An exact reduction of the master equation to a strictly stable system with an explicit expression for the stationary distribution

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Abstract
The evolution of a continuous time Markov process with a finite number of states is usually calculated by the Master equation - a linear differential equations with a singular generator matrix. We derive a general method for reducing the dimensionality of the Master equation by one by using the probability normalization constraint, thus obtaining a affine differential equation with a (non-singular) stable generator matrix. Additionally, the reduced form yields a simple explicit expression for the stationary probability distribution, which is usually derived implicitly. Finally, we discuss the application of this method to stochastic differential equations.

1 Introduction
Let $X (t)$ be a continuous time Markov process with discrete states $\{1, 2, ..., M\}$, where $1 < M < \infty$, with $A_{ij}$ being the (non-negative) transition rate from state $j$ to state $i$. We define $p_i (t) \in [0, 1]$ to be the probability to be in state $i$ at time $t$, the probability vector

$$p (t) \triangleq (p_1 (t), ..., p_M (t))^\top \in [0, 1]^M,$$

(1.1)

and the rate matrix $A$, so that

$$(A)_{ij} \triangleq \begin{cases} A_{ij}, & \text{if } i \neq j \\ -\sum_{j \neq i} A_{ji}, & \text{if } i = j \end{cases}$$

(1.2)

and

$$\frac{dp (t)}{dt} = Ap (t)$$

(1.3)

is the corresponding master equation, with solution

$$p (t) = \exp (At) p (0).$$

(1.4)
From the normalization of the probability, \( p(t) \) must be constrained at all time by
\[
\mathbf{e}^\top p(t) = 1; \quad \mathbf{e} \triangleq (1, 1, ..., 1)^\top.
\] (1.5)

Note that from the properties of \( A \) (specifically, the fact that \( \mathbf{e}^\top A = 0 \)), if we start from an initial condition \( p_0 \in [0, 1]^M \) so that \( \mathbf{e}^\top p_0 = 1 \), then, \( \forall t \), \( \mathbf{e}^\top p(t) = 1 \) automatically - though this is not immediately obvious from the above notation.

In order to improve the interpretability of the above notation, we combine Eq. 1.5 directly with Eq. 1.3. We shall henceforth assume that \( X(t) \) is irreducible, and reduce the dimensionality of the problem from \( M \) to \( M - 1 \) (section 2). Note that if instead \( X(t) \) is reducible with \( K \) connected components, then the method suggested here can be applied to each component separately, reducing the dimensionality of the problem from \( M \) to \( M - K \) (see appendix A). The reduced form of the master equation (Eq. 2.3 or Eq. 4.3) has some “nice” properties. For example, in section 3 we prove that the reduced form is strictly contracting; in section 4 we show it is easy to find a novel explicit form for the stationary (invariant) distribution using this reduced form (for the relation with previous stationary distribution expressions see appendix B); and in section 5 we discuss the application of this method to stochastic differential equations (SDE) based on a population of independent Markov processes.

Note that similar reduction methods are rather popular for the special case of a two state system \( x \leftrightarrow 1 - x \), in the context of deterministic kinetic equations, which are the limit of the SDE equations for an infinite population (e.g. [3]). In a few special cases they were also used in SDE descriptions of specific systems with more than one state [2].

## 2 Reduction of the Master Equation

First, we make a few additional definitions:

1. \( \mathbf{I}_M \) is the \( M \times M \) identity matrix
2. \( \mathbf{J} \) is \( \mathbf{I}_M \) with it last row removed: \( \mathbf{J} = \begin{pmatrix}
  1 & 0 & 0 & \cdots & 0 & 0 \\
  0 & 1 & 0 & \cdots & 0 & 0 \\
  \vdots & \vdots & \vdots & \ddots & \vdots & 0 \\
  0 & 0 & 0 & \cdots & 1 & 0 
\end{pmatrix}, \dim(J) = (M - 1) \times M 
\)
3. \( \mathbf{e}_M \triangleq (0, 0, ..., 1)^\top 
\)
4. \( \mathbf{H} \triangleq (\mathbf{I}_M - \mathbf{e}_M \mathbf{e}^\top) \mathbf{J}^\top = \begin{pmatrix}
  1 & 0 & 0 & \cdots & 0 \\
  0 & 1 & 0 & \cdots & 0 \\
  \vdots & \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & 0 & \cdots & 1 \\
  -1 & -1 & -1 & -1 & -1 
\end{pmatrix}, \dim(H) = M \times (M - 1)
\)
5. \( \dot{\mathbf{p}}(t) = \mathbf{J} \mathbf{p}(t), \dim(\dot{\mathbf{p}}) = (M - 1) \times 1 
\)
Note that $\tilde{p}(t) \in [0, 1]^{M-1}$, and the “hard” normalization constraint has been lifted (instead we remain with a “soft” constraint $e^T J^T \tilde{p}(t) \leq 1$). Using these definitions, we can use \ref{eq:1.5} to write

