * (u(a) + \beta * V^*(s))]\} \tag{18.4}$$

Using value iteration, we found $V^* = [1, 1, 1, 0]$ in the example above. We find $\pi(0)$ by

$$\begin{aligned}
\pi(0) &= \text{argmax}_{1,2}\{p(1) * (u(1) + V^*(1)), p(2) * (u(2) + V^*(2))\} \\
&= \text{argmax}\{1 * (-1 + 1), 1 * (0 + 1)\} \\
&= \text{argmax}\{0, 1\} \\
&= 2.
\end{aligned}$$

So when the robot is in state 0, he should take action 2, moving *Right*. This avoids the -1 penalty for moving *Down* into square 2. Similarly,

$$\pi(1) = \text{argmax}_{0,1}\{1 * (0 + 1), 1 * (1 + 1)\} = \text{argmax}\{1, 2\} = 1.$$

The policy corresponding to the optimal reward is $[2, 1, 2, 0]$. The robot should move to square 3 if possible, avoiding 2 because it has a negative reward. Since 3 is terminal, it does not matter what $\pi(3)$ is. We set it to 0 for convenience.

Problem 2. Write a function called `extract_policy()` that will accept a dictionary P representing the decision process, the number of states, the number of actions, an array representing the value function, and a discount factor $\beta \in (0, 1)$, defaulting to 1. Return the policy vector corresponding to V^*. Test your code on the example with $\beta = 1$.

Policy Iteration

For dynamic programming problems, it can be shown that value function iteration converges relative to the discount factor β. As β approaches 1, the number of iterations increases dramatically. As mentioned earlier β is usually close to 1, which means this algorithm can converge slowly. In value iteration, we used an initial guess for the value function, V_0 and used (**??**) to iterate towards the true value function. Once we achieved a good enough approximation for V^*, we recovered the true policy function π. Instead of iterating on our value function, we can instead make an initial guess for the policy function, π_0, and use this to iterate toward the true policy function, called policy iteration. We do so by taking advantage of the definition of the value function, where we assume that our policy function yields the most optimal result.

That is, given a specific policy function π_k, we can modify (**??**) by assuming that the policy function is the optimal choice. This process, called *policy evaluation*, evaluates the value function for a given policy.

$$V_k(s) = \max_{a \in [A_s]} \{\Sigma([p(a) * (u(a) + \beta V^*(s))]\} = \max_{a \in [A_s]} \Sigma([p(\pi(s)) * (u(\pi(s)) + \beta * V^*(\pi(s)))]\} \quad (18.5)$$

The last equality occurs because in state s, the robot should choose the action that maximizes reward, which is $\pi(s)$ by definition.

Problem 3. Write a function called `compute_policy_v()` that accepts a dictionary P representing the decision process, the number of states, the number of actions, an array representing a policy, a discount factor $\beta \in (0, 1)$ defaulting to 1, and a tolerance amount ε defaulting to $1e^-8$,. Return the value function corresponding to the policy. Test your code on the policy vector generated from `extract_policy` for the example. The result should be the same value function array from `value_iteration`.

Now that we have the value function for our policy, we can take the value function and find a better policy. Called policy improvement, this step is the same method used in value iteration to find the policy.

Thus, given an initial guess for our policy function, π_0, we calculate the corresponding value function using (18.5), and then use (18.4) to improve our policy function. The algorithm for policy function iteration can be summarized as follows:

Algorithm 18.2 Policy Iteration

procedure POLICY ITERATION FUNCTION(P, nS, nA, β, tol, maxiter)
  $\pi_0 \leftarrow [\pi_0(w_0), \pi_0(w_1), \ldots, \pi_0(w_N)]$ ▷ Common choice is $\pi_0(w_i) = w_{i-1}$ with $\pi_0(0) = 0$
  for $i = 1, 2, \ldots,$ `maxiter` **do** ▷ Iterate only `maxiter` times at most.
    for $s \in S$ **do** ▷ Policy evaluation
      $V_k(s) = \max_{a \in A_s}\{\Sigma[p(\pi(s)) * (u(\pi(s)) + \beta * V^*(\pi(s)))]\}$ ▷ compute_policy_v.
    for $s \in S$ **do** ▷ Policy improvement.
      $\pi_{k+1}(s) = \text{argmax}_{a \in A_s}\{\Sigma[p(a) * (u(a) + \beta * V_k * (s))]\}$ ▷ extract_policy.
    if $||\pi_{k+1} - \pi_k|| < \varepsilon$ **then**
      `break` ▷ Stop iterating if the policy doesn't change enough.
  return V_k, π_{k+1}

