Supplementary Information Text and Figures of "*Roles of network topology in the relaxation dynamics of simple chemical reaction network models*"

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1 A necessary condition for networks with $\delta = 0$ to have no conserved quantities

Recall that the number of conserved quantities is the dimension of left-nullspace of the chemical reaction network. Here, we introduce some notations. We denote the internal reaction network S_0, and

$$\begin{aligned} S_1 &= (S_0|\vec{U}^{(0)}|\vec{U}^{(1)}|\cdots\vec{U}^{(N_{\rm nut}-1)}), \\ S_2 &= (S_1|\vec{W}), \end{aligned}$$

where $\vec{U}^{(i)}$'s are the stoichiometry of the uptake reaction, having only a single non-zero element for each. $\vec{W}$ represents the growth reaction. $W_i = 1$ if the ith chemical is one of the growth factors, and else W_i is set to zero. With this notation, we claim the following

Proposition: For any network which has at least one polymer consisting of different numbers of monomer species, if the rank gap of the network $\delta = {\rm rank}S_2 - {\rm rank}S_1$ equals to zero,

$$\text{dim ker } S_2^T \geq M - N_{\rm in}$$

holds.

Proof: From the dimension theorem, and the condition $\delta = 0$, the following holds;

$$\begin{aligned} \text{dim Ker } S_2^T &= N - {\rm rank}S_2^T \\ &= N - {\rm rank}S_2 \\ &= N - {\rm rank}S_1, \end{aligned} \tag{1}$$

where N is the number of polymers in the network. Since the internal reaction network conserves, at least, the number of monomers of each M monomer

species, dim $\ker S_0^T \geq M$ holds[1]. Again, from the dimension theorem, we obtain $\mathrm{rank} S_0 = N - \dim \ker\, S_0 \leq N - M$.

Recall that the expanded matrix S_1 is obtained by adding N_{in} vectors to S_0, and thus, the difference of the rank between S_1 and S_0 is, at most, N_{in}. Therefore, $\mathrm{rank} S_1 \leq N - M + N_{\mathrm{in}}$ holds. By substituting this to Eq.(1), we get

$$\begin{aligned} \dim \mathrm{Ker}\, S_2^T &= N - \mathrm{rank} S_1 \\ &\geq N - (N - M + N_{\mathrm{in}}) \\ &= M - N_{\mathrm{in}}. \end{aligned}$$

□

As a straightforward corollary, the following holds; it is impossible for models to have no conserved quantities if the number of inputs is less than the number of monomers and $\delta = 0$.

[1]For this part, we need that at least one polymer consists of different number of monomers, and otherwise, the basis of the left nullspace of S_0 becomes linearly dependent.

