Information Geometry and its Applications IV

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In honor of Professor Amari

Information geometry associated with two generalized means

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Outline

Information geometry

(e-geodesic, m-geodesic, KL-divergence)

Generalized information geometry

Kolmogorov - Nagumo mean

Generalized (e-geodesic, m-geodesic, KL-divergence)

Quasi divergence

The other generalized KL divergence

The core of information geometry $\mathscr{F} = \{f: f(x) \ge 0, \int f(x)dP(x) = 1\}$ m-geodesic $C_{f,g}^{(m)} = \{f_t^{(m)}(x) := (1-t)f(x) + tg(x) : t \in [0,1]\}$

e-geodesic $C_{f,g}^{(e)} = \{ f_t^{(e)}(x) := e^{(1-t)\log f(x) + t\log g(x) - \kappa(t)} : t \in [0,1] \}$

KL divergence $D(f,g) = E_f(\log f - \log g)$



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Metric and connections

Let
$$M = \{ f_{\theta}(x) : \theta = (\theta_1, \dots, \theta_d) \in \Theta \}$$
 with $\Theta \subseteq \mathbb{R}^d$



Conjugate

$$\frac{\partial}{\partial \theta_k} G_{ij}(\theta) = \Gamma_{ik,j}^{(m)}(\theta) + \Gamma_{jk,i}^{(e)}(\theta)$$

Rao (1945), Dawid (1975), Amari (1982)

Exponential model

Let us fix a canonical statistic $\mathbf{t} = (t_1, \dots, t_K)$.

Exponential model	$M^{(e)} = \{ f_{\theta}^{(e)}(\boldsymbol{x}) := \exp\{\boldsymbol{\theta}^{\mathrm{T}}\boldsymbol{t}(\boldsymbol{x}) - \boldsymbol{\kappa}(\boldsymbol{\theta})\} : \boldsymbol{\theta} \in \boldsymbol{\Theta} \}$
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Mean parameter
$$\eta = \mathbb{E}_{f_{\theta}^{(e)}} \{ t(X) \} = \frac{\partial}{\partial \theta} \kappa(\theta)$$

Remark 1 θ and η are affine parameterswrt $\Gamma^{(e)}$ and $\Gamma^{(m)}$. $(M^{(e)}$ is dually flat.)Amari (1982)

Remark 2 $M^{(e)}$ is totally e-gedesic.

(The e-geodesic curve connecting any two densities in $M^{(e)}$ is always in $M^{(e)}$.)

Minimum KL leaf

Exponential model $M^{(e)} = \{ f_{\theta}^{(e)}(x) : \theta \in \Theta \}$

Mean equal space $\mathscr{Q}(f) = \{ g \in \mathscr{F} : E_g \{ t(X) \} = E_f \{ t(X) \} \}$

$$f^* \in M^{(e)} \implies D(g, f) = D(g, f^*) + D(f^*, f) \ (\forall g \in \mathscr{Q}(f^*), \forall f \in M^{(e)})$$



Pythagoras foliation

$$\{\mathscr{Q}(f): f \in M^{(e)}\} \text{ is a foliation, i.e.}$$
(i) $f_1 \neq f_2 \Rightarrow \mathscr{Q}(f_1) \cap \mathscr{Q}(f_2) = \phi$
(ii) $\mathscr{F} = \bigcup_{f \in M^{(e)}} \mathscr{Q}(f)$



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KL divergence (revisited)

e-geodesic
$$f_t^{(e)}(x) = \exp\{(1-t)\log f(x) + t\log g(x) - \kappa(t)\}$$

The normalizing constant

$$\kappa(t) = \log\left[\int \exp\{(1-t)\log f(x) + t\log g(x)\}dP(x)\right]$$

We observe

$$-\frac{d\kappa(0)}{dt} = E_f(\log f - \log g) = D(f,g)$$

$$0$$

$$1$$

$$K(t)$$

 $\mathbf{\Lambda}$

KL divergence is induced by e-geodesic

Cf. the canonical divergence, Amari-Nagaoka (2001)



$$f = \exp(\log(f))$$

$$exp((1-t)\log f(x) + t\log g(x) - \kappa_t)$$

$$(1-t)f(x) + tg(x)$$

$(\log, \exp) \rightarrow (\phi, \psi)$

where ϕ is a concave function on $(0, \infty)$ and ψ is the inverse of ϕ .