Problem 4. Write a function called `policy_iteration()` that will accept a dictionary P representing the decision process, the number of states, the number of actions, a discount factor $\beta \in (0, 1)$, defaulting to 1, the tolerance amount ε defaulting to $1e^{-}8$, and the maximum number of iterations `maxiter` defaulting to 3000. Perform policy iteration until $\|\pi_{k+1} - \pi_k\| < \varepsilon$ or $k >$ `maxiter`. Return the final vector representing V_k, the optimal policy π_k, and the number of iterations. Test your code on the example given above and compare your answers to the results from 1 and 2.

The Frozen Lake Problem

For the rest of the lab, we will be using the OpenAi Gym environments. It can be installed using conda or pip.

```
$ pip install gym[all]
```

In the Frozen Lake problem, you and your friends tossed a frisbee onto a mostly frozen lake. The lake is divided into an $N \times N$ grid where the top left hand corner is the start, the bottom right hand corner is the end, and the other squares are either frozen or holes. To retrieve the frisbee, you must successfully navigate around the melted ice without falling. The possible actions are left, right, up, and down. Since ice is slippery, you won't always move in the intended direction. If you fall, your reward is 0. If you succeed, your reward is 1. There are two scenarios: $N = 4$ and $N = 8$. To run the 4×4 scenario, use `env_name='FrozenLake-v0'`. For the 8×8 scenario, use `env_name='FrozenLake8x8-v0'`.

Using Gym

To use gym, we import it and create an environment based on the built-in gym environment. The FrozenLake environment has 3 important attributes, P, nS, and nA. P is a dictionary where $P[s][a] = [(probability, nextstate, reward, is\_terminal)...]$. Notice that this is the same P we used in the previous problems. nS and nA are the number of states and actions respectively.

We can calculate the optimal policy using value iteration or policy iteration. Since the ice is slippery, this policy will not always result in a reward of 1. The gym environments have built-in functions that allow us to simulate each step of the environment. Before running a scenario in gym, always put it in the starting state by calling `env.reset()`. To simulate moving, call `env.step`.

```
$ import gym
$ from gym import wrappers
$ env_name  = 'FrozenLake-v0'
$ env = gym.make(env_name).env
$ number_of_states = env.nS
$ obs = env.reset()
$ obs, reward, done, _ = env.step(int(policy[obs]))
```

The step function returns four values: observation, reward, done, info. The observation is an environment-specific object representing the observation of the environment. For FrozenLake, this is the current state. When we step, or take an action, we get a new observation, or state, as well as the reward for taking that action. If we fall into a hole or reach the frisbee, the simulation is over so we are done. The info value is a dictionary of diagnostic information. It will not be used in this lab.

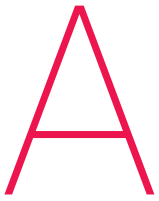
Problem 5. Write a function that runs `value_iteration` and `policy_iteration` on FrozenLake. It should accept a boolean `basic_case` defaulting to `True` that indicates whether to run the 4×4 or 8×8 scenario and an integer n defaulting to 1000 that indicates how many times to run the simulation. Calculate the value function and policy for the environment using both value iteration and policy iteration. Return the policies generated by value iteration and the policy and value function generated by policy iteration. Set the mean total rewards to 0 and return them as well.

Problem 6. Write a function `run_simulation()` that takes in the environment `env`, a policy `policy`, a discount factor β defaulting to 1, and a boolean `render` defaulting to False. Calculate the total reward for the policy for one simulation using `env.reset` and `env.step()`. Stop the simulation when *done* is $True$. (Hint: When calculating reward, use β^k.)

Modify `frozen_lake()` to run `run_simulation` for both the value iteration policy and the policy iteration policy M times. Return the policy generated by value iteration, the mean total reward for the policy generated by value iteration, the policy generated by policy iteration, and the mean total reward for the policy generated by policy iteration.

