IGAIA 4 Bohemia

# **Information Geometry**

### --- Historical Episodes and Future with Recent Developments

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### **Prehistory --- Riemannian Geometry**

H. Hotteling 1929 Riemannian metric and Fisher information location-scale model : constant curvature

P. Ch. Maharanobis 1936 Euclidean distance (multivariate-Gaussian)

C. R. Rao 1945 Cramer-Rao Theorem; Riemannian

H. Jeffreys 1946 Bayesian theory and Jeffreys invariant prior

# **Dual Geometry, Invariance**

N. Chentsov 1972 invariance,  $\{g, T\}$ ,  $\alpha$ -connection

B. Efron 1975 (A. P. Dawid) statistical curvature; higher-order asymptotics

O. Barndorff-Nielsen 1976 exponential family; Legendre transform

S. Amari 1982 duality; curvature and statistics (M. Kumon)

H. Nagaoka and S. Amari 1982 duality, Pythagorean theorem

# Amari's personal history

### 1958: statistics seminar (master course at U Tokyo)

S. Kullback, "Information and Statistics" Riemannian metric (suggested by S. Moriguti)

**Gausssian**  $N(\mu, \sigma^2)$  : geodesic, constant curvature (Poincare-half plane)

### beautiful structure $\rightarrow$ essential meaning?

mathematical engineering graph and topology of networks: homology non-Riemannian geometry of materials manifold: dislocations information systems, learning and neural networks

### **Statistical curvature and higher-order inference**

### B. Efron, 1975

**Fisher's idea; exponential connection and mixture connection** A. P. Dawid, 1975 e- and m-connections

**S. Amari :** 
$$\alpha$$
-geometry  $Error^2 = \frac{1}{n}G^{-1} + \frac{1}{n^2}(H_e^2 + H_m^2 + \Gamma_m^2) + \frac{1}{n^3}K$ 

(Rao, Kano K? Fisher's dream)

Amari and M.Kumon higher-order power of statistical test

### Amari paper : Ann. Statist. 1982

**Reviewers (S. Lauritzen and A.P. Dawid)** 

**Chentsov work (handwritten manuscript)** 

 H. Nagaoka and S. Amari 1982 (Technical Report)
 Ann. Probability Theory 7 reviewers
 Zeitshrift fur Wahrsceinlichkeitstheorie und VerwandteGebiete geometry has nothing to do with statistics
 IEEE Trans. Inf. Theory Shannon Theory, now well-known

# London Workshop: 1984 (D. Cox)

### Cox visited Japan in 1983 patron of information geometry

Rao, Efron, Dawid, Barndorff-Nielsen, Lauritzen Kass, Eguchi many others

Dodson, Critchley, Marriot, Komaki, Zhang, Ay, Pistone, Giblisco, Nielsen, ...

## **Information Geometry --- lucky naming**

### **Applications area:**

statistics, time-series and systems, machine learning, signal processing, optimization brain theory, consciousness physics, economics, mathematics (Banach manifold, affine differential geometry and beyond) quantum information, Tsallis entropy

# **International Conferences**

### IGAIA series; GSIS series, ...

Many monographs new journal (Jun Zhang); where to publish mailing list and society

still small community; united and cooperative, blessed by all

# My recent works

- 1. Systems complexity and consciousness (IIT)
- 2. Geometry of score matching (Hyvarinen score)
- 3. Natural gradient descent and topology of deep learning)
- 4. Canonical divergence
- 5. Multi-terminal statistical inference
- 6. Information geometry and Wasserstein distance

Information Integration and Complexity of Systems

-- Stochastic approach



$$p(\mathbf{x}, \mathbf{y}) = p(\mathbf{x}) p(\mathbf{y} \mid \mathbf{x})$$

x: state of the brain

y: next state of the brain

### Integrated Information Theory G. Tononi



**Necessary condition; sufficient?** 



full model:  $S_F = \{p(\mathbf{x}, \mathbf{y})\}$  Disconnected model:  $S_{dis} = \{q(\mathbf{x}, \mathbf{y})\} \quad q(\mathbf{y} | \mathbf{x}) = \Pi q(y_i | x_i)$ 

