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Module DataFit: Data analysis and modelling – Tutorial / workshop 1b

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Introduction

This additional workshop will not be formally assessed, but you will need to show that you have completed all the problems outlined in this worksheet. These are designed to give you some practice in data simulation and fitting, and are an essential part of the course.

These exercises should ideally be carried out with the scientific data analysis software IGOR Pro, but you can use other packages / environments if you wish, though without any help.

To solve these problems, you can use online help and ask the postgraduate demonstrator to get you started.

You may also need to refer to your notes from the lectures.

A common task in data analysis involves the identification and fitting of peaks in spectra. Typically, three parameters per peak are sought: the position (peak centre), the amplitude and the width. However, the functional form of peaks can vary. We will study two of the most common forms, Gaussian and Lorentzian, and a combined form called a simple Voigt profile.

The Gaussian peak function, which arises for example in spectroscopy as a result of Doppler broadening, is also a good starting point for any peak fitting. The Lorentzian peak function arises in spectroscopy from natural lifetime broadening (as a results of Heisenberg's Uncertainty Principle). Often, observed line shapes are a combination of both these forms, or more strictly, a convolution of the two, called a Voigt profile.

Problem

1) Obtain the functional forms for Gaussian, Lorentzian and pseudo-Voigt profiles (internet / Igor manual research). Check that you have the right forms with your tutor.

2) Generate files containing Gaussian, Lorentzian, and (Pseudo) Voigt profiles (as a function of x over the range x = 95 to 105) centred at x_0 = 100, with a peak amplitude of 1 and full width at half maximum of 1. Add Gaussian noise to each (with an average amplitude of 0.1).

3) Create your own fitting functions to fit each of the profiles obtained.

4) For the Voigt profile, compare the residuals obtained using Gaussian, Lorentzian and Voigt fits.

5) For a bonus, in the Gaussian case, generate and fit a file with three peaks centred at x = 98, 100 and 101 with amplitudes of 1, 2 and 0.5, and widths of 0.5 FWHM