

Coarse-graining and reconstruction for Markov matrices

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Abstract

We present a coarse-graining (or model order reduction) procedure for stochastic matrices by clustering. The method is consistent with the natural structure of Markov theory, preserving positivity and mass, and does not rely on any tools from Hilbert space theory. The reconstruction is provided by a generalized Penrose-Moore inverse of the coarse-graining operator incorporating the inhomogeneous invariant measure of the Markov matrix. As we show, the method provides coarse-graining and reconstruction also on the level of tensor spaces, which is consistent with the notion of an incidence matrix and quotient graphs, and, moreover, allows to coarse-grain and reconstruct fluxes. Furthermore, we investigate the connection with functional inequalities and Poincaré-type constants.

1 Introduction

Coarse-graining or model reduction is a fundamental procedure that reduces the complexity of a physical model. It is a well-established tool used in many branches of applied mathematics including analysis, modeling and numerics. In this paper we are interested in coarse-graining for physical systems on a finite state space described by Markov matrices.

Let us first describe the mathematical setting. Fixing a finite state spaces $\mathcal{Z} = \{1, \dots, n\}$, $n \in \mathbb{N}$, the statistical states are given by the set of probability vectors

$$\text{Prob}(\mathcal{Z}) = \left\{ p \in \mathbb{R}^n : p_i \geq 0, \sum_{i=1}^n p_i = 1 \right\} \subset \mathbb{R}^n := X^*.$$

Important is the distinction between primal X and dual spaces X^* (although both are isomorphic to the \mathbb{R}^n as real-vector spaces), where the first contains functions on \mathcal{Z} equipped with the supremum-norm, and the second contains probabilities on \mathcal{Z} equipped with the 1-norm. Dual pairing is denoted by $\langle \cdot, \cdot \rangle$. Apart from X being a vector space, it has a natural order, i.e. $x \geq y$ if the pointwise estimate $x_i \geq y_i$ holds for all $i \in \mathcal{Z}$. Moreover, it is an algebra, i.e. product of two elements x and y is given by $(x \cdot y)_i = x_i \cdot y_i$ by pointwise multiplication.

The change of statistical states is described by a Markov matrix (or operator) $K : X \rightarrow X$, which, by definition, satisfies $K_{ij} \geq 0$ and $\sum_{j \in \mathcal{Z}} K_{ij} = 1$ for all $i \in \mathcal{Z}$. Equivalently, K maps non-negative elements in X to non-negative and $K \mathbb{1} = \mathbb{1}$, where $\mathbb{1}_X = (1, \dots, 1)^T$ is the constant one-vector. The invariant vector $\pi \in \text{Prob}(\mathcal{Z}) \subset X^*$ of K^* is defined by satisfying $\sum_i \pi_i K_{ij} = \pi_j$, or, equivalently, by $\pi^T K = \pi^T$, or $K^* \pi = \pi$. Throughout the paper, we assume that the invariant vector is unique and positive. (See e.g. [Nor97] for introductory reading on Markov matrices.) We remark that for further generalizations to infinite and continuous state spaces (in which case X and X^* are infinite dimensional) we denote by $B^* : Y^* \rightarrow X^*$ the dual (or adjoint) operator of $B : X \rightarrow Y$, which is just the (real) transpose in matrix representation.

The aim of the paper is to present an operator-theoretic and structure preserving approach to coarse-graining for Markov matrices. In contrast to classical model order reduction procedures, it does not rely on tools from Hilbert space theory like orthonormal projections or symmetry, as for example Krylov subspace projection methods and so on (see e.g. [SvdVR08]). In general, Hilbert space projections will not preserve positivity of the measures, which is unphysical. Here, the approach is more direct and based on clusters. Reduction methods based on clusters as [ChS20, CY*20] preserve the graph theoretical structure for Markov chains, but do not distinguish between primal and dual spaces. With that, the theory is based on homogenous Euclidean spaces, which are not canonical for Markov matrices as the invariant measure $\pi \in \text{Prob}(\mathcal{Z})$ is in general not homogenous and the natural Hilbert space would be $L^2(\pi)$.

Here, the coarse-graining procedure is based on the structural duality between X and X^* . Implicitly, the involved operators (maybe in a modified form) have been used in literature (see e.g. [ChS20, PMK06]) and we recall technical results from [MiS20] in Section 2. However, to the author's knowledge no structural study has been done so far. Heuristically, the reconstruction procedure rebuilds the information from the coarser system back to the finer system using the local information of the invariant probability vector π . The reconstruction operators can be understood as generalized Penrose-Moore inverse of the coarse-graining operator respecting the (in general inhomogeneous) invariant measure π . This procedure has many different mathematical advantages, which become clear in the following. First, it is consistent with the graph-theoretic notion of a incidence matrix (or operator) and quotient graph (see Section 3). Moreover, it provides tools for reconstructing functions on tensor spaces (e.g. fluxes defined on edges) as well (see Section 4.2 for more details).

Another important question regarding coarse-graining is the question how eigenvalues depend on the reduction procedure. The first nontrivial eigenvalue defines the spectral gap and provides information regarding asymptotical decay of the process (see e.g. [BoT06]). In the last decades, functional inequalities for Markov processes on discrete states spaces have been studied intensively [BoT06, ErM12, Joh17, FaS18, FaF21]. In Section 5, we derive the connection between coarse-graining and energy functionals. In particular, we derive estimates for functional inequalities and discrete Poincaré-type constants (like the Poincaré constant, or log-Sobolev constant).

2 Coarse-graining

We present the operator theoretic framework for capturing the collection of states, which has also been introduced in [MiS20].

2.1 Operator theoretic coarse-graining

For two finite state spaces $\mathcal{Z} = \{1, \dots, n\}$, $\hat{\mathcal{Z}} = \{1, \dots, \hat{n}\}$ with $\hat{n} < n$, we assume that there is a given surjective function $\phi : \mathcal{Z} \rightarrow \hat{\mathcal{Z}}$, which plays the role of a coarse-graining or clustering map. We define the *coarse-graining operator* $M : \hat{X} \rightarrow X$ by $(M\hat{x})_i = \hat{x}_{\phi(i)}$ for all $\hat{x} \in \hat{X}$. One easily sees that M is a deterministic Markov matrix since the adjoint (or dual) matrix $M^* : X^* \rightarrow \hat{X}^*$ maps pure states (or dirac-measures) to pure states. In fact the dual operator M^* should be called *coarse-graining operator* because it maps statistical states in X^* to coarser states in \hat{X}^* . Since M is a deterministic Markov matrix we have that for all $\hat{x}, \hat{y} \in \hat{X}$ it holds $M(\hat{x} \cdot \hat{y}) = M\hat{x} \cdot M\hat{y}$, where the multiplication is meant pointwise. (By the way, this characterizes all deterministic Markov matrices.)

Fixing a positive probability vector $\pi \in X^*$, we may define the multiplication operator given by the

diagonal matrix $Q_\pi : X \rightarrow X^*$, i.e. $(Q_\pi x)_i = \pi_i x_i$. We observe that Q_π is symmetric and its inverse is given by $Q_\pi^{-1} : X^* \rightarrow X$, $p \mapsto \rho = (p_i/\pi_i)_i$. One easily sees that the multiplication operator satisfies $\langle x, Q_\pi y \rangle = \langle x \cdot y, \pi \rangle$ for all $x, y \in X$. Although the spaces are finite-dimensional and isomorphic, we remark that the parameter π of Q_π is an element of the dual space and the inverse $Q_\pi^{-1} : p \mapsto \rho$ maps a probability vector p to the relative density ρ of p with respect to π as a discrete analogue of the Radon-Nikodym derivative.

We define a new coarse-grained measure $\hat{\pi}$ by $\hat{\pi} = M^* \pi$. We easily observe that $\hat{\pi}$ is also positive. We have the following characterization of a deterministic Markov matrix.

Lemma 2.1 ([MiS20, Lemma 2.4]). *We have $\hat{\pi} = M^* \pi$ if and only if $Q_{\hat{\pi}} = M^* Q_\pi M$.*

Proof. Evaluating $Q_{\hat{\pi}} = M^* Q_\pi M$ at $\hat{\mathbb{1}}$, we have $\hat{\pi} = Q_{\hat{\pi}} \hat{\mathbb{1}} = M^* Q_\pi M \hat{\mathbb{1}} = M^* Q_\pi \mathbb{1} = M^* \pi$, which is one direction of the claim.

