Supplementary Material to EMBM Paper: "Multicellular Pattern Formation: Parameter Estimation for ODE-based Gene Regulatory Network Models"

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Here, we give a detailed list of the optimized parameters for the to test systems given by Eq. 5, Eq. 6, Eq. 7, and Eq. 8. In Tab. 1 we list the optimized parameters for the first test system (an activator inhibitor kinetic) and in Tab. 1 we list the optimized parameters for the second test system (two independent activator inhibitor kinetics regulating a single response gene).

The proposed method was able to identify suitable parameters in most of the optimization runs. Still, the found solutions show significant variations in some of the optimized parameters, e.g., in Tab. 1 parameter sets two and three. This can occur due to the fact that for the considered non-linear systems in principle different regions in the parameter space can result in qualitatively similar behavior. Therefore, the fact that the proposed method is capable of identifying parameter sets from different regions illustrates the explorative power of the approach which is a desirable feature: When starting with a system hypothesis, only the desired outcome behavior is known. If there are different parameter sets resulting in that behavior one is interested in learning about as many as possible of these parameter sets. The conclusion one can draw from the fact that there are different parameter sets resulting in the desired behavior are twofold: (i) The fact that parameter sets resulting in the desired target behavior are found indicates that the assumed network in principle can result in the desired behavior. (ii) Further control experiments are needed in order to reduce the set of different parameter settings to a single parameter set.

κ_a	μ_a	σ_a	ρ_a	μ_h	σ_h	ρ_h	D_a	D_h
0.005057	0.030557	0.007620	0.751801	0.010509	0.527146	2.865511	0.013792	0.153323
0.313687	13.110143	3.443316	3.410343	0.162290	0.027667	0.018318	0.000233	0.308771
1.245785	0.064232	0.149503	15.925325	0.000284	1.681174	1.274759	0.001362	0.105593
3.064560	0.590503	0.149366	6.430855	0.009670	0.001004	1.454994	0.007292	0.118458
0.017284	0.382926	2.015209	1.067923	0.002181	0.001572	0.000680	0.006598	0.147123
0.837505	0.863320	0.132459	2.655199	0.042563	0.001054	0.246167	0.001661	0.252623
0.013461	0.000115	1.376548	1.416244	0.128737	2.445894	0.196909	0.212664	2.279555
0.004660	0.000131	0.598908	2.232890	0.778805	2.432500	3.292868	0.106765	1.441187
0.948179	0.873367	0.339654	0.929988	0.003530	0.143911	0.092189	0.006341	0.129367
0.372366	0.095918	0.031939	0.580111	0.020077	0.000083	0.007800	0.000006	0.196483
0.285967	0.183579	0.008729	0.556811	0.604547	1.009067	0.059068	0.014436	0.038818
0.006329	0.000747	0.328384	0.720893	0.422809	0.609701	1.407671	0.105759	1.738038

Table 1: Parameter sets identified during twelve optimization runs for the first test system.

κ_{a_1}	μ_{a_1}	σ_{a_1}	ρ_{a_1}	μ_{h_1}	σ_{h_1}	ρ_{h_1}	D_{a_1}	D_{h_1}
0.524852	0.000140	1.498977	0.152896	2.602764	2.101099	1.120183	0.002150	1.146289
0.008375	0.000724	0.352744	0.926963	3.872010	0.801008	3.970773	0.000012	2.194969
1.127918	0.001221	0.000085	0.108886	0.033755	1.442974	0.000001	0.004295	1.400775
0.067285	0.000197	1.081540	0.427426	0.194993	2.256961	2.494726	0.002895	1.197297
0.728980	0.000065	0.001444	0.698879	0.000230	0.970562	0.707323	0.000263	1.892159
0.170372	0.569345	0.162767	0.327087	0.248477	0.622060	0.333700	0.003414	0.103632
0.331356	0.000522	1.298993	1.194589	0.349307	2.110977	0.022343	0.022327	2.353656
0.392112	0.003962	0.002259	0.424309	0.103788	2.756224	0.308160	0.000005	1.136900
0.786539	0.000324	0.001116	0.063926	0.554125	1.229055	1.453876	0.001152	0.124796
0.468660	0.004986	0.001833	0.409889	0.319640	1.657598	0.001355	0.009893	2.277225
1.733929	0.000900	0.001103	1.299437	0.048523	1.246063	0.057416	0.015717	1.395827
0.444937	0.000033	0.120527	3.030510	0.020045	2.565782	2.009904	0.000467	1.614265

κ_{a_2}	μ_{a_2}	σ_{a_2}	ρ_{a_2}	μ_{h_2}	σ_{h_2}	ρ_{h_2}	D_{a_2}	D_{h_2}
0.003022	0.001672	0.000381	0.076987	0.231612	0.416058	1.823799	0.002151	1.146289
0.370368	0.000040	0.017093	2.229681	0.105087	5.852413	0.005142	0.000012	2.194969
0.774421	0.000232	0.185404	0.628469	0.058507	1.627462	0.517737	0.004295	1.400775
0.005657	0.000032	0.071264	0.342676	2.181970	3.319910	0.004435	0.002895	1.197297
4.213250	0.000004	0.073181	0.093304	2.660325	3.443585	1.888077	0.000263	1.892159
0.056386	2.801579	0.077322	0.141560	0.336346	0.000373	0.104789	0.003414	0.103632
0.838473	0.000316	3.486151	0.085493	2.011771	0.006169	0.031426	0.022327	2.353656
2.508779	0.000003	0.554998	0.008436	1.058622	1.275221	1.036778	0.000005	1.136900
0.256345	1.804145	0.172242	0.161243	0.026342	0.962410	0.025815	0.001152	0.124796
1.223686	0.000044	1.955755	0.002793	0.705979	0.004568	2.924878	0.009893	2.277225
0.063759	0.000880	0.004244	0.113517	2.317535	2.484761	0.026547	0.015717	1.395827
0.055354	0.000800	1.576046	0.574824	0.227830	0.489102	0.001581	0.000467	1.614265

Table 2: Parameter sets identified during twelve optimization runs for the second test system. The parameters labeled with the subscript 1 belong to the first of the independent activator inhibitor kinetics and the parameters labeled with the subscript 2 belong to the second of the independent activator inhibitor kinetics, respectively.