A

Maximum Likelihood Estimation of Reaction Rates

Hereafter, we solve the following optimization problem:

$$\hat{\mathbf{k}} = \underset{\mathbf{k}}{\operatorname{argmax}}\ \mathcal{L}(\mathbf{k}|e_1, \ldots, e_n) = \underset{\mathbf{k}}{\operatorname{argmax}} f(e_1, \ldots, e_n|\mathbf{k}). \tag{A.1}$$

where $\mathcal{L}(\mathbf{k}|e_1, \ldots, e_n)$ is the likelihood of the rate vector $\mathbf{k}$ given the sequence of observed events $(e_1, \ldots, e_n)$.

We can write the probability $f(e_i|\mathbf{k})$ of a single event e_i as follows:

$$\begin{aligned} f(e_i|\mathbf{k}) &= a_{R_i}(\mathbf{x}_i) \cdot e^{-a_{R_i}(\mathbf{x}_i)\cdot t_i} \cdot \prod_{R_j \neq R_i} \int_{t_i}^{\infty} a_{R_j}(\mathbf{x}_i) \cdot e^{-a_{R_j}(\mathbf{x}_i)\cdot t} \cdot dt \\ &= a_{R_i}(\mathbf{x}_i) \cdot e^{-a_{R_i}(\mathbf{x}_i)\cdot t_i} \cdot \prod_{R_j \neq R_i} -e^{-a_{R_j}(\mathbf{x}_i)\cdot t} \Big|_{t=t_i}^{t=\infty} \\ &= a_{R_i}(\mathbf{x}_i) \cdot e^{-a_{R_i}(\mathbf{x}_i)\cdot t_i} \cdot \prod_{R_j \neq R_i} e^{-a_{R_j}(\mathbf{x}_i)\cdot t_i} \\ &= a_{R_i}(\mathbf{x}_i) \cdot \prod_{R_j} e^{-a_{R_j}(\mathbf{x}_i)\cdot t_i} = a_{R_i}(\mathbf{x}_i) \cdot e^{-a_0(\mathbf{x}_i)\cdot t_i} \end{aligned} \tag{A.2}$$

where

$$a_0(\mathbf{x}) \triangleq \sum_{R_j \in \mathcal{R}} a_{R_j}(\mathbf{x}). \tag{A.3}$$

Since we assume independence of events (Markovian property), we can write:

$$\begin{aligned} \mathcal{L}(\mathbf{k}|e_1, \ldots, e_n) &= f(e_1, \ldots, e_n|\mathbf{k}) \\ &= f(e_1|\mathbf{k}) \cdot \ldots \cdot f(e_n|\mathbf{k}) \\ &= \prod_{i=1}^{n} a_{R_i}(\mathbf{x}_i) \cdot e^{-a_0(\mathbf{x}_i)\cdot t_i}. \end{aligned} \tag{A.4}$$

For the sake of simplicity, we will omit the arguments of $\mathcal{L}$ in the sequel.

Now, we can try to solve the optimization problem formulated by Equation A.1. To make our problem simpler (both from an analytical and a numerical standpoint), we work with the natural logarithm of the likelihood function:

$$\ln \mathcal{L} = \ln\Bigg(\prod_{i=1}^{n} a_{R_i}(\mathbf{x}_i)\cdot e^{-a_0(\mathbf{x}_i)\cdot t_i}\Bigg) = \sum_{i=1}^{n}\Bigg(\ln a_{R_i}(\mathbf{x}_i) - a_0(\mathbf{x}_i)\cdot t_i\Bigg). \tag{A.5}$$

First, we need to compute the gradient of the log-likelihood function $\ln \mathcal{L}$:

$$\nabla \ln \mathcal{L} = \left(\frac{\partial \ln \mathcal{L}}{\partial k_{R_1}}, \ldots, \frac{\partial \ln \mathcal{L}}{\partial k_{R_N}}\right) \tag{A.6}$$

with

$$\begin{aligned}\frac{\partial \ln \mathcal{L}}{\partial k_{R_j}} &= \sum_{i=1}^{n}\left(\frac{\partial \ln a_{R_i}(\mathbf{x}_i)}{\partial k_{R_j}} - \frac{\partial a_0(\mathbf{x}_i)\cdot t_i}{\partial k_{R_j}}\right)\\ &= \sum_{i=1}^{n}\left(\frac{1}{a_{R_i}(\mathbf{x}_i)}\frac{\partial a_{R_i}(\mathbf{x}_i)}{\partial k_{R_j}} - \frac{\partial a_0(\mathbf{x}_i)}{\partial k_{R_j}}\cdot t_i\right)\end{aligned} \tag{A.7}$$