For the other claim, we introduce the multiplication operator $\Pi_{\hat{y}} : \hat{X} \rightarrow \hat{X}$ by $(\Pi_{\hat{y}} \hat{x})_j = \hat{y}_j \hat{x}_j$ with the dual operator $\Pi_{\hat{y}}^* : \hat{X}^* \rightarrow \hat{X}^*$ given by $\Pi_{\hat{y}}^* \hat{c} = Q_{\hat{c}} \hat{y}$. Using that M is a deterministic operator we have $M \Pi_{\hat{y}} = \Pi_{M \hat{y}} M$, which implies by dualizing $\Pi_{\hat{y}}^* M^* = M^* \Pi_{M \hat{y}}^*$. So we get for any \hat{x} that $Q_{\hat{\pi}} \hat{x} = \Pi_{\hat{x}}^* \hat{\pi} = \Pi_{\hat{x}}^* M^* \pi = M^* \Pi_{M \hat{x}}^* \pi = M^* Q_\pi M \hat{x}$. \square

This important relation does not hold if M is not a deterministic operator. Moreover, it implies that the following diagram commutes:

$$\begin{array}{ccc} \hat{X} & \xrightarrow{M} & X \\ Q_{\hat{\pi}} \downarrow & & \downarrow Q_\pi \\ \hat{X}^* & \xleftarrow{M^*} & X^* \end{array}$$

Since $Q_{\hat{\pi}}$ is invertible, it is now possible to “invert” the coarse-graining operator M , by defining the so-called *reconstruction operator* $N : X \rightarrow \hat{X}$:

$$N = Q_{\hat{\pi}}^{-1} M^* Q_\pi : X \rightarrow \hat{X}, \quad N^* = Q_\pi M Q_{\hat{\pi}}^{-1} : \hat{X}^* \rightarrow X^*. \quad (2.1)$$

$$\begin{array}{ccc} \hat{X} & \xrightleftharpoons{M} & X \\ Q_{\hat{\pi}} \downarrow & \begin{array}{c} N \\ M^* \end{array} & \downarrow Q_\pi \\ \hat{X}^* & \xrightleftharpoons{N^*} & X^* \end{array}$$

The operator N^* reconstructs the coarser statistical states in \hat{X}^* respecting the measure $\pi \in X^*$. Before summarizing properties of N in the next proposition, we introduce the notion of *detailed balance*.

Definition 2.2. A Markov matrix K is said to satisfy the *detailed balance condition* with respect to its positive invariant measure π , if $K^* Q_\pi = Q_\pi K$.

Proposition 2.3 ([MiS20, Lemma 2.5, Proposition 2.7]). *Let $M : \hat{X} \rightarrow X$ be a deterministic Markov matrix and let $\pi \in X^*$ be a given positive probability vector. Let N and N^* be defined by (2.1). Then the following holds:*

- 1 N is a Markov matrix and $N^*\hat{\pi} = \pi$, i.e. N^* inverts with respect to π .
- 2 $NM = \text{id}_{\hat{X}}$ and $MN =: P$ is a (Markov) projection on X . We have the splitting $X = \text{Range}(P) + \text{Ker}(P) = \text{Range}(M) + \text{Ker}(N)$. The adjoint P^* has π as its stationary measure and satisfies detailed balance.

Proof. Clearly N is nonnegative and $N\mathbb{1} = Q_{\hat{\pi}}^{-1}M^*Q_{\pi}\mathbb{1} = Q_{\hat{\pi}}^{-1}M^*\pi = Q_{\hat{\pi}}^{-1}\hat{\pi} = \hat{\mathbb{1}}$. Hence, N is a Markov matrix. Moreover we have $N^*\hat{\pi} = Q_{\pi}MQ_{\hat{\pi}}^{-1}\hat{\pi} = Q_{\pi}M\hat{\mathbb{1}} = \pi$.

For the second claim, we use Lemma 2.1, which implies that $M^*N^* = M^*Q_{\pi}MQ_{\hat{\pi}}^{-1} = \text{id}_{\hat{X}^*}$. Hence, $NM = \text{id}_{\hat{X}}$ and $P = MN$ is a projection. This provides the decomposition of X since N is surjective and M is injective. Since it is the composition of Markov matrices P is again a Markov matrix and obviously $P^*\pi = \pi$. To see that P satisfies detailed balance, we observe

$$Q_{\pi}P = Q_{\pi}MN = Q_{\pi}MQ_{\hat{\pi}}^{-1}M^*Q_{\pi} = N^*M^*Q_{\pi} = P^*Q_{\pi}.$$

□

Remark 2.4. We remark that in [Ste13] inverse operators for general Markov operators have been introduced and their relation to the direction of time has been investigated.

Finally, we investigate the connection between the “inverse” operator N and the Penrose-Moore inverse of linear algebra. First, we see that $N : X \rightarrow \hat{X}$ is a pseudo inverse of $M : \hat{X} \rightarrow X$, because $MNM = M$ and $NMN = N$ by Proposition 2.3. Recall that for an injective $M : \hat{X} \rightarrow X$, the Penrose-Moore inverse of M can be defined by

$$M^+ = (M^*M)^{-1}M^*.$$

The next proposition shows, that this formula provides exactly N , if the adjoint operator M^* is understood in the space $L^2(\pi)$. In particular, if $\pi = \frac{1}{N}(1, \dots, 1)^T$, we have that $N = M^+$. To see this, we define the $L^2(\pi)$ -inner product in X by

$$(x, y)_{\pi} := \langle x, Q_{\pi}y \rangle = \langle x \cdot y, \pi \rangle.$$

Proposition 2.5. *The reconstruction operator $N = Q_{\hat{\pi}}^{-1}M^*Q_{\pi}$ is the $L^2(\pi)$ -adjoint of M . In particular, N is generalized Penrose-Moore inverse of M in $L^2(\pi)$.*

Proof. We have that

$$(M\hat{x}, y)_{\pi} = \langle \hat{x}, M^*Q_{\pi}y \rangle = \langle \hat{x}, Q_{\hat{\pi}}Ny \rangle = (\hat{x}, Ny)_{\hat{\pi}}.$$

□

We note that the notion of *detailed balance* from Definition 2.2 means that the Markov matrix K is symmetric in $L^2(\pi)$.

2.2 Example

For an example, we consider $Z = \{1, 2, 3\}$ and $\hat{Z} = \{\hat{1}, \hat{2}\}$ and define $\phi(1) = \hat{1}$, $\phi(2) = \phi(3) = \hat{2}$. In matrix representation, the coarse-graining operator has the form

$$M = \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}, \quad M^* = \begin{pmatrix} 1 & & \\ & 1 & 1 \end{pmatrix}.$$

Setting $\pi = (\pi_1, \pi_2, \pi_3)^\top$ we obtain $\hat{\pi} = (\pi_1, \pi_2 + \pi_3)^\top$, and hence

$$N = \begin{pmatrix} 1 & & \\ & \frac{\pi_2}{\pi_2 + \pi_3} & \frac{\pi_3}{\pi_2 + \pi_3} \end{pmatrix}, \quad P = MN = \begin{pmatrix} 1 & & \\ & \frac{\pi_2}{\pi_2 + \pi_3} & \frac{\pi_3}{\pi_2 + \pi_3} \\ & \frac{\pi_2}{\pi_2 + \pi_3} & \frac{\pi_3}{\pi_2 + \pi_3} \end{pmatrix}.$$

2.3 Coarse-graining for Markov matrices

Let a Markov matrix $K : X \rightarrow X$ be given. We assume that its adjoint K^* has a unique invariant measure π , i.e. $K^*\pi = \pi$. We define the coarse-grained Markov matrix \hat{K} by contracting K via

$$\hat{K} = NKM : \hat{X} \rightarrow \hat{X}.$$

The next proposition shows that \hat{K} can indeed be understood as a coarse-grained version of K .

Theorem 2.6. *Let a Markov matrix $K : X \rightarrow X$ with an invariant measure π be given. Let M be a deterministic Markov matrix, and reconstruction operator N be defined by (2.1). Let $\hat{K} := NKM : \hat{X} \rightarrow \hat{X}$. Then, we have*

- 1 \hat{K} is a Markov matrix on \hat{X} .
- 2 \hat{K}^* has $\hat{\pi}$ as its invariant measure.
- 3 Define the Markov chain $p_{k+1} = K^*p_k$, $p_0 \in X^*$. If there is an equilibration of the form $p_k = N^*\hat{p}_k$ for $\hat{p}_k \in \hat{X}$ and all $k \geq 0$, then the probability vectors \hat{p}_k satisfy the coarse-grained Markov chain $\hat{p}_k = \hat{K}^*\hat{p}_{k-1}$.
- 4 If K satisfies the detailed balance condition with respect to π , then does \hat{K} with respect to $\hat{\pi}$.

