A Short Guide to Using Python For Data Analysis In Experimental Physics

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Abstract

Common signal processing tasks in the numerical handling of experimental data include interpolation, smoothing, and propagation of uncertainty. A comparison of experimental results to a theoretical model further requires curve fitting, the plotting of functions and data, and a determination of the goodness of fit. These tasks often typically require an interactive, exploratory approach to the data, yet for the results to be reliable, the original data needs to be freely available and resulting analysis readily reproducible. In this article, we provide examples of how to use the Numerical Python (Numpy) and Scientific Python (SciPy) packages and interactive Jupyter Notebooks to accomplish these goals for data stored in a common plain text spreadsheet format. Sample Jupyter notebooks containing the Python code used to carry out these tasks are included and can be used as templates for the analysis of new data.

Navigation Tip: For a handy table of contents, select **Table of Contents** from the **Document** V pull down menu (upper left of this page). Clicking on an item in the table of contents will take you to that section.

1 Introduction

1.1 About this guide

This is a short guide to using Python to accomplish some commonly needed tasks when working with data acquired in an experimental physics lab, including data import/export, plotting with error bars, curve fitting of functions to data, testing the goodness of fit of these functions to the data (taking into account the uncertainty in the measurements), the interpolation, smoothing, and differentiation of data , the propagation of "error" in calculated quantities, and numerical calculations of data including units and/or uncertainty. A careful discussion of how to import needed functions from the Numerical Python (numpy) and Scientific Python (SciPy) libraries — what Python calls 'packages' — is also included. The examples presented here rely heavily on functions from these packages to simplify various analysis tasks in the examples below. The focus here is on using Python as a scientific and graphing calculator for experimental data, but more experienced Python users should still find the functions and methods presented here useful in their own programs.

The goal of this guide is for you to be carry out each of the analysis steps illustrated here using your own data, and to be able to do so by making at most only a few small changes (such as the names of data files and columns of data) to the templates included with each example. Beginners will need to know a few basic

Python rules and syntax — for example, that x^2 is written `x**2` and NOT as `x^2`— but will not need to already be experienced programmers. For Recommendations on how to get started with Python, see below.

1.2 How to get started

1.2.1 Python

If Python is new to you, we recommend the getting started with Python tutorials developed by our friends and rivals in the Wellesley College Physics Department. Go Smith College Pioneers! These highly focused, highly practical tutorials are in the form of interactive Jupyter notebooks (see below) that allow you to try Python out as you learn; we use them in our own courses and they form the foundation for the methods presented here. We also recommend the unusually lucidly written (and most generously, freely provided) introductory chapter Python programming for physicists from Mark Newman's Numerical Python-based textbook Computational Physics (Newman, 2013). Newman's text provides "an introduction to the Python language at a level suitable for readers with no previous programming experience" with an emphasis on the application of computational methods to typical theoretical problems in undergraduate physics.

1.2.2 Jupyter Notebooks

The examples provided in this guide run Python within user friendly but somewhat oddly named Jupyter notebooks mentioned above. In some ways they look and act like Mathematica® notebooks, including the use of 'cells' (paragraphs of text, equations, or code) and the use of the `shift+enter` keys to execute the code in a cell. Jupyter notebooks are a spin-off of what is known as interactive Python (iPython) and in older examples on the web, you will still encounter references to iPython Notebook instead of Jupyter. This is also why Jupyter is spelled with a 'py' and why Jupyter notebook filenames still end with `.ipynb`.

If the Jupyter notebook (formerly iPython notebook) interface is new to you, take time now to try the on-line interactive tutorial on how to run Python inside Jupyter notebooks. Go ahead, we'll wait. The most important web pages in that tutorial are the first two: Notebook Basics andiPython: beyond plain Python. Once you are ready to learn how to add your own text and equations to Jupyter notebooks, see the third page (on Markdown Cells).

Note that Jupyter notebooks are not the only way to write and run Python code. A bare-bones command line editor called IDLE is used by many beginning computer science students (and in the text Computational Physics) and a MATLAB® style interface called Spyder (again with the 'py'!) is used by many advanced Python programmers. The Python programs provided here will run in any of these environments. But this also means you can run Python programs encountered elsewhere within Jupyter notebooks!

Within the Physics Department here at Smith College, we use the Jupyter notebook interface for two primary reasons: (1) running Python within the notebook provides a reproducible, self-documenting method of analyzing collected data, and (2) the ability to add explanatory notes, tables, figures, and equations within Jupyter notebooks means we can also use them as electronic lab notebooks for courses.

1.2.3 Try it out!

On a webserver

Jupyter notebooks are viewed and run using a web browser such as Firefox (just like this article in Authorea). That means they can also be run on a webserver that you access from a web browser and, as a result, it isn't necessary to have Python installed on your own computer (provided you have internet access and all the Python packages you wish to use are already installed on the webserver).

To try out the Python programs presented here using a Jupyter webserver hosted by Authorea, click the `</> Code` button found to the left of many of the figures in this guide. This will reveal the `.ipynb` Jupyter notebook (and associated data files) containing the Python code used to generate that figure. Clicking on the notebook file name will launch the notebook in a new tab or window within your web browser . Clicking within a 'cell' (a block of text, equations, and or code, outlined by a rectangular border) and hitting SHIFT-ENTER will run any code in that cell and advance to the next one. Alternatively, you can make edits to the code in notebook (for example, adjust a smoothing parameter or change the name of a file) then select `Run All` from the `Cell` menu or `Restart & Run All` from the `Kernel` menu to rerun the program. For additional help, see the online interactive tutorial on how to run Python inside Jupyter notebooks.

Many institutions *host and configure their own Jupyter webservers* suitable for Python programming. For example, Smith College physics students can upload and run any of the Jupyter notebooks included in this guide on the webserver `https://jove.smith.edu`, as this particular webserver has all the packages used here preinstalled. (Note to Smith students: contact the course instructor for an account).

On your own computer

The Authorea server will work for all of the examples except the (aptly named) Python packages Pint and Uncertainties used for numerical calculations using units and/or uncertainties, as those packages are not currently installed on that server (but maybe someday?). That said, you will want to write, run, and store your own data and programs on your own system. If you don't have access to a local Jupyter webserver with the packages you need, you will want to install and run Python and Jupyter on your own computer. The good news is that everything needed is available for free (except the computer)! See Section 9: Installing Python for instructions on how to do this.

2 Importing and exporting data

There are many ways to import, export, and represent data in files. Here we provide just enough to get you started but it might very well be all you need. In these examples, we assume you have first entered the data into a spreadsheet program, then exported that data in 'CSV' (comma separated variable) file format. We use the CSV file format here because it is ubiquitous: all spreadsheets have the ability to export and import data in the CSV file format. Data in other common plain text file formats (such as tab delimited) can also be imported by making a few small modifications to the examples provided below.

2.1 CSV spreadsheet file format

Let's look at a particular CSV data file titled `Calibration_650nm.csv` . The file consists of a single header row of text which we need to skip over when loading the numerical data, followed by three columns of data, one for each measured variable.

Here's what the data looks like in spreadsheet form (grid lines not shown):

angle	V_pd	V_pd_error
0.0e+00	3.24e+01	2.49e-02
1.5e+01	3.01e+01	1.54e-01
3.0e+01	2.4e+01	2.53e-01
4.5e+01	1.59e+01	2.85e-01
6.0e+01	7.78e+00	2.41e-01
7.5e+01	1.96e+00	1.33e-01
9.0e+01	3.57e-02	1.64e-02
1.05e+02	2.58e+00	1.53e-01
1.2e+02	8.95e+00	2.52e-01
1.35e+02	1.74e+01	2.85e-01
1.5e+02	2.56e+01	2.41e-01
1.65e+02	3.13e+01	1.34e-01
1.8e+02	3.3e+01	2.49e-02
1.95e+02	3.03e+01	1.54e-01
2.1e+02	2.39e+01	2.53e-01
2.25e+02	1.56e+01	2.85e-01
2.4e+02	7.55e+00	2.41e-01
2.55e+02	1.88e+00	1.33e-01
2.7e+02	3.38e-02	1.64e-02
2.85e+02	2.46e+00	1.53e-01
3.0e+02	8.51e+00	2.52e-01
3.15e+02	1.66e+01	2.85e-01
3.3e+02	2.47e+01	2.41e-01
3.45e+02	3.05e+01	1.34e-01
3.6e+02	3.25e+01	2.49e-02

Table 1: This is a caption

Here's what the first few lines of the same CSV spreadsheet file looks like when opened in a text editor (notice the commas separating the values within each row):

```
angle, V_pd, V_pd_error

0.000000000000000000e+00,3.236249999999999716e+01,2.492398249033692462e-02

1.500000000000000000e+01,3.008079999999999998e+01,1.536232648449061544e-01

3.000000000000000000e+01,2.402850000000000108e+01,2.527732747539992997e-01
```

2.2 loading data from a CSV file

We are now going to use the Numerical Python (numpy) command `loadtxt` to load data from this CSV text file. Each column of data will become a Numerical Python (`numpy`) array.

The process consists of two steps:

1. importing the `loadtxt` command from Numerical Python
2. using the `loadtxt` command to transfer the data from the file

2.2.1 importing commands

`loadtxt` is not part of the core Python language but is instead part of the Numerical Python package (`numpy`). We must therefore "import" it into our program before using. There are two common methods of doing this.

In the first method, each individual function or module (such as `loadtxt` from `numpy`) is imported as needed . We call this the **direct numpy import style**.

``` # example: direct import method

from numpy import loadtxt #import just the numpy command loadtxt #from numpy import * #an alternative method that imports *all* numpy commands. Be careful!

This method is used, for example, in the excellent Python-based textbook Computational Physics by Mark Newman (Newman, 2013).

Here is another example:

```
#example: direct import method
from numpy import sin, cos, array, pi   # import a few needed functions from the numpy package

angle_in_degrees = array([0, 30, 60, 90]) # create an array with elements corresponding to 0, 30, 60, a
angle_in_radians = angle_in_degrees * pi / 180   # convert to radians
x = cos(angle_in_radians)   # calculate cosine for each element in array, assign values t
y = sin(angle_in_radians)   # calculate sine for each element in array, assign values to

print(y)
```

with result

```
[0. 0.5 0.8660254   1.]
```

In the second method, we first import all of the `numpy` package (and, optionally, provide an abbreviation for `numpy` such as `np.`) We then add `numpy.` (or the abbreviation `np.`) as a prefix when using a function from the `numpy` package. We call this the **traditional import style**.

```
# example: traditional import method

import numpy as np # if you include 'as np', 'numpy' is replaced with the abbreviation 'np'
```

We call this the **traditional** method because this is what you will find in the examples included in the official numpy user guide and quickstart tutorials.
```

The key to using the traditional method is to be sure to specify that you are using a function or module from the numpy package by preceding it either with `numpy` or the abbreviation of your choice (such as `np`). This is why the `loadtxt` commands used in the examples below are written `np.loadtxt` instead of `loadtxt`.

