

**Machine Learning SS: Kyoto U.**

# **Information Geometry and Its Applications to Machine Learning**

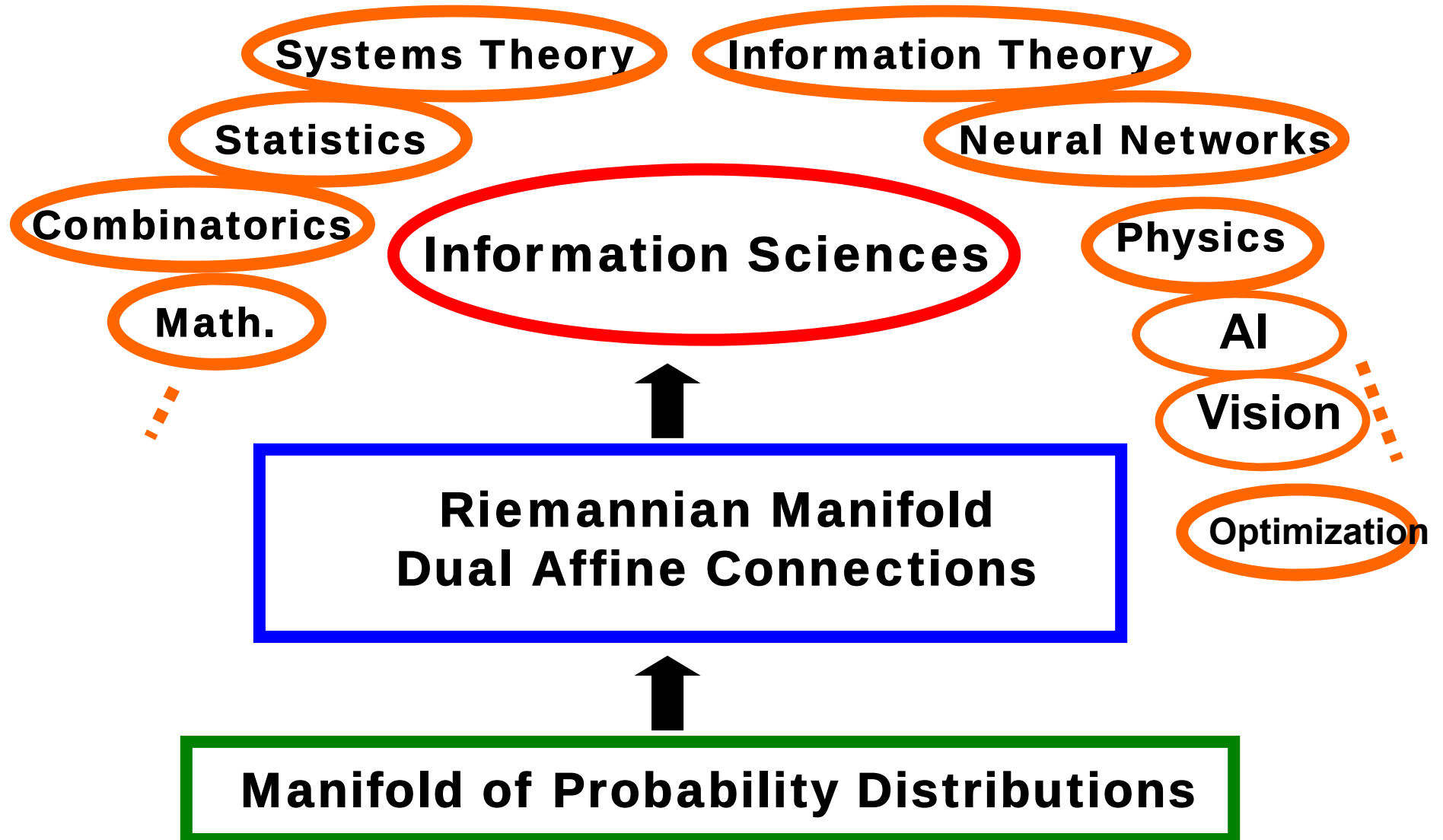
**Shun-ichi Amari**  
**RIKEN Brain Science Institute**

# Information Geometry

-- Manifolds of  
Probability Distributions

$$M = \{p(\mathbf{x})\}$$

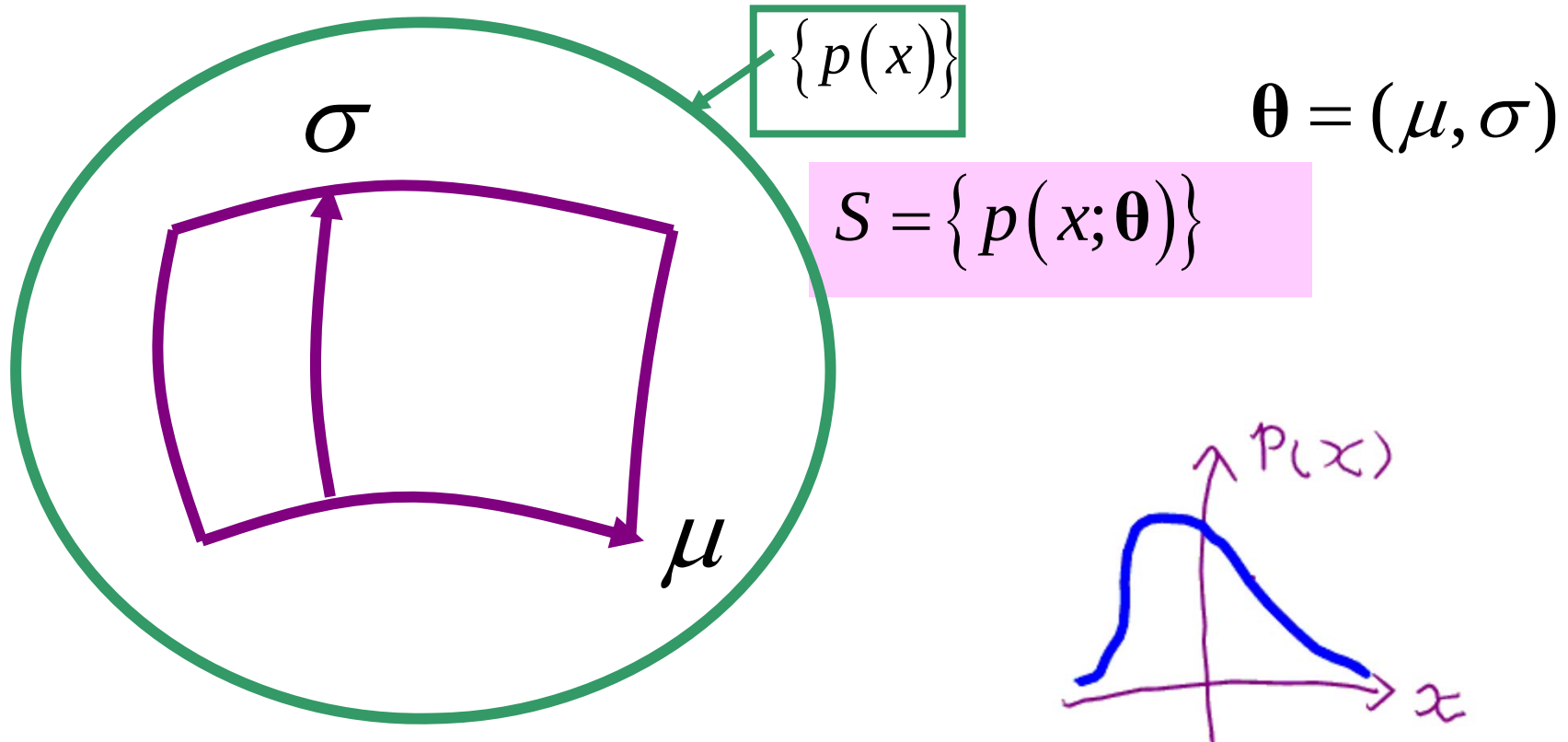
# **Information Geometry**



# Information Geometry ?

## Gaussian distributions

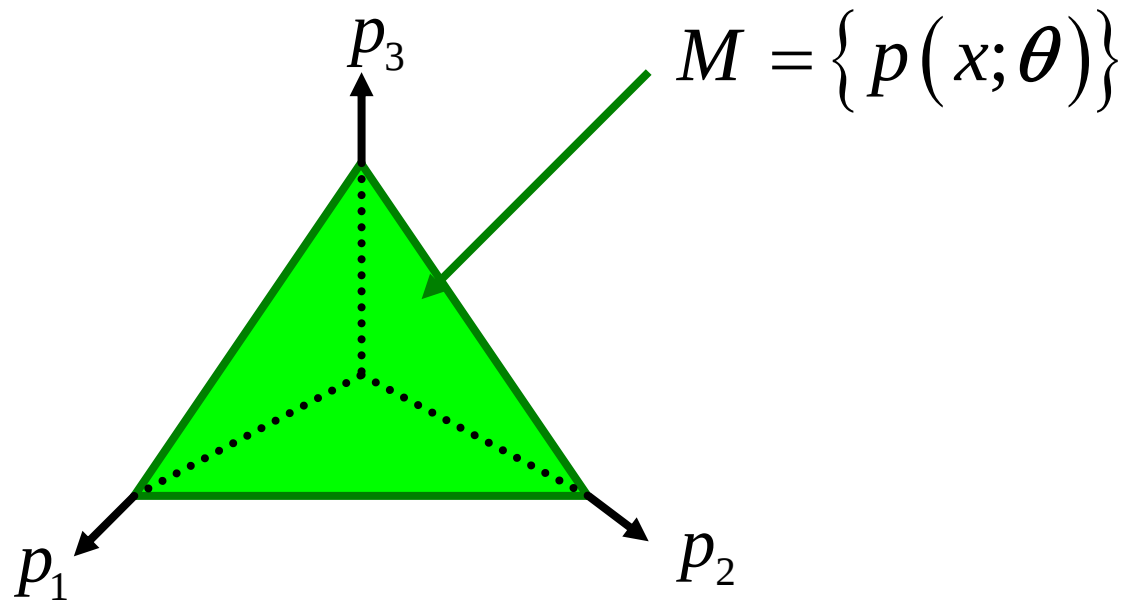
$$S = \{p(x; \mu, \sigma)\} \quad p(x; \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}$$



# Manifold of Probability Distributions

$$x = 1, 2, 3 \quad S_n = \{p(x)\}$$

$$\mathbf{p} = (p_1, p_2, p_3) \quad p_1 + p_2 + p_3 = 1$$



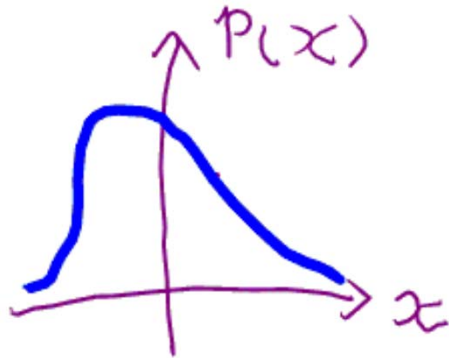
# Invariance

$$S = \{p(x, \theta)\}$$

*Invariant under different representation*

$$y = y(x), \quad \bar{p}(y, \theta)$$

**sufficient statistics**



$$\int |p(x, \theta_1) - p(x, \theta_2)|^2 dx \\ \neq \int |\bar{p}(y, \theta_1) - \bar{p}(y, \theta_2)|^2 dy$$

# Two Geometrical Structures

*Riemannian metric*

*affine connection --- geodesic*

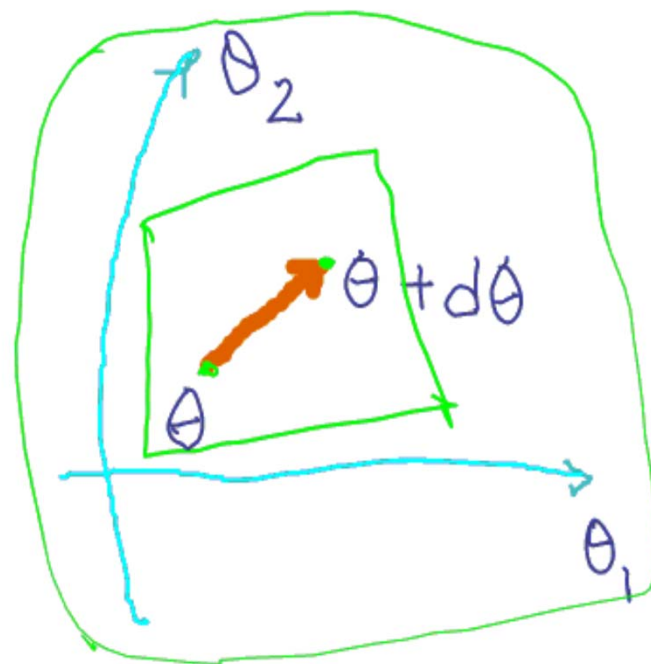
$$ds^2 = \sum g_{ij}(\theta) d\theta_i d\theta_j$$

*Fisher information*

$$g_{ij} = E \left[ \frac{\partial}{\partial \theta_i} \log p \frac{\partial}{\partial \theta_j} \log p \right]$$

**Orthogonality: inner product**

$$\langle d_1 \theta, d_2 \theta \rangle = d_1 \theta^T G d_2 \theta$$



# Affine Connection

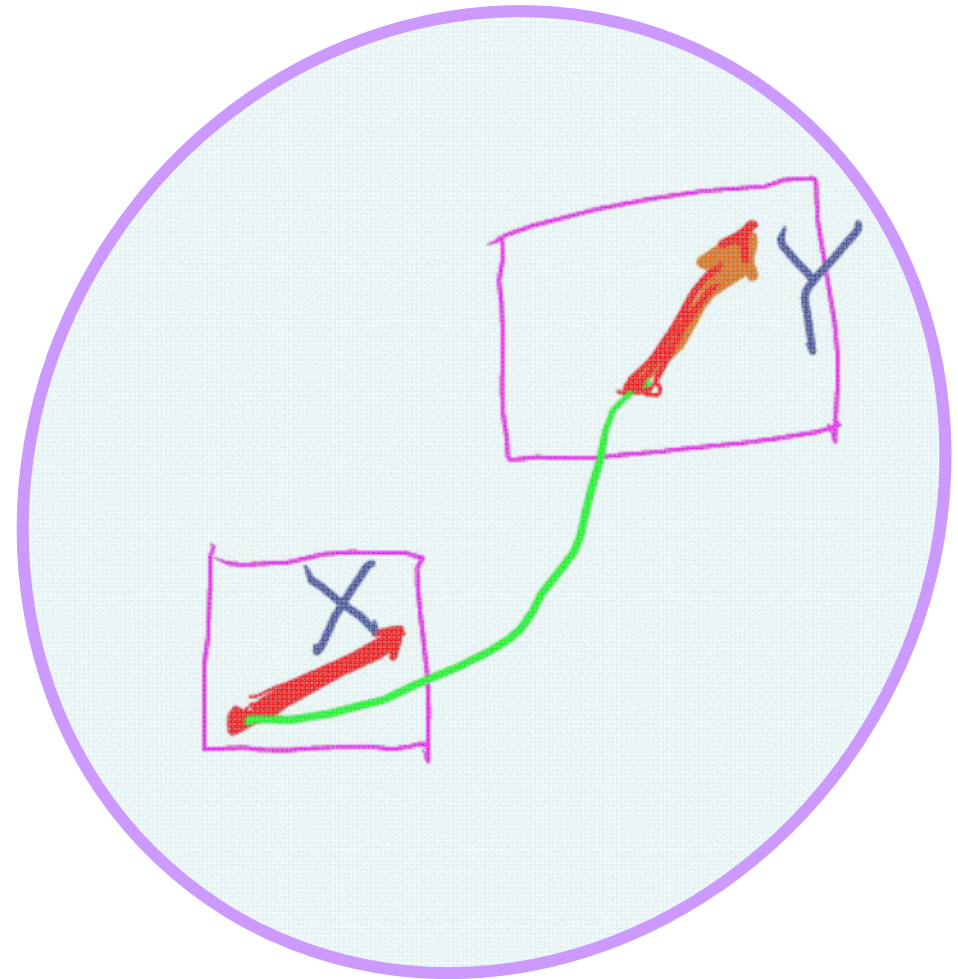
**covariant derivative; parallel transport**

