Scientific Python: Using SciPy for Optimization

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When you want to do scientific work in Python, the first library you can turn to is SciPy. As you'll see in this tutorial, **SciPy** is not just a library, but a whole **ecosystem** of libraries that work together to help you accomplish complicated scientific tasks quickly and reliably.

In this tutorial, you'll learn how to:

- **Find** information about all the things you can do with SciPy

- **Install** SciPy on your computer

Help

- **Use** SciPy to cluster a dataset by several variables
- **Use** SciPy to find the optimum of a function

You can follow along with the examples in this tutorial by downloading the source code available at the link below:

> **Get Sample Code: Click here to get the sample code you'll use** to learn about SciPy in this tutorial.

Differentiating SciPy the Ecosystem and SciPy the Library

When you want to use Python for scientific computing tasks, there are several libraries that you'll probably be advised to use, including:

- NumPy
- SciPy
- Matplotlib
- IPython
- SymPy
- Pandas

Collectively, these libraries make up the **SciPy ecosystem** and are designed to work together. Many of them rely directly on NumPy arrays to do computations. This tutorial expects that you have some familiarity with creating NumPy arrays and operating on them.

> **Note:** If you need a quick primer or refresher on NumPy, then you can check out these tutorials:
>
> - Look Ma, No `for` Loops: Array Programming With NumPy
> - NumPy `arange()`: How to Use `np.arange()`
> - MATLAB vs. Python: An Overview of Basic Array Operations

In this tutorial, you'll learn about the **SciPy library**, one of the core components of the SciPy ecosystem. The SciPy library is the fundamental library for scientific computing in Python. It provides many efficient and user-friendly interfaces for tasks such as numerical integration, optimization, signal processing, linear algebra, and more.

Understanding SciPy Modules

The SciPy library is composed of a number of **modules** that separate the library into distinct functional units. If you want to learn about the different modules that SciPy includes, then you can run `help()` on `scipy`, as shown below:

Python

```python
>>> import scipy
>>> help(scipy)
```

This produces some help output for the entire SciPy library, a portion of which is shown below:

Text

```
 Subpackages
 -----------

 Using any of these subpackages requires an explicit import.  For example,
 ``import scipy.cluster``.

 ::

  cluster                  --- Vector Quantization / Kmeans
  fft                      --- Discrete Fourier transforms
  fftpack                  --- Legacy discrete Fourier transforms
  integrate                --- Integration routines
 ...
```

This code block shows the `Subpackages` portion of the help output, which is a list of all of the available modules within SciPy that you can use for calculations.

Note the text at the top of the section that states, `"Using any of these subpackages requires an explicit import."` When you want to use functionality from a module in SciPy, you need to import the module that you want to use **specifically**. You'll see some examples of this a little later in the tutorial, and guidelines for importing libraries from SciPy are shown in the [SciPy documentation](#).

Once you decide which module you want to use, you can check out the SciPy [API reference](#), which contains all of the details on each module in SciPy. If you're looking for something with a little more exposition, then the [SciPy Lecture Notes](#) are a great resource to go in-depth on many of the SciPy modules.

Later in this tutorial, you'll learn about `cluster` and `optimize`, which are two of the modules in the SciPy library. But first, you'll need to install SciPy on your computer.

Installing SciPy on Your Computer

As with most [Python packages](#), there are two main ways to install SciPy on your computer:

1. [Anaconda](#)
2. [PyPI and `pip`](#)

Here, you'll learn how to use both of these approaches to install the library. SciPy's only direct dependency is the NumPy package. Either installation method will automatically install NumPy in addition to SciPy, if necessary.

Anaconda

Anaconda is a popular **distribution** of Python, mainly because it includes pre-built versions of the most popular scientific Python packages for Windows, macOS, and Linux. If you don't have Python installed on your computer at all yet, then Anaconda is a great option to get started with. Anaconda comes pre-installed with SciPy and its required dependencies, so once you've installed Anaconda, you don't need to do anything else!

You can download and install Anaconda from their [downloads page](#). Make sure to download the most recent Python 3 release. Once you have the installer on your computer, you can follow the default setup procedure for an application, depending on your platform.

> **Note:** Make sure to install Anaconda in a directory that **does not require administrator permissions** to modify. This is the default setting in the installer.

If you already have Anaconda installed, but you want to install or update SciPy, then you can do that, too. Open up a [terminal](#) application on macOS or Linux, or the Anaconda Prompt on Windows, and type one of the following lines of code:

Shell

```
$ conda install scipy
$ conda update scipy
```

You should use the first line if you need to install SciPy or the second line if you just want to update SciPy. To make sure SciPy is installed, run Python in your terminal and try to import SciPy:
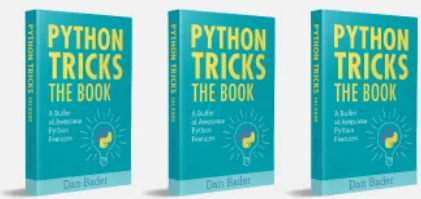
```Python
>>> import scipy
>>> print(scipy.__file__)
/.../lib/python3.7/site-packages/scipy/__init__.py
```

In this code, you've imported `scipy` and printed the location of the file from where `scipy` is loaded. The example above is for macOS. Your computer will probably show a different location. Now you have SciPy installed on your computer ready for use. You can skip ahead to the next section to get started using SciPy!