# measure of interaction : N. Ay information integration : Tononi Barrett and Seth Many other $\Phi$

# Measure of information integration, or system complexity $\Phi$



### **Definition of** $\Phi$ : **Postulates**

1) 
$$\Phi = \min_{q} D[p(x, y) : q(x, y)], \quad q \in S_{dis}$$

**2)** 
$$D = D_{KL}[p:q] = \int p(x,y) \log \frac{p(x,y)}{q(x,y)}$$

3) Disconnected model: S<sub>dis</sub> Markov conditions



(1->2) branch deleted: Markov condition:  $X_1 \rightarrow X_2 \rightarrow Y_2$ 

$$p(x_1, y_2 \mid x_2) = p(x_1 \mid x_2) p(y_2 \mid x_2)$$
  

$$X_1 - X_2 - Y_2$$
  

$$X_2 - X_1 - Y_1$$

$$S_{dis}$$
: all  $x_i \to y_j$   $(i \neq j)$  deleted

### Why KL-divergence?

1) 
$$D[p:q] \ge 0$$
, = 0, when and only when  $p = q$ 

2) D[p:q] invariant under transformations of **X** 

3) 
$$D[p:q] = \sum_{i} d[p(x_i), q(x_i)]$$

4) D[p:q] induces flat structure dually

### **Geometric degree of information integration**

$$\Phi_{geo} = \min_{q} D_{KL}[p(x, y): q(x, y)], \quad q \in S_{dis}$$



$$\mathbf{y} = A\mathbf{x} + \mathbf{e} \qquad \Sigma = \mathbf{E}[\mathbf{e}\mathbf{e}^T]$$
$$\mathbf{y} = A'\mathbf{x} + \mathbf{e}' \qquad \Sigma' = \mathbf{E}[\mathbf{e}'\mathbf{e}'^T] \qquad A': \text{diagonal}$$

$$\Phi_{geo} = \log \frac{|\Sigma'|}{|\Sigma|}$$



$$\mathbf{y} = A\mathbf{x} + \mathbf{e} \qquad \Sigma = \mathbf{E}[\mathbf{e}\mathbf{e}^T]$$
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$$\Phi_{geo} = \log \frac{|\Sigma'|}{|\Sigma|}$$

### Many other definitions of $\Phi$

Full model Disconnected models





 $p(\mathbf{x}, \mathbf{y}) = \exp\left\{\sum \theta_i^X x_i + \sum \theta_i^Y y_i + \theta_{12}^X x_1 x_2 + \theta_{12}^Y y_1 y_2 + \sum \theta_{ij}^{XY} x_i y_j + \text{higher-order terms } -\psi(\boldsymbol{\theta})\right\}$ **exponential family** 

 $\theta$ -coordinates  $\theta$  $\eta$ -coordinates  $\eta_i^X = E[x_i], \dots, \eta_{ij}^{XY} = E[x_iy_j], \dots$ 

### There are many disconnected models!!

### Split Model $S_H$ : Ay, Barrett & Seth



### **Mixed Coordinates :**

$$\boldsymbol{\xi} = \left(\eta_i^X, \eta_{12}^X, \eta_i^Y, \eta_{11}^{XY}, \eta_{22}^{XY}; \theta_{12}^{XY}, \theta_{21}^{XY}, \theta_{12}^Y\right)$$
$$\hat{q} = \prod p = q\left(\boldsymbol{x}, \boldsymbol{y}; \hat{\boldsymbol{\xi}}\right)$$

**problem**  $0 \le \Phi[p] \le I[X:Y]$  $p_{ind} = p_X(x)p_Y(y) \Rightarrow I = 0, \quad \Phi > 0$ 

Markovian Condition  $Y_1 - X_1 - X_2 - Y_2 \implies$  $X_1 - X_2 - Y_2; Y_1 - X_1 - X_2$ 