Here is another example:

```
#example: traditional import method

import numpy as np                            # you only need to type this once in each program

angle_in_degrees = np. array([0, 30, 60, 90]) # create an array with elements corresponding to 0, 30, 6
angle_in_radians = angle_in_degrees * np.pi / 180      # convert to radians
x = np.cos(angle_in_radians)                  # calculate cosine for each element in array, assign valu
y = np.sin(angle_in_radians)                 # calculate sine for each element in array, assign values 

print(y)
```

with the same result as before:

```
[0. 0.5 0.8660254 1.]
```

One one hand, the direct import method has the advantage of being lean, clean, and easy to read. Computer scientists love it. On the other hand, it does not work well if we need to use multiple packages containing identically named functions. For example, the math package `math`, the complex mathematics package `cmath`, the numerical python package `numpy`, and the numerical calculation of uncertainties package `uncertainties` all have trigonometric functions called `sin` and `cos`. To keep clear which function we are using from which package, and when, we will usually use the traditional import style for packages.

2.2.2 importing the data file

We now show how to use `loadtxt`to import the csv format spreadsheet file `Calibration_650nm.csv`. Unless specified otherwise, the data file is assumed to be in the same file folder as the Python program.

The loadtxt command:

```
# example: traditional import method

import numpy as np # only need this once per program

file_name = 'Calibration_650nm.csv'               # replace with the name of your csv data file

file_folder = ''                                  # use this if your data file is in the same folder as

#file_folder = '/Users/nfortune/data'             # use this if data file is in a folder called 'data'
                                                  # inside the folder 'nfortune' within the 'Users' dir
                                                  # such as when using the Jupyter webserver jove.smith
                                                  # this is called 'absolute addressing'

#file_folder = 'data_subfolder/'                  # you can use this if data file is in a _subfolder_ c
```

```
                                                     # this is called 'relative addressing'
data_file = file_folder + file_name

angle, V_pd, V_pd_error  = np.loadtxt(data_file, delimiter = ',', skiprows = 1, usecols = (0, 1, 2), un
```

What these commands do:

`data_file = file_folder + file_name` tells Python what the name of the file is and where to find it! Tip: If you have trouble determining how to specify the file_folder location for your data, an easy workaround is to first put the data in the same folder as your Python program, then either (a) set `file_folder = ''` as in the example above or (b) replace `np.loadtxt(file_folder + file_name, ...)` with `np.loadtxt(file_name, ...)` .

`delimiter = ','` tells `loadtxt` that your data is in comma separated variable format (CSV). The character used to separate one column of data from another is called the 'delimiter.' See the numpy.loadtxt manual page for details.

`skiprows = 1` tells `loadtxt` *to skip over one row* of text in the CSV file before looking for data to load into arrays. This is because the first row of text contains names for each column of data instead of data values (as shown in Table 1).

`unpack = True` tells `loadtxt` that the data is in a 'packed' data format (in which each *variable* corresponds to a different *column* instead of to a different *row*)and therefore needs to be 'unpacked' when loaded. This is the typical arrangement for data in spreadsheets. Use `unpack = False` if the data is in an 'unpacked' data format (in which each *variable* corresponds to a different *row* instead of a different *column*).

`usecols = (0, 1, 2)` says the data you are looking for is in the first 3 columns, which are numbered 0, 1, and 2 (because Python always starts from zero when counting). In our case, since there are only 3 columns of data and we want to use all three, this command is unnecessary. You could leave it out and everything would work just fine for this particular data file. If, however, you wanted to load data from a file with many columns but only needed data from column number 0, column number 3, and column number 4, you would need to include `usecols = (0,3,4)` within the `loadtxt` command.

`angle, V_pd, V_pd_error = np.loadtxt(...)` tells Numerical Python to create an array called `angle` and fill it with values from the first column of data in the CSV spreadsheet file, then create an array called `V_pd` and fill it with values from the second column of data, and finally create an array called `V_pd_error` and fill it with values from the third column of data. The result is three shiny new numpy data arrays we can use in our calculations.

What if your data is in a different text file format (such as tab delimited)? In that case you can still use `loadtxt` to import your data as long as you modify the `delimiter`command to match the file format. See the numpy.loadtxt manual page for details.

2.3 saving data to a CSV file

For completeness, we now provide an example of how to use the `savetxt` command from `numpy` to *save data* in csv format. There are many ways to save files in spreadsheet format but this is the simplest method we've found so far using `numpy`.

Direct numpy import style:

```
from numpy import savetxt, array                 #assumes you haven't already imported these commands

output_filename = 'output.csv'                   #provide a name for the new file
header_row_text = 'angle, V_pd, V_pd_error'      #make first row of file be a list of column names. Opti
comment_text = ''                                #do not start header row with a '#'. Optional.
#comment_text = '#'                              #start the header row with a '#' . Default setting.

data = array([angle, V_pd, V_pd_error]).T        #create a 2D matrix and transpose rows and columns (cle
savetxt(output_filename, data, delimiter = ',', header = header_row_text, comments = comment_text)
```

Traditional numpy import style:

```
import numpy as np                               #don't import numpy again if already done once before

output_filename = 'output.csv'                   #provide a name for the new file
header_row_text = 'angle, V_pd, V_pd_error'      #make first row of file be a list of column names. Opti
comment_text = ''                                #do not start header row with a '#'. Optional.
#comment_text = '#'                              #start the header row with a '#' . Default setting.

data = np.array([angle, V_pd, V_pd_error]).T     #create a 2D matrix and transpose rows and columns (cle
np.savetxt(output_filename, data, delimiter = ',', header = header_row_text, comments = comment_text)
```

Why do we need the line `data = array([angle, V_pd]).T` ? We need it because ordinarily `savetxt` would save the data in what Python calls 'unpacked' format, a format in which each *variable* corresponds to a different *row* instead of to a different *column*. This is often convenient but is *not* what we wanted in this particular case. We therefore did the following **clever trick** before saving the data to a file: we created a 2D matrix of our data with the numpy command `array([angle, V_pd])`, then used the `.T` command to transpose the matrix , thereby flipping the rows and columns.

2.4 Other file handling methods

For more advanced data handling of spreadsheet data files, large data sets, and/or the handling of binary data, you may wish to try the commands provided by the very popular Python Data Analysis Library package pandas or the big data Hierarchical Data Format (HDF5) using the Python interface package h5py (instead of those provided by numpy).

3 Plotting data using error bars

The most commonly used plotting package in Python is Matplotlib. Here's an example of how to use it to generate plots with error bars representing the uncertainty in each data point. We use `angle` from the file `650 nm calibration.csv` for the x-axis values, we use `V_pd` for the y-axis values, and we use `V_pd_delta` for the uncertainty in the y-axis values.

```
%matplotlib inline

import matplotlib as mpl
from matplotlib import pyplot as plt #this is the traditional method

mpl.rc('xtick', labelsize = 18)      #use 18 point font for numbering on x axis
mpl.rc('ytick', labelsize = 18)      #use 18 point font for numbering on y axis

plt.figure(figsize = (7,5))          #specify figure size as 7 x 5 inches
                                     #for default size, type plt.figure()

plt.xlabel(r"$\theta$ [degrees]", fontsize = 18) #label axis (using LaTeX commands)
plt.ylabel(r"$V_{pd}$ [volts]", fontsize = 18)   #use 18 point font for label text

plt.errorbar(angle, V_pd,
    xerr=None, yerr=V_pd_error,
    linestyle = 'none',
    color = 'blue',
    capsize = 3, capthick = 1)

plt.show()
```

The result is shown in Fig.1 below.

What these commands do:

`%matplotlib inline` is an interactive Python (iPython) 'magic command' used when running Python within a Jupyter notebook. It allows the display of data plots within the notebook.

Tip: When running Jupyter notebooks within Authorea , the`%matplotlib inline` command must precede the `from matplotlib import pyplot` command.

`plt.figure()` signifies the beginning of the plotting instructions specific to that figure.

`plt.errorbar(angle, V_pd, xerr = None, yerr=V_pd_delta)` is the command that instructs matplotlib to generate a x-y plot with error bars (as opposed to a bar graph or scatter plot, for example). All four parameters (`x, y, xerr, yerr`) are required.

`linestyle` and `color` are used to customize the appearance of the data points. `Linestyle = None` means there are no connecting lines between points. `Color` means the color of the error bar lines and caps. The standard colors are blue, green, red, cyan, magenta, yellow, black, and white (with corresponding abbreviations 'b', 'g', 'r', 'c', 'm', 'y', 'k', and 'w').

`capsize`, and `capthick` are used to customize the appearance of the error bars. `capsize =3` sets the width of the error bars to '3' (in typesetter points), and `capthick=1`sets the thickness of the drawn bars to '1' (again in typesetter points). Note that if the `capsize` and `capthick` commands are omitted, matplotlib will draw lines indicating the given uncertainty but will omit the bars!

`plt.show()` signifies the end of the plotting instructions and causes matplotlib to plot the data.

For additional examples and information about other commands and options (including grid lines, tick marks, semilog plots, and log-log plots), please click on the links supplied here or search the online matplotlib.pyplot documentation.

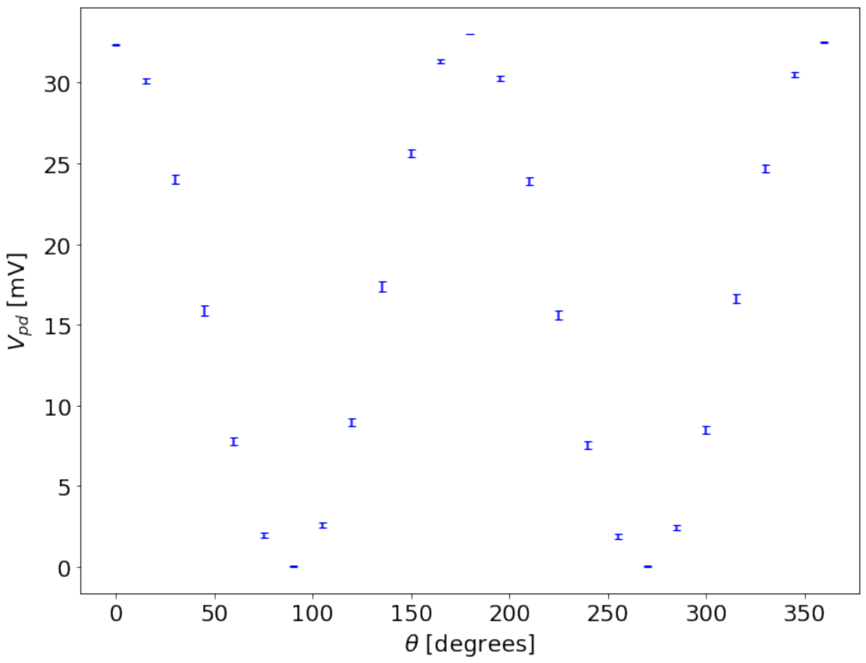


Figure 1: Photodiode voltage as a function of relative polarizer angle for light at 650 nm passing through two polarizers. V_{pd} corresponds to the voltage measured across a resistor placed in series with a photodiode and is linearly proportional to light intensity under these conditions. A change in polarization angle of the light (due to the Faraday effect, for example) can be detected as a change in photodiode voltage but the size of the change in voltage for a given change in polarization angle depends on the relative orientation of the two polarizers.

