



Information Geometry of Reversible Markov Chains

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Introduction & Preliminaries

Information geometry

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Regard family $\mathcal{M} = \{m_q : q \in \mathbb{Q}\} \subset P(X)$ as a smooth manifold.

Fisher information metric g and dual affine connections $r^{(e)}, r^{(m)}$

$$g_{ij}(m_q) = \int_{x \in X} m_q(x) \eta_i \log m_q(x) \eta_j \log m_q(x),$$

$$G_{ij,k}^{(e)}(m_q) = \int_{x \in X} \eta_i \eta_j \log m_q(x) \eta_k m_q(x),$$

$$G_{ij,k}^{(m)}(m_q) = \int_{x \in X} \eta_i \eta_j m_q(x) \eta_k \log m_q(x).$$

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Wide range of applications

1. Higher-order efficiency analysis of estimator
2. Information decomposition / projection
3. Natural gradient algorithms

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What about Markov models?

Irreducible Markov chains

Notation

$E \subseteq X^2$ such that (X, E) **strongly connected**.

Functions and positive functions over E : $F(X, E)$, $F_+(X, E)$.

Irreducible row-stochastic matrices over (X, E) : $W(X, E)$.

Often we will take $E = X^2$.

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Discrete-time, time-homogeneous Markov chain

$$P(X_1 = x_1, \dots, X_k = x_k) = m(x_1) \prod_{t=1}^{k-1} P(x_t, x_{t+1}),$$

$$(m, P) \in (P(X), W(X, E)).$$

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Stationary distribution: $\rho P = \rho$.

Edge-measure: $Q(x, x^\ell) = \rho(x)P(x, x^\ell) = P_\rho(X_t = x, X_{t+1} = x^\ell)$.

Reversible Markov chains

Notation

Time-reversal: $P^?(x, x^0) = p(x^0)P(x^0, x) / p(x)$.

Reversible: $p(x)P(x, x^0) = p(x^0)P(x^0, x)$ (detailed balance).

$W_{\text{rev}}(X, E)$ the set of all reversible kernels.

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Numerous interesting properties (e.g.)

Spectrum is **real** and **stable**.

Mixing time is governed by **spectral gap**.

Stationary distribution is easy to compute.

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Historical remarks

Inspiration & origin Schrödinger (1931).

First treatment for MCs Kolmogorov (1936, 1937).

Tribute and historical summary Dobrushin et al. (1988).

Exponential tilting (ET)

ET of distribution

$X \sim m \in \mathcal{P}([m]), f: X \rightarrow \mathbb{R}$. Construct **exponential family**:

$$m_q(x) = m(x) e^{qf(x) - k(q)}, \quad k(q) = \log \mathbb{E} e^{qf(X)} \quad (\text{CGF}).$$

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$$I > E[f], \lim_{k \rightarrow \infty} \frac{1}{k} \log P \left(\frac{1}{k} \sum_{t=1}^k f(X_t) > I \right) = k^*(I), \quad \sup_{q \in \mathbb{R}} qI - k(q).$$

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$$I > E[f], \lim_{k \rightarrow \infty} \frac{1}{k} \log P \left(\frac{1}{k} \sum_{t=1}^k f(X_t) > I \right) = -k^*(I), \quad k^*(I) = \sup_{q \in \mathbb{R}} [qI - Z(q)].$$

ET of stochastic matrix

$$P \in \mathcal{W}, f: \mathcal{X} \rightarrow \mathbb{R}, \mathbb{P}_q(x, x^0) = P(x, x^0) \exp(qf(x^0)),$$

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$P \in \mathbb{W}, f: X \rightarrow \mathbb{R}, \mathbb{P}_q(x, x^0) = P(x, x^0) \exp(qf(x^0)), \mathbb{P}_q = s(\mathbb{P}_q)$, with Perron-Frobenius (PF) rescaling (Miller, 1961),

$$s: F_+(X, E) \rightarrow \mathbb{W}(X, E), \mathbb{P}(x, x^0) \mapsto P(x, x^0) = \frac{\mathbb{P}(x, x^0) v(x^0)}{r v(x)},$$

where r, v are the **PF root and right PF eigenvector** of

Exponential tilting (ET)

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$P \in W, f : X \rightarrow \mathbb{R}, \mathbb{P}_q(x, x') = P(x, x') \exp(qf(x))$, $P_q = s(\mathbb{P}_q)$, with Perron-Frobenius (PF) rescaling (Miller, 1961),

