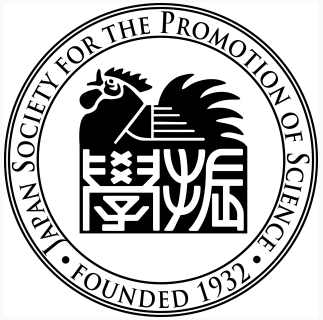

Information Geometry of Reversible Markov Chains

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Introduction & Preliminaries

Information geometry

Finite space $\mathcal{X} \cong [m]$. Simplex over $\mathcal{X}$: $\mathcal{P}(\mathcal{X})$.

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

$$\mathfrak{g}_{ij}(\mu_\theta) \triangleq \sum_{x \in \mathcal{X}} \mu_\theta(x) \partial_i \log \mu_\theta(x) \partial_j \log \mu_\theta(x),$$

$$\Gamma^{(e)}_{ij,k}(\mu_\theta) \triangleq \sum_{x \in \mathcal{X}} \partial_i \partial_j \log \mu_\theta(x) \partial_k \mu_\theta(x),$$

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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

$\mathcal{E} \subset \mathcal{X}^2$ such that $(\mathcal{X}, \mathcal{E})$ strongly connected.

Functions and positive functions over $\mathcal{E}$: $\mathcal{F}(\mathcal{X}, \mathcal{E})$, $\mathcal{F}_+(\mathcal{X}, \mathcal{E})$.

Irreducible row-stochastic matrices over $(\mathcal{X}, \mathcal{E})$: $\mathcal{W}(\mathcal{X}, \mathcal{E})$.

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Discrete-time, time-homogeneous Markov chain

$$\mathbb{P}\left(X_1 = x_1, \ldots, X_k = x_k\right) = \mu(x_1) \prod_{t=1}^{k-1} P(x_t, x_{t+1}),$$

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

Edge-measure: $Q(x, x') = \pi(x)P(x, x') = \mathbb{P}_\pi\left(X_t = x, X_{t+1} = x'\right)$.

Reversible Markov chains

Notation

Time-reversal: $P^\star(x, x') = \pi(x')P(x', x)/\pi(x)$.

Reversible: $\pi(x)P(x, x') = \pi(x')P(x', x)$ (detailed balance).

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

$$\mu_\theta(x) = \mu(x) e^{\theta f(x) - \kappa(\theta)}, \qquad \kappa(\theta) = \log \mathbb{E} e^{\theta f(X)} \qquad \text{(CGF)}.$$

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$$\mathfrak{s}\colon \mathcal{F}_+(\mathcal{X},\mathcal{E}) \to \mathcal{W}(\mathcal{X},\mathcal{E}), \ \widetilde{P}(x,x') \mapsto P(x,x') = \frac{\widetilde{P}(x,x')v(x')}{\rho v(x)},$$

where ρ, v are the PF root and right PF eigenvector of $\widetilde{P}$.

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Information Geometry of Markov Chains

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1. Large deviations: Miller (1961); Donsker and Varadhan (1975); Gärtner (1977)
2. Information projection: Csiszár 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)

Information Geometry of Markov Chains (Nagaoka, 2005)

Distributions

$\mathcal{P}(\mathcal{X})$

D

KL divergence

$$D\left(\mu_\theta || \mu_{\theta'}\right) = \mathbb{E}_{\mu_\theta} \log \frac{\mu_\theta(x)}{\mu_\theta(x')}$$

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Distributions
$\mathcal{P}(\mathcal{X})$

Markov chains
$\mathcal{W}(\mathcal{X}, \mathcal{E})$

$$X_1, X_2, \ldots, X_t \sim P$$

$D \longrightarrow D$

KL divergence

KL divergence rate

$$\lim_{t\to\infty} \frac{1}{t} D\left(X_1, \ldots, X_t \sim P_\theta || X'_1, \ldots, X'_t \sim P_{\theta'}\right) = \mathbb{E}_{(X,X')\sim Q_\theta} \log \frac{P_\theta(X,X')}{P_{\theta'}(X,X')}$$

$$\triangleq D\left(P_\theta || P_{\theta'}\right)$$

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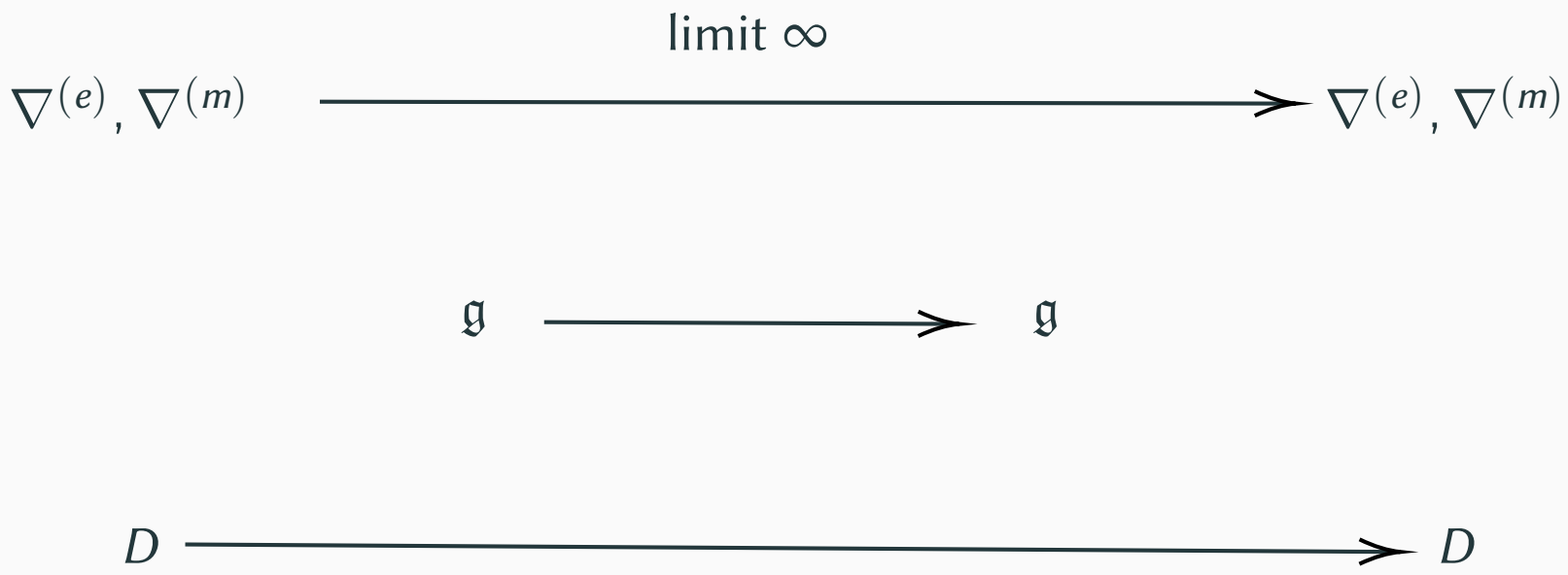

