

APPROXIMATING SELECTED NON-DOMINANT TIMESCALES BY MARKOV STATE MODELS

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Abstract

We consider time-continuous, reversible Markov processes on large or continuous state space. For a practical analysis of such processes it is often necessary to construct low dimensional approximations, like Markov State Models (MSM). MSM have been used for this purpose in several applications, particularly in molecular dynamics, see [16] for an example. One of the main goals of MSMs is the correct approximation of slow processes in the system. Recently, it was possible to understand under which conditions a MSM inherits the most dominant timescales of the original Markov process [6, 7]. However, all rigorous statements known have yet been concerned with the approximation of the absolutely slowest processes in the system, i.e., its dominant timescales. In this article, we will show that it is also possible to design MSMs to reproduce selected non-dominant timescales and which approximation quality can be achieved.

INTRODUCTION

Markov State Models (MSM) have been used as finite Markov chain approximations for ergodic, time-continuous Markov processes for many years [20, 21, 22, 5, 24, 4]. Usually, one assumes that the process of interest exhibits metastable dynamical behavior. That is, there exist sets in state space in which the process stays for a long period of time, compared to the typical transition times between these sets. The goal of an MSM approximation is to construct a Markov jump process with the metastable sets as discrete states so that the MSM process inherits essential information from the original continuous Markov process. For multiscale systems, e.g., this essential information is the timescale associated with important slow processes in the system. For example, in molecular dynamics applications these processes could correspond to protein folding [11, 12], conformational rearrangements between native protein substates [9, 15], or ligand binding [17]. In this context, the MSM process should model the conformation dynamics of the system, i.e., it should reproduce the transition rates between its most important conformations [21, 14, 10, 22].

The sets representing the Markov states in a MSM can have two different forms. In *standard MSMs* they form a full partition of state space; a guideline to the construction of such MSM is provided in [18]. A recently developed alternative

MSM variant does not require the sets to form a full partition. It is rather based on so called core sets and milestoning [23, 3] and will be called *core set MSM* subsequently. Both methods share that their construction can be interpreted in the sense of a projected transfer operator [19]. That is, the choice of n sets corresponds one-to-one to the choice of a basis of an n -dimensional subspace D , and the transition matrix of the MSM to the operator QTQ , where T is the transfer operator of the original Markov process and Q the orthogonal projection onto D . Therefore, rigorous results from [6, 7] concerning the approximation quality of MSMs apply. Its simplest form states that the longest m timescales of the original Markov process are correctly reproduced by the MSM under consideration if the projection error

$$\delta_m := \max_{i=1, \dots, m} \|Q^\perp u_i\|, \quad Q^\perp = Id - Q \quad (1)$$

is small enough. The set $\{u_i\}_{i=1, \dots, m}$ here denotes the eigenvectors of the original transfer operator T which correspond to the m largest eigenvalues; via Q the projection error δ_m depends on the sets chosen. In the next section, we will present the exact formulation of this statement. We will see that the drawback of the Theorem is that it aims at the approximation of the m longest, i.e., the absolutely dominant timescales, only. Nevertheless, in many application one is interested in events that happen on a particular timescale, that may not be dominant in the above sense.

Such timescales will be called *non-dominant* in the following. As we will show in this article it is possible to construct a MSM so that it reproduces a particular non-dominant timescale without having to describe (or know) all more dominant timescales of the system. Furthermore we will present an estimate of the projection error; the interpretation induced by it allows to understand when the projection error can be expected small.