Equilibration $p_k = N^*\hat{p}_k$ means that the densities of p_k and \hat{p}_k with respect to π or $\hat{\pi}$, respectively are equilibrated, i.e.

$$p_k = Q_\pi M Q_{\hat{\pi}}^{-1} \hat{p}_k \quad \Leftrightarrow \quad \rho_k = M \hat{\rho}_k,$$

where $\rho_k = Q_\pi^{-1} p_k$, $\hat{\rho}_k = Q_{\hat{\pi}}^{-1} \hat{p}_k$. In particular, this makes clear why \hat{K} is the natural coarse-graining Markov matrix of K .

Proof. Since \hat{K} is the composition of Markov matrices it is itself a Markov matrix. Moreover, we see that $\hat{\pi}$ is the invariant measure of \hat{K} , because

$$\hat{K}^*\hat{\pi} = M^*K^*N^*\hat{\pi} = M^*K^*\pi = M^*\pi = \hat{\pi}.$$

Considering the Markov chain, let $p_k = K^* p_{k-1}$ be given. Assuming that $p_k = N^* \hat{p}_k$, we conclude that $\hat{p}_k = M^* N^* \hat{p}_k = M^* p_k$. Hence,

$$\hat{p}_k = M^* p_k = M^* K^* p_{k-1} = M^* K^* N^* \hat{p}_{k-1} = \hat{K}^* \hat{p}_{k-1}.$$

Finally, if K satisfies detailed balance with respect to π then $Q_\pi K = K^* Q_\pi$, and hence, we have

$$Q_\pi \hat{K} = Q_\pi N K M = M^* Q_\pi K M = M^* K^* Q_\pi M = M^* K^* N^* Q_\pi = \hat{K}^* Q_\pi.$$

□

Conversely, if $\hat{p}_{k+1} = \hat{K}^* \hat{p}_k$, and $\hat{K} = N K M$, then a direct computation shows that $p_k := N^* \hat{p}_k$ solves the projected Markov chain $p_{k+1} = P^* K^* P^* p_k$, which in general is different to $p_{k+1} = K^* p_k$. In this sense, the projection P describes the information loss going from a coarser system to a finer system.

Remark 2.7. Theorem 2.6 naturally generalizes to continuous time Markov processes (see for example [MiS20]). Let $p(t) = e^{tA} p_0$ or equivalently p solving $\dot{p} = A^* p$ be given, where A is a Markov generator such that e^{tA} is a semigroup of Markov matrices. If $p(t) = N^* \hat{p}(t)$, then the coarse-grained probability vectors \hat{p} satisfies the coarse-grained Markov process $\dot{\hat{p}} = \hat{A}^* \hat{p}$, with the coarse-grained Markov generator

$$\hat{A} = N A M.$$

3 Coarse-grained network

Graph theoretically, a Markov matrix K defines a directed graph $G = G(V, E)$, with vertices given by the state space \mathcal{Z} and edges between states z_i and z_j whenever $K_{ij} > 0$. An equivalence relation given by the coarse-graining map $\phi : \mathcal{Z} \rightarrow \hat{\mathcal{Z}}$ (i.e. $z_i \sim z_j$ iff $\phi(z_i) = \phi(z_j)$), defines a partition of the the graph into blocks. By definition, these blocks define the vertices of the so-called *quotient graph* \hat{G} . The edges in the quotient graph are defined as follows: two blocks B_1 and B_2 are adjacent if some vertex in B_1 is adjacent to some vertex in B_2 with respect to the edges in the starting graph. That means if on $G = G(V, E)$ there is an equivalence relation \sim then \hat{G} has vertices $\hat{V} = V / \sim$ and edges $\{([u]_\sim, [v]_\sim) : (u, v) \in E\}$. In particular, the edges in each equivalence class (or block) vanish (see e.g. [Bo198]).

Since we are interested in functions that are defined on the edges (e.g. fluxes), we translate the above state-based coarse-graining procedure to edges. For this it is convenient to introduce tensor spaces.

3.1 Coarse-graining in tensor spaces

Naturally the space over the edges can be identified by matrices or equivalently by the tensor product space $X \otimes X \simeq L(X^*, X)$. In particular, we use both formulations and switch between them whenever necessary. In principle, also multi-tensor spaces can be considered for example to capture cycles between several states. However, we restrict ourselves to tensors of second order.

Importantly the tensor space $X \otimes X$ is consistent with the concept of Markov matrices capturing positivity and duality. Positivity is again defined pointwise. The constant 1-element in $X \otimes X$ is given

by $\mathbb{1} \otimes \mathbb{1}$ and will be denoted by $\mathbb{1}_\otimes$. The dual space of $L(X^*, X)$ is given by $L(X^*, X)^* \simeq L(X^{**}, X^*) \simeq L(X, X^*) \simeq X^* \otimes X^*$. The duality mapping is given by

$$A \in L(X, X^*) \mapsto \text{Tr}(A^* \cdot) \in L(X^*, X)^*.$$

In the following we will denote the dual pairing between $L(X^*, X)$ and $L(X, X^*)$ by

$$\langle\langle A, B \rangle\rangle := \text{Tr}(A^* B) = \text{Tr}(A B^*) = \sum_{i,j} A_{ij} B_{ij},$$

which is just the usual dual pairing by pointwise multiplication if the matrices are understood as $n \times n$ -vectors.

We may also define multiplication operators with elements of the dual space. For a given matrix $m \in L(X, X^*) \simeq X^* \otimes X^*$ we define the (diagonal) multiplication operator by

$$Q_m : L(X^*, X) \rightarrow L(X, X^*), \quad Q_m b = (m_{ij} b_{ij})_{ij}$$

by pointwise multiplication. Clearly, we have that $Q_m \mathbb{1}_\otimes = m$. Indeed, the target space of Q_m makes sense which can be seen from the following observation that Q_m is symmetric:

$$\langle\langle c, Q_m b \rangle\rangle = \sum_{i,j} m_{ij} b_{ij} c_{ij} = \sum_{i,j} m_{ij} c_{ij} b_{ij} = \langle\langle b, Q_m c \rangle\rangle.$$

Of great importance for us is the element $m = Q_\pi K \in L(X, X^*) \simeq X^* \otimes X^*$, which can be understood as a weight function defined on the edges.

For the coarse-grained state space \hat{X} , we analogously define $\hat{X} \otimes \hat{X} \simeq L(\hat{X}^*, \hat{X})$ and $\hat{X}^* \otimes \hat{X}^* \simeq L(\hat{X}, \hat{X}^*)$ by replacing X by \hat{X} . We define a coarse-graining operator on $L(X^*, X)$ by

$$\begin{aligned} \widetilde{M} : L(\hat{X}^*, \hat{X}) &\simeq \hat{X} \otimes \hat{X} && \rightarrow L(X^*, X) \simeq X \otimes X \\ \hat{b} &&& \mapsto \widetilde{M} \hat{b} := M \hat{b} M^*. \end{aligned}$$

Proposition 3.1. *The operator \widetilde{M} has the following properties:*

1 \widetilde{M} is again a deterministic Markov operator.