The `pip` Package Manager

If you already have a version of Python installed that isn't Anaconda, or you don't want to use Anaconda, then you'll be using `pip` to install SciPy. To learn more about what `pip` is, check out Using Python's `pip` to Manage Your Projects' Dependencies and A Beginner's Guide to `pip`.

> **Note:** `pip` installs packages using a format called **wheels**. In the wheel format, code is compiled before it's sent to your computer. This is nearly the same approach that Anaconda takes, although wheel format files are slightly different than the Anaconda format, and the two are not interchangeable.

To install SciPy using `pip`, open up your terminal application, and type the following line of code:

```Shell
$ python -m pip install -U scipy
```

The code will install SciPy if it isn't already installed, or upgrade SciPy if it is installed. To make sure SciPy is installed, run Python in your terminal and try to import SciPy:

```Python
>>> import scipy
>>> print(scipy.__file__)
/.../lib/python3.7/site-packages/scipy/__init__.py
```

In this code, you've imported `scipy` and printed the location of the file from where `scipy` is loaded. The example above is for macOS using pyenv. Your computer will probably show a different location. Now you have SciPy installed on your computer. Let's see how you can use SciPy to solve a couple of problems you might encounter!

Using the Cluster Module in SciPy

Clustering is a popular technique to categorize data by associating it into groups. The SciPy library includes an implementation of the k-means clustering algorithm as well as several hierarchical clustering algorithms. In this example, you'll be using the k-means algorithm in `scipy.cluster.vq`, where `vq` stands for **vector quantization**.

First, you should take a look at the dataset you'll be using for this example. The dataset consists of 4827 real and 747 spam text (or SMS) messages. The raw dataset can be found on the UCI Machine Learning Repository or the authors' web page.

> **Note:** The data was collected by Tiago A. Almeida and José María Gómez Hidalgo and published in an article titled "Contributions to the Study of SMS Spam Filtering: New Collection and Results" in the *Proceedings of the 2011 ACM*

> *Symposium on Document Engineering (DOCENG'11)* hosted in Mountain View, CA, USA in 2011.

In the dataset, each message has one of two labels:

1. `ham` for legitimate messages

2. `spam` for spam messages

The full text message is associated with each label. When you scan through the data, you might notice that spam messages tend to have a lot of numeric digits in them. They often include a phone number or prize winnings. Let's predict whether or not a message is spam based on the number of digits in the message. To do this, you'll **cluster** the data into three groups based on the number of digits that appear in the message:

1. **Not spam:** Messages with the smallest number of digits are predicted not to be spam.

2. **Unknown:** Messages with an intermediate number of digits are unknown and need to be processed by more advanced algorithms.

3. **Spam:** Messages with the highest number of digits are predicted to be spam.

Let's get started with clustering the text messages. First, you should import the libraries you'll use in this example:

Python
```
1  from pathlib import Path
2  import numpy as np
3  from scipy.cluster.vq import whiten, kmeans, vq
```

You can see that you're importing three functions from `scipy.cluster.vq`. Each of these functions accepts a NumPy array as input. These arrays should have the **features** of the dataset in the columns and the **observations** in the rows.

A feature is a [variable](#) of interest, while an observation is created each time you record each feature. In this example, there are 5,574 observations, or individual messages, in the dataset. In addition, you'll see that there are two features:

1. **The number of digits** in a text message
2. **The number of times** that number of digits appears in the whole dataset

Next, you should load the data file from the UCI database. The data comes as a text file, where the class of the message is separated from the message by a tab character, and each message is on its own line. You should read the data into a [list](#) using [`pathlib.Path`](#):

Python
```
4  data = Path("SMSSpamCollection").read_text()
5  data = data.strip()
6  data = data.split("\n")
```

In this code, you use `pathlib.Path.read_text()` to read the file into a string. Then, you use `.strip()` to remove any trailing spaces and split the [string](#) into a list with `.split()`.

Next, you can start **analyzing** the data. You need to count the number of digits that appear in each text message. Python includes `collections.Counter` in the standard library to collect counts of objects in a dictionary-like structure. However, since all of the functions in `scipy.cluster.vq` expect NumPy arrays as input, you can't use `collections.Counter` for this example. Instead, you use a NumPy array and implement the counts manually.

Again, you're interested in the number of digits in a given SMS message, and how many SMS messages have that number of digits. First, you should create a NumPy array that associates the number of digits in a given message with the result of the message, whether it was ham or spam:

Python
```
7  digit_counts = np.empty((len(data), 2), dtype=int)
```

In this code, you're creating an empty NumPy array, `digit_counts`, which has two columns and 5,574 rows. The number of rows is equal to the number of messages in the dataset. You'll be using `digit_counts` to associate the number of digits in the message with whether or not the message was spam.

You should create the array before entering the loop, so you don't have to allocate new memory as your array expands. This improves the efficiency of your code. Next, you should process the data to record the number of digits and the status of the message:

Python

```python
 8   for i, line in enumerate(data):
 9       case, message = line.split("\t")
10       num_digits = sum(c.isdigit() for c in message)
11       digit_counts[i, 0] = 0 if case == "ham" else 1
12       digit_counts[i, 1] = num_digits
```

Here's a line-by-line breakdown of how this code works:

- **Line 8:** Loop over `data`. You use `enumerate()` to put the value from the list in `line` and create an index `i` for this list. To learn more about `enumerate()`, check out [Python enumerate(): Simplify Loops That Need Counters](#).

- **Line 9:** Split the line on the tab character to create `case` and `message`. `case` is a string that says whether the message is `ham` or `spam`, while `message` is a string with the text of the message.