where

$$\frac{\partial a_{R_i}(\mathbf{x}_i)}{\partial k_{R_j}} = \frac{\partial k_{R_i}\cdot \widetilde{a}_{R_i}(\mathbf{x}_i)}{\partial k_{R_j}} = \begin{cases}\widetilde{a}_{R_i}(\mathbf{x}_i) & \text{if } R_j = R_i\\ 0 & \text{otherwise}\end{cases} \tag{A.8}$$

and

$$\frac{\partial a_0(\mathbf{x}_i)}{\partial k_{R_j}}\cdot t_i = \frac{\partial a_{R_j}(\mathbf{x}_i)}{\partial k_{R_j}}\cdot t_i = t_i\cdot \widetilde{a}_{R_j}(\mathbf{x}_i). \tag{A.9}$$

Replacing these terms into Equation A.7, we obtain

$$\frac{\partial \ln \mathcal{L}}{\partial k_{R_j}} = \sum_{i=1}^{n}\left(\frac{\mathbf{1}_{R_i=R_j}}{k_{R_i}} - t_i\cdot \widetilde{a}_{R_j}(\mathbf{x}_i)\right) \tag{A.10}$$

where $\mathbf{1}_{R_i=R_j}$ is the indicator function. A local extremum of the function $\ln \mathcal{L}$ corresponds to a zero of the gradient

$$\nabla \ln \mathcal{L} = \big(0, \ldots, 0\big) \tag{A.11}$$

which is equivalent to writing

$$\begin{aligned}\sum_{i=1}^{n}\frac{\mathbf{1}_{R_i=R_j}}{k_{R_i}} &= \sum_{i=1}^{n}\Big(t_i\cdot \widetilde{a}_{R_j}(\mathbf{x}_i)\Big)\\ \frac{1}{k_{R_j}}\cdot\sum_{i=1}^{n}\mathbf{1}_{R_i=R_j} &= \sum_{i=1}^{n}\Big(t_i\cdot \widetilde{a}_{R_j}(\mathbf{x}_i)\Big)\\ \widehat{k}_{R_j} = k_{R_j} &= \frac{\sum_{i=1}^{n}\mathbf{1}_{\{R_i=R_j\}}}{\sum_{i=1}^{n}\big(t_i\cdot \widetilde{a}_{R_j}(\mathbf{x}_i)\big)}\end{aligned} \tag{A.12}$$

for $j = 1, \ldots, N$. Importantly, the rate of the reaction $R = R_j$ also depends on events that do not involve R.

For this point to be a maximum of $\ln \mathcal{L}$, we need the Hessian matrix

$$H(\ln \mathcal{L}) = \begin{pmatrix} \frac{\partial^2 \ln \mathcal{L}}{\partial k_{R_1}^2} & \frac{\partial^2 \ln \mathcal{L}}{\partial k_{R_1} \partial k_{R_2}} & \cdots & \frac{\partial^2 \ln \mathcal{L}}{\partial k_{R_1} \partial k_{R_N}} \\ \frac{\partial^2 \ln \mathcal{L}}{\partial k_{R_2} \partial k_{R_1}} & \frac{\partial^2 \ln \mathcal{L}}{\partial k_{R_2}^2} & \cdots & \frac{\partial^2 \ln \mathcal{L}}{\partial k_{R_2} \partial k_{R_N}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 \ln \mathcal{L}}{\partial k_{R_N} \partial k_{R_1}} & \frac{\partial^2 \ln \mathcal{L}}{\partial k_{R_N} \partial k_{R_2}} & \cdots & \frac{\partial^2 \ln \mathcal{L}}{\partial k_{R_N}^2} \end{pmatrix} = \begin{pmatrix} H_1 & 0 & \dots & 0 \\ 0 & H_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & H_N \end{pmatrix} \tag{A.13}$$

to be negative-definite, which is clearly the case for all $\mathbf{k} \in \mathbb{R}_+^N$ since we have that

$$H_j = -\sum_{i=1}^{n} \frac{\mathbf{1}_{R_i = R_j}}{k_{R_j}^2}. \tag{A.14}$$

Importantly, the Hessian matrix can be used to compute the variance-covariance matrix of the estimated parameters, which is defined as the inverse of the Fisher information matrix $\mathcal{I}$, which is itself the negative of the expected value of the Hessian matrix:

$$\operatorname{var}(\mathbf{k}) = \big[\mathcal{I}(\mathbf{k})\big]^{-1} = \Big(- E\big[H(\ln \mathcal{L})\big]\Big)^{-1}. \tag{A.15}$$

