# PHY480: Activities 11

*Online handouts: Pendulum power spectrum graphs, listings of ode_test_class.cpp and classes, multifit_test.cpp and multimin_test.cpp.*

In this Activities, we'll take a look at nonlinear least-squares fitting with GSL.

*Your goals for today:*

- Take a quick look at some pendulum power spectra.
- Try out and extend the adaptive ode code with classes.
- Try out nonlinear minimization on a demonstration problem.
- Try out nonlinear least-squares fitting on a demonstration problem.

Please work in pairs (more or less). The instructors will bounce around and answer questions.

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## Pendulum Power Spectra [Activities 10 Follow-up]

Look at the handout with the three rows of plots showing the time dependence of a pendulum on the left and the corresponding power spectrum on the right plotted in terms of frequency = 1/period.

1. *How can you most accurately determine the single frequency in the first row from the graph on the left?*
I personally would find the weighted average of the two points given and use that. As long as it is near .15 you are on the right track.

2. Identify (and write down) two of the frequencies in the second row *from the plot on the left*. Do they agree with the plot on the right?
On the left, I see a .04 and .12 frequency. This does match up with the power spectrum.

3. *What is the characteristic of the power spectrum in the third row that is consistent with a chaotic signal?*
It is more continuous than it is discrete. Very few values are near 0.

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## Multidimensional Minimization with GSL Routines

The basic problem is to find a minimum of the scalar function f(xvec) [scalar means that the result of evaluating the function is just a number] where xvec = (x_0, x_1, ... , x_N) is an N-dimensional vector. This is a much harder problem for N > 1 than for N=1. The GSL library offers several algorithms; the best one to use depends on the problem to be solved. Therefore, it is useful to be able to switch between different choices to compare results. GSL makes this easy. Here we'll try a sample problem. For more details, see the online GSL manual under "Multidimensional Minimization" (linked on 6810 page).

The routines used here find *local* minima only, and only one at a time. They have no way of determining whether a minima is a global one or not (we'll return to this point later).

1. Look at the test code "multimin_test.cpp" and compare it to the online GSL documentation under "Multidimensional Minimization" (there is also a handout copy). Identify the steps in the minimization process. *What classes might you introduce for this code?* Definitely a minimizer class to clean up those inputs, and maybe a vector manipulation class.

2. Compile and link the program with "make_multimin_test" and run it. Your results may differ from what is in the comments of the code. *Adjust the program so that your answer is good to $10^{-6}$ accuracy. What is it that is found to that accuracy? (E.g., is it the positions of the minimum or something else?)* It is the norm of the gradient. Essentially, a value that if you are beneath, the point you are on is flat enough. (and hopefully a minimum, if you are unlucky it might be possible to "land" on a maximum or saddle point and technically converge.)

3. Modify the function minimized so it is a function of three variables (e.g., x, y, z), namely a three-dimensional paraboloid with your choice of minimum. Change the code so that the dimension of `xvec` is a parameter. (Be sure to change ALL of the relevant functions.) *Is the minimum still found?* Yes.

4. *What algorithm is used initially to do the minimization? Modify the code to try steepest_descent and then one of the other algorithms. Which is "best" for this problem?* This is the Fletcher-Reeves conjugate gradient algorithm. Steepest descent fails, but bfgs2 (Broyden-Fletcher-Goldfarb-Shanno) works extremely well. Found the minimum in 3 steps!

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## Nonlinear Least-Squares Fitting with GSL Routines

Using the nonlinear least-squares fitting routines from GSL is similar to using the GSL minimizer (and involves a special case of minimization). Your main job is to figure out from the documentation (see 6810 page) and this example from GSL (only slightly modified from what you will find in the documentation) how to use the routines. Here we briefly explore the sample problem, which also illustrates how to create a "noisy" (i.e., realistic) test case ("pseudo-data").

The model is that of a weighted exponential with a constant background:

$y = A\, e^{-\lambda t} + b$

You'll generate pseudo-data at a series of time steps $t_i$ (in practice, $t_i$ is taken to be 0, 1, 2, ...). Noise is added to each $y_i$ in the form of a random number distributed like a gaussian with a given standard deviation $\text{sigma}_i$. We'll revisit the GSL functions that generate this random distribution in the next Activities; for now just accept that it works.

1. Take a look at the multifit_test.cpp code (there is a printout), run it (compile and link with make_multifit_test) and figure out the flow of the program. *What is the fitting ("objective") function to be minimized? What role does $\text{sigma}_i$ play?* We are trying to fit data to the form A * exp(\lambda * t) + b Sigma is essentially a weight factor based on the expected error of the data, the smaller the error, the more "certain" that point is, and it gets priority over data values with higher error. Also this code does not work with latest version of GSL.
2. *What is the "Jacobian" for? (Check the online documentation for the answer!)* The jacobian creates a symbolic gradient (I mean, it is literally a gradient, but the jacobian doesn't have to rely on physical space is what I was trying to say) that we can use to decide on the direction and length our variables travel.
3. *Modify the code so that you can plot both the initial data and the fit curve using gnuplot. Look up how to add error bars for the data in gnuplot. [Hint: Try "help set style", "help errors", and "help plot errorbars" for some clues.] Did it work??.* I am out of time so I just copied the data over to a file. But I did plot it!, Just, no .dat file is generated sorry.

