The exponential family of Markov chains
and its information geometry

Hiroshi Nagaoka *

Abstract — We introduce a new definition of exponential family of Markov chains, and show that many characteristic properties of the usual exponential family of probability distributions are properly extended to Markov chains. The method of information geometry is effectively applied to our framework, which enables us to characterize the divergence rate of Markov chain from a differential geometric viewpoint.

Keywords — exponential family, Markov chain, Markov process, information geometry

1 Introduction

A d-dimensional parametric family

\[ \{ p_\theta \mid \theta = (\theta^1, \ldots, \theta^d) \in \Theta \}, \quad \Theta \subset \mathbb{R}^d \]

of probability density functions on a measure space \((\mathcal{X}, \mathcal{B}, \nu)\) is called an exponential family with a natural parameter \(\theta = (\theta^\nu)\) (e.g. \([2]\)) when there exist \(d + 1\) \(\mathbb{R}\)-valued functions \(C, F_1, \ldots, F_d\) on \(\mathcal{X}\) and an \(\mathbb{R}\)-valued function \(\psi\) on \(\Theta\) such that

\[
\log p_\theta(x) = C(x) + \sum_{i=1}^d \theta^i F_i(x) - \psi(\theta). \tag{1}
\]

The notion of exponential family is very important in various fields such as the theory of statistical inference (parameter estimation, hypothesis testing, etc.), large deviations, information theory, etc., and a dualistic viewpoint of the information geometry ([6, 7, 8]) works effectively to understand the structure of exponential families in a unified and elegant manner. The present paper is aimed at demonstrating that many characteristic properties of exponential families ([1] are preserved by families of Markov kernel densities of the form

\[
\log w_\psi(y|x) = C(x,y) + \sum_{i=1}^d \theta^i F_i(x,y) \\
+ K_\psi(y) - K_\psi(x) - \psi(\theta). \tag{2}
\]

In particular, we show that the family is dually flat just as is the case for ([1], which enables us to apply the general theory for dually flat spaces to investigation of the information-geometrical structure of the family. In order to avoid being involved with functional analytic arguments and to concentrate upon geometric and algebraic aspects, we mostly confine ourselves to the case where \(\mathcal{X}\) is a finite set and \(\nu\) is the counting measure, whereas the essence of the arguments can be extended to the general case by putting proper regularity conditions.

Several attempts have been made so far to extend the definition of exponential families to Markov processes or more general stochastic processes (e.g. \([3, 4, 5]\)). Although they share the common criterion that an exponential family should have a finite dimensional (exact or asymptotic) sufficient statistic, the definitions given there are diverse, reflecting their respective backgrounds. The authors of such papers as ([9, 11] had essentially the same concept on exponential families of Markov chains as ours when they said that the totality of strictly positive Markov chains of a fixed order is asymptotically regarded as an exponential family in an approximate sense. We refine the concept so that the general definition of exponential families of Markov kernels is given without appealing to asymptotic settings, although the significance of the definition is made clear through some asymptotic arguments. This non-asymptotic treatment enables us to develop the information geometry of Markov chains in a transparent and systematic way.

This article is essentially based on the technical report ([14]. The proofs of the theorems are omitted for want of space.

2 Definition and an example

Let \(\mathcal{X}\) be a finite set with \(|\mathcal{X}| \geq 2\). We denote the totality of positive probability distributions on \(\mathcal{X}\) by \(\mathcal{P} = \mathcal{P}(\mathcal{X})\). A Markov kernel (transition matrices) on \(\mathcal{X}\) is a map \(w : \mathcal{X}^2 \rightarrow [0, 1]\) \((x, y) \mapsto w(y|x))\) satisfying \(\sum_{y \in \mathcal{X}} w(y|x) = 1\) for every \(x \in \mathcal{X}\). Suppose that we are given a subset \(\mathcal{E} \subset \mathcal{X}^2 \times \mathcal{X}\) for which the directed graph \((\mathcal{X}, \mathcal{E})\) is strongly connected; i.e., for any \((x, y) \in \mathcal{X}^2\) there exists a sequence \((x_1, x_2), (x_2, x_3), \ldots, (x_{n-1}, x_n)\) in \(\mathcal{E}\) such that \(x_1 = x, x_n = y, n \geq 2\). Let the totality of irreducible Markov kernels \(w\) on \(\mathcal{X}\) such that \(\{(x, y) \mid w(y|x) > 0\} = \mathcal{E}\) be denoted by \(\mathcal{W} = \mathcal{W}(\mathcal{X}, \mathcal{E})\). This includes the set of strictly positive Markov kernels \(\mathcal{W}(\mathcal{X}, \mathcal{X}^2)\) as a special case.