 $\psi(\phi(f)) = f$ $\psi'(\phi(f))\phi'(f) = 1$

Kolmogorov-Nagumo mean

K-N mean is $\psi((1-t)\phi(f) + t\phi(g))$ for positive numbers f and g.

Cf. Kolmogorov(1930), Nagumo (1930), Naudts (2009)

(1)
$$\phi(s) = s$$
 arithmetic mean : $(1-t)f + tg$
(2) $\phi(s) = \log s$ geometric mean : $\exp((1-t)f + tg)$
(3) $\phi(s) = \frac{1}{s}$ harmonic mean : $\frac{1}{(1-t)\frac{1}{f} + t\frac{1}{g}}$

Generalized e-geodesic

$$C_{f,g}^{(e\phi)} = \{ f_t^{(e\phi)}(x) : t \in [0,1] \}$$

$$f_t^{(e\phi)}(x) := \psi((1-t)\phi(f(x)) + t\phi(g(x)) - \kappa^{(\phi)}(t))$$

where $\kappa^{(\phi)}(t)$ is a constant to satisfy
$$\int \psi((1-t)\phi(f) + t\phi(g) - \kappa^{(\phi)}(t)) dP = 1$$

Remark Let $C_{f_1,\dots,f_k}^{(e\phi)} = \{ \psi(\pi_1\phi(f_1) + \dots + \pi_k\phi(f_k) - \kappa(\pi)) : \pi \in S_{k-1} \}.$

If
$$f, g \in C_{f_1, \dots, f_k}^{(e\phi)}$$
, then $C_{f,g}^{(e\phi)}$ is always in $C_{f_1, \dots, f_k}^{(e\phi)}$
($C_{f_1, \dots, f_k}^{(e\phi)}$ is totally $e\phi$ -geodesic)

Generalized KL-divergence

$$D^{(\phi)}(f,g) = E_{\xi(f)} \{ \phi(f) - \phi(g) \}$$
where $\xi(f) = \frac{\overline{\phi'(f)}}{\int \frac{dP}{\phi'(f)}}$ ($\psi'(\phi(f)) = \frac{1}{\phi'(f)}$)

Remember $\kappa^{(\phi)}(t)$ defined to satisfy

$$\int \psi((1-t)\phi(f) + t\phi(g) - \kappa^{(\phi)}(t)) dP = 1$$

Then $-\frac{d\kappa^{(\phi)}(0)}{dt} = \frac{\int \psi'(\phi(f))\{\phi(f) - \phi(g)\}dP}{\int \psi'(\phi(f)) dP}$
$$= \frac{\int \frac{\phi(f) - \phi(g)}{\phi'(f)}}{\int \frac{dP}{\phi'(f)}} \quad (\quad \psi'(\phi(f))\phi'(f) = 1)$$



Generalized m-geodesic

$$C_{f,g}^{(m\phi)} = \{ f_t^{(m\phi)}(x) : t \in [0,1] \}$$

where $f_t^{(m\phi)} = \xi^{-1}((1-t)\xi(f) + t\xi(g)).$

Remark

(i)
$$\operatorname{E}_{\xi(f)}\{S(X)\} = \operatorname{E}_{\xi(g)}\{S(X)\} = \tau \Longrightarrow \operatorname{E}_{\xi(f_t^{(m\phi)})}\{S(X)\} = \tau \ (\forall t \in (0,1))$$

(ii)
$$f_t^{(m\phi)} = \phi'^{-1} \left(\frac{1}{(1-t)\frac{1}{\phi'(f)} + t\frac{1}{\phi'(g)}} \right)$$
 (quasi-harmonic mean)

(iii)
$$C_{f_1,\dots,f_k}^{(m\phi)}$$
 is $m\phi$ - totally geodesic

Metric and connections by $D^{(\phi)}$

 $D^{(\phi)}(f,g) \approx \int \xi(f)\phi(g)dP$ cf. Eguchi (1992)

Riemannian metric
$$G_{ij}^{(\phi)}(\theta) = \int \frac{\partial \xi(f_{\theta})}{\partial \theta_i} \frac{\partial \phi(f_{\theta})}{\partial \theta_j} dP$$
Generalized m-connection $\Gamma_{ij,k}^{(m\phi)}(\theta) = \int \frac{\partial^2 \xi(f_{\theta})}{\partial \theta_i \partial \theta_j} \frac{\partial \phi(f_{\theta})}{\partial \theta_k} dP$ Generalized e-connection $\Gamma_{ij,k}^{(e\phi)}(\theta) = \int \frac{\partial \xi(f_{\theta})}{\partial \theta_k} \frac{\partial^2 \phi(f_{\theta})}{\partial \theta_k} dP$