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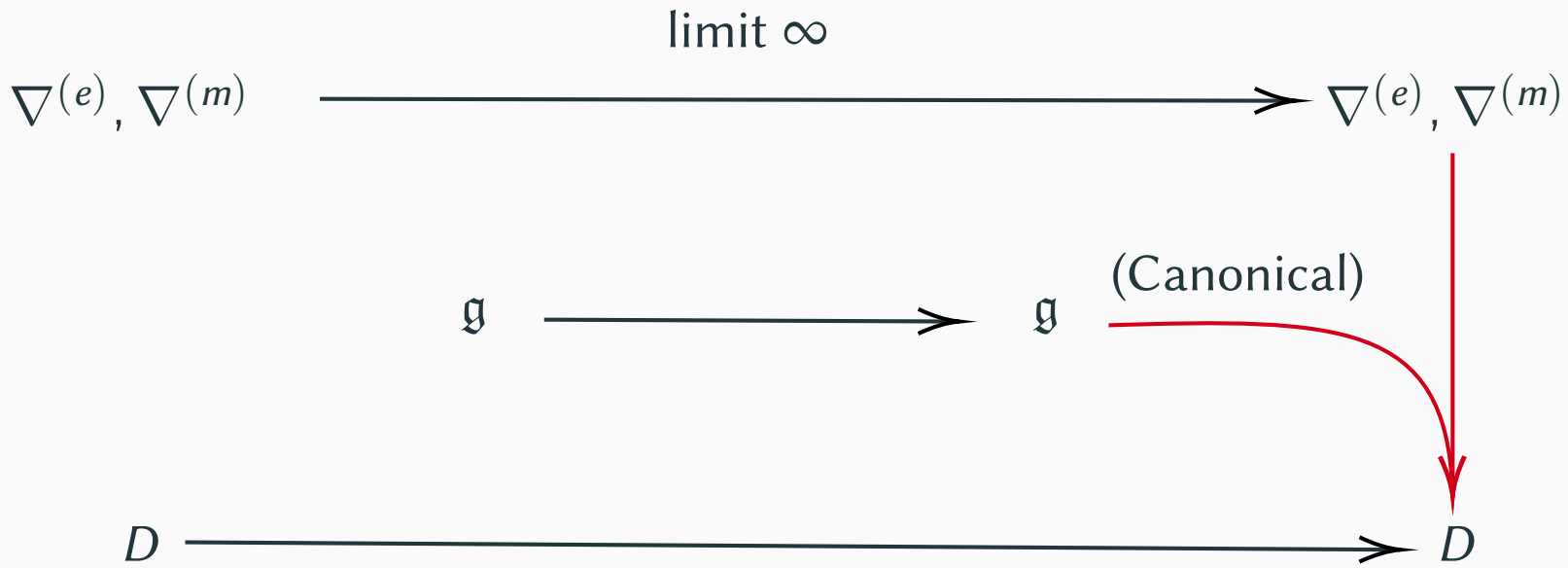

Information geometry Markov chains (Nagaoka, 2005)

View $\mathcal{W}(\mathcal{X}, \mathcal{E})$ as a smooth manifold.

Fisher information metric $\mathfrak{g}$

$$\mathfrak{g}_{ij}(P_\theta) \triangleq \sum_{(x,x')\in\mathcal{E}} Q_\theta(x,x')\partial_i \log P_\theta(x,x')\partial_j \log P_\theta(x,x').$$

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

$$\Gamma^{(e)}_{ij,k}(P_\theta) \triangleq \sum_{(x,x')\in\mathcal{E}} \partial_i\partial_j \log P_\theta(x,x')\partial_k Q_\theta(x,x'),$$

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Exponential families of transition kernels (Nagaoka, 2005)

Let $\Theta \subseteq \mathbb{R}^d$, open connected parameter space.

$$\mathcal{V}_e = \left\{ P_\theta : \theta = (\theta^1, \ldots, \theta^d) \in \Theta \right\} \subset \mathcal{W}$$

is an e-family with natural parameter θ, whenever there exist functions $K, R_\theta, \psi_\theta, g_1, \ldots, g_d$ such that

$$\log P_\theta(x, x') = K(x, x') + \sum_{i=1}^{d} \theta^i g_i(x, x') + \underbrace{R_\theta(x') - R_\theta(x) - \psi_\theta}_{\text{rescaling terms}}.$$

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Example 1 (Nagaoka, 2005)

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

$$\log P(x, x') = \sum_{i=1}^{|\mathcal{X}|} \sum_{\substack{j=1 \\ j \neq x_\star}}^{|\mathcal{X}|} \overbrace{\log \frac{P(i,j)P(j,x_\star)}{P(i,x_\star)P(x_\star,x_\star)}}^{\theta^{ij}} \overbrace{\delta_i(x)\delta_j(x')}^{g_{ij}(x,x')} + \log P(x, x_\star) - \log P(x', x_\star) + \log P(x_\star, x_\star).$$

Mixture families (Nagaoka, 2005)

We say that $\mathcal{V}_m$ is a mixture family when there exists functions $C, F_1, \ldots, F_d$, such that $C, C + F_1, \ldots, C + F_d$ are affinely independent,

$$\sum_{x,x' \in \mathcal{X}} C(x, x') = 1, \qquad \sum_{x,x' \in \mathcal{X}} F_i(x, x') = 0, \forall i \in [d],$$

and

$$\mathcal{V}_m = \left\{ P_\xi \in \mathcal{W} \colon Q_\xi = C + \sum_{i=1}^{d} \xi^i F_i, \xi \in \Xi \right\}$$

where $\Xi = \left\{ \xi \in \mathbb{R}^d \colon Q_\xi(x, x') > 0, \forall (x, x') \in \mathcal{X}^2 \right\}$, and Q_ξ is the edge measure that pertains to P_ξ.

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Example 2
$\mathcal{W}_{\text{bis}}$ (doubly stochastic) forms an m-family (Hayashi and Watanabe, 2016).

Applications – Inference in Markov chains

Geometric approach has recently lead to finite sample analysis for:

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Extension of known concepts... but also new structures emerge!

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What about families of fixed points?

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Theorem (Kolmogorov's criterion (Kolmogorov, 1936))
Let P irreducible, and Γ the set of finite directed closed-paths, i.e. $\gamma \in \Gamma$, when $\gamma\colon [n] \to \mathcal{E}$, $\gamma(t) = (x_t, x_{t+1})$ with $x_{n+1} = x_1$. Write $\gamma^\star$ the time-reversed path. P is reversible if and only if for all $\gamma \in \Gamma$,

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Log-reversible function
A function $h \in \mathcal{F}$ is log-reversible whenever it satisfies that for all $\gamma \in \Gamma$,

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Characterization of reversible e-families

Theorem 2
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Lemma 2 (Polynomial time procedure for reversibility checking)
Let $h \in \mathcal{F}_+$ (more generally irreducible). $\log[h]$ is log-reversible if and only if $\Pi_h \circ h^\intercal$ is a symmetric matrix, with $\Pi_h = v_h^\intercal u_h$ the PF projection of h, where u_h and v_h are respectively the left and right PF eigenvectors of h, normalized such that $u_h v_h^\intercal = 1$.

Affine structures

Lemma 4 (Vector space of log-reversible functions)

$$\mathcal{F}_{\text{rev}} \triangleq \{h \in \mathcal{F} \colon h \text{ is log-reversible}\},$$
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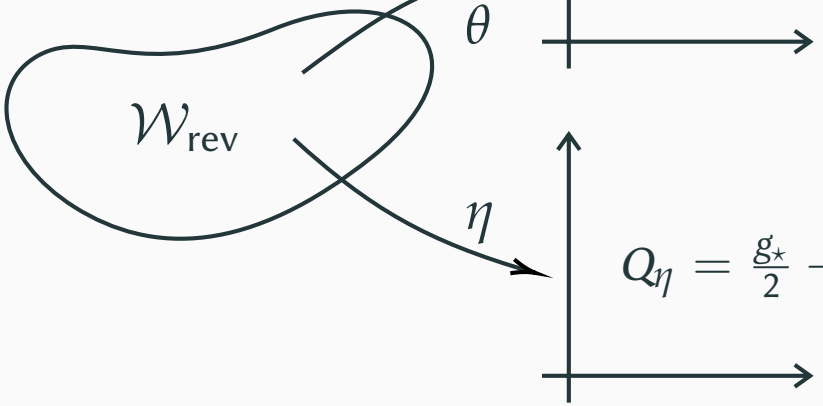
(*iii*) $\dim \mathcal{W}_{\text{rev}} = |T|$.