2 The adjoint operator is given by

$$\widetilde{M}^* : L(X, X^*) \rightarrow L(\hat{X}, \hat{X}^*), \quad \widetilde{M}^* b = M^* b M.$$

3 Let $m := Q_\pi K$. Then $\hat{m} := \widetilde{M}^* m = Q_{\hat{\pi}} \hat{K}$.

Proof. Clearly, \widetilde{M} is again positive. Moreover, it maps to constant 1-function $\hat{\mathbb{1}}_\otimes = \hat{\mathbb{1}} \otimes \hat{\mathbb{1}}$ in $\hat{X} \otimes \hat{X}$ to the constant 1-function $\mathbb{1}_\otimes = \mathbb{1} \otimes \mathbb{1}$ in $X \otimes X$ because we have

$$\widetilde{M} \left(\hat{\mathbb{1}} \otimes \hat{\mathbb{1}}^* \right) = M \left(\hat{\mathbb{1}} \otimes \hat{\mathbb{1}} \right) M^* = M \hat{\mathbb{1}} \otimes M \hat{\mathbb{1}} = \mathbb{1} \otimes \mathbb{1}.$$

Hence, \widetilde{M} is a Markov operator. To see that it is deterministic, we use the representation of the adjoint operator \widetilde{M}^* which is the second claim and proved below. Using that, we have $\widetilde{M}^* (e_i \otimes e_j) = M^* e_i \otimes M^* e_j$ which is again a pure state in $\hat{X}^* \otimes \hat{X}^*$

To compute the adjoint operator \widetilde{M}^* we have for $\hat{b} \in L(\hat{X}^*, \hat{X})$ and $c \in L(X, X^*)$ that

$$\langle\langle \widetilde{M}\hat{b}, c \rangle\rangle = \text{Tr} \left(\left(M\hat{b}M^* \right)^* c \right) = \text{Tr} \left(M\hat{b}^*M^*c \right) = \text{Tr} \left(M^*cM\hat{b}^* \right) = \langle\langle M^*cM, \hat{b} \rangle\rangle,$$

where we used that the trace is invariant under commuting matrices. Hence, $\widetilde{M}^*c = M^*cM$.

For the last claim, we observe that $\hat{m} = \widetilde{M}^*m = M^*Q_\pi KM = Q_{\hat{\pi}}NKM = Q_{\hat{\pi}}\hat{K}$. \square

Proposition 3.1 shows that the (dual) deterministic coarse-graining operator \widetilde{M}^* maps the weights $m = Q_\pi K$ on the coarse-grained weight $\hat{m} = Q_{\hat{\pi}}\hat{K}$. This allows to define a reconstruction operator \widetilde{N} as the inverse operator of \widetilde{M} with respect to m as in Section 2. We define

$$\widetilde{N} : L(X^*, X) \rightarrow L(\hat{X}^*, \hat{X}), \quad \widetilde{N} = Q_{\hat{m}}^{-1}\widetilde{M}^*Q_m. \quad (3.1)$$

Again, we have that $\widetilde{N}\mathbb{1}_\otimes = \hat{\mathbb{1}}_\otimes$. Its adjoint (with respect to $\langle\langle \cdot, \cdot \rangle\rangle$) is given by

$$\widetilde{N}^* : L(\hat{X}, \hat{X}^*) \rightarrow L(X, X^*), \quad \widetilde{N}^* = Q_m\widetilde{M}Q_{\hat{m}}^{-1}.$$

Clearly, the operator \widetilde{N}^* maps \hat{m} to m . The definition of reconstruction operator \widetilde{N} has two advantages. First it allows to define a coarse-grained incidence matrix as we will see next. The incidence matrix will be crucial for estimating Poincaré-type constants in Section 5. Moreover, it can be used to reconstruct fluxes, which are functions on edges (see Section 4).

3.2 Coarse-graining of the incidence matrix

The connection between X and $X \otimes X$ is given by the incidence matrix (or operator) $D : X \rightarrow L(X^*, X) \approx X \otimes X$ for the complete graph of the vertices V , which is (in coordinates) defined by

$$De_i = \sum_j (e_i \otimes e_j - e_j \otimes e_i) \in X \otimes X.$$

We remark that this definition distinguish between outgoing and ingoing edges.

To define the adjoint operator, we fix the canonical basis in the dual space $e_k^* \in X^*$ with $\langle e_k^*, e_i \rangle = \delta_{ik}$. This also defines a basis $\{e_k^* \otimes e_l^*\}_{k,l}$ in the tensor space $X^* \otimes X^*$ such that it holds $\langle\langle e_k^* \otimes e_l^*, e_i \otimes e_j \rangle\rangle = \delta_{ijkl}$. The adjoint operator D^* is given by

$$\begin{aligned} D^* : X^* \otimes X^* &\rightarrow X^*, \\ D^* (e_i^* \otimes e_j^*) (e_l) &= \langle\langle De_l, e_i^* \otimes e_j^* \rangle\rangle = \sum_k \langle\langle e_l \otimes e_k - e_k \otimes e_l, e_i^* \otimes e_j^* \rangle\rangle \\ &= \sum_k \langle\langle e_l \otimes e_k - e_k \otimes e_l, e_i^* \otimes e_j^* \rangle\rangle = \begin{cases} 0 & l \neq i, l \neq j \\ 1 & l = i \\ -1 & l = j \end{cases}, \end{aligned} \quad (3.2)$$

whenever $i \neq j$, and otherwise it is zero.

The next result shows that the coarse-graining procedure is consistent with the definition of the incidence matrix and the quotient graph.

Theorem 3.2. Let $M : \hat{X} \rightarrow X$ be given as above, which is in local coordinates $M\hat{e}_k = \sum_{i \in \phi^{-1}(k)} e_i$. Let $m \in X^* \otimes X^*$ be arbitrary and fixed, and let \tilde{N} be defined by (3.1). The operator $\hat{D} : \hat{X} \rightarrow L(\hat{X}^*, \hat{X})$ defined by

$$\hat{D} = \tilde{N}DM : \hat{X} \rightarrow L(\hat{X}^*, \hat{X})$$

is an incidence matrix, i.e. we have

$$\hat{D}\hat{e}_k = \sum_l (\hat{e}_k \otimes \hat{e}_l - \hat{e}_l \otimes \hat{e}_k).$$

Moreover, it holds $\tilde{M}\hat{D} = DM$.

Remarkably, the form of \hat{D} is independent of the $m \in X \otimes X$. We note that the second claim does not follow immediately from $\hat{D} = \tilde{N}DM$, which would imply $\tilde{M}\hat{D} = \tilde{P}DM$ with the projection $\tilde{P} = \tilde{M}\tilde{N}$ on $X \otimes X$. The relation $\tilde{M}\hat{D} = DM$ is finer and provides that the coarse-graining procedure is consistent with the definition of the quotient graph.

Proof. For the proof, we compute $\hat{D}\hat{e}_k$ explicitly. We have $M\hat{e}_k = \sum_{i \in \phi^{-1}(k)} e_i$ and hence,

$$DM\hat{e}_k = \sum_j M\hat{e}_k \otimes e_j - e_j \otimes M\hat{e}_k = \sum_j \sum_{i \in \phi^{-1}(k)} e_i \otimes e_j - e_j \otimes e_i.$$

Moreover, we have that $\tilde{N} = Q_m^{-1}\tilde{M}^*Q_m$. To evaluate $\tilde{N}(e_i \otimes e_j)$, we observe that $\tilde{M}^*(e_i \otimes e_j) = \hat{e}_{\phi(i)} \otimes \hat{e}_{\phi(j)}$ which implies that

$$\begin{aligned} \tilde{M}^*Q_mDM\hat{e}_k &= \sum_j \sum_{i \in \phi^{-1}(k)} m_{ij}\tilde{M}^*(e_i \otimes e_j) - m_{ji}\tilde{M}^*(e_j \otimes e_i) \\ &= \sum_j \sum_{i \in \phi^{-1}(k)} m_{ij}\hat{e}_{\phi(i)} \otimes \hat{e}_{\phi(j)} - m_{ji}\hat{e}_{\phi(j)} \otimes \hat{e}_{\phi(i)} \\ &= \sum_{l_j} \sum_{j \in \phi^{-1}(l_j)} \sum_{i \in \phi^{-1}(k)} m_{ij}\hat{e}_{\phi(i)} \otimes \hat{e}_{\phi(j)} - m_{ji}\hat{e}_{\phi(j)} \otimes \hat{e}_{\phi(i)} \\ &= \sum_{l_j} \hat{m}_{kl_j}\hat{e}_k \otimes \hat{e}_{l_j} - \hat{m}_{l_jk}\hat{e}_{l_j} \otimes \hat{e}_k, \end{aligned}$$

where we have used the definition of $\hat{m} = \tilde{M}^*m$ given by $\hat{m}_{kl} = \sum_{j \in \phi^{-1}(l)} \sum_{i \in \phi^{-1}(k)} m_{ij}$. Hence, we conclude that

$$\hat{D}\hat{e}_k = \tilde{N}DM\hat{e}_k = Q_m^{-1}\tilde{M}^*Q_mDM\hat{e}_k = \sum_l \hat{e}_k \otimes \hat{e}_l - \hat{e}_l \otimes \hat{e}_k,$$

which is the desired formula.

