

EXERCISE 1: ML ESTIMATION OF THE d_N/d_S (ω) RATIO "BY HAND"

Objectives: Use codeml to evaluate the likelihood the *GstD1* sequences for a variety of ω values. Plot log-likelihood scores against the values of ω and determine the maximum likelihood estimate of ω . Check your finding by running codeml's hill-climbing algorithm.

Step-by-step guide:

1. Find the files for Exercise 1 on the web-site (`ex1_codeml.ctl`, `ex1_seqfile.txt`) and familiarize yourself with them. Pay close attention to the modified control file called "`ex1_codeml.ctl`". When you are ready to run CODEML, delete the "`ex1_`" prefix (the control file must be called "`codeml.ctl`").
2. Create a directory where you want your results to go, and place all your files within it. Now open a terminal, move to the directory that contains your files, and run CODEML.
3. Familiarize yourself with the results. If you have not edited the control file the results will be written to a file called "`results.txt`". Identify the line within the results file that gives the likelihood score for the example dataset.
4. Now change the control files and re-run CODEML. The objective is to compute the likelihood of the example dataset given a fixed value of omega.
 - a. Change the name of your result file (via "`outfile =`" in the control file) or you will overwrite your previous results!
 - b. Change the fixed value for ω by changing the value for "`omega =`" in the control file. The values for this exercise are provided as comments at the bottom of the example control file that has been provided to you.
5. Repeat step 4 for each value of ω given in the comments of the example control file.
6. Use your favorite spread sheet or statistical package to plot the likelihood score (y-axis) against the fixed value for ω (x-axis). Use a logarithmic scale for the x-axis (do not transform ω).
7. From the plot, try to guess the value of omega that will maximize the likelihood score (*i.e.*, the MLE).
8. Now change the control file so that CODEML will use its hill-climbing algorithm to find the MLE; set "`fix_omega = 0`" in the control file. Compare the result to your guess from step 7.