SETTING AND FORMER RESULT

In the following we analyze an ergodic and reversible Markov process (X_t) on state space E with unique invariant measure μ . We consider its transfer operator $T = T_\tau$ for a fixed lag time $\tau > 0$ to act on the space $L^2_\mu(E) = \{v : E \rightarrow \mathbb{R} \mid \int_E v^2 d\mu < \infty\}$, that is, on a Hilbert space equipped with the scalar product

$$\langle v, w \rangle = \int_E v w d\mu, \quad (2)$$

so that the operator T associated with (X_t) is self-adjoint; details can be found in [6, 7], including the following Theorem:

Theorem 1 *Let $1 = \lambda_0 > \lambda_1 > \dots > \lambda_{m-1}$ be the m dominant eigenvalues of T , i.e., for every other eigenvalue λ it holds $\lambda < \lambda_{m-1}$. Let u_0, u_1, \dots, u_{m-1} be the corresponding normalized eigenvectors, $D \subset L^2_\mu(E)$ a subspace with*

$$\mathbf{1} \in D \quad \dim(D) =: n \geq m \quad (3)$$

and Q the orthogonal projection onto D .

Let $1 = \hat{\lambda}_0 > \hat{\lambda}_1 > \dots > \hat{\lambda}_{m-1}$ be the dominating eigenvalues of the projected operator QTQ . Then

$$\max_{i=1, \dots, m-1} |\lambda_i - \hat{\lambda}_i| \leq \lambda_1 (m-1) \delta_{m-1}^2, \quad (4)$$

where

$$\delta_{m-1} = \max_{i=1, \dots, m-1} \|Q^\perp u_i\|$$

is the maximal projection error of the eigenvectors to the space D .

As already said the projected transfer operator QTQ is equivalent to the transition or rate matrices of the respective MSMs; for standard MSMs, the subspace D would be spanned by stepfunctions each being constant on the partitioning sets, and for core set MSMs, it would be spanned by the committors [8, 13] with respect to the core sets chosen. Thus the eigenvalues $\hat{\lambda}_1 > \dots > \hat{\lambda}_{m-1}$ encode the timescales incorporated in the MSM and the $\lambda_1 > \dots > \lambda_{m-1}$ the dominant timescales of the original Markov process. So, as promised in the introduction, Theorem 1 tells us that the MSM will approximate the

dominant timescales of the original Markov process if the projection error (1) is small enough. Unfortunately, it does not contain information about how to approximate a process on a selected non-dominant timescale of interest without taking care of all slower processes as well.

MAIN THEOREM

The subsequent theorem will show that there is no need to resolve all slower processes by a MSM if one is interested in particular events taking place on a non-dominant timescale (for its proof see the appendix):

Theorem 2 *Let T be a self-adjoint transfer operator and Q the orthogonal projection to a subspace D with $\mathbf{1} \in D$. Let λ be any eigenvalue of T and u a corresponding normalized eigenvector and set $\delta = \|Q^\perp u\|$. Then there exists an eigenvalue $\hat{\lambda}$ of the projected transfer operator QTQ with*

$$|\lambda - \hat{\lambda}| \leq \lambda_1 \delta (1 - \delta^2)^{-\frac{1}{2}}. \quad (5)$$

To simplify the right-hand side, note that for $\delta^2 < \frac{3}{4}$, which must be the case for any reasonable approximation, we have $(1 - \delta^2)^{-\frac{1}{2}} < 2$. Then, (5) reads

$$|\lambda - \hat{\lambda}| \leq 2\lambda_1 \delta. \quad (6)$$

This statement shows that, if we select a timescale of the original process encoded by the eigenvalue λ of T with associated eigenvector u , and construct the MSM from sets (i.e., via a projection Q) such that $\|Q^\perp u\|$ is small enough, then the MSM will approximate the selected timescale well.

Remark 3 *If the eigenvalue is degenerate, i.e., if it is not simple, we are allowed to set $\delta = \min_u \|Q^\perp u\|$, where the minimum is taken over all normalized vectors from the associated eigenspace. This fact can be deduced from the proof of Theorem 2 since it shows that the inequality (5) holds for every normalized eigenvector related to the eigenvalue of interest.*

Remark 4 *The dimension of the approximation subspace D may be greater than two such that QTQ has more than one nontrivial eigenvalue. Theorem 2 only states that one of these eigenvalues is close to the desired one if the associated projection error δ is small. However, one will not know which eigenvalue of QTQ is the one without knowing for which eigenvector δ is small. Therefore we may want to consider $m = \dim(D) = 2$ only (or small m in general) which seems to be a severe limitation. However, we will see in Thm. 5*

below that $m = 2$ has additional advantages, and our subsequent numerical examples will illustrate that the general case perhaps should be approached by means of a successive refinement strategy with $m = 2$ in each refinement step.