Now we prove $\tilde{M}\hat{D} = DM$ again by direct calculation. We have $\tilde{M}(\hat{e}_k \otimes \hat{e}_l) = M\hat{e}_k \otimes M\hat{e}_l$ and hence,

$$\tilde{M}\hat{D}\hat{e}_k = \sum_l M\hat{e}_k \otimes M\hat{e}_l - M\hat{e}_l \otimes M\hat{e}_k = \sum_l \sum_{j \in \phi^{-1}(l)} M\hat{e}_k \otimes e_j - e_j \otimes M\hat{e}_k = DM\hat{e}_k,$$

which we wanted to show. \square

Remark 3.3. We finally remark that the coarse-graining procedure can also be applied to undirected graphs. Introducing the space $X \odot X \simeq L_{\text{sym}}(X^*, X)$ containing the symmetric tensors (or matrices), the coarse-graining operator \tilde{M} respect the symmetric structure. Moreover, if $m = Q_\pi K$ is symmetric then also \tilde{N} maps into symmetric tensors. In the following we will treat the case of symmetric m with more detail but we will not consider undirected graphs.

4 Detailed balance Markov matrices

A special situation occurs if the operator K satisfies detailed balance meaning that $m_{ij} = \pi_i K_{ij} = \pi_j K_{ji} = m_{ji}$. We define the associated Markov generator A by $A = K - \text{id}$ and investigate the following evolution system in X^* :

$$\dot{c} = A^* c.$$

In the next lemma, we recall that assuming that K (or equivalently A) satisfies detailed balance, the system $\dot{c} = A^* c$ can be written as a gradient flow expressed via the incidence operator

$$\begin{aligned} \dot{c} &= -D^* b, \\ b &= \frac{1}{2} Q_m D \rho, \\ \rho &= Q_\pi^{-1} c, \end{aligned}$$

where the first equation is a continuity equation between the fluxes b and the concentrations c , the last equation defines the relative densities ρ of c with respect to π and the second equation is the constitutive relation between the relative densities ρ and the fluxes b , which uses the tensor valued diagonal operator Q_m . Note that there is a factor $\frac{1}{2}$ because the incidence operator D counts every edge twice.

Lemma 4.1. *Let K (or equivalently A) satisfy the detailed balance condition. Then we have $A^* = -\frac{1}{2} D^* Q_m D Q_\pi^{-1}$.*

Proof. By direct computation, we have for $\rho = \sum_i \rho_i e_i$ that

$$D\rho = \sum_i \rho_i D e_i = \sum_{i,j} \rho_i (e_i \otimes e_j - e_j \otimes e_i).$$

Hence, we get that $Q_m D\rho = \sum_{i,j} \rho_i m_{ij} e_i^* \otimes e_j^* - \rho_i m_{ji} e_j^* \otimes e_i^*$, which implies

$$-D^* Q_m D\rho = -\sum_{i,j} \rho_i m_{ij} D^* (e_i^* \otimes e_j^*) + \rho_i m_{ji} D^* (e_j^* \otimes e_i^*).$$

Evaluating both sides at e_l and using the explicit formula (3.2), we get that

$$\begin{aligned} (-D^* Q_m D\rho) e_l &= -\sum_{i,j} \rho_i m_{ij} D^* (e_i^* \otimes e_j^*) e_l + \sum_{i,j} \rho_i m_{ji} D^* (e_j^* \otimes e_i^*) e_l \\ &= -\sum_j \rho_l m_{lj} + \sum_i \rho_i m_{il} + \sum_i \rho_i m_{li} - \sum_j \rho_l m_{jl} \\ &= -\rho_l \sum_j (m_{lj} + m_{jl}) + \sum_i \rho_i (m_{il} + m_{li}). \end{aligned}$$

Using that $m_{il} = m_{li} = \pi_i A_{il} = \pi_l A_{li}$ and $\rho_i = c_i / \pi_i$, we get

$$\left(-\frac{1}{2} D^* Q_m D\rho \right) e_l = -c_l \sum_j m_{lj} / \pi_l + \sum_i c_i m_{il} / \pi_i = -c_l \sum_j A_{lj} + \sum_i c_i A_{il},$$

which implies that $A^* c = -\frac{1}{2} D^* Q_m D Q_\pi^{-1} c$ for all $c \in X$. \square

4.1 Coarse-graining for detailed balance Markov operators

We are going to show that the above gradient flow decomposition is also consistent with the coarse-graining procedure. Crucial for that result is the relation $DM = \widetilde{M}\hat{D}$.

Theorem 4.2. *Let us assume that there is an equilibration of the concentrations $c = N^*\hat{c}$. Then the coarse-grained concentrations \hat{c} solves the coarse-grained evolution equation of the form*

$$\begin{aligned}\dot{\hat{c}} &= -\hat{D}^*\hat{b}, \\ \hat{b} &= \frac{1}{2}Q_{\hat{m}}\hat{D}\hat{\rho}, \\ \hat{\rho} &= Q_{\hat{\pi}}^{-1}\hat{c}.\end{aligned}$$

In particular, we have an equilibration of the fluxes $b = \widetilde{N}^*\hat{b}$.

Proof. Since $\widetilde{M}^*N^* = \text{id}_{X^*}$, we observe that $M^*c = \hat{c}$. By Theorem 3.2 we have that $DM = \widetilde{M}\hat{D}$. Hence, we obtain

$$\dot{\hat{c}} = M^*\dot{c} = -M^*D^*b = -\hat{D}^*\widetilde{M}^*b,$$

Defining $\hat{b} := \widetilde{M}^*b$ (which implies that $b = \widetilde{N}^*\hat{b}$) and using that $\widetilde{M}^*Q_m = Q_{\hat{m}}\widetilde{N}$ and $Q_{\hat{\pi}}^{-1}N^* = MQ_{\hat{\pi}}^{-1}$, we get

$$\hat{b} = \widetilde{M}^*b = \frac{1}{2}\widetilde{M}^*Q_mDQ_{\hat{\pi}}^{-1}N^*\hat{c} = \frac{1}{2}Q_{\hat{m}}\widetilde{N}DMQ_{\hat{\pi}}^{-1}\hat{c} = \frac{1}{2}Q_{\hat{m}}\hat{D}\hat{\rho},$$

where we have introduced the coarse-grained relative density $\hat{\rho} = Q_{\hat{\pi}}^{-1}\hat{c}$. \square

4.2 Flux reconstruction

Theorem 4.2 provides that an equilibration of the fluxes necessarily occurs if concentrations equilibrate. In practice, often the converse question arises, namely how fluxes on the large graph can be reconstructed out of the coarse-grained quantities like concentrations and fluxes. As one would guess $b = \widetilde{N}^*\hat{b}$ is not the desired flux because additional fluxes between coarse-grained states are needed.

The next proposition provides an affirmative answer and shows that for a given pair (\hat{c}, \hat{b}) satisfying the continuity equation $\dot{\hat{c}} = -\hat{D}^*\hat{b}$, then there is a reconstructed flux b such that $c = N^*\hat{c}$ solves $\dot{c} = -D^*b$ and the reconstructed flux consists of two parts $b = b_1 + b_2$ such that $b_1 = \widetilde{N}^*\hat{b}$ and $b_2 \in \text{Ker}\hat{D}^*\widetilde{M}^*$. Moreover, b depends linearly on \hat{b} .