(*iv*) *Basis:* $\left\{g_{ij} \triangleq \delta_i^{\mathsf{T}} \delta_j + \delta_j^{\mathsf{T}} \delta_i \colon (i, j) \in T\right\}$.

Parametrization of $\mathcal{W}_{\text{rev}}$ (Theorem 5)

$$g_{ij} = \delta_i^\intercal \delta_j + \delta_j^\intercal \delta_i$$
$$g_\star = \delta_m^\intercal \delta_1 + \delta_1^\intercal \delta_m$$



$$\log P_\theta(x, x') = \sum_{(i,j)\in T} \overbrace{\frac{1}{2(1+\delta_i(j))} \log \frac{P(i,j)P(j,i)}{P(m,1)P(1,m)}}^{=\theta^{ij}} g_{ij}(x, x') + \tfrac{1}{2}\log \pi(x') - \tfrac{1}{2}\log \pi(x) + \tfrac{1}{2}\log P(m,1)P(1,m)$$

$$Q_\eta = \tfrac{g_\star}{2} + \sum_{(i,j)\in T} (g_{ij} - g_\star) \tfrac{Q(i,j)}{1+\delta_i(j)}$$

$$\theta^i(\eta) = \sum_{x,x'\in\mathcal{E}} \left(\frac{Q_\eta(x,x')}{\partial \eta_i} \right) \log P_\eta(x, x')$$

$$\eta_i(\theta) = \sum_{x,x'\in\mathcal{E}} Q_\theta(x, x') g_i(x, x')$$

Reversible e/m-projections

Closest reversible chain

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

1. $(P + P^\star)/2$, the additive reversiblization of P.
2. $PP^\star$, the multiplicative reversiblization of P (Fill, 1991).
3. $\mathscr{S}_\pi(P)$, the reversible dilation of P (Wolfer and Kontorovich, 2022).

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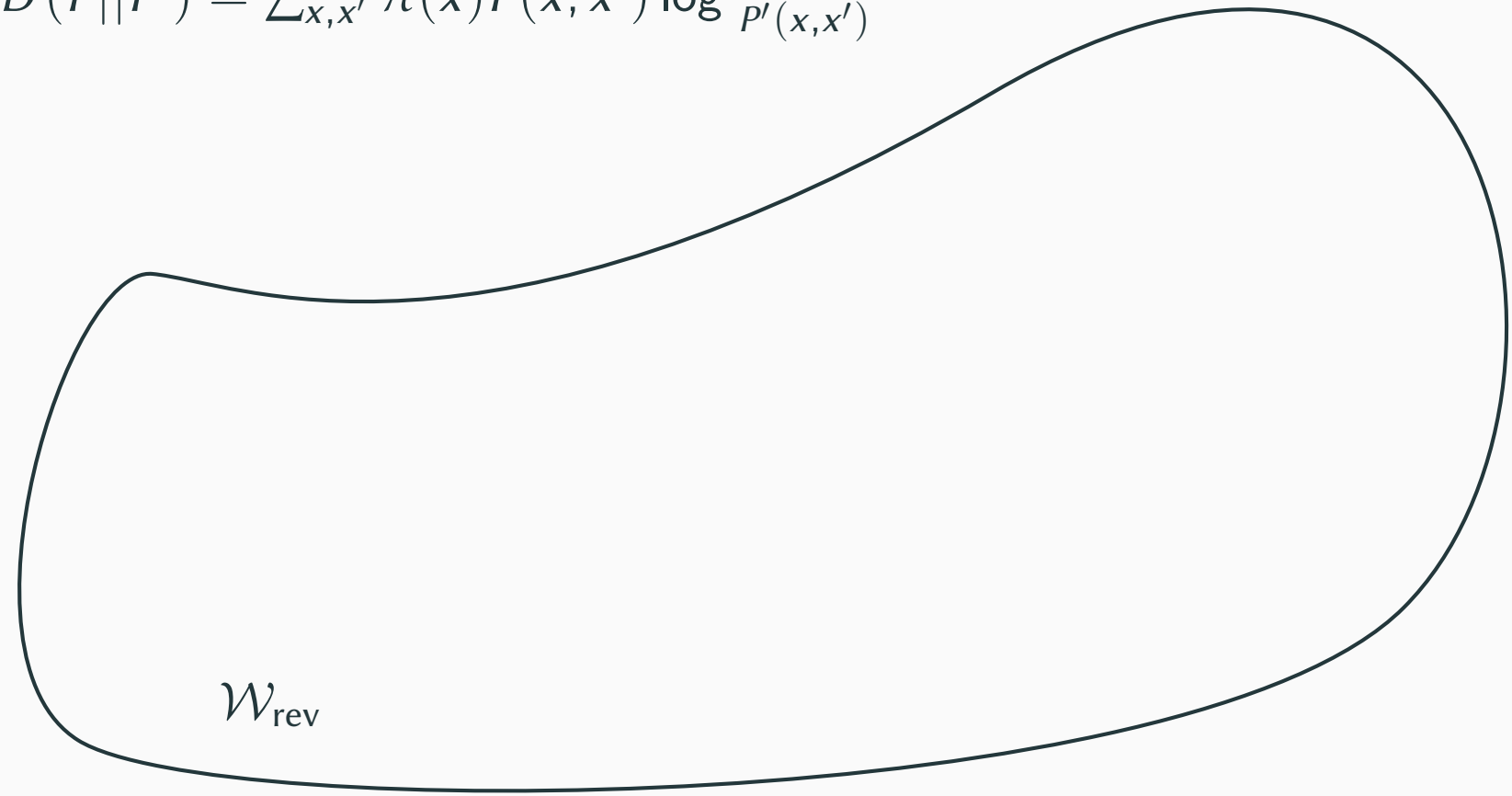
Related work
Analyzed by Nielsen and Weber (2015) for matrix norms induced by scalar products (unique, obtained by solving a convex minimization problem).