DISCUSSION AND EXAMPLES

Let us consider a diffusion, i.e. the stochastic differential equation

$$dX_t = -\nabla V(X_t)dt + \sigma dB_t, \quad (7)$$

where V denotes the one-dimensional potential illustrated in Fig. 1, $\sigma = 0.8$ denotes the noise intensity, and B_t scalar Brownian motion.

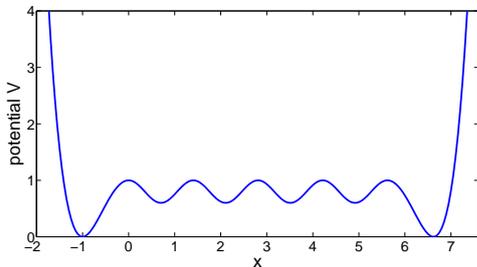


FIGURE 1: Potential V

For a lag time $\tau = 1$, we find the following dominant spectrum of the transfer operator T :

$$\begin{array}{ccccc} \lambda_0 & \lambda_1 & \lambda_2 & \lambda_3 & \lambda_4 \\ 1.0000 & 0.9885 & 0.9247 & 0.7911 & 0.6289. \end{array}$$

We will now compare different core set MSMs with respect to the approximation of these eigenvalues. First, with two core sets that are chosen as in Fig. 2,

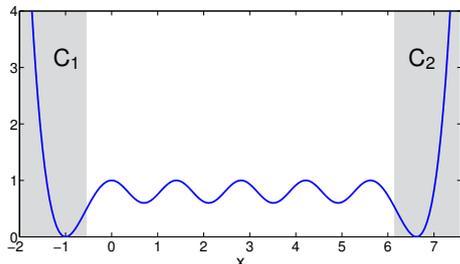


FIGURE 2: Two good core sets to approximate the first timescale.

we get a very precise approximation of the first eigenvalue $|\lambda_1 - \hat{\lambda}_1| < 10^{-4}$ by the dominant eigenvalue $\hat{\lambda}_1$ of the MSM operator QTQ . This is due to the small projection error $\delta_1 = \|Q^\perp u_1\| = 0.0164$. Now, let us assume that we are rather interested in the second slowest process in the system that describes the event

of going from the center of the transition region into the two main wells and back. This process is connected to λ_2 . In order to build an MSM that captures this process, we have to introduce another set in the middle of the transition region. Two choices are presented in Fig. 3.

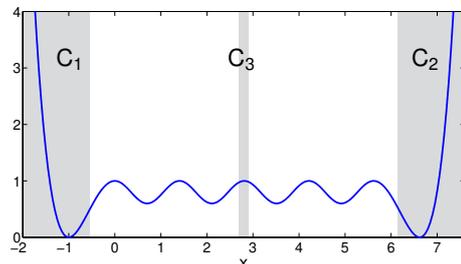
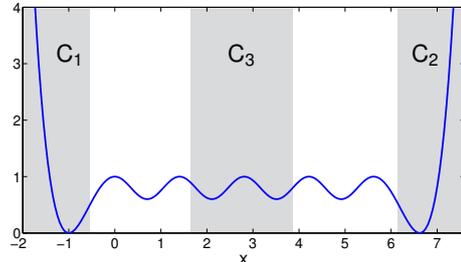