From the irreducibility, each \(w \in \mathcal{W}\) has the unique stationary distribution in \(\mathcal{P}\), which is denoted by \(p_w\). We introduce the notation

\[
p^{(n)}_w(x_1, \ldots, x_n) = p_w(x_1)w(x_2|x_1) \cdots w(x_n|x_{n-1})
\]

\((p^{(1)}_w(x) = p_w(x)\) and \(p^{(2)}_w(x,y) = p_w(x)w(y|x)\) in particular, which will be used in later sections.
A $d$-dimensional parametric family

\[ M = \{ w_\theta \mid \theta = (\theta^1, \ldots, \theta^d) \in \mathbb{R}^d \} \subset \mathcal{W} \]

is called an exponential family (or a full exponential family) following the terminology of [2] of Markov kernels on $(\mathcal{X}, \mathcal{E})$ with a natural (or canonical) parameter $\theta$, when there exist functions $C, F^1, \ldots, F^d : \mathcal{X} \to \mathbb{R}$, $K : \mathcal{X} \times \mathbb{R}^d \to \mathbb{R}$, $\psi : \mathbb{R}^d \to \mathbb{R}$ such that equation (2) holds for every $\theta \in \mathbb{R}^d$ and every $(x, y) \in \mathcal{E}$.

When a family of initial distributions, say $\{ q_\theta \mid \theta \in \mathbb{R}^d \}$, is specified, the family of joint probability distributions for $x^n = (x_1, \ldots, x_n)$ satisfying $(x_t, x_{t+1}) \in \mathcal{E} \ (\forall t)$ is determined by

\[ q_\theta^{(n)}(x^n) = q_\theta(x_1)w_\theta(x_2|x_1) \cdots w_\theta(x_n|x_{n-1}), \]  

for which we have from (2)

\[ \log q_\theta^{(n)}(x^n) = \log q_\theta(x_1) + \sum_{t=1}^{n-1} \left\{ C(x_t, x_{t+1}) + \sum_{i=1}^{d} \theta^i F(x_t, x_{t+1}) - \psi(\theta) \right\} + K_\theta(x_1) - K_\theta(x_1) 
\]

\[ = \sum_{t=1}^{n-1} C(x_t, x_{t+1}) + \sum_{i=1}^{d} \theta^i \left( \sum_{t=1}^{n-1} F(x_t, x_{t+1}) - (n-1)\psi(\theta) - O(1) \right). \]  

This shows that the family $\{ q_\theta^{(n)} \mid \theta \in \mathbb{R}^d \}$ is asymptotically an exponential family in the usual sense.

**Example 1**  For any $w \in \mathcal{W} = \mathcal{W}(\mathcal{X}, \mathcal{E}^2)$, we have

\[ \log w(y|x) = \sum_{i=0}^{\lvert \mathcal{X} \rvert - 1} \sum_{j=1}^{\lvert \mathcal{X} \rvert - 1} \log \frac{w(j|i)w(0|0)}{w(0|i)w(0|0)} \delta_{i,j}(x, y) 
\]

\[ + \log w(0|x) - \log w(0|y) + \log w(0|0), \]

where $\delta_{i,j}(x, y) = 1$ if $(i, j) = (x, y)$ and $= 0$ otherwise. We can easily verify this identity by respectively calculating the RHS for the two cases $y \neq 0$ and $y = 0$. This shows that $\mathcal{W}$ is an exponential family with $\dim \mathcal{W} = \lvert \mathcal{X} \rvert - (\lvert \mathcal{W} \rvert - 1)$.

