

Introduction to Computational Physics (PHYS105)

Lecture 7: Good Practice and Debugging

Carl Gwilliam

(C.Gwilliam@liverpool.ac.uk)



UNIVERSITY OF
LIVERPOOL

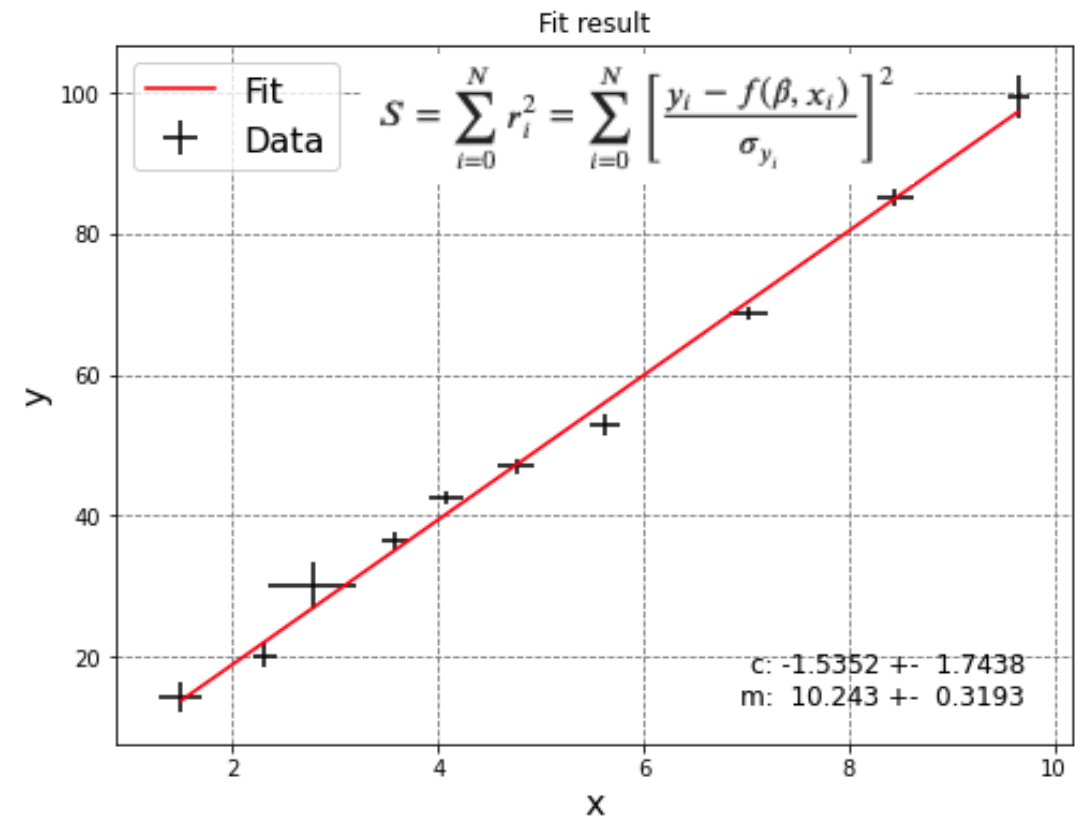
Lecture 6: Recap

- Last week we started the second part of the course, using python for real physics problems!

- Started with fitting a functional form to data.

- Read in data from files (using `np.loadtxt`)
 - Plot to check sensible
 - Find initial params
- Define necessary functions
 - Functional form and its differential
 - Point-by-point residuals
- Run `least_squares()` from `scipy.optimize`
 - Check fit succeeds and get fitted params
- Calculate χ^2 test statistic from the residuals
 - Check fit is good e.g. $0.25 < \chi^2/\text{NDF} < 4$
- Calculate parameter errors
 - Print best-fit parameters and associated error
- Plot data and fitted function
 - Passing best fit params to functional form