- **Line 10:** Calculate the number of digits in the message by using the [sum()](#) of a comprehension. In the comprehension, you check each character in the message using [isdigit()](#), which returns `True` if the element is a numeral and `False` otherwise. `sum()` then treats each `True` result as a 1 and each `False` as a 0. So, the result of `sum()` on this comprehension is the number of characters for which `isdigit()` returned `True`.

- **Line 11:** Assign values into `digit_counts`. You assign the first column of the `i` row to be 0 if the message was legitimate (`ham`) or 1 if the message was spam.

- **Line 12:** Assign values into `digit_counts`. You assign the second column of the `i` row to be the number of digits in the message.

Now you have a NumPy array that contains the number of digits in each message. However, you want to apply the **clustering algorithm** to an array that has the number of messages with a certain number of digits. In other words, you need to create an array where the first column has the number of digits in a message, and the second column is the number of messages that have that number of digits. Check out the code below:

Python

```python
13   unique_counts = np.unique(digit_counts[:, 1], return_counts=True)
```

[np.unique()](#) takes an array as the first argument and returns another array with the unique elements from the argument. It also takes several optional arguments. Here, you use `return_counts=True` to instruct `np.unique()` to also return an array with the number of times each unique element is present in the input array. These two outputs are returned as a tuple that you store in `unique_counts`.

Next, you need to transform `unique_counts` into a shape that's suitable for clustering:

Python

```python
14   unique_counts = np.transpose(np.vstack(unique_counts))
```

You combine the two 1xN outputs from `np.unique()` into one 2xN array using `np.vstack()`, and then transpose them into an Nx2 array. This format is what you'll use in the clustering functions. Each row in `unique_counts` now has two elements:

1. **The number of digits** in a message
2. **The number of messages** that had that number of digits

A subset of the output from these two operations is shown below:

Text

```
[[   0 4110]
 [   1  486]
 [   2  160]
 ...
 [  40    4]
 [  41    2]
 [  47    1]]
```

In the dataset, there are 4110 messages that have no digits, 486 that have 1 digit, and so on. Now, you should apply the k-means clustering algorithm to this array:

Python

```
15  whitened_counts = whiten(unique_counts)
16  codebook, _ = kmeans(whitened_counts, 3)
```

You use `whiten()` to normalize each feature to have unit variance, which improves the results from `kmeans()`. Then, `kmeans()` takes the whitened data and the number of clusters to create as arguments. In this example, you want to create 3 clusters, for **definitely ham**, **definitely spam**, and **unknown**. `kmeans()` returns two values:

1. **An array with three rows and two columns representing the centroids of each group:** The `kmeans()` algorithm calculates the optimal location of the centroid of each cluster by minimizing the distance from the observations to each centroid. This array is assigned to `codebook`.

2. **The mean Euclidian distance from the observations to the centroids:** You won't need that value for the rest of this example, so you can assign it to _.

Next, you should determine which cluster each observation belongs to by using `vq()`:

Python

```
17  codes, _ = vq(whitened_counts, codebook)
```

`vq()` assigns codes from the `codebook` to each observation. It returns two values:

1. **The first value** is an array of the same length as `unique_counts`, where the value of each element is an integer representing which cluster that observation is assigned to. Since you used three clusters in this example, each observation is assigned to cluster 0, 1, or 2.

2. **The second value** is an array of the Euclidian distance between each observation and its centroid.

Now that you have the data clustered, you should use it to make predictions about the SMS messages. You can inspect the counts to determine at how many digits the clustering algorithm drew the line between definitely ham and unknown, and between unknown and definitely spam.

The clustering algorithm randomly assigns the code 0, 1, or 2 to each cluster, so you need to identify which is which. You can use this code to find the code associated with each cluster:

Python

```
18  ham_code = codes[0]
19  spam_code = codes[-1]
20  unknown_code = list(set(range(3)) ^ set((ham_code, spam_code)))[0]
```

In this code, the first line finds the code associated with ham messages. According to our hypothesis above, the ham messages have the fewest digits, and the digit array was sorted from fewest to most digits. Thus, the ham message cluster starts at the beginning of `codes`.

Similarly, the spam messages have the most digits and form the last cluster in `codes`. Therefore, the code for spam messages will be equal to the last element of `codes`. Finally, you need to find the code for unknown messages. Since there are only 3 options for the code and you have already identified two of them, you can use the `symmetric_difference` operator on a [Python set](#) to determine the last code value. Then, you can print the cluster associated with each message type:

Python

```
21   print("definitely ham:", unique_counts[codes == ham_code][-1])
22   print("definitely spam:", unique_counts[codes == spam_code][-1])
23   print("unknown:", unique_counts[codes == unknown_code][-1])
```

In this code, each line is getting the rows in `unique_counts` where `vq()` assigned different values of the codes. Since that operation returns an array, you should get the last row of the array to determine the highest number of digits assigned to each cluster. The output is shown below:

Text

```
definitely ham: [0  4110]
definitely spam: [47  1]
unknown: [20 18]
```

In this output, you see that the **definitely ham** messages are the messages with zero digits in the message, the **unknown** messages are everything between 1 and 20 digits, and **definitely spam** messages are everything from 21 to 47 digits, which is the maximum number of digits in your dataset.