$$\nabla_X Y, \quad \Pi_c X = Y$$

$$\text{geodesic } \Pi \dot{X} = \dot{X} \quad X = X(t)$$

$$s = \int \sqrt{\sum g_{ij}(\theta) d\theta^i d\theta^j}$$

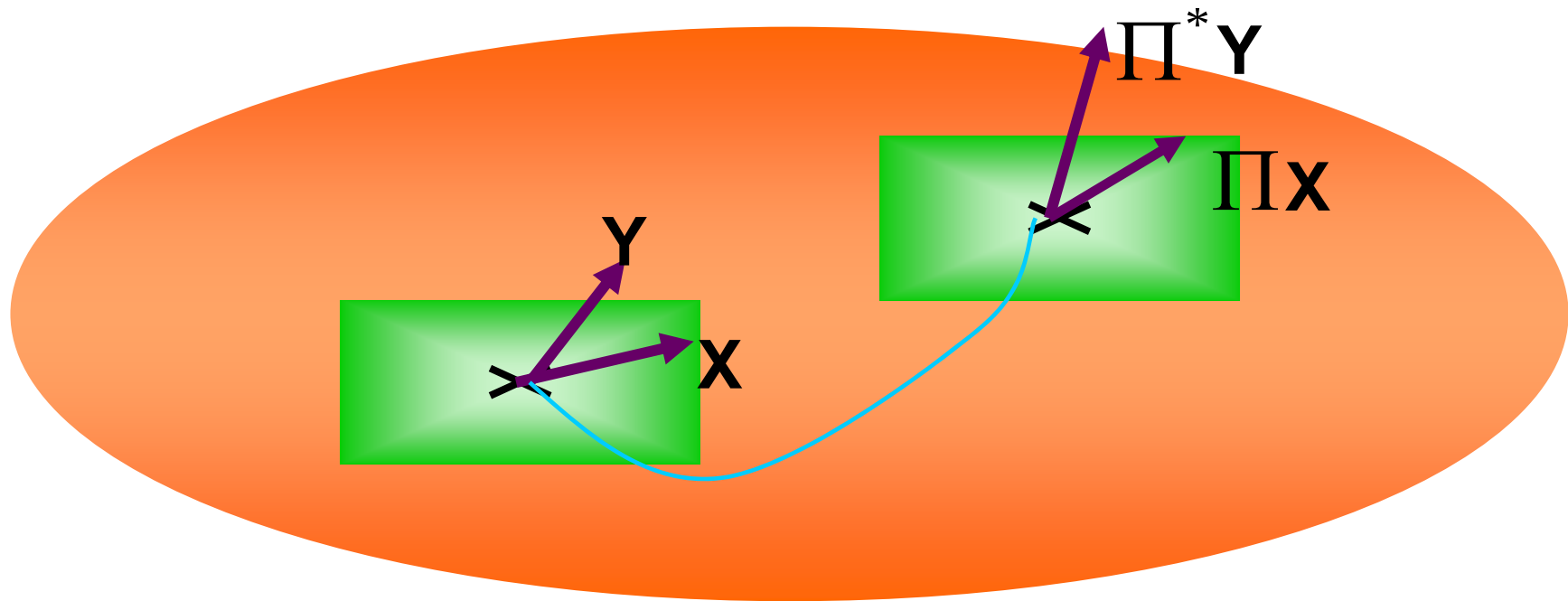
**minimal distance**  
**straight line**



# Duality: two affine connections

$$\{S, g, \nabla, \nabla^*\}$$

$$\langle X, Y \rangle = \langle \Pi X, \Pi^* Y \rangle \quad \langle X, Y \rangle = \sum g_{ij} X^i Y^j$$



Riemannian geometry:  $\Pi = \Pi^*$

# Dual Affine Connections $(\nabla, \nabla^*)$

$$(\Pi, \Pi^*)$$

*e-geodesic*

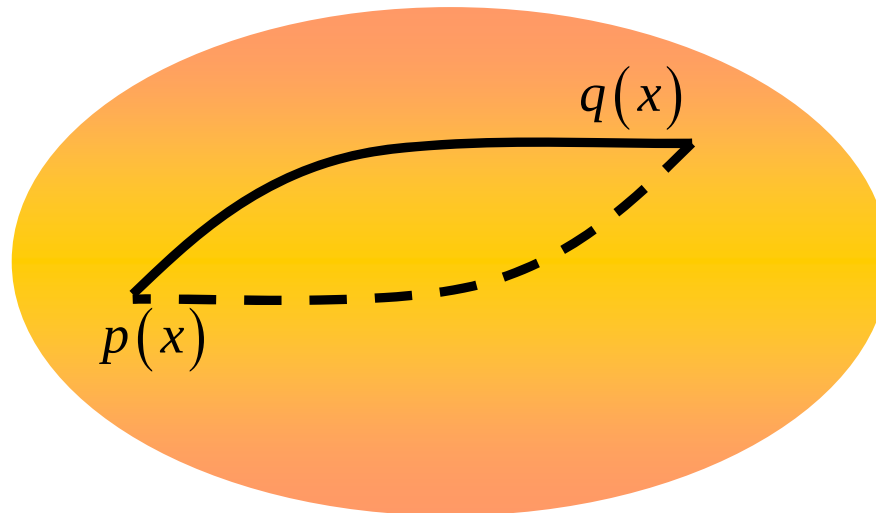
$$\log r(x, t) = t \log p(x) + (1-t) \log q(x) + c(t)$$

*m-geodesic*

$$r(x, t) = tp(x) + (1-t)q(x)$$

$$\nabla_{\dot{x}} \dot{x}(t) = 0$$

$$\nabla^*_{\dot{x}} \dot{x}(t) = 0$$



# Mathematical structure of $S = \{p(x, \xi)\}$

$$g_{ij}(\xi) = E[\partial_i l \partial_j l]$$

$$T_{ijk}(\xi) = E[\partial_i l \partial_j l \partial_k l]$$

$$\{\mathbf{M}, \mathbf{g}, \mathbf{T}\}$$

$$l = \log p(x, \xi); \quad \partial_i = \frac{\partial}{\partial \xi^i}$$

$\alpha$  -connection

$$\Gamma_{ijk}^\alpha = \{i, j; k\} - \alpha T_{ijk}$$

$$\nabla^\alpha \leftrightarrow \nabla^{-\alpha} : \text{dually coupled}$$

$$X \langle Y, Z \rangle = \langle \nabla_X Y, Z \rangle + \langle Y, \nabla_X^* Z \rangle$$

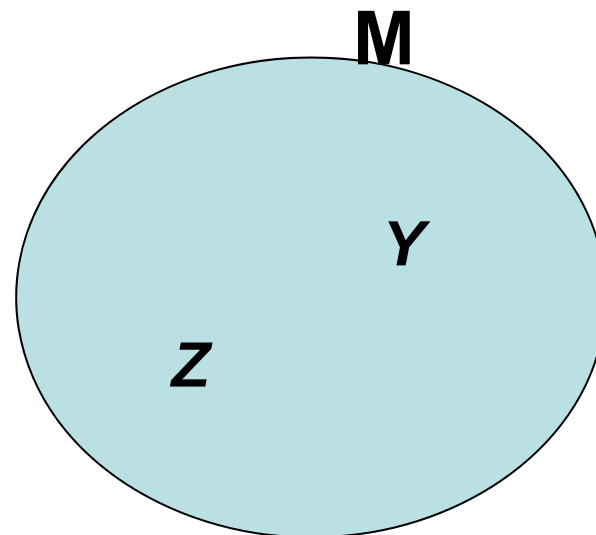
# Divergence: $D[z : y]$

$$D[z : y] \geq 0$$

$$D[z : y] = 0, \quad \text{iff } z = y$$

$$D[z : z + dz] = \sum g_{ij} dz_i dz_j$$

**positive-definite**



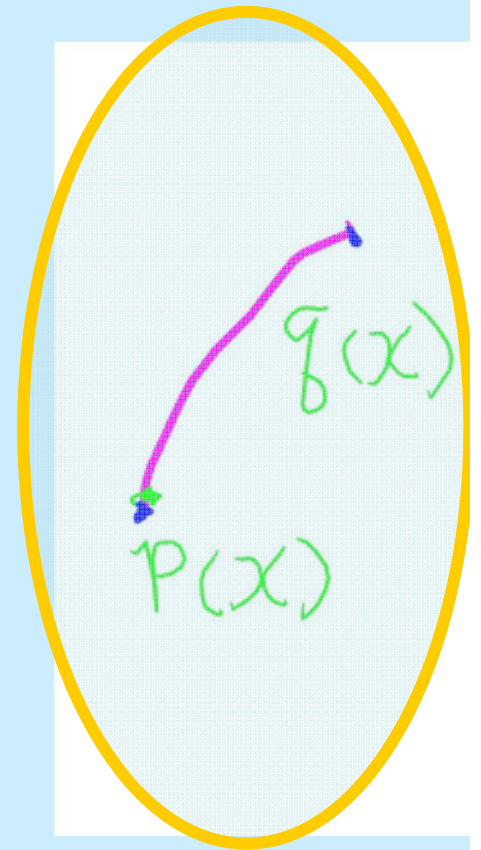
# Kullback-Leibler Divergence

quasi-distance

$$D[p(x) : q(x)] = \sum_x p(x) \log \frac{p(x)}{q(x)}$$

$$D[p(x) : q(x)] \geq 0 \quad = 0 \text{ iff } p(x) = q(x)$$

$$D[p : q] \neq D[q : p]$$



# $f$ divergence of $\tilde{S}$

$$\tilde{S} = \{\tilde{\boldsymbol{p}}\}, \quad \tilde{p}_i > 0 : (\sum \tilde{p}_i = 1 \text{ nn holds})$$

$$D_f[\tilde{\boldsymbol{p}} : \tilde{\boldsymbol{q}}] = \sum \tilde{p}_i f\left(\frac{\tilde{q}_i}{\tilde{p}_i}\right) \geq 0 \quad D_f[\tilde{\boldsymbol{p}} : \tilde{\boldsymbol{q}}] = 0 \Leftrightarrow \tilde{\boldsymbol{p}} = \tilde{\boldsymbol{q}}$$

$$\text{not invariant under } \tilde{f}(u) = f(u) - c(u-1)$$

# $\alpha$ divergence

$$D_{\alpha}[\tilde{p} : \tilde{q}] = \sum \left\{ \frac{1-\alpha}{2} \tilde{p}_i + \frac{1+\alpha}{2} \tilde{q}_i - \tilde{p}_i^{\frac{1-\alpha}{2}} \tilde{q}_i^{\frac{1+\alpha}{2}} \right\}$$

## KL-divergence

$$D[\tilde{p} : \tilde{q}] = \sum \left\{ \tilde{p}_i \log \frac{\tilde{p}_i}{\tilde{q}_i} + \tilde{p}_i - \tilde{q}_i \right\}$$

## $(\alpha, \beta)$ – divergence

$$D_{\alpha, \beta}[p : q] = \sum \left\{ \frac{\alpha}{\alpha + \beta} p_i^{\alpha + \beta} + \frac{\beta}{\alpha + \beta} q_i^{\alpha + \beta} - p_i^\alpha q_i^\beta \right\}$$

$\beta = -\alpha$ :  $\alpha$  – divergence

$\alpha = 1$ :  $\beta$ -divergence

# Metric and Connections Induced by Divergence

## Riemannian metric

(Eguchi)

$$g_{ij}(\mathbf{z}) = \partial_i \partial_j D[\mathbf{z} : \mathbf{y}]|_{\mathbf{y}=\mathbf{z}} : D[\mathbf{z} : \mathbf{z} + d\mathbf{z}] = \frac{1}{2} g_{ij}(\mathbf{z}) dz_i dz_j$$

## affine connections

$\{\nabla, \nabla^*\}$

$$\Gamma_{ijk}(\mathbf{z}) = -\partial_i \partial_j \partial'_k D[\mathbf{z} : \mathbf{y}]|_{\mathbf{y}=\mathbf{z}} \quad \partial_i = \frac{\partial}{\partial z_i}, \quad \partial'_i = \frac{\partial}{\partial y_i}$$

$$\Gamma_{ijk}^*(\mathbf{z}) = -\partial'_i \partial'_j \partial_k D[\mathbf{z} : \mathbf{y}]|_{\mathbf{y}=\mathbf{z}}$$

**Duality:**  $X \langle Y, Z \rangle = \langle \nabla_X Y, Z \rangle + \langle Y, \nabla_X^* Z \rangle$

$$\partial_k g_{ij} = \Gamma_{kij} + \Gamma_{kji}^*$$

$$\Gamma_{ijk} = \Gamma_{ijk}^* - T_{ijk}$$

$$\{M, g, T\}$$

# Dually flat manifold

exponential family; mixture family;  $\{p(x); x \text{ discrete}\}$

$$p(x, \theta) = \exp\left\{\sum \theta_i x_i - \psi(\theta)\right\} : \text{exponential family}$$

$\theta$ -coordinates : affine coordinates, flat, geodesics



$\eta$ -coordinates: (dual) affine coordinates, flat, geodesics

**not Riemannian flat**

canonical divergence  $D(P: P') : KL - \text{divergence}$

# Dually flat manifold

potential functions  $\psi(\theta), \varphi(\eta)$

$$\eta_i = \frac{\partial}{\partial \theta_i} \psi(\theta); \quad \theta_i = \frac{\partial}{\partial \eta_i} \varphi(\eta): \quad \text{Legendre transformation}$$

$$\psi(\theta) + \varphi(\eta) - \sum \theta_i \eta_i = 0$$

$$g_{ij}(\theta) = \frac{\partial^2}{\partial \theta_i \partial \theta_j} \psi(\theta) \cdots g^{ij} = \frac{\partial^2}{\partial \eta_i \partial \eta_j} \varphi(\eta)$$

$$p(x, \theta) = \exp \left\{ \sum \theta_i x_i - \psi(\theta) \right\} : \text{exponential family}$$

$\psi$  : cumulant generating function

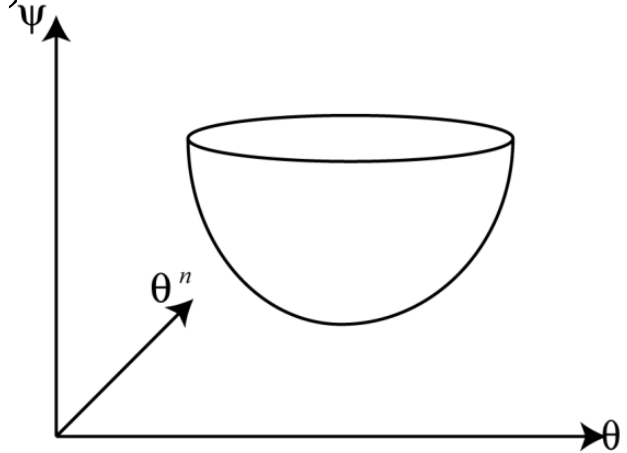
$\varphi$  : negative entropy

$$\text{canonical divergence } D(P: P') = \psi(\theta) + \varphi(\eta') - \sum \theta_i \eta_i'$$

# Manifold with Convex Function

$S$  : coordinates  $\theta = (\theta^1, \theta^2, \dots, \theta^n)$

$\psi(\theta)$  : convex function



$$\psi(\theta) = \frac{1}{2} \sum (\theta^i)^2$$

**negative entropy**

$$\varphi(p) = \int p(x) \log p(x) dx$$

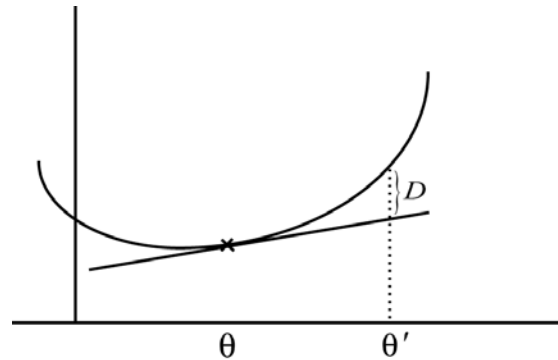
# Riemannian metric and flatness

(affine structure)

