

The following is a user guide for the MATLAB tool TRS which is based on the methodology described in the paper “Inferring transcriptional logic from multiple dynamic experiments” by Giorgos Minas, Dafyd Jenkins, David Rand and Bärbel Finkenstädt.

The tool is contained in four folders: (1) inputs (2) scripts (3) functions (4) outputs.

The user is required to provide the inputs in the format described in section 1 and run the scripts in the order described in section 2. The scripts use the MATLAB functions contained in folder (3) to derive the output that can then be found in folder (4).

The tool contains the data (input and output) used for the simulation and real examples provided in the above paper and this can be used as a guidance.

In the following we provide a more detailed description of the tool.

## **1. Inputs**

The following files need to be provided by the user.

### **(1) base network file**

*Description:* Provides the base interactions to be tested and parameterised by TRS

*Format:* cvs file with 3 columns.

- First column: regulator name
- Second Column: interaction type
- Third Column: target name

*Name:* basenetNetworkName.csv

**Note:** *The file can contain base interactions to more than one target and more than one type*

### **(2) names of target and candidate regulators file**

*Description:* In case the regulators have multiple names, GST ids etc. this can be provided here.

*Format:* cvs file with columns the different names of each regulator

*Name:* namesNetworkName.csv

**NOTE:** *If only a single name is used please provide a file with a single column*

### **(3) data file:**

*Description:* Provides the data for the regulators and target(s) of each experiment

*Format:* csv file with rows the data of each regulator or target participating in the base network in a single column. Replicates follow one after the other.

\*\*\*\* **IMPORTANT NOTE:** the order of the rows should be the same as the order of the names in namesNetworkName.csv file \*\*\*\*

*Name:* data\_ExperimentName.csv

*NOTE:* Data of each experiment are provided in separate files. Data of each replicate of the same experiment are in the same file (see format).

## 2. Scripts:

The user needs to run the scripts in the following order: (1) createNetworkScript (2) createDatasetScript (3) createSmoothProfilesScript (4) createProfilesPriorsAndProposalDistrsScript (5) trsScript

The scripts should be run from the parent TRS directory.

## 3. Outputs:

(1) basenetNetworkNameInteractionType.mat

*Description:* mat file containing a structure with the names of the regulators and targets in the NetworkName that are related by the InteractionType provided in the script createNetworkScript.m

(2) data\_ExpName.mat

*Description:* mat file containing a structure with the data provided in data\_ ExpName.csv

(3) smoothProfiles\_ExpName1\_ExpName2\_...\_ExpNameK.mat

*Description:* mat file containing a structure with the smooth profiles and various other variables for the data in experiments with name ExpName1, ExpName2,..., ExpNameK as provided in the script createSmoothProfilesScript.m

(4) prof\_priors\_prop\_ExpName1\_ExpName2\_...\_ExpNameKTargetName.mat

*Description:* mat file containing the smoothed profiles of the candidate regulators of TargetName in experiments ExpName1, ExpName2,..., ExpNameK as well as the prior distributions for the parameters of TRS and various parameters related to the proposal distributions used in the RJMCMC implemented in TRS.

(5) finalOutput\_ ExpName1\_ExpName2\_...\_ExpNameKTargetName.mat

*Description:* mat file containing a structure with the results of applying TRS to the data of the specified experiments and with the base network provided. This includes the MCMC chains of various parameters and the posterior distributions for various parameters including:

- (1) the number of regulators
- (2) the regulation set including the probability of selecting each parent under any regulation set

**Plots/tables:**

- (1) The script createSmoothProfilesScript creates a plot with all regulator's data, their smooth profiles and their Bootstrap confidence envelopes
- (2) The script createProfilesPriorsAndProposalDistrsScript creates plots with the prior distribution for the number of regulators, for the regulators to be selected in any regulation set and for their activation threshold.
- (3) The script trsScript creates an interactive plot of the TRS results with the regulators present on the plot and taking part in regulation being selected by the user with information provided by the script. Two regulation sets can be plotted at the same time.

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