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New theorems of Laplace Kernels with Radon measures in Galerkin Markov-State Models: about time evolution of eigenvalues and about errors

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Abstract

New theorems apt to the methods of the Markov-State Models in the Galerkin representation are derived directly from the Markov-chains theories. The analytical expressions of the time evolution of the eigenvalues and those of the relative error are derived. The new theorems are descended from measure-theory methodologies. The newly-written theorems therefore provide wit the analytical expressions of the time evolution of the eigenvalues and with that of the relative error from the measure-theoretical foundations of the Markov-chains models; the applications to protein folding are originated form the orthogonality of the committor functions in the appropriate description(s). The newly-found theorems are indicated of use for the other necessitated errors calculations. The modellisation used is one apt to recover the items of information about the originating chains.
Markov-chains models offer the suitable tools of a wide range of investigation branches: protein-folding, catalysis, polymeric materials, further molecular-dynamics processes, kinetic-network models, electron spin resonance, etc.

Keywords:

Markov chains; Markov-State Models; transition kernels; projection error; relative error; coarse-graining error.

1 Introduction

Continuous-time Markov chains are considered in [1].
For a chosen subset of of Markov states,the total reward can be calculated of the time spent of the system in the chosen subset.
The expected values of the rewards can be calculated after these formulations.
From these derivations, the Laplace Kernels can be calculated of the distributions corresponding to the rewards.
As far as Markov chains admitting a finite state space are concerned, the results are understood as being applications of the distributions of the first passage times.
In the particular case when a single state is of interest, the distributions are found to be independent and identically-distributed. From [2], the rewards are expected to admit the same distributions as far as the modified chains.
The applications will be considered elsewhere, when the sojourn times of homogenous finite Markov processes in a chosen subset of states are given: they can be investigated both in the discrete-time case and int he continuous-time case.
The mapping of the 'pseudo aggregation is defined, of the pertinent measure spaces.
The infinitesimal generators of the processes can be found.
From a uniformised Markov chain, the homogenous Markov chain of the chosen subset is defined; the probability vector of the opportune $(n - th)$ transition is well-defined.
The time spent in a give state of a chosen subset of the of the phase space can be assigned a random variable.
As far as Markov irreducible chains are concerned, the the existence is proven of an infinity of sojourns with probability 1. Further perspective application are defined in Section 9.
The aim of the present paper is the understanding of this latter hypothesis.

The reward is calculated after a measure which is invariant under the Markov chain. The operators needed are recapitulated with the necessitated measures. From the rewards, the expected values of the rewards are calculated. The calculations allow one to establish the projections (i.e. and the maximal projection) of the errors.
Within these tools, is it possible to formulate new theorems about the time evolution of the eigenvalues, which are initially formulated, for the sake of understanding the basic guidelines of the dynamics, in the Galerkin representation.
From the new theorems about the time evolution of the eigenvalues, as the following successive step, the corresponding new theorems are retrieved after the items of information be recuperated about the spectral gap from the 'lag times', about the errors.
From the analysis in the Galerkin representation, the expressions of the stated theorems in the formulations of the Markov chains are newly retrieved. In Section 2, the measures used in the calculations of Markov chains are recapitulated.

In Section 3, the path-integral formulation of the kernels for the calculation of the expected values of the rewards are reviewed, and the expressions of the maximal projection of the errors are reviewed.
In Section 5, new theorems about eigenvalues in the Galerkin representation are stated.
In Section 6, new theorems about errors in the Galerkin representation are stated.
In Section 7, the errors calculations are given.
In Section 8, the calculation are newly written of the new theorems as far as the original chains are concerned form the ’lag time’ and for the ’spectral gap.

2 Definition of the measures of the Markov processes

As from [3], the following definitions of integrations and measures are applied to the different integration techniques of the rewards (which define the application of the transition) in the opportune spaces, where the measures are proven as invariant under the Markov(-chain) process, from which the m-states MSM are originated.
For the $n-th$ transition probability, the integration is of the Radon-Stieltjes type.
An m-nonsingular transition is defined on a Banach space; the measure is therefore Radon-Nikodym.

Proposition 1 *After an m-nonsingular transition probability, an operator U is defined (after the reward), in $\mathcal{L}^\infty(m)$ into itself: U is the adjoint operator of the operator T, and is linear, positive and bounded (with norm 1).*

For the operator U induced after a Markov process, the following properties hold.