4 Curve fitting

4.1 mathematical modeling

Curve fitting requires a mathematical model, initial estimates for the adjustable parameters in the model, and estimates of the uncertainty in the values of each data point. Here, we construct a mathematical model based on "Malus's Law" to describe light passing through two linear polarizers, as measured by a powered photodiode:

$$I(\theta) = I_0 \cos^2(\theta - \theta_0) + C = \frac{1}{2} I_0 \left[1 + \cos(2(\theta - \theta_0))\right] + C \tag{1}$$

where θ_0 is the (fixed) angle of the first (reference) linear polarizer, θ is the (variable) angle of the second linear polarizer, $\theta - \theta_0$ is the relative angle between them, and I_0 is the maximum intensity of the light passing through both polarizers (which occurs when $\theta = \theta_0$). The offset C represents any 'dc' offset in the signal from the photo-detector (resulting in a nonzero signal in the absence of light), any additional light reaching the photo-detector that didn't pass through the polarizers, and if the polarizers are not perfect (ideal), the fraction of light passing through but not polarized by both polarizers.

Rewriting in terms of the measured output photodiode voltage V_{pd} , the relative polarizer angle $\phi = \theta - \theta_0$, and assuming a linear response between the photo-detector output voltage and light intensity, we have

$$V_{pd}(\phi) = V_0 \cos^2(\phi) + V_1 = \frac{1}{2} V_0 \left[1 + \cos(2\phi)\right] + V_1 \tag{2}$$

If, in addition, the variables V_0,V_1, θ and $\theta_0$and ϕ are independent of each other (which will be the case for ideal polarizers), then to first order, the uncertainty δV_{pd} is given by (Hughes and Hase, 2010)

$$(\delta V_{pd}) = \sqrt{\left(\frac{\partial V_{pd}}{\partial V_0}\right)^2 (\delta V_0)^2 + \left(\frac{\partial V_{pd}}{\partial \phi}\right)^2 (\delta \phi)^2 + \left(\frac{\partial V_{pd}}{\partial V_1}\right)^2 (\delta V_1)^2} \tag{3}$$

where $\delta\phi = \sqrt{(\delta\theta)^2 + (\delta\theta_0)^2}$ and which we will approximate as $\delta\theta$ as we are holding θ_0 constant.

Evaluating the partial derivatives in Eq. 3,

$$\delta V_{pd} = V_0 \sqrt{(\cos\phi)^4 \left(\frac{\delta V_0}{V_0}\right)^2 + (-2\cos\phi\sin\phi)^2 (\delta\phi)^2 + \left(\frac{\delta V_1}{V_0}\right)^2} \tag{4}$$

The corresponding Python functions are

```
# import numpy as np

def polarization_model( phi_array, V_0, phi_0, V_1):
    return V_0 * (1 + np.cos(2 * (phi_array - phi_0)))/2 + V_1
```

and

```
# import numpy as np

def photodiode_error(phi_array, delta_V_0, delta_phi, delta_V_1, V_0, phi_0):
    V_0_error= (delta_V_0 / V_0) * (np.cos(phi_array - phi_0))**2
    phi_error = (delta_phi) * (2 * np.cos(phi_array- phi_0) * np.sin(phi_array - phi_0))
    V_1_error= (delta_V_1 / V_0)
    fractional_error = np.sqrt(V_0_error **2 + phi_error **2 + V_1_error **2)
    return fractional_error * V_0
```

We can determine δV_1 and δV_0 experimentally by measuring the statistical spread in the minimum and maximum values of V_{pd} (when $\phi = \frac{\pi}{2}$ radians and $\phi = 0$, respectively). The polarizer angle θ is mechanically set, so the uncertainty $\delta\phi$ depends on the accuracy of a nominally 15° step change in angle θ with the apparatus at hand.

Now we encounter an apparent conundrum: we want to use the curve fit to determine a best estimate for V_0 but solving for δV requires us to already have a numerical value for V_0. How do we determine the numerical values for $\delta V_{pd}(\theta)$ needed to find a best estimate of V_0 if we don't already know V_0? This, however, is not the impasse that it might seem. The curve fitting algorithm already requires that we supply an initial guess for the parameters. In this situation, then, we can carry out the curve fitting algorithm a second or third time instead of just once, each time using the best fit values output by the algorithm in the previous fit as our new initial values for the new fit. Once the output values match the input values (within uncertainty), we stop. When the output values match the input values, we say the results are *self-consistent.*

Here is the procedure for finding self-consistent 'best fit' values from curve-fitting:

1. Make a rough initial guess for the parameters V_0, V_1, and θ_0 from a graph of the data.
2. Use the values of V_0, V_1, and θ_0 output by the curve-fitting routine as a new 'initial guess'
3. Repeat the curve fit (using each output as a new input) until V_0 stops changing.

Note: if you know how to do programming in Python, this would be a great place to simplify your life by introducing a **while loop** into the code that repeats the curve fit until the results become self-consistent. We plan to add a section illustrating how to do that in a future version of this guide.

4.2 fitting the model to data

4.2.1 calculating best fit values

We now turn to the actual Python code for non-linear curve fitting. Notice that this is a "weighted" fit, in that the stated uncertainty of each data point is taken into account during the fit. Practically speaking, this means the curve-fitting routine tries harder to match the model to the data at points with a smaller uncertainty (although it may not succeed) because those points are given greater importance ('weight'). This is as it should be, and is also needed to calculate a numerically accurate chi-square value for a determination of the "goodness of fit."

Here we assume that values have already been experimentally determined for uncertainties in V_0, V_1, and θ. We will therefore leave these unchanged throughout the curve-fitting process.

```
# measured uncertainties
delta_V0 = 0.020           # mV, after averaging
delta_V1 = 0.014           # mV, after averaging
delta_theta = 0.5 * np.pi / 180  # 0.5 degrees, in radians
```

Now let's take care of the initial setup:

```
# initial guess for polarization models
V0 = 30.0    #initial guess, in mV
V1 = 0.02    #initial guess, in mV

theta = angle * np.pi / 180    # convert from degrees to radians

theta0 = -2.0 * np.pi / 180   #initial guess for offset angle of 2 degree, in radians
```

```
initial_guess = np.array([V0, theta0, V1])
initial_error = np.array([delta_V0, delta_theta, delta_V1])
old_fit = np.copy(initial_guess)  # save a copy to compare new with old

estimated_error = photodiode_error(theta, delta_V0, delta_theta, delta_V1,
    V0, theta0)    #propagate uncertainty using initial values
```

Finally let's run the curve fit command:

```
# load curve_fit routine from scipy
from scipy.optimize import curve_fit # import method used here

# alternative method (as recommended in https://docs.scipy.org/doc/scipy/reference.api.html)
#from scipy import optimize
#fit, covariance = optimize.curve_fit(...)

#run curve_fit for polarization_model
fit, covariance = curve_fit(polarization_model, theta, V_pd,
                            p0 = initial_guess,
                            sigma = estimated_error, absolute_sigma = True)

error = np.sqrt(np.diag(covariance))

print(old_fit)
print(fit)

old_fit = np.copy(fit)

print()
print('V_0    = ','{:.3f}'.format(fit[0]), '±', '{:.3f}'.format(error[0]), ' mV')
print('V_1 = ','{:.4f}'.format(fit[2]), '±', '{:.3f}'.format(error[2]), ' mV')
print('theta_0  = ','{:.4f}'.format(fit[1]), '±', '{:.4f}'.format(error[1]), 'radian')
print('       = ','{:.4f}'.format(fit[1]*180/np.pi), '±', '{:.4f}'.format(error[1]*180/np.pi), 'degrees
```

Here are the results after the first iteration:

```
V_0     =  32.631  ± 0.024  mV
V_1     =   0.023  ± 0.016  mV
theta_0 =  -0.0203 ± 0.0018 radian
        =  -1.162  ± 0.102 degrees
```

We now use the output values for V_0 and V_1 as the new input values and recalculate the estimated error for each $V_{pd}\left(\theta\right)$ value:

```
new_initial_values = np.array([fit[0], fit[1], fit[2]])

estimated_error = photodiode_error(theta, delta_V0, delta_theta, delta_V1,
    fit[0], fit[1]) # propagate error using new values for V0, etc

fit, covariance = curve_fit(polarization_model, theta, V_pd,
                            p0 = new_initial_values,
                            sigma = estimated_error, absolute_sigma = True)

error = np.sqrt(np.diag(covariance))
```

```
print(old_fit)
print(fit)

old_fit = np.copy(fit)

V_pd_model = polarization_model(theta, fit[0], fit[1], fit[2])
residual = V_pd - V_pd_model

data_uncertainty = photodiode_error(theta, delta_V0, delta_theta, delta_V1, fit[0], fit[1])

chisq = sum((residual/ data_uncertainty)**2) #typo corrected
degrees_of_freedom = len(residual) - len(initial_guess)
reduced_chisq = chisq / degrees_of_freedom  # this should be close to one
CDF = chi2.cdf(chisq, degrees_of_freedom)   # this should be close to 50 percent

print('chi-square         = ',chisq)
print('degrees of freedom = ',degrees_of_freedom)
print('reduced chi-square = ',reduced_chisq)
print('fractional probability of chisq \selectlanguage{english}[?]', chisq, 'for ', degrees_of_freedom,
```

and continue in this way until the value V_0 stops changing.

4.2.2 graphing the results

Our final numerical results are:

```
V_0     =  32.629  +- 0.020  mV
V_1     =   0.022  +- 0.013  mV
theta_0 =  -0.0202 +- 0.0020 radian
        =  -1.155  +- 0.112 degrees
```

We can now graphically compare the original data with our model (Eq. 2) using the best fit values for the parameters:

```
plt.figure(figsize = (11,8))                  #specify figure size as 7 x 5 inches
                                             #for default size, type plt.figure()

plt.xlabel(r"$\theta$ [degrees]", fontsize = 18) #label axis (using LaTeX commands)
plt.ylabel(r"$V_{pd}$ [volts]", fontsize = 18)   #use 18 point font for label text

# plot the data as before in blue
plt.errorbar(angle, V_pd,
    xerr=None, yerr=V_pd_error,
    linestyle = 'none',
    color = 'blue',
    capsize = 3, capthick = 1, label = "data")

#create curve showing fit to data
angle_fit = np.linspace(0, 360, 180)
theta_fit = angle_fit * np.pi / 180
V_pd_fit = polarization_model(theta_fit, fit[0], fit[1], fit[2])

#plot the curve fit in red
```

```
plt.errorbar(angle_fit, V_pd_fit, xerr = None, yerr = None, color = 'red', label = 'fit' )
plt.xlim(-15, 375)
plt.ylim(-2.5, 40)
plt.xticks([0,   30, 60, 90, 120, 150, 180, 210, 240, 270, 300, 330, 360],
           ('0', '', '', 90,  '',  '', 180,  '',  '', 270,  '',  '', 360))
plt.legend(loc = 'best')

plt.show()
```

The results are plotted in Fig. 2 below.