$\{S, \psi(\theta), \theta\}$

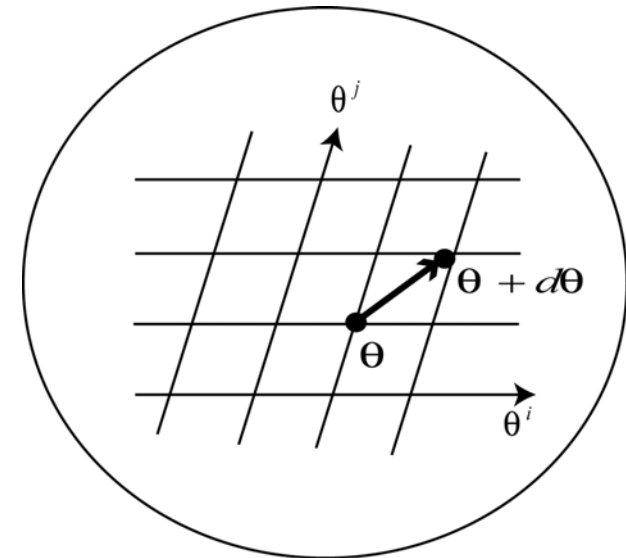
Bregman divergence

$$D(\theta, \theta') = \psi(\theta') - (\theta' - \theta) \cdot \text{grad } \psi(\theta)$$



$$D(\theta, \theta + d\theta) = \frac{1}{2} \sum g_{ij}(\theta) d\theta^i d\theta^j$$

$$g_{ij} = \partial_i \partial_j \psi(\theta), \quad \partial_i = \frac{\partial}{\partial \theta^i}$$



Flatness (affine)  $\theta$  : **geodesic** (not Levi-Civita)

# Legendre Transformation

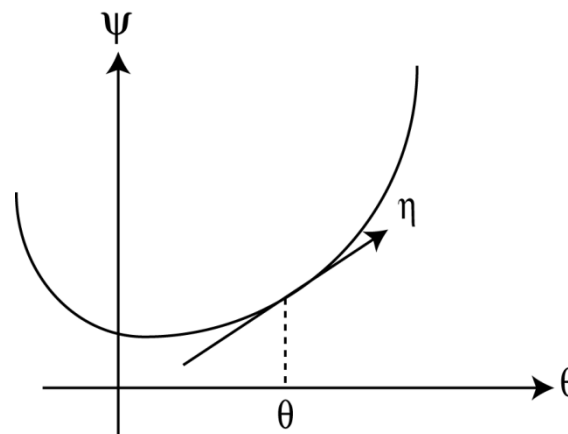
$$\eta_i = \partial_i \psi(\theta)$$

$$\theta \leftrightarrow \eta \quad \text{one-to-one}$$

$$\varphi(\eta) + \psi(\theta) - \theta_i \eta^i = 0$$

$$\theta^i = \partial^i \varphi(\eta), \quad \partial^i = \frac{\partial}{\partial \eta_i}$$

$$D(\theta, \theta') = \psi(\theta) + \varphi(\eta') - \theta \cdot \eta'$$



$$\varphi(\eta) = \max_{\theta} \{ \theta^i \eta_i - \psi(\theta) \}$$

# Two affine coordinate systems $(\theta, \eta)$

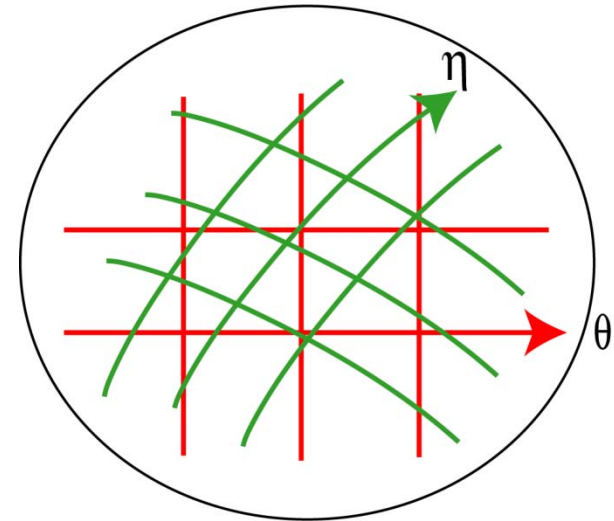
$\theta$  : geodesic (e-geodesic)

$\eta$  : dual geodesic (m-geodesic)

“dually orthogonal”

$$\langle \partial_i, \partial^j \rangle = \delta_i^j$$

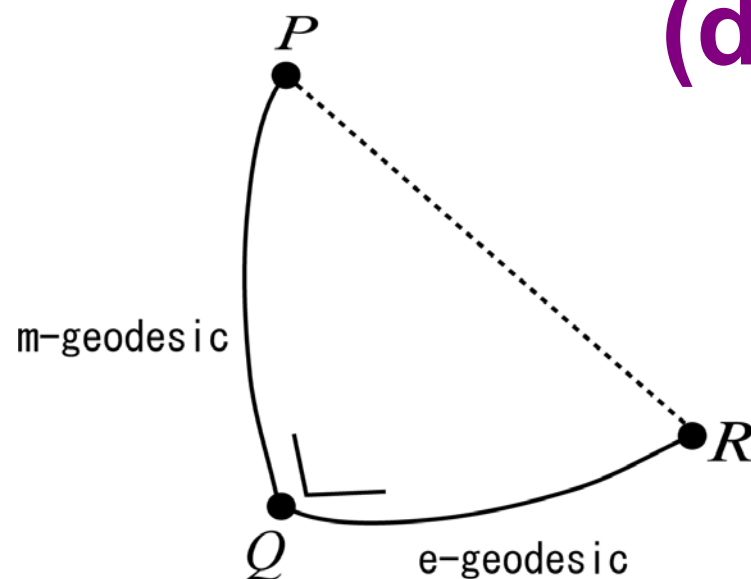
$$\partial_i = \frac{\partial}{\partial \theta^i}, \quad \partial^i = \frac{\partial}{\partial \eta_i}$$



$$X \langle Y, Z \rangle = \langle \nabla_X Y, Z \rangle + \langle Y, \nabla_X^* Z \rangle$$

# Pythagorean Theorem

(dually flat manifold)



$$D[P:Q] + D[Q:R] = D[P:R]$$

**Euclidean space: self-dual**

$$\theta = \eta$$

$$\psi(\theta) = \frac{1}{2} \sum (\theta_i)^2$$

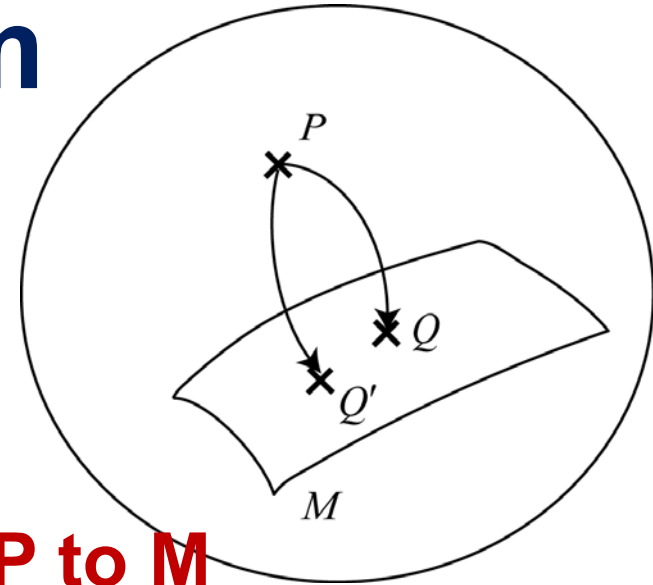
# Projection Theorem

$$\min_{Q \in M} D[P : Q]$$

**Q = m-geodesic projection of P to M**

$$\min_{Q \in M} D[Q : P]$$

**Q' = e-geodesic projection of P to M**



# Two Types of Divergence

**Invariant divergence** (Chentsov, Csiszar)

**f-divergence: Fisher- $\alpha$  structure**

$$D[p : q] = \int p(x) f\left\{\frac{q(x)}{p(x)}\right\} dx$$

**Flat divergence** (Bregman) – convex function

**KL-divergence belongs to**

**both classes: flat and invariant**

# divergence

$S = \{p\}$  : space of probability distributions

**invariance**

**dually flat space**

**invariant divergence**

**Flat divergence**

**F-divergence**  
**Fisher inf metric**  
**Alpha connection**

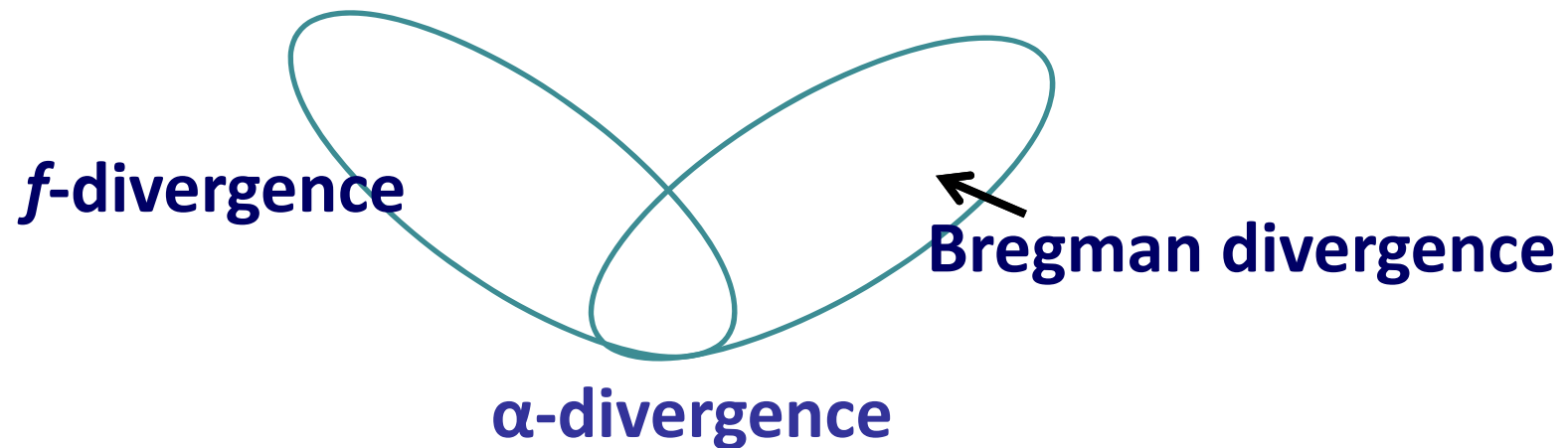
**KL-divergence**

**convex functions**  
**Bregman**

$$D[p : q] = \int p(x) \log \left\{ \frac{p(x)}{q(x)} \right\} dx$$

# Space of positive measures : vectors, matrices, arrays

$$\tilde{S} = \{\tilde{\boldsymbol{p}}\}, \quad \tilde{p}_i > 0 : (\sum \tilde{p}_i = 1 \text{ holds})$$



# Applications of Information Geometry

Statistical Inference

Machine Learning and AI

Computer Vision

Convex Programming

Signal Processing (ICA; Sparse)

Information Theory, Systems Theory

Quantum Information Geometry

# Applications to Statistics

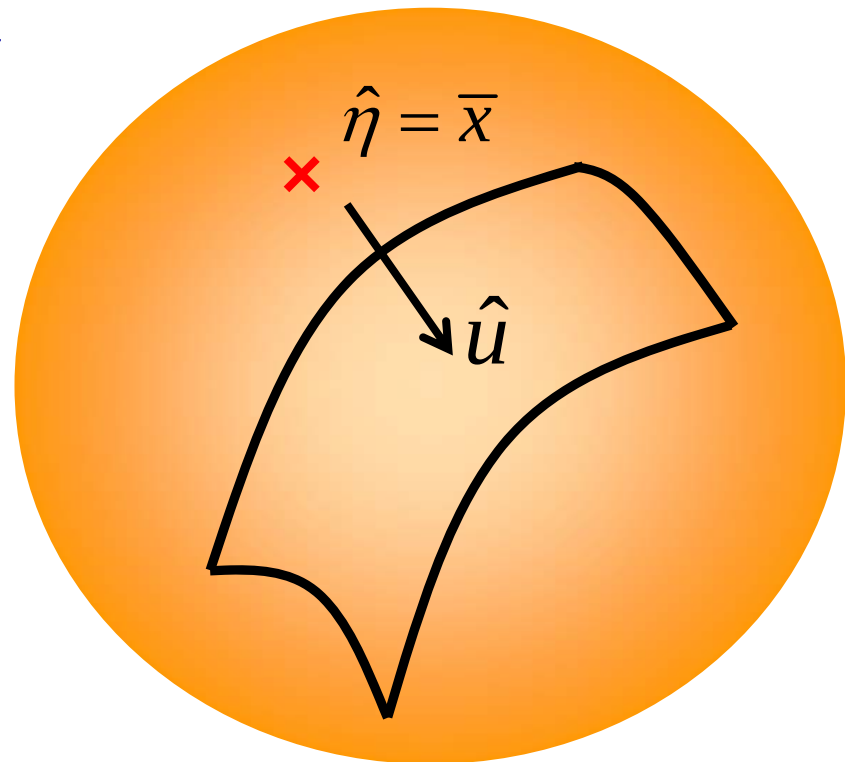
curved exponential family:

$$p(x, u) \propto x_1, x_2, \dots, x_n \quad p(x, \theta) = \exp\{\theta \cdot x - \psi(\theta)\}$$

$$p(x, u) = \exp\{\theta(u) \cdot x - \psi(\theta(u))\}$$

$\hat{u}(x_1, \dots, x_n)$  : estimator

$$\bar{x} = \frac{1}{n} \sum_{k=1}^n x_k$$



**x : discrete     $X = \{0, 1, \dots, n\}$**

**$S_n = \{p(x) \mid x \in X\}$  : exponential family**

$$p(x) = \sum_{i=0}^n p_i \delta_i(x) = \exp\left[\sum_{i=1}^n \theta^i x_i - \psi(\theta)\right]$$

$$\theta^i = \log p_i - \log p_0; \quad x_i = \delta_i(x); \quad \psi(\theta) = -\log p_0$$

**statistical model :  $p(x, u)$**

# High-Order Asymptotics

$$p(x, \theta(u)) \quad : x_1, \dots, x_n$$

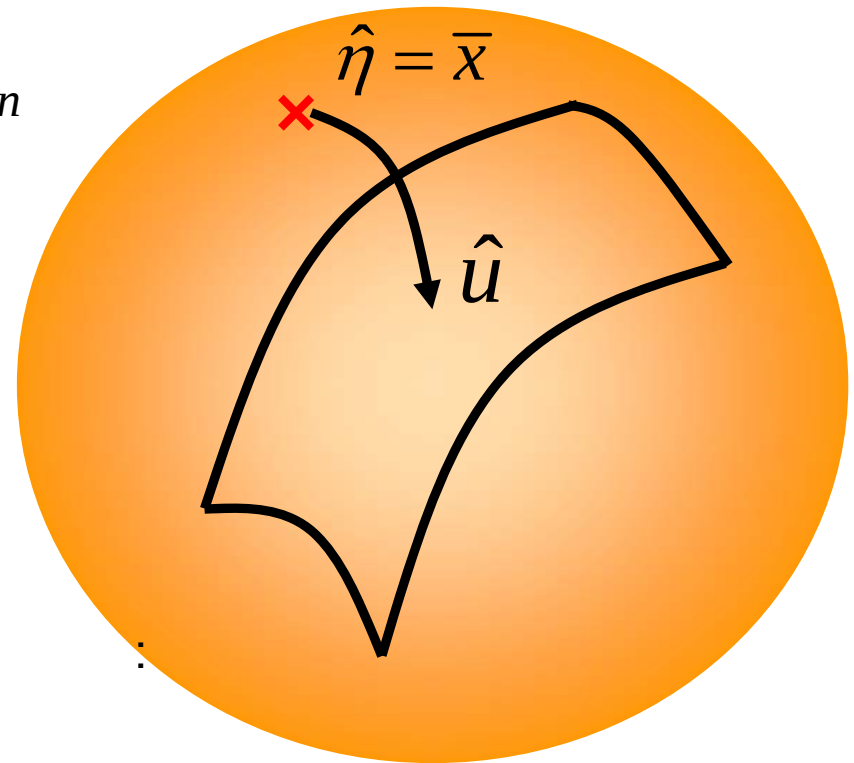
$$\hat{u} = u(x_1, \dots, x_n)$$

$$e = E[(\hat{u} - u)(\hat{u} - u)^T]$$

$$e = \frac{1}{n} G_1 + \frac{1}{n^2} G_2$$

$$G_1 \geq G^{-1} \quad : \text{Cramér-Rao: linear theory}$$

$$G_2 = H_M^{(e)^2} + H_A^{(m)^2} + \Gamma^{(m)^2} \quad \text{quadratic approximation}$$



# Information Geometry of Belief Propagation

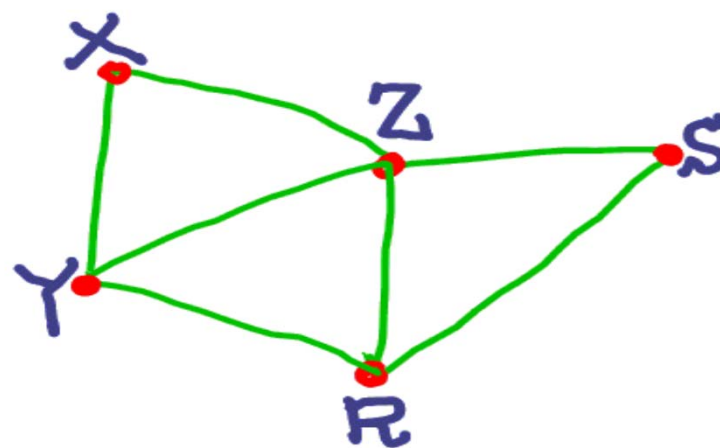
- Shun-ichi Amari (RIKEN BSI)
- Shiro Ikeda (Inst. Statist. Math.)
- Toshiyuki Tanaka (Kyoto U.)

