Applied Mathematics Letters 22 (2009) 1471–1475

Contents lists available at ScienceDirect

Applied Mathematics Letters

journal homepage: www.elsevier.com/locate/aml

Bounding the lumping error in Markov chain dynamics

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ARTICLE INFO

Article history:
Received 5 February 2008
Received in revised form 10 March 2009
Accepted 30 March 2009

Keywords:
Markov chain
Coarse graining error
Lumped states
State space dynamics
Lumped dynamics

ABSTRACT

Forming lumped states in a Markov chain is a very useful device leading to a coarser level of description. The Markov chain on these lumped states is often taken as an approximation for the time evolution of the unlumped chain. In the present work we derive a bound on the error in this approximation.

1. Introduction

Markov chains are a standard modeling tool used in applications ranging from business [1,2] and sociology [3] to chemistry [4], physics [5,6], biology [7], computer science [8], and statistics [9]. The models in which such chains occur involve discrete stochastic dynamics represented by a matrix of transition probabilities. It is often convenient to partition the states of a chain into aggregates or lumps and to view the dynamics at a coarser level as the system of interest moves among the lumps. Examples of such aggregation include a weather model lumping the states "drizzle", "rain" and "snow" into one state called "precipitation" or a physical model aggregating the microstates of a physical system into so-called coarse grained "mesostates" each representing many microstates. Although the dynamics moving between the lumps is not even Markovian in general [10], there is a natural choice for a Markov chain model on the set of lumped states. This choice [10–13] matches the time evolution of the original unlumped chain started at equilibrium. In the present work we bound the error of the dynamics predicted by this lumped chain considered as a model of the unlumped chain. Our goal in this letter is to analyze the accuracy of such coarse grained models as compared to the exact microscopic behavior, i.e., to bound the error in a coarse grained description.

2. Lumped Markov chains

Let Ω be a finite set of states, and let p be a probability distribution on Ω viewed as a vector $p = (p_1, p_2, \ldots, p_N)$ with non-negative entries, where p_x is the probability that the system is in state $x \in \Omega$. The dynamics is given by

$$p(n+1) = p(n)G, \tag{1}$$

where G is the transition probability matrix and n denotes the (discrete) time. In the present work, we restrict our attention to Markov chains that are regular, time-homogeneous, and reversible. The time-homogeneous assumption says that G does

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0893-9659/$ – see front matter © 2009 Published by Elsevier Ltd
doi:10.1016/j.aml.2009.03.016

not depend on n. Regular means that there exists an n_0 such that G^{n_0} has all positive entries and this in turn guarantees that G has a unique stationary distribution π such that

$$\pi = \pi G. \tag{2}$$

Reversible ensures that

$$\pi_x G_{xy} = \pi_y G_{yx} \quad \forall x, y \in \Omega. \tag{3}$$

Our goal is to analyze the quantitative errors made in using a lumped Markov chain model [10] compared with the unlumped chain. Let $\{L_j\}$, $j = 1, \ldots, M$ be a partition of Ω. We introduce the collecting matrix C with

$$C_{xj} = \begin{cases} 1 & \text{if } x \in L_j \\ 0 & \text{otherwise.} \end{cases} \tag{4}$$

The matrix C serves to specify the lumped probability distribution $\hat{p} = pC$ on $\mathcal{O} = \{1, 2, \ldots, M\}$ corresponding to a distribution p on Ω. C collects the probability of the states belonging to each of the lumped states j. We also introduce the distributing matrix D with

$$D_{jx} = \begin{cases} \tilde{\pi}_x^j & \text{if } x \in L_j \\ 0 & \text{otherwise,} \end{cases} \tag{5}$$

where $\tilde{\pi}_x^j = \pi_x / \sum_{x \in L_j} \pi_x$ is the stationary distribution restricted to L_j and renormalized such that its entries add to 1. Note that for any probability distribution q in the lumped space, its image qD is locally equilibrated, i.e., qD restricted to any element L_j of our partition equals the stationary distribution π restricted to L_j and renormalized to add up to q_j. With $\hat{\pi} = \pi C$ we find

$$D_{jx} = C_{xj} \frac{\pi_x}{\hat{\pi}_j} \quad \forall x \in \Omega, j \in \mathcal{O}. \tag{6}$$

Next we consider the local equilibration operator CD. The name is justified by considering its action. Starting from any distribution p on Ω, CD collects the probability in each L_j and then redistributes this much probability $(pC)_j$ among the states $x \in L_j$ as $(pC)_j \tilde{\pi}_x^j$. In particular,

$$\pi = \pi CD. \tag{7}$$

On the other hand $DC = I$, since C collects back exactly what D distributes.