### **Problem: Gaussian channel** $p(x, y): y = Ax + \varepsilon \implies \hat{q}: y = \hat{A}x + \varepsilon' \in S_G$

$$p(\mathbf{x}, \mathbf{y}) = \exp\left[-\frac{1}{2}\left\{\mathbf{x}' \sum_{x}^{-1} \mathbf{x} + (\mathbf{y} - A\mathbf{x})' \sum_{\varepsilon}^{-1} (\mathbf{y} - A\mathbf{x}) - \psi\right\}\right]$$

 $\hat{A}$  is not diagonal  $\leftarrow \theta_{12}^{XY} = \theta_{21}^{XY} = 0$ 



**Mismatched Decoding Model**  $S_M$ 

$$\mathbf{y} \to \hat{\mathbf{x}}$$
$$x_1 \longrightarrow y_1$$

Best mismatched decoding from y to x

$$x_2 \longrightarrow y_2$$

$$S_{M} = \{q_{\beta}(\mathbf{x}, \mathbf{y}) = p(\mathbf{x}) p_{\beta}(\mathbf{y}) \prod p(\mathbf{y}_{i} | \mathbf{x}_{i})^{\beta} \}$$
$$\Phi^{*} = D_{KL}[p:S_{M}]$$

$$S_H \subset S_{Gr}, S_{Geo} : S_{Gr}, S_H$$
 dually flat  
 $S_M \subset S_{Gr} : S_M, S_{Geo}$  not flat



### **Transfer Entropy; Granger causality**

 $TE[x_i \rightarrow y_j] = \min D_{KL}[p:q] \quad q \in (i \rightarrow j) \text{ disconnected}$  $= H[Y_j \mid X - X_i] - H[Y_j \mid X]$  $x_1 \circ \xrightarrow{y_1}$  $x_2 \circ \xrightarrow{y_2}$ 

### **Non-additive**

 $TE[x_i \to y_j; x_k \to y_m] \neq TE[x_i \to y_j] + TE[x_k \to y_m]$ 

### **Hierarchy: transfer entropy**



### **Information Geometry of Hyvärinen Game Score**

#### Following Grinwald, Dawid, Parry, Lauritzen, Hyvärinen

$$L(p,q) = E_{p(x)} [l(x,a)]: a = q(x)$$
  

$$S(x,q) = l(x,q) \qquad l(x,q) = \log q(x)$$
  
S-entropy 
$$H_{s} [p:q] = E_{p} [S(x,q)]$$
  
S-divergence 
$$D_{s} [p:q] = H_{s} [p:q] - H_{s} [p:p]$$

### Hyvärinen score

$$S(x,q) = \ddot{l}(x,\xi) + \frac{1}{2} \{\dot{l}(x,\xi)\}^{2}$$
$$D_{s}[p:q] = \frac{1}{2} E_{p} \left[ \frac{d}{dx} \{\log p(x) - \log q(x,\theta)\}^{2} \right]$$
$$D[p:cq] = D[p:q]$$
$$s(x,\xi) = \partial_{\xi} \ddot{l}(x,\xi) + \dot{l}(x,\xi) \partial_{\xi} \dot{l}(x,\xi)$$



**Information geometry of**  $D_s[p:q]$ 

### **Asymptotic Analysis of estimator**

$$E\left[\Delta\boldsymbol{\xi}\Delta\boldsymbol{\xi}^{T}\right] = \frac{1}{N}K^{-1}VK^{-T} \ge G^{-1}$$

$$K = E\left[\partial_{\xi} s\left(x,\xi\right)\right]$$
$$V = E\left[s\left(x,\xi\right)s\left(x,\xi\right)^{T}\right] \to G$$

$$E\left[\Delta\xi\Delta\xi^{T}\right] = G^{-1}AG^{-1}$$
$$A = E\left[a(x,\xi)a(x,\xi)^{T}\right]$$
$$s(x,\xi) = c\left\{\partial_{\xi}\log(x,\xi) + a(x,\xi)\right\}$$