$$p(t) = e_M + H\tilde{p}(t) \quad (2.1)$$

Substituting this into Eq. \ref{eq:1.3} we obtain

$$H \frac{d\tilde{p}(t)}{dt} = Ae_M + AH\tilde{p}(t)$$

Multiplying this by $J$ from the left, we obtain

$$JH \frac{d\tilde{p}(t)}{dt} = J Ae_M + JAH\tilde{p}(t).$$

Using the fact that

$$JH = J (I - e_M e^T) J^T = J J^T = I_{M-1}, \quad (2.2)$$

where we used $Je_M = 0$ in the second equality. Defining $\hat{A} \triangleq JAH, \hat{b} \triangleq JAe_M$, we can write our first reduced form of Eq. \ref{eq:1.3}

$$\frac{d\tilde{p}(t)}{dt} = \hat{b} + \hat{A}\tilde{p}(t). \quad (2.3)$$

3 Properties of $\hat{A}$

Since $A$ is a rate matrix of an irreducible process, it has a single zero eigenvalue and all the other eigenvalues have negative real parts \cite{6}. Given this, we can find the eigenvalues of $\hat{A}$.

**Theorem 1.** Assume $X(t)$ is an irreducible process, then $\hat{A}$ has the same eigenvalues as $A$ - except its (unique) zero eigenvalue.

**Proof.** To find the eigenvalues of $\hat{A}$, we examine the characteristic polynomial

$$|\hat{A} - \lambda I_{M-1}| = |JAH - \lambda I_{M-1}|$$

$$\quad \equiv (1) \lambda^{M-1} |\lambda^{-1} JA (I - e_M e^T) J^T - I_{M-1}|$$

$$\quad \equiv (2) \lambda^{M-1} |\lambda^{-1} (I - e_M e^T) J^T JA - I_M|$$

$$\quad \equiv (3) \lambda^{-1} |(I - e_M e^T) (I - e_M e_M^T) A - \lambda M|$$

$$\quad \equiv (4) \lambda^{-1} |A - \lambda M|$$

$$\quad \equiv (5) \lambda^{-1} \prod_{i=1}^{M} (\lambda - \lambda_i)$$

$$\quad = \prod_{i=2}^{M} (\lambda - \lambda_i)$$
where in (1) we used the definition of $H$ and the fact that $|\lambda X| = \lambda^M |X|$ for any $M \times M$ matrix and scalar $\lambda$, in (2) we used Sylvester’s determinant theorem ($|I_p + BC| = |I_p + CB|$ for all $B, C$ matrices of size $p \times n$ and $n \times p$ respectively), in (3) we used $J^T J = (I - e_M e_M^T)$ and $|\lambda X| = \lambda^M |X|$ again, in (4) we used $e^T e_M = 1$ and $e^T A = 0$ and in (5) we denoted by $\{\lambda_i\}_{i=1}^M$ the eigenvalues of $A$, with $\lambda_1 = 0$. The last line concludes the proof.

Remark. Although the eigenvalues of $A$ and $\tilde{A}$ are the same, their corresponding eigenvectors $v_m$ and $\tilde{v}_m$ are not tied by a simple projection, namely $\tilde{v}_m \neq Jv_m$.

Recall again that a rate matrix $A$ of an irreducible process has a single zero eigenvalue and all the other eigenvalues have negative real parts [6]. Using theorem 1 this immediately gives

**Corollary 2.** $\tilde{A}$ is a stable matrix - i.e. all its eigenvalues have a strictly negative real part.

Specifically, since $\tilde{A}$ does not have any zero eigenvalues,

**Corollary 3.** $\tilde{A}$ is a non-singular matrix, and therefore, invertible.

## 4 Stationary Distribution

Recall ([6]) that if $X(t)$ is irreducible then $p(t) \to p_\infty$, a stationary distribution which is the (unique) zero eigenvector of the matrix $A$,

$$0 = Ap_\infty.$$  \hspace{1cm} (4.1)

This is an implicit equation for $p_\infty$. However, using the our reduced version, it is easy to find an explicit expression for the stationary distribution.

