Geometry on Positive Definite Matrices Induced from V-Potentials -Foliated Structure and an Application-

Atsumi Ohara University of Fukui & Shinto Eguchi Institute of Statistical Mathematics 統計多様体の幾何学とその周辺, 北海道大学 2014 Jan. 11

1. Introduction



• $PD(n, \mathbf{R})$: the set of <u>P</u>ositive <u>D</u>efinite real symmetric matrices

• logarithmic characteristic func. on $PD(n, \mathbf{R})$ [Vinberg 63], [Faraut & Koranyi 94]

$$\varphi(P) = -\log \det P, \quad P \in PD(n; \mathbb{R})$$

$\phi(P)$ = -log det *P* appears in



- Semidefinite Programming (SDP)
 self-concordant barrier function
- Multivariate Analysis (Gaussian dist.) log-likelihood function

(structured covariance matrix estimation)

- Symmetric cone: log characteristic function
- Information geometry on $PD(n, \mathbf{R})$

a potential function in standard case

Information geometry on ${\cal M}$



Dualistic geometrical structure $Xg(Y,Z) = g(\nabla_X Y,Z) + g(Y,\nabla_X^* Z)$

X, Y and Z: arbitrary vector fields on \mathcal{M} g:Riemannian metric

 ∇ , ∇^* :a pair of dual affine connections

standard IG on $PD(n, \mathbf{R})$



[O,Suda & Amari LAA96]

 $\varphi(P)$ plays a role of potential function

- g : Riemannian metric is the Hesse matrix

of $\varphi(P)$ (Fisher for Gaussian)

- ∇ , ∇^* :related to the third derivatives of $\varphi(P)$

Nice properties: $GL(n, \mathbf{R})$ -invariant (unique),

KL-divergence, Pythagorean theorem, etc



Purpose of this presentation

• The other convex potentials V-potential functions

$$\varphi^{(V)}(P) = V(\det P)$$

- Their different and/or common geometric structures
 - Structure of submanifolds
 - Decomposition properties of divergences
 - Application to non-Gaussian pdf's

Outline



Review

- Dualistic geometry induced by V-potentials
- Foliated structures
 - Submanifold of constant determinant
 - Decomposition of divergence
- Applications to multivariate elliptic pdf's
 - GL(n)-invariance of geometry of q-Gaussian family induced by beta-divergence

2. Preliminaries and Notation



- $Sym(n; \mathbf{R})$: the set of *n* by *n* real symmetric matrix vec. sp. of dimension N(=n(n+1)/2)
- $\{E_i\}_{i=1}^N$: arbitrary set of basis matrices
- (primal) affine coordinate system

$$Sym(n; \mathbf{R}) \ni X = \sum_{i=1}^{N} x^i E_i$$

• Identification

$$T_P PD(n) \ni (\partial/\partial x^i)_P \equiv E_i \in Sym(n)$$



V-potential function

Def. $\varphi^{(V)}(P) = V(\det P), \qquad V(s): \mathbf{R}_+ \to \mathbf{R}$

-The standard case:

$$V(s) = -\log s \Longrightarrow \varphi(P) = -\log \det P$$

Def.

$$\nu_i(s) = \frac{d\nu_{i-1}(s)}{ds}s, \quad i = 1, 2, \cdots, \text{ where } \nu_0(s) = V(s)$$
Rem. The standard case V= -log:

$$\nu_1(s) = -1, \nu_k(s) = 0, \quad k \ge 2$$

Prop.1 (convexity conditions)

The Hessian matrix of the V-potential is positive definite on $\ PD(n,{\bf R}) \$ if and only if

For
$$\forall s > 0$$
,
i) $\nu_1(s) < 0$, ii) $\beta^{(V)}(s) < \frac{1}{n}$, where $\beta^{(V)}(s) = \frac{\nu_2(s)}{\nu_1(s)}$



- Riemannian metric is $g_P^{(V)}(X,Y)$ $= -\nu_1(\det P) \operatorname{tr}(P^{-1}XP^{-1}Y) + \nu_2(\det P) \operatorname{tr}(P^{-1}X) \operatorname{tr}(P^{-1}Y)$ Here,

X, Y in $sym(n, \mathbf{R}) \sim tangent vectors at <math>P$

<u>Rem</u>. The standard case V= -log: $g_P^{(V)}(X,Y) = \operatorname{tr}(P^{-1}XP^{-1}Y)$

Prop. (affine connections)