Remark

$$G_{ij}^{(\phi)}(\theta) \propto G_{ij}(\theta) \quad (\text{ conformal })$$
$$\frac{\partial}{\partial \theta_k} G_{ij}^{(\phi)}(\theta) = \Gamma_{ik,j}^{(e\phi)}(\theta) + \Gamma_{jk,i}^{(m\phi)}(\theta) \quad (\text{ conjugate })$$

Generalized two geodesic curves



ø Pythagorean theorem

Pythagoras theorem

$$C_{f,g}^{(m\phi)} \perp_g C_{g,h}^{(e\phi)} \Leftrightarrow D^{(\phi)}(f,h) = D^{(\phi)}(f,g) + D^{(\phi)}(g,h)$$



$$\phi(s) = \log s \implies \psi(t) = \exp t, \ \xi(s) = s,$$
$$(f_t^{(e\phi)}, f_t^{(m\phi)}, D^{(\phi)}) = (f_t^{(m)}, f_t^{(e)}, D)$$

Power-log function

$$\phi(s) = \frac{s^{\beta} - 1}{\beta} \implies \psi(t) = (1 + \beta t)^{\frac{1}{\beta}}, \ \xi(s) = s^{1 - \beta}$$

$$f_t^{(e\phi)}(x) = ((1 - t)f(x)^{\beta} + tg(x)^{\beta} - \kappa_t)^{\frac{1}{\beta}}$$

$$f_t^{(m\phi)}(x) = ((1 - \kappa_{\beta t})f(x)^{1 - \beta} + \kappa_{\beta t}g(x)^{1 - \beta})^{\frac{1}{1 - \beta}}$$

$$D^{(\phi)}(f, g) = \frac{1}{\beta \int f^{1 - \beta} dP} \{1 - \int f^{1 - \beta}g^{\beta}dP\}$$

Generalized exponential model

G-exponential model

$$M^{(e\phi)} = \{ f_{\theta}^{(e\phi)}(x) := \psi(\theta^{\mathrm{T}} t(x) - \kappa^{(\phi)}(\theta)) : \theta \in \Theta \}$$

where $\kappa^{(\phi)}(\theta)$ is a normalizing constant.

Mean parameter
$$\eta = E_{\xi(f_{\theta}^{(e\phi)})} \{t(X)\} = \frac{\partial}{\partial \theta} \kappa^{(\phi)}(\theta)$$
 Cf. Naudts (2010)

Remark 1 θ and η are affine parameters wrt $\Gamma^{(e\phi)}$ and $\Gamma^{(m\phi)}$. ($M^{(e\phi)}$ is dually flat.) Cf. Matsuzoe-Henmi (2014)

Remark 2 $M^{(e\phi)}$ is totally $(e\phi)$ - geodesic.

(The generalized e-geodesic curve connecting any two densities in $M^{(e\phi)}$ is always in $M^{(\phi e)}$.)

Minimum GKL leaf

G-exponential model $M^{(e\phi)} = \{ f_{\theta}^{(e\phi)}(x) : \theta \in \Theta \}$

Mean equal space $\mathscr{Q}^{(\xi)}(f) = \{g : \mathcal{E}_{\xi(g)}\{t(X)\} = \mathcal{E}_{\xi(f)}\{t(X)\}\}$ $f^* \in M^{(e)} \Rightarrow$ $D^{(\phi)}(g, f) = D^{(\phi)}(g, f^*) + D^{(\phi)}(f^*, f) \quad (\forall g \in \mathscr{Q}^{(\xi)}(f^*), \forall f \in M^{(e)})$



Generalized Pythagoras foliation

$$\{\mathscr{Q}^{(\xi)}(f): f \in M^{(e\phi)}\} \text{ is a foliation}$$

(i) $f_1 \neq f_2 \Rightarrow \mathscr{Q}^{(\xi)}(f_1) \cap \mathscr{Q}^{(\xi)}(f_2) = \phi$
(ii) $\mathscr{F} = \bigcup_{f \in M^{(e\phi)}} \mathscr{Q}^{(\xi)}(f)$



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If $(\phi, \psi) \neq (\log, \exp)$, then

(i) the geometry depends on the choice of P, Cf. Newton (2012) (ii) the minimum $D^{(\phi)}$ estimation is not feasible.