Proposition 2 $\exists$ *a finite equivalent invariant measure ν.*
The operator U sends $\mathcal{L}^1(\nu)$ into $\mathcal{L}^1(\nu)$; and $\mathcal{L}^\infty(\nu)$ into $\mathcal{L}^\infty(\nu)$.
$\mathcal{L}^\infty(\nu)$ is identical with $\mathcal{L}^\infty(m)$.
U has $\mathcal{L}^1(\nu)$-norm equal to 1.
U has $\mathcal{L}^\infty(\nu)$-norm equal to 1.

Corollary 1 $\Rightarrow \exists$ *a finite, equivalent invariant measure of the Markov process in a finite-measure space, or in a σ-finite-measure space.*

3 The path-integral formulation

The derivations of [4] and [1] are here followed.
Be $(X(t), t \geq 0)$ a continuous-time Markov chain, which takes values in $\mathbb{N}_0$,

defined after the states $S = (0, 1, ...)$ of the state space, and be A a fixed subset of S.
Be f an application $F : A \to [0, \infty)$.
The time τ is defined as the 'first exit time' as

$$\tau \equiv inf\{t > 0 : X(t) \notin A\}. \tag{1}$$

The function f_i is the reward per unit time of the stay in the state i of the Markov landscape.
The total reward Γ calculated over the time duree during which the system is in A is calculated as

$$\Gamma = \int_0^\tau f_{X(t)} dt. \tag{2}$$

The Markov chain $X(t)$ is assumed a stable, conservative chain.
Be $\hat{Q}$ the matrix of the transition rates. The matrix $\hat{Q}$ is assumed to be regular.
The entry q_{ij} of $\hat{Q}$ correspond to the transition rate from the state i to the state j.
The total rate of exiting the state i is q_i defined as

$$q_i \equiv -q_{ii} = \sum_{j \neq i} q_{ij}. \tag{3}$$

The regularity of the matrix $\hat{Q}$ implies that there exist many processes within the given set of states; nevertheless, the minimal chain $(X(t), t \geq 0)$ is here chosen.
The hypothesis is taken, that

$$q_{ij} > 0 \forall j \in A. \tag{4}$$

From [4], the path integral Γ_0 is defined as

$$\Gamma_0(f) = \int_0^{\tau_0} f(X(t)) dt \tag{5}$$

with $\tau_0 \equiv inf\{t > 0 : X(t) = 0\}$ being the 'first hitting time' of the state $0 \in S$, and f non-decreasing.
The expected value $E_i(\Gamma_0(f)) \mid X(0) = i$ with $i \geq 1$ is considered.

3.1 Laplace transforms

The Laplace transform of Γ is worked out as follows.
Be y_i defined as

$$y_i(\theta) \equiv E_i(e^{-\Gamma\theta}), \tag{6}$$

with $y_i(\theta) = 1$ for $i \notin A$.
The characterization of the hitting times is here extended as

$$E_i(e^{-\Gamma\theta}) = \int_0^\infty \sum_{k \neq i} e^{thetaf_i u} E_k e^{-\Gamma\theta} \frac{q_{ik}}{q_i} q_i e^{-q_i u} du. \tag{7}$$

Given $z = (z_i, i \in S)$ such that

$$0 \leq z_j \leq 1, \quad j \in A, \tag{8a}$$
$$z_j = 1, \quad j \notin A, \tag{8b}$$

z_i is a solution of

$$\sum_{j \in S} q_{ij} z_j = \theta f_i z_i, \quad i \in A. \tag{9}$$

Thus,

$$y_i(\theta) \geq z \ \ \forall i \in S. \tag{10}$$

The probability matrix $\hat{P}$ is defined from the entries $p_{ij}(t), i, j \in S$ as the 'minimal solution' which satisfies the Kolmogorov backward equations. In particular, the entries $p_{ij}(t)$ are such that

$$p_{ij}(t) = (ProbX(t) = j, N(t) < \infty \mid X(0) = i) \tag{11}$$

wit $N(t)$ the requested number of jumps until the time t.