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

$$D(P||P') = \sum_{x,x'} \pi(x) P(x, x') \log \frac{P(x,x')}{P'(x,x')}$$



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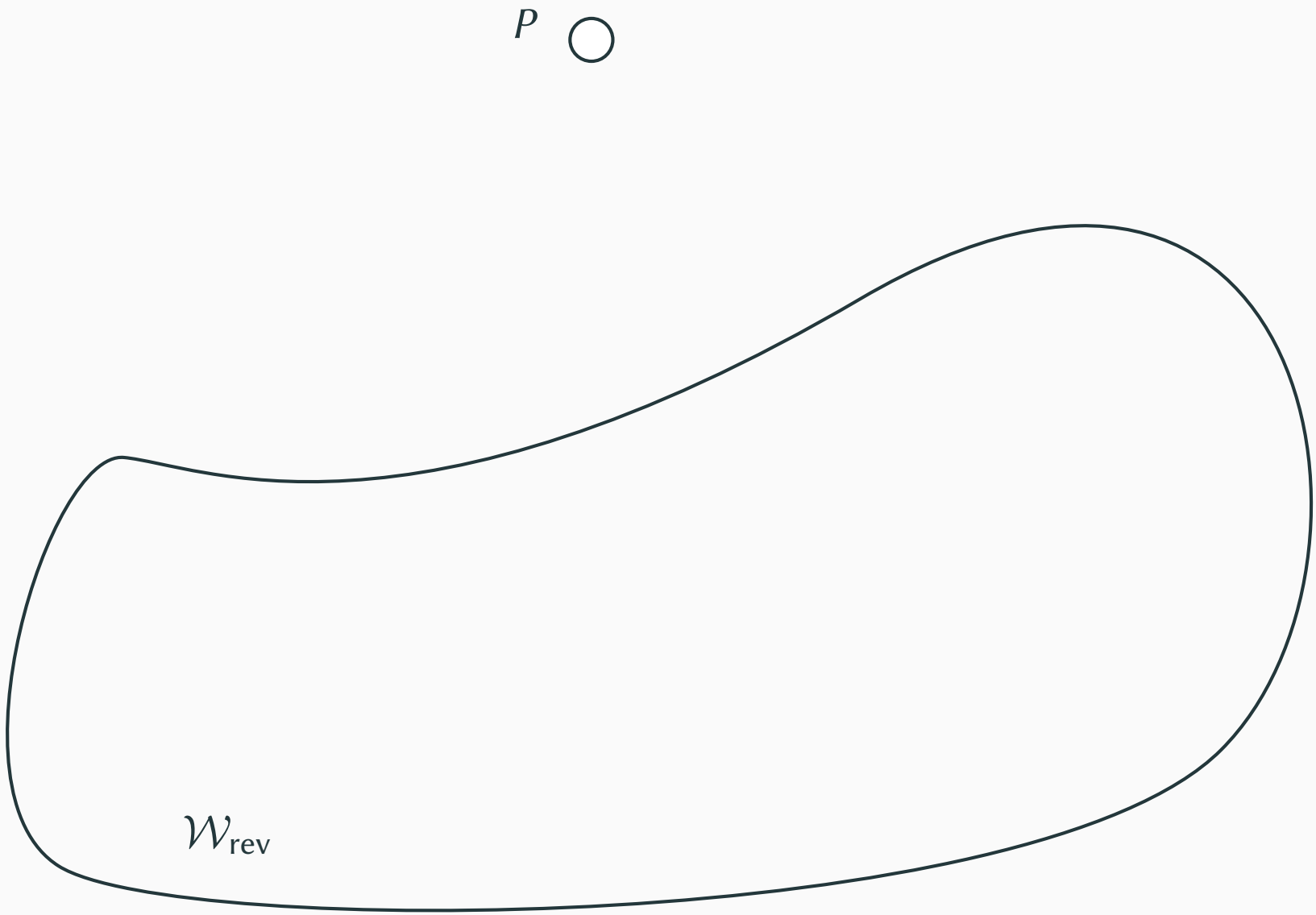

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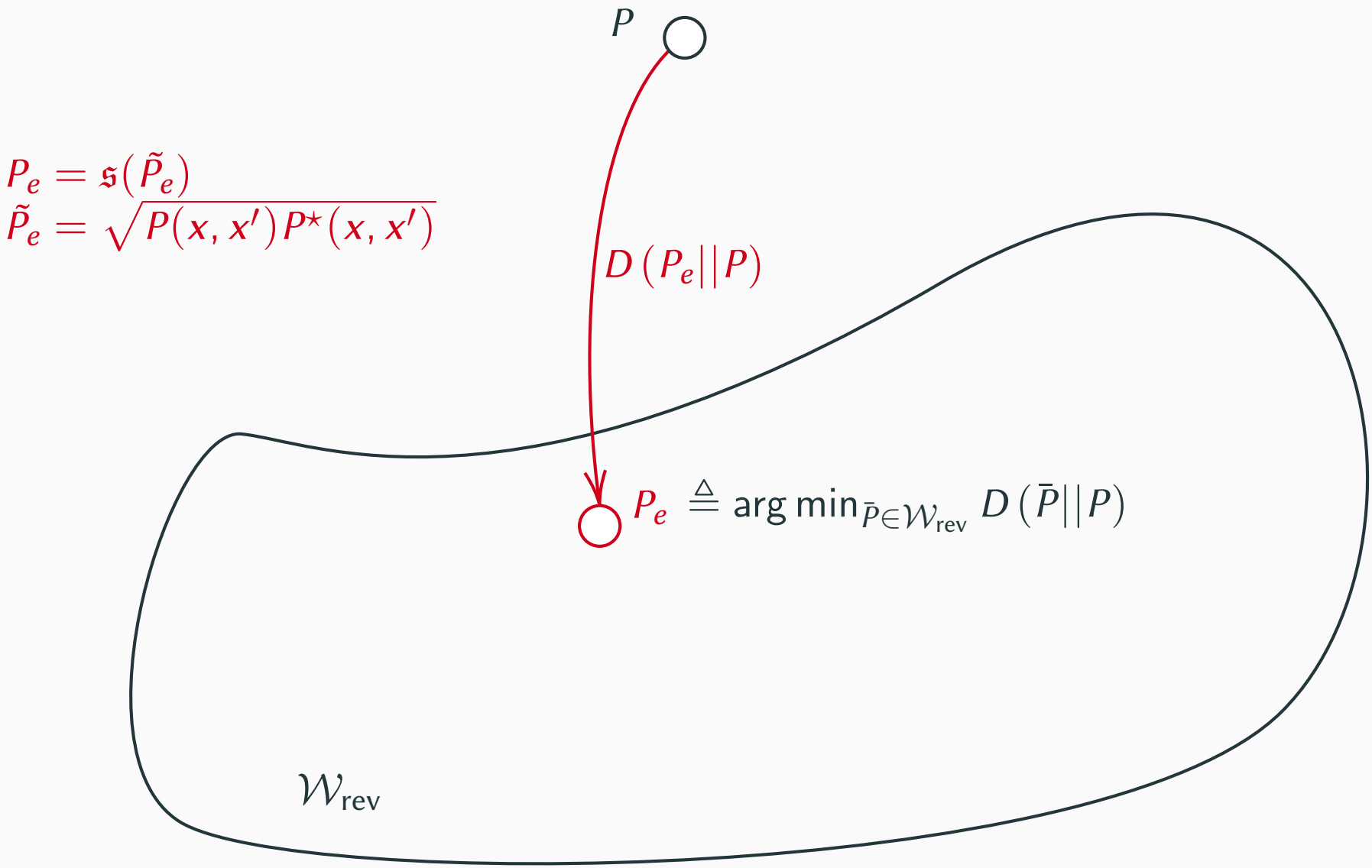