# Stochastic Reasoning

$$p(x, y, z, r, s)$$

$$p(x, y, z | r, s)$$

$$x, y, z, \dots = 1, -1$$



# Stochastic Reasoning

$q(x_1, x_2, x_3, \dots | \text{observation})$

$\mathbf{X} = (x_1 \ x_2 \ x_3 \ \dots)$      $x = 1, -1$

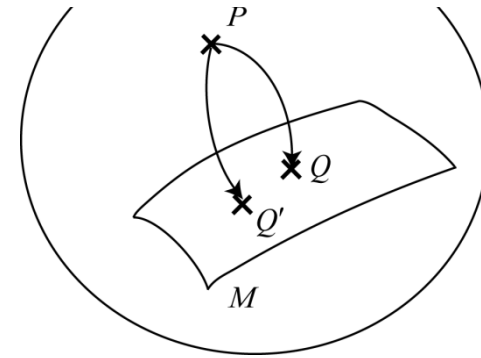
$\mathbf{X} = \text{argmax } q(x_1, x_2, x_3, \dots)$     maximum likelihood

$X_i = \text{sgn } E[x_i]$     least bit error rate estimator

# Mean Value

Marginalization:

projection to independent distributions



$$\Pi_0 q(\mathbf{x}) = q_1(x_1)q_2(x_2)\dots q_n(x_n) = q_0(\mathbf{x})$$

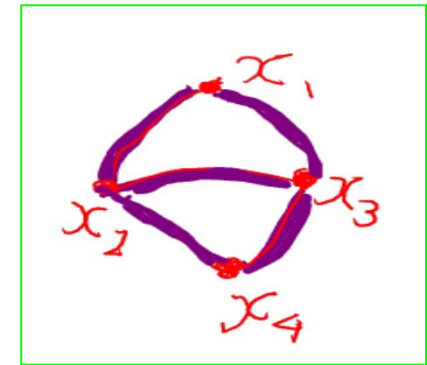
$$q_i(x_i) = \int q(x_1, \dots, x_n) dx_1 \dots d\tilde{x}_i \dots dx_n$$

$$\boldsymbol{\eta} = \mathbf{E}_q[\mathbf{x}] = \mathbf{E}_{q_0}[\mathbf{x}]$$

$$q(\mathbf{x}) = \exp \left\{ \sum k_i \cdot x_i + \sum_{r=1}^L c_r(\mathbf{x}) - \psi_q \right\}$$

$$c_r(\mathbf{x}) = c_r x_{i_1} \cdots x_{i_s}, \quad r = (i_1 \cdots i_s)$$

$$x_i = \{1, -1\} \quad r = (i_1, i_2)$$



Boltzmann machine, spin glass, neural networks  
Turbo Codes, LDPC Codes

# Computationally Difficult

$$q(\mathbf{x}) \rightarrow \eta = E[\mathbf{x}]$$

$$q(\mathbf{x}) = \exp \left\{ \sum c_r(\mathbf{x}) - \psi_q \right\}$$

**mean-field approximation**

**belief propagation**

**tree propagation, CCCP (convex-concave)**

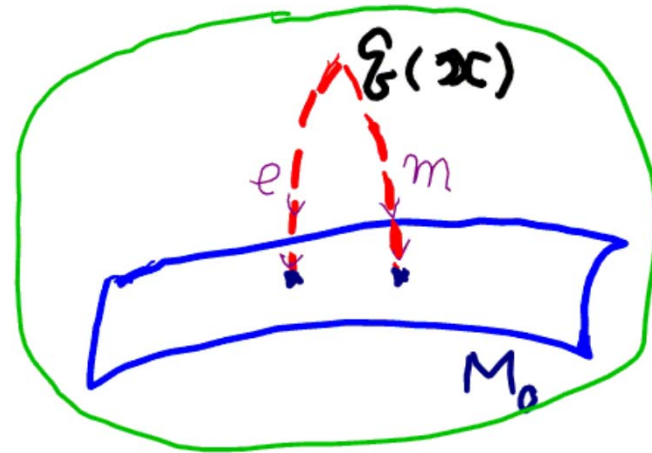
# Information Geometry of Mean Field Approximation

- m-projection
- e-projection

$$D[q:p] = \sum_x q(x) \log \frac{q(x)}{p(x)}$$

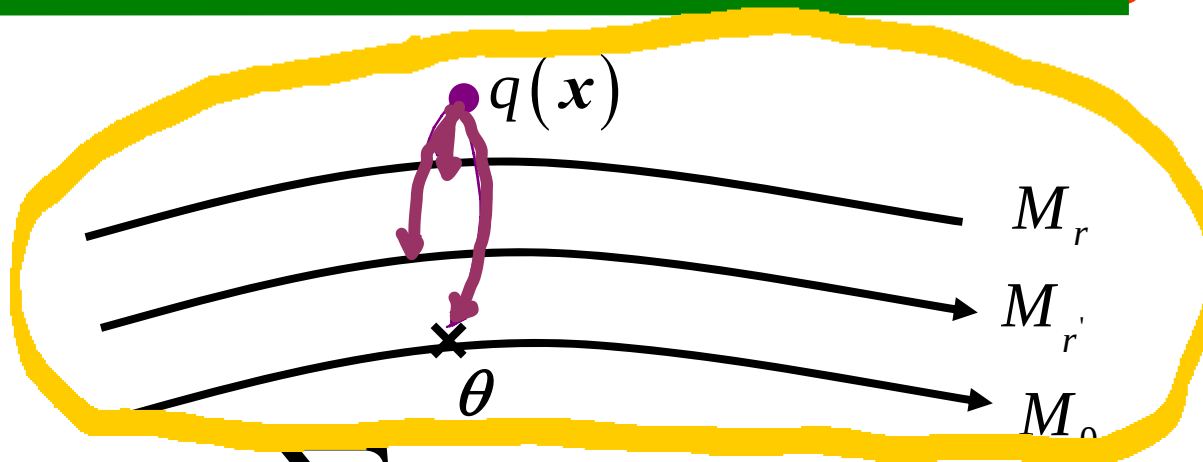
$$\Pi_0^m q = \operatorname{argmin} D[q:p]$$

$$\Pi_0^e q = \operatorname{argmin}_{p(x) \in M_0} D[p:q]$$



$$M_0 = \{\Pi_i p_i(x_i)\}$$

# Information Geometry



$$q(x) = \exp \left\{ \sum c_r(x) - \phi \right\}$$

$$M_0 = \{ p_0(\mathbf{x}, \boldsymbol{\theta}) \} = \exp \{ \boldsymbol{\theta} \cdot \mathbf{x} - \psi_0 \}$$

$$M_r = \left\{ p_r(\mathbf{x}, \boldsymbol{\xi}_r) = \exp \left\{ c_r(\mathbf{x}) + \boldsymbol{\xi}_r \cdot \mathbf{x} - \psi_r \right\} \right\}_{r=1, \dots, L}$$

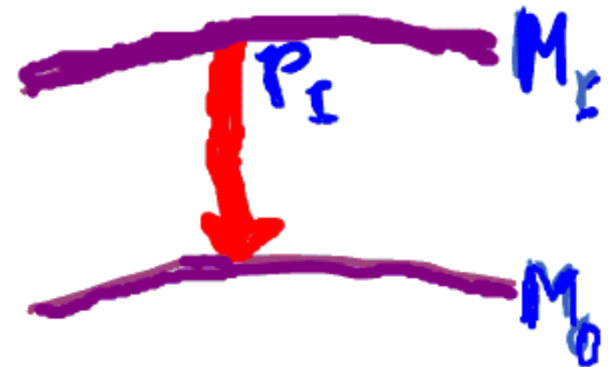
# Belief Propagation

$$M_r : p_r(\mathbf{x}, \xi_r) = \exp\{c_r(\mathbf{x}) + \xi_r \cdot \mathbf{x} - \psi_r\}$$

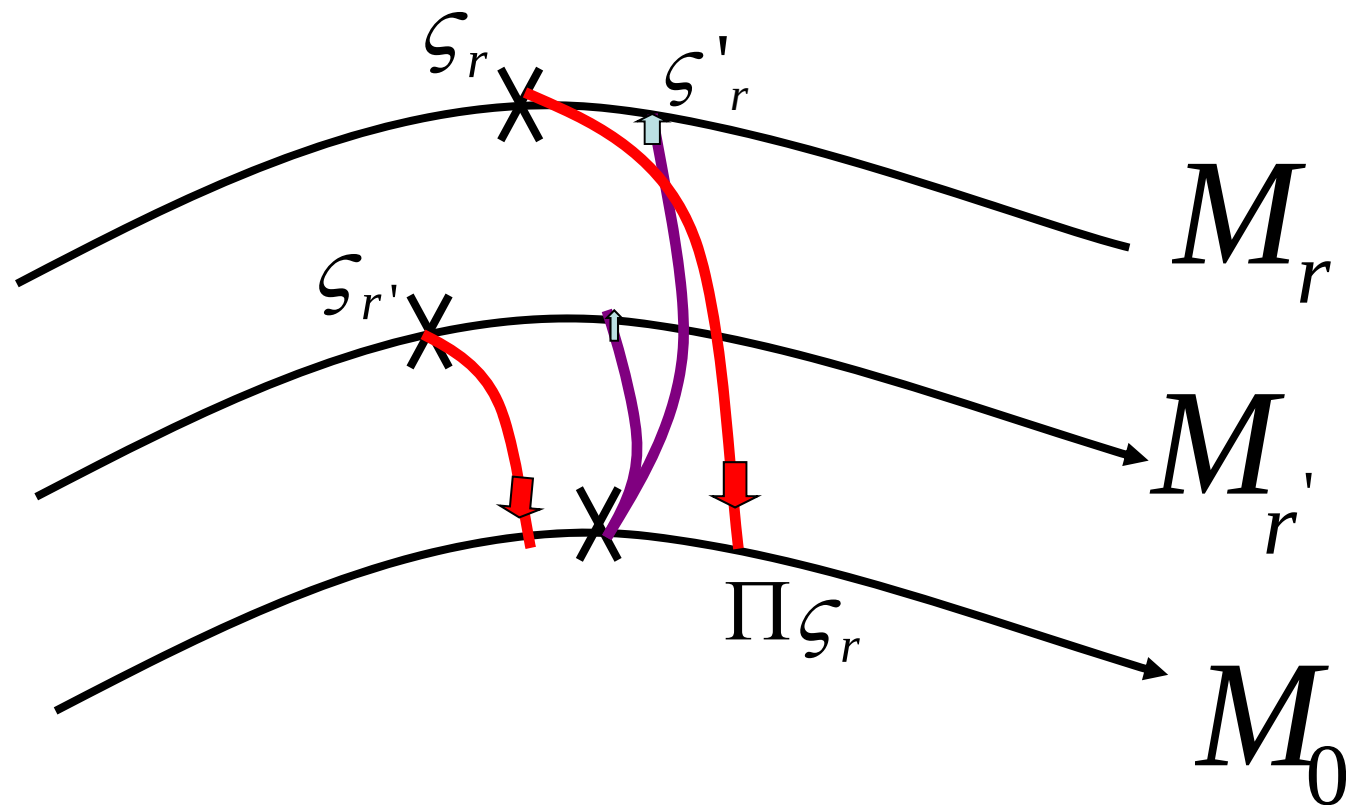
$$\Pi_0 p_r(x, \xi_r^t)$$

$$\theta_r^{t+1} = \Pi_0 p_r(x, \xi_r^t) - \xi_r^t : \text{belief for } c_r(x)$$

$$\theta^{t+1} = \sum \theta_r^{t+1}$$



# Belief Prop Algorithm

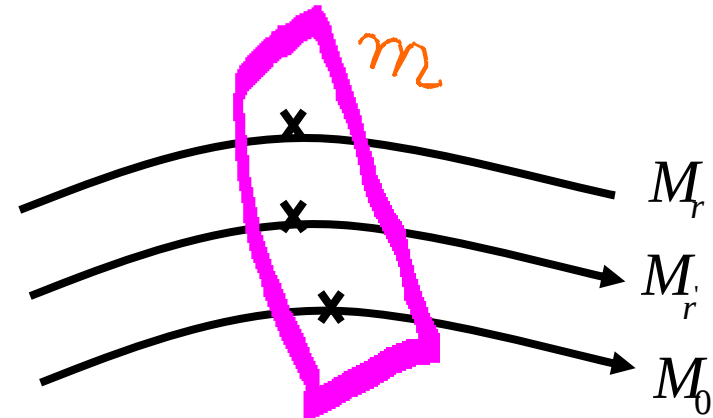


# Equilibrium of BP $(\theta^*, \xi_r^*)$

## 1) $m$ -condition

$$\theta^* = \Pi_0 p_r(x, \xi_r^*)$$

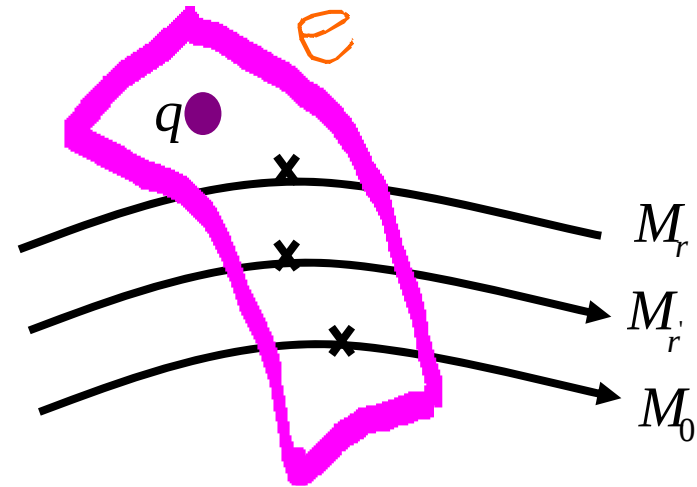
$m$ -flat submanifold  $M(\theta^*)$   
 $\xi_1(\theta^*)$