FIGURE 3: Large and small third core set

For the small third core set we get

$$\|Q^\perp u_1\| = 0.0339 \quad \|Q^\perp u_2\| = 0.1024$$

and exactly the other way around for the large third core set

$$\|Q^\perp u_1\| = 0.1302 \quad \|Q^\perp u_2\| = 0.0444.$$

So, Theorem 2 yields that the second non-trivial eigenvalue λ_2 should be better reproduced by the MSM using the larger core set, paying with a possible loss in accuracy of the dominant timescale. Actual computation of the eigenvalues of the 3×3 projected transfer operator QTQ in fact results in the following values:

$$\text{small third core set: } \hat{\lambda}_1 = 0.9883, \hat{\lambda}_2 = 0.9203,$$

$$\text{large third core set: } \hat{\lambda}_1 = 0.9847, \hat{\lambda}_2 = 0.9235,$$

that perfectly exhibit the predicted tendency.

Theorem 1 cannot describe this effect since it gives a statement about the joint projection error only:

$$\text{small third core set: } \delta_2 = 0.1024,$$

$$\text{large third core set: } \delta_2 = 0.1302.$$

Since we already have a good MSM for the reproduction of the slowest timescale, why not design a two state MSM just for the reproduction of the second slowest one? This can be done by choosing core sets as shown in Fig.4.

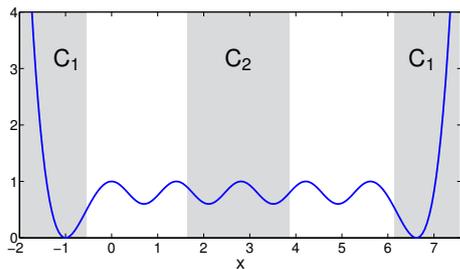


FIGURE 4: Two core sets for approximation of the second slowest timescale.

This choice leads to a MSM operator QTQ that acts on a two dimensional subspace D ; its two eigenvalues

$$\hat{\lambda}_0 = 1, \hat{\lambda}_1 = 0.9235,$$

are only describing the dynamics of the second slowest process. For this special case, we can also prove a slightly better approximation quality.

Theorem 5 *Let T be a self-adjoint transfer operator and Q the orthogonal projection to a two-dimensional subspace D with $\mathbf{1} \in D$. Let λ be an eigenvalue of T and u the corresponding normalized eigenvector and set $\delta = \|Q^\perp u\|$. Let the smallest eigenvalue of T be given by λ^- . Then for the non-trivial eigenvalue $\hat{\lambda}$ of the projected transfer operator QTQ it holds*

$$|\lambda - \hat{\lambda}| \leq \max\{\lambda_1 - \lambda, \lambda - \lambda^-\} \delta^2 (1 - \delta^2)^{-1}. \quad (8)$$

Again, one can simplify the statement without loss of generality for $\delta^2 < \frac{1}{2}$:

$$|\lambda - \hat{\lambda}| \leq 2\lambda_1 \delta^2. \quad (9)$$

Our above example seems to indicate that one always has to resolve the dominant timescales in order to be able to approximate smaller timescales. Our next example indicates that this is *not* the case in general. We again consider a diffusion process of form (7) but this time in the three-well energy landscape shown in Fig. 5 with $\sigma = 0.65$.

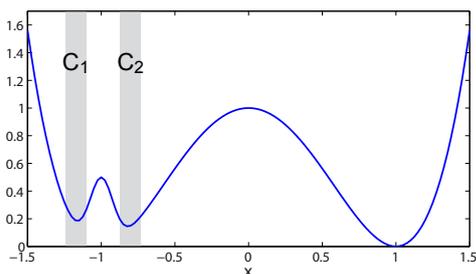


FIGURE 5: Potential V

For a lag time $\tau = 0.1$, we find the following dominant spectrum of the transfer operator T :

$$\begin{array}{cccc} \lambda_0 & \lambda_1 & \lambda_2 & \lambda_3 \\ 1.0000 & 0.9979 & 0.7943 & 0.6061. \end{array}$$