Expected *\phi* density

Consider

 $\mathrm{E}_{f}\left\{-\phi(g)\right\}$

Let $g_{\text{opt}} \coloneqq \argmin_{g \in \mathscr{F}} E_f \{-\phi(g)\}$

Then
$$\frac{\partial}{\partial \varepsilon} \mathbf{E}_f \{ \phi((1-\varepsilon)g_{\text{opt}} + \varepsilon h) \} |_{\varepsilon=0}$$

$$= \int \{ \underline{f \phi'(g_{\text{opt}})}(h - g_{\text{opt}}) \} dP = 0 \text{ for all } h \text{ of } \mathcal{F}$$

Therefore $f(x)\phi'(g_{opt}(x)) = c$ with a constant *c*, that is,

$$g_{\text{opt}}(x) = \zeta(f(x))$$
 where $\zeta(f) = (\phi')^{-1} \left(\frac{c}{f}\right)$

$$\mathbf{E}_{f} \{-\phi(\zeta(f))\} = \min_{g \in \mathcal{F}} \mathbf{E}_{f} \{-\phi(g)\}$$

Quasi divergence

Remark

$$\xi(\zeta(f)) = \frac{\frac{1}{\phi'(\zeta(f))}}{\int \frac{dP}{\phi'(\zeta(f))}} = \frac{\frac{f}{c}}{\int \frac{f}{c}dP} = f$$

because
$$\xi(f) = \frac{1}{\phi'(f)} / \int \frac{dP}{\phi'(f)}$$
 and $\zeta(f) = (\phi')^{-1} (\frac{c}{f})$

Let
$$D_0(f,g) = \mathcal{E}_f \{-\phi(g)\} - \min_{f \in \mathscr{F}} \mathcal{E}_f \{-\phi(g)\}.$$

Then $D_0(f,g) = E_f \{ \phi(\xi^{-1}(f)) - \phi(g) \}$

$$D_0(f,g) \ge 0$$
 with equality iff $g = \xi^{-1}(f)$

Another generalization of KL-divergence

One adjustment

$$D^{(\phi)}(f,g) = D_0(\xi(f),g) = \mathcal{E}_{\xi(f)}\{\phi(f) - \phi(g)\}$$

The other adjustment

$$\Delta^{(\phi)}(f,g) = D_0(f,\xi^{-1}(g)) = \mathcal{E}_f \{ \phi(\xi^{-1}(f)) - \phi(\xi^{-1}(g)) \}$$

Remark

(i)
$$\Delta^{(\phi)}(f,g) = D^{(\phi)}(\xi(f),\xi(g))$$

(ii) $\Delta^{(\phi)}(f,g)$ is a unique divergence defined by the standard expectation in the class of corrected quasi divergence

Gamma divergence

$$\phi(f) = \frac{f^{\beta} - 1}{\beta} \implies \qquad \xi(g(x)) = \frac{g(x)^{1 - \beta}}{\int g^{1 - \beta} dP},$$

$$\xi^{-1}(g(x)) = \frac{g(x)^{\frac{1}{1 - \beta}}}{\int g^{\frac{1}{1 - \beta}} dP}$$

$$\Delta^{(\phi)}(f,g) = -\frac{\mathrm{E}_f(g^{\frac{\beta}{1-\beta}})}{\left(\int g^{\frac{1}{1-\beta}}dP\right)^{\beta}} + \left(\int f^{\frac{1}{1-\beta}}dP\right)^{1-\beta}$$

Remark $\Delta^{(\phi)}$ is γ -divengence with $\gamma = \frac{\beta}{1-\beta}$ Fujisawa-Eguchi (2008)



Metric and connections by $\Delta^{(\phi)}$

$$\Delta^{(\phi)}(f,g) \approx \int f \, \Phi(g) dP$$

Riemannian metric $G_{ij}^{(\Phi)}(\theta) = \int \frac{\partial f_{\theta}}{\partial \theta_{i}} \frac{\partial \Phi(f_{\theta})}{\partial \theta_{j}} dP$ Generalized m-connection $\Gamma_{ij,k}^{(m\Phi)}(\theta) = \int \frac{\partial^{2} f_{\theta}}{\partial \theta_{i} \partial \theta_{j}} \frac{\partial \Phi(f_{\theta})}{\partial \theta_{k}} dP$ Generalized e-connection $\Gamma_{ij,k}^{(e\phi)}(\theta) = \int \frac{\partial f_{\theta}}{\partial \theta_{k}} \frac{\partial^{2} \Phi(f_{\theta})}{\partial \theta_{i} \partial \theta_{j}} dP$