4 Summary and review of techniques about eigenvalues

Following [5], the following definition is given

Definition 1 *Be χ_A characteristic functions of the set a. The orthogonal projector Q is defined on the n-dimensional space of the step functions D_n, where the latter has an orthonormal basis.*

The projector $\hat{P}$ on the transfer operator T and on D_n is defined as

$$\hat{P} = QTQ, \tag{12}$$

such that $\mathcal{L}^2_\mu \to D_n \subset \mathcal{L}^2_\mu$.
The transition matrix of the MSM Markov chain coincides with the matrix representation of the projected transfer operator $\hat{P}$.
As an operator on a finite-dimensional space, $\hat{P}$ admits a matrix representation.
The following definition is recalled.

Definition 2 *the $\tilde{\lambda}$ the eigenvalue of QTQ Eq. (12) is written as*

$$\hat{T}r = \hat{\lambda}Mr. \tag{13}$$

In Eq. (13), the operator $\hat{T}$ is spelled as

$$\hat{T_{ij}} = \frac{< q_i, Tq_j >}{\hat{\rho(i)}}, \tag{14}$$

with the specification

$$\hat{\rho}_i \equiv|| q_i || \tag{15}$$

and the mass matrix M_{ij} as

$$M_{ij} \equiv \frac{< q_i, q_j >}{\hat{\rho}(i)}. \tag{16}$$

From [6], the orthogonality of the step functions ensures that M_{ij} is

$$M_{ij} = \frac{< q_i, q_j >}{\hat{\mu}_i} = 1, \quad i = j, \tag{17a}$$

$$M_{ij} = \frac{< q_i, q_j >}{\hat{\mu}_i} = 0, \quad i \neq j. \tag{17b}$$

From [5], a continuous-time process is chosen.
From Eq. (13), the eigenfunction chosen can be the committors.
The matrices $\hat{T_{ij}}$ and M_{ij} are taken from [6].
As a result, the committor functions become therefore orthogonal in the chosen Garlenkin description.

Summary and review of techniques about errors From [6], the Th. 2.2 from [7] is used, according to which the transfer operator is demonstrated to be self-adjoint; Th. 4.2 from [6] is here recalled as

Theorem 1 *Given the m-states MSM, under the dominant-eigenvalues hypothesis, the chosen m dominant eigenvalues are ordered as*

$$1 = \lambda_0 < \lambda_1 < ... < \lambda_{m-1} \tag{18}$$

and the corresponding eigenvectors w_i are considered, which live in $D \subset \mathcal{L}^2_\mu$ (whose corresponding algebra can be rendered unital); Q is the direction orthogonal to D.
The set

$$1 = \hat{\lambda}_0 < \hat{\lambda}_1 < ... < \hat{\lambda}_{m-1} \tag{19}$$

are the corresponding eigenvalues of QTQ Eq. (12).
Given a δ as

$$\delta = max_{i=1,...,m-1} || Q^{\perp} w_i, \tag{20}$$

the maximal projection error $E(\delta)$ of the eigenvalues of D is majorised with

$$E(\delta) \equiv max_{i=1,...,m-1} \mid \lambda_i - \hat{\lambda}_i \mid \leq \lambda_1 (m-1)\delta^2 \tag{21}$$

Let the error $E(\delta)$ be defined as

$$E(\delta) = max_{i=1,...,m-1} \mid \lambda_i - \hat{\lambda}_i \mid \leq \lambda_i (m-1)\delta^2 \tag{22}$$

being

$$\delta = max_{i=1,...,m-1} || Q^{\perp} u_i || . \tag{23}$$

5 New theorems about eigenvalues

Form the guidelines in Section 5, the following new theorems hold.
From the comments on Definition 1,

Theorem 2 *The scalar products of the projection (also) of the right eigenfunctions remain invariant from the Markov chain to the MSM.*

Proof:
As a projector, P is idempotent and selfadjoint. □

Theorem 3 *The time evolution of the eigenvalues* $\tilde{\lambda}_{i,\ \tau}$ *is written as*

$$\tilde{\lambda}_{i,\ \tau} = \int_0^\infty e^{-\Lambda_i(t+\tau)} e^{-\theta\delta\Lambda_i} d\theta \tag{24}$$

Proof:
By definition of the orthogonal committors after Proposition 1. □

Theorem 4 *For a discretised MSM, the time evolution of the eigenvalues in the Galerkin description is written as*

$$\lambda_{i,n\tau} = \int_0^\infty e^{-\theta\Lambda_i(t+n\tau)} e^{-\theta\delta_n\Lambda_i} \tag{25}$$