Using Eq. 2.3 and Corollary 3 we define

$$\tilde{p}_\infty \triangleq -\tilde{A}^{-1}\tilde{b}$$ \hspace{1cm} (4.2)

and re-write Eq. 2.3 as

$$\frac{d\tilde{p}(t)}{dt} = \tilde{A}(\tilde{p}(t) - \tilde{p}_\infty),$$ \hspace{1cm} (4.3)

which is our second reduced form of Eq. 1.3

Since $\tilde{A}$ is stable, $p(t) \to \tilde{p}_\infty$, and so the solution of (4.3) is

$$\tilde{p}(t) = \tilde{p}_\infty + (\tilde{p}(0) - \tilde{p}_\infty)e^{\tilde{A}t}.$$

And so, we found an explicit expression for the steady state distribution in the reduced form

$$\tilde{p}_\infty = -(JAH)^{-1}JAe_M.$$

Returning to the original form, using Eq. 2.1 we obtain the explicit expression

$$p_\infty = (I_M - H(JAH)^{-1}JA)e_M.$$ \hspace{1cm} (4.4)

In section B we compare this expression with previous results. Note that for a discrete time Markov chain with transition matrix $P$, we can again find the stationary distribution by substituting $A = I - P$ in either Eq. 1.3 or B.2.
5 The reduction methods in stochastic differential equations

Consider a population of identical, irreducible and independent Markov processes $\{X_n(t)\}_{n=1}^N$, where each process has states $\{1, 2, ..., M\}$, where $1 < M < \infty$. Also, for all processes, $A_{ij}$ is the transition rate from state $j$ to state $i$, and $A$ is the corresponding matrix. We denote by $x_i(t)$ the fraction of processes that are in state $i$ at time $t$ (not following convention of using upper case only for random variables). Formally

$$x_i(t) \triangleq \frac{1}{N} \sum_{n=1}^N I[X_n(t) = i],$$

where $I[\cdot]$ is the indicator function. Also, we denote $x = (x_1, ..., x_M)\top$. From normalization,

$$e\top x(t) = 1 ; \quad e \triangleq (1, 1, ..., 1). \quad (5.1)$$

As derived in [4], for large enough $N$ we can approximate the dynamics of $x$ by the following $n$-dimensional stochastic differential equation (SDE)

$$\dot{x}(t) = Ax(t) + B(x(t))\xi(t) \quad (5.2)$$

where $\xi$ is a vector of $M(M - 1)/2$ independent white noise processes with zero mean and correlation $\langle \xi(t)\xi(t') \rangle = \delta(t - t')$ ($\langle \cdot \rangle$ denotes ensemble expectation), and $B$ is a (sparse) $M \times M(M - 1)/2$ matrix, with

$$B_{ik} = \frac{1}{\sqrt{N}} \text{sgn}(i - m_{ik}) \sqrt{A_{im ik} x_m ik + A_{m ik} i x_i}$$

where $k$ is the index of a transition pair $(i \leftrightarrow j)$ and $m_{ik}$ is index of the state connected to state $i$ by transition pair $k$. Note that since $N$ is large, any Ito correction would be of size $O(N^{-2})$, and is therefore neglected here.

We can reduce the form of Eq. 5.2 using 5.1 in a similar way as we did for the Markov process. Defining $A = JAH$ (as before), $B = JB$ (with $x_K$ replaced by $1 - x_1 - x_2 - ... - x_{K-1}$) and $\tilde{x}_\infty \triangleq \tilde{p}_\infty = (A)^{-1} JAE_M$, we obtain the following equation for the reduced state vector $\hat{x} = Jx$

$$\frac{d\hat{x}(t)}{dt} = \tilde{A} (\hat{x}(t) - \tilde{x}_\infty) + \tilde{B} (\hat{x}(t))\xi(t). \quad (5.3)$$

As before $\tilde{A}$ is a stable matrix. Additionally, the reduced diffusion matrix $D \triangleq BB\top$ is positive definite (in contrast to $D = BB\top$, which is only semi-definite). This stems from the combination of the following facts: (1) $D = BB\top$ is symmetric (2) The rank of $B$ is $M - 1$ (for irreducible $X_n(t)$) (3) For any real matrix $X$, rank $(XX\top) = \text{rank}(X)$ [1].
Appendix

A Generalization to a reducible processes

Assume now that \( X(t) \) is a reducible process, with \( K \) connected components \( C_k \), \( k = \{1, 2, \ldots, K\} \), where \( C_k \) contains \( M^{(k)} \) states. In this case, we can write

\[
A = \begin{pmatrix}
A^{(1)} & 0 & \cdots & 0 \\
0 & A^{(2)} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & A^{(K)}
\end{pmatrix}.
\]

Also, the normalization condition (Eq. 1.5) can be expanded to each component separately,

\[
\forall k : u_k^T p(t) = q_k ; \quad (u_k)_m \triangleq \mathbb{I} [m \in C_k]
\]

where \( \sum_k q_k = 1 \). In order to derive the reduced form of Eq. 1.3 in this case, we just have to find the reduced form for each component separately, and then concatenate the equations, reducing the dimensionality from \( M \) to \( M - K \). Formally, we define:

1. \( a_k \) is the index of the last \( (M^{(k)}) \) state in \( C_k \).
2. \( L \) is \( \mathbf{I}_M \) with the rows corresponding to \( \{a_k\}_{k=1}^K \) removed.
3. \( f \) is an length-\( M \) vector for which all the indices \( \{a_k\}_{k=1}^K \) equal \( q_k \) and all the rest equal 0.
4. \( H_m \) as \( \mathbf{H} \) with \( M = m \).
5. \( G \) as

\[
G = \begin{pmatrix}
H^{(1)} & 0 & \cdots & 0 \\
0 & H^{(2)} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & H^{(K)}
\end{pmatrix}
\]

6. \( \tilde{p}(t) = Jp(t) \)

Using these definitions, we can use 1.5 to write

\[
p(t) = f + G \tilde{p}(t) . \tag{A.1}
\]

Substituting this into Eq. 1.3 we obtain

\[
G \frac{d\tilde{p}(t)}{dt} = Af + AG \tilde{p}(t) .
\]

Multiplying this by \( J \) from the left, we obtain

\[
LG \frac{d\tilde{p}(t)}{dt} = LAf + LAG \tilde{p}(t) .
\]
Using the fact that

\[ \mathbf{LG} = \mathbf{I}_{M-K}, \quad (A.2) \]

and defining \( \hat{\mathbf{A}} \triangleq \mathbf{LAF}, \hat{\mathbf{b}} \triangleq \mathbf{LAF}, \) we can write our first reduced form of Eq. 1.3

\[ \frac{d\hat{\mathbf{p}}(t)}{dt} = \tilde{\mathbf{b}} + \hat{\mathbf{A}}\hat{\mathbf{p}}(t). \quad (A.3) \]

which has dimension \( M - K. \) All the other results we derived for the irreducible case (i.e. the properties of \( \hat{\mathbf{A}}, \) the stationary distribution, etc.) can be similarly proven.

**B Relations to previous results - stationary distribution expression**

In the main text (Eq. 4.4) we derived an expression for the stationary distribution

\[ \mathbf{p}_\infty = \left( \mathbf{I}_M + \mathbf{H}(\mathbf{JAH})^{-1}\mathbf{JA} \right) \mathbf{e}_M. \quad (B.1) \]

Note however, that this is not the first explicit form suggested for the solution of Eq. 4.1. For example, [5] proved that

\[ \mathbf{p}_\infty = (\mathbf{A} + \mathbf{ve}^\top)^{-1}\mathbf{v} \quad (B.2) \]

for any \( \mathbf{v} \) such that \( \mathbf{e}^\top\mathbf{v} \neq 0. \)

Both Eq. 4.1 and Eq. B.2 must be equal and behave similarly if we vary \( \mathbf{A}. \) For example, Eq. B.1 immediately implies that \( \mathbf{p}_\infty \) does not change if we scale \( \mathbf{A} \rightarrow c\mathbf{A} \) by some non-zero constant, as implied by Eq. 4.1. This can be seen also in Eq. B.2 if we scale \( \mathbf{v} \rightarrow c\mathbf{v} \) simultaneously with the scaling in \( \mathbf{A}. \)

To prove that both equations coincide (for any choice of \( \mathbf{v} \)), we equate them, expecting to derive an identity:

\[
\mathbf{v} = (\mathbf{A} + \mathbf{ve}^\top)\left( \mathbf{I}_M + \mathbf{H}(\mathbf{JAH})^{-1}\mathbf{JA} \right) \mathbf{e}_M
\]

\[
= \mathbf{Ae}_M + \mathbf{AH}(\mathbf{JAH})^{-1}\mathbf{JAe}_M + \mathbf{ve}^\top\mathbf{e}_M + \mathbf{ve}^\top\mathbf{H}(\mathbf{JAH})^{-1}\mathbf{JAe}_M
\]

Since \( \mathbf{e}^\top\mathbf{e}_M = 1 \) and \( \mathbf{e}^\top\mathbf{H} = 0, \) we obtain

\[ 0 = \mathbf{Ae}_M + \mathbf{AH}(\mathbf{JAH})^{-1}\mathbf{JAe}_M \]

multiplying this by \( \mathbf{J} \) from the left we get \( 0 = 0, \) as expected. Multiplying by \( \mathbf{e}^\top \) from the left also gives \( 0 = 0, \) since \( \mathbf{e}^\top\mathbf{A} = 0. \) Since the row vectors of \( \mathbf{J}, \) combined with \( \mathbf{e}^\top, \) span the vector space \( \mathbb{R}^M, \) this concludes our proof.
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