### 3 Affine structures

The gist of the definition will be clarified by a fundamental relation between the affine structure of functions on $\mathcal{E}$ and the Markov kernels on $\mathcal{E}$ as shown below. Let $\mathcal{F} = \mathcal{F}(\mathcal{X}, \mathcal{E})$ be the totality of functions on $\mathcal{E}$, which is a $\lvert \mathcal{E} \rvert$-dimensional linear space. An element $f$ of $\mathcal{F}$ is sometimes identified with its extension to a function on $\mathcal{X}^2$ by letting $f(x, y) = 0$ for any $(x, y) \in \mathcal{X}^2 \setminus \mathcal{E}$. For a $f \in \mathcal{F}$ we define the functions $f(\cdot, \cdot)$ and $f(\cdot, +)$ on $\mathcal{X}$ by

\[ f(\cdot, x) = \sum_{y \in \mathcal{X}} f(y, x) \quad \text{and} \quad f(\cdot, +) = \sum_{y \in \mathcal{X}} f(y, x). \]

A function $f \in \mathcal{F}$ is said to be shift-invariant if $f(\cdot, \cdot) = f(\cdot, +)$, and the totality of shift-invariant functions is denoted by $\mathcal{F}^S = \mathcal{F}^S(\mathcal{X}, \mathcal{E})$. A function $f \in \mathcal{F}$ is said to be anti-shift-invariant if there exists a function $\kappa$ on $\mathcal{X}$ such that $f(x, y) = \kappa(y) - \kappa(x)$ for any $(x, y) \in \mathcal{E}$, and the totality of anti-shift-invariant functions is denoted by $\mathcal{F}^A = \mathcal{F}^A(\mathcal{X}, \mathcal{E})$. The linear subspaces $\mathcal{F}^S$ and $\mathcal{F}^A$ of $\mathcal{F}$ are the orthogonal complements of each other with respect to the inner product on $\mathcal{F}$ defined by $(f_1, f_2) = \sum_{(x,y) \in \mathcal{E}} f_1(x, y)f_2(x, y)$, which follows from

\[ \sum_{(x,y) \in \mathcal{E}} f(x, y)(\kappa(y) - \kappa(x)) = \sum_{x\in \mathcal{X}} (f(\cdot, x) - f(\cdot, +))\kappa(x). \]

We thus have the direct sum decomposition $\mathcal{F} = \mathcal{F}^S \oplus \mathcal{F}^A$. In addition, from the assumption that $(\mathcal{X}, \mathcal{E})$ is strongly connected, the necessary and sufficient condition for two functions $\kappa_1, \kappa_2$ to define the same element of $\mathcal{F}^A$ is that $\kappa_1 - \kappa_2$ is constant on $\mathcal{X}$. This leads to $\dim \mathcal{F}^A = \lvert \mathcal{X} \rvert - 1$ and $\dim \mathcal{F}^S = \dim \mathcal{F} - \dim \mathcal{F}^A = \lvert \mathcal{E} \rvert - \lvert \mathcal{X} \rvert + 1$.

Let

\[ \mathcal{F}^+ = \mathcal{F}^+(\mathcal{X}, \mathcal{E}) \defeq \{ f \mid f : \mathcal{E} \to \mathbb{R}^+ \} \subset \mathcal{F}, \]

where $\mathbb{R}^+ = (0, \infty)$. Then we have the following theorem, which is a direct consequence of the Perron-Frobenius theorem for irreducible nonnegative matrices.

**Theorem 1** For any $f \in \mathcal{F}^+$, there exist $w \in \mathcal{W}$, $Z > 0$ and $\gamma : \mathcal{X} \to \mathbb{R}^+$ such that

\[ \forall (x, y) \in \mathcal{E}, \quad w(y|x) = \frac{1}{Z} \gamma(y) f(x, y). \]

Here $w$ and $Z$ are unique, and $\gamma$ is unique up to a constant factor.

Denoting the correspondence between $f$ and $w$ in (6) by $w = \Gamma(f)$, we define the mapping $\Gamma : \mathcal{F}^+ \to \mathcal{W}$. Note that $\mathcal{W} \subset \mathcal{F}^+$ and $\Gamma(w) = w$ for any $w \in \mathcal{W}$.