Let ∇ be the canonical flat connection on $PD(n, \mathbf{R})$. Then the V-potential defines the following dual connection $*\nabla^{(V)}$ with respect to $g^{(V)}$:

$$\begin{split} \left({}^{*} \nabla^{(V)}_{\frac{\partial}{\partial x^{i}}} \frac{\partial}{\partial x^{j}} \right)_{P} &= -E_{i} P^{-1} E_{j} - E_{j} P^{-1} E_{i} - \Phi(E_{i}, E_{j}, P) - \Phi^{\perp}(E_{i}, E_{j}, P), \\ \Phi(X, Y, P) &= \frac{\nu_{2}(s) \operatorname{tr}(P^{-1}X)}{\nu_{1}(s)} Y + \frac{\nu_{2}(s) \operatorname{tr}(P^{-1}Y)}{\nu_{1}(s)} X, \\ \Phi^{\perp}(X, Y, P) &= \frac{(\nu_{3}(s)\nu_{1}(s) - 2\nu_{2}^{2}(s)) \operatorname{tr}(P^{-1}X) \operatorname{tr}(P^{-1}Y) + \nu_{2}(s)\nu_{1}(s) \operatorname{tr}(P^{-1}XP^{-1}Y)}{\nu_{1}(s)(\nu_{1}(s) - n\nu_{2}(s))} P \end{split}$$

 $(g^{(V)}, \nabla, {}^*\nabla^{(V)})$: Dually flat structure on $PD(n, \mathbf{R})$ induced by the V-potential

divergence function

$$D^{(V)}(P,Q) = \varphi^{(V)}(P) + \varphi^{(V)*}(Q^*) - \langle Q^*, P \rangle$$

= V(det P) - V(det Q) + \langle Q^*, Q - P \langle.

$$P^* = \operatorname{grad} \varphi^{(V)}(P) = \nu_1(\det P)P^{-1}$$
$$\varphi^{(V)*}(P^*) = n\nu_1(\det P) - \varphi^{(V)}(P).$$

- a variant of relative entropy,
- Pythagorean type decomposition

3. Group Invariance of the structure $(g^{(V)}, \nabla, *\nabla^{(V)})$ on $PD(n, \mathbf{R})$

• Linear transformation on $PD(n, \mathbf{R})$ congruent transformation: $\tau_G P = GPG^T, G \in GL(n, \mathbf{R}),$ the differential: $(\tau_G)_* X = GXG^T$

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- Invariance
 - metric: $g_{\widetilde{P}}(\widetilde{X},\widetilde{Y}) = g_P(X,Y)$
 - connections: $(\tau_G)_* (\nabla_X Y)_P = (\nabla_{\widetilde{X}} \widetilde{Y})_{\widetilde{P}}$ and the same for $\nabla^{(V)}$

where

$$\widetilde{P} = \tau_G P, \widetilde{X} = (\tau_G)_* X, \widetilde{Y} = (\tau_G)_* Y$$

Prop.



The largest group that preserves the dualistic structure $(g^{(V)}, \nabla, {}^*\nabla^{(V)})$ invariant is

$$\tau_G$$
 with $G \in SL(n, \mathbf{R})$

except in the standard case.

<u>**Rem</u></u>. the standard case: \tau_G with G \in GL(n, \mathbf{R})</u>**

<u>Rem</u>. The power potential of the form:

$$V(s) = c_1 + c_2 s^\beta$$

has a special property.

2. Foliated structures



The following foliated structure features the dualistic geometry $(g^{(V)}, \nabla, *\nabla^{(V)})$ induced from every V-potential.

$$PD(n, \mathbf{R}) = \bigcup_{s>0} \mathcal{L}_s, \quad \mathcal{L}_s = \{P|P>0, \det P = s\}.$$
 leaf



<u>Prop.</u> Each leaf \mathcal{L}_s and ray \mathcal{R}_P are orthogonal to each other with respect to $g^{(V)}$.



<u>Prop.</u> Every \mathcal{R}_P is simultaneously a ∇ - and * $\nabla^{(V)}$ -geodesic for an arbitrary V-potential.



Induced geometry on \mathcal{L}_s from $(g^{(V)}, \nabla, *\nabla^{(V)})$

<u>Prop</u>. For any V, the followings hold: i)Riemannian metric: $\tilde{g}^{(V)} = -\nu_1(s)\tilde{g}^{(-\log)}$ ii)Divergence: $D^{(V)}(P,Q) = -\nu_1(s)D^{(-\log)}(P,Q)$ iii)Dual connection: $*\tilde{\nabla}^{(V)} = \tilde{\nabla}^{(-\log)}$