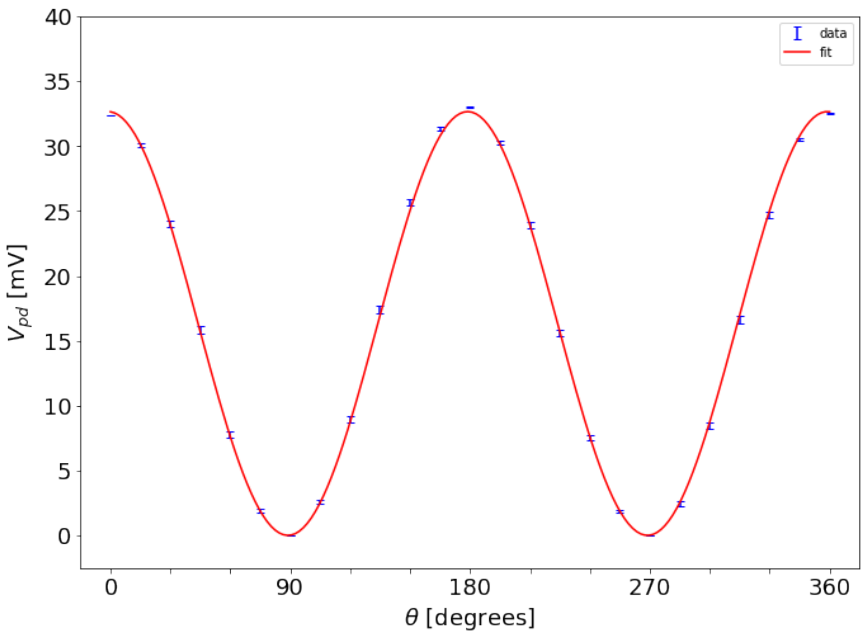


Figure 2: Curve fit of Eq. 2 to calibration data for 650 nm using best-fit values for parameters.

At first glance, the model appears to describe the data quite well, with the possible exception of the points where $V_{pd}(\theta)$ is a maximum. To quantify the goodness of fit, however, we will need to evaluate the fit residuals and chi-square test goodness of fit. See section 4.3.

Note: there are additional features of the curve_fit function not demonstrated here, including the ability to set lower and upper bounds on each of the adjustable parameters. For example, setting the option `bounds = ([0, -np.pi,  -1.0], [np.inf, +np.pi, 1.0])`

would then force the best fit parameters to stay in the range $0 \leq I_0$, $-\pi \leq \theta_0 \leq \pi$ in rad, and $-1 \leq$ offset $\leq +1$. See the scipy.optimize.curve_fit documentation for details.

4.3 Evaluating the goodness of fit

We now have a best fit of the model to the data. How good a fit is it? That is, how well does the model describe the data, taking into account the uncertainty in each data point? Two quick ways to test the goodness of fit of the model to the data are through calculations of the residuals and the reduced chi-square value. See (Hughes and Hase, 2010) and (Berendsen, 2011).

4.3.1 residuals

The calculation of the residual errors is easy once the model is defined and the fitting parameters determined. Here is an example:

```
# theta = angle * np.pi / 180  # convert to radians

V_pd_model = polarization_model_1(theta, fit[0], fit[1], fit[2])
residual = V_pd - V_pd_model
```

The corresponding plot is shown in Fig. 3 below.

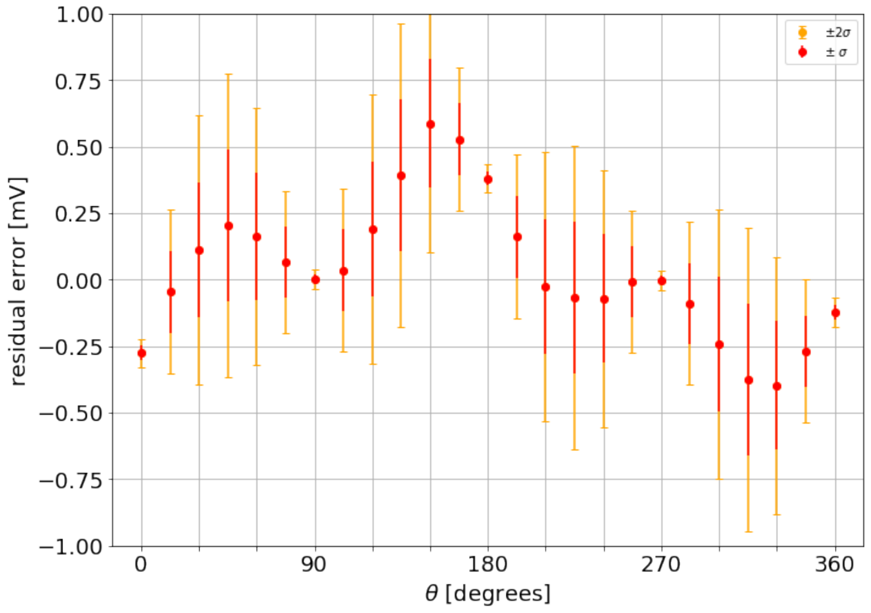


Figure 3: residual error compared with estimated measurement uncertainty for $\pm\sigma$ (in red) and $\pm 2\sigma$ (in orange). Most points are within one or two standard deviations of zero residual error, as expected for a good fit to the data using Malus's law, but the points do not appear randomly distributed. Instead, there is a weak angular dependence suggesting a small uncorrected systematic misalignment of the light source and/or polarizers with respect to the detector.

The residuals are generally within one standard deviation of zero but do not appear randomly distributed. Instead there is a weak residual angular dependence. One possibility is that light beam, polarizers, and detector are not perfectly centered and the polarization is not completely uniform across the entire surface of the polarizer. Malus's law does not however appear to be in question. Rather, the residuals indicate a small level of polarizer-angle dependent systematic error.

4.3.2

4.3.3 chi-square test

Once the residuals have been calculated, the determination of the corresponding chi-square value for goodness of fit is straightforward. Here is an example:

```
from scipy.stats import chi2          # 'chi-square' goodness of fit calculation

chisq = sum((residual/ data_uncertainty)**2)  # typo corrected 2/1/2019
degrees_of_freedom = len(residual) - len(initial_guess)
reduced_chisq = chisq / degrees_of_freedom  # this should be close to one
CDF = chi2.cdf(chisq, degrees_of_freedom)   # this should be close to 50 percent

print('chi-square         = ',chisq)
print('degrees of freedom = ',degrees_of_freedom)
print('reduced chi-square = ',reduced_chisq)
print('fractional probability of chisq [?]', chisq, 'for ', degrees_of_freedom, 'dof is', CDF)
```

Ideally, if the model describes the data AND the estimated uncertainty of each point has been accurately determined, the reduced chi-square value would be approximately equal to one (for large ν) and the fractional probability of χ^2 values larger and smaller than that measured would both be approximately 50%. Statistically, however, we expect some reasonable random variation from the expected mean value of ν for $\chi^2_{\rm min}$, meaning that statisticians generally will not reject the "null hypothesis" (that the model describes the data and all deviations can be reasonably attributed to expected random variation) as long as $\chi^2_{\rm min}$ is within 2 standard deviations (2σ) of the mean value. Here, $\chi^2_{mean} = \nu$ and $\sigma_\nu = \sqrt{2\nu}$ (Hughes and Hase, 2010) , so the criterion can be reexpressed as

$$\nu - 2\sqrt{2\nu} \leq \chi^2{}_{min} \leq \nu + 2\sqrt{2\nu} \tag{5}$$

Here are the results for the fit shown in Fig. 2:

chi-square test value $\chi^2_{\rm min}$ = 15.3

degrees of freedom ν = 25 - 3 = 22

reduced chi-square = 0.694

fractional probability of χ^2 [?] 15.3 is 15.0%

fractional probability of $\chi^2 >$ 15.3 is 85.0%

Here, $\sigma = \sqrt{2\,\nu} = 6.6$, $\chi^2_{mean} - \sigma = 15.4$, and $\chi^2_{mean} + \sigma = 28.6$, indicating that our result is very slightly outside one standard deviation of the mean but well within two standard deviations. We conclude that we have acceptably good agreement between model and experiment at this level of experimental precision but that further improvements in apparatus design, measurement method, and reduction in uncertainty are merited.

5 Data Smoothing and Differentiation

5.1 Savitzky-Golay filters

Data smoothing is a way of reducing time varying noise in measured data so as to reveal the underlying dependence of the measured variable on a different variable (such as an applied voltage or an external magnetic field). In most cases, the computer is acting as a digital low pass filter. It differs from an analog low pass output filter in that the filtering is done by us using a computer after the measurement is complete rather than by the instrument itself. Like the signal averaging done by a digital oscilloscope — the point by point averaging of a periodic signal — data smoothing seeks to separate random noise from a reproducible signal, but here the measured 'signal' to be smoothed is not assumed to be periodic and is in fact usually a function of a variable other than time. An example would be the measurement of current as a function of applied voltage for a non-ohmic device.

The SciPy (for scientific python) package offers an exhaustive list of signal processing functions useful for the digital filtering. If you have some programming experience in Python, you may wish to design your own filter, perhaps using the lower level scipy.signal filter design tools. There are, for example, a wide variety of spectral analysis and peak finding routines for frequency data that we will not explore further here.

In this getting start guide, we will focus on the use of a particularly useful and easy to use ready-made filter for **data smoothing** of $y(x_i)$ data equally spaced in x: the Savitzky-Golay low pass filter (Savitzky and Golay, 1964; Steinier et al., 1972). This filter works by fitting a subset of data points adjacent to a particular data point with a low-degree polynomial, evaluating the polynomial at that point, and then repeating the process for each data point. The set of points centered about a particular data point is called the 'filter window' and the number of points in the filter window is called the *window length* (although *width* would seem more apt). The picture here might be of a small window in a cabin looking out upon a nearby data stream. The window reveals a small subset of points at a time as the data "streams" by. The fit is carried out on the points seen through the window, and repeated for each point in the stream.

As a bonus, the SciPy Savitzky-Golay filter function `scipy.signal.savgol_filter` can also be used to numerically **differentiate the smoothed data** (again, provided the data is "equally spaced"). This is a particularly useful feature. For example, we might directly measure $I(V)$ for a particular non-ohmic device (such as a light bulb or LED) but be more interested theoretically in the differential current $\frac{dI}{dV}$ as a function of applied voltage V. Experimentally, the noise fluctuations in a measurement of I as a function of V might preclude a direct calculation of $\frac{dI}{dV}$. By first smoothing the data using a Savitzky-Golay filter to reduce the noise, a meaningful calculation of $\frac{dI}{dV}$ as a function of V can now be carried out.

There are a few practical constraints:

1. the window length must be an odd number
2. the polynomial order (1, 2, 3, . . .) must be less than the window length
3. the data points are assumed to be "evenly spaced" (for example in time, voltage, or magnetic field)

For example, when measuring current I as a function of applied voltage V from -10 to +30 V in equal steps of 0.1 volts, specifying a window length of 21 points and a second order polynomial fit would correspond to a fitting a quadratic function to a set of 21 points spanning a 2 V range centered about a particular data point (including that point), then repeating that process for each subsequent data point. In the SciPy implementation, this repeated fitting over a moving data stream is done automatically for us.

As noted above, the number of points included in the subset and the order of the polynomial must be specified by the user. In all data smoothing routines, there is a tradeoff between the degree of smoothing and the ability to resolve small features in the underlying signal; data smoothing is not a substitute for working as carefully as possible to minimize the measurement noise and maximize the accuracy and precision of the originally measured data! In the end, the 'best values' for these parameters are usually determined by trial and error. Keep track of the values used when determining the resolution of your experiment!