Following [14], we now introduce the lumped dynamics with transition matrix $\hat{G} = DGC$. This choice of the transition matrix together with the choice of D insures that the distribution $\hat{\pi} = \pi C$ is the stationary distribution of $\hat{G}$ since multiplying (7) by GC we have

$$\pi CDGC = \pi GC \tag{8}$$

$$\pi C\hat{G} = \pi C. \tag{9}$$

We note that $\hat{G}$ is also reversible and thus $\hat{\pi}$ is its unique stationary distribution.

3. Bounding coarse graining errors

Starting from a distribution p_0 on Ω, its time evolution among the aggregates L_j with the unlumped dynamics is $\hat{p}(t) = p_0 G^t C$ while its time evolution with the lumped dynamics is $q(t) = p_0 C \hat{G}^t$. The main question considered here is how different these two dynamics can be. To facilitate this consideration, we define the norm $\|\cdot\|_\pi$ with

$$\|v\|_\pi = \|vU_\pi\|_2 = \sqrt{\sum_x v_x^2/\pi_x}, \tag{10}$$

where $U_\pi = \mathrm{diag}(1/\sqrt{\pi_1}, 1/\sqrt{\pi_2}, \ldots, 1/\sqrt{\pi_N})$ and $\|\cdot\|_2$ is the 2-norm. The corresponding operator norm is

$$\|A\|_\pi = \max_{\|v\|_\pi = 1} \|vA\|_\pi = \max_{\|vU_\pi\|_2 = 1} \|vU_\pi U_\pi^{-1} A U_\pi\|_2 \tag{11}$$

$$= \max_{\|w\|_2 = 1} \|wU_\pi^{-1} A U_\pi\|_2 = \|U_\pi^{-1} A U_\pi\|_2. \tag{12}$$

Returning to our goal of bounding how different the two dynamics can be, we see that for one time step the difference is

$$\begin{aligned} \|p_0 C\hat{G} - p_0 GC\|_\pi &= \|p_0 CDGC - p_0 GC\|_\pi \\ &= \|p_0 (CDG - G)C\|_\pi. \end{aligned} \tag{13}$$

The difference for n steps can be similarly rearranged to give

$$\begin{aligned}\|p_0C\hat{G}^n - p_0G^nC\|_\pi &= \|p_0C(DGC)^n - p_0G^nC\|_\pi \\ &= \|p_0CDGCD\cdots GCDGC - p_0G^nC\|_\pi \\ &= \|p_0(CDG)^nC - p_0G^nC\|_\pi \\ &= \|p_0((CDG)^n - G^n)C\|_\pi. \end{aligned} \tag{14}$$

We see from (13) and (14) the prominent role of the operator CDG. While many authors [14,12,13] have considered the lumped matrix $\hat{G}$, specifying the lumped dynamics on the aggregates $\{L_1, \ldots, L_M\}$, less attention has been paid to the matrix $CDG \equiv H$ which specifies the lumped dynamics on the original states Ω.

Our goal will be to bound the n-step difference $\|H^n - G^n\|_\pi$ in terms of the one-step difference $\|H - G\|_\pi$. The general behavior of the n-step difference is that it can grow for a while, but must eventually decline to zero as, by construction, the lumped and the unlumped chain converge to the same equilibrium distribution. Bounding how large the difference can get along the way in terms of the one-step difference is the content of our theorem.