Now, you should check how accurate your predictions are on this dataset. First, create some masks for `digit_counts` so you can easily grab the `ham` or `spam` status of the messages:

Python

```
24   digits = digit_counts[:, 1]
25   predicted_hams = digits == 0
26   predicted_spams = digits > 20
27   predicted_unknowns = np.logical_and(digits > 0, digits <= 20)
```

In this code, you're creating the `predicted_hams` mask, where there are no digits in a message. Then, you create the `predicted_spams` mask for all messages with more than 20 digits. Finally, the messages in the middle are `predicted_unknowns`.

Next, apply these masks to the actual digit counts to retrieve the predictions:

Python

```
28   spam_cluster = digit_counts[predicted_spams]
29   ham_cluster = digit_counts[predicted_hams]
30   unk_cluster = digit_counts[predicted_unknowns]
```

Here, you're applying the masks you created in the last code block to the `digit_counts` array. This creates three new arrays with only the messages that have been clustered into each group. Finally, you can see how many of each message type have fallen into each cluster:

Python

```
31   print("hams:", np.unique(ham_cluster[:, 0], return_counts=True))
32   print("spams:", np.unique(spam_cluster[:, 0], return_counts=True))
33   print("unknowns:", np.unique(unk_cluster[:, 0], return_counts=True))
```

This code prints the counts of each unique value from the clusters. Remember that `0` means a message was `ham` and `1` means the message was `spam`. The results are shown below:

Text

```
hams: (array([0, 1]), array([4071,   39]))
spams: (array([0, 1]), array([  1, 232]))
unknowns: (array([0, 1]), array([755, 476]))
```

From this output, you can see that 4110 messages fell into the **definitely ham** group, of which 4071 were actually ham and only 39 were spam. Conversely, of the 233 messages that fell into the **definitely spam** group, only 1 was actually ham and the rest were spam.

Of course, over 1200 messages fell into the **unknown** category, so some more advanced analysis would be needed to classify those messages. You might want to look into something like natural language processing to help improve the accuracy of your prediction, and you can use Python and Keras to help out.
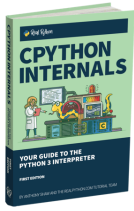
Using the Optimize Module in SciPy

When you need to **optimize** the input parameters for a function, `scipy.optimize` contains a number of useful methods for optimizing different kinds of functions:
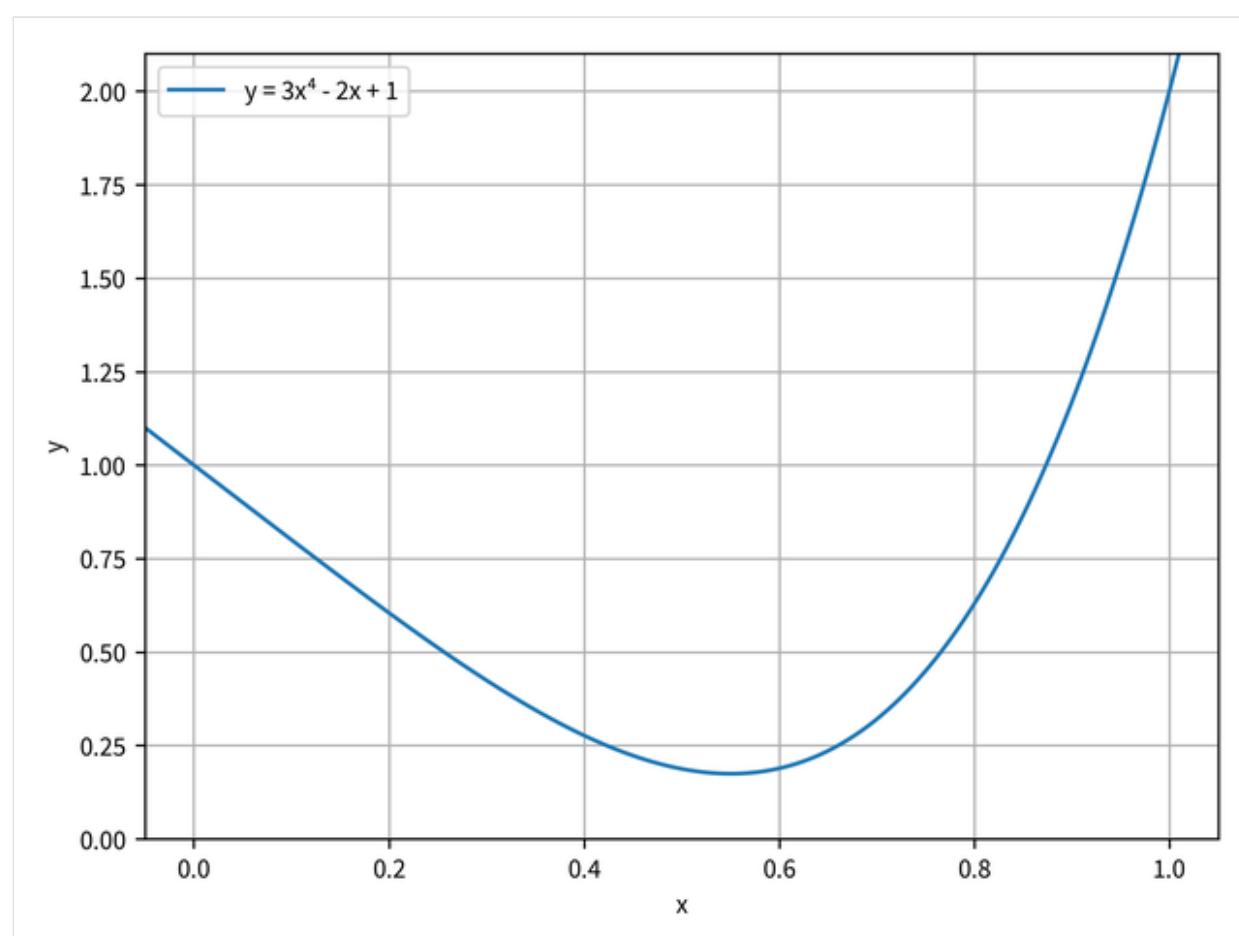
- `minimize_scalar()` and `minimize()` to minimize a function of one variable and many variables, respectively
- `curve_fit()` to fit a function to a set of data
- `root_scalar()` and `root()` to find the zeros of a function of one variable and many variables, respectively
- `linprog()` to minimize a linear objective function with linear inequality and equality constraints