5.1.1 Scipy.Signal.Savgol_filter

This filter can be implemented in Python with just two lines of code: one to import from the `scipy.signal` module the function `savgol_filter`, and one more to carry out the data smoothing.

We first need to specify two parameters:

1. *window_length*, the number of adjacent data points we wish to include in the fit
2. *polyorder*, the order of the polynomial fit (where 0 = constant, 1 = linear, 2 = quadratic, and 3 = cubic)

If we also want to calculate the slope of the data at each point by taking a derivative, we then need to specify two additional parameters :

1. *deriv*, the order of the derivative (where 0 = no derivative, 1 = first derivative, 2 = 2nd derivative,. . .)
2. *delta*, the spacing of the samples to which the filter will be applied.

As an example, suppose we want again to determine $\frac{dI}{dV}$ from a measurement of $I(V)$ for applied voltages between -10 V and +30 V and that measurements were made evenly spaced in voltage with a step size of 0.1 V. If so, we then specify that deriv = 1 and delta = 0.1 within the `savgol_filter` function.

Finally, for the computed derivative to be physically and quantitatively meaningful,

1. the order of the polynomial fit needs to be greater than the order of derivative (!)
2. The delta value needs to be correctly specified. If unspecified, it is assumed that delta = 1.

As usual, there are additional optional settings, including options for how to handle data near the endpoints (see `mode`): the default (`mode = interp`) is to fit the last window_length / 2 points to a polynomial of order polyorder. For this and other details, see the Scipy reference manual page.

5.1.2 Sample Python code

Here is an example of how to use the SciPy function `savgol_filter` for data smoothing.

```
from scipy.signal import savgol_filter

window_width = 25      # set number of points over which data is fit and smoothed equal to 25
                       # window_width must be an odd number
polynomial_order = 2   # set order of polynominal used to fit data equal to 2
                       # polynomial_order must be less than window_width

data_spacing = 0.1     # data_spacing = x_1 - x_0 for data y(x_0), y(x_1), ....

smoothed_data   = savgol_filter(noisy_data, window_width, polynomial_order) #smooth data
data_derivative = savgol_filter(noisy_data, window_width, polynomial_order, deriv = 1, delta = 0.1) #ta
```

An example of data smoothing using the Savitzky-Golay low pass filter is shown in Fig 4. Since for real experimental data the original 'clean signal' is unknown, the degree of smoothing is always a matter of judgement. A comparison of several different smoothing values (not shown) can be useful in discerning the best choice of parameters and the effective resolution of your processed data (and any derivatives) .

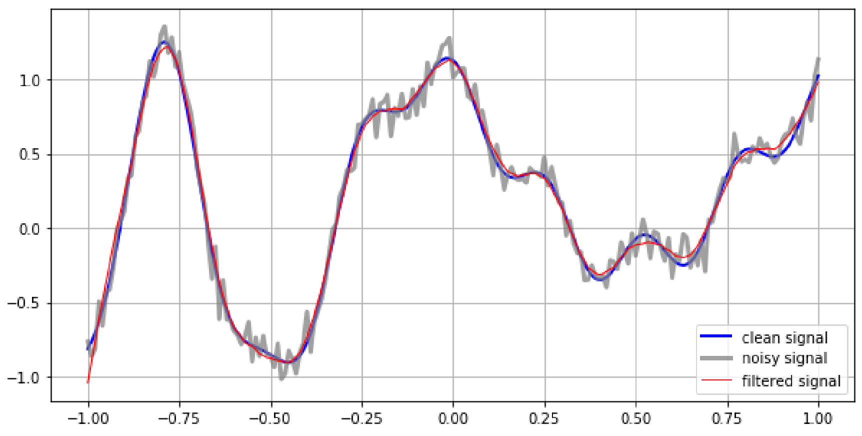


Figure 4: Use of a Savitzky-Golay low pass filter to smooth (artificially generated) noisy data.

In general, increasing the window width increases the degree of smoothing, causing small features in the original 'clean signal' to disappear; decreasing the window width decreasing the degree of smoothing, causing artificial features (arising from the noise) to emerge. Increasing the order of the polynomial while holding the window width constant decreases the degree of noise reduction but is needed for if there is significant data curvature over the width of the smoothing window. To see this for yourself, this click first on the </> Code button, then on the file name `Smooth_and_differentiate.ipynb` to open and view the underlying Jupyter notebook containing the Python code used to generate this figure. Once opened, you can vary the smoothing parameters and re-run the notebook to see the changes. You can also download the notebook to your own computer as a template.

5.2 Butterworth filters

Everyone has there own favorite low pass filter smoothing routine. The Savitky-Golay method presented here is a useful and intuitive place to start but it is not necessarily better or worse than any other smoothing routine. For more advanced filtering methods and examples, see the SciPy Cookbook and the SciPy signal processing reference guide.

Two examples of particular interest from the SciPy Cookbook involve Butterworth filters, which are designed to have as flat a frequency response as possible over the range of frequencies to be passed while still filtering out unwanted frequencies (such as high frequency noise):

1. a Butterworth bandpass filter to filter out high frequency noise, low frequency noise, and dc drift
2. a Butterworth low pass filter for general data smoothing

Note: The use of a Butterworth filter requires the specification of a cutoff frequency (or frequencies). For a digital Butterworth filter, varying the value of the normalized Nyquist_frequency between zero and one will change the degree of smoothing provided. Lower values produce greater smoothing of the data.

The example in Fig. 5 below uses a 3rd order digital Butterworth low-pass filter with a Nyquist frequency of 0.13 (see attached code) to smooth the same signal as in Fig. 4 ; the originalSciPy cookbook example uses a frequency of 0.05. See the SciPy cookbook and the Jupyter notebook attached to this figure for additional details.

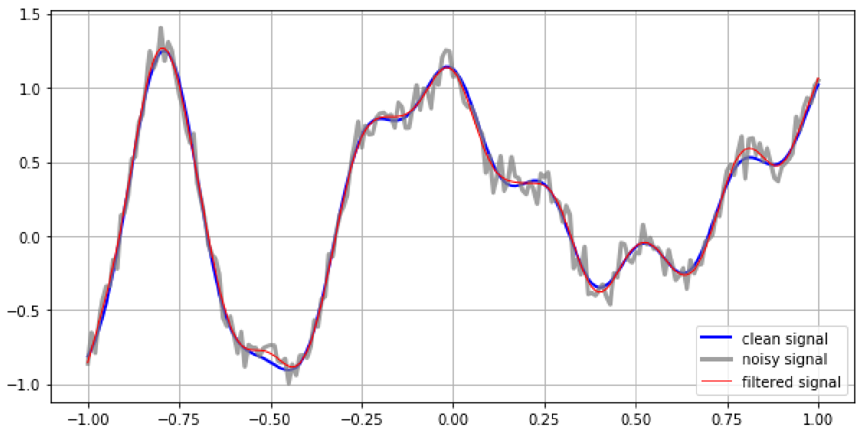


Figure 5: Use of a digital Butterworth low-pass filter (and some fancy footwork) to smooth the same data as in Fig. 4.

5.3 Differentiation

One of the most common reasons for data smoothing is to then be able to differentiate the data. As noted earlier in section 5.1.1, one of the advantages of using `scipy.signal.savgol_filter` is that the data smoothing and differentiation can be done in a single step (when working with evenly spaced data). Here is an example (for the data originally shown in Fig. 4):

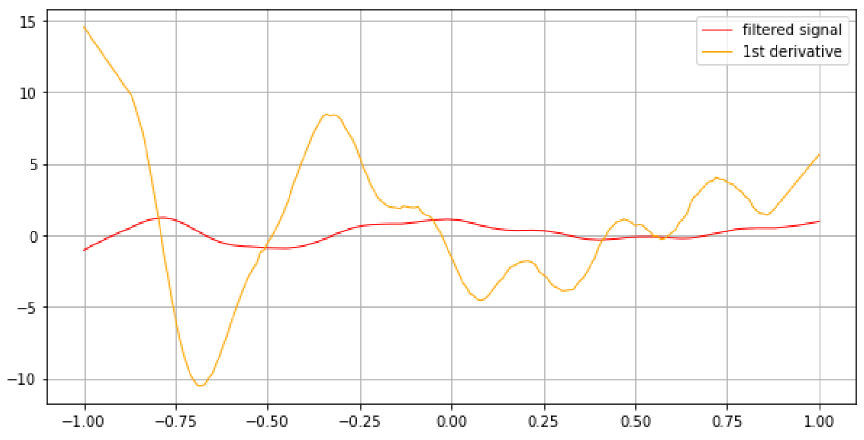


Figure 6: Filtered signal and first derivative of data shown in FIg. 4 . Numerical results calculated (from noisy signal) using the SciPy Savitzky-Golay filter function (window width = 25, polyorder = 2).

More generally, however, the numerical derivative of a suitably filtered signal $y(x)$ can also be evaluated at each x value using the `numpy` function `gradient` where for a 1D array of data the gradient will be the same as the derivative $\frac{dy}{dx}$. According to the `numpy.gradient` reference page , this function "calculates the gradient using second order accurate central differences in the interior points and either first or second order accurate one-sides (forward or backwards) differences at the boundaries. " It also has the advantage of not requiring equally spaced data values. See the reference page for further examples and details.

Here is a simple example of how to use `gradient` to numerically calculate $\frac{df}{dx}$ from smoothed $f(x_i)$ data without knowledge of the function $f(x)$, assuming that the data is equally spaced with a sample distance dx of 0.1:

```
import numpy as np

data_derivative_array = np.gradient(smoothed_data_array, 0.1)
```

Gradient can also used with unequally spaced values, if those values are provided. Here is one example:

```
import numpy as np

x = np.array([0., 1., 1.5, 3.5, 4., 6.], dtype = float)
f = np.array([1, 2, 4, 7, 11, 16], dtype = float)

dfdx = np.gradient(f,x)
```

For a more general guide to numerical differentiation and integration (in which you also learn how to code your own routines using numpy), see Chapter 5: Integrals and Derivatives from the Python-based textbook Computational Physics by Mark Newman (Newman, 2013).

6 Interpolation and Peak Finding

6.1 interp1d

Perhaps the most commonly used interpolating function in python is `scipy.interpolate.interp1d`. The default option is linear interpolation but for sparsely separated data a cubic spline is often preferable. See the interp1d manual page for additional options and details.

Here is an example of how to use interp1d to construct a cubic spline interpolation of sparse data.