## 2) $e$ -condition

$$\theta^* = \frac{1}{L-1} \sum_r^* \xi_r^*$$

$q(x) \in e$ -flat submanifold



# Free energy:

$$F(\theta, \zeta_1, \dots, \zeta_L) = D[p_0 : q] - \sum D[p_0 : p_r]$$

*critical point*

$$\frac{\partial F}{\partial \theta} = 0 \quad : e\text{-condition}$$

$$\frac{\partial F}{\partial \zeta_r} = 0 \quad : m\text{-condition}$$

*not convex*

# Belief Propagation

**e-condition OK**

$$(\boldsymbol{\theta}; \xi_1, \xi_2, \dots, \xi_L), \quad \boldsymbol{\theta}' = \frac{1}{L-1} \sum \xi'_r$$

$$(\xi_1, \xi_2, \dots, \xi_L) \rightarrow (\xi'_1, \xi'_2, \dots, \xi'_L)$$

**CCCP**      **m-condition OK**

$$\boldsymbol{\theta} \rightarrow \boldsymbol{\theta}'$$

$$\xi_1(\boldsymbol{\theta}'), \xi_1(\boldsymbol{\theta}'), \dots, \xi_1(\boldsymbol{\theta}')$$

$$\boldsymbol{\theta}' = \Pi_0 p_r(\mathbf{x}, \xi'_r) : \quad \xi' = \Pi_r p_0(\mathbf{x}, \boldsymbol{\theta}')$$

$$\xi_r^{t+1} = \Pi_r \boldsymbol{\theta}^{t+1} = \Pi_r p_0 \left( \boldsymbol{x}, \boldsymbol{\theta}^{t+1} \right)$$

$$\boldsymbol{\theta}^{t+1} = L \boldsymbol{\theta}^t - \sum \xi_r^{t+1}$$

# Convex-Concave Computational Procedure (CCCP) Yuille

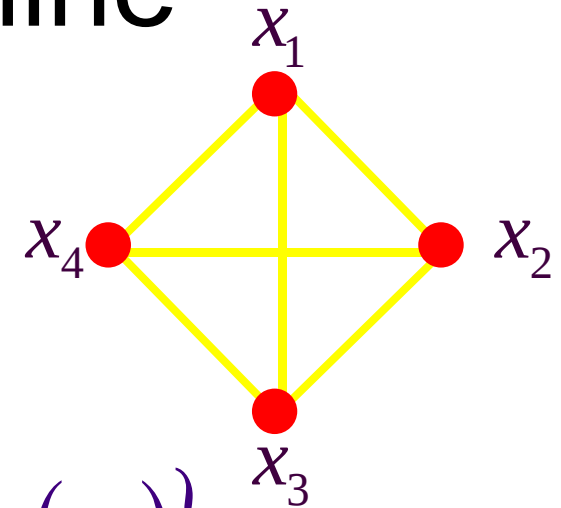
$$F(\theta) = F_1(\theta) - F_2(\theta)$$

$$\nabla F_1(\theta^{t+1}) = \nabla F_2(\theta^t)$$

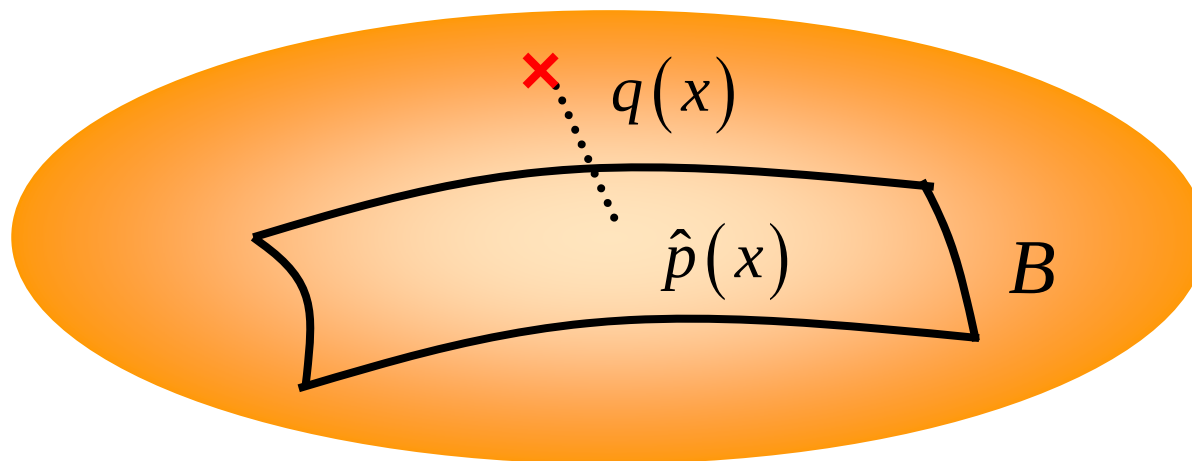
Elimination of double loops

# Boltzmann Machine

$$p(x_i = 1) = \varphi\left(\sum w_{ij}x_j - h_i\right)$$



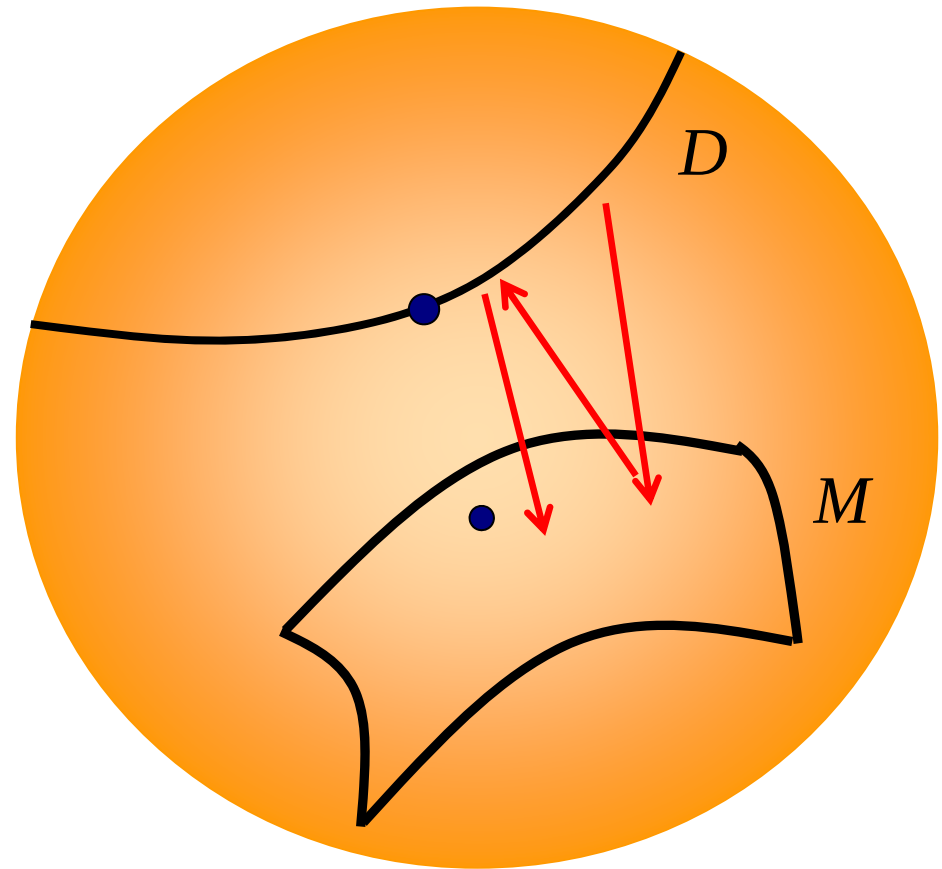
$$p(x) = \exp\left\{\sum w_{ij}x_ix_j - \sum h_ix_i - \psi(w)\right\}$$



# Boltzmann machine

---hidden units

- EM algorithm
- e-projection
- m-projection



# EM algorithm

hidden variables

$$p(\mathbf{x}, \mathbf{y}; \mathbf{u})$$

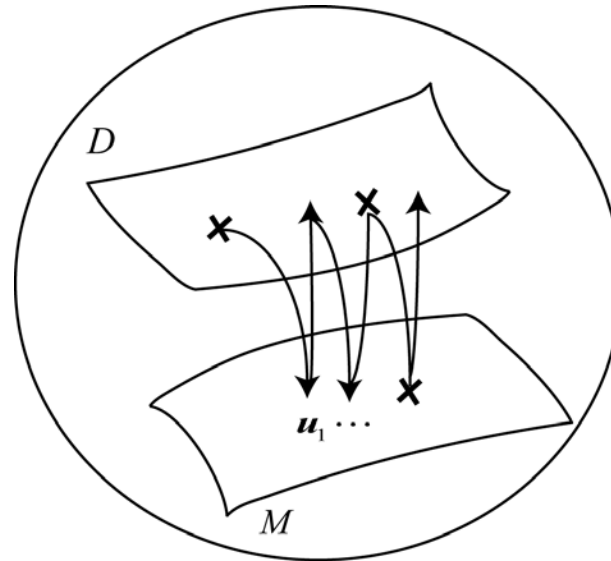
$$D = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$$

$$M = \{p(\mathbf{x}, \mathbf{y}; \mathbf{u})\}$$

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

$$\min KL[\hat{p}(\mathbf{x}, \mathbf{y}) : p \in M] \quad \text{m-projection to} \quad M$$

$$\min KL[p \in D : p(\mathbf{x}, \mathbf{y}; \hat{\mathbf{u}})] \quad \text{e-projection to} \quad D$$



# SVM : support vector machine

**Embedding**  $z_i = \phi_i(x)$   
 $f(x) = \sum w_i \phi_i(x) = \sum \alpha_i y_i K(x_i, x)$

**Kernel**  $K(x, x') = \sum \phi_i(x) \phi_i(x')$

## Conformal change of kernel

$$K(x, x') \longrightarrow \rho(x) \rho(x') K(x, x')$$

$$\rho(x) = \exp\{-\kappa |f(x)|^2\}$$

# Signal Processing

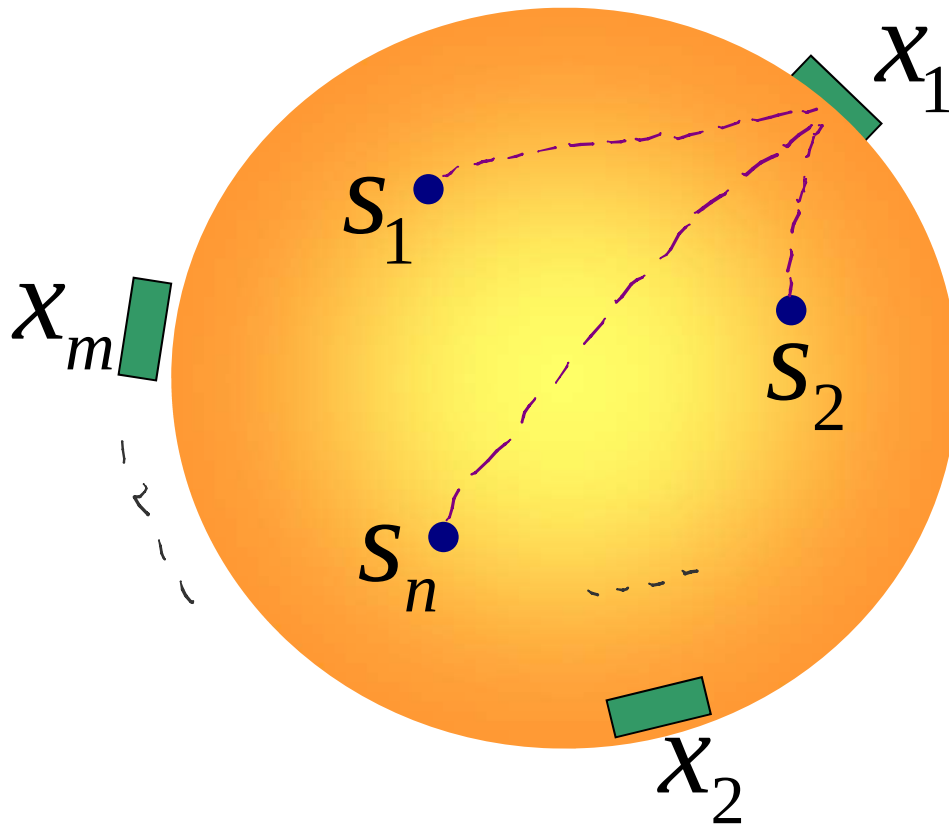
**ICA : Independent Component Analysis**

$$\mathbf{x}_t = A\mathbf{s}_t \qquad \mathbf{x}_t \rightarrow \mathbf{s}_t$$

**sparse component analysis**

**positive matrix factorization**

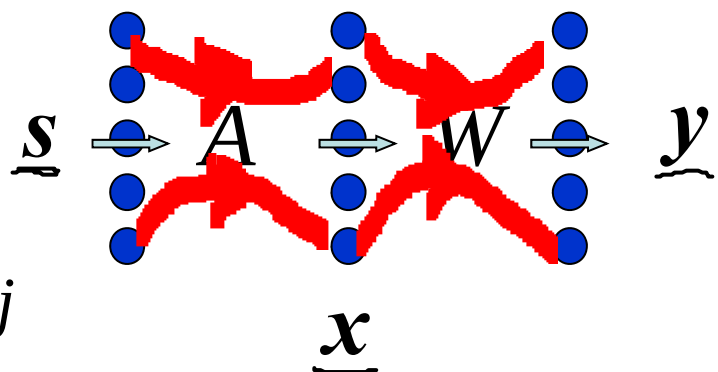
# mixture and unmixture of independent signals



$$x_i = \sum_{j=1}^n A_{ij} s_j$$

$$\mathbf{x} = \mathbf{A}\mathbf{s}$$

# Independent Component Analysis

$$\mathbf{x} = \mathbf{A}\mathbf{s} \quad x_i = \sum A_{ij} s_j$$


$$\mathbf{y} = \mathbf{W}\mathbf{x} \quad \mathbf{W} = \mathbf{A}^{-1}$$

observations:  $\mathbf{x}(1), \mathbf{x}(2), \dots, \mathbf{x}(t)$

recover:  $\mathbf{s}(1), \mathbf{s}(2), \dots, \mathbf{s}(t)$

**Example of color image separation :**

Five original images (but unknown to the neural net)