In practice, all of these functions are performing **optimization** of one sort or another. In this section, you'll learn about the two minimization functions, `minimize_scalar()` and `minimize()`.

Minimizing a Function With One Variable

A mathematical function that accepts one number and results in one output is called a **scalar function**. It's usually contrasted with multivariate functions that accept multiple numbers and also result in multiple numbers of output. You'll see an example of optimizing multivariate functions in the next section.

For this section, your scalar function will be a **quartic polynomial**, and your objective is to find the **minimum value** of the function. The function is $y = 3x^4 - 2x + 1$. The function is plotted in the image below for a range of x from 0 to 1:

In the figure, you can see that there's a minimum value of this function at approximately $x = 0.55$. You can use `minimize_scalar()` to determine the exact x and y coordinates of the minimum. First, import `minimize_scalar()` from `scipy.optimize`. Then, you need to define the objective function to be minimized:

Python

```
1   from scipy.optimize import minimize_scalar
2
3   def objective_function(x):
4       return 3 * x ** 4 - 2 * x + 1
```

`objective_function()` takes the input `x` and applies the necessary mathematical operations to it, then returns the result. In the function definition, you can use any mathematical functions you want. The only limit is that the function must return a single number at the end.

Next, use `minimize_scalar()` to find the minimum value of this function. `minimize_scalar()` has only one required input, which is the name of the objective function definition:

Python

```
5   res = minimize_scalar(objective_function)
```

The output of `minimize_scalar()` is an instance of [OptimizeResult](). This class collects together many of the relevant details from the optimizer's run, including whether or not the optimization was successful and, if successful, what the final result was. The output of `minimize_scalar()` for this function is shown below:

Text

```
      fun: 0.17451818777634331
    nfev: 16
     nit: 12
 success: True
       x: 0.5503212087491959
```

These results are all attributes of `OptimizeResult`. `success` is a [Boolean value]() indicating whether or not the optimization completed successfully. If the optimization was successful, then `fun` is the value of the objective function at the optimal value `x`. You can see from the output that, as expected, the optimal value for this function was near x = 0.55.

Note: As you may know, **not every function has a minimum**. For instance, try and see what happens if your objective function is y = x^3. For `minimize_scalar()`, objective functions with no minimum often result in an `OverflowError` because the optimizer eventually tries a number that is too big to be calculated by the computer.

On the opposite side of functions with no minimum are **functions that have several minima**. In these cases, `minimize_scalar()` is not guaranteed to find the global minimum of the function. However, `minimize_scalar()` has a `method` keyword argument that you can specify to control the solver that's used for the optimization. The SciPy library has three built-in methods for scalar minimization:

1. `brent` is an implementation of [Brent's algorithm](). This method is the default.
2. `golden` is an implementation of the [golden-section search](). The [documentation]() notes that Brent's method is usually better.
3. `bounded` is a bounded implementation of Brent's algorithm. It's useful to limit the search region when the minimum is in a known range.

When `method` is either `brent` or `golden`, `minimize_scalar()` takes another argument called `bracket`. This is a sequence of two or three elements that provide an initial guess for the bounds of the region with the minimum. However, these solvers do not guarantee that the minimum found will be within this range.