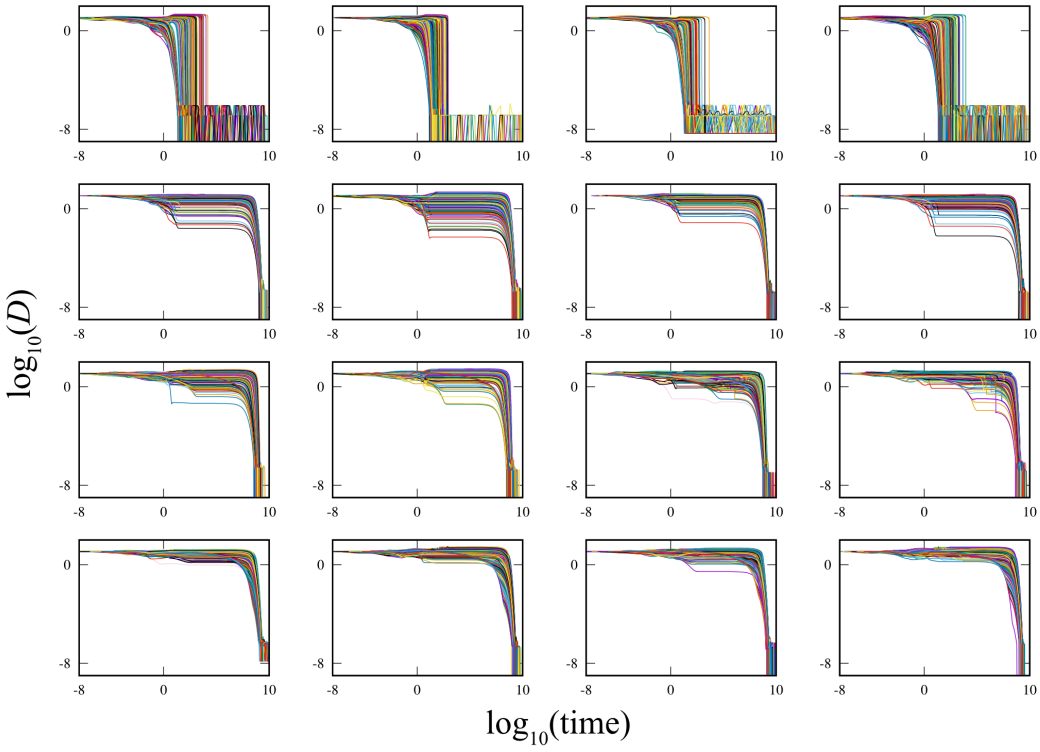

Figure S1: The relaxation dynamics of the Euclidean distance between the state at a given time $\boldsymbol{x}(t)$ and the trajectory average of the final concentration $\langle \boldsymbol{x}(T) \rangle$, $D(t) = \| \langle \ln \boldsymbol{x}(T) \rangle - \ln \boldsymbol{x}(t) \|$. The first, second, third, and fourth rows show the dynamics of the 256 trajectories of four typical model instances of type I, II, III, and IV, respectively.