Prop. Each leaf $(\mathcal{L}_s, \tilde{g}^{(V)})$ is a Riemannian symmetric space

$$\mathcal{L}_s \simeq SL(n, \mathbf{R}) / SO(n)$$

 $\iota_s: \mathcal{L}_s \to \mathcal{L}_s$: Involutive isometry of $(\mathcal{L}_s, \tilde{g}^{(V)})$

$$\iota_s P = -\left(\frac{s}{s^*}\right)^{\frac{1}{n}} \operatorname{grad} \varphi^{(V)}(P) = s^{\frac{2}{n}} P^{-1}, \quad s^* = \frac{(-\nu_1(s))^n}{s}.$$

- Level surface of both $\varphi^{(V)}$ and $\varphi^{(V)*} \implies \mathsf{ADG}$
- Normal vector field N

$$\begin{split} N &= -\frac{1}{d\varphi^{(V)}(E)}E. \\ g^{(V)}(X,E) &= d\varphi^{(V)}(X), \quad \forall X \in \mathcal{X}(PD(n,\mathbf{R})) \end{split}$$

• Centro-affine immersion

$$\nabla_X Y = \tilde{\nabla}_X Y + h(X, Y)N,$$

$$\nabla_X N = -A(X) + \tau(X)N.$$

$$h = \tilde{g}^{(V)}, \quad \tau = 0$$
²¹



Lemma [UOF 00]

- The submfd $(\mathcal{L}_s, \tilde{\nabla}, \tilde{g}^{(V)})$ is 1-conformally flat.
- Assume

$$P,Q\in\mathcal{L}_s,R\in\mathcal{R}_Q,R=\lambda Q,\lambda>0.$$
 Then

$$D^{(V)}(P,R) = \mu D^{(V)}(P,Q) + D^{(V)}(Q,R),$$

where

$$R^* = \mu Q^*, \ i.e., \ \mu = \lambda^{-1} \nu_1(\det R) / \nu_1(\det Q) > 0.$$



+ Illustration: decomposition of divergence (1)

If $P, Q \in \mathcal{L}_s$ and $R \in \mathcal{R}_Q$ with $R = \lambda Q, \ \lambda > 0$, $PD(n, \mathbf{R})$ $R = \mu D^{(V)}(P, Q) + D^{(V)}(Q, R)$ then $D^{(V)}(P, R) = \mu D^{(V)}(P, Q) + D^{(V)}(Q, R)$

where $\mu = \lambda^{-1} \nu_1 (\det R) / \nu_1 (\det Q) > 0^{23}$



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Each leaf \mathcal{L}_s is a homogeneous space of constant negative curvature $k_s = 1/(\nu_1(s)n)$. $R(X,Y)Z = k_s \{g(Y,Z)X - g(X,Z)Y\}.$

Shown by Gauss eq. and $A = k_s I$

Lemma (modified Pythagorean)[Kurose94] $P, Q, R \in \mathcal{L}_s \quad \tilde{\gamma}_{PQ} \perp \tilde{\gamma}_{QR}^* \text{ at } Q \Rightarrow$ $D^{(V)}(P,R) = D^{(V)}(P,Q) + D^{(V)}(Q,R) - k_s D^{(V)}(P,Q) D^{(V)}(Q,R).$

Decomposition of divergences (2)

+ Combining the two decomposition results

<u>Prop.</u> If $\tilde{\nabla}$ -geodesic $\tilde{\gamma}$ and $\tilde{\nabla}$ -geodesic $\tilde{\gamma}^*$ are orthogonal at R, then

$$D^{(V)}(P,S) = D^{(V)}(P,R) + \kappa D^{(V)}(R,S)$$

$$\kappa = \lambda \{ 1 - k_s D^{(V)}(Q, R) \} > 0$$
$$Q \in \mathcal{L}_s \cap \mathcal{R}_P$$



3. Application to multivariate statistics

- Non Gaussian distribution (generalized exponential family)
 - Robust statistics
 - beta-divergence,
 - Machine learning, and so on
 - Nonextensive statistical physics
 - Power distribution,
 - generalized (Tsallis) entropy, and so on





U-model and U-divergence

U-model Def.

Given a convex function U on \mathbf{R} and set u=U', U-model is a family of elliptic pdf's specified by P:

$$\mathcal{M}_{U} = \left\{ f(x, P) = u \left(-\frac{1}{2} x^{T} P x - c_{U} (\det P) \right) : P \in PD(n, \mathbf{R}) \right\}$$

 $c_U(\det P)$:normalizing const.



<u>Rem</u>. When $U=\exp$, the U-model is the family of Gaussian distributions.

<u>U-divergence</u>:

Natural closeness measure on the U-model $D_U(f,g) = \int U(\xi(g)) - U(\xi(f)) - \{\xi(g) - \xi(f)\} f dx,$ $f,g \in \mathcal{M}_U$

where ξ is the inverse function of u.