On the other hand, when `method` is `bounded`, `minimize_scalar()` takes another argument called `bounds`. This is a sequence of two elements that strictly bound the search region for the minimum. Try out the `bounded` method with the function y = x^4 - x^2. This function is plotted in the figure below:
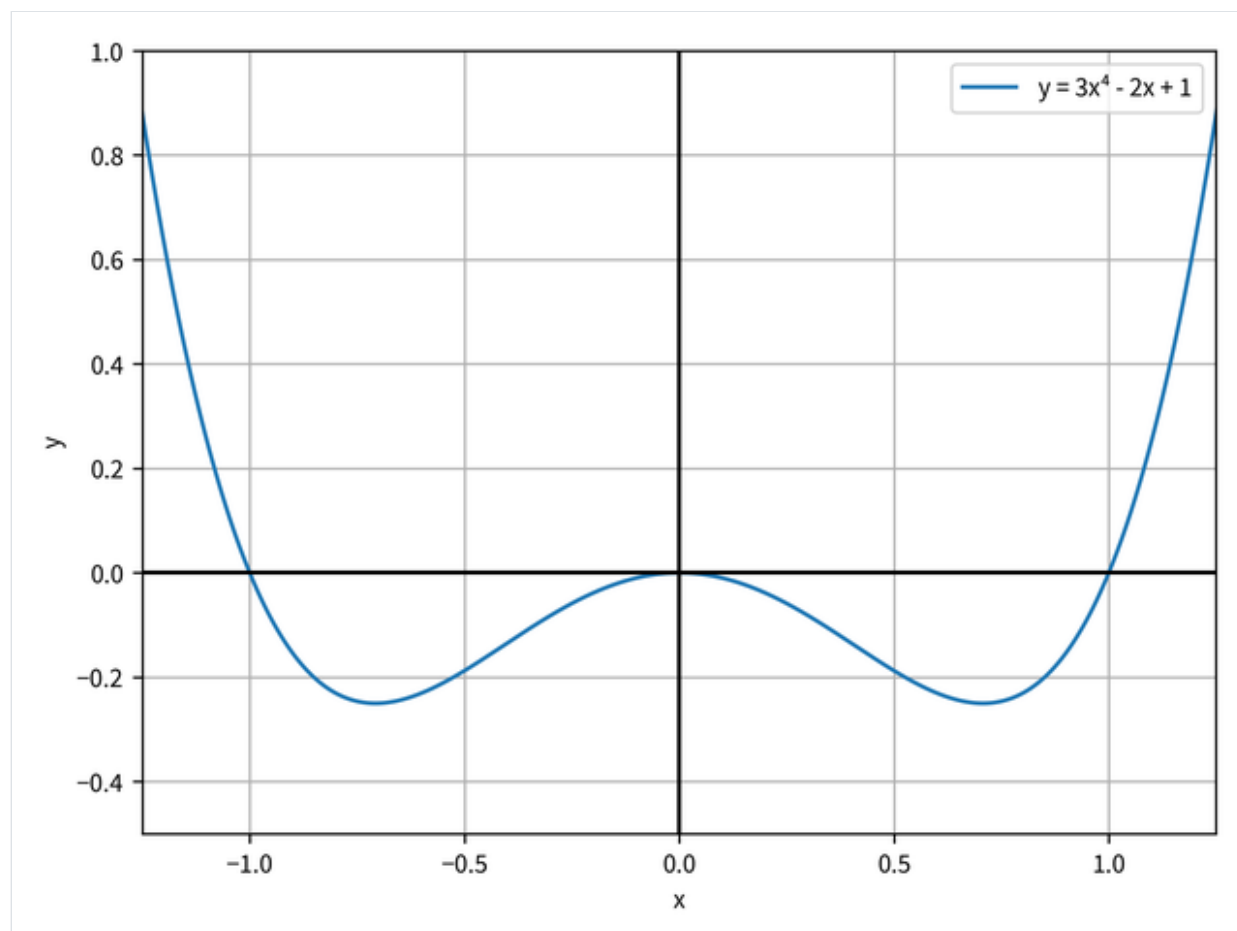
Using the previous example code, you can redefine `objective_function()` like so:

Python

```
7  def objective_function(x):
8      return x ** 4 - x ** 2
```

First, try the default `brent` method:

Python

```
9  res = minimize_scalar(objective_function)
```

In this code, you didn't pass a value for `method`, so `minimize_scalar()` used the `brent` method by default. The output is this:

Text

```
    fun: -0.24999999999999994
   nfev: 15
    nit: 11
success: True
      x: 0.7071067853059209
```

You can see that the optimization was successful. It found the optimum near x = 0.707 and y = -1/4. If you [solved for the minimum](#) of the equation analytically, then you'd find the minimum at $x = 1/\sqrt{2}$, which is extremely close to the answer found by the minimization function. However, what if you wanted to find the **symmetric minimum** at $x = -1/\sqrt{2}$? You can return the same result by providing the `bracket` argument to the `brent` method:

Python

```
10  res = minimize_scalar(objective_function, bracket=(-1, 0))
```

In this code, you provide the sequence `(-1, 0)` to `bracket` to start the search in the region between -1 and 0. You expect there to be a minimum in this region since the objective function is **symmetric** about the y-axis. However, even with `bracket`, the `brent` method still returns the minimum at $x = +1/\sqrt{2}$. To find the minimum at $x = -1/\sqrt{2}$, you can use the `bounded` method with `bounds`:

Python

```
11  res = minimize_scalar(objective_function, method='bounded', bounds=(-1, 0))
```

In this code, you add `method` and `bounds` as arguments to `minimize_scalar()`, and you set `bounds` to be from -1 to 0. The output of this method is as follows:

Text

```
     fun: -0.24999999999998732
 message: 'Solution found.'
    nfev: 10
  status: 0
 success: True
       x: -0.707106701474177
```

As expected, the minimum was found at x = -1/√2. Note the additional output from this method, which includes a `message` attribute in `res`. This field is often used for more detailed output from some of the minimization solvers.

Minimizing a Function With Many Variables

`scipy.optimize` also includes the more general `minimize()`. This function can handle **multivariate** inputs and outputs and has more complicated optimization algorithms to be able to handle this. In addition, `minimize()` can handle **constraints** on the solution to your problem. You can specify three types of constraints:

1. `LinearConstraint`: The solution is constrained by taking the inner product of the solution x values with a user-input array and comparing the result to a lower and upper bound.

2. `NonlinearConstraint`: The solution is constrained by applying a user-supplied function to the solution x values and comparing the return value with a lower and upper bound.

3. `Bounds`: The solution x values are constrained to lie between a lower and upper bound.

When you use these constraints, it can limit the specific choice of optimization method that you're able to use, since not all of the available methods support constraints in this way.

Let's try a demonstration on how to use `minimize()`. Imagine you're a stockbroker who's interested in **maximizing the total income** from the sale of a fixed number of your stocks. You have identified a particular set of buyers, and for each buyer, you know the price they'll pay and how much cash they have on hand.