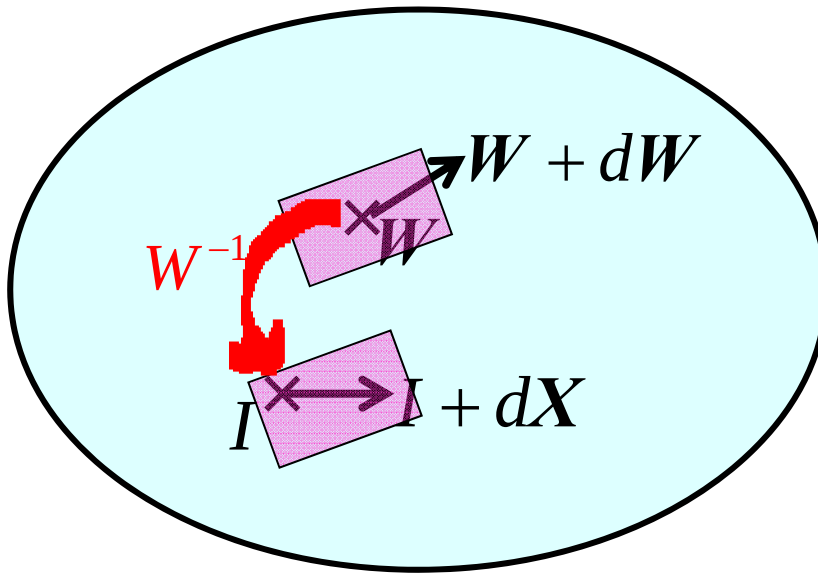


Five mixed images for separation



Final (stable states) of five separated images

# Space of Matrices : Lie group



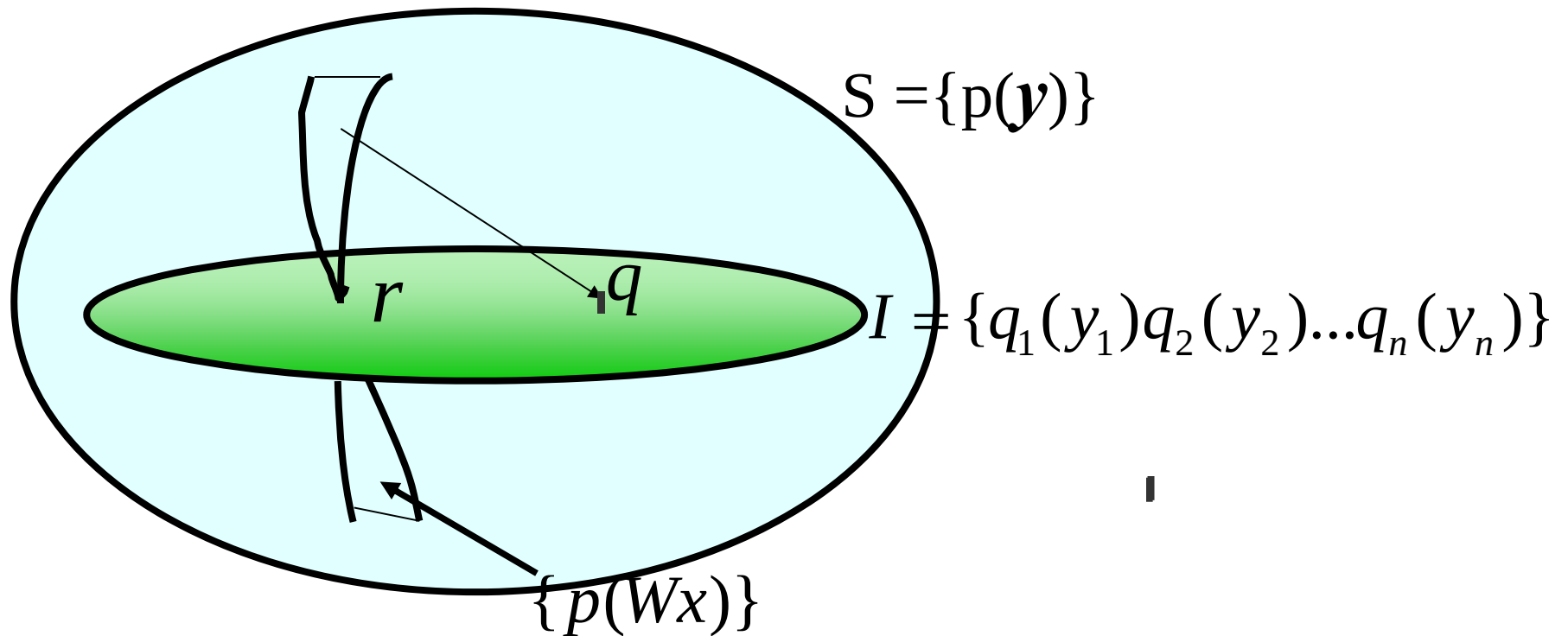
$$dX = dW W^{-1}$$

$$|dW|^2 = \text{tr}(dX dX^T) = \text{tr}(dW W^{-1} W^{-T} dW^T)$$

$$\nabla l = \frac{\partial l}{\partial W} W^T W$$

$dX$  : non-holonomic basis

# Information Geometry of ICA



**natural gradient**  
**estimating function**  
**stability, efficiency**

$$l(\mathbf{W}) = KL[p(\mathbf{y}; \mathbf{W}) : q(\mathbf{y})]$$

$r(\mathbf{y})$

# Semiparametric Statistical Model

$$p(\mathbf{x}; \mathbf{W}, r) = |\mathbf{W}| r(\mathbf{W}\mathbf{x})$$

$$\mathbf{W} = \mathbf{A}^{-1}, \quad r(s): \text{ unknown} \quad r = \prod r_i$$

$$x(1), x(2), \dots, x(t)$$

# Natural Gradient

$$\Delta W = -\eta \frac{\partial l(y, W)}{\partial W} W^T W$$

# Basis Given: overcomplete case

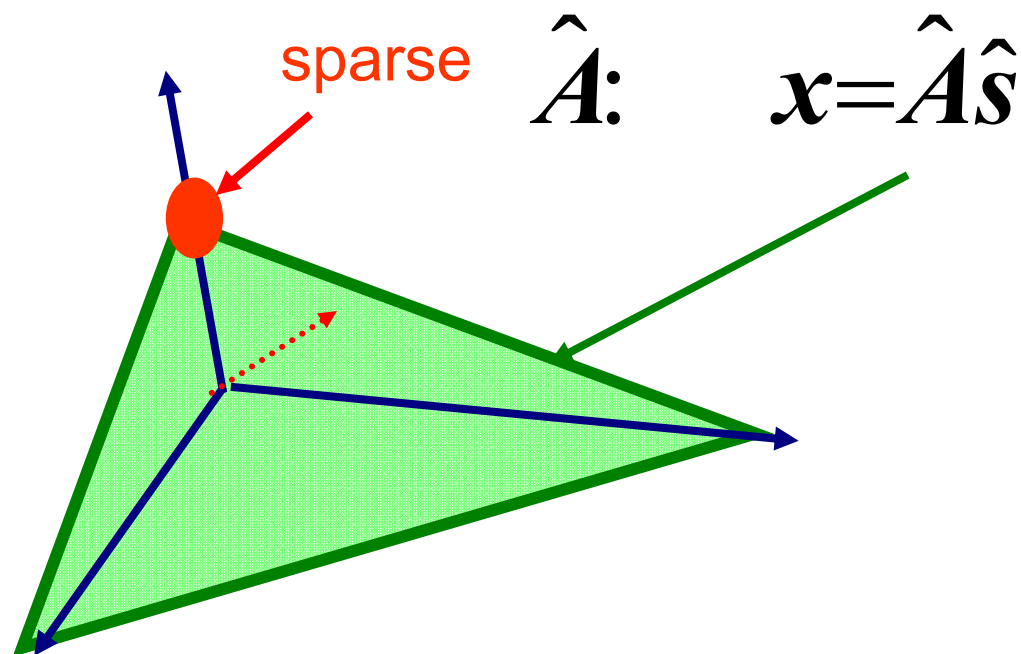
## Sparse Solution

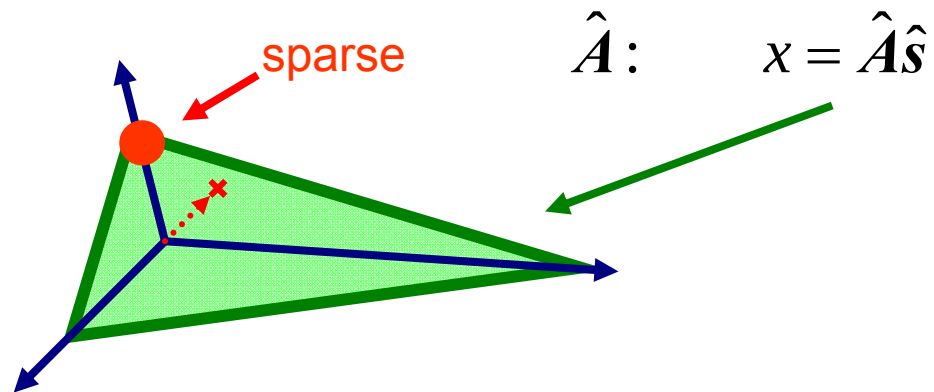
$$\mathbf{x} = \mathbf{A}\mathbf{s} = \sum s_i \mathbf{a}_i$$

many solutions

many  $s_i \rightarrow 0$

$$\mathbf{x}_t = \hat{\mathbf{A}}\mathbf{s}_t$$



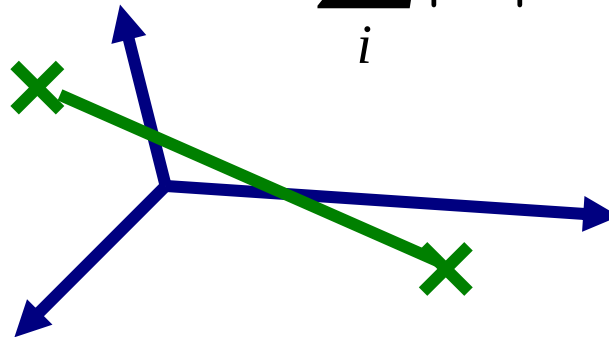


generalized inverse

$L_2$ -norm:  $\min \sum |\hat{s}_i|^2$

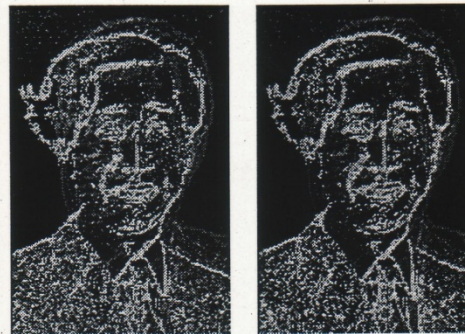
sparse solution

$L_1$ -norm:  $\min \sum |\hat{s}_i|$





(a) Three binary edge images (reverse images are used in the experiment)



(b) Two edge image mixtures



(c) Reconstructed binary edge images (after reversion)

**Fig. 5:** Example of edge image image reconstruction: (a) the three binary edge images (reverse image copies are supplied for processing) , (b) their two mixtures, (c) the three extracted edge images (after reversion).

# Overcomplete Basis and Sparse Solution

$$\mathbf{x} = \sum s_i \mathbf{a}_i = A\mathbf{s}$$

$$\min \|\mathbf{s}\|_1 = \sum |s_i|$$

$$\min \|\mathbf{A}\mathbf{s} - \mathbf{x}\|_p + \alpha \|\mathbf{s}\|_p,$$

non-linear denoising

# Sparse Solution

$$\min \varphi(\beta)$$

$$\text{penalty } F_p(\beta) = \sum |\beta_i|^p \quad : \text{ Bayes prior}$$

$$F_0(\beta) = \#1[\beta_i \neq 0] : \text{ sparsest solution}$$

$$F_1(\beta) = \sum |\beta_i| : L_1 \text{ solution}$$

$$F_p(\beta) : 0 \leq p \leq 1 \quad \text{Sparse solution: overcomplete case}$$

$$F_2(\beta) = \sum |\beta_i|^2 : \text{ generalized inverse solution}$$

# Optimization under Sparsity Condition

$$\begin{cases} \min \varphi(\boldsymbol{\beta}) & : \text{convex function} \\ \text{constraint} & F(\boldsymbol{\beta}) \leq c \end{cases}$$

**typical case:**

$$\varphi(\boldsymbol{\beta}) = \frac{1}{2} \|\mathbf{y} - X\boldsymbol{\beta}\|^2 = \frac{1}{2} (\boldsymbol{\beta} - \boldsymbol{\beta}^*)^T G (\boldsymbol{\beta} - \boldsymbol{\beta}^*)$$
$$F(\boldsymbol{\beta}) = \frac{1}{p} \sum |\beta_i|^p \quad ; \quad p = 2, \quad p = 1, \quad p = 1/2$$

# L1-constrained optimization

$P_c$  Problem  $\min \varphi(\beta) \quad \text{under } F(\beta) \leq c$  **LASSO**  
solution  $\beta^*(c) : c = 0 \rightarrow \infty$   
 $\beta_c^* = 0 \rightarrow \beta^*$

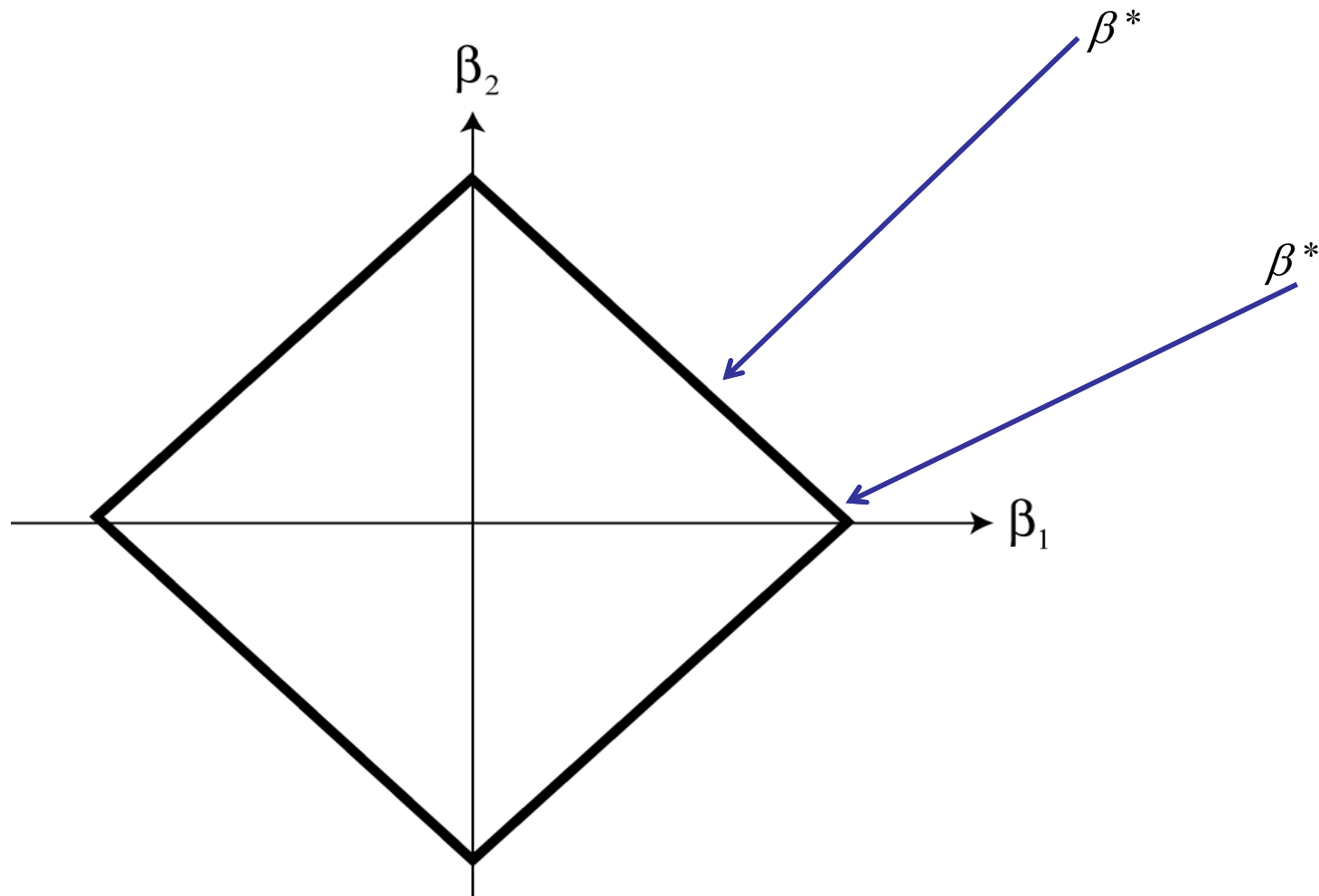
$P_\lambda$  Problem  $\min \varphi(\beta) + \lambda F(\beta)$  **LARS**  
solution  $\beta^*(\lambda) \quad \lambda = \infty \rightarrow 0$   
 $\beta_\lambda^* = 0 \rightarrow \beta^*$

solutions  $\beta_c^*$  and  $\beta_\lambda^*$  : coincide,  $\lambda = \lambda(c)$ ,  $p \geq 1$