Proof:
From Theorem 3 after discretisation, the properties of the eigenfunctions coincide with those of the continuous system. □

Corollary 2 *The time evolution of the discretised two-states Markov model is written as*

$$\tilde{\lambda}_{2,n\tau} = \int_0^\infty e^{-\theta\Lambda(t+n\tau)} e^{-\theta\tilde{\delta_n}\Lambda} d\theta. \tag{26}$$

Proof*:*
After the definition of Theorem 4. □

The auxiliary time variable θ in newly-obtained Laplace kernels is chosen not to coincide with the exit times.

6 New theorems about errors

Theorem 5 *The relative error is therefore newly analytically calculated from Eq. (22) as*

$$\tilde{E} = max_{i=1,\ldots,m-1} \mid \tilde{\lambda}_i - \hat{\lambda}_i \mid \tag{27}$$

Proof:
The definition Eq. (22) is here upgraded. □.
The new constant $\hat{\delta}$ is newly calculated and its estimation proven to be improved.

7 Errors calculations

From [6], the propagation error is newly calculated from Eq. (12) as

$$\tilde{E}_k = \| QT^kT - (QTQ)^k \| \tag{28}$$

From [5], the error for coarse-grained transfer operator is newly rewritten as

$$\hat{E}_k = \| QT^kT - Q(TQ)^k \| \tag{29}$$

8 Calculations from the original chains

The study original Markov-chain process analysed is accomplished after the assumption of the 'dominant-eigenvalues' m-states MSM, i.e. one where the eigenvalues chosen are real, of limited number, and ordered, i.e. as from Assumption 2.2 of [5].
In [5], the orthonormal basis of eigenvectors u_j, $j = 1, ..., m$ is therefore selected in the way such that, with the associated eigenvalues λ_j, the evolution is codified as

$$Tu_j = \lambda_j u_j. \tag{30}$$

Moreover, the hypothesis is taken, that the remainder of the spectrum of the operator T is in a neighbourhood $B_r(\mathbb{C})$ of radius $r < \lambda_m$.
Within this description, the the study of the 'lag time' τ is requested, under the 'rates' r from λ_j defined as

$$\lambda_j = e^{-\Lambda_j \tau}, \tag{31}$$

i.e.

$$r = e^{-r\tau}, \tag{32}$$

with

$$\frac{r}{\lambda_1} = e^{-\tau(R-\Lambda_1)} = e^{-\Delta\tau}, \tag{33}$$

where Δ is named the 'spectral gap'.

9 Outlook and perspectives

In the present paper, new theorems are stated in particular representations of Markov chains, about the time evolution of the eigenvalues and about that or errors.
As perspective studies, sojourn time in the continuous-time Markov chains are considered for the irreducible homogenous Markov chains on a finite state space, i.e. as form [2].
The generators of the process are written when the representation of the output rates of the states are found the representation of.
Transition-probability matrix representations can be given of the 'uniformised chain' [8].

The relations between the infinitesimal generators are found on the appropriate (normed) spaces.
From this respect, the ’pseudo-aggregation’ process of homogenous irreducible Markov chains are found.
The calculations f the sojourn times of the pseudo aggregated states can be formulated, after which, in the continuous-time case, analogous results are found between the properties of the sojourn times in the chosen properties of the Markov chains and the pertinent ’holding times’ in the ’pseudo-aggregated’ processes properties.
Buffer states and the processors can be further considered.
The systems can be assumed, at which the processors and the buffers are operational.
The states are of interest, which belong to a set in which the system is operational.

The techniques to retrieve the pertinent qualities of the originating Markov chains are here provided with.
The paper is organised as follows.
In Section 2, the measure-theoretical arguments about Markov chains are recalled.
I Section 3, the path-integral formulation is recalled, for the aim of recovering the expressions of maximal projection of the error.
In Section 5, new theorems about eigenvalues are stated in the Galerkin representation.
In Section 6, new theorems about errors in the Galerkin representation are stated.
In Section 7, some errors calculations are inidicated.
In Section 8, the formulation of these theorems from the original Markov chain is newly retrieved.
Outlook and perspectives follow in Section 9.

Conflicts of interests

Not applicable.

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