Remark

$$\Gamma^{(\mathbf{m}\Phi)}_{ij,k} = \Gamma^{(\mathbf{m})}$$

Minimum $\Delta^{(\phi)}$ estimation

Model	$M = \{ f_{\theta} : \theta \in \Theta \}$
Data set	$\{X_i\} \sim_{\text{i.i.d.}} f_{\theta}(x)$
Loss function	$L^{(\Phi)}(\theta) = -\frac{1}{n} \sum_{i=1}^{n} \Phi(f_{\theta}(X_i))$
Proposed estimator	$\hat{\theta}^{(\Phi)} = \underset{\theta \in \Theta}{\arg\min} L^{(\Phi)}(\theta)$
Expected loss	$\mathbb{L}^{(\Phi)}(\theta) = \mathbb{E}_{f} \{-\Phi(f_{\theta})\} \text{ if } \{X_{i}\} \sim f(x)$
consistency	$\hat{\theta}^{(\Phi)} \rightarrow \theta \text{ if } f = f_{\theta}$

Estimation selection, Robustness, Spontaneous data learning

Non-convex learning

Model

$$f_{\theta}(x) = \frac{1}{2\pi^{d/2}} \exp\left\{-\frac{1}{2}(x-\theta)^T(x-\theta)\right\}$$

Loss function

$$L^{(\Phi)}(\theta) = -\frac{1}{n} \sum_{i=1}^{n} \exp\left\{-\frac{\gamma}{2} (x_i - \theta)^{\mathrm{T}} (x_i - \theta)\right\}$$



Spontaneous data learning

The consistent class of estimators $\{\hat{\theta}^{(\Phi)} \text{ with } L^{(\Phi)}(\theta)\}_{\Phi}$



Estimation selection than model selection

Concluding remarks



	expectation	metric
$D^{(\phi)}$	$\mathrm{E}_{\xi(f)}$	$\propto G$
$\Delta^{(\phi)}$	E_f	$\not \sim G$

$$(\phi, \psi) = (\log, \exp) \implies \Delta^{(\phi)} = D^{(\phi)} = D$$

Τηανκ ψου

Welcome to any comments: eguchi@ism.ac.jp

U-divergence

Let U be a function satisfying $U(s) = \int_0^s \psi(t) dt$

U-cross-entropy $C_U(f,g) = \int \{-f \phi(g) + U(\phi(g))\} d\mu$

*U***-entropy** $H_U(f) = C_U(f, f)$

U-divergence $D_U(f,g) = C_U(f,g) - H_U(f)$

Note $C_U(f,g) \ge H_U(f)$ or $D_U(f,g) \ge 0$

Exm Let
$$U_{\beta}(s) = \frac{1}{1+\beta} (1-\beta s)^{\frac{1+\beta}{\beta}}$$
.

Then power entropy $C_{U_{\beta}}(f,g) = -\frac{1}{\beta} \int f g^{\beta} d\mu + \frac{1}{\beta+1} \int g^{\beta+1} d\mu$

beta divergence $D_{U_{\beta}}(f,g) = \frac{1}{\beta} \int f(f^{\beta} - g^{\beta}) d\mu + \frac{1}{\beta+1} \int (f^{\beta+1} - g^{\beta+1}) d\mu$ 34

Generalized exponential model (ver. 2)

Let us fix a canonical statistic $\mathbf{t} = (t_1, \dots, t_K)$.

G-exponential model

$$M^{(e\Phi)} = \{ f_{\theta}^{(e\Phi)}(x) := \Phi^{-1}(\theta^{T}t(x) - \kappa^{(\Phi)}(\theta)) : \theta \in \Theta \}$$

where $\kappa^{(\Phi)}(\theta)$ is a normalizing constant.

Mean parameter
$$\boldsymbol{\eta} = \mathbb{E}_{f_{\boldsymbol{\theta}}^{(e\Phi)}} \{\boldsymbol{t}(\boldsymbol{X})\} = \frac{\partial}{\partial \boldsymbol{\theta}} \kappa^{(\Phi)}(\boldsymbol{\theta})$$

Remark 1 θ and η are affine parameters wrt $\Gamma^{(e\Phi)}$ and $\Gamma^{(m)}$. ($M^{(e\Phi)}$ is dually flat.)

Remark 2 $M^{(e\Phi)}$ is totally gedesic wrt $\Gamma^{(e\Phi)}$.