<u>Rem</u>. When $U=\exp$, the U-divergence is the Kullback-Leibler divergence (relative entropy).

Example: beta-model and betadivergence (1)

• Beta-model \mathcal{M}_{β}

• For
$$\beta \neq 0$$
 and $\beta \neq -1$

$$U(s) = \begin{cases} \frac{1}{\beta+1} (1+\beta s)^{(\beta+1)/\beta}, & s \in I_{\beta} = \{s \in \mathbf{R} | 1+\beta s > 0\} \\ 0, & \text{otherwise} \end{cases}$$

$$u(s) = \begin{cases} \frac{dU(s)}{ds} = (1+\beta s)^{1/\beta} & s \in I_{\beta} = \{s \in \mathbf{R} | 1+\beta s > 0\} \\ 0, & \text{otherwise} \end{cases}$$

$$\xi(t) = \frac{t^{\beta} - 1}{\beta}, \quad t > 0$$

q-exponential and q-logarithmic functions

Example: beta-model and betadivergence (2)

• Beta-divergence

$$D_{\beta}(f,g) = \int \frac{g(x)^{\beta+1} - f(x)^{\beta+1}}{\beta+1} - \frac{f(x)\{g(x)^{\beta} - f(x)^{\beta}\}}{\beta} dx$$

IG induced from divergences

• Divergence induces stat mfd structure.
$$\begin{split} g^{(D)}(X,Y) &= -D(X|Y), \\ g^{(D)}(\nabla^{(D)}_XY,Z) &= -D(XY|Z), \\ g^{(D)}(^*\nabla^{(D)}_XY,Z) &= -D(Z|XY), \end{split}$$

where

 $D(X_1 \cdots X_n | Y_1 \cdots Y_m)(p) = (X_1)_p \cdots (X_n)_p (Y_1)_q \cdots (Y_m)_q D(p,q)|_{p=q}$



Relation between the U- and Vgeometries Prop.

IG on \mathcal{M}_U induced from D_U coincides with $(g^{(V)}, \nabla, {}^*\nabla^{(V)})$ derived from the following V-potential function:

$$V(s) = s^{-\frac{1}{2}} \int U\left(-\frac{1}{2}x^T x - c_U(s)\right) dx + c_U(s), \quad s > 0.$$

Group invariance for the power potentials $V(s) = c_1 + c_2 s^{\beta}$



Prop.

- V is of the power form \iff
- 1) Orthogonality is GL(n)-invariant.
- 2) The dual affine connections derived from the power potentials are GL(n)-invariant.

Hence,

• Both ∇ - and * $\nabla^{(V)}$ -projections are GL(n) -invariant.



<u>Thm</u> [O & Eguchi 13] IG on \mathcal{M}_{β} induced from D_{β} coincides with $(q^{(V)}, \nabla, *\nabla^{(V)})$ on $PD(n, \mathbf{R})$ induced from $V(s) = \begin{cases} \frac{1}{\beta} + c^{+} s^{1/(2n_{\beta})}, & \beta > 0\\ \frac{1}{\beta} + c^{-} s^{1/(2n_{\beta})}, & -\frac{2}{n+2} < \beta < 0 \end{cases}$

<u>Implication</u>: statistical inference on \mathcal{M}_{β} using D_{β} is GL(n)-invariant.

Conclusions

- Derived dualistic geometry is invariant under the SL(n,R)-group actions.
 - For power function, dual connections and orthogonality are GL(n,R)-invariant.
- Each leaf is a homogeneous manifold with a negative constant curvature.
- Decomposition of the divergence function
- Correspondence between the U- and V-geometries
 - Statistical inference on Beta-model using dual projections are GL(n,R)-invariant.

Main References



- A. Ohara, N. Suda and S. Amari, Dualistic Differential Geometry of Positive Definite Matrices and Its Applications to Related Problems, *Linear Algebra and its Applications*, Vol.247, 31-53 (1996).
- A. Ohara and S. Eguchi, Geometry on positive definite matrices and V-potential function, Research Memorandum No. 950, The Institute of Statistical Mathematics, Tokyo, July (2005).
- T. Kanamori and A. Ohara,

A Bregman Extension of quasi-Newton updates I: An Information Geometrical Framework, *Optimization Methods and Software*, Vol. **28**, No. 1, 96-123 (2013).

 A. Ohara and S. Eguchi, Group Invariance of Information Geometry on q-Gaussian Distributions Induced by Beta-Divergence, *Entropy*, Vol. 15, 4732-4747 (2013).