In our case, since $H(\ln \mathcal{L})$ is diagonal, we have:

$$\operatorname{var}(\mathbf{k}) = \begin{pmatrix} -\big(E[H_1]\big)^{-1} & 0 & \dots & 0 \\ 0 & -\big(E[H_2]\big)^{-1} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & -\big(E[H_N]\big)^{-1} \end{pmatrix}, \tag{A.16}$$

which translates into

$$\operatorname{var}(k_{R_j}) = -\Big(E[H_j]\Big)^{-1} = \left(E\left[\sum_{i=1}^{n} \frac{\mathbf{1}_{R_i = R_j}}{k_{R_j}^2}\right]\right)^{-1} = \frac{E[k_{R_j}^2]}{\sum_{i=1}^{n} \mathbf{1}_{R_i = R_j}}. \tag{A.17}$$

To avoid to compute the expectation of the squared reaction rate, one can use the following approximation for large sample sizes:

$$\operatorname{var}(k_{R_j}) \simeq -\left(\frac{\partial^2 \mathcal{L}(k_{R_j} | e_1, \dots, e_n)}{\partial k_{R_j}^2} \bigg|_{k_{R_j} = \widehat{k}_{R_j}} \right)^{-1} = \frac{\widehat{k}_{R_j}^2}{\sum_{i=1}^{n} \mathbf{1}_{R_i = R_j}}. \tag{A.18}$$

These terms are of course similar to the diagonal terms of the Hessian matrix.

B

Proof of Theorem 9.12

Theorem 9.12 (Continuous-discrete phase mapping). *Given a finite set of interactions $\mathcal{I}$, there exists a function $\Omega : \mathbb{S} \rightarrow \mathcal{V}^{ext}$, which maps each extended state $\mathbf{x} \in \mathbb{S}$ to a corresponding extended mode $\boldsymbol{\xi} \in \mathcal{V}^{ext}$, such that $\boldsymbol{\xi}$ is the active control mode whenever the system is in state $\mathbf{x}$.*

Proof. First, we show the *existence* of an image $\boldsymbol{\xi} \in \mathcal{V}^{\text{ext}}$ for each $\mathbf{x} \in \mathbb{S}$. By construction, each extended state $\mathbf{x}$ corresponds to a unique arrangement of the particles in $\mathbb{X}$. Given this arrangement, the control mode of each particle P_i is completely and uniquely determined by the status of the interactions in which P_i is involved. Whether an interaction $I \in \mathcal{I}$ is active depends solely on the predicate *cond*, which is completely and uniquely determined by $\mathbf{x}$, and the functions $\mathcal{D}_1$ and $\mathcal{D}_2$, which may depend on the status of other interactions. The property of monotonicity (Remark 9.7) and the finiteness of the set $\mathcal{I}$ ensures that any dependency chain is finite (in particular, if any cyclic dependency exists, all of its constitutive interactions will always remain inactive). As a result, given the position of each particle in $\mathbb{X}$, one can determine the status of each interaction, which in turn determines the interaction configuration of each particle, and the extended mode $\boldsymbol{\xi} \in \mathcal{V}^{\text{ext}}$.

Second, we show the *uniqueness* of $\boldsymbol{\xi}$. Let the extended state $\mathbf{x}$ have two images $\boldsymbol{\xi}_1$ and $\boldsymbol{\xi}_2$. If these two extended modes are different, then the status of at least one interaction, say I_1, must be different in either modes. Since the predicate *cond* of I_1 is completely determined by $\mathbf{x}$, this difference must originate from the dependency of I_1 (given by either $\mathcal{D}_1$ or $\mathcal{D}_2$) on another interaction, say I_2, whose status is also different $\boldsymbol{\xi}_1$ and $\boldsymbol{\xi}_2$. A similar argument can then be applied to I_2, which in turn depends on I_3, and so on, until the end of the dependency chain. In presence of cyclic dependencies, no interaction could have become active in the first place, in which case $\boldsymbol{\xi}_1$ equals $\boldsymbol{\xi}_2$. In absence of cyclic dependencies, the only cause for $\boldsymbol{\xi}_1$ and $\boldsymbol{\xi}_2$ being different is that the predicate *cond* of some interaction I_i is different in either modes, which is impossible since it is fully determined by $\mathbf{x}$. Therefore, we have $\boldsymbol{\xi}_1 = \boldsymbol{\xi}_2$.