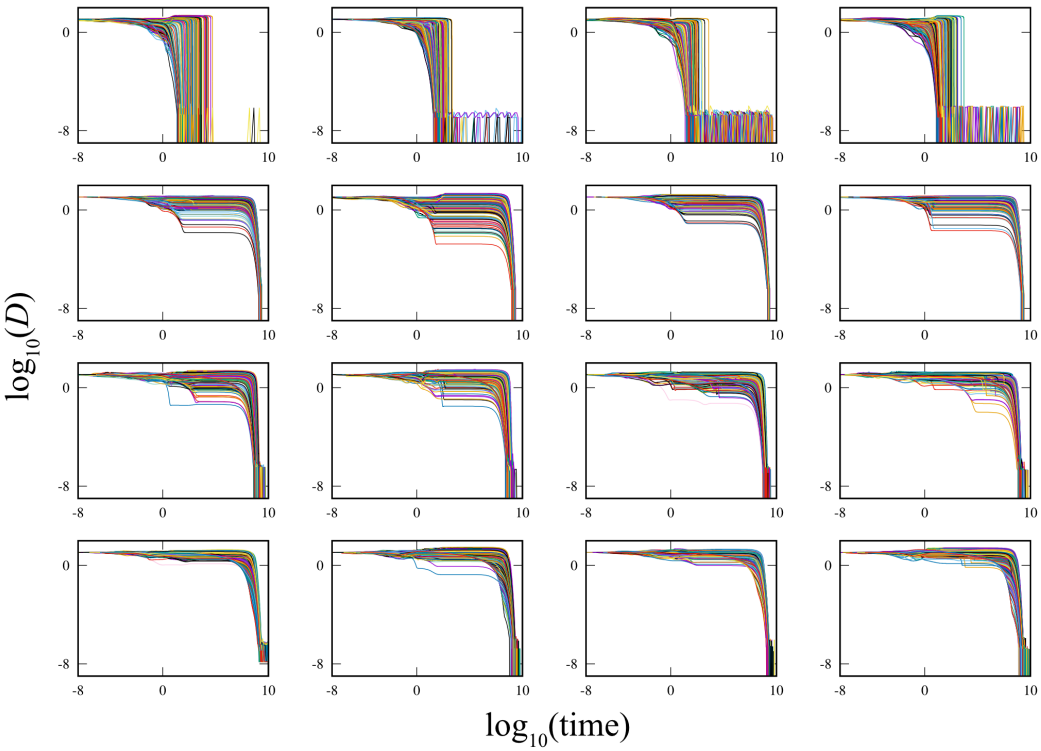

Figure S2: The relaxation dynamics of the Euclidean distance between the state at a given time $\boldsymbol{x}(t)$ and the trajectory average of the final concentration $\langle \boldsymbol{x}(T) \rangle$, $D(t) = \| \langle \ln \boldsymbol{x}(T) \rangle - \ln \boldsymbol{x}(t) \|$ in the random parameter models. The first, second, third, and fourth rows show the dynamics of the 256 trajectories of four typical model instances of type I, II, III, and IV, respectively. The reaction rate constants v are randomly generated as $v = 10^r$, where $r \sim U(-1, 1)$, while the spontaneous degradation rate ϕ is as in the original model.

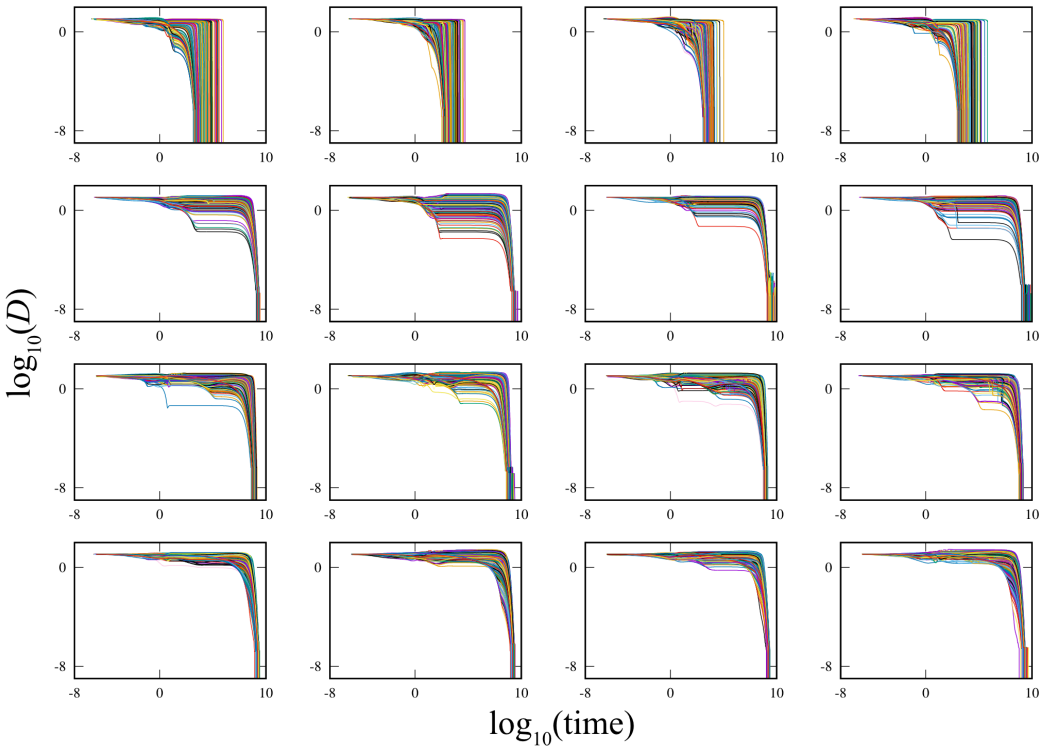

Figure S3: The relaxation dynamics of the Euclidean distance between the state at a given time $\boldsymbol{x}(t)$ and the trajectory average of the final concentration $\langle \boldsymbol{x}(T) \rangle$, $D(t) = \| \langle \ln \boldsymbol{x}(T) \rangle - \ln \boldsymbol{x}(t) \|$ of the model with the Michaelis-Menten rate equation. The first, second, third, and fourth rows show the dynamics of the 256 trajectories of four typical model instances of type I, II, III, and IV, respectively. The reaction rate equation is given by $J = v(x_{s_1} x_{s_2} - x_p)/(K + x_{s_1} x_{s_2} + x_p)$, where s_i and p are the substrates and product, respectively. The rate constant v is set to unity, while the Michaelis-Menten constant K is randomly chosen to be $K = 10^k, k \sim U(0, 2)$.