In this case, the dominant nontrivial eigenvalue λ_1 encodes the dominant timescale $t = -\tau/\log(\lambda_1) \approx 48$ of switches between the two small wells on the left hand side of the main energy barrier at $x = 0$ and the larger one on the right hand side. The next relevant timescale corresponds to the switching between the two smaller wells left of the main energy barrier. We want to approximate this timescale. Therefore, we ignore the large well on the right hand side of $x = 0$ and choose the two core sets C_1 and C_2 shown in Fig. 5. Based on the committors associated with these core sets we compute QTQ and find eigenvalues

$$\hat{\lambda}_0 = 1, \hat{\lambda}_1 = 0.7946.$$

In view of Thm. 5 the small error $|\lambda_2 - \hat{\lambda}_1| = 3 \cdot 10^{-4}$ is in good agreement with the projection error $\delta = \|Q^\perp u_2\| = 0.0187$ of the relevant eigenvalue u_2 of T .

The example demonstrates that one does not necessarily have to resolve the whole structure of the state space if one is interested in the dynamics on a particular timescale. The important condition to allow for a low-dimensional approximation of a non-dominant timescale is that one can approximate an associated eigenvector well by committor functions corresponding to only few core sets. This raises hopes for a hierarchical refinement strategy, which would try to approximate every timescale separately by a different set of core sets resolving only the relevant part of state space. In general, an approximation using only two core sets for every timescale may require the use of more sophisticated refinement strategies introducing an additional weighting between core sets.

ESTIMATING THE PROJECTION ERROR

Next we will give an estimate of the projection error $\delta = \|Q^\perp u\|$ that appears in our above theorems for a specific subspace D . Therefore we first introduce the committors q_1, \dots, q_m that are induced by the m core sets C_1, \dots, C_m under consideration: The committor q_j is given by the linear equation

$$\begin{aligned} (Id - T)q_j &= 0, \text{ on } C \\ q_j &= g_j, \text{ on } E \setminus C, \end{aligned}$$

with $g_j = 1$ on C_j and $g_j = 0$ on all other core sets, and $C = E \setminus \cup_j C_j$. The space spanned by

the committors can be written as

$$\begin{aligned} D &= \text{span}\{q_1, \dots, q_m\} \\ &= \{v \mid v \text{ is constant on each set } C_j, \\ &\quad Tv = v \text{ on } C\}. \end{aligned}$$

Now we can estimate the projection error $\|Q^\perp u\|$ for any eigenvector u .

Theorem 6 *Take the setting from above, but let D be the space spanned by committors. Denote with Q the orthogonal projection onto D . Let λ be an eigenvalue of T and u the corresponding, normalized eigenvector. Then*

$$\|Q^\perp u\| \leq p(u) + 2\mu(C)p_{max}(u) + r(C)(1 - \lambda)c(u)$$

with

$$\begin{aligned} r(C) &= \sup_{\substack{\|v\|=1, \\ v=0 \text{ on } E \setminus C}} \left(\frac{1}{\int_C (v - Tv)^2 d\mu} \right)^{1/2} \\ p(u) &= \|P^\perp u\| \\ p_{max}(u) &= \|P^\perp u\|_\infty \\ (Pu)(x) &= \begin{cases} u(x), & \text{if } x \in C, \\ \frac{1}{\mu(C_j)} \int_{C_j} u d\mu, & \text{if } x \in C_j. \end{cases} \\ c(u) &= \left(\int_C u^2 d\mu \right)^{\frac{1}{2}} \end{aligned} \tag{10}$$

INTERPRETATION

In order to achieve a small bound we have to make sure that the two summands

$$r(C)(1 - \lambda)c(u), \text{ and } p(u) + 2\mu(C)p_{max}(u) \tag{11}$$

are small. For given λ the first summand consists of objects that depend on the set C only. If we let Π denote the projection onto the space of $v \in L^2_\mu(E)$ with $v|_{E \setminus C} = 0$ then $r(C) = \|\Pi(Id - T)\Pi\|$ so that we get from [1, 2], that

$$r(C) \leq \sup_{z \in C} \mathbb{E}_z(\tau(\cup_j C_j)),$$

where $\tau(A)$ denote the first entry time of $(X_{nt})_{n \in \mathbb{N}}$ into the set A . That is, $r(C)$ is small whenever the process quickly leaves the set C . Therefore the first summand is small whenever λ is close to one and the process leaves the set quickly. In order to have a small second summand the eigenvector u just has to be almost constant on the sets C_1, \dots, C_m .