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Information Geometry of Markov Chains

1. Large deviations: Miller (1961); Donsker and Varadhan (1975); Gärtner (1977)
2. Information projection: Csizsar et al. (1987)
3. Asymptotic e-families: Ito and Amari (1988); Takeuchi and Barron (1998); Takeuchi and Kawabata (2007); Takeuchi and Nagaoka (2017)
4. One-parameters exponential families: Nakagawa and Kanaya (1993)
5. Dually flat structure: Nagaoka (2005)

Distributions

$P(X)$

D

KL divergence

$$D(m_{q|j} || m_{q|0}) = E_{m_q} \log \frac{m_q(x)}{m_q(x^0)}$$

Information Geometry of Markov Chains (Nagaoka, 2005)

Distributions

$P(X)$

Markov chains

$W(X, E)$

$X_1, X_2, \dots, X_t \quad P$

$D \xrightarrow{\hspace{15em}} D$

KL divergence

KL divergence rate

$$\lim_{t \rightarrow \infty} \frac{1}{t} D(X_1, \dots, X_t \mid P_{q|j} X_1^0, \dots, X_t^0 \mid P_{q^0}) = E_{(X, X^0)} \left[\log \frac{P_q(X, X^0)}{P_{q^0}(X, X^0)} \right]$$

$$, \quad D(P_{q|j} \mid P_{q^0})$$

Information Geometry of Markov Chains (Nagaoka, 2005)

Distributions
 $P(X)$

Markov chains
 $W(X, E)$

$r^{(e)}, r^{(m)}$ $\xrightarrow{\text{limit } \neq}$ $r^{(e)}, r^{(m)}$

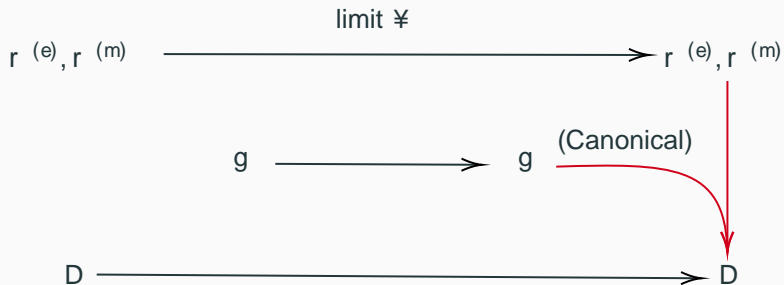
$g \longrightarrow g$

$D \longrightarrow D$

Information Geometry of Markov Chains (Nagaoka, 2005)

Distributions
 $P(X)$

Markov chains
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View $W(X, E)$ as a **smooth manifold**.

Fisher information metric g

$$g_{ij}(P_q) = \int_{(x, x^0) \in E} \dot{a} Q_q(x, x^0) \mathbb{1}_i \log P_q(x, x^0) \mathbb{1}_j \log P_q(x, x^0).$$

Dual affine connections $r^{(e)}, r^{(m)}$

$$G_{j,k}^{(e)}(P_q) = \int_{(x, x^0) \in E} \dot{a} \mathbb{1}_i \mathbb{1}_j \log P_q(x, x^0) \mathbb{1}_k Q_q(x, x^0),$$

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Exponential families of transition kernels (Nagaoka, 2005)

Let $Q \subset \mathbb{R}^d$, open connected **parameter space**.

$$V_e = \{P_q : q = (q^1, \dots, q^d) \in Q\} \subset \mathcal{W}$$

is an **e-family** with **natural parameter** q , whenever there exist functions $K, R_q, y_q, g_1, \dots, g_d$ such that

$$\log P_q(x, x^0) = K(x, x^0) + \sum_{i=1}^d q^i g_i(x, x^0) + \underbrace{\frac{R_q(x^0)}{R_q(x)}}_{\text{rescaling terms}} \underbrace{y_q}_{\text{}}.$$

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Example 1 (Nagaoka, 2005)

$\mathcal{W}(X, E)$ forms an **e-family** of dimension $|E| = |X|$. For $E = X^2$,

$$\begin{aligned} \log P(x, x^0) &= \sum_{i=1}^{|X|} \sum_{j=1}^{|X|} \log \frac{P(i, j) P(j, x^0)}{P(i, x^0) P(x^0, x^0)} + \log P(x, x^0) \\ &\quad + \log P(x, x^0) - \log P(x^0, x^0) + \log P(x^0, x^0). \end{aligned}$$