4. The covariance matrix of the best-fit parameters can be used to extract information about how good the fit is (see notes). *How is it used in the program to estimate the uncertainties in the fit parameters? How do*

*these uncertainties scale with the magnitude of the noise? Do they scale with the number of time-steps used in the fit?* (I.e., if you change the "amplitude" of the gaussian noise, how do the errors in the fit parameters change?) The covariance should give the uncertainties of the fit parameters, and I am pretty sure the more noisy it is, the more uncertain it is, though I couldn't get the program running (as it now needs a workspace and I tried fudging it instead of rewriting it, wasting hours, so I gave up.) (I FIXED IT! Had to dig through those header files though.) The higher sigma is, the more the covariance factors increase. More points does change it, but it does not look like it scales by a factor of any kind.

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## GSL Adaptive ODE Solver Revisited

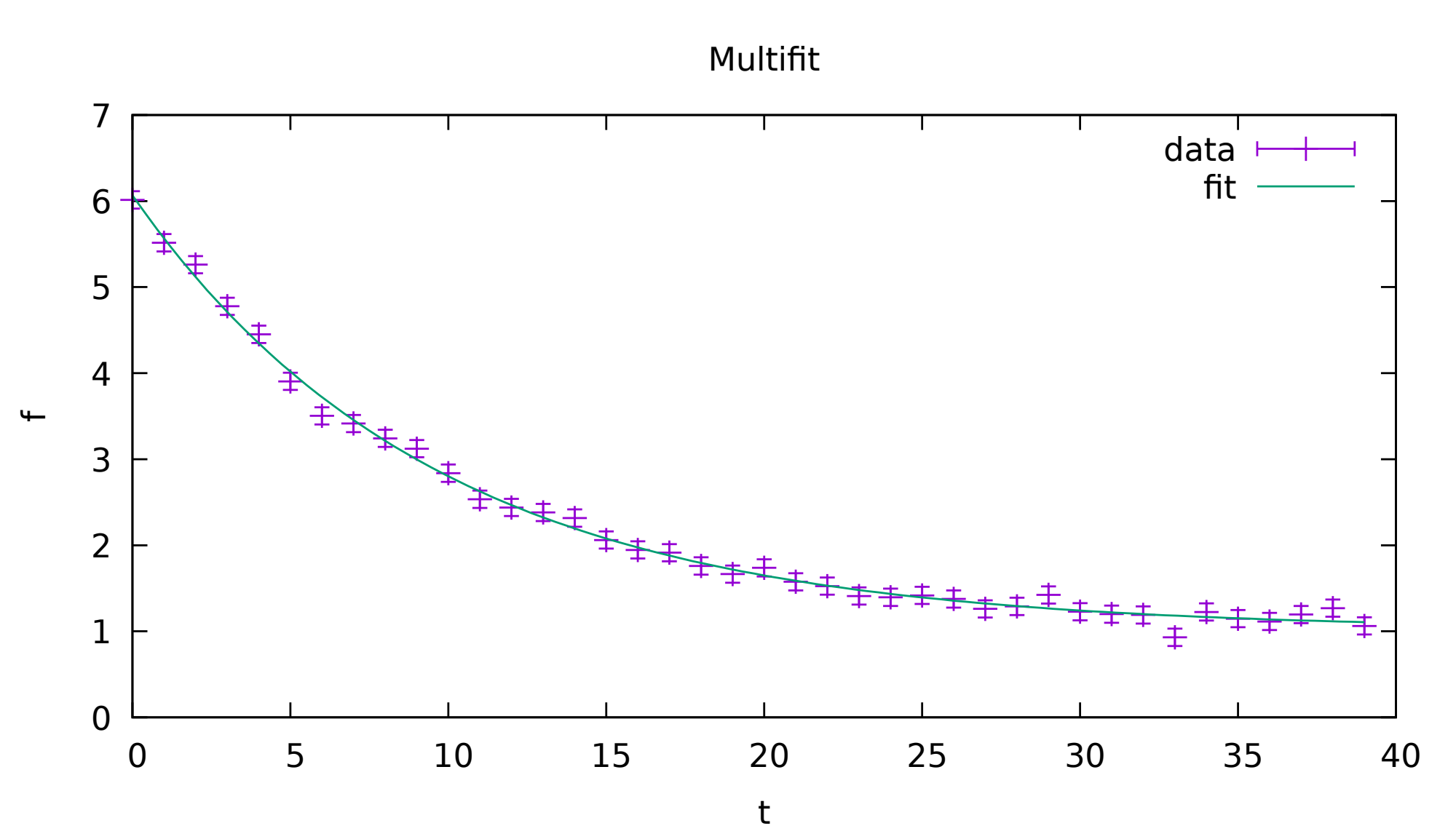
In Activities 10, we took a quick look at `ode_test.cpp`, which implemented the GSL adaptive differential equation solver on the Van der Pol oscillator. Here we look at a rewrite that uses classes.