Since $\exp(f(x, y))$ defines an element of $\mathcal{F}^+$ for every $f$, we obtain a mapping

\[ \Delta \defeq \Gamma \circ \exp : \mathcal{F} \to \mathcal{W}, \quad f \mapsto \Gamma(\exp(f)). \]

Noting that $w = \Delta(f) = \Gamma(\exp(f))$ is written as $w(y|x) = \exp(f(x, y))\gamma(y)/Z\gamma(x)$ from (6), we have

\[ \log w(y|x) = f(x, y) + \kappa(y) - \kappa(x) - \psi, \]

where $\kappa(x) = \log \gamma(x)$ and $\psi = \log Z$. This means that $\log w \equiv f$ mod $\mathcal{F}^A \oplus \mathbb{R}$, where a real constant is identified with the corresponding constant function in $\mathcal{F}$. Moreover, $\Delta$ gives a diffeomorphism from the quotient linear space $\mathcal{F}/(\mathcal{F}^A \oplus \mathbb{R})$ to $\mathcal{W}$. Now we have the following theorem.
A subset $M$ of $W$ is an exponential family if and only if there exists an affine subspace $V$ of $F$ such that $M = \Delta(V) \triangleq \{ \Delta(f) \mid f \in V \}$, and we have $\dim M = \dim V$. Moreover, the correspondence between exponential families and affine subspaces is one-to-one.

From this theorem, we have the following corollaries.

**Corollary 1** $W$ itself is an exponential family of dimension $|E| - |X'|$.

Remember that in Example 1 we have verified the above fact for the case of complete graph $E = X^2$ by a little complicated calculation.

**Corollary 2** The 1-dimensional exponential family $\{ w_t \mid t \in \mathbb{R} \}$ passing through given two kernels $w_0, w_1 \in W$ is written in the form $w_t = \Gamma(w_1^i w_0^{-i})$, or equivalently

$$w_t(y|x) = \frac{\gamma_t(y)}{\sum_{t'} \gamma_t(y)} \{w_1(y|x)\}^t \{w_0(y|x)\}^{1-t}.$$ (8)

A 1-dimensional exponential family is called an $e$-geodesic.

**Corollary 3** A subset $M$ of $W$ is an exponential family if and only if for any two points $w_0$ and $w_1$ in $M$ the $e$-geodesic $\{ \Gamma(w_1^i w_0^{-i}) \mid t \in \mathbb{R} \}$ lies in $M$.

### 4 Fisher information

For an arbitrary $d$-dimensional parametric family $M = \{ w_0 \mid \theta = (\theta^i) \in \Theta \} \subset W$, where $\Theta$ is an open subset of $\mathbb{R}^d$, the Fisher information matrix $G_\theta = [g_{ij}(\theta)] : d \times d$ (with respect to the parameter $(\theta^i)$) is defined by

$$g_{ij}(\theta) \triangleq \sum_{(x,y) \in E} p_\theta(x,y) \left( \partial_i \log w_\theta(y|x) \right) \left( \partial_j \log w_\theta(y|x) \right),$$ (9)

where $p_\theta(x,y) = p^{(2)}_w(x,y) = p_w(x) w_\theta(y|x)$ and $\partial_i = \partial / \partial \theta^i$. This definition is commonly used because of the following fact. Let $\{ q_\theta \mid \theta \in \Theta \}$ be an arbitrary family of probability distributions on $X$ (possibly being independent of $\theta$) and consider the joint distributions

$$q_\theta^{(n)}(x^n) = q_\theta(x_1) w_\theta(x_2|x_1) \cdots w_\theta(x_n|x_{n-1}).$$

Letting $G_\theta^{(n)} = [g_{ij}^{(n)}(\theta)]$ be the Fisher information matrix (in the usual sense) of the family $\{ q_\theta^{(n)} \mid \theta \in \Theta \}$, we have

$$g_{ij}(\theta) = \lim_{n \to \infty} \frac{1}{n} g_{ij}^{(n)}(\theta).$$ (10)

From the information-geometric viewpoint, the Fisher information is regarded as a Riemannian metric $g$ through the relation $g(\partial_i, \partial_j) = g_{ij}$ and is called the Fisher metric.