Mixture families (Nagaoka, 2005)

We say that V_m is a **mixture family** when there exists functions C, F_1, \dots, F_d , such that $C, C + F_1, \dots, C + F_d$ are affinely independent,

$$\int_{x, x^0 \in X} C(x, x^0) = 1, \quad \int_{x, x^0 \in X} F_i(x, x^0) = 0, \quad \forall i \in [d],$$

and

$$V_m = \left\{ P_x \in \mathcal{W} : Q_x = C + \sum_{i=1}^d x^i F_i \right\}$$

where $X = \{x \in \mathbb{R}^d : Q_x(x, x^0) > 0, \forall (x, x^0) \in X^2\}$, and Q_x is the edge measure that pertains to P_x .

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where $X = \{x \in \mathbb{R}^d : Q_x(x, x^0) > 0, \forall (x, x^0) \in X^2\}$, and Q_x is the edge measure that pertains to P_x .

Example 2

W_{bis} (doubly stochastic) forms an m -family (Hayashi and Watanabe, 2016).

Geometric approach has recently lead to finite sample analysis for:

1. Parameter estimation problem in Markov chains in HMMs
[Hayashi and Watanabe \(2016\)](#); [Hayashi \(2022\)](#).

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Extension of known concepts^ but also new structures emerge!

Time-reversal families

Definition

Let $V \subseteq W$.

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What about **families of fixed points**?

Reversible e-families

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V is reversible when P is reversible $\forall P \in V$.

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V is reversible when P is reversible $\Leftrightarrow P \perp V$.

Example 3

Unbiased lazy random walks on the cycle form a reversible e-family.

Reversible e-families

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V is reversible when P is reversible $\Leftrightarrow P \in \mathcal{R}(V)$.

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Problem: How to determine whether a given e-family is reversible ?

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V is reversible when P is reversible on V .

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Theorem (Kolmogorov's criterion (Kolmogorov, 1936))

Let P irreducible, and G the set of finite directed closed-paths, $g \in G$

wheng: $[n] \rightarrow E$, $g(t) = (x_t, x_{t+1})$ with $x_{n+1} = x_1$. Write $g^?$ the

time-reversed path. P is reversible if and only if $\forall g \in G$

$$\prod_{t=1}^{|g|} P(g(t)) = \prod_{t=1}^{|g|} P(g^?(t)).$$

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time-reversed path. P is reversible if and only if for all $g \in \mathcal{G}$

$$\prod_{t=1}^{|g|} P(g(t)) = \prod_{t=1}^{|g|} P(g^?(t)).$$

Log-reversible function

A function $h \in \mathbb{R}^E$ is **log-reversible** whenever it satisfies that for all $g \in \mathcal{G}$

$$\prod_{t=1}^{|g|} h(g(t)) = \prod_{t=1}^{|g|} h(g^?(t)).$$

Characterization of reversible e-families

Theorem 2

Let V be e-family of kernels generated by K and $\mathbb{K}_{i2[d]}$. The two statements are equivalent:

Characterization of reversible e-families

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Let V be e-family of kernels generated by $K \in \mathcal{K}_{i_2[d]}$. The two statements are equivalent:

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Let V be e-family of kernels generated by K and $\mathcal{G}_i^2[d]$. The two statements are equivalent:

- (i) V is **reversible**.
- (ii) V is such that K and $\mathcal{G}_i^2[d]$ are all **log-reversible functions** (and $E = E^?$ for more general irreducible kernels).

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Naively, the number of distinct equations that must be checked would be large

$$(d+1) \sum_{k=3}^{j \times j} \frac{j \times j}{k} \frac{(k-1)!}{2}.$$

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Lemma 2 (**Polynomial time** procedure for reversibility checking)

Let $h \in F_+$ (more generally irreducible) **$\log[h]$ is log-reversible** if and only if **$P_h = h^l$ is a symmetric matrix**, with **$P_h = v_h^l u_h$ the PF projection of h** , where u_h and v_h are respectively the left and right PF eigenvectors of h , normalized such that $u_h^l v_h = 1$.

Lemma 4 (Vector space of log-reversible functions)

F_{rev} , $f, h \in F$: h is log-reversible,

\mathbb{N} , $h \in F$: $\exists(c, f), h(x, x^0) = f(x^0) + f(x) + c$.