- Encapsulated all this in a reusable function



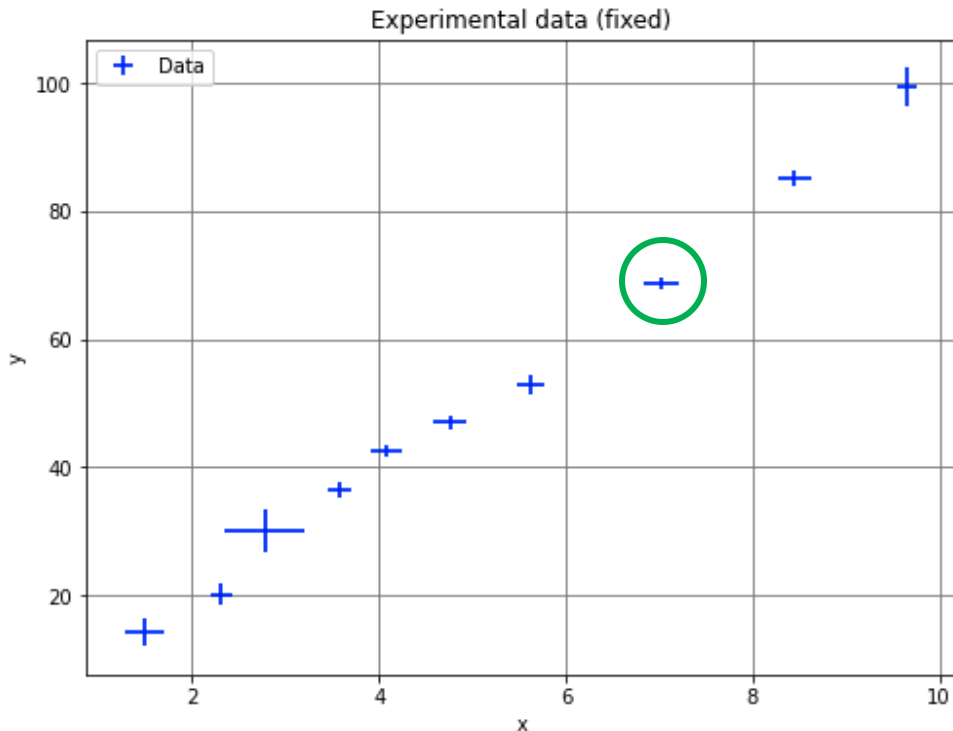
- You will use this over-and-over in labs
 - Will create your own python module for this in the last week of PHYS105

Lecture 6: Formative problem solutions

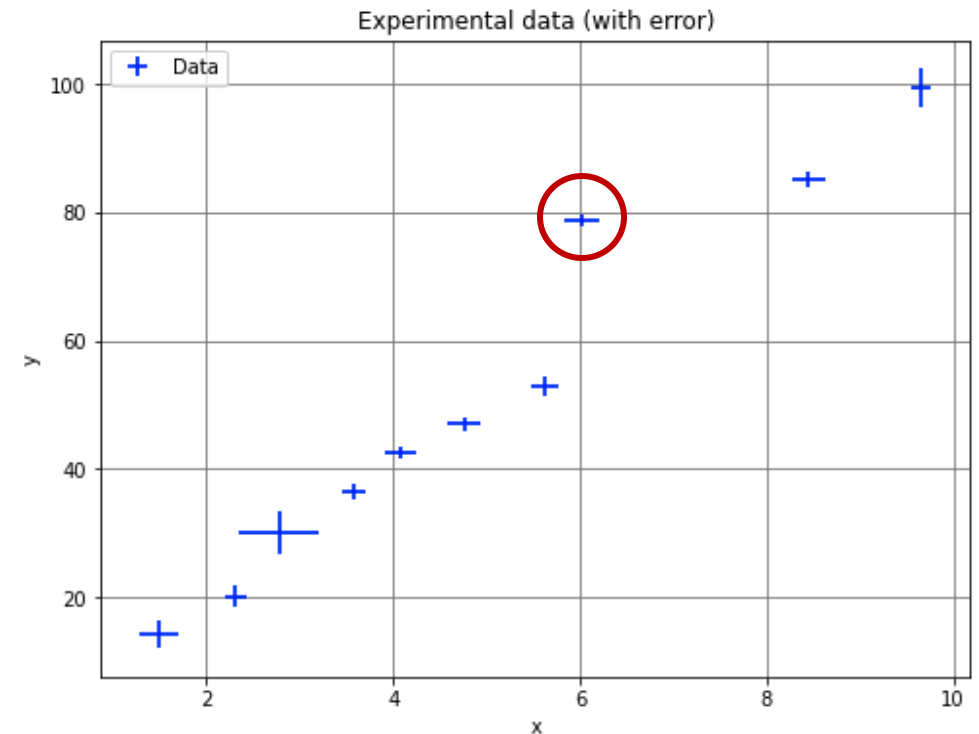
- Exercise 1: Plot the experimental data and fix any errors compared to the table above
 - Plot data read from csv file using `errorbar()`
 - Clear that 8th point is incorrect → fix by updating array value at **index 7** and replot

```
import matplotlib.pyplot as plt
%matplotlib inline

plt.figure(figsize = (8, 6))
plt.title("Experimental data (with error)")
plt.xlabel("x")
plt.ylabel("y")
plt.errorbar(xdata, ydata, xerr=xerror, yerr=yerror,
             color = 'b', linestyle = '', label = 'Data')
plt.grid(color = 'grey')
plt.legend(loc = 2)
plt.show()
```