1. The details of `ode_test_class.cpp` and the `Ode` and `Rhs` classes are described in detail in the Activities 11 notes. Look at the printout while you go through the notes. *What questions do you have?* I don't know much about virtual functions but I can figure it out.

2. Add two additional calls to `evolve_and_print` so that all three initial conditions from Activities 10, [x0=1.0, v0=0.0], [x0=0.1, v0=0.0], and [x0=-1.5, v0=2.0], are generated with the same run. *Did the three output files get generated? (You can try plotting to check correctness.)* Yeps.

3. Add another instance of the `Rhs_VdP` class called `vdp_rhs_2` with mu=3 and generate results for the same initial conditions. *Plot these. Is it still an isolated attractor?* Yep.

4. [Bonus. Come back to this if you finish everything else.] Add another class `Rhs_Pendulum` that implements the pendulum differential equation with natural frequency omega0 and a driving force with amplitude f_ext and frequency omega_ext. (You will want to modify or replace `evolve_and_print`.)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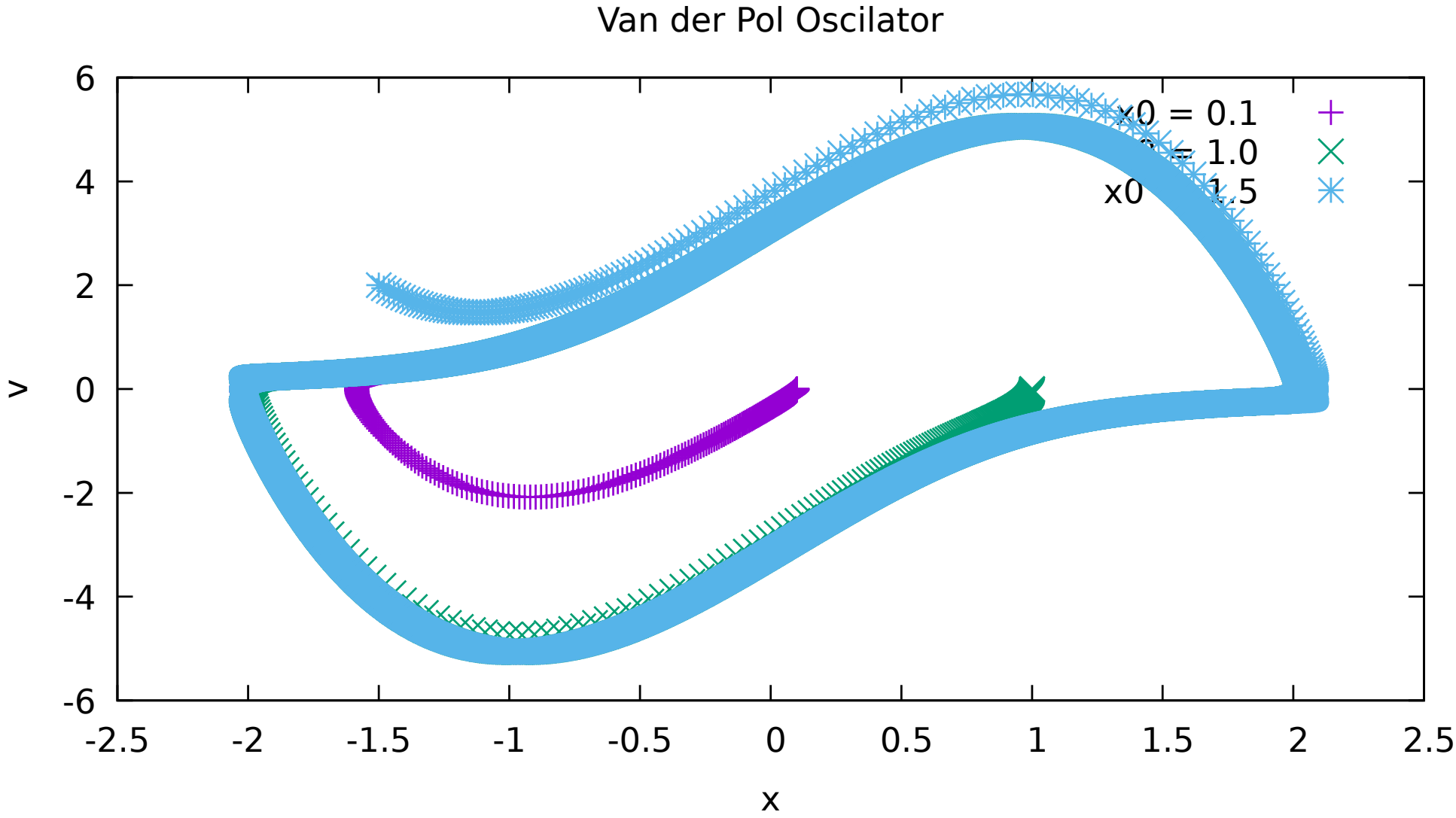


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