Lemma 4 (Vector space of log-reversible functions)

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N , $h \in F$: $\exists(c, f), h(x, x^0) = f(x^0) - f(x) + c$.

$N \subset F_{\text{rev}} \subset F$ (vector space inclusions)

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quotient space: $G_{\text{rev}}, F_{\text{rev}}/N$

$D(G_{\text{rev}}) = W_{\text{rev}}$, with $D(f)$, $s(\exp[f])$ diffeomorphism

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Theorem 3 & 4

Let $T = f(x) - x^0 \in \mathfrak{g}(m, 1)$, $\|T\| = \|x\|(\|x\| + 1)/2 + 1$.

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Theorem 3 & 4

Let $T = \{x^0, \dots, x^n\} \in (m, 1)^n$, $|T| = \binom{n}{j} = \frac{n!}{j!(n-j)!}$.

(i) G_{rev} is a $|T|$ -dimensional vector space.

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Theorem 3 & 4

Let $T = \int_{x^0}^x f(x) dx$, $T_j = \int_{x^0}^x f(x) dx$, $jT_j = jX_j(jX_j + 1)/2 - 1$.

- (i) G_{rev} is a jT_j -dimensional vector space.
- (ii) W_{rev} is an **e-family**, and is an **m-family**.

Lemma 4 (Vector space of log-reversible functions)

F_{rev} , $f \in F$: f is log-reversible,

N , $h \in F$: $h(x, x^0) = f(x^0) - f(x) + c$.

$N \subset F_{\text{rev}} \subset F$ (vector space inclusions)

quotient space: $G_{\text{rev}}, F_{\text{rev}}/N$

$D(G_{\text{rev}}) = W_{\text{rev}}$, with $D(f)$, $s(\exp[f])$ diffeomorphism

Theorem 3 & 4

Let $T = \{x^0, \dots, x^m\}$, $f \in (m, 1)g$, $|T| = j$, $|T_j| = (j-1)/2 + 1$.

- (i) G_{rev} is a $|T_j|$ -dimensional vector space.
- (ii) W_{rev} is an **e-family**, and is an **m-family**.
- (iii) $\dim W_{\text{rev}} = |T_j|$.

Lemma 4 (Vector space of log-reversible functions)

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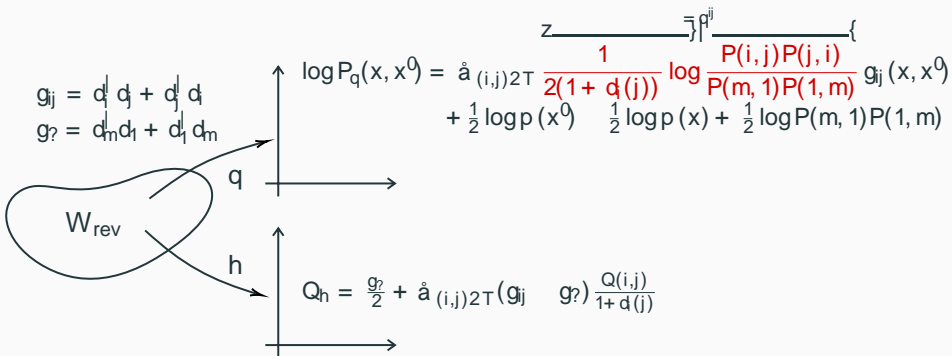
$D(G_{\text{rev}}) = W_{\text{rev}}$, with $D(f)$, $s(\exp[f])$ diffeomorphism

Theorem 3 & 4

Let $T = \{x^j : 0 \leq j \leq n\} \subset \mathbb{R}^n$, $J_T = (j+1) \binom{n}{j}$.

- (i) G_{rev} is a J_T -dimensional vector space.
- (ii) W_{rev} is an **e-family**, and is an **m-family**.
- (iii) $\dim W_{\text{rev}} = J_T$.
- (iv) Basis: $g_j, d_j^i + d_j^i : (i, j) \in T$.

Parametrization of W_{rev} (Theorem 5)



$$q^i(h) = \sum_{x, x^0 \in E} \frac{Q_h(x, x^0)}{q^i(h)} \log P_h(x, x^0)$$

$$h_i(q) = \sum_{x, x^0 \in E} Q_q(x, x^0) g_i(x, x^0)$$

Reversible e/m-projections

Closest reversible chain

Reversiblization

Given an irreducible (non-reversible) P , we can construct

1. $(P + P^T) / 2$, the **additive** reversiblization of P .
2. PP^T , the **multiplicative** reversiblization of P (Fill, 1991).
3. $S_p(P)$, the **reversible dilation** of P (Wolfer and Kontorovich, 2022).