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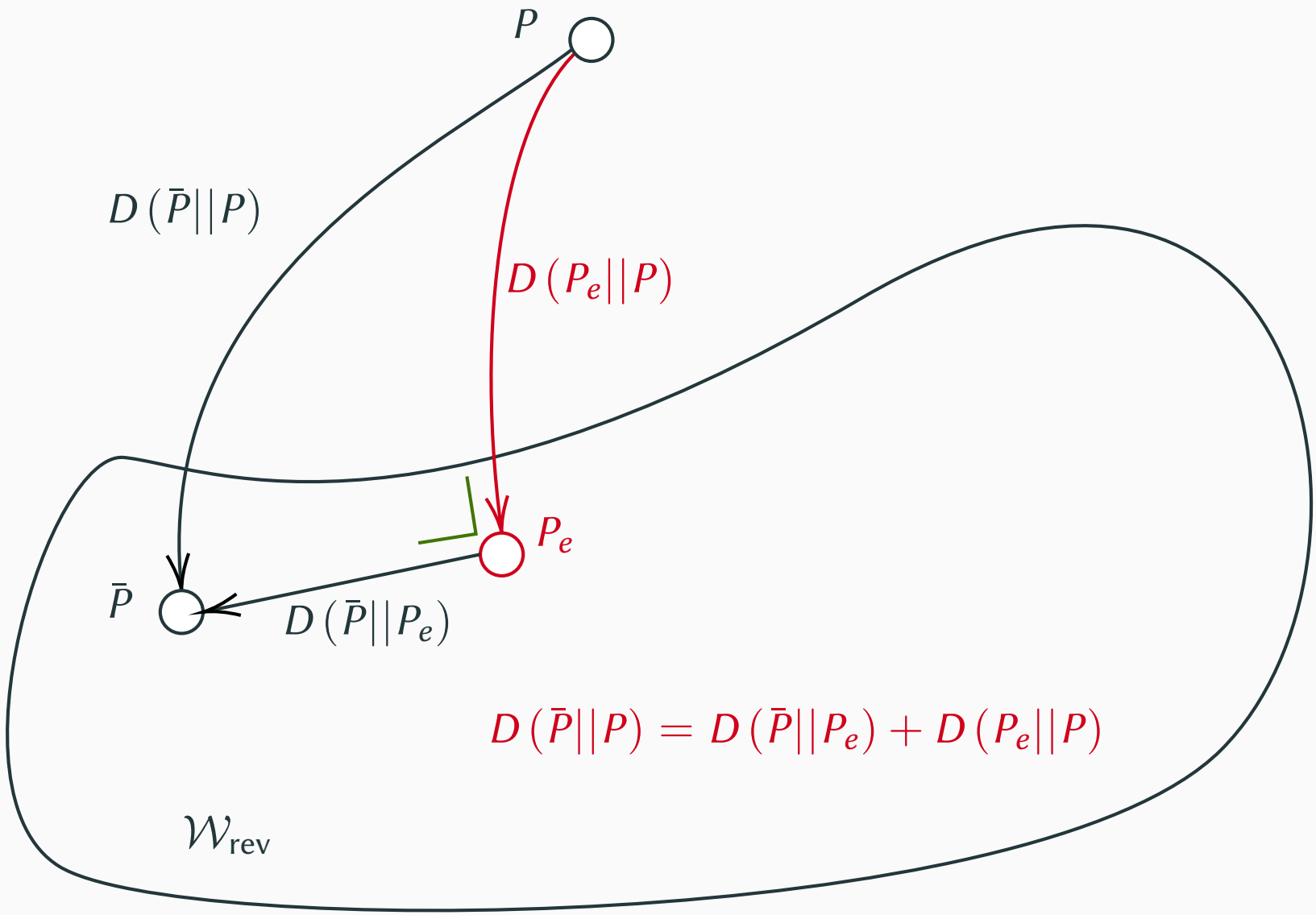

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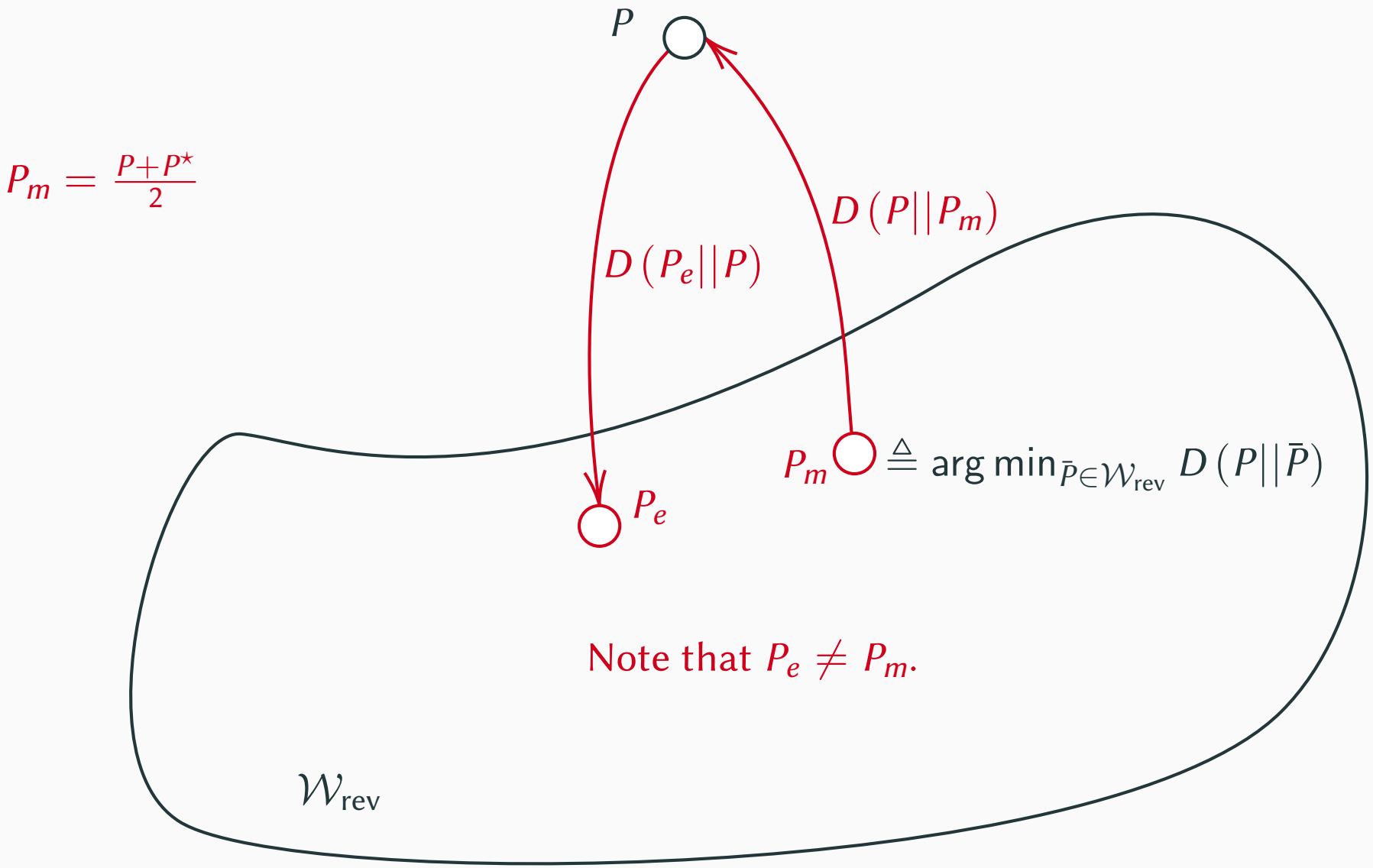