$p < 1$  :  $\lambda = \lambda(c)$  multiple, noncontinuous

stability different

**Projection from  $\beta^*$  to  $F = c$  (information geometry)**



# Convex Cone Programming

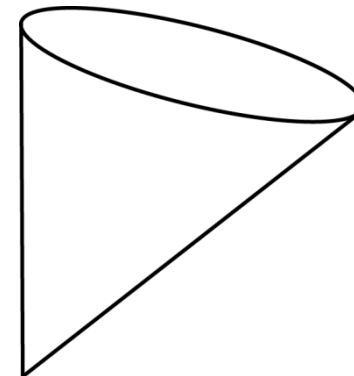
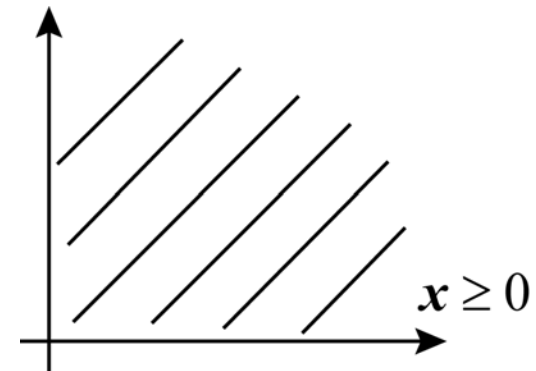
$P$  : positive semi-definite matrix

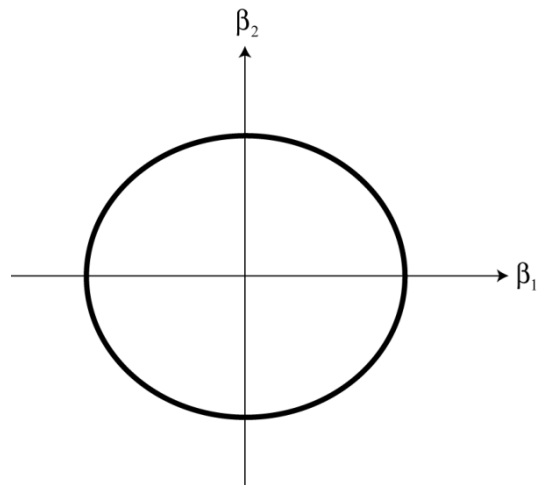
convex potential function

dual geodesic approach

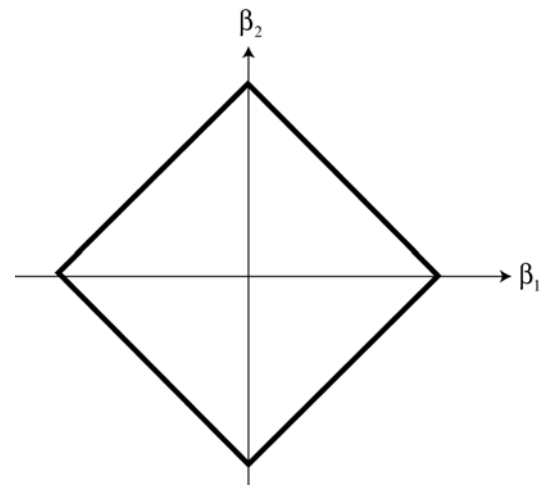
$$A\mathbf{x} = \mathbf{b}, \quad \min \mathbf{c} \cdot \mathbf{x}$$

Support vector machine

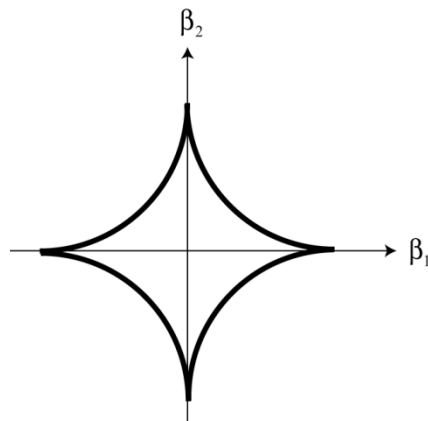




a)  $R_c : n = 2, p > 1$



b)  $R_c : n = 2, p = 1$



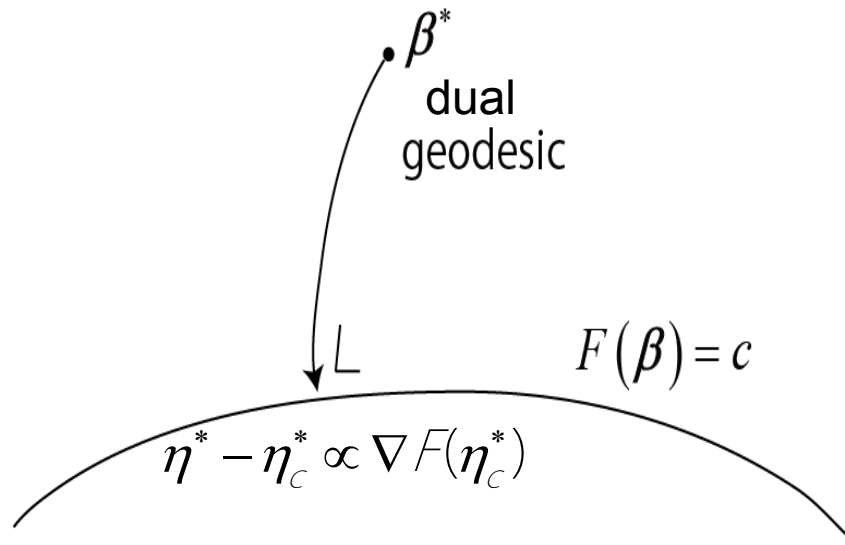
c)  $R_c : n = 2, p < 1$

**non-convex**

Fig. 1

orthogonal projection, dual projection

$\min \varphi(\beta) = \mathbf{D}[\beta : \beta^*], \quad F(\beta) = c : \text{dual geodesic projection}$



$$\eta_c^* \propto \nabla F(\eta_c^*)$$

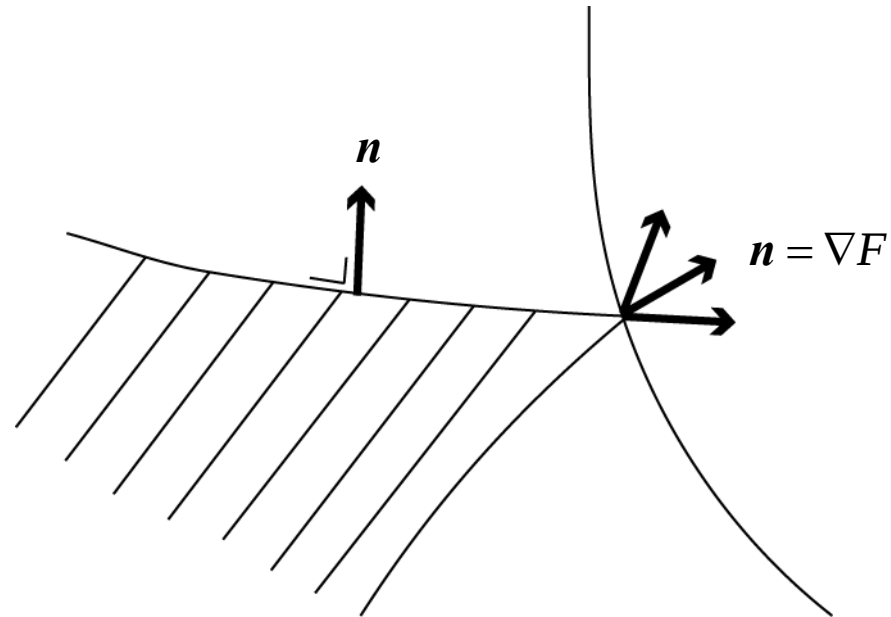


Fig. 5 subgradient

# LASSO path and LARS path (stagewise solution)

$$\min \varphi(\beta) \quad : \quad F(\beta) = c$$

$$\min \varphi(\beta) + \lambda F(\beta)$$

$$\beta^*(c), \beta^*(\lambda) \quad \quad \mathbf{c} \Leftrightarrow \lambda \text{ correspondence}$$

# Active set and gradient

$$A(\boldsymbol{\beta}) = \{i \mid \beta_i \neq 0\}$$

$$\nabla F_p(\boldsymbol{\beta}) = \begin{cases} \operatorname{sgn}(\beta_i) |\beta_i|^{-(1-p)}, & i \in A \\ (-\infty, \infty), & i \notin A \\ [-1, 1] \end{cases}$$

# Solution path

$$\nabla_A \varphi(\beta_c^*) + \lambda_c \nabla_A F(\beta_c^*) = 0, \quad \beta_c^*$$

$$\left\{ \nabla_A \nabla_A \varphi(\beta_c^*) + \lambda_c \nabla_A \nabla_A F(\beta_c^*) \right\} \cdot \dot{\beta}_c = -\dot{\lambda}_c \nabla_A F(\beta_c)$$

$$\dot{\beta}_c = -\dot{\lambda}_c K^{-1} \nabla_A F(\beta_c^*) \quad ; \quad \dot{\beta}_c = \frac{d}{dc} \beta_c$$

$$K = G(\beta_c^*) + \lambda_c \nabla \nabla F(\beta_c^*)$$

$$(\nabla \nabla F_1 = 0; \quad \nabla F_1 = (\text{sgn } \beta_i) : L_1)$$

# **Solution path in the subspace of the active set**

$$\nabla_A \varphi(\beta_\lambda^*) + \lambda \nabla_A F(\beta_\lambda^*) = 0 \quad \nabla_A : \text{active direction}$$

$$\dot{\beta}_\lambda^* = -K_A^{-1} \nabla_A F(\beta_\lambda^*)$$

**turning point     $\mathbf{A} \rightarrow \mathbf{A}'$**

# Gradient Descent Method

$$\min L(x+a): \quad g_{ij}a^i a^j = \varepsilon^2$$

$$\nabla L = \left\{ \frac{\partial}{\partial x_i} L(x) \right\}: \quad \text{covariant}$$

$$\tilde{\nabla} L = \left\{ \sum g^{ji} \frac{\partial}{\partial x_i} L(x) \right\}: \quad \text{contravariant}$$

$$x_{t+1} = x_t - c \nabla L(x_t)$$

# Extended LARS ( $p = 1$ ) and Minkovskian grad

$$\text{norm } \|\mathbf{a}\|_p = \sum |a_i|^p$$

$$\max \psi(\boldsymbol{\beta} + \varepsilon \mathbf{a}) \quad \text{under } \|\mathbf{a}\|_p = 1$$

$$\psi(\boldsymbol{\beta} + \varepsilon \mathbf{a}) - \lambda \|\mathbf{a}\|_p$$

$$p = 1^+$$

$$\nabla_1 \psi(\boldsymbol{\beta}) = \mathbf{1}_A \begin{cases} \text{sgn } \eta_i, & |\eta_i| = \max \{|\eta_1|, \dots, |\eta_N|\} \\ 0, & \text{otherwise} \end{cases}$$

$$\boldsymbol{\eta} = \nabla \psi(\boldsymbol{\beta})$$

$$i^* = \arg \max |f_i|$$

$$\max |f_i| = |f_{i^*}| = |f_{j^*}|$$

$$(\tilde{\nabla} F)_i = \begin{cases} 1, & \text{for } i = i^* \text{ and } j^*, \\ 0 & \text{otherwise.} \end{cases}$$

$$\beta_{t+1} = \beta_t - \eta \tilde{\nabla} F$$

**LARS**

$$\tilde{\nabla} F = \nabla f \quad \text{Euclidean case}$$

$$\tilde{\nabla} F = c \left( \operatorname{sgn} f_i \right) \left| f_i \right|^{\frac{1}{p-1}}$$

$$\tilde{\nabla} F = c \left( \operatorname{sgn} f_{i^*} \right) \begin{bmatrix} 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad \alpha \rightarrow 1$$

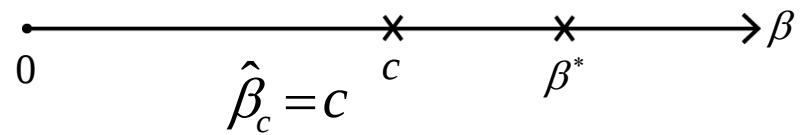
# L1/2 constraint: non-convex optimization

$\lambda$ -trajectory and -trajectory

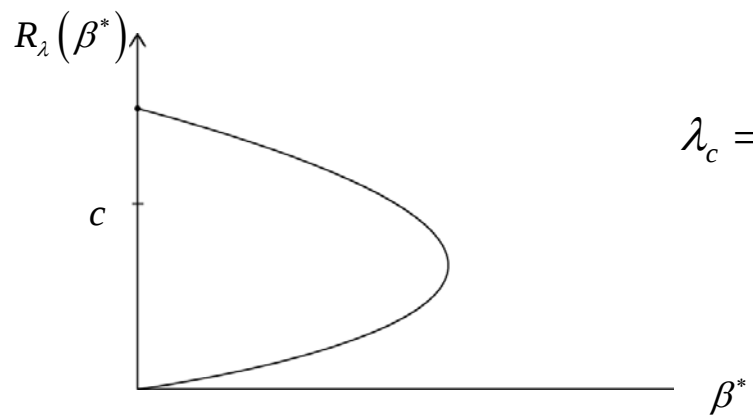
**Ex. 1-dim**  $\varphi(\beta) = \frac{1}{2}(\beta - \beta^*)^2$

$$f_\lambda(\beta) = \phi + \lambda F = \frac{1}{2}(\beta - 2)^2 + 2\lambda\sqrt{\beta}$$

$$P_c : \min (\beta - \beta^*)^2, \quad |\beta| \leq c$$



$$P_\lambda : \nabla f_\lambda = 0 \quad \beta - \beta^* + \frac{\lambda}{\sqrt{\beta}} = 0 \quad \hat{\beta} = R_\lambda(\beta^*) \quad : \text{ Xu Zongben's operator}$$



$\lambda$

**ICCN-Huangshan(黄山)**

# **Sparse Signal Analysis**

**Shun-ichi Ammari (甘利俊一)**

**RIKEN Brain Science Institute**

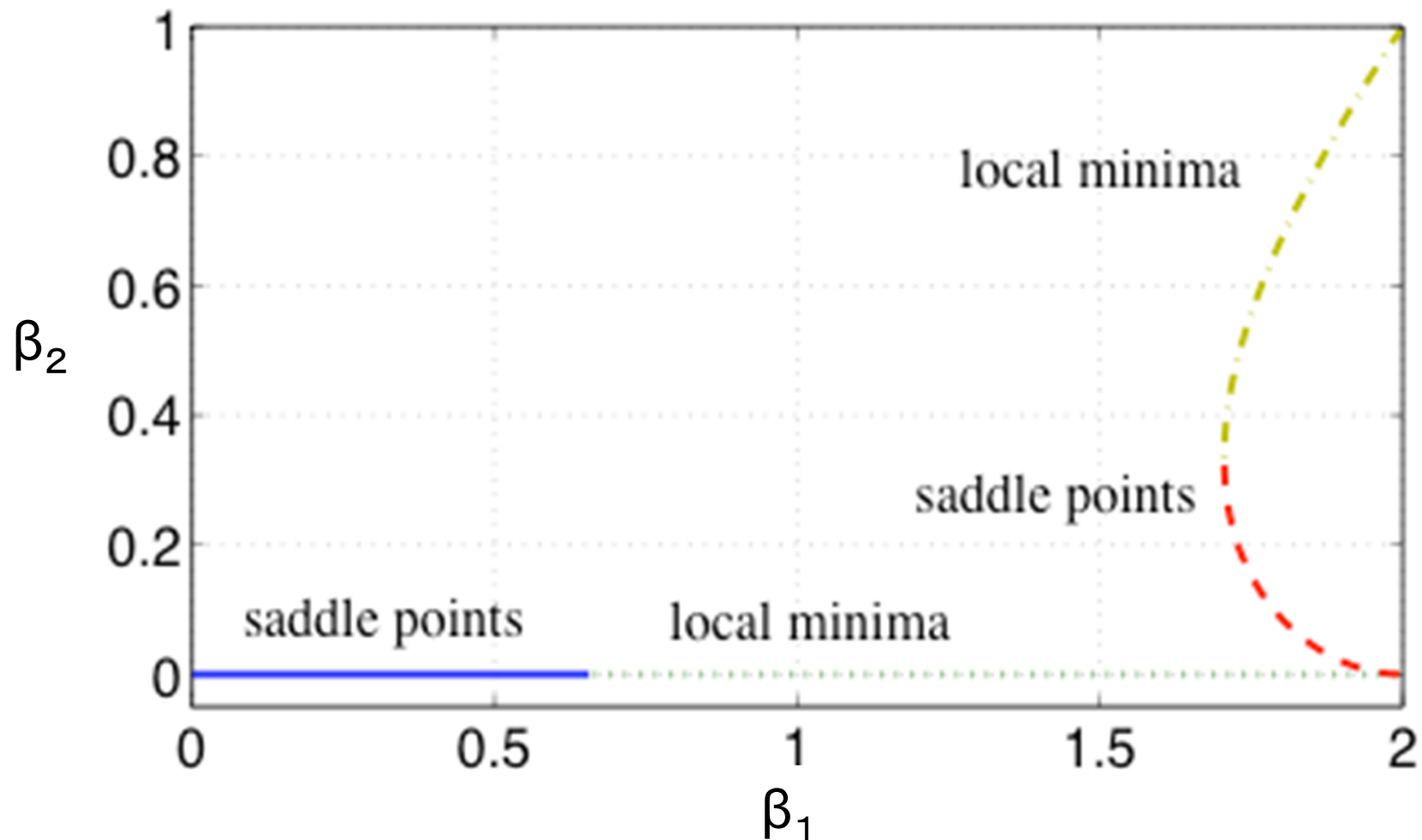
**(Collaborator: Masahiro Yukawa, Niigata University)**

