Analyzing gene regulatory networks by comparing the dynamics obtained via DSGRN (Dynamic Signatures Generated by Regulatory Networks) and RACIPE (Random Circuit Perturbation)

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Week Five

Important Inputs and Stability Percentages

		Both
/		80
	[Available options:	20
	-h : Show all available options.	100
	-maxtime : Maximum time for the simulation (Default 23.5 h).	100
	-solver : The integrator method (1> cuter of 2> KK45) to solve the ODEs equations (Default 1).	
	e simulation).	
	-KDID : Gene or link (See their ID in the .cfg file) to be knocked down.	
	-OEID : Gene (See their ID in the .cfg file) to be overexpressed. (follow by -OEFD).	
	-OEFD : Fold change to overexpress a gene (-OEID must be first set in the option, the value need to b	Both
/	e bigger than 1). (Default 1) if the corresponding OEFD is not set, it will be set to 1.	
	-DEFD : Gene (see them in the stry inter to be downexpressed. (introv by -DEFD).	35.48
	bigger than 1). (Default 1) if the corresponding DEFD is not set, it will be set to 1.	
	-dist : Distribution used for randomization	54.84
	1> Uniform Distribution (Default)	0.00
	2> Guassian Distribution	9.68
	-SE> Exponential Distribution	100
	be smaller than 1 (Default 1).	100
	-num_findT : The number of simulations used to estimate the thresholds (Default 10000).	
	-num_paras : The number of RACIPE models to generate (Default 100).	
	-num_ode : The number of Random initial values to solve ODEs (Default 100).	
	-num_stability : The maximum number of stable states to save for one RACIPE model (Default 10).	
	-Ind : Cutoff for Convergence of Steady States for numerically softing ODEs (Default 1.0).	Both
	-stepsize : Stepsize for solving ODEs (Default 0.1).	
	-maxiters : The maximum number of iterations for solving ODEs at each random initial condition (Default 2	14.82
	0).	
	-Toggle_T_test : Test the threshold assumption or not (Default 1 (yes)).	39.95
	-SBML_MODEL : UUTPUT a model in the SBML format. The parameter will be the 1D of the model (start from 1) t	00.54
	-seed : random seed (Default 1).	32.54
	-minP : Minimum production rate (Default 1.0)	10.05
		10.05
		2.65
		2.05

100

Progress

This week we started messing with the customizable options in RACIPE. This includes the likes of the number of models generated, the range of the Hill coefficient, and random initial values for the ODEs. We chose to simulate TS2SA, the toggle switch with two self-activating edges, because it exhibits the most interesting behavior and the highest levels of stability of the three toggle switch motifs. Since we found the exact DSGRN percentages last week (based on essential parameters and their neighbors), we spent this week affecting the RACIPE simulations with customized values and ranges chosen by Konstantin and Marcio. We also made tables in which we varied the number of models generated and the Hill coefficient range.

Essential Nodes and Their Neighbors





Results for Toggles Switches

Both	
4	
1	
5	
Both	
22	
34	
6	
62	
Both	
112	
302	
246	
76	
20	
756	

Both
80
20
100
Both
35.48
54.84
9.68
100
Both
14.82
39.95
32.54
10.05
2.65
100



RACIPE TS2SA Simulations



(Euler ODE solver)

model	num_paras	minN/maxN	num_ode	stable: 1 #	stable: 2 #	stable: 3 #	stable: 4 #	stable: 5 #	stable: 1 %	stable: 2 %	stable: 3 %	stable: 4 %	stable: 5 %
TS2SA	1000	2	1000	438	528	34	0	0	43.8	52.8	3.4	0	0
TS2SA	1000	6	1000	106	613	265	16	0	10.6	61.3	26.5	1.6	0
TS2SA	1000	10	1000	93	538	336	29	4	9.3	53.8	33.6	2.9	0.4
TS2SA	1000	14	1000	91	492	383	24	10	9.1	49.2	38.3	2.4	1
TS2SA	1000	18	1000	66	505	386	34	9	6.6	50.5	38.6	3.4	0.9
TS2SA	1000	22	1000	75	470	413	38	4	7.5	47	41.3	3.8	0.4
TS2SA	1000	26	1000	85	452	411	41	11	8.5	45.2	41.1	4.1	1.1
TS2SA	1000	30	1000	90	454	407	37	12	9	45.4	40.7	3.7	1.2
TS2SA	10000	2	1000	4234	5369	394	3	0	42.34	53.69	3.94	0.03	0
TS2SA	10000	6	1000	1183	5863	2825	111	18	11.83	58.63	28.25	1.11	0.18
TS2SA	10000	10	1000	927	5399	3420	226	28	9.27	53.99	34.2	2.26	0.28
TS2SA	10000	14	1000	885	5062	3730	261	62	8.85	50.62	37.3	2.61	0.62
TS2SA	10000	18	1000	843	4877	3919	296	65	8.43	48.77	39.19	2.96	0.65
TS2SA	10000	22	1000	817	4687	4059	344	93	8.17	46.87	40.59	3.44	0.93
TS2SA	10000	26	1000	870	4596	4041	387	106	8.7	45.96	40.41	3.87	1.06
TS2SA	10000	30	1000	806	4521	4196	370	107	8.06	45.21	41.96	3.7	1.07
TS2SA	DSGRN (756	Essential + N	leighbors)	112	302	246	76	20	14.8148148	39.9470899	32.5396825	10.0529101	2.64550265

What's Next?

We will now analyze the data (the percentages) generated and generate the final table, which will include the RK45 solver and more. There are already some observable trends in some of the stabilities with the increasing of the Hill coefficient range (where the range is set to a fixed number). We will consider the impact of factors like the Hill coefficient range and the number of models generated. Additionally, the running times of the simulations were recorded, so we can include those too. In general, we want to consider the range of models that can be input, computational cost, time cost, and more factors when comparing DSGRN and RACIPE. These percentages as well as the time data should be quite useful for generating the final table.

Thank You for Listening!

and

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