 $a \perp \partial_{\xi} \log q$ : efficient

### Hyvärinen score

$$S(x,q) = \ddot{l}(x,\xi) + \frac{1}{2} \{\dot{l}(x,\xi)\}^{2}$$
$$D_{s}[p:q] = \frac{1}{2} E_{p} \left[ \frac{d}{dx} \{\log p(x) - \log q(x,\theta)\}^{2} \right]$$
$$D[p:cq] = D[p:q]$$
$$s(x,\xi) = \partial_{\xi} \ddot{l}(x,\xi) + \dot{l}(x,\xi) \partial_{\xi} \dot{l}(x,\xi)$$
### **Hyvärinen estimator**

**Fisher efficient**  $\iff$  *q* multivariate Gaussian

**Discrete case** :  $x \in$  graph nodes



$$S(\mathbf{x},q) = \left\{ \frac{\Delta q(\mathbf{x})}{q(\mathbf{x})} \right\}^{2} - 2\Delta \left\{ \frac{\Delta q(\mathbf{x})}{q(\mathbf{x})} \right\}$$
$$D_{S}[\boldsymbol{\xi}:\boldsymbol{\xi}'] = E_{q(x,\boldsymbol{\xi})} \left\{ \frac{\Delta q(x,\boldsymbol{\xi})}{q(x,\boldsymbol{\xi})} - \frac{\Delta q(x,\boldsymbol{\xi}')}{q(x,\boldsymbol{\xi}')} \right\}^{2}$$
$$\sum_{x} \Delta f(\mathbf{x})h(\mathbf{x}) = \sum_{x} f(\mathbf{x})\Delta'h(\mathbf{x}) \qquad f,h \to 0$$
$$\int f'(x)h(x)dx = -\int f(x)h'(x)dx \qquad x \to \pm \infty$$

## Deep Learning

#### Self-Organization + Supervised Learning

**RBM: Restricted Boltzmann Machine** Auto-Encoder, Recurrent Net





Dropout Contrastive divergence bi-directional convolution

#### **Mathematical Neurons**

$$y = \varphi \left( \sum w_i x_i - h \right) = \varphi \left( \boldsymbol{w} \cdot \boldsymbol{x} \right)$$



#### **Multilayer Perceptrons**



 $\theta = (w_1, \dots, w_m; v_1, \dots, v_m)$ 



#### **Backpropagation --- stochastic gradient learning**







Geometry of singular model



# model: 2 hidden neurons

$$f(\boldsymbol{x},\boldsymbol{\theta}) = w_1 \varphi (\boldsymbol{J}_1 \cdot \boldsymbol{x}) + w_2 \varphi (\boldsymbol{J}_2 \cdot \boldsymbol{x})$$

$$y = f(\boldsymbol{x}, \boldsymbol{\theta}) + \boldsymbol{\varepsilon}$$

$$\varphi(u) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{u} e^{-\frac{t^2}{2}} dt$$

loss function: 
$$l(\mathbf{x}, y; \boldsymbol{\theta}) = \frac{1}{2} \{ y - f(\mathbf{x}, \boldsymbol{\theta}) \}^2$$

y: teacher signal:  $\theta_0$  stochastic descent learning

$$\dot{\boldsymbol{\theta}} = -\eta \left\langle \frac{\partial l(\boldsymbol{x}_t, \boldsymbol{y}_t, \boldsymbol{\theta}_t)}{\partial \boldsymbol{\theta}} \right\rangle$$
 backprop: vanilla gradient

**Natural Gradient Stochastic Descent** 

 $\dot{\boldsymbol{\theta}} = -\eta G^{-1}(\boldsymbol{\theta}_t) \left\langle \nabla_{\boldsymbol{\theta}}(\boldsymbol{x}_t, \boldsymbol{y}_t, \boldsymbol{\theta}_t) \right\rangle$ 

$$\nabla_{\theta} = \frac{\partial}{\partial \theta}$$

 $G(\boldsymbol{\theta}) = \langle \nabla_{\boldsymbol{\theta}} l \nabla_{\boldsymbol{\theta}} l \rangle$  : Fisher Information Matrix

invarint; steepest descent

# Natural gradient is superior

**Steepest descent; invariant** Yan Ollivier

**Fisher-efficient** 

Natural gradient is non-vanishing even in multiple layers

Good at singular regions (avoid plateaus: Milnor attractor)