**Theorem 3** When $M = \{ w_\theta \mid \theta \in \mathbb{R}^d \}$ is an exponential family of the form (2), the Fisher information matrix with respect to the natural parameter $(\theta^i)$ is given by

$$g_{ij}(\theta) = \partial_i \partial_j \psi(\theta).$$ (11)

### 5 Expectation parameters

For an exponential family $M = \{ w_\theta \mid \theta \in \mathbb{R}^d \}$ of the form (2), we define

$$\eta_i(\theta) \triangleq \sum_{(x,y) \in E} p_w^{(2)}(x,y) F_i(x,y).$$ (12)

Then $\eta = (\eta_1, \ldots, \eta_d)$ forms another coordinate system for $M$, which we call the expectation parameter corresponding to the representation (2).

**Theorem 4** We have:

$$\eta_i = \partial_i \psi,$$ (13)

$$\partial_i \psi_j = g_{ij},$$ (14)

$$\partial^i \psi_j = g^{ij},$$ (15)

$$[g^{ij}] = [g_{ij}]^{-1},$$ (16)

where $\partial^i = \partial / \partial \eta_i$, and $[g^{ij}]$ denotes the Fisher information matrix with respect to the dual parameter ($\eta_i$).

Moreover, if we define $\varphi = \sum \theta^i \eta_i - \psi$, we have

$$\theta^i = \partial^i \varphi,$$ (17)

$$g^{ij} = \partial^i \partial^j \varphi.$$ (18)

### 6 A dually flat structure

For an arbitrary $d$-dimensional parametric family $M = \{ w_\theta \mid \theta = (\theta^i) \in \Theta \} \subset W$, the exponential connection (or $e$-connection for short) $\nabla^{(e)}$ and the mixture connection (or $m$-connection for short) $\nabla^{(m)}$ are defined as follows.

$$\Gamma^{(e)}_{i,j,k} = g(\nabla^{(e)}_{\partial_i} \partial_j, \partial_k) = \sum_{(x,y) \in E} \partial_i \partial_j \log w_\theta(y|x) \partial_k p_\theta(x,y),$$ (19)

$$\Gamma^{(m)}_{i,j,k} = g(\nabla^{(m)}_{\partial_i} \partial_j, \partial_k) = \sum_{(x,y) \in E} \partial_i \partial_j p_\theta(x,y) \partial_k \log w_\theta(y|x),$$ (20)

where $g$ is the Fisher metric. Then $\nabla^{(e)}$ and $\nabla^{(m)}$ are dual with respect to $g$ in the sense that $X g(Y,Z) = g(\nabla^{(e)}_{X} Y, Z) + g(Y, \nabla^{(m)}_{X} Y)$ holds for any vector fields $X,Y,Z$.

**Theorem 5** For an exponential family $M = \{ w_\theta \mid \theta = (\theta^i) \in \mathbb{R}^d \}$ of the form (2), both $\nabla^{(e)}$ and $\nabla^{(m)}$ are flat, and $[\theta^i]$ and $[\eta_i]$ are affine coordinate systems of these connections, respectively.

**Theorem 6** Suppose that $M$ is an exponential family and $N$ is a submanifold of $M$. Then $N$ is an exponential family if and only if $N$ is auto-parallel with respect to the $e$-connection of $M$.

Let

$$\mathcal{P}^{(2)} = \mathcal{P}(E) \cap F^{S} = \left\{ p^{(2)} \in \mathcal{P}(E) \mid \forall y, \sum_x p^{(2)}(x,y) = \sum_x p^{(2)}(y,x) \right\}. $$

Then $w \mapsto p^{(2)}_w$ gives a diffeomorphism from $W$ to $\mathcal{P}^{(2)}$.
Theorem 7 The m-connection of $\mathcal{W}$ is the natural flat connection induced from the convexity of $\mathcal{P}^{(2)}$. In particular, the m-geodesic (i.e., the auto-parallel curve with respect to the m-connection) connecting given two points $w_0$ and $w_1$ in $\mathcal{X}$ is represented as

$$p_w^{(2)} = tp_w^{(1)} + (1-t)p_w^{(1)}.$$  \hfill (21)