You can phrase this problem as a **constrained optimization problem**. The objective function is that you want to maximize your income. However, `minimize()` finds the minimum value of a function, so you'll need to multiply your objective function by -1 to find the x-values that produce the largest negative number.

There is one **constraint** on the problem, which is that the sum of the total shares purchased by the buyers does not exceed the number of shares you have on hand. There are also **bounds** on each of the solution variables because each buyer has an upper bound of cash available, and a lower bound of zero. Negative solution x-values mean that you'd be paying the buyers!

Try out the code below to solve this problem. First, import the modules you need and then set variables to determine the number of buyers in the market and the number of shares you want to sell:

Python

```python
1  import numpy as np
2  from scipy.optimize import minimize, LinearConstraint
3
4  n_buyers = 10
5  n_shares = 15
```

In this code, you import `numpy`, `minimize()`, and `LinearConstraint` from `scipy.optimize`. Then, you set a market of 10 buyers who'll be buying 15 shares in total from you.

Next, create arrays to store the price that each buyer pays, the maximum amount they can afford to spend, and the maximum number of shares each buyer can afford, given the first two arrays. For this example, you can use random number generation in `np.random` to generate the arrays:

Python

```python
6    np.random.seed(10)
7    prices = np.random.random(n_buyers)
8    money_available = np.random.randint(1, 4, n_buyers)
```

In this code, you set the seed for NumPy's random number generators. This function makes sure that each time you run this code, you'll get the same set of random numbers. It's here to make sure that your output is the same as the tutorial for comparison.

In line 7, you generate the array of prices the buyers will pay. `np.random.random()` creates an array of random numbers on the half-open interval [0, 1]. The number of elements in the array is determined by the value of the argument, which in this case is the number of buyers.

In line 8, you generate an array of integers on the half-open interval from [1, 4), again with the size of the number of buyers. This array represents the total cash each buyer has available. Now, you need to compute the maximum number of shares each buyer can purchase:

Python

```python
 9    n_shares_per_buyer = money_available / prices
10    print(prices, money_available, n_shares_per_buyer, sep="\n")
```

In line 9, you take the ratio of the `money_available` with `prices` to determine the maximum number of shares each buyer can purchase. Finally, you print each of these arrays separated by a newline. The output is shown below:

Text

```
[0.77132064 0.02075195 0.63364823 0.74880388 0.49850701 0.22479665
 0.19806286 0.76053071 0.16911084 0.08833981]
[1 1 1 3 1 3 3 2 1 1]
[ 1.29647768 48.18824404  1.57816269  4.00638948  2.00598984 13.34539487
 15.14670609  2.62974258  5.91328161 11.3199242 ]
```

The first row is the array of prices, which are floating-point numbers between 0 and 1. This row is followed by the maximum cash available in integers from 1 to 4. Finally, you see the number of shares each buyer can purchase.

Now, you need to create the **constraints** and **bounds** for the solver. The constraint is that the sum of the total purchased shares can't exceed the total number of shares available. This is a constraint rather than a bound because it involves more than one of the solution variables.

To represent this mathematically, you could say that `x[0] + x[1] + ... + x[n] = n_shares`, where `n` is the total number of buyers. More succinctly, you could take the dot or inner product of a vector of ones with the solution values, and constrain that to be equal to `n_shares`. Remember that `LinearConstraint` takes the dot product of the input array with the solution values and compares it to the lower and upper bound. You can use this to set up the constraint on `n_shares`:

Python

```python
11    constraint = LinearConstraint(np.ones(n_buyers), lb=n_shares, ub=n_shares)
```

In this code, you create an array of ones with the length `n_buyers` and pass it as the first argument to `LinearConstraint`. Since `LinearConstraint` takes the dot product of the solution vector with this argument, it'll result in the sum of the purchased shares.

This result is then constrained to lie between the other two arguments:

1. The lower bound `lb`
2. The upper bound `ub`

Since `lb = ub = n_shares`, this is an **equality constraint** because the sum of the values must be equal to both `lb` and `ub`. If `lb` were different from `ub`, then it would be an **inequality constraint**.

Next, create the bounds for the solution variable. The bounds limit the number of shares purchased to be 0 on the lower side and `n_shares_per_buyer` on the upper side. The format that `minimize()` expects for the bounds is a sequence of tuples of lower and upper bounds:

Python

```
12  bounds = [(0, n) for n in n_shares_per_buyer]
```

In this code, you use a [comprehension](#) to generate a list of tuples for each buyer. The last step before you run the optimization is to define the objective function. Recall that you're trying to maximize your income. Equivalently, you want to make the negative of your income as large a negative number as possible.

The income that you generate from each sale is the price that the buyer pays multiplied by the number of shares they're buying. Mathematically, you could write this as `prices[0]*x[0] + prices[1]*x[1] + ... + prices[n]*x[n]`, where `n` is again the total number of buyers.

