MPB311 coursework 1: Neural networks
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When handing in this coursework, please submit one document, containing the answers to the exercises, through the module Learn page. The deadline is 13:00, Wednesday 23rd November.

The bulk modulus of a material is one of its most basic elastic properties and corresponds to the elastic constant relating to uniform compression or expansion of the material in the linear regime. You will investigate a reasonably large dataset which contains the bulk modulus for a number of Al containing compounds, including both metallic alloys and ceramics, the aim is to predict the bulk modulus based upon the other information supplied.

You have been provided with a data set which contains eight labelled columns, one of these is given only for information, the formula of the compound. The other data include the formation energy (eV), the density (g/cm^3), the band gap (eV), the magnetic moment, the bulk modulus (GPa), the shear modulus (GPa) and the elastic anisotropy.

1. State which are the input and output parameters.

(2 marks)

2. Perform a multiple linear regression on the data provided using a straight-line fit of the form $y = \sum_i m_i x_i + c$, where y is the output parameter, x_i are the input parameters, and m_i and c are free parameters. Give the equation for the straight line, and comment on its quality.

(4 marks)

3. Perform a multiple linear regression on the data provided using a quadratic form including cross terms. Give the equation for the fit, and comment on its quality and its appropriateness for this problem.

(8 marks)

4. Train a neural network on the data provided and refine it to be a good fit. Discuss the quality of the final fit and the steps you took to improve it.

(14 marks)

5. Investigate whether all of the input parameters contribute to the quality of the fit and whether it is appropriate to exclude one or more of them. Do this by training a neural network on the data provided excluding the input variables one by one and one, and refine it to be a good fit. Discuss the quality of the final fit, the steps you took to improve it, and how it compares to the neural network fit carried out using all the quantities.

(22 marks)