Theorem. *Let G be a transition probability matrix, and let C and D be collecting and distributing matrices as introduced above. Define*

$$\delta = \|CDG - G\|_\pi. \tag{15}$$

Then

$$\|(CDG)^n - G^n\|_\pi < K(n)\delta < \hat{K}\delta, \tag{16}$$

with $K(n) = n|\lambda_2|^{n-1}$, where λ_2 is the second-largest eigenvalue of G, and $\hat{K} = \frac{-1}{\lambda_2 e \ln(\lambda_2)}$.

Proof. We start by noting that

$$\|H^n - G^n\|_\pi = \|(H - G)H^{n-1} + G(H^{n-1} - G^{n-1})\|_\pi. \tag{17}$$

Iterating, we find

$$\|H^n - G^n\|_\pi = \left\|\sum_{k=0}^{n-1} G^k(H - G)H^{n-k-1}\right\|_\pi \tag{18}$$

$$\leq \sum_{k=0}^{n-1} \|G^k(H - G)H^{n-k-1}\|_\pi. \tag{19}$$

To proceed further, we make use of the fact that H and G have the common stationary distribution π. Accordingly, we define the projection $P_\pi = e^{\mathrm{T}}\pi$, where e is the vector $e = (1, 1, \ldots, 1) \in R^N$. The complementary projection $P_\sigma = I - P_\pi$. P_σ projects any vector onto the subspace $\Sigma = \{v | ve^{\mathrm{T}} = 0\}$. Σ is invariant under the action of any stochastic matrix. We end up with the following representation of G and H:

$$G = (P_\pi + P_\sigma)G = P_\pi + P_\sigma G, \tag{20}$$

and

$$H = (P_\pi + P_\sigma)H = P_\pi + P_\sigma H. \tag{21}$$

From (20) and (21) we obtain $H - G = P_\sigma H - P_\sigma G$, and $P_\pi P_\sigma G = P_\sigma G P_\pi = P_\pi P_\sigma H = P_\sigma H P_\pi = 0$. We note that $\|CDG - G\|_\pi = \|P_\sigma H - P_\sigma G\|_\pi = \delta$. Then for integers k, n,

$$\|G^k(H - G)H^{n-k-1}\|_\pi \tag{22}$$

$$= \|(P_\pi + P_\sigma G)^k(P_\sigma H - P_\sigma G)(P_\pi + P_\sigma H)^{n-1-k}\|_\pi \tag{23}$$

$$= \|(P_\sigma G)^k(P_\sigma H - P_\sigma G)(P_\sigma H)^{n-1-k}\|_\pi \tag{24}$$

$$\leq \|P_\sigma G\|_\pi^k \delta \|P_\sigma H\|_\pi^{n-k-1}. \tag{25}$$

Combining (14), (19) and (25) we thus find

$$\begin{aligned}\|(CDG)^n - G^n\|_\pi &\leq \sum_{k=0}^{n-1} \|G^k(H - G)H^{n-k-1}\|_\pi \\ &\leq \sum_{k=0}^{n-1} \|_\pi\, P_\sigma G\|_\pi^k \delta \|P_\sigma H\|_\pi^{n-k-1}. \end{aligned} \tag{26}$$

The manipulations thus far are valid for any submultiplicative matrix norm. We now make use of our special choice of norm, in particular of the fact that $\|A\|_\pi = \|U_\pi^{-1} A U_\pi\|_2$. By reversibility, (3), $U_\pi^{-1} G U_\pi$ is a symmetric matrix. Therefore, its 2-norm is its dominant eigenvalue. In fact, as shown below, the matrix U_π also symmetrizes P_π, $P_\pi G$, $P_\sigma G$, and CD, and thus their norm also equals their dominant eigenvalue.

To start with, a direct calculation shows $\pi U_\pi = e U_\pi^{-1}$. Thus we have $U_\pi^{-1} P_\pi U_\pi = U_\pi^{-1} e^{\mathrm{T}} \pi U_\pi = (e U_\pi^{-1})^{\mathrm{T}} (\pi U_\pi) = (\pi U_\pi)^{\mathrm{T}} (\pi U_\pi) = ((\pi U_\pi)^{\mathrm{T}} (\pi U_\pi))^{\mathrm{T}} = (U_\pi^{-1} P_\pi U_\pi)^{\mathrm{T}}$ which proves that P_π is symmetrized by U_π.