Proposition 4.3. *Let (\hat{c}, \hat{b}) satisfying the continuity equation $\dot{\hat{c}} = -\hat{D}^*\hat{b}$. Define the reconstructed concentrations by $c = N^*\hat{c}$. Then there is a reconstructed flux b , which solves the macroscopic continuity equation $\dot{c} = -D^*b$ and b is given by $b = b_1 + b_2$ with $b_1 = \widetilde{N}^*\hat{b}$ and $b_2 \in \text{Ker}\hat{D}^*\widetilde{M}^*$, which depends linear on \hat{b} .*

Proof. Let $b_1 = \widetilde{N}^*\hat{b}$. Then we have to construct $b_2 \in X^* \otimes X^*$ such that

$$\dot{c} = -D^*(b_1 + b_2) = -D^*(\widetilde{N}^*\hat{b} + b_2).$$

Since $c = N^*\hat{c}$, which implies $\dot{c} = N^*\dot{\hat{c}} = -N^*\hat{D}^*\hat{b}$, we get that b_2 has to satisfy the linear equation

$$D^*b_2 = \left(N^*\hat{D}^* - D^*\widetilde{N}^*\right)\hat{b} =: x^* \in X^*. \quad (4.1)$$

Using Fredholm's alternative, this equation is solvable if for all $x \in \text{Ker}(D)$ we have that $\langle x, x^* \rangle = 0$. So let $x \in \text{Ker}(D) \subset X$. Hence,

$$\langle x, x^* \rangle = \langle x, (N^* \hat{D}^* - D^* \tilde{N}^*) \hat{b} \rangle = \langle \hat{D} N x, \hat{b} \rangle.$$

Using Proposition 2.3, we decompose $x \in X = \text{Ker}(N) + \text{Range}(M)$. Hence, for proving that $\langle x, x^* \rangle = 0$, we may assume that $x \in \text{Range}(M)$, i.e. $M \hat{x} = x$. Using that $\hat{b} = \tilde{M}^* b_1$ and that $NM = \text{id}_{\hat{X}}$, we compute

$$\langle x, x^* \rangle = \langle \hat{D} N M \hat{x}, \tilde{M}^* b_1 \rangle = \langle \tilde{M} \hat{D} \hat{x}, b_1 \rangle = \langle D M \hat{x}, b_1 \rangle = \langle D x, b_1 \rangle = 0,$$

where we have used that $\tilde{M} \hat{D} = D M$. Hence, there exists b_2 with $D^* b_2 = (N^* \hat{D}^* - D^* \tilde{N}^*) \hat{b}$, which implies that $b = b_1 + b_2$ solves $\dot{c} = -D^* b$. By (4.1) we see that b_2 depends linearly on \hat{b} .

To see that $b_2 \in \text{Ker}(\hat{D}^* \tilde{M}^*)$, we observe that

$$\hat{D}^* \tilde{M}^* b_2 = M^* D^* b_2 = M^* (N^* \hat{D}^* - D^* \tilde{N}^*) \hat{b} = (M^* N^* M^* D^* \tilde{N}^* - M^* D^* \tilde{N}^*) \hat{b} = 0.$$

□

Remark 4.4. We note that the existence of b_2 as well as the linear dependence on \hat{b} as been used in [Ste21] to coarse-grain fast-slow linear reaction-diffusion systems.

5 Functional inequalities and Poincaré constants

In this section we apply the coarse-graining procedure to derive estimates between functionals on X and \hat{X} . First we observe the following for the expectations

$$\mathbb{E}_\pi(x) := \sum_{i \in \mathcal{Z}} \pi_i x_i = \langle x, \pi \rangle, \quad \mathbb{E}_{\hat{\pi}}(\hat{x}) := \sum_{j \in \hat{\mathcal{Z}}} \hat{\pi}_j \hat{x}_j = \langle \hat{x}, \hat{\pi} \rangle.$$

Lemma 5.1. *If $\hat{x} = N x$ or $x = M \hat{x}$, then $\mathbb{E}_\pi(x) = \mathbb{E}_{\hat{\pi}}(\hat{x})$.*

Proof. If $\hat{x} = N x$, we have $\mathbb{E}_{\hat{\pi}}(\hat{x}) = \langle \hat{\pi}, \hat{x} \rangle = \langle \hat{\pi}, N x \rangle = \langle N^* \hat{\pi}, x \rangle = \langle \pi, x \rangle = \mathbb{E}_\pi(x)$. If $x = M \hat{x}$ we conclude that $N x = \hat{x}$. □

5.1 Coarse-graining for energy functionals

For any strictly convex and non-negative function $\Phi : \mathbb{R} \rightarrow [0, \infty[$ we define the associated energy functional on X by

$$\mathcal{E}_\Phi(x) = \mathbb{E}_\pi \Phi(x) - \Phi(\mathbb{E}_\pi x) = \langle \Phi(x), \pi \rangle - \Phi(\langle x, \pi \rangle),$$

where for a vector $x \in X \simeq \mathbb{R}^n$ the function $\Phi(x) \in X$ is defined componentwise, i.e. $\Phi(x)_i = \Phi(x_i)$. Note, that the measure $\pi \in X^*$ is fixed and implicitly given in the definition of \mathcal{E}_Φ .

Lemma 5.2. *The functional \mathcal{E}_Φ is non-negative and its minimum is attained on constant vectors. Moreover, we have for the rescaled function $\tilde{\Phi}(r) = \Phi(r) + cr + d$ that $\mathcal{E}_{\tilde{\Phi}} = \mathcal{E}_\Phi$.*

Proof. The first claim follows directly by Jensen's inequality since Φ is strictly convex. Moreover, a direct computation shows that

$$\begin{aligned}\mathcal{E}_{\tilde{\Phi}}(x) &= \mathbb{E}_{\pi} \tilde{\Phi}(x) - \tilde{\Phi}(\mathbb{E}_{\pi} x) = \langle \Phi(x) + cx + d, \pi \rangle - \Phi(\mathbb{E}_{\pi} x) - c \mathbb{E}_{\pi} x - d = \\ &= \langle \Phi(x), \pi \rangle + c \langle x, \pi \rangle + d \langle \mathbb{1}, \pi \rangle - \Phi(\mathbb{E}_{\pi} x) - c \mathbb{E}_{\pi} x - d = \mathcal{E}_{\Phi}(x).\end{aligned}$$

□

Typical examples for the function Φ are:

- 1 $\Phi(r) = \frac{1}{2}r^2$. Then $\mathcal{E}_{\Phi}(x) = \frac{1}{2}(\langle x^2, \pi \rangle - \langle x, \pi \rangle^2)$ corresponds to the quadratic energy or statistical variance.
- 2 $\Phi(r) = r \log r - r + 1$. Then \mathcal{E}_{Φ} corresponds to the free energy of Boltzmann type, which will be denoted by Ent_{π} in the following.

Remark 5.3. There are several remarks in order.

- 1 Often functionals of the form $\mathcal{E}^*(p) = \langle \Psi(p/\pi), \pi \rangle$ as relative energies or entropies are considered. In contrast to \mathcal{E}_{Φ} , which is defined on X , functionals of the latter form are defined on probability vectors as elements of the dual space X^* . However, they are related via the Legendre transform. To see this, forgetting about the normalization term $-\Phi(\mathbb{E}_{\pi} x)$, the Legendre transform of the functional $\tilde{\mathcal{E}}_{\Phi}, \tilde{\mathcal{E}}_{\Phi}(x) := \langle \Phi(x), \pi \rangle$ is given by

$$\tilde{\mathcal{E}}_{\Phi}^*(p) = \sup_{x \in X} \left(\langle p, x \rangle - \tilde{\mathcal{E}}_{\Phi}(x) \right) = \sup_{x \in X} \left(\langle p, x \rangle - \langle \Phi(x), \pi \rangle \right).$$

Introducing the relative density g of p with respect to the positive probability vector π , we get that

$$\begin{aligned}\tilde{\mathcal{E}}_{\Phi}^*(p) &= \sup_{x \in X} \left(\langle g\pi, x \rangle - \langle \Phi(x), \pi \rangle \right) = \sup_{x \in X} \left(\langle g \cdot x, \pi \rangle - \langle \Phi(x), \pi \rangle \right) \\ &= \sup_{x \in X} \langle g \cdot x - \Phi(x), \pi \rangle = \langle \sup_{x \in X} (g \cdot x - \Phi(x)), \pi \rangle = \langle \Phi^*(g), \pi \rangle = \langle \Phi^* \left(\frac{p}{\pi} \right), \pi \rangle,\end{aligned}$$

which is exactly the desired form.

- 2 We could also investigate functionals of the form $\tilde{\mathcal{E}}_{\Phi}(x) = \langle \Phi(x - \mathbb{E}_{\pi} x), \pi \rangle$ as a generalization of the variance $\Phi(r) = r^2$. These functionals have the property that they are always convex. However, we will restrict to the above form.

Analogously, we define $\hat{\mathcal{E}}_{\Phi}$ on \hat{X} by replacing x by \hat{x} and π by $\hat{\pi}$. The functionals \mathcal{E}_{Φ} on X and $\hat{\mathcal{E}}_{\Phi}$ on \hat{X} can be estimated as follows.