#### **Adaptive Natural Gradient**

#### **Singular Region in Parameter Space**

$$R(w, \boldsymbol{J}) = \left\{ \boldsymbol{\theta} \middle| \boldsymbol{J}_1 = \boldsymbol{J}_2 = \boldsymbol{J}, w_1 + w_2 = w \right\}$$

$$\bigcup \left\{ \boldsymbol{\theta} \middle| w_1 = 0, w_2 = w, \boldsymbol{J}_2 = \boldsymbol{J} \right\}$$

$$\bigcup \left\{ \boldsymbol{\theta} \middle| w_1 = w, w_2 = 0, \boldsymbol{J}_1 = \boldsymbol{J} \right\}$$

$$f(\boldsymbol{x},\boldsymbol{\theta}) = w_1 \varphi (\boldsymbol{J}_1 \cdot \boldsymbol{x}) + w_2 \varphi (\boldsymbol{J}_2 \cdot \boldsymbol{x})$$

### **Coordinate transformation**

$$\boldsymbol{v} = \frac{W_1 \boldsymbol{J}_1 + W_2 \boldsymbol{J}_2}{W_1 + W_2},$$

$$w = w_1 + w_2,$$

$$\boldsymbol{u}=\boldsymbol{J}_2-\boldsymbol{J}_1,$$

$$z = \frac{w_2 - w_1}{w_1 + w_2}$$

$$\boldsymbol{\xi} = (\boldsymbol{v}, \boldsymbol{w}, \boldsymbol{u}, \boldsymbol{z})$$

#### Singular Region $R(w, J) = \{u = 0\} \cup \{z = \pm 1\}$



#### Milnor attractor



Fig. 5. Critical set with local minima and plateaus.



Fig. 2: trajectories

# Saddle and plateau





#### **Topology of singular R**

blow-down coordinates :  $\boldsymbol{\alpha} = (\tau, \sigma, \boldsymbol{e})$ 

$$\tau = c_1 \left( 1 - z^2 \right) u^2, \qquad \qquad u = |\boldsymbol{u}|$$

$$\sigma = c_2 z \left(1 - z^2\right) u^3,$$

$$\boldsymbol{e} = \frac{\boldsymbol{u}}{|\boldsymbol{u}|} \in S_n, \qquad |\boldsymbol{e}| = 1$$

#### Singular Region $R(w, J) = \{u = 0\} \cup \{z = \pm 1\}$





# Sphere Sn and Projective space Pn



#### natural gradient learning near singularity

$$\frac{d}{dt} \begin{pmatrix} \tau \\ \sigma \end{pmatrix} = -\eta \begin{pmatrix} \tau \\ \sigma \end{pmatrix}$$

: true model  $\in R$ 

$$\frac{d}{dt} \begin{pmatrix} \tau \\ \sigma \end{pmatrix} = O(1)$$

: true model  $\notin R$ 

Milnor attractor

# Canonical Divergence in Manifold of Dual Affine Connections

Nihat Ay and S. Amari

### **Divergence and metric**

$$D[p:q] \ge 0$$
  
$$D[\boldsymbol{\xi}:\boldsymbol{\xi} + d\boldsymbol{\xi}] = \frac{1}{2}g_{ij}(\boldsymbol{\xi})d\boldsymbol{\xi}^{i}d\boldsymbol{\xi}^{j} + O(|d\boldsymbol{\xi}|^{3})$$