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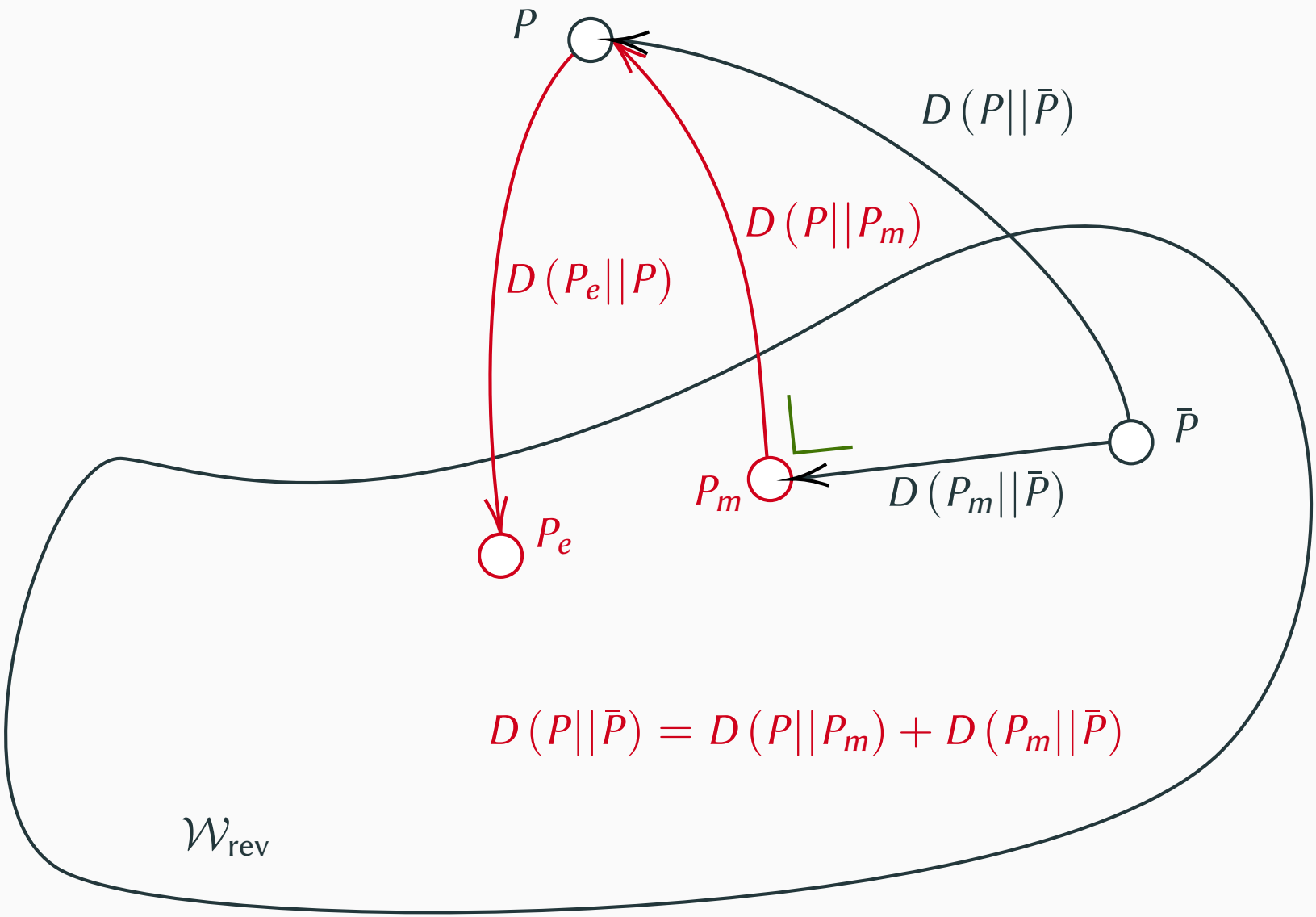

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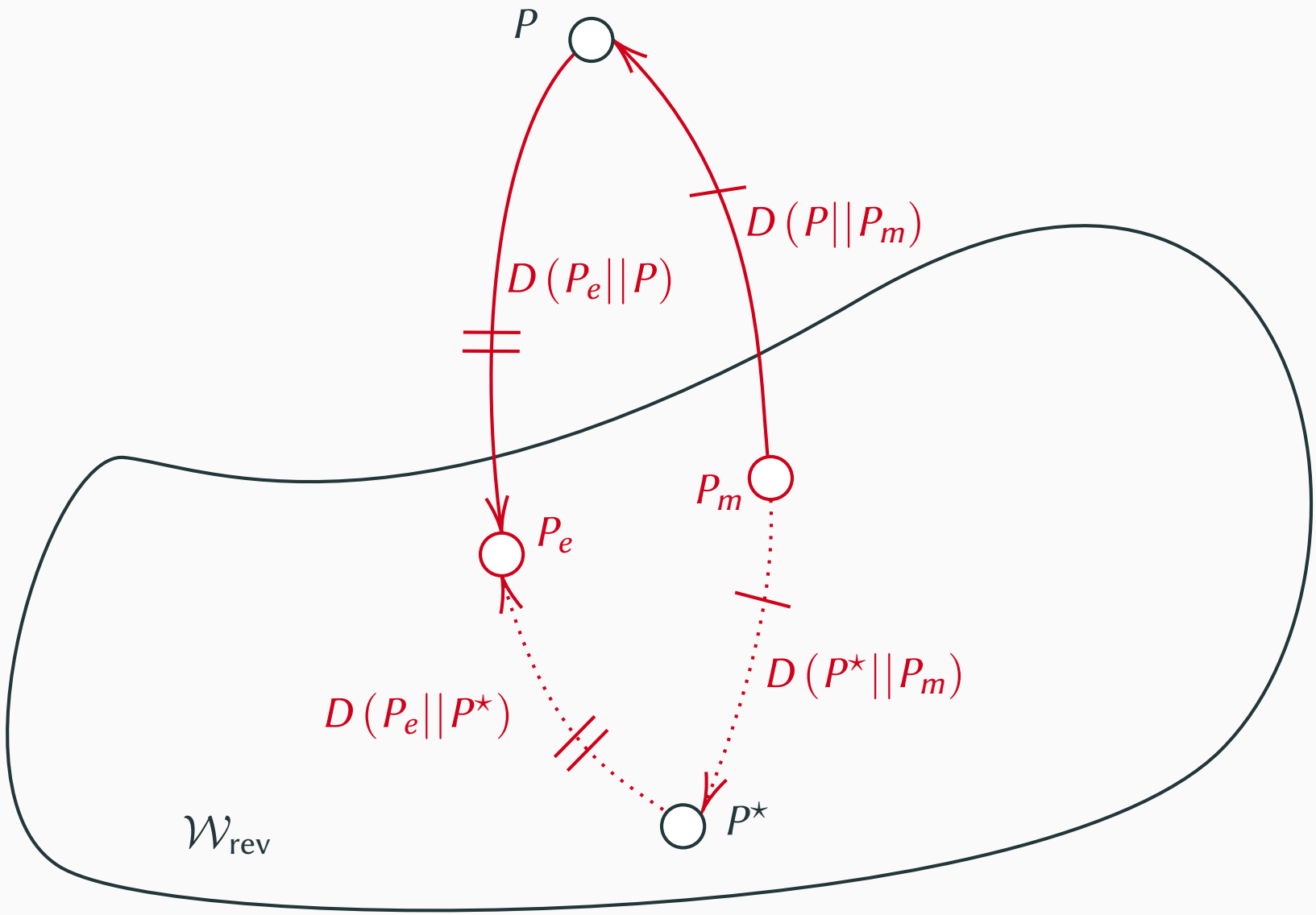

Usual families of kernels

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$\mathcal{W}_{\text{bis}}$: bi-stochastic kernels ($P^\intercal \in \mathcal{W}$)

$\mathcal{W}_{\text{sym}}$: symmetric kernels ($P = P^\intercal$)

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Mfd.	m-family	e-family	Dimension
$\mathcal{W}$	✓	✓	$\lvert\mathcal{X}\rvert\,(\lvert\mathcal{X}\rvert - 1)$
$\mathcal{W}_{\text{rev}}$	✓	✓	$\lvert\mathcal{X}\rvert\,(\lvert\mathcal{X}\rvert + 1)/2 - 1$
$\mathcal{W}_{\text{bis}}$	✓	✗	$(\lvert\mathcal{X}\rvert - 1)^2$
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$\mathcal{W}_{\text{iid}}$	✗	✓	$\lvert\mathcal{X}\rvert - 1$

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$\mathcal{W}_{\text{sym}}$	✓	✗	$\lvert\mathcal{X}\rvert\,(\lvert\mathcal{X}\rvert - 1)/2$
$\mathcal{W}_{\text{iid}}$	✗	✓	$\lvert\mathcal{X}\rvert - 1$