Once again, you can represent this more succinctly with the inner product, or `x.dot(prices)`. This means that your objective function should take the current solution values `x` and the array of prices as arguments:

Python

```
13  def objective_function(x, prices):
14      return -x.dot(prices)
```

In this code, you define `objective_function()` to take two arguments. Then you take the dot product of `x` with `prices` and return the negative of that value. Remember that you have to return the negative because you're trying to make that number as small as possible, or as close to negative infinity as possible. Finally, you can call `minimize()`:

Python

```
15  res = minimize(
16      objective_function,
17      x0=10 * np.random.random(n_buyers),
18      args=(prices,),
19      constraints=constraint,
20      bounds=bounds,
21  )
```

In this code, `res` is an instance of `OptimizeResult`, just like with `minimize_scalar()`. As you'll see, there are many of the same fields, even though the problem is quite different. In the call to `minimize()`, you pass five arguments:

1. **`objective_function`**: The first positional argument must be the function that you're optimizing.

2. **`x0`**: The next argument is an initial guess for the values of the solution. In this case, you're just providing a random array of values between 0 and 10, with the length of `n_buyers`. For some algorithms or some problems, choosing an appropriate initial guess may be important. However, for this example, it doesn't seem too important.

3. **`args`**: The next argument is a tuple of other arguments that are necessary to be passed into the objective function. `minimize()` will always pass the current value of the solution `x` into the objective function, so this argument serves as a place to collect any other input necessary. In this example, you need to pass `prices` to `objective_function()`, so that goes here.

4. **`constraints`**: The next argument is a sequence of constraints on the problem. You're passing the constraint you generated earlier on the number of available shares.

5. **`bounds`**: The last argument is the sequence of bounds on the solution variables that you generated earlier.

Once the solver runs, you should inspect `res` by printing it:

Text

```
     fun: -8.783020157087478
     jac: array([-0.7713207 , -0.02075195, -0.63364828, -0.74880385,
       -0.49850702, -0.22479665, -0.1980629 , -0.76053071, -0.16911089,
       -0.08833981])
 message: 'Optimization terminated successfully.'
    nfev: 204
     nit: 17
    njev: 17
  status: 0
 success: True
       x: array([1.29647768e+00, 2.78286565e-13, 1.57816269e+00,
       4.00638948e+00, 2.00598984e+00, 3.48323773e+00, 3.19744231e-14,
       2.62974258e+00, 2.38121197e-14, 8.84962214e-14])
```

In this output, you can see `message` and `status` indicating the final state of the optimization. For this optimizer, a status of `0` means the optimization terminated successfully, which you can also see in the `message`. Since the optimization was successful, `fun` shows the value of the objective function at the optimized solution values. You'll make an income of $8.78 from this sale.

You can see the values of `x` that optimize the function in `res.x`. In this case, the result is that you should sell about 1.3 shares to the first buyer, zero to the second buyer, 1.6 to the third buyer, 4.0 to the fourth, and so on.

You should also check and make sure that the constraints and bounds that you set are satisfied. You can do this with the following code:

Python

```python
22 print("The total number of shares is:", sum(res.x))
23 print("Leftover money for each buyer:", money_available - res.x * prices)
```

In this code, you print the sum of the shares purchased by each buyer, which should be equal to `n_shares`. Then, you print the difference between each buyer's cash on hand and the amount they spent. Each of these values should be positive. The output from these checks is shown below:

Text

```
The total number of shares is: 15.000000000000002
Leftover money for each buyer: [3.08642001e-14 1.00000000e+00
 3.09752224e-14 6.48370246e-14 3.28626015e-14 2.21697984e+00
 3.00000000e+00 6.46149800e-14 1.00000000e+00 1.00000000e+00]
```

As you can see, all of the constraints and bounds on the solution were satisfied. Now you should try changing the problem so that the solver *can't* find a solution. Change `n_shares` to a value of 1000, so that you're trying to sell 1000 shares to these same buyers. When you run `minimize()`, you'll find that the result is as shown below:

Text

```
     fun: nan
     jac: array([nan, nan, nan, nan, nan, nan, nan, nan, nan, nan])
 message: 'Iteration limit exceeded'
    nfev: 2182
     nit: 101
    njev: 100
  status: 9
 success: False
       x: array([nan, nan, nan, nan, nan, nan, nan, nan, nan, nan])
```

Notice that the `status` attribute now has a value of `9`, and the `message` states that the iteration limit has been exceeded. There's no way to sell 1000 shares given the amount of money each buyer has and the number of buyers in the market. However, rather than raising an error, `minimize()` still returns an `OptimizeResult` instance. You need to make sure to check the status code before proceeding with further calculations.

Conclusion

In this tutorial, you learned about the **SciPy ecosystem** and how that differs from the **SciPy library**. You read about some of the modules available in SciPy and learned how to install SciPy using Anaconda or `pip`. Then, you focused on some examples that use the clustering and optimization functionality in SciPy.

In the **clustering** example, you developed an algorithm to sort spam text messages from legitimate messages. Using `kmeans()`, you found that messages with more than about 20 digits are extremely likely to be spam!

In the **optimization** example, you first found the minimum value in a mathematically clear function with only one variable. Then, you solved the more complex problem of maximizing your profit from selling stocks. Using `minimize()`, you found the optimal number of stocks to sell to a group of buyers and made a profit of $8.79!

SciPy is a huge library, with many more modules to dive into. With the knowledge you have now, you're well equipped to start exploring!

You can follow along with the examples in this tutorial by downloading the source code available at the link below:

Get Sample Code: Click here to get the sample code you'll use to learn about SciPy in this tutorial.

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```
1 # How to merge two dicts
2 # in Python 3.5+
3
4 >>> x = {'a': 1, 'b': 2}
5 >>> y = {'b': 3, 'c': 4}
6
7 >>> z = {**x, **y}
8
9 >>> z
10 {'c': 4, 'a': 1, 'b': 3}
```

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