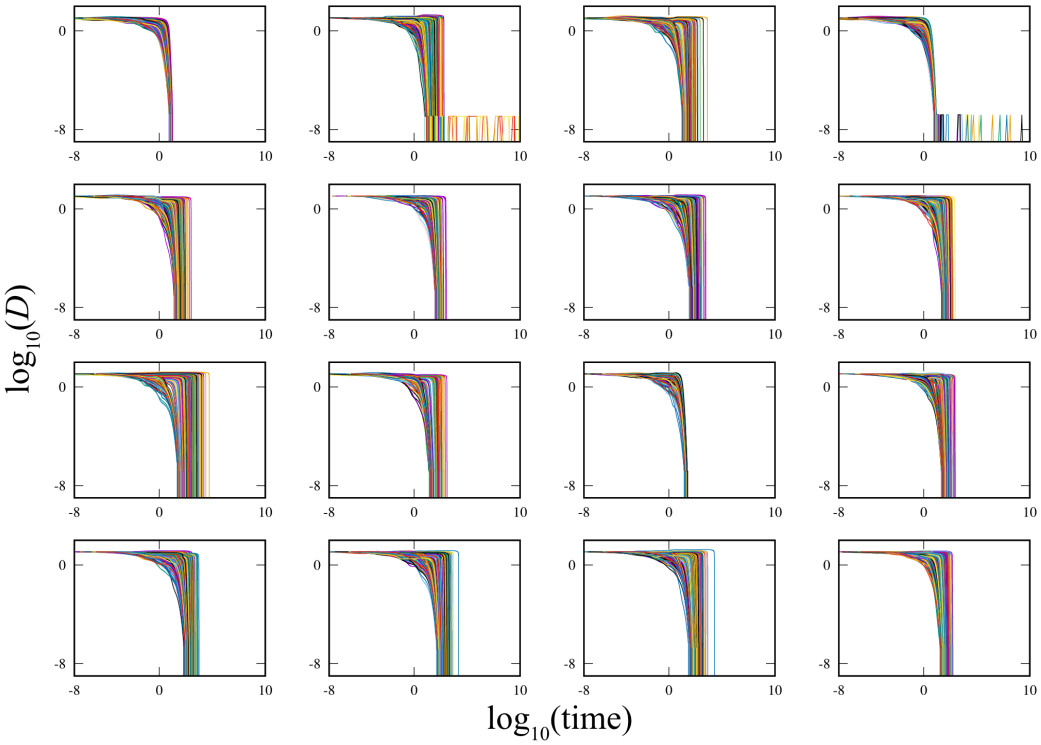

Figure S4: The relaxation dynamics of the Euclidean distance between the state at a given time $\boldsymbol{x}(t)$ and the trajectory average of the final concentration $\langle \boldsymbol{x}(T) \rangle$, $D(t) = \| \langle \ln \boldsymbol{x}(T) \rangle - \ln \boldsymbol{x}(t) \|$ of non-minimal network models. The first, second, third, and fourth rows show the dynamics of the 256 trajectories of four typical model instances of type I, II, III, and IV, respectively. After generating a minimal network of R reactions, $\lceil R/2 \rceil$ random uni-uni reactions are added. Mass action kinetics is used and the parameters are chosen to be unity.