C

Expectation of the Second-Order Error

We derive the expectation of the second-order error $\mathcal{E}_2$ between the steady state predictions of macro-stochastic and macro-deterministic models. Indeed, the finiteness of the population introduces a steady state error that grows as the number of agents decreases; an infinite number of agents makes both approaches equivalent. However, since we have a finite number N of agents, we expect to see some difference between the desired and actual distribution of agents, even after convergence. This steady state error has to be characterized in order to determine whether the given distribution has converged or not. In our case, we define the second-order error $\mathcal{E}_2$ as the square of the l^2-norm between the actual distribution and the desired distribution of agents:

$$\mathcal{E}_2 = \|\mathbf{x}^{N_0} - \mathbf{x}^{\infty}\|^2 = \sum_{i=1}^{N_S} \left(x_i^{N_0} - x_i^{\infty} \right)^2 . \tag{C.1}$$

Assume that the system is at equilibrium, and $x_i = \sum_{j=1}^{N_0} \mathbf{1}_{j,i}/N_0$ with

$$\mathbf{1}_{j,i} = \begin{cases} 1 \text{ if agent } j \text{ is in state } i \text{ at steady state,} \\ 0 \text{ otherwise.} \end{cases} \tag{C.2}$$

In the thermodynamic limit, each agent is in state i with probability x_i^{∞}. Also, each agent moves independently of the others. Hence, variables $\mathbf{1}_{j,i}$ are independent for each agent[1]. Therefore, we have (assuming $t \to \infty$):

$$\begin{aligned} E[\mathcal{E}_2] &= E\left[\sum_{i=1}^{N_S} (x_i^{N_0} - x_i^{\infty})^2 \right] = \sum_{i=1}^{N_S} E\left[(x_i^{N_0} - x_i^{\infty})^2 \right] \\ &= \sum_{i=1}^{N_S} E\left[(x_i^{N_0})^2 - 2\, x_i^{N_0}\, x_i^{\infty} + (x_i^{\infty})^2 \right] \\ E[x_i] &= E\left[\frac{\sum_{j=1}^{N_0} \mathbf{1}_{j,i}}{N_0} \right] = x_i^{\infty} \end{aligned} \tag{C.3}$$

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[1] Actually, they have to follow the additional constraint $\sum_{i=1}^{N_S} \sum_{j=1}^{N_0} \mathbf{1}_{j,i} = N_0$ to conserve the number of agents. However, they are independent for each agent, which is the property used.

$$E[x_i^2] = E\left[\frac{\sum_{l,k} \mathbf{1}_{l,i} \cdot \mathbf{1}_{k,i}}{N_0^2}\right] = \frac{1}{N_0}\left(\sum_j E\left[\frac{\mathbf{1}_{j,i}^2}{N_0}\right] + \sum_{k \neq l} E\left[\frac{\mathbf{1}_{l,i} \cdot \mathbf{1}_{k,i}}{N_0}\right]\right)$$
$$= \frac{1}{N_0}\left(x_i^\infty + (N_0 - 1) \cdot (x_i^\infty)^2\right). \tag{C.4}$$

Hence, $$E[\mathcal{E}_2] = \frac{1}{N_0}\sum_{i=1}^{N}(x_i^\infty - (x_i^\infty)^2) = \frac{1 - \sum_{i=1}^{N}(x_i^\infty)^2}{N_0} \tag{C.5}$$

Equation C.5 can be computed for a any given state distribution and number of agents, but it accounts only for the contribution of small copy numbers to the overall error exhibited by macro-deterministic models.

Glossary

ABM	Agent-Based Model
CAD	Computer-Aided Design
CFD	Computational Fluid Dynamics
CME	Chemical Master Equation
CMM	Canonical Microscopic Model
CRN	Chemical Reaction Network
CRNT	Chemical Reaction Network Theory
CRW	Correlated Random Walk
DES	Discrete Event Simulation
DOF	Degree of Freedom
FSM	Finite State Machine
GA	Genetic Algorithm
IR	Infrared
KS	Kolmogorov-Smirnov
MCM	Monte-Carlo Method
MDP	Markov Decision Process
MEMS	Micro-Electro-Mechanical System
MLE	Maximum Likelihood Estimation
MLMM	Multi-Level Modeling Methodology
ODE	Ordinary Differential Equation
PDE	Partial Differential Equation
PDF	Probability Density Function
PSO	Particle Swarm Optimization
SA	Self-Assembly
SMP	Smart Minimal Particle
SSA	Stochastic Simulation Algorithm

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