Proposition 5.4. *We have the following relation for the functionals regarding coarse-graining and reconstruction.*

- 1 For all $\hat{x} \in \hat{X}$, $x = M\hat{x}$ implies $\mathcal{E}_{\Phi}(x) = \hat{\mathcal{E}}_{\Phi}(\hat{x})$. This holds even for all functions $\Phi : \mathbb{R} \rightarrow \mathbb{R}$ not necessarily convex.
- 2 For all $x \in X$, $\hat{x} = Nx$ implies $\hat{\mathcal{E}}_{\Phi}(\hat{x}) \leq \mathcal{E}_{\Phi}(x)$.

Proof. For the first claim, take any $\hat{x} \in \hat{X}$. Then we have with Lemma 5.1 that

$$\begin{aligned} \mathcal{E}_\Phi(x) &= \mathcal{E}_\Phi(M\hat{x}) = \sum_i \pi_i \Phi((M\hat{x})_i) - \Phi(\mathbb{E}_\pi(M\hat{x})) = \sum_{j \in \hat{Z}} \sum_{i=\phi^{-1}(j)} \pi_i \Phi((M\hat{x})_i) - \mathbb{E}_{\hat{\pi}} \hat{x} \\ &= \sum_{j \in \hat{Z}} \sum_{i=\phi^{-1}(j)} \pi_i \Phi(\hat{x}_{\phi(i)}) - \mathbb{E}_{\hat{\pi}} \hat{x} = \sum_{j \in \hat{Z}} \Phi(\hat{x}_j) \sum_{i=\phi^{-1}(j)} \pi_i - \mathbb{E}_{\hat{\pi}} \hat{x} \\ &= \sum_{j \in \hat{Z}} \hat{\pi}_j \Phi(\hat{x}_j) - \mathbb{E}_{\hat{\pi}} \hat{x} = \hat{\mathcal{E}}_\Phi(\hat{x}), \end{aligned}$$

where we used that $\hat{\pi}_j = \sum_{i=\phi^{-1}(j)} \pi_i$.

For the second claim, take any $x \in X$. Using Jensen's inequality for the convex function Φ , which means that we have the pointwise inequality $\Phi(Nx) \leq N\Phi(x)$, we obtain

$$\begin{aligned} \hat{\mathcal{E}}_\Phi(Nx) &= \langle \hat{\pi}, \Phi(Nx) \rangle - \mathbb{E}_{\hat{\pi}}(Nx) \leq \langle \hat{\pi}, N\Phi(x) \rangle - \mathbb{E}_\pi(x) = \\ &= \langle N^* \hat{\pi}, \Phi(x) \rangle - \mathbb{E}_\pi(x) = \langle \pi, \Phi(x) \rangle - \mathbb{E}_\pi(x) = \mathcal{E}_\pi(x). \end{aligned}$$

□

The log-Sobolev constant is defined by estimating $\mathcal{E}_\Phi(x^2)$ where $\Phi(r) = r \log r$, i.e. $\text{Ent}_\pi(x^2)$. From the above proposition it is not clear that is possible to obtain estimates between $\text{Ent}_{\hat{\pi}}((\hat{x})^2)$ and $\text{Ent}_\pi((M\hat{x})^2)$. In fact, we prove that this is possible even for general convex functions not necessarily quadratic.

Proposition 5.5. *Let $g : \mathbb{R} \rightarrow [0, \infty[$ be convex and satisfy $g(x) > 0$ if $x \neq 0$ and $g(0) = 0$. Then we have*

$$\forall \hat{x} \in \hat{X} \quad : \quad \text{Ent}_{\hat{\pi}}(g(\hat{x})) \leq \text{Ent}_\pi(g(M\hat{x})),$$

where again with a small abuse of notation $g(x)$ is meant component-wise, i.e. $g(x)_i = g(x_i)$.

Proof. The proof is done in two steps. First, we shift the function $\Phi(r) = r \log r$ to incorporate g . Secondly, we derive the estimate.

1. Step: Clearly, we have equality for $\hat{x} = 0$. So let us take $\hat{x} \neq 0$. Then, $g(\hat{x}) > 0$ and because $\pi > 0$, there is a constant $C > 0$ such that $\langle g(M\hat{x}), \pi \rangle \geq C > 0$. Let us define $c > 0$ by $c := e^{-(1+C)}$. We define $\tilde{\Phi}(r) = r \log r + cr$, which has its minimum at $r = C$. So we have $\tilde{\Phi}(r_1) \geq \tilde{\Phi}(r_2)$ for $r_1 \geq r_2 \geq C$. Recalling that the energy functional is invariant under affine shifts (Lemma 5.2), we have that $\text{Ent}_\pi(x) = \mathcal{E}_{\tilde{\Phi}}(x)$ and analogously also for the coarse-grained states \hat{x} . So we are going to show $\hat{\mathcal{E}}_{\tilde{\Phi}}(g(\hat{x})) \leq \mathcal{E}_{\tilde{\Phi}}(g(M\hat{x}))$, or, equivalently,

$$\langle \tilde{\Phi}(g(\hat{x})), \hat{\pi} \rangle - \tilde{\Phi}(\langle g(\hat{x}), \hat{\pi} \rangle) \leq \langle \tilde{\Phi}(g(M\hat{x})), \pi \rangle - \tilde{\Phi}(\langle g(M\hat{x}), \pi \rangle).$$

2. Step: We observe that (completely similar to the proof of Proposition 5.4)

$$\begin{aligned} \langle \tilde{\Phi}(g(M\hat{x})), \pi \rangle &= \sum_i \tilde{\Phi}(g(M\hat{x})_i) \pi_i = \sum_i \tilde{\Phi}(g(M\hat{x})_i) \pi_i = \sum_{j \in \hat{Z}} \sum_{i=\phi^{-1}(j)} \pi_i \tilde{\Phi} \circ g(\hat{x}_{\phi(i)}) \\ &= \sum_{j \in \hat{Z}} \hat{\pi}_j \tilde{\Phi} \circ g(\hat{x}_j) = \langle \tilde{\Phi}(g(\hat{x})), \hat{\pi} \rangle. \end{aligned}$$

Hence, it suffices to prove that $\tilde{\Phi}(\langle g(\hat{x}), \hat{\pi} \rangle) \geq \tilde{\Phi}(\langle g(M\hat{x}), \pi \rangle)$. To see this we use Jensen's inequality which states that $g(M\hat{x}) \leq Mg(\hat{x})$ for all Markov matrices M and convex functions g . Hence, we get $\langle g(M\hat{x}), \pi \rangle \leq \langle Mg(\hat{x}), \pi \rangle = \langle g(\hat{x}), M^*\pi \rangle = \langle g(\hat{x}), \hat{\pi} \rangle$. Since $\langle g(M\hat{x}), \pi \rangle \geq C$ and the function $\tilde{\Phi}$ is monotone for arguments larger than C by construction, we conclude that also $\tilde{\Phi}(\langle g(M\hat{x}), \pi \rangle) \leq \tilde{\Phi}(\langle g(\hat{x}), \hat{\pi} \rangle)$. Hence, the claim is proved. \square

5.2 Dirichlet forms and Poincaré-type estimates

To estimate Poincaré-type constants, we introduce the Dirichlet form (or dissipation) for K and \hat{K} by

$$\mathcal{D}_K(x) = \frac{1}{2} \sum_{i,j} \pi_i K_{ij} (x_i - x_j)^2, \quad \mathcal{D}_{\hat{K}}(x) = \frac{1}{2} \sum_{i,j} \hat{\pi}_i \hat{K}_{ij} (x_i - x_j)^2.$$

Without loss of generality, we assume that K and \hat{K} satisfy detailed balance, because the Dirichlet form takes into account only the symmetric part of $Q_m K$. Using $m = Q_\pi K$ and $\hat{m} = Q_{\hat{\pi}} \hat{K}$, the Dirichlet form is related to the generator $A = K - \text{id}$ by

$$\mathcal{D}_K(x) = \frac{1}{2} \langle \langle Dx, Q_m Dx \rangle \rangle = \frac{1}{2} \langle x, D^* Q_m Dx \rangle = -\langle x, A^* Q_\pi x \rangle = -\langle Ax, Q_\pi x \rangle = -\langle x \cdot Ax, \pi \rangle.$$

Moreover, we have $\mathcal{D}_{\hat{K}}(\hat{x}) = \frac{1}{2} \langle \langle \hat{D}\hat{x}, Q_{\hat{m}} \hat{D}\hat{x} \rangle \rangle = -\langle \hat{x} \cdot \hat{A}\hat{x}, \hat{\pi} \rangle$.