CONCLUSION

In this article, we have shown that it is not necessary for a MSM to resolve *all* slow processes of the approximated system. We proved that it is possible to design special MSMs for the approximation of selected non-dominant timescales, in principle. By the way of doing this we also gave an estimate for the projection error that appears in previous estimates of the MSM approximation error, as e.g. in Thm. 1.

Concerning the algorithmic question of how to choose a good core sets, our results seem to indicate that a multilevel identification strategy that resolves timescale after timescale may not only be possible but also superior to the simultaneous reproduction of many timescales with many core sets.

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APPENDIX

PROOF OF THEOREM 2

Proof. For $\lambda = 1$ it is trivial, so $\lambda < 1, u \neq \mathbf{1}$. Since T is self-adjoint, also QTQ is self-adjoint on a finite dimensional space. Therefore, we have an orthonormal basis of eigenvectors $\hat{u}_1, \dots, \hat{u}_n$ and real eigenvalues $\hat{\lambda}_1, \dots, \hat{\lambda}_n$ and

$$QTQ u = \sum_{i=1}^n \hat{\lambda}_i \langle u, \hat{u}_i \rangle \hat{u}_i.$$

On the other hand we have

$$\begin{aligned} QTQ u &= QTu - QTQ^\perp u = \lambda Qu - QTQ^\perp u \\ &= \lambda \sum_{i=1}^n \langle u, \hat{u}_i \rangle \hat{u}_i - QTQ^\perp u. \end{aligned}$$

Putting both equations together we get

$$QTQ^\perp u = \sum_{i=1}^n (\lambda - \hat{\lambda}_i) \langle u, \hat{u}_i \rangle \hat{u}_i.$$

Therefore,

$$\begin{aligned} \|QTQ^\perp u\|^2 &= \sum_{i=1}^n (\lambda - \hat{\lambda}_i)^2 \langle u, \hat{u}_i \rangle^2 \\ &\geq \min_{i=1, \dots, n} \{(\lambda - \hat{\lambda}_i)^2\} \sum_{i=1}^n \langle u, \hat{u}_i \rangle^2 \\ &= \min_{i=1, \dots, n} \{(\lambda - \hat{\lambda}_i)^2\} \|Qu\|^2 \\ &= \min_{i=1, \dots, n} \{(\lambda - \hat{\lambda}_i)^2\} (1 - \delta^2). \end{aligned}$$

So, there exists an eigenvalue $\hat{\lambda}$ with

$$(\lambda - \hat{\lambda})^2 \leq \|QTQ^\perp u\|^2 (1 - \delta^2)^{-1}.$$

Moreover,

$$\|QTQ^\perp u\|^2 \leq \|QTQ^\perp\|^2 \|Q^\perp u\|^2 \leq \lambda_1^2 \delta^2,$$

since $Q^\perp u_0 = Q^\perp \mathbb{1} = 0$. Taking the square root completes the proof. \square