First, import the necessary python packages and data:

```
#setup Jupyter notebook
%matplotlib inline
```

```
#import packages and functions
import matplotlib as mpl
import matplotlib.pyplot as plt
import numpy as np
from scipy.interpolate import interp1d  # this is the 1d iterpolation function

#specify data file location
file_name = 'Calibration_650nm_result.csv'
file_folder = '/Users/nfortune/data/'

#import data from CSV text file
angle, V_pd, data_uncertainty  = np.loadtxt(
    file_folder + file_name,
    delimiter = ',', skiprows = 1,
    usecols = (0, 1, 2), unpack = True)
```

Second, construct an interpolating function from the data, then use it to generate new (interpolated) values

```
#construct an interpolating function from the data
interpolating_function = interp1d(angle, V_pd, kind = 'cubic') # create interpolation function

#create array of new angle values for interpolation
new_angle_values = np.linspace(0, 360, 180)   # in degrees

#evaluate at new angle values
interpolated_data = interpolating_function(new_angle_values)
```

Third, graph the results:

```
plt.figure(figsize = (11,8))                  #specify figure size as 7 x 5 inches
                                             #for default size, type plt.figure()

plt.errorbar(angle, V_pd, xerr=None, yerr=data_uncertainty,
    linestyle = 'none', color = 'blue',  capsize = 3, capthick = 2,
    label = "original data points")

plt.errorbar(new_angle_values, interpolated_data, xerr = None, yerr = None,
    color = 'black',
    label = 'cubic spline interpolation')

plt.xlabel(r"$\theta$ [degrees]", fontsize = 18) #label axis (using LaTeX commands)
plt.ylabel(r"$V_{pd}$ [mV]", fontsize = 18)   #use 18 point font for label text
plt.xlim(-15, 375)
plt.ylim(-2.5, 40)
plt.xticks([0,   30, 60, 90, 120, 150, 180, 210, 240, 270, 300, 330, 360],
           ('0', '', '', 90,  '',  '', 180,  '',  '', 270,  '',  '', 360))
plt.legend(loc = 'best')

plt.show()
```

The results are shown in Fig. 7.

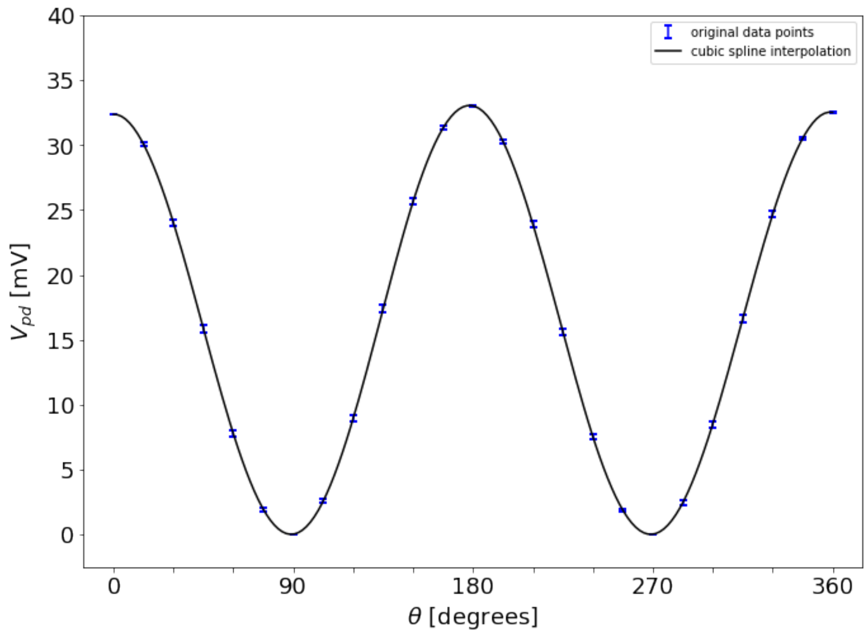


Figure 7: cubic spline interpolation of 650 nm calibration data using scipy.interpolate.interp1d

6.2 InterpolatedUnivariateSpline

Not surprisingly, the function `interp1d` is just one of many spline functions and classes, one-dimensional (univariate) and multidimensional (multivariate) interpolation classes, and Lagrange, Taylor, and Pade polynomial interpolators. For a comprehensive list, see the scipy.interpolate reference manual.

Two of these might be of particular interest to you in the analysis of 1D data:

1. UnivariateSpline, which constructs a 1D smoothing spline of degree k to the provided x,y data
2. InterpolatedUnivariateSpline, which constructs a 1D spline that passes through all data points

Their advantages include

- the ability to construct a new spline representing the derivative of the original spline
- the ability to construct a new spline representing an integral of the original spline
- and for 3rd order splines, the ability to find the roots (zero crossings) of the spline

Note: these 'object-oriented' interpolating functions are technically what Python calls classes rather than functions. For us that just means there are a few differences in syntax and usage we will need to pay attention to, but in exchange, we get a much more powerful interpolation routine.

Here we show how to use `InterpolatedUnivariateSpline` to interpolate the same data as before using a 4th order spline, find a (3rd order) derivative, find the roots of that derivative, and then use that information to identify the extrema for the original interpolating spline. For corresponding examples using `UnivariateSpline`, see the reference manual page.

Let us assume we have imported the data as before and are now ready to interpolate the data. Interpolation is again a two-step process: construct an interpolating function, then apply it to generate new data values.

```
from scipy.interpolate import InterpolatedUnivariateSpline

#construct interpolating function
InterpolatingUnivariateSpline_function = InterpolatedUnivariateSpline( angle, V_pd, k = 4) # 4th order

#create array of new angle values for interpolation
new_angle_values = np.linspace(0, 360, 180)   # in degrees

# generate new data values
IUS_interpolated_data = InterpolatingUnivariateSpline_function(angle_fit)
```

When graphed, the new interpolated spline fit is indistinguishable from the previous one using interp1d:

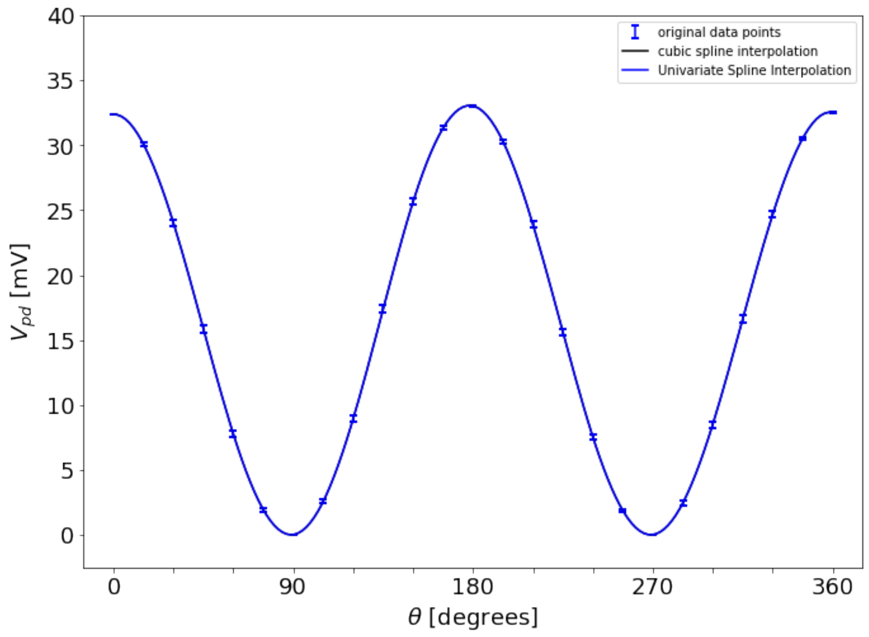


Figure 8: Comparison of two spline interpolations with data. The two methods give nearly equivalent results (so the interp1d cubic spline interpolation is black is largely overwritten by the InterpolatingUnivariateSpline 4th order interpolation in blue).

As will be shown below, the true value of the InterpolatingUnivariateSpline method is in the ability to find derivatives and roots. Here we first construct a generating function for the 1st derivative of the original univariate spline, then use that to evaluate the derivative at the same points as before:

```
spline_derivative_function = InterpolatingUnivariateSpline_function.derivative()

data_derivative = spline_derivative_function(angle_fit)
```

Next, we find the roots of the derivative and the corresponding extrema of the original interpolating spline:

```
zero_crossings = InterpolatingUnivariateSpline_function.derivative().roots()
extrema_values = InterpolatingUnivariateSpline_function(zero_crossings)

zero_values = np.zeros(len(zero_crossings))  # generate an array of zeros
```

The results are shown in Fig 9 for the derivative

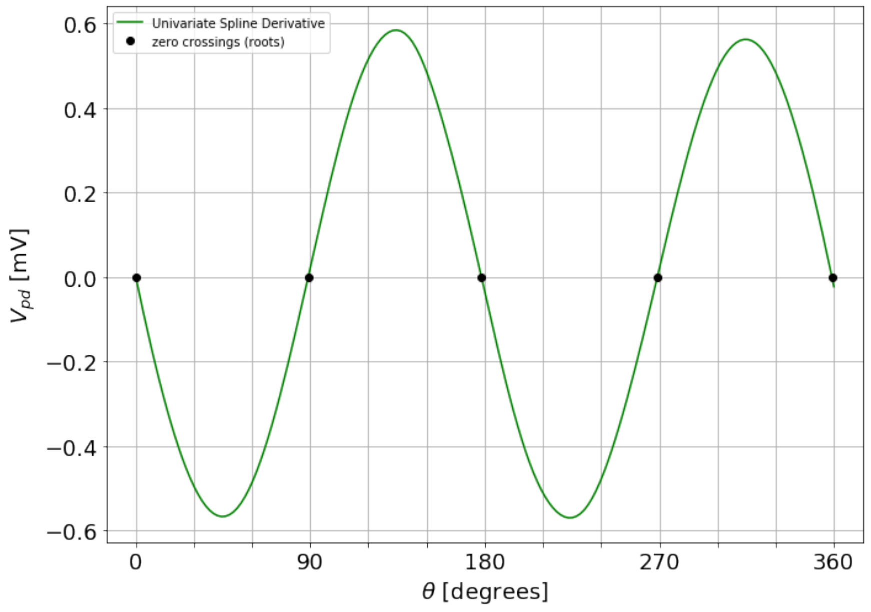


Figure 9: Derivative of the interpolating spline function

and in FIg. 10 for the original interpolating spline:

6.3 peak finding

This can be a handy way to peaks and valleys in your data but depending on the noise level it may identify a sequence of points rather than a single value. You may be able to address this by smoothing the data before interpolation, but for more advanced peak finding routines (including determination of peak widths and relative degree of prominence), see the links to the **peak finding routines** on the `scipy.signal` reference manual page. Examples can be found at the bottom of the reference pages for each function.

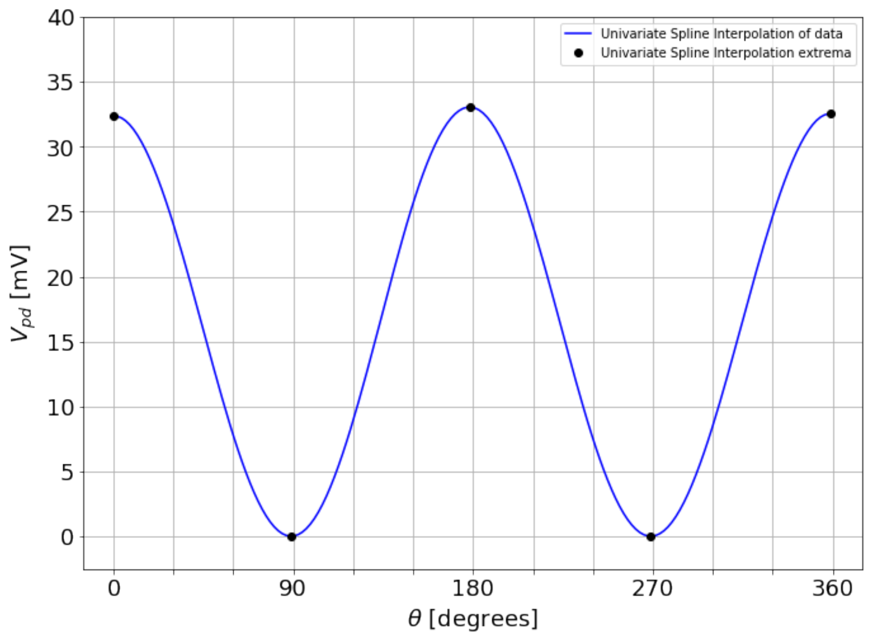


Figure 10: Locations of extrema (peaks and valleys) for the interpolated data

7

8 Working with units and uncertainties

When using Python in place of a calculator, we have the ability to directly include information about dimensions, units and uncertainties in the calculations. When used, these abilities offer the advantage of allowing us to check algebraic calculations, automatically propagate uncertainties in calculated quantities, and avoid unit conversion errors, but the necessary Python modules are not included in the standard Anaconda Navigator Python installation and must be added by hand if needed.