xdata[7] = 7.02
ydata[7] = 68.8



Lecture 6: Formative problem solutions (2)

- Exercise 2: Fit extended data

```
# Extend data
import numpy as np
xdata2 = np.append(xdata, [10.25, 11.85])
ydata2 = np.append(ydata, [110.5, 122.1])
xerror2 = np.append(xerror, [0.21, 0.41])
yerror2 = np.append(yerror, [3.1, 3.3])
```

Read data

```
import numpy as np
from scipy.optimize import least_squares
from scipy.stats import chi2 as stats_chi2
import matplotlib.pyplot as plt
%matplotlib inline

# Set initial params
init_params = [0.0, 10.0]

# Run fit
result = least_squares(minimise, init_params,
                      args=(xdata2, ydata2, xerror2, yerror2))

# Check fit succeeds
if not result.success or result.status < 1:
    print ("ERROR: Fit failed with message {}".format(result.message))
    print ("Please check the data and initial parameter estimates")
else:
    print ("Fit succeeded")

# Get fitted parameters
final_params = result.x
c = final_params[0]
m = final_params[1]
nparams = len(final_params)
```

Run fit and
check it
succeeds

New data

Get fitted
parameters

```
# Calculate chi2
chi2_array = result.fun ** 2
chi2 = sum(chi2_array)
npoints = len(xdata)
reduced_chi2 = chi2 / (npoints - nparams)
chi2_prob = stats_chi2.sf(chi2, (npoints - nparams))

# Print chi2
np.set_printoptions(precision = 3)
print("\n=== Fit quality ===")
print("chisq per point = \n", chi2_array)
print("chisq = {:7.5g}, ndf = {}, chisq/NDF = {:7.5g}, chisq prob = {:7.5g}\n".
      format(chi2, npoints-nparams, reduced_chi2, chi2_prob))

if reduced_chi2 < 0.25 or reduced_chi2 > 4:
    print("WARNING: chi2/ndf suspiciously small or large."
          "Please check the data and initial parameter estimates")

if chi2_prob < 0.05:
    print("WARNING: chi2 probability for given degrees of freedom less than 0.05."
          "Please check the data and initial parameter estimates")
```

Calculate χ^2
and check
fit is good

```
# Calculate errors
jacobian = result.jac
jacobian2 = np.dot(jacobian.T, jacobian)
determinant = np.linalg.det(jacobian2)

if determinant < 1E-32:
    print(f"Matrix singular (determinant = {determinant}, error calculation failed.")
    param_errors = np.zeros(nparams)
else:
    covariance = np.linalg.inv(jacobian2)
    param_errors = np.sqrt(covariance.diagonal())

print ("c = {:7.5g} +- {:7.5g}".format(final_params[0], param_errors[0]))
print ("m = {:7.5g} +- {:7.5g}".format(final_params[1], param_errors[1]))
```

Calculate param
errors and print

Lecture 6: Formative problem solutions (3)

- Exercise 2 (cont): Fit extended data

```
# Calculate fitted function values
yfit = straight_line(final_params, xdata2)

# Visualise result
fig = plt.figure(figsize = (8, 6))
plt.title('Fit result')
plt.xlabel('x', fontsize=16)
plt.ylabel('y', fontsize=16)
plt.grid(color = 'grey', linestyle="--")

plt.errorbar(xdata2, ydata2, xerr = xerror2, yerr = yerror2, fmt='k',
             linestyle = '', label = "Data")
plt.plot(xdata2, yfit, color = 'r', linestyle = '-', label = "Fit")

plt.legend(loc = 2, fontsize=16)

text = "c: {:.7.5g} +- {:.7.5g}\n".format(final_params[0], param_errors[0])
text += "m: {:.7.5g} +- {:.7.5g}\n".format(final_params[1], param_errors[1])
plt.text(0.95, 0.0, text, transform = fig.axes[0].transAxes, ha = "right",
        va = "bottom", fontsize=12)

plt.show()
```

Evaluate best fit y and plot

New data!