#### *G* : Riemannian metric, positive-definite

#### **Divergence and dual affine connections**

$$\begin{split} &\Gamma_{ijk} \sim \nabla \qquad \Gamma^*_{ijk} \sim \nabla^* \\ &\Gamma_{ijk} = -\partial_i \partial_j \partial'_k D \big[ \boldsymbol{\xi} : \boldsymbol{\xi}' \big]_{\boldsymbol{\xi}' = \boldsymbol{\xi}} \\ &\Gamma^*_{ijk} = -\partial'_i \partial'_j \partial_k D \big[ \boldsymbol{\xi} : \boldsymbol{\xi}' \big]_{\boldsymbol{\xi}' = \boldsymbol{\xi}} \\ &\partial_i = \frac{\partial}{\partial \boldsymbol{\xi}^i}; \qquad \partial'_j = \frac{\partial}{\partial \boldsymbol{\xi}'^j} \end{split}$$

# **Dual geometry**

$$\begin{split} &\left\{M,g,\nabla,\nabla^*\right\}\\ &X\left\langle Y,Z\right\rangle = \left\langle\nabla_X Y,Z\right\rangle + \left\langle Y,\nabla_X^* Z\right\rangle\\ &\left\{M,g,T\right\}, \qquad T_{ijk} = \Gamma_{ijk}^* - \Gamma_{ijk}\\ &\Gamma_{ijk}^{\pm\alpha} = \Gamma_{ijk}^o \mp \frac{\alpha}{2}T_{ijk} \qquad \Gamma^o: \text{Levi-Civita connection} \end{split}$$

### 

 $M: \text{ dually flat } : \exists \psi(\theta), \varphi(\eta)$  $D[\theta:\theta'] = \psi(\theta) + \varphi(\eta') - \theta \cdot \eta'$ 

#### **Bregman divergence**

## **Exponential map :** $\xi(t)$ geodesic



# **Exponential map divergence**

$$D[p:q] = \|X(p:q)\|^{2}$$
  

$$\alpha \text{-divergence}$$

$$q$$

$$D_{\alpha}[p:q] = \left\| X_{\alpha}(p:q) \right\|^{2}$$

**Theorem 1.** Exponential map divergence induces  $\alpha = -3$  geometry

**Theorem 2.**  $\alpha = -\frac{1}{3}$  exponential map divergence recovers the original geometry

**Standard divergence:**  $D_{\text{stan}}[p:q] = ||X_{-1/3}(p,q)||^2$ 

$$D[p:q] = \int_0^1 \langle X_t(q,p), \dot{\xi}_{q,p}(t) \rangle dt$$
$$= \int_0^1 t \| \dot{\xi}_{q,p}(t) \|^2 dt$$

$$\int_0^1 w(t) \| \dot{\xi}_{q,p}(t) \|^2 dt$$

## **Divergence and projection**


**IEEE ISIT-2011 Sankt Petersburg** 

Data Compression in Multiterminal Statistical Inference

Shun-ichi Amari RIKEN Brain Science Institute

# A long standing problem

T.Berger; Csiszar, Ahlswede, Burnashev, Han, Amari

correlated sources X, Y

data compression and statistical inference p(x, y; q); *iid*  $\begin{array}{c}
X : x_1 x_2 \cdots x_n & \hline k_x \text{ bits} \\
Y : y_1 y_2 \cdots y_n & \hline k_y \text{ bits} \\
\end{array}$ 

$$p(x, y;q)$$
; *iid*  $\operatorname{Prob} \{x = y\} = q$ 

binary : x, y = 0,1 ; Prob 
$$\{x = 1\}$$
 = Prob  $\{y = 1\}$  =  $\frac{1}{2}$ 

#### **Encoding : data compression**



## **One-bit helper case**

 $k_x = 1, \quad k_y = n$  $c = \operatorname{sgn}(a \cdot x)$ 



Is single-bit encoding optimal?
It is optimal
when q = 1/2 (x, y independent),

but not for general q.

**Fisher information**:  $k_x = 1$ ,  $k_y = n$ 



# Kingo Kobayashi: parity encoding



Information Geometry and Transportation Problem (Wasserstein distance)

entropic relaxation : min <c, p> - a{-H(p)} dual

**New Paper** 

### S. Pal and T-K L. Wong, Exponentially concave function and a new information geometry

Portfolio theory, transportation problem and information geometry (dually projectively flat)