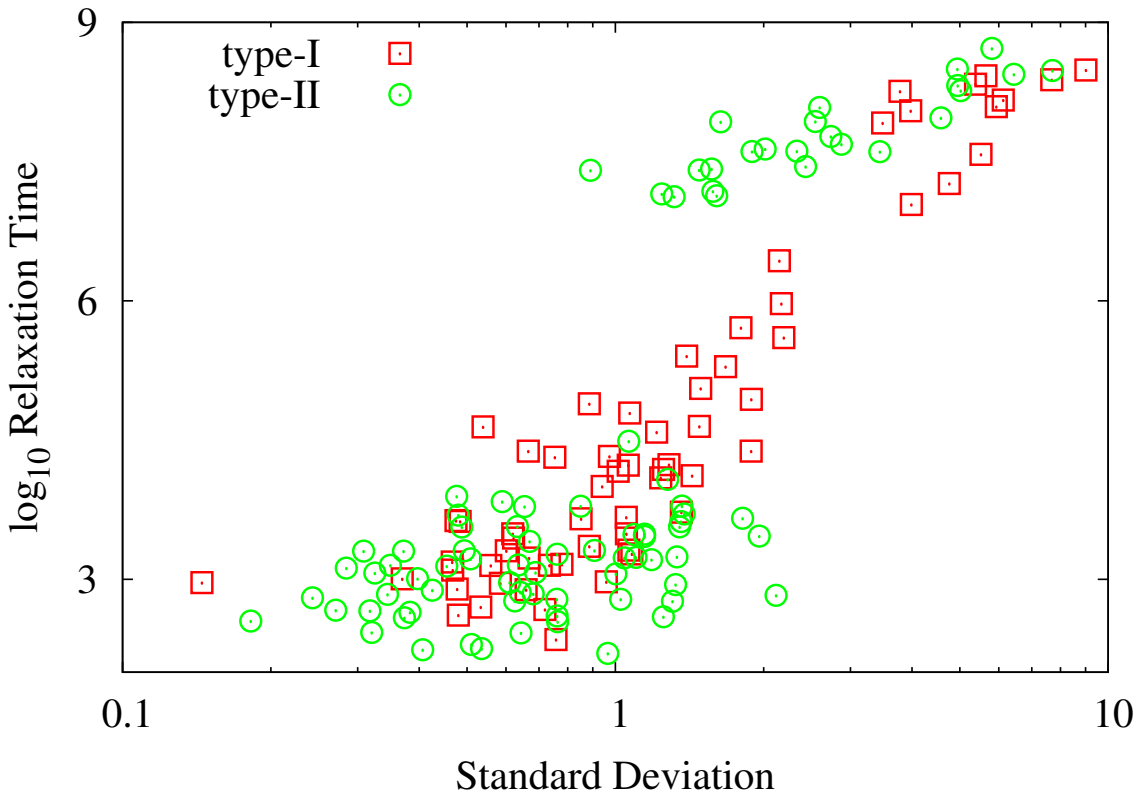

Figure S5: The relationship between the standard deviation of the concentration at the attractor and the relaxation time. Here, the relaxation time is defied as the time that the norm of the time derivative $|d\boldsymbol{x}/dt|$ becomes smaller than 0.01, and the standard deviation is computed in the natural logarithmic scale.