Hierarchies

$$\mathcal{W}_{\text{iid}} \overset{\text{e-family}}{\subsetneq} \mathcal{W}_{\text{rev}} \overset{\text{e-family}}{\subsetneq} \mathcal{W},$$

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$$\mathcal{W}_{\text{sym}} \overset{\text{m-family}}{\subsetneq} \mathcal{W}_{\text{bis}} \overset{\text{m-family}}{\subsetneq} \mathcal{W}.$$

Generation of reversible kernels

Generation of the reversible family from $\mathcal{W}_{\text{iid}}$

Definition 4 (Mixture hull)
Let $\mathcal{V} \subset \mathcal{W}$.

$$\text{m-hull}(\mathcal{V}) = \left\{ P \colon Q \in \mathcal{Q}, Q = \sum_{i=1}^{k} \alpha_i Q_i, k \in \mathbb{N}, \alpha_1, \ldots, \alpha_k \in \mathbb{R}, P_1, \ldots, P_k \in \mathcal{V} \right\},$$

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

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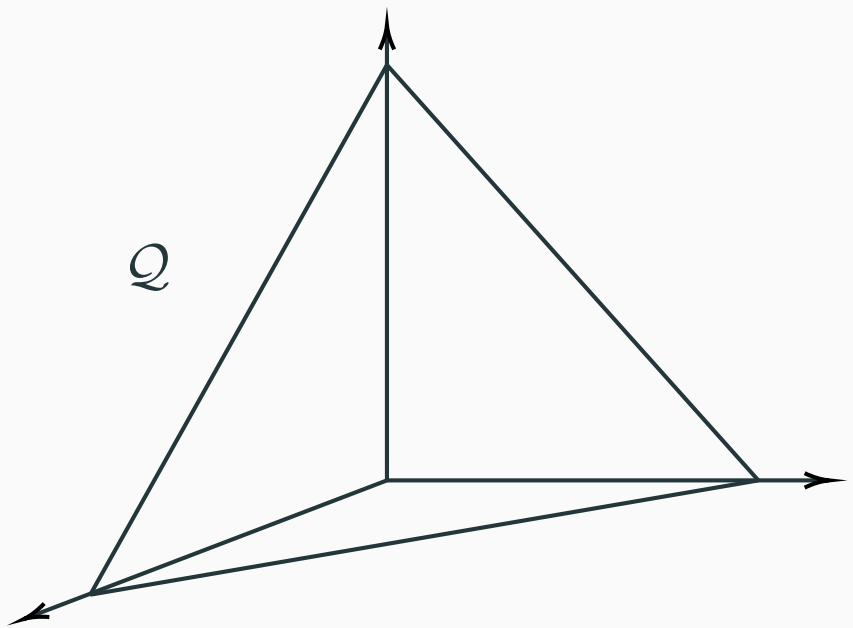

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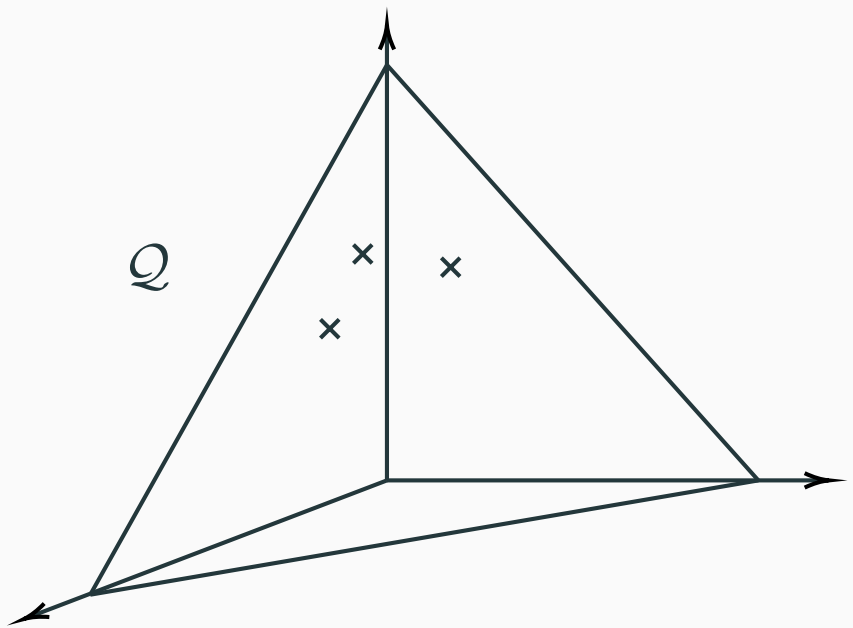

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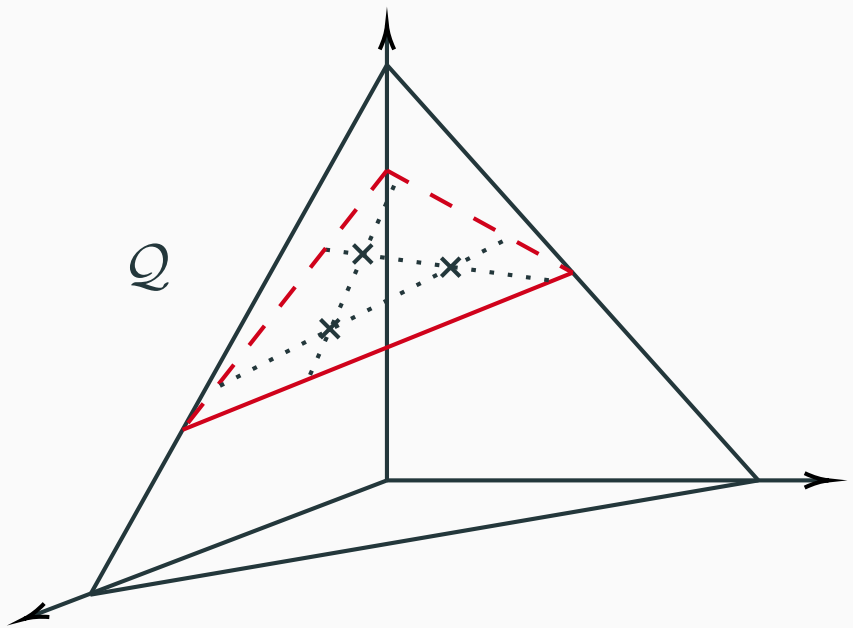

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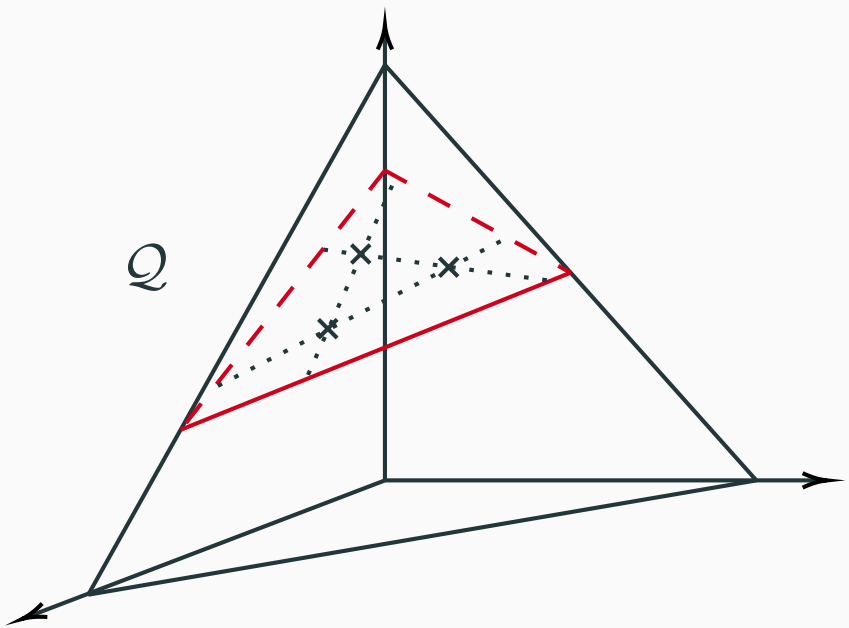

Theorem 10

$$\text{m-hull}(\mathcal{W}_{\text{iid}}) = \mathcal{W}_{\text{rev}}.$$

Generation of the reversible family from $\mathcal{W}_{\mathrm{sym}}$

Definition 5 (Exponential hull)
Let $\mathcal{V} \subset \mathcal{W}$.