7 Canonical Divergence

Let $M$ be an exponential family of the form (2). Then the canonical divergence $D : M \times M \to \mathbb{R}$ with respect to the dually flat structure $(g, \nabla^{(m)}, \nabla^{(e)})$ is defined by

$$D(w_1 | w_2) = \varphi(w_1) + \psi(w_2) - \sum_{i=1}^{d} \eta_i(w_1) \theta^i(w_2).$$  \hfill (22)

The divergence $D$ is also characterized by the following property: let $\gamma$ be an m-geodesic such that $\gamma(1) = w_1$ and $\gamma(0) = w_2$, and $\delta$ be an e-geodesic such that $\delta(1) = w_3$ and $\delta(0) = w_2$, which intersect at $w_2$. Then we have

$$D(w_1 | w_2) + D(w_2 | w_3) = D(w_1 | w_3) = g(\gamma(0), \dot{\gamma}(0)).$$  \hfill (23)

where the RHS means the inner product between the tangent vectors of $\gamma$ and $\delta$ at the intersecting point $w_2$.

Theorem 8 $D$ is represented as

$$D(w_1 | w_2) = \sum_{(x,y) \in \mathcal{E}} p_{w_1}^{(2)}(x,y) \frac{w_1(y|x)}{w_2(y|x)}.$$  \hfill (24)

This is nothing but the divergence rate of Markov chains. Actually, we have

$$D(w_1 | w_2) = \lim_{n \to \infty} \frac{1}{n} D(q_1^{(n)} | q_2^{(n)}),$$  \hfill (25)

where $q_i^{(n)}$, $i = 1, 2$ are defined as

$$q_i^{(n)}(x_1, \ldots, x_n) = q_i(x_1)w(x_2|x_1)\cdots w(x_n|x_{n-1})$$

by arbitrary distributions $q_i$ on $\mathcal{X}$.

8 Remaining subjects

The following subjects can also be treated in the present framework or its obvious extension.

- Application to the large deviation theory.
- Some variant of Cramér-Rao inequality, and an estimation-theoretic characterization of exponential families.
- Extension to higher-order Markov chains, and a hierarchy of exponential families: $\mathcal{P} = \mathcal{W}_0 \subset \mathcal{W} = \mathcal{W}_1 \subset \mathcal{W}_2 \subset \cdots$.
- Extension to general measureable spaces, and autoregressive models as an example.

References

[1] H. Nagaoka, “Exponential families of Markov chains and their information geometry,” IS Technical Reports, UEC-IS-2003-6, Univ. of Electro-Communications, 2003.
[2] O.E. Barndorff-Nielsen, Information and Exponential Families in Statistical Theory, Wiley, 1978.
[3] P. D. Feigin, “Conditional exponential families and a representation theorem for asymptotic inference,” Ann. Statist., vol.9, no.3, 597–603, 1981.
[4] U. Küchler and M. Sørensen, “On exponential families of Markov processes,” J. Statist. Planning and Inference, vol.66, 3-19, 1998.
[5] U. Küchler and M. Sørensen, Exponential Families of Stochastic Processes, Springer-Verlag, 1997.
[6] S. Amari, Differential-Geometrical Methods in Statistics (Lecture Notes in Statistics 28), Springer-Verlag, 1985.
[7] S. Amari and H. Nagaoka, Methods of Information Geometry, AMS&Oxford Univ. Press, 2000.
[8] H. Nagaoka and S. Amari, “Differential geometry of smooth families of probability distributions”, METR 82-7, Univ. of Tokyo, 1982.
[9] H. Ito and S. Amari, “Geometry of information sources,” Proceedings of the 11th Symposium on Information Theory and Its Applications (SITA ’88), 57–60, 1988 (in Japanese).
[10] N. Merhav, “The estimation of the model order in exponential families,” IEEE Trans. on Inform. Theory, vol.35, no.5, 1109–1114, 1989.
[11] S. Amari, “Information geometry on hierarchy of probability distributions,” IEEE Trans. on Inform. Theory, vol.47, no.5, 1701–1711, 2001.