Part II

Appendices



NumPy Visual Guide

Lab Objective: *NumPy operations can be difficult to visualize, but the concepts are straightforward. This appendix provides visual demonstrations of how NumPy arrays are used with slicing syntax, stacking, broadcasting, and axis-specific operations. Though these visualizations are for 1- or 2-dimensional arrays, the concepts can be extended to n-dimensional arrays.*

Data Access

The entries of a 2-D array are the rows of the matrix (as 1-D arrays). To access a single entry, enter the row index, a comma, and the column index. Remember that indexing begins with 0.

$$A[0] = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix} \qquad A[2,1] = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix}$$

Slicing

A lone colon extracts an entire row or column from a 2-D array. The syntax `[a:b]` can be read as "the ath entry up to (but not including) the bth entry." Similarly, `[a:]` means "the ath entry to the end" and `[:b]` means "everything up to (but not including) the bth entry."

$$\texttt{A[1]} = \texttt{A[1,:]} = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix} \qquad \texttt{A[:,2]} = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix}$$

$$\texttt{A[1:,:2]} = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix} \qquad \texttt{A[1:-1,1:-1]} = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix}$$

Stacking

`np.hstack()` stacks sequence of arrays horizontally and `np.vstack()` stacks a sequence of arrays vertically.

$$A = \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix} \qquad B = \begin{bmatrix} * & * & * \\ * & * & * \\ * & * & * \end{bmatrix}$$

$$\texttt{np.hstack((A,B,A))} = \begin{bmatrix} \times & \times & \times & * & * & * & \times & \times & \times \\ \times & \times & \times & * & * & * & \times & \times & \times \\ \times & \times & \times & * & * & * & \times & \times & \times \end{bmatrix}$$

$$\texttt{np.vstack((A,B,A))} = \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ * & * & * \\ * & * & * \\ * & * & * \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix}$$

Because 1-D arrays are flat, `np.hstack()` concatenates 1-D arrays and `np.vstack()` stacks them vertically. To make several 1-D arrays into the columns of a 2-D array, use `np.column_stack()`.

$$x = \begin{bmatrix} \times & \times & \times & \times \end{bmatrix} \qquad y = \begin{bmatrix} * & * & * & * \end{bmatrix}$$

$$\texttt{np.hstack((x,y,x))} = \begin{bmatrix} \times & \times & \times & \times & * & * & * & * & \times & \times & \times & \times \end{bmatrix}$$

$$\texttt{np.vstack((x,y,x))} = \begin{bmatrix} \times & \times & \times & \times \\ * & * & * & * \\ \times & \times & \times & \times \end{bmatrix} \qquad \texttt{np.column\_stack((x,y,x))} = \begin{bmatrix} \times & * & \times \\ \times & * & \times \\ \times & * & \times \\ \times & * & \times \end{bmatrix}$$

Broadcasting

NumPy automatically aligns arrays for component-wise operations whenever possible. See `http://docs.scipy.org/doc/numpy/user/basics.broadcasting.html` for more in-depth examples and broadcasting rules.

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \\ 1 & 2 & 3 \end{bmatrix} \qquad x = \begin{bmatrix} 10 & 20 & 30 \end{bmatrix}$$

$$\texttt{A + x} = \begin{bmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \\ 1 & 2 & 3 \end{bmatrix} + \begin{bmatrix} 10 & 20 & 30 \end{bmatrix} = \begin{bmatrix} 11 & 22 & 33 \\ 11 & 22 & 33 \\ 11 & 22 & 33 \end{bmatrix}$$

$$\texttt{A + x.reshape((1,-1))} = \begin{bmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \\ 1 & 2 & 3 \end{bmatrix} + \begin{bmatrix} 10 \\ 20 \\ 30 \end{bmatrix} = \begin{bmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{bmatrix}$$

Operations along an Axis

Most array methods have an `axis` argument that allows an operation to be done along a given axis. To compute the sum of each column, use `axis=0`; to compute the sum of each row, use `axis=1`.

$$A = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \end{bmatrix}$$

$$\texttt{A.sum(axis=0)} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \end{bmatrix} = \begin{bmatrix} 4 & 8 & 12 & 16 \end{bmatrix}$$

$$\texttt{A.sum(axis=1)} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 4 \end{bmatrix} = \begin{bmatrix} 10 & 10 & 10 & 10 \end{bmatrix}$$