Fit succeeded

=== Fit quality ===

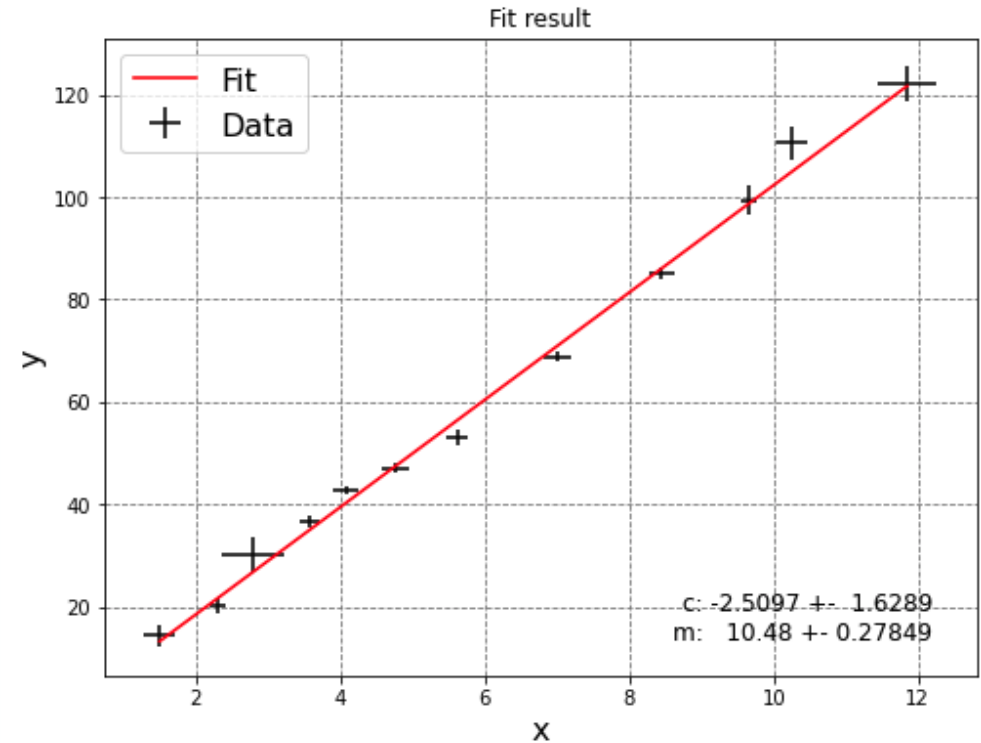
chisq per point =

[0.128 0.533 0.387 0.724 1.507 0.016 2.579 1.072 0.156 0.062 2.159 0.006]

chisq = 9.329, ndf = 10, chisq/NDF = 0.9329, chisq prob = 0.50119

c = -2.5097 +- 1.6289

m = 10.48 +- 0.27849



Lecture 6: Formative problem solutions (4)

- Exercise 3: Does straight line still fit the data
 - Yes, as shown by χ^2 :
 - χ^2/ndf between $\frac{1}{4}$ and 4 `chisq/NDF = 1.1661`
 - χ^2 prob greater than 5% `chisq prob = 0.3153`
- Have the gradient or intercept changed significantly?
 - No, values are still compatible within errors
 - Quantify by "Consistency Check" (as in labs)