Note for Smith students: these additional modules are already installed on the classroom computers for PHY 350 and the Smith Physics Jupyter webserver at `https://jove.smith.edu`. (The https is necessary).

8.1 Calculations with units

In the PHY350 Experimental Physics course here at Smith College, we make extensive use of the Python module Pint by Hernan Greco. A tutorial for Pint is available here.

Here is an example of using Pint for calculator-like calculations with units:

```
import numpy as np
import pint

unit = pint.UnitRegistry()  # for clarity, we use 'unit' instead of the default 'ureg'
Q_ = unit.Quantity
```

```
g  = 9.8  * unit.newton / unit.kg # define quantities with units
m = Q_(1.0, 'kg')  # an alternative method

force = m * g  #define calculated quantity

print(force)
9.8 newton  # sample output
```

Pint also includes support for numpy arrays, as shown in this example:

```
>>> mass_magnitudes = np.array([0.1, 0.2, 0.5, 1.0, 2.0, 5.0, 10.0])
>>> masses = mass_magnitudes * unit.kg
>>> print('{:~P}'.format(masses))
[  0.1   0.2   0.5   1.    2.    5.   10. ] kg

>>> masses.magnitude
array([  0.1,   0.2,   0.5,   1. ,   2. ,   5. ,  10. ])

>>> print('{:~P}'.format(masses * g))
[  0.98   1.96   4.9    9.8   19.6   49.    98.   ] N
```

You can view the complete notebook by clicking on the </> Code button to the left of Fig. below, then clicking on the file named PintTest.ipynb . Doing so will open up the notebook in Jupyter webserver hosted by Authorea.

Note: in some cases, Python notebooks such as these can be run and modified within the Authorea Jupyter notebook webserver. In this case, however, you must first download the code to your own computer, as Pint is not yet included in the Authorea's python installation. Note about print formatting commands: the ˜ command instructs Pint to output units in abbreviated form. The P command adds subscript and superscript formatting. See the Pint tutorial.

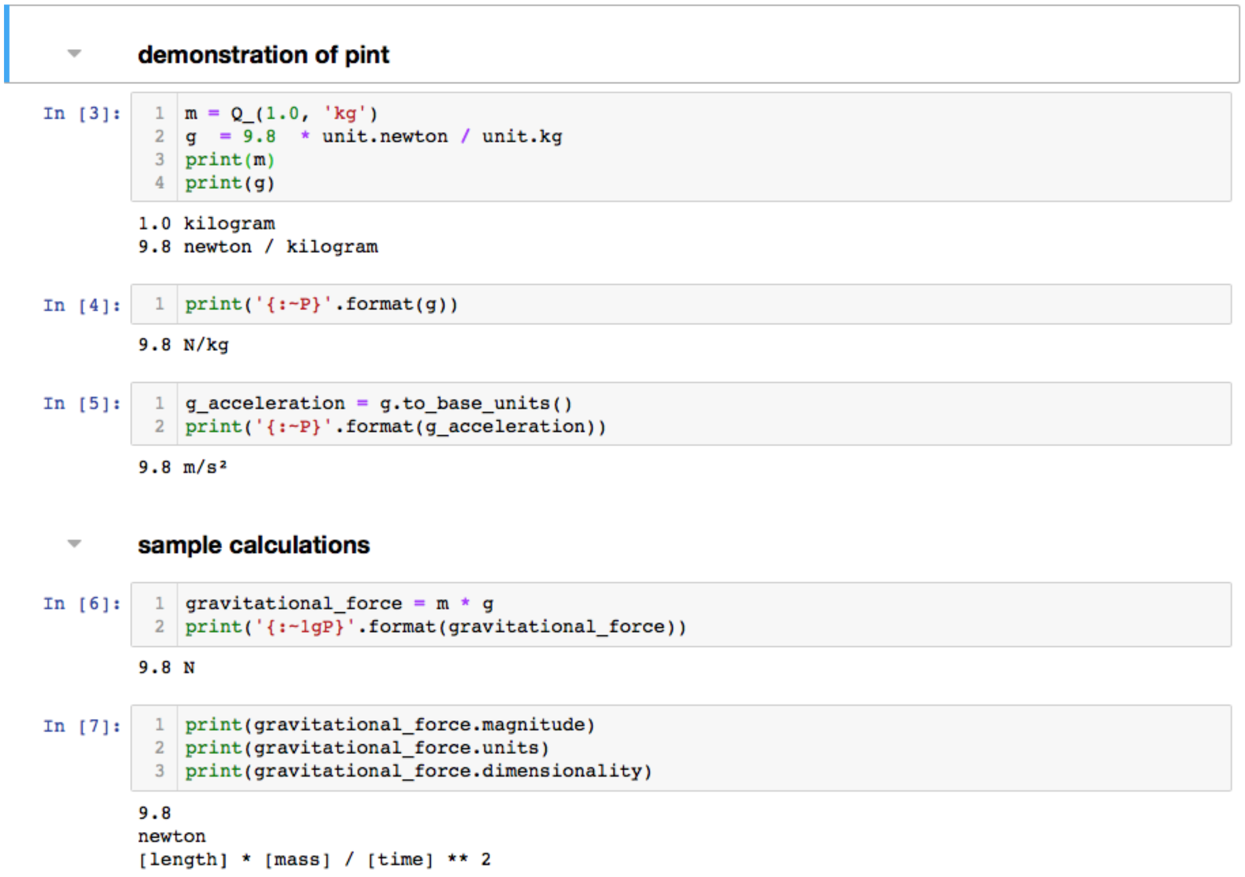
8.2 Calculations with uncertainties

For simple first-order ('linear') error propagation involving quantities with units, you can use Pint's handy plus_minus() operator. It allows absolute and relative uncertainties:

```
import numpy as np
from pint import UnitRegistry
unit = UnitRegistry()
width = (10. * unit.centimeter).plus_minus(.1, relative=True) # 10 percent uncertainty
length = (20. * unit.centimeter).plus_minus(2.) # 2 cm uncertainty
area = length * width

print(width)
print(length)
print('{:~P}'.format(area))

(10.0 +/- 1.0) centimeter
(20.0 +/- 2.0) centimeter
(200 \selectlanguage{ngerman}± 28) cm²
```


demonstration of pint

```
In [3]:
m = Q_(1.0, 'kg')
g  = 9.8  * unit.newton / unit.kg
print(m)
print(g)
```

```
1.0 kilogram
9.8 newton / kilogram
```

```
In [4]:
print('{:~P}'.format(g))
```

```
9.8 N/kg
```

```
In [5]:
g_acceleration = g.to_base_units()
print('{:~P}'.format(g_acceleration))
```

```
9.8 m/s²
```

sample calculations

```
In [6]:
gravitational_force = m * g
print('{:~1gP}'.format(gravitational_force))
```

```
9.8 N
```

```
In [7]:
print(gravitational_force.magnitude)
print(gravitational_force.units)
print(gravitational_force.dimensionality)
```

```
9.8
newton
[length] * [mass] / [time] ** 2
```

Figure 11: an extract of the Jupyter notebook PintTest.ipynb demonstrating the use of Pint to do calculations in Python using units.

For details, see the Pint measurements tutorial.

For general propagation of uncertainty tasks , we use Uncertainties: a Python package written by Eric. O. Lebigot, the same package Pint uses "under the hood" for calculations invoking `.plus_minus()`. The uncertainties module returns its result with the uncertainty specified by linear error propagation theory, taking into account any direct correlations between variables. Quoting from the uncertainties website,

> The standard deviations and nominal values calculated by this package are thus meaningful approximations as long as **uncertainties are "small"**. A more precise version of this constraint is that the final calculated functions must have **precise linear expansions in the region where the probability distribution of their variables is the largest**. Mathematically, this means that the linear terms of the final calculated functions around the nominal values of their variables should be much larger than the remaining higher-order terms over the region of significant probability (because such higher-order contributions are neglected).
>
> For example, calculating `x*10` with `x` = 5±3 gives a *perfect result* since the calculated function is linear... Another example is `sin(0+/-0.01)`, for which `uncertainties` yields a meaningful standard deviation since the sine is quite linear over 0±0.01. However, `cos(0+/-0.01)`, yields an approximate standard deviation of 0 because it is parabolic around 0 instead of linear; this

might not be precise enough for all applications.

Here we provide a demonstration of how to use Uncertainties to calculate the uncertainty values (error bars) for the data shown in Fig. 1).

First, *import the data and assign values, including specification of uncertainties* to the input parameters V_0, V_1, θ_0 and the data array θ.

```
%matplotlib inline

#import packages
from matplotlib import pyplot as plt
from numpy import *
from uncertainties import ufloat, unumpy  # these are extensions of numpy floating point numbers and ar

#import x, y data
filename = 'Calibration_650nm.csv'
angle_data, V_pd_data = loadtxt(filename, delimiter = ',', skiprows = 1, usecols = (1, 2), unpack = Tru

#specify directly measured values, including uncertainties:  V_0 ± delta_V_0, V_1 ± delta_V_1, etc
V_0 = ufloat(32.631, 0.024) # first element is the nominal value, the second is the standard dev, both 
V_1 = ufloat(0.023, 0.016) # first element is the nominal value, the second is the standard dev, both i
theta_0 = ufloat(-1.16, 0.11) * pi / 180  # convert from degrees to radians

#convert to radians for use in trigonometric functions
theta_data = angle_data * pi / 180
delta_theta = 0.5 * pi / 180

# create an array of angle values with uncertainty
theta_array = unumpy.uarray(theta_data, delta_theta)
```

Next, use uncertainties to *automatically propagate uncertainty.* The uncertainties package automatically calculates derivatives as needed (see, for example, Eq. 3), following the standard rules for propagation of error:

```
#to calculate values while also automatically taking into account uncertainties, use unumpy instead of 
V_pd_theory = (1/2)*V_0 * (1 + unumpy.cos(2*(theta_array - theta_0 ))) + V_1 #notice use of unumpy.cos

values = unumpy.nominal_values(V_pd_array)  #creates an array with best estimates of V_pd
uncertainties = unumpy.std_devs(V_pd_array) #creates an array with uncertainties for V_pd
```