PROOF OF THEOREM 5

Proof. From the proof of Theorem 2 we get

$$\begin{aligned} QTQ^\perp u &= (\lambda - \hat{\lambda}) \langle u, \hat{u} \rangle \hat{u} \\ &= (\lambda - \hat{\lambda}) Qu, \end{aligned}$$

where \hat{u} is the eigenvector to the only non-trivial eigenvalue $\hat{\lambda}$. On the other hand,

$$\langle Qu, \mathbb{1} \rangle = \langle u, Q\mathbb{1} \rangle = \langle u, \mathbb{1} \rangle = 0,$$

which means, that $\{1, \frac{Qu}{\|Qu\|}\}$ is an orthonormal basis of D . Therefore,

$$\begin{aligned} QTQ^\perp u &= \langle TQ^\perp u, \mathbb{1} \rangle \mathbb{1} + \frac{1}{\|Qu\|^2} \langle TQ^\perp u, Qu \rangle Qu \\ &= \frac{1}{\|Qu\|^2} \langle TQ^\perp u, Qu \rangle Qu. \end{aligned}$$

Combination with the first equation yields

$$\begin{aligned} \lambda - \hat{\lambda} &= \frac{1}{\|Qu\|^2} \langle TQ^\perp u, Qu \rangle \\ &= \frac{1}{\|Qu\|^2} \langle Q^\perp u, Q^\perp TQ u \rangle \\ &= \frac{1}{\|Qu\|^2} (\langle Q^\perp u, Q^\perp T u \rangle - \langle Q^\perp u, Q^\perp T Q^\perp u \rangle) \\ &= \frac{1}{\|Qu\|^2} (\lambda \|Q^\perp u\|^2 - \langle Q^\perp u, TQ^\perp u \rangle) \\ &\leq \frac{1}{\|Qu\|^2} (\lambda - \lambda^-) \|Q^\perp u\|^2 \\ &= (\lambda - \lambda^-) \delta^2 (1 - \delta^2)^{-1}. \end{aligned}$$

Moreover,

$$\begin{aligned} \hat{\lambda} - \lambda &= \frac{1}{\|Qu\|^2} (\langle Q^\perp u, TQ^\perp u \rangle - \lambda \|Q^\perp u\|^2) \\ &\leq (\lambda_1 - \lambda) \delta^2 (1 - \delta^2)^{-1}. \end{aligned}$$

\square

PROOF OF THEOREM 6

In the proof of Theorem 6 the following maximum principle will be needed:

Lemma 7 Let $v \in L_\mu^2(E)$ be the solution of

$$\begin{aligned} (Id - T)v &= 0, \text{ on } C \\ v &= g, \text{ on } E \setminus C, \end{aligned} \quad (12)$$

with $g \in L^\infty(\mu), g \neq 0$ on $E \setminus C$. Then,

$$\begin{aligned} \|v\|_\infty &:= \max_{y \in E} |v(y)| \\ &\leq \max_{y \in E \setminus C} |g(y)|. \end{aligned}$$

For a proof of this Lemma please visit [19], Sec. 3.3.

Proof. Take the projection P onto the space $V = \{v \in L_\mu^2(E) | v(x) = c_j \forall x \in C_j, c_j \in \mathbb{R}, j = 1, \dots, n\}$ of functions, which are constant on the core sets.

First, $\|Q^\perp u\| = \|u - Qu\| \leq \|u - q\|$ for every $q \in D$, as Qu is the best approximation. Take the interpolating $q \in D$, that is a solution of

$$\begin{aligned} Tq &= q \text{ on } C, \\ q &= Pu, \text{ on } E \setminus C. \end{aligned} \quad (13)$$

As $q \in V$ we have $Pq = q$. Therefore (13) is equivalent to

$$\begin{aligned} PTPq &= q \text{ on } C, \\ q &= Pu, \text{ on } E \setminus C. \end{aligned} \quad (14)$$

Moreover, for the projection Pu

$$PTPu = PTu - PTP^\perp u = \lambda Pu - PTP^\perp u.$$

Therefore the error $e := Pu - q$ solves

$$\begin{aligned} (Id - PTP)e &= (1 - \lambda)Pu + PTP^\perp u \text{ on } C, \\ e &= 0, \text{ on } E \setminus C. \end{aligned}$$

