PH2150 Scientific Computing Skills

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1 Introduction

In this problem sheet we are introducing arrays as a *Python* construct. In the class using the *%timeit* statement we compared how long *Python* takes to add 1 to a million points in a list, with adding 1 to a million points in an array. In which the array was much faster. [remember: *timeit?* returns help file , list = range(1000000), array = arange(1000000)]

Also the *NumPy* package contains *ufuncs* (Universal functions that act on arrays) further reducing the time to operate on arrays.

2 PS3 Ex1: Creating Arrays

Write code to create and print the following arrays:

a) A two dimensional floating point array with 4 rows and 4 columns all filled with 0.0, call this array EX1a.

b) A two dimensional floating point array with 4 rows and 4 columns filled with the range of numbers 1-16, call this array EX1b.

c) A two dimensional floating point array with 4 rows and 4 columns filled with random numbers, call this array EX1c.

d) Use linspace() to create a two dimensional array with 4 rows and 4 columns. The first row containing numbers between 1 and 17, the second row containing numbers between 1 and 2, the third row containing numbers between 100 and 200, the fourth row should be equal to the 3rd row rounded to two decimal places. Call this array EX1d.

The next exercises are to demonstrate how basic arithmetic works on arrays:

e) Add EX1a to EX1b to EX1c, call the answer EX1e, return the element that is 4 across on the third row.

f) Multiply EX1b by itself, return EX1f take the dot product of EX1b with itself and calculate the difference from EX1f, comment on what these two operations are doing.

g) Calculate sin(x)**2 for each element of EX1c, return as EX1g.

h) Transpose the elements of EX1c.

i) Return the diagonal() of EX1c.

j) Create a (8,4)array by stacking EX1a and EX1b.

k) Create a (4,8) array by stacking EX1a and EX1c.

3 PS3 Ex2: Plotting with Arrays

The file stars.dat on moodle (twiki) contains a catalog of temperatures and magnitudes for 7860 nearby stars, create an array using this data, use the NumPy function np.loadtxt() to read the data from the file. Then plot a Hertzsprung-Russell diagram using this catalog, look at online examples of HR diagrams to see the convetions of how the axes should be displayed etc.

4 PS3 Ex3: Advanced Plotting with Arrays

The file stm.dat contains a grid of values from a scanning tunneling microscope measurement of the [111] surface of silicon. The STM is a device that measures the shape of a surface at the atomic level by tracking a sharp tip over the surface and measuring quantum tunneling current as a function of position. The end result is a grid of values that represent the height of the surface. Use imshow() to create a density plot to represent the surface of the silicon, explore the options to create a clear image of the surface.