Transanalysis IPython Notebooks and Functions

John Thomas Sauls

16 December 2013

IPython Notebooks

- import_block Hold some common start up stuff, import models, loading transcription data, etc.
- reaction_connectedness Looks at either iJO or the core model, the minspans within them. Finds minspans each reaction is in, and the size of the minspans. FPKM averages for minspans can be calculated while excluding highly connected reactions
- minspan_shifts Explores how the average FPKM value changes per minspan under the different conditions we have. Also finds most differentially regulated minspans under aerobic vs anaerobic conditions and maps this with Visbio.
- core_minspans Looks at just the core minspans as calculated from the core model. Still uses iJO as the model in order to associate the FPKM data.
- core_flux This investigates explores how the FBA solution for the core model stacks up with the FPKM data, in the context of minspans.
- ijo_flux Same thing for iJO1366. Note this script and the one above, flux per minspan is calculated with the projection, or just a simple averaging.
- find_bottlenecks Solves iJO under pFBA and E-flux, and sees where individual reactions are over constrained. Is a precursor for the relax_eflux script.
- relax_eflux This script finds the bottlenecks as above, and then relaxes
 those bounds in a recursive manner so E-flux does not over constrain the
 model.
- compare_fpkms_reactions Combining FPKM data per reaction, compares two FPKM datasets to see how correlated they are under similar and disparate conditions.
- microarray_vs_fpkm Does a comparison by reactions like above, but uses data from the microarrays as well.

transAnalysis Functions

These functions have descriptions, as well as input and outputs in their docstring.

- make_gene_fpkm_dict Makes a dictionary from an FPKM tracking file with genes as keys and FPKM levels as values
- make_reaction_fpkm_dict Using the GPRs associations, makes a dictionary with reactions as keys and combined fpkm values for the related genes as values.
- make_minspan_list Creates a list of minspans from the excel file which contains them. Either for iJO or core model as tested.
- make_minspan_fpkm_list Averages FPKM values of the reactions for each minspan. Can choose a cut off value to exclude highly connected reactions.
- rank_reactions Rank reactions based on FPKM value as computed through the GPRs.
- fpkm_comparison Takes two FPKM filenames, a model, and a list of minspans and outputs a graph and correlation values for how the minspans line up in terms of their FPKM values.
- Eflux Perform E-flux as per the Colijn et al. paper. Modified form the script the Danish guys sent.
- relax-bounds Takes a model with an E-flux solution and recursively releases the bounds to find over-constrained reactions.
- make_minspan_k_dict A dictionary with minspan IDs as keys and the involved reactions in a list as values.
- make_reaction_k_dict A dictionary with reaction IDs as keys and involved minspans in a list as values.
- make_reaction_k_dict1 Same as above, but draws the reaction list from the minspans, so only reactions that are involved in minspans end up in the dictionary.
- run_pfba Solve the model using pFBA, modified from Teddy's script.
- make model irrev Used for run pfba