Here are the first three calculated values of V_{pd} corresponding to $\theta = 0,\ 15,\ 30$ degrees that result (including the calculated uncertainty) :

```
print(angle_data[0:3])
[ 0. 15. 30.]

print(V_pd_theory[0:3])
[32.64055493822073+/-0.03115762246979197
 30.125380043639208+/-0.1578587386098956
 23.916021775219797+/-0.25858767540002414]
```

and a corresponding graph comparing the data (in blue) with the calculated values (in red), including calculated uncertainties (shown as error bars):

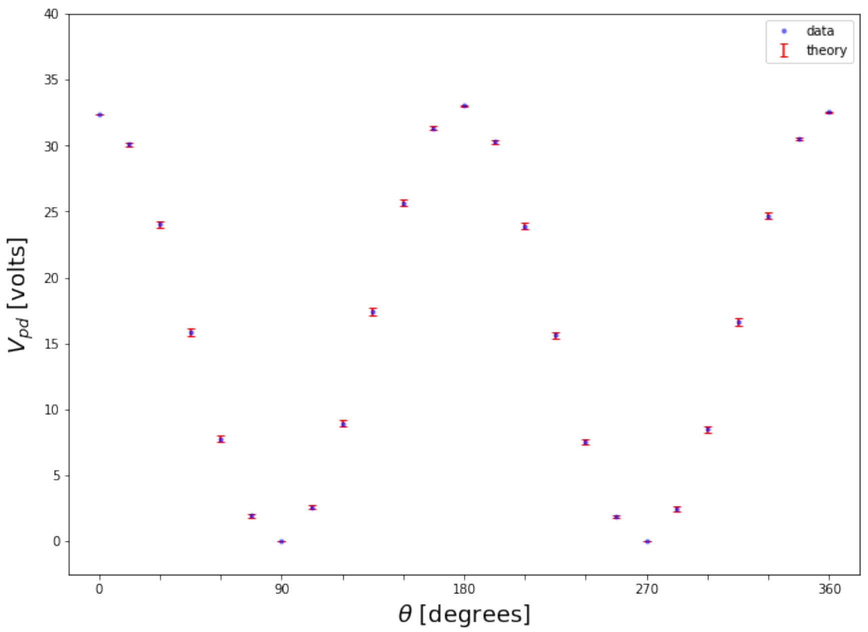


Figure 12: Comparison of data (in blue) with calculated values for $V_{pd}(\theta)$ from Eq. 2. Error bars for calculated values were determined automatically from the uncertainties in the input parameters (using the uncertainties package and Eq. 2 instead of Eq. 4).

Notice that our original approach in section 4.1 of explicitly calculating the uncertainty in V_{pd} from Eq. 4 and this new approach of using the `uncertainties` package give equivalent results, but that in both cases we needed a good estimate of $V_0 \pm \delta V_0$ to determine $V_{pd} \pm \delta V_{pd}$ at each value of θ.

In general, either of these two approaches will be sufficient for most of our work with data, but notice that because both involve linear expansions of functions about their nominal values, both yield an unrealistically low uncertainty of zero for small variations in V_0 and ϕ (neglecting δV_1 for now) at $\phi = \theta - \theta_0 = 0$. This is because an Taylor expansion of $\cos(\phi)$ around $\phi = 0$ yields $\cos(0 \pm \delta\phi) = 0 + 0 \cdot \delta\phi + \frac{1}{2} \cdot (\delta\phi)^2 + \ldots = 0$ in the linear approximation limit (which treats terms of order $(\delta\phi)^2$ and higher as being negligibly small).

If you need still more advanced approaches topropagation of uncertainty, the author of uncertainties recommends looking at soerp and mcerp. According to the uncertainties website, ”the soerp package performs *second-order* error propagation: this is still quite fast, but the standard deviation of higher-order functions like f(x) = x^3 for x = 0±0.1 is calculated as being exactly zero (as with `uncertainties`). The mcerp package performs Monte-Carlo calculations, and can in principle yield very precise results, but calculations are much slower than with approximation schemes.”

9 Installing Python

This section is only relevant if you are planning on running Python on your own computer. If you are running Python within a Jupyter notebook on a webserver or a computer account which has already been configured for your use (such as `https://jove.smith.edu` for Smith College physics) , this section can be skipped.

9.1 Python distributions

Our focus in this article is on the use of Python to expedite the analysis of your experimental data and not, for example, the specifics of various Python distributions and their relative merits for computational physics in terms of speed, accuracy, and memory requirements.

We therefore recommend that if you need to install a Python distribution for scientific data analysis in physics on your own computer, you choose an installer that will automatically install Python, interactive Python (iPython) and Jupyter notebooks, scientific python development environments (editing, testing, debugging) such as Spyder or Canopy, and essential Scientific Python packages (such as numpy, matplotlib and scipy) in a single step, rather than building this from scratch. This provides ease of installation, ease of use, and a comprehensive curated set of preinstalled and easily added packages.

Two of the most popular distributions and installers are from Anaconda and Enthought. Both are freely available for Mac OS, Linux, and Windows . Either should do what you need. That said, the examples presented below for installation of additional Python packages assume the use of Anaconda Navigator.

Also, if you are using this for a Smith Physics course, we ask you to use Anaconda Navigator if you wish us to be able to provide support with installation and programming (since that is what we are using).

9.1.1 Installing Anaconda Navigator

Download the latest version of Anaconda Navigator here. Be sure to chose the Python 3.x version of Python (and not the older version 2.7), as all of the examples provided here assume the use of Python 3. After installation, restart and launch the Anaconda Navigator app. You should then be able to launch a Jupyter notebook from either the graphical interface or environments tab (see Figure 13) to be officially off and running.

OK, you also need to install some supplementary packages if you want to be able to do calculations that include units and/or uncertainties. But it isn't difficult within Anaconda to do that. See section 9.3 below.

9.1.2 Building your own distribution

Still prefer to build your own clean, lean, and mean Python installation and willing to blaze (and maintain) your own trail ? Here's a guide to getting started that results in an exceptionally lean installation suitable for use in computational physics. If you want to run the example code provided here on your own computer, however, you will also want to install the iPython, Jupyter, and Scipy packages (at a minimum). Other packages may be needed as well; one tried and true but tedious way to do this is to attempt to run the code and then let the computer tell you what you are missing!

Finally, if you are an experienced and independent-minded Python programmer (and would you have read the previous paragraph if you weren't?), you may ask, "Why Jupyter?" Why not use the Python or iPython command line directly, use a bare-bones editor such as IDLE , or a more comprehensive MATLAB like programming environment like Spyder? If you are in one of our Smith Physics courses, the answer is because we use Jupyter notebooks not only to run Python code but also to generate a partially "self-documenting" electronic lab notebook as we do so. If you are doing a lot of programming requiring extensive re-writing and debugging, you may prefer to first work in development environment like Spyder, then run the finished product within Jupyter to generate a notebook version of the data analysis, but in experimental physics, you still need to keep an comprehensive electronic notebook of your instrument setup, measurement, and data analysis steps! Finally, note that the command line is convenient for quick calculations and tests of code but is inadequate for serious editing and debugging, and does not provide a reproducible record of your results. As a calculator it is great but as a notebook it is not! There's really no good reason as an experimental physicist with a computer at your disposal not to use an electronic notebook instead of a calculator in the first place. Get with the program! :)

9.2 Using the Anaconda installer

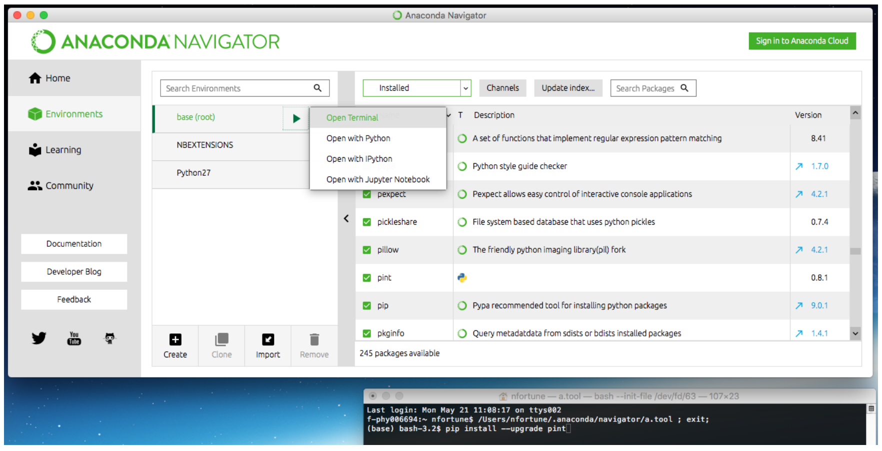
Packages included in the Anaconda Python distribution can be installed and updated using the Anaconda Navigator installer. This has an easy to use graphical interface. As a bonus, any needed auxiliary files will updated at the same time . Potential conflicts between packages will also be identified ahead of time. See the section of the Getting Starting guide provided by Anaconda titled Managing Packages for step by step instructions.

9.3 Using command line installers

Packages not included in the standard Anaconda Navigator installer can still be installed using Anaconda Navigator. To do so,

1. **open a terminal window** from with Anaconda Navigator (see figure 13 below)
2. **issue the installation command**. See below for examples using **conda** (section 9.3.1) and **pip** (section 9.3.2)

Be sure to closely follow the installation instructions provided with the documentation for the package. In most cases it is straightforward but sometimes extensions are also needed. If the package can be installed using either **conda** or **pip**, choose **conda** (as **conda** will also install needed extensions).



	T	Description	Version
		A set of functions that implement regular expression pattern matching	8.41
		Python style guide checker	1.7.0
pexpect		Pexpect allows easy control of interactive console applications	4.2.1
pickleshare		File system based database that uses python pickles	0.7.4
pillow		The friendly python imaging library(pil) fork	4.2.1
pint			0.8.1
pip		Pypa recommended tool for installing python packages	9.0.1
pkginfo		Query metadatdata from sdists or bdists installed packages	1.4.1

245 packages available

nfortune — a.tool — bash --init-file /dev/fd/63 — 107×23

```
Last login: Mon May 21 11:08:17 on ttys002
f-phy006694:~ nfortune$ /Users/nfortune/.anaconda/navigator/a.tool ; exit;
(base) bash-3.2$ pip install --upgrade pint
```

Figure 13: How to open a terminal window within Anaconda Navigator.

9.3.1 conda install

Here is an example of how to use the **conda** command while in the terminal window to install Pint, a Python package written by Hernan E. Grecco to define, operate and manipulate physical quantities: the product of a numerical value and a unit of measurement.

```
conda install -c conda-forge pint
```

9.3.2 pip install

Here is an example of how to use the **pip** command while in the terminal window to install uncertainties, a Python package written by Eric. O. Lebigot that **transparently** handles calculations with **numbers with uncertainties** (like 3.14±0.01).

```
pip install --upgrade uncertainties
```

Upgrades can be done in a similar way. To upgrade Pint, for example, type the following while in a terminal window:

```
pip install -U pint
```

Note that you shouldn't be running any notebooks within Anaconda when you do this! Best practice is to restart Anaconda Navigator first, then install upgrades, then open a Jupyter notebook to launch Python.

References

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