$$\text{Significance} = \frac{|x_1 - x_2|}{\underbrace{\sqrt{\sigma_{x_1}^2 + \sigma_{x_2}^2}}_{\text{Total error}}} < 3$$

```
from math import sqrt

def sigma(x1, x2, e1, e2):
    "Calculate number of standard deviations"
    return abs(x1-x2)/sqrt(e1**2 + e2**2)

final_params_10pts = [-1.535, 10.243]
param_errors_10pts = [1.744, 0.319]

csig = sigma(final_params[0], final_params_10pts[0],
             param_errors[0], param_errors_10pts[0])
msig = sigma(final_params[1], final_params_10pts[1],
             param_errors[1], param_errors_10pts[1])

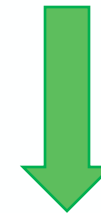
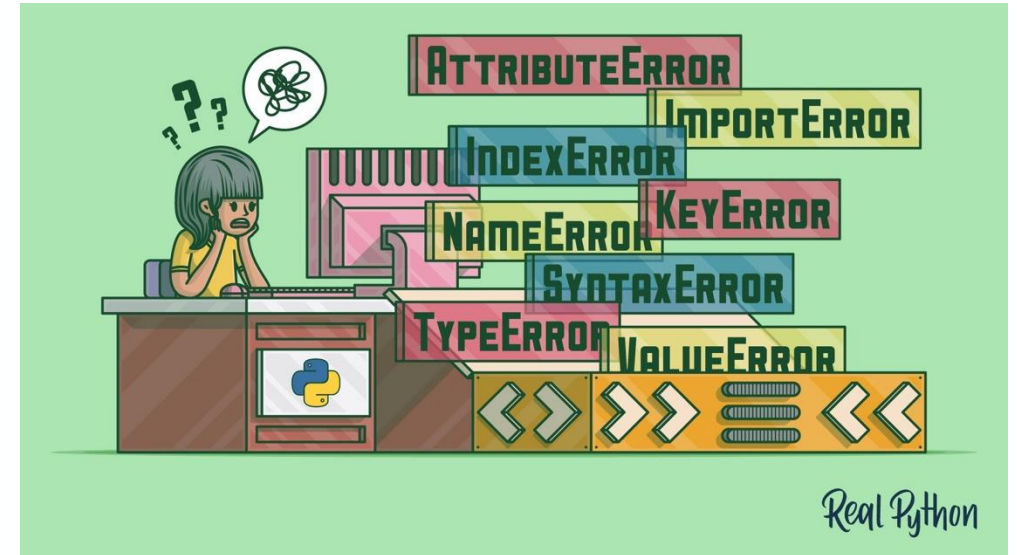
print (f"Significance for c = {csig:.2f} and m = {msig:.2f}")
if csig < 3 and msig < 3:
    print("Values are consistent")
```

Significance for c = 0.41 and m = 0.56
Values are consistent

- Now that we have developed our first real physics program, it is time to take a step back ...

Python errors

- At many points during the course you will have come across issues with your code
 - Where python has given you a big fat error message or you get the wrong result
- We can try to avoid these via good coding practice
 - Using sensible variable names,
 - Writing useful comments,
 - Checking inputs/values, etc
- But no matter how good we are, as we write more complex programs we'll encounter them more often
- There are several different types of error we may encounter
 - Code that is syntactically incorrect and therefore won't parse at all
 - Programs that start but give a run-time error and don't complete
 - Programs that run but produce incorrect results
- This week, we are going to look in detail at how to understand these errors and debug them



Harder to debug

Understanding and debugging error messages

- Real example saw during week 4 PC class

```
1 def rectPrismParams(width, length, height):
2     """
3     Return volume, surface area and length of edges of
4     rectangular prism given its width,length and height
5     """
6     vol = width * length * height
7     area = 2 * (width * length + width * height + length * height)
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11 w,l,h = 0.3,0.17,0.25
12 V, A, s = rectPrismParams(w, l, h)
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14 print(f"Volume = {V:.2f}")
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- Can turn on line numbers by
View → Line Numbers → Show

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 - Python is telling us the type of the object is incorrect

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 - In this case python thinks we are trying to call an integer (like we would do a function)

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- The “traceback”, showing how the code got to the point of the error through various function calls, going from most recent at the bottom to least recent at the top.
 - The lines indicated by the ‘--->’ are the ones called; the others are for context.
 - In this case it calls `rectPrimsPamas (...)` on L12 & then gives an error in calculating the area on L7

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- So, what's the mistake in the code here?

- We are missing a multiplication sign * between the integer and the brackets!
- Python sees this as trying to call a function: 2 ()
- But you can't call an integer, hence the error

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- The best way to get familiar with this is practice → let's look at some in a notebook now ...

Summary

- This week we looked at various python errors and how to understand and debug them
- In particular, in the lecture we looked at:
 - Errors that prevent the program running at all
 - Programs that start but don't complete
- Learnt more about how to read python error messages
 - And practiced this with several different error types
- In this week's notebook you will explore errors further:
 - How to reduce the scope for errors with good coding practice
 - Debugging more of the above errors yourself
 - Finally, some programs that run but give the incorrect result!
- You will make coding mistakes (I still make many!)
 - But with practice you can find and fix them quicker!