So $U_\pi^{-1} G U_\pi$ and $U_\pi^{-1} P_\pi U_\pi$ are symmetric and commute with each other as G and P_π commute. Thus $U_\pi^{-1} P_\pi G U_\pi = U_\pi^{-1} P_\pi U_\pi U_\pi^{-1} G U_\pi$ is symmetric.

It follows that $U_\pi^{-1} P_\sigma G U_\pi = U_\pi^{-1} (I - P_\pi) G U_\pi$ is symmetric as well.

Finally, from (6) we have $D = U_{\hat\pi}^2 C^{\mathrm{T}} U_\pi^{-2}$ or $U_{\hat\pi}^{-1} D U_\pi = U_{\hat\pi} C^{\mathrm{T}} U_\pi^{-1}$ and thus

$$U_\pi^{-1} C D U_\pi = (U_\pi^{-1} C U_{\hat\pi})(U_{\hat\pi}^{-1} D U_\pi) \tag{27}$$

$$= (U_\pi^{-1} C U_{\hat\pi})(U_{\hat\pi} C^{\mathrm{T}} U_\pi^{-1}) \tag{28}$$

$$= (U_\pi^{-1} C U_{\hat\pi})(U_\pi^{-1} C U_{\hat\pi})^{\mathrm{T}}. \tag{29}$$

As the rhs is a matrix times its transpose, we conclude that CD is symmetrized by U_π.

Since $U_\pi^{-1} P_\sigma G U_\pi$ is symmetric and based on the definition of the norm we have

$$\|P_\sigma G\|_\pi = |\lambda_2|, \tag{30}$$

where λ_2 is the second-largest eigenvalue of G. To bound $\|P_\sigma H\|_\pi$, we proceed as follows:

$$\|P_\sigma H\|_\pi = \|CDG - P_\pi\|_\pi = \|CDG - CDP_\pi\|_\pi \tag{31}$$

$$= \|CD(G - P_\pi)\|_\pi \le \|P_\sigma G\|_\pi \|CD\|_\pi = |\lambda_2| \|CD\|_\pi. \tag{32}$$

Now noting that CD is a stochastic matrix and U_π symmetrizes CD, we conclude that $\|CD\|_\pi = 1$.

Thus our bound becomes

$$\|H^n - G^n\|_\pi \le n|\lambda_2|^{n-1} \delta = K(n)\delta \tag{33}$$

with $K(n) = n|\lambda_2|^{n-1}$. $K(n)$ can be bound from above by maximizing over n to give

$$K(n) \le \hat K = \frac{-1}{\lambda_2 \mathrm{e} \ln(\lambda_2)}, \tag{34}$$

where e is the base of the natural logarithm. Note that this last relation gives an n-independent bound for the deviation of our lumped dynamics and completes our proof. □

4. Conclusion

Above, we presented the first quantitative bound on the errors made by using a lumped Markov chain instead of the unlumped chain. The bounds presented depend on the second-largest eigenvalue of the transition probability matrix. The important finding is that in a mesoscopic description the deviations from a microscopic description can indeed be uniformly bounded in terms of the deviation between the two descriptions in one time step. We find that the deviations decay as a power of the second-largest eigenvalue of the transition matrix. This is to be expected for any asymptotic bound since the asymptotic convergence of the chain to its equilibrium must go as powers of the modulus of the second-largest eigenvalue, known in this context as the coefficient of ergodicity [15]. The achievement of the present work derives from the fact that our bounds hold for all time and are not just asymptotic.

The main technique making our bound possible concerned the use of a carefully chosen norm, which induced operator norms that are given by eigenvalues of our matrices. The technique depends on the fact that for reversible Markov chains the transition matrices are diagonally similar to symmetric matrices and thus we can find a norm that equals the dominant eigenvalue. While it is generally possible to choose matrix norms that come arbitrarily close to the dominant eigenvalue [15], it is not clear whether our arguments would carry through for Markov chains not satisfying the reversibility condition since different norms would be needed for the different operators in our expansion.

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