We are interested in estimating the spectral gap $\lambda = \lambda(K, \Phi)$, which is defined by the largest constant $c > 0$ that satisfies the discrete Poincaré-type inequality

$$\mathcal{D}_K(x) \geq c \mathcal{E}_\Phi(x), \quad \text{i.e.} \quad \lambda(K, \Phi) = \inf \left\{ \frac{\mathcal{D}_K(x)}{\mathcal{E}_\Phi(x)} : \forall x \mathcal{E}_\Phi(x) \neq 0 \right\}.$$

Analogously, we define $\hat{\lambda} = \hat{\lambda}(\hat{K}, \Phi) = \inf \left\{ \frac{\mathcal{D}_{\hat{K}}(\hat{x})}{\hat{\mathcal{E}}_\Phi(\hat{x})} : \forall \hat{x} \hat{\mathcal{E}}_\Phi(\hat{x}) \neq 0 \right\}$. We also define the log-Sobolev constants $\lambda_{g,LS} = \inf \left\{ \frac{\mathcal{D}_K(x)}{\text{Ent}_\pi(g(x))} : \text{Ent}_\pi(g(x)) \neq 0 \right\}$ and analogously $\hat{\lambda}_{g,LS}$.

Theorem 5.6. *With the above notation, we have the following:*

- 1 For all $\hat{x} \in \hat{X}$ we have that $\mathcal{D}_K(M\hat{x}) = \mathcal{D}_{\hat{K}}(\hat{x})$.
- 2 For all functions Φ we have that $\lambda(K, \Phi) \leq \lambda(\hat{K}, \Phi)$.
- 3 We have for the log-Sobolev constants that $\lambda_{g,LS} \leq \hat{\lambda}_{g,LS}$.

Proof. We have

$$\begin{aligned} \mathcal{D}_K(M\hat{x}) &= \frac{1}{2} \langle \langle DM\hat{x}, Q_m DM\hat{x} \rangle \rangle = -\langle M\hat{x}, A^* Q_\pi M\hat{x} \rangle \\ &= -\langle \hat{x}, M^* A^* N^* Q_{\hat{\pi}} \hat{x} \rangle = -\langle \hat{x}, \hat{A}^* Q_{\hat{\pi}} \hat{x} \rangle = \frac{1}{2} \langle \hat{x}, \hat{D}^* Q_{\hat{m}} \hat{D}\hat{x} \rangle = \mathcal{D}_{\hat{K}}(\hat{x}), \end{aligned}$$

which is the first claim. Hence, we obtain the following relations for the functional inequalities

$$\begin{aligned} \lambda &= \inf \left\{ \frac{\mathcal{D}_K(x)}{\mathcal{E}_\Phi(x)} : \mathcal{E}_\Phi(x) \neq 0 \right\} \leq \inf \left\{ \frac{\mathcal{D}_K(M\hat{x})}{\mathcal{E}_\Phi(M\hat{x})} : \mathcal{E}_\Phi(M\hat{x}) \neq 0 \right\} \\ &= \inf \left\{ \frac{\mathcal{D}_{\hat{K}}(\hat{x})}{\mathcal{E}_\Phi(M\hat{x})} : \mathcal{E}_\Phi(M\hat{x}) \neq 0 \right\}. \end{aligned}$$

For the second claim, we use Proposition 5.4 which implies that $\mathcal{E}_\Phi(M\hat{x}) = \hat{\mathcal{E}}_\Phi(\hat{x})$ and hence, $\lambda \leq \hat{\lambda}$. For the third claim we use $\text{Ent}_{\hat{\pi}}(g(\hat{x})) \leq \text{Ent}_\pi(g(M\hat{x}))$ by Proposition 5.5 to obtain the bound $\lambda_{g,LS} \leq \hat{\lambda}_{g,LS}$. \square

Proposition 5.4 states that we have $\mathcal{E}_\pi(x) \geq \mathcal{E}_{\hat{\pi}}(Nx)$ for all $x \in X$. So naturally the question arises whether it is possible to obtain uniform estimates between $\mathcal{D}_K(x)$ and $\mathcal{D}_{\hat{K}}(Nx)$. The counterexample in the next section shows that this is in general not true.

5.3 Counterexample

We compute and compare $\mathcal{D}_{\hat{K}}(Nx)$ and $\mathcal{D}_K(x)$ for a fixed $x \in X$. We have

$$\begin{aligned} \mathcal{D}_{\hat{K}}(Nx) &= \frac{1}{2} \langle \hat{D}Nx, Q_{\hat{m}}\hat{D}Nx \rangle = \frac{1}{2} \langle x, N^*\hat{D}^*Q_{\hat{m}}\hat{D}Nx \rangle = -\langle x, P^*A^*Q_\pi Px \rangle = \\ &= -\langle Px, Q_\pi APx \rangle = -\langle Px \cdot APx, \pi \rangle. \end{aligned}$$

Recall, that we have $\mathcal{D}_K(x) = -\langle x \cdot Ax, \pi \rangle$. It is clear that $\mathcal{D}_K(x) \geq \mathcal{D}_{\hat{K}}(Nx)$ holds for all $x \in \text{Range}(P)$ (because then the inequality is a trivial equality) and also for all $x \in \text{Range}(\text{id} - P) = \text{Ker}(P)$ (because $\mathcal{D}_{\hat{K}}(Nx) = 0$). In particular, we always have $\mathcal{D}_K(x) \geq \mathcal{D}_{\hat{K}}(Nx)$ in the simple case of $Z = \{1, 2\}$.

For $a \geq 0$, we define on \mathbb{R}^3 the parameter dependent Markov generator

$$A_a = \begin{pmatrix} -8 & 4 & 4 \\ 1 & -2 & 1 \\ a & a & -2a \end{pmatrix}.$$

Then A_a^* has the stationary measure $\pi_a = \frac{1}{5a+4}(a, 4a, 4)^\top$. One easily checks that A_a satisfies detailed balance with respect to π_a . As in the example from Section 2.2, we define the coarse-graining function $\phi : Z \rightarrow \hat{Z}$ with $\phi(1) = \hat{1}$ and $\phi(2) = \phi(3) = \hat{2}$. The corresponding Markov operator

$M : \hat{X} \rightarrow X$ is given by $M = \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}$. The coarse-grained stationary measure is given by $\hat{\pi}_a =$

$M^*\pi_a = \frac{1}{5a+4}(a, 4a+4)^\top$. The inverse operator $N_a : X \rightarrow \hat{X}$ and the projection $P_a : X \rightarrow X$ are given by

$$N_a = Q_{\hat{\pi}_a}^{-1}M^*Q_{\pi_a} = \begin{pmatrix} 1 & & \\ & \frac{a}{a+1} & \frac{1}{a+1} \\ & & \frac{1}{a+1} \end{pmatrix}, P_a = MN_a = \begin{pmatrix} 1 & & \\ & \frac{a}{a+1} & \frac{1}{a+1} \\ & \frac{a}{a+1} & \frac{1}{a+1} \end{pmatrix}.$$

We compute $\mathcal{D}_{K_a}(x)$ and $\mathcal{D}_{\hat{K}_a}(N_ax)$ for $x = (3, 1, 2)^\top$. We have $-\langle x \cdot A_ax, \pi_a \rangle = \frac{24a}{5a+4}$. Moreover, we have $-\langle P_ax \cdot A_aP_ax, \pi_a \rangle = \frac{8a(1+2a)^2}{(a+1)^2(5a+4)}$. Hence we have that $\mathcal{D}_{K_a}(x) \geq \mathcal{D}_{\hat{K}_a}(N_ax)$ is

equivalent to

$$\frac{24a}{5a+4} \geq \frac{8a(1+2a)^2}{(a+1)^2(5a+4)} \Leftrightarrow (1+2a)^2 \leq 3(a+1)^2 \Leftrightarrow a \leq 1 + \sqrt{3} =: a_*.$$

In particular, we have for $x = (3, 1, 2)^T$ that $\mathcal{D}_{K_a}(x) \geq \mathcal{D}_{\hat{K}_a}(N_a x)$ for $a \in [0, a^*]$ and that $\mathcal{D}_{K_a}(x) \leq \mathcal{D}_{\hat{K}_a}(N_a x)$ for $a \in [a_*, \infty[$. Summarizing, it is not possible to have uniform estimates between \mathcal{D}_{K_a} and $\mathcal{D}_{\hat{K}_a}(N_a \cdot)$. Hence, no inequality for the Poincaré-type constants can be expected.

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