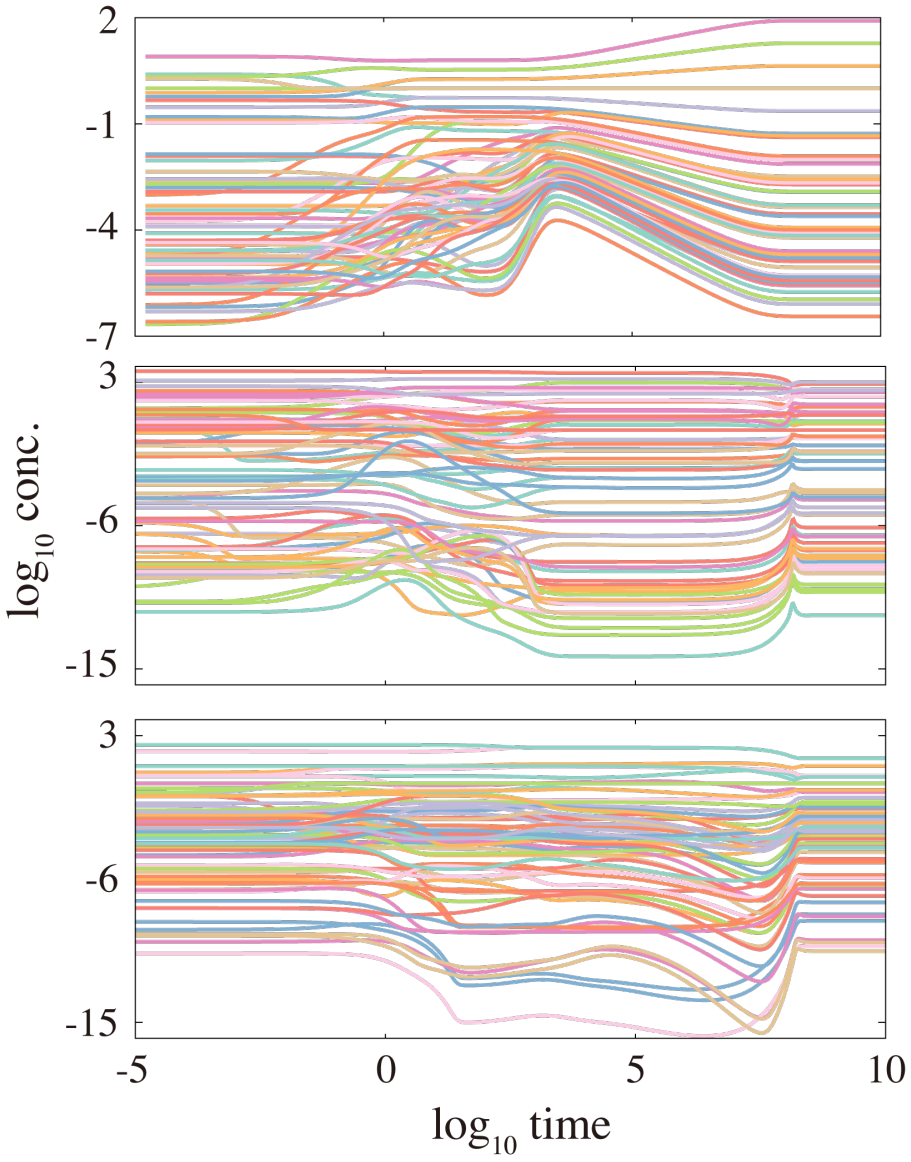

Figure S6: Three example time courses from three different large networks. The dynamics shown in the top and middle panels can be termed as the power-law and the plateau relaxation, respectively, while that in the bottom panel is more complicated.

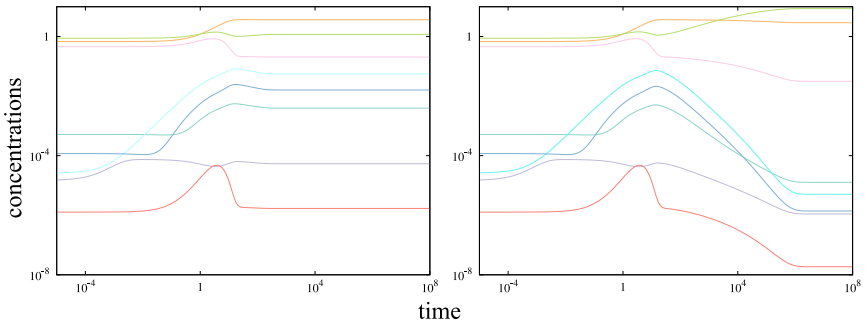

Figure S7: Dynamics of the metabolic model of glucose fermentation in *Lactococcus lactis*. All rate constant except the NOX reaction are set to be unity. The rate constant of the NOX reaction is 10^2 in the left panel and 10^{-2} in the right panel.