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Given an irreducible P , what is the reversible kernel that is the closest to P ?

Closest reversible chain

Reversibilization

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Properties of reversible chains are powerful but **brittle**

(e.g. real spectrum, Weyl's inequality).

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Related work

Analyzed by **Nielsen and Weber (2015)** for matrix norms induced by scalar products (unique, obtained by solving a convex minimization problem).

Reversible e-projection / m-projection (Theorem 7)

$$D(P||P^0) = \int_{x,x^0} p(x) P(x, x^0) \log \frac{P(x, x^0)}{P^0(x, x^0)}$$



W_{rev}

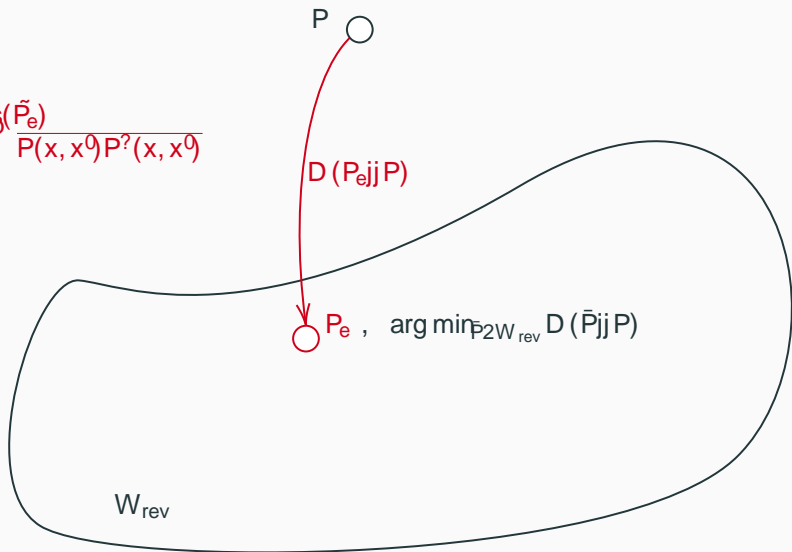
Reversible e-projection / m-projection (Theorem 7)

P ○

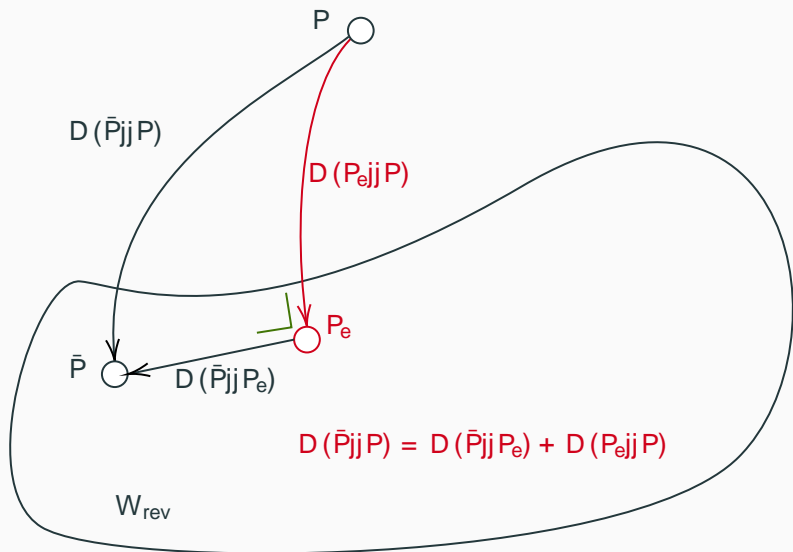


Reversible e-projection / m-projection (Theorem 7)

$$P_e = \mathcal{P}(\tilde{P}_e)$$
$$\tilde{P}_e = \frac{P(x, x^0)P^*(x, x^0)}{P(x, x^0)P^*(x, x^0)}$$