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P $\times$ $\quad$ P' $\times$

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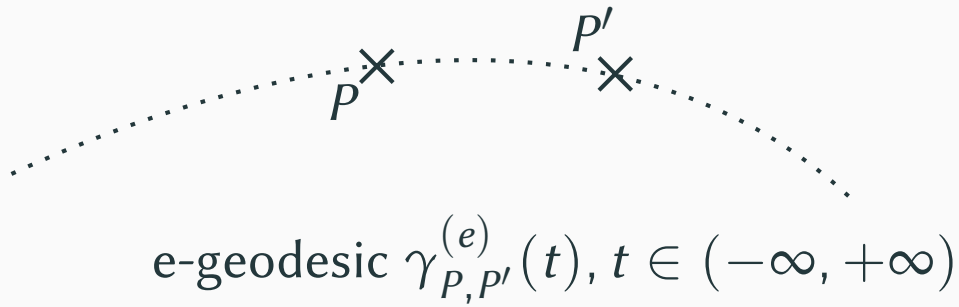

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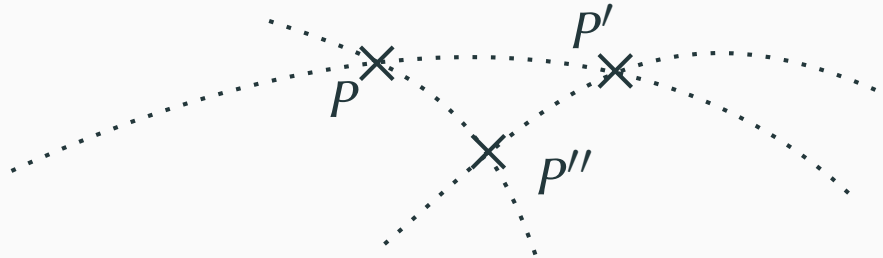

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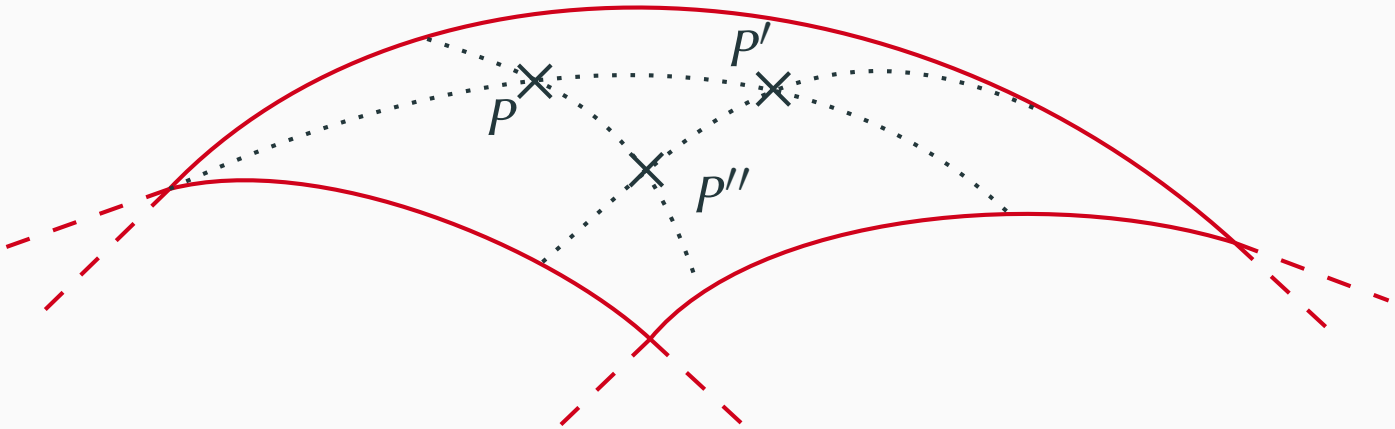

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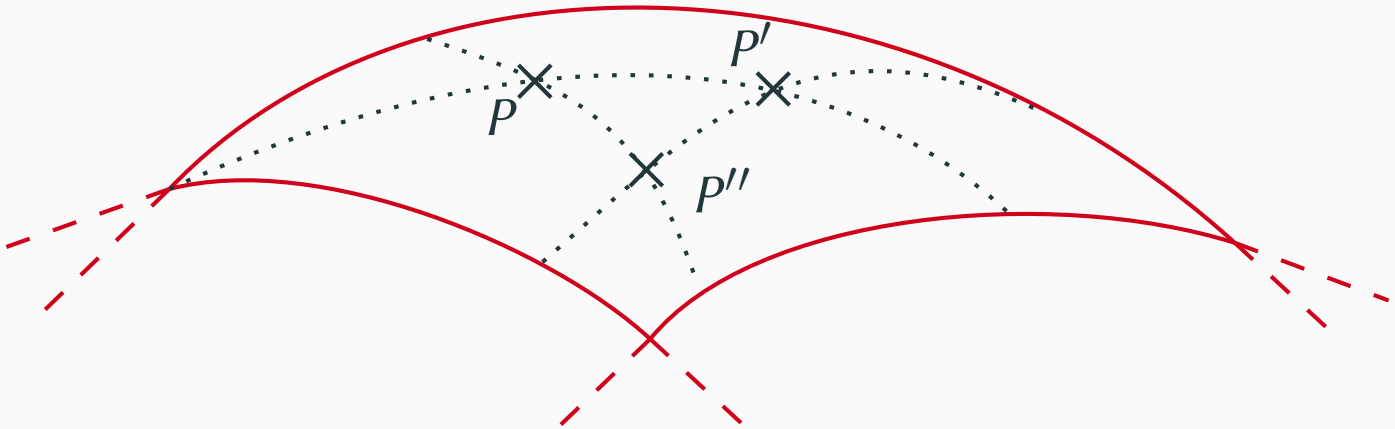

Theorem 9

$$|\mathcal{X}| \geq 3 \implies \text{e-hull}(\mathcal{W}_{\text{sym}}) = \mathcal{W}_{\text{rev}}.$$

Reversible edge measures

Reversible family of edge measures

Edge-measures

P reversible $\implies$ $Q \triangleq \operatorname{diag}(\pi)P$ is symmetric.

$$\mathcal{Q} = \left\{ Q\colon \sum_{x' \in \mathcal{X}} Q(x, x') = \sum_{x' \in \mathcal{X}} Q(x', x) \right\},$$

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Theorem 8

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

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(*iii*) $\mathcal{Q}$ *is not e-family in* $\mathcal{P}(\mathcal{X}^2)$ *(except when* $|\mathcal{X}| = 2$*).*

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, $\mathcal{W}_{\text{rev}}$ 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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