**Solution Path :**  $\lambda \leftrightarrow c$

**not continuous, not-monotone  
jump**

$$\beta_\lambda \Leftrightarrow \beta_c$$

# An Example of the greedy path

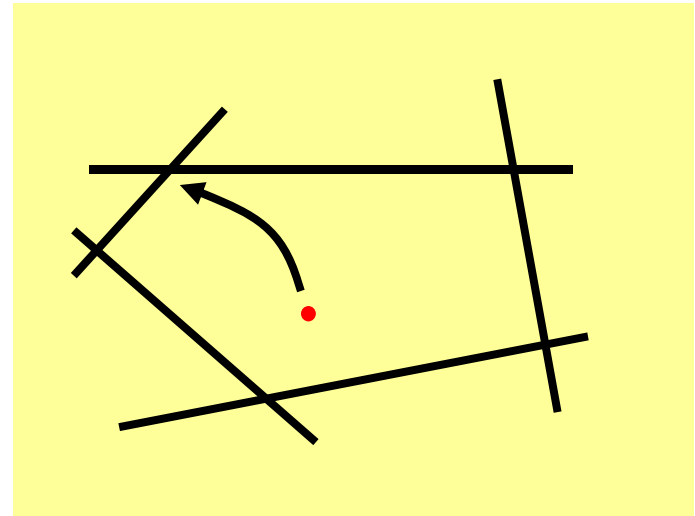


# Linear Programming

$$\sum A_{ij}x_j \geq b_i$$

$$\max \sum c_i x_i$$

$$\psi(\mathbf{x}) = \sum_i \log\left(\sum A_{ij}x_j - b_i\right)$$



# Convex Programming

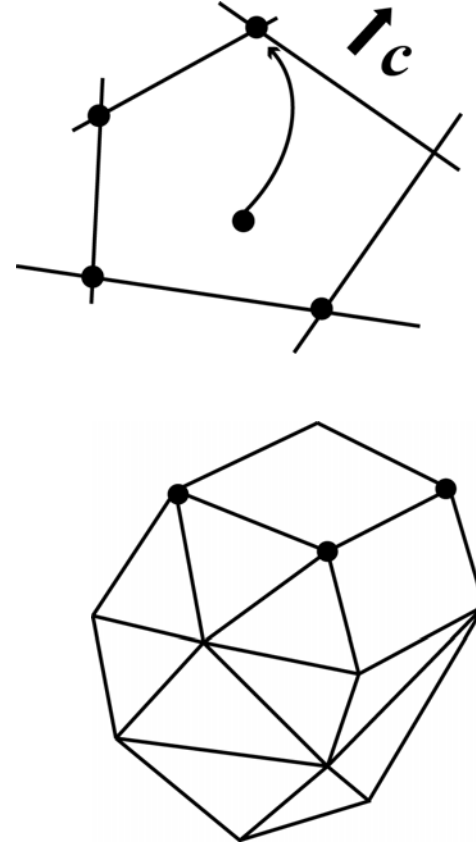
## — Inner Method

$$LP : A\mathbf{x} \geq \mathbf{b}, \quad \mathbf{c} \cdot \mathbf{x} \geq 0$$

$$\min \quad \mathbf{c} \cdot \mathbf{x}$$

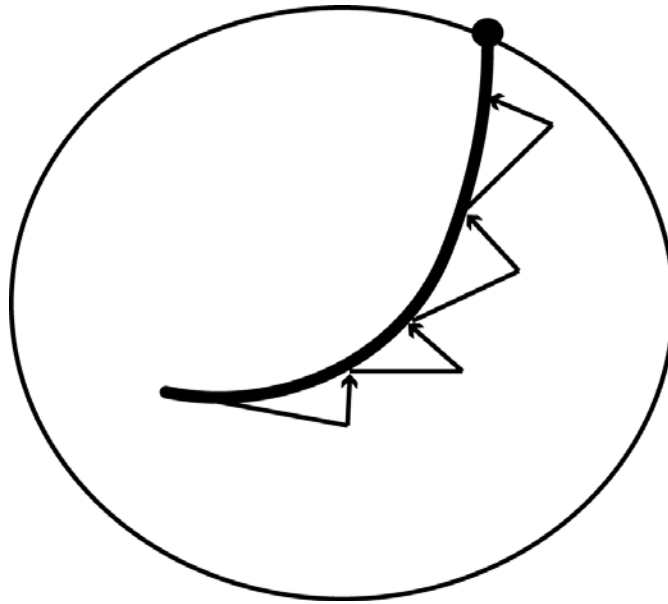
$$\psi(\mathbf{x}) = \sum \log\left(\sum A_{ij}x_j - b_i\right) + \sum \log x_i$$

$$\boldsymbol{\eta} = \partial_i \psi(\mathbf{x})$$



**Simplex method ; inner method**

# Polynomial-Time Algorithm



**curvature : step-size**

$$\left| H^{(m)} \right|^2$$

$$\min : t\mathbf{c} \cdot \mathbf{x} + \psi(\mathbf{x}) \quad \mathbf{x} = \delta(t) \quad \nabla^* - \text{geodesic}$$

# Neural Networks

## **Multilayer Perceptron**

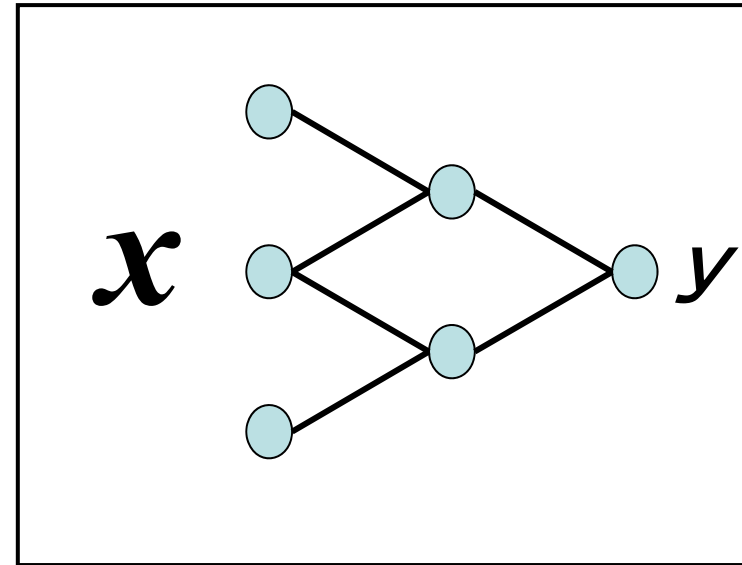
*Higher-order correlations*

*Synchronous firing*

# Multilayer Perceptrons

$$y = \sum v_i \varphi(\mathbf{w}_i \cdot \mathbf{x}) + n$$

$$\mathbf{x} = (x_1, x_2, \dots, x_n)$$

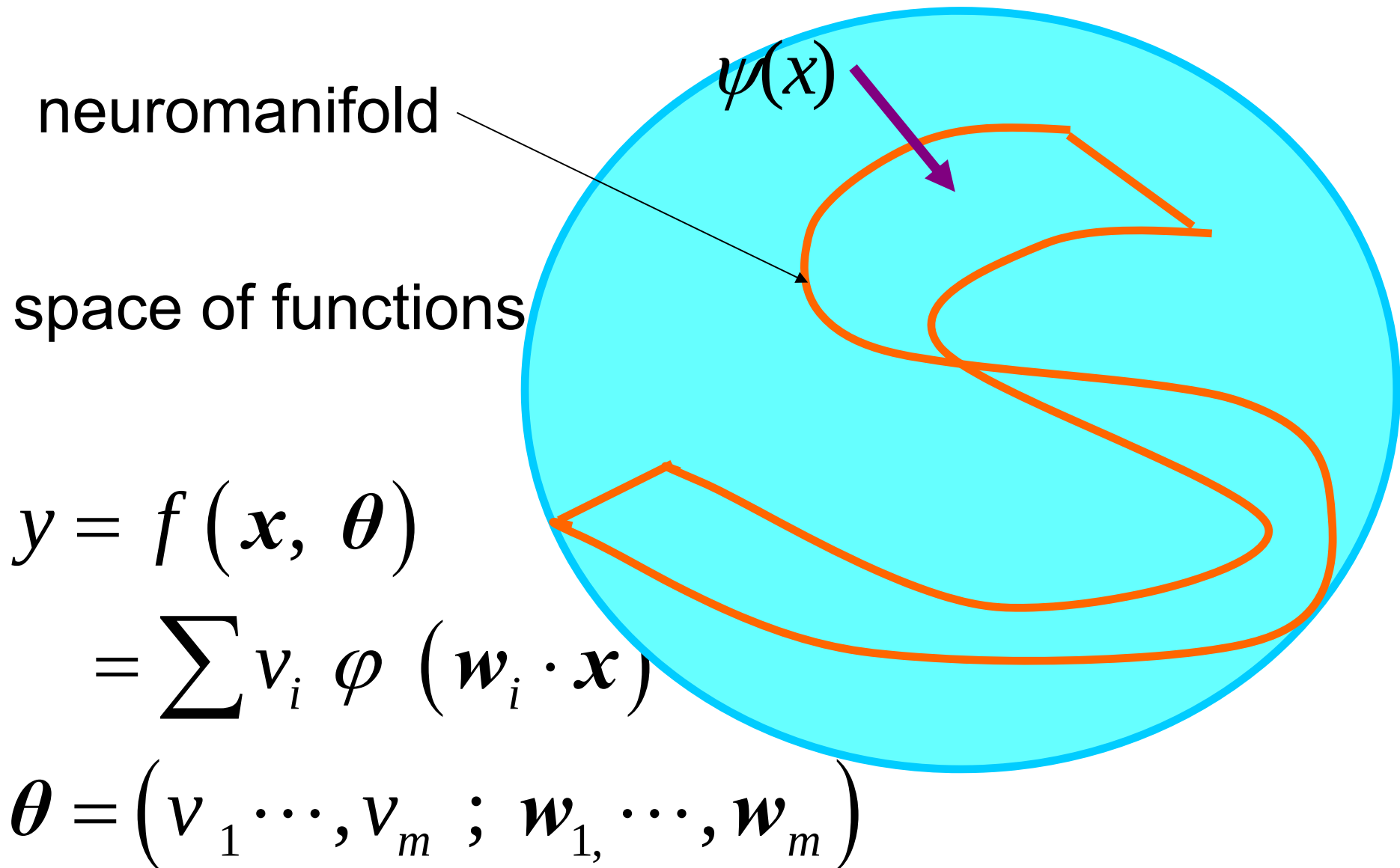


$$p(y|\mathbf{x};\boldsymbol{\theta}) = c \exp \left\{ -\frac{1}{2} (y - f(\mathbf{x}, \boldsymbol{\theta}))^2 \right\}$$

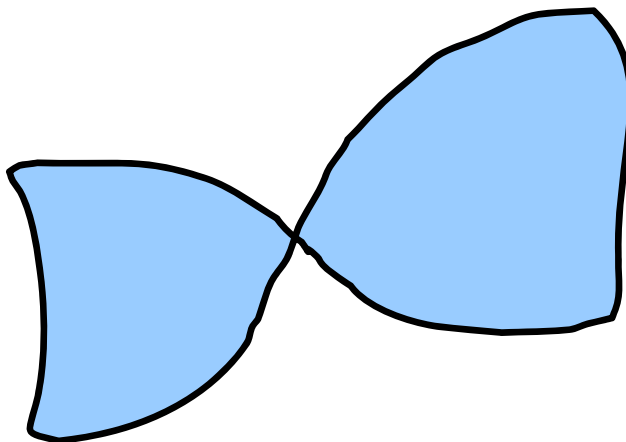
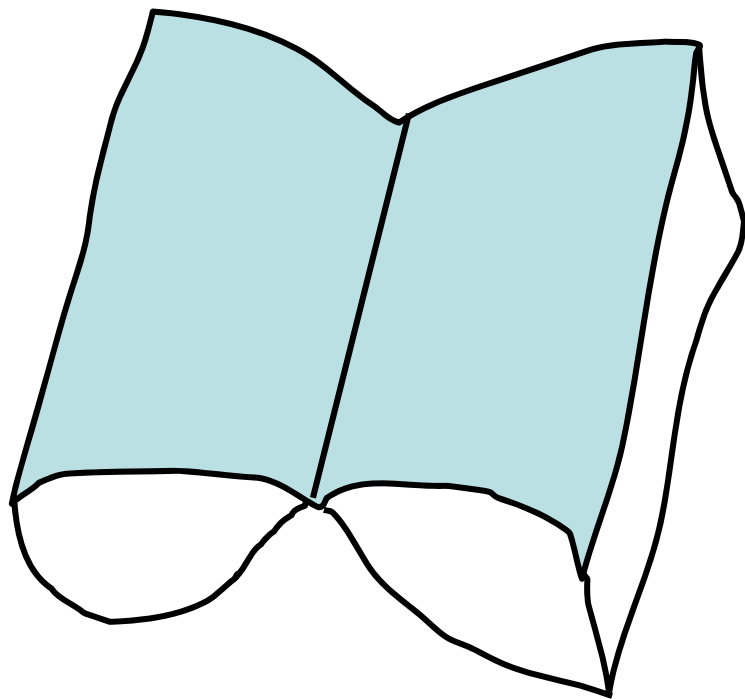
$$f(\mathbf{x}, \boldsymbol{\theta}) = \sum v_i \varphi(\mathbf{w}_i \cdot \mathbf{x})$$

$$\boldsymbol{\theta} = (\mathbf{w}_1, \dots, \mathbf{w}_m; v_1, \dots, v_m)$$

# Multilayer Perceptron



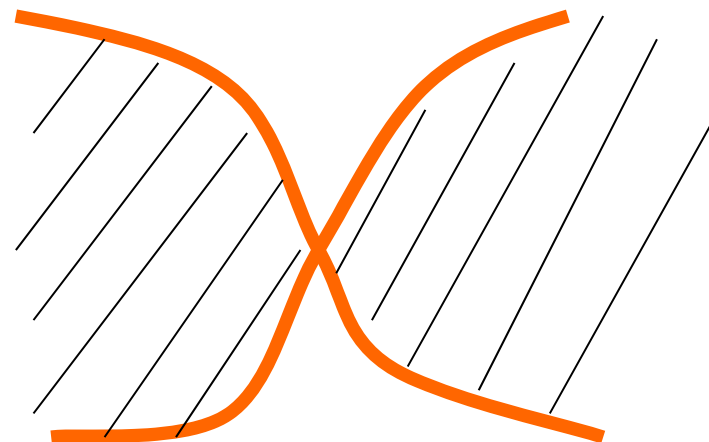