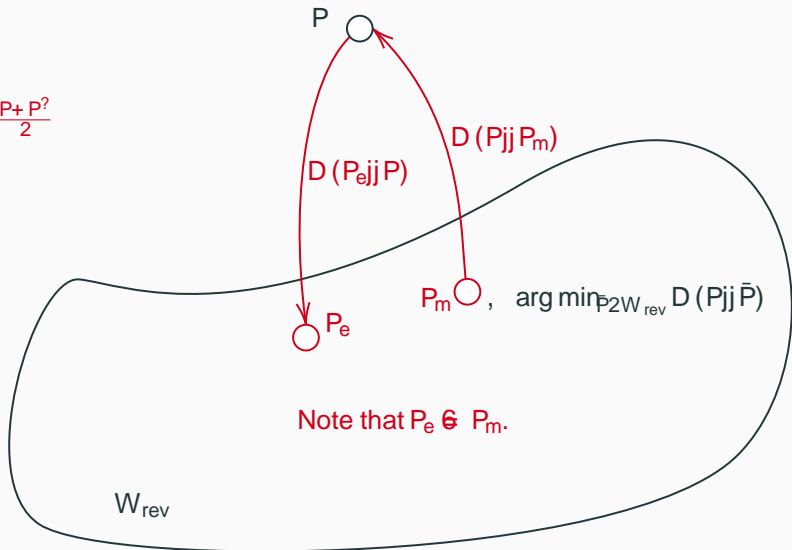


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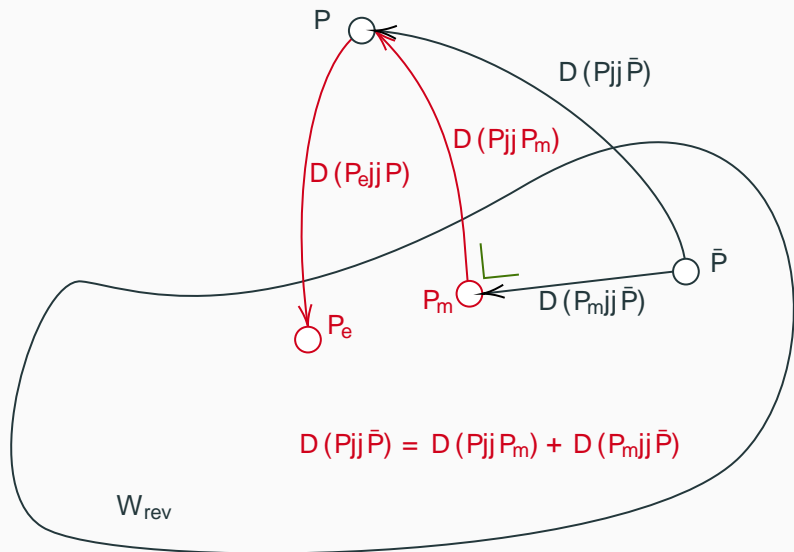


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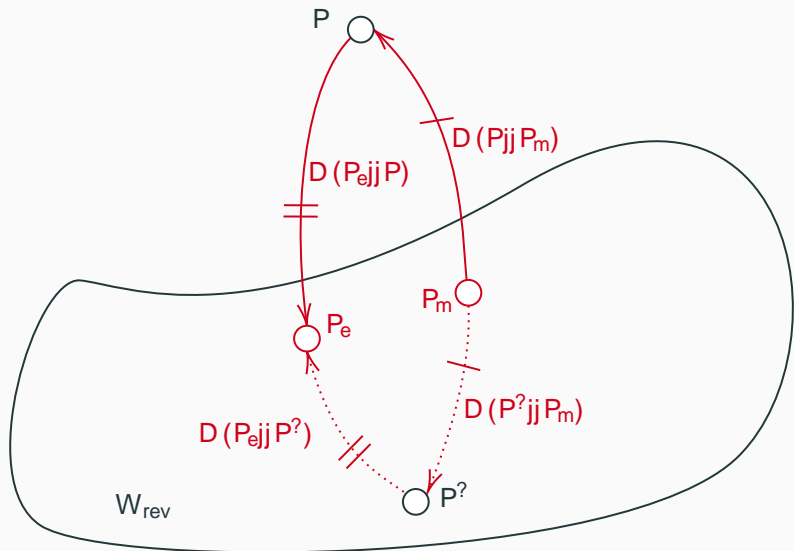
$$P_m = \frac{P + P^e}{2}$$



Reversible e-projection / m-projection (Theorem 7)



Reversible e-projection / m-projection (Theorem 7)



Usual families of kernels

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W_{bis} : bi-stochastic kernels ($\mathbb{R}^I \times \mathbb{R}^J$)