This means, $e \in E_\Theta = \{v | v(x) = 0, x \in E \setminus C\} \subset E$ fulfills

$$\Theta(Id - PTP)\Theta e = (1 - \lambda)\Theta Pu + \Theta PTP^\perp u \quad (15)$$

with

$$\Theta v(x) = \begin{cases} v(x), & x \in C \\ 0, & x \in E \setminus C \end{cases}.$$

Obviously it holds $P\Theta = \Theta P = \Theta$. Thus, (15) is equivalent to

$$Re := \Theta(Id - T)\Theta e = (1 - \lambda)\Theta u + \Theta TTP^\perp u \quad (16)$$

Now R has to be invertible on E_Θ because if it was not, there would be some $v \in E_\Theta$ satisfying

$$Rv = 0,$$

which would imply

$$\begin{aligned} Tv &= v \text{ on } C, \\ v &= 0, \text{ on } E \setminus C. \end{aligned}$$

But then it must hold $Tv = 0$ on $E \setminus C$, because otherwise we would have $\|Tv\| > \|v\|$. This would imply $Tv = v$ on E , which is a contradiction to

the unique, positive invariant measure.
So we can write

$$e = R^{-1}(1 - \lambda)\Theta u + R^{-1}\Theta TP^\perp u.$$

R is self-adjoint, because T is, and therefore $\|R^{-1}\| = \frac{1}{\kappa}$, where κ is the smallest eigenvalue of R , i.e. there is a vector $v \in E_\Theta$, $\|v\| = 1$ with

$$\Theta(Id - T)\Theta v = \kappa v.$$

Now we have

$$\begin{aligned} \kappa^2 &= \int_E (\kappa v)^2 d\mu = \int_E (\Theta(Id - T)\Theta v)^2 d\mu \\ &= \int_C ((Id - T)v)^2 d\mu. \end{aligned}$$

This implies

$$\|R^{-1}\| \leq \frac{1}{\min_{v \in E_\Theta, \|v\|=1} \left(\int_C (v - Tv)^2 d\mu \right)^{\frac{1}{2}}}.$$

Moreover, $\Theta TP^\perp = \Theta(T - Id)P^\perp$, which gives

$$\|R^{-1}\Theta TP^\perp u\| = \|R^{-1}\Theta(Id - T)P^\perp u\| = \|\Theta f\|,$$

where Θf solves

$$R\Theta f = \Theta(Id - T)\Theta f = \Theta(Id - T)P^\perp u$$

which is equivalent to

$$\Theta(Id - T)(\Theta f - P^\perp u) = 0.$$

That is, $w := \Theta f - P^\perp u$ is the solution of

$$\begin{aligned} (Id - T)w &= 0 \text{ on } C \\ w &= -P^\perp u \text{ on } E \setminus C \end{aligned}$$

Lemma 7 now implies that $\|w\|_\infty = \|P^\perp u\|_\infty$ and therefore

$$\begin{aligned} \|R^{-1}\Theta TP^\perp u\| &= \|\Theta f\| \leq \mu(C)\|P^\perp u\| \\ &\quad + \|w\|_\infty \leq 2\mu(C)\|P^\perp u\|_\infty. \end{aligned}$$

So,

$$\begin{aligned} \|e\| &= \|R^{-1}(1 - \lambda)\Theta u + R^{-1}\Theta TP^\perp u\| \\ &\leq \|R^{-1}\|(\|(1 - \lambda)\Theta u\| + \|R^{-1}\Theta TP^\perp u\|) \\ &= r(C)(1 - \lambda) \left(\int_C u^2 d\mu \right)^{\frac{1}{2}} + 2\mu(C)\|P^\perp u\|_\infty. \end{aligned}$$

Further,

$$\begin{aligned} \|Q^\perp u\| &= \|u - Qu\| \leq \|u - q\| \\ &\leq \|u - Pu\| + \|Pu - q\| = p(u) + \|e\|. \end{aligned}$$

Putting all together completes the proof. \square

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