W_{sym} : symmetric kernels ($\mathbb{R}^I = \mathbb{R}^I$)

W_{iid} : memoryless kernels ($\mathbb{R}^I = \mathbb{R}^I \times \mathbb{R}^J$)

Usual families of kernels

W_{bis} : bi-stochastic kernels $(\mathbb{R}^J \times \mathbb{R}^J \rightarrow \mathbb{R})$

W_{sym} : symmetric kernels $(\mathbb{R}^J \times \mathbb{R}^J \rightarrow \mathbb{R})$

W_{iid} : memoryless kernels $(\mathbb{R}^J \times \mathbb{R}^J \rightarrow \mathbb{R})$

Mfd.	m-family	e-family	Dimension
W	3	3	$j \times j (j \times j - 1)$
W_{rev}	3	3	$j \times j (j \times j + 1) / 2 - 1$
W_{bis}	3	7	$(j \times j - 1)^2$
W_{sym}	3	7	$j \times j (j \times j - 1) / 2$
W_{iid}	7	3	$j \times j - 1$

Usual families of kernels

W_{bis} : bi-stochastic kernels $(\mathbb{R}^I \times \mathbb{R}^I \rightarrow \mathbb{R})$

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W_{sym}	3	7	$j \times j (j \times j - 1) / 2$
W_{iid}	7	3	$j \times j - 1$

Hierarchies

$$W_{\text{iid}} \begin{matrix} \text{e-family} \\ \left(\right. \end{matrix} W_{\text{rev}} \begin{matrix} \text{e-family} \\ \left(\right. \end{matrix} W,$$

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Generation of reversible kernels

Definition 4 (Mixture hull)

Let $V \subseteq W$.

$$m\text{-hull}(V) = \left(P: Q \subseteq Q, Q = \sum_{i=1}^k a_i Q_i, k \in \mathbb{N}, a_1, \dots, a_k \in \mathbb{R}, P_1, \dots, P_k \in V \right),$$

where Q (resp. Q_i) pertains to P (resp. P_i).

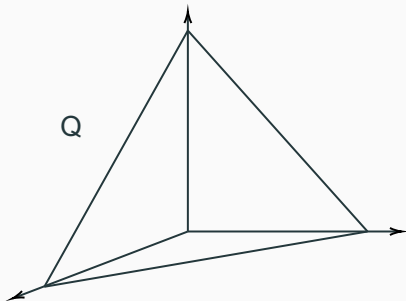
Generation of the reversible family from W_{iid}

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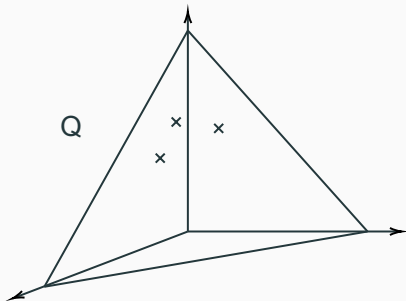


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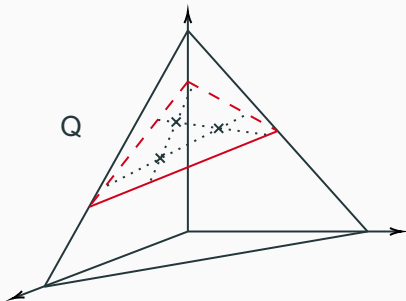


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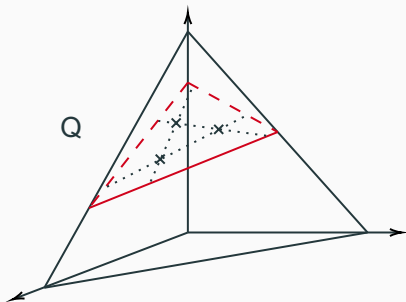
Generation of the reversible family from W_{iid}

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where Q (resp. Q_i) pertains to P (resp. P_i).



Theorem 10

$$m\text{-hull}(W_{iid}) = W_{rev}.$$

Definition 5 (Exponential hull)

Let $V \subseteq W$.

$$\begin{aligned}
 \text{e-hul}(V) = & \left(s(\mathcal{P}) : \log[\mathcal{P}] = \sum_{i=1}^k a_i \log[P_i], \right. \\
 & \left. k \in \mathbb{N}, a_1, \dots, a_k \in \mathbb{R}, \sum_{i=1}^k a_i = 1, P_1, \dots, P_k \in V \right).
 \end{aligned}$$

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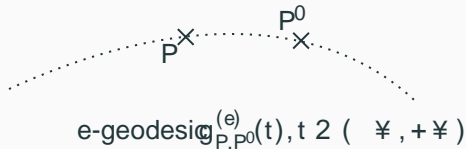
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 \end{aligned}$$

$$\begin{matrix}
 P^X & P^0 \\
 X & X
 \end{matrix}$$

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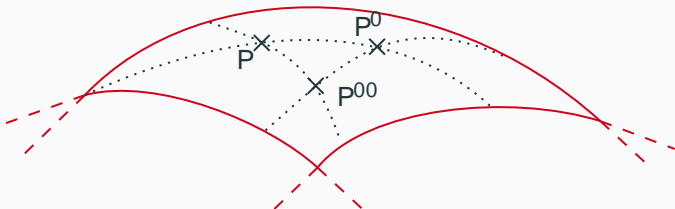
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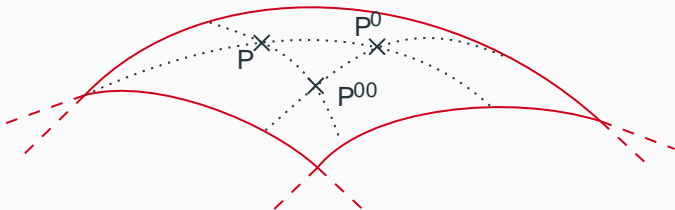


Generation of the reversible family from W_{sym}

Definition 5 (Exponential hull)

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Theorem 9

$$j \times j \quad 3 \Rightarrow e\text{-hul}(W_{\text{sym}}) = W_{\text{rev.}}$$

Reversible edge measures

Reversible family of edge measures

Edge-measures

P reversible $\Rightarrow Q, \text{diag}(p)P$ is symmetric.

$$Q = \left(\begin{array}{c} Q: \int_{x^0 \in X} Q(x, x^0) = \int_{x^0 \in X} Q(x^0, x) \end{array} \right),$$
$$Q_{\text{rev}} = f Q \text{ } 2 \text{ } Q : Q^? = Qg.$$

Reversible family of edge measures

Edge-measures

P reversible $\Rightarrow Q, \text{diag}(p)P$ is symmetric.

$$Q = \sum_{x, x^0 \in X} Q(x, x^0) \begin{pmatrix} \vdots \\ \vdots \\ \vdots \end{pmatrix} \begin{pmatrix} \vdots \\ \vdots \\ \vdots \end{pmatrix}^T$$

$$Q_{\text{rev}} = \frac{1}{2} (Q + Q^T) = Qg.$$

Lemma 6

$$Q_{\text{rev}} = P \frac{jXj(jXj + 1)}{2},$$

where \equiv denotes Markov equivalence.

Reversible family of edge measures

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$$Q = \sum_{x, x^0 \in X} Q(x, x^0) = \sum_{x, x^0 \in X} Q(x^0, x),$$

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Theorem 8

(i) Q_{rev} is **e-family** and **m-family** of $\mathcal{P}(X^2)$.

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- (i) Q_{rev} is **e-family** and **m-family** of $\mathcal{P}(X^2)$.
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Reversible family of edge measures

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Theorem 8

- (i) Q_{rev} is **e-family** and **m-family** of $\mathcal{P}(X^2)$.
- (ii) $\dim Q_{\text{rev}} = jXj(jXj + 1)/2 - 1$.
- (iii) Q is **not e-family** in $\mathcal{P}(X^2)$ (except when $jXj = 2$).

Summary

- (i) Property of being an e/m-family is **invariant** under **time-reversal** operation.
- (ii) We introduce **reversible e-families**, and provide a **characterization** (efficiently verifiable).
- (iii) Perhaps surprisingly, W_{rev} **forms an e/m-family**. We further construct a basis, and derive an **explicit parametrization**.
- (iv) We show that **e/m-projections**, possess **closed-form** expressions that verify **Pythagorean** identities, and are always **equidistant** from an irreducible Markov kernel and its time-reversal (**bisection property**).
- (v) We characterize the **reversible family** as both the **minimal exponential family** that comprises **symmetric** kernels, and the **smallest mixture family** that contains **memoryless** Markov kernels.
- (vi) We show that, unlike the set of all irreducible edge measures, the restriction to **reversible edge measures** forms an **e-family** (in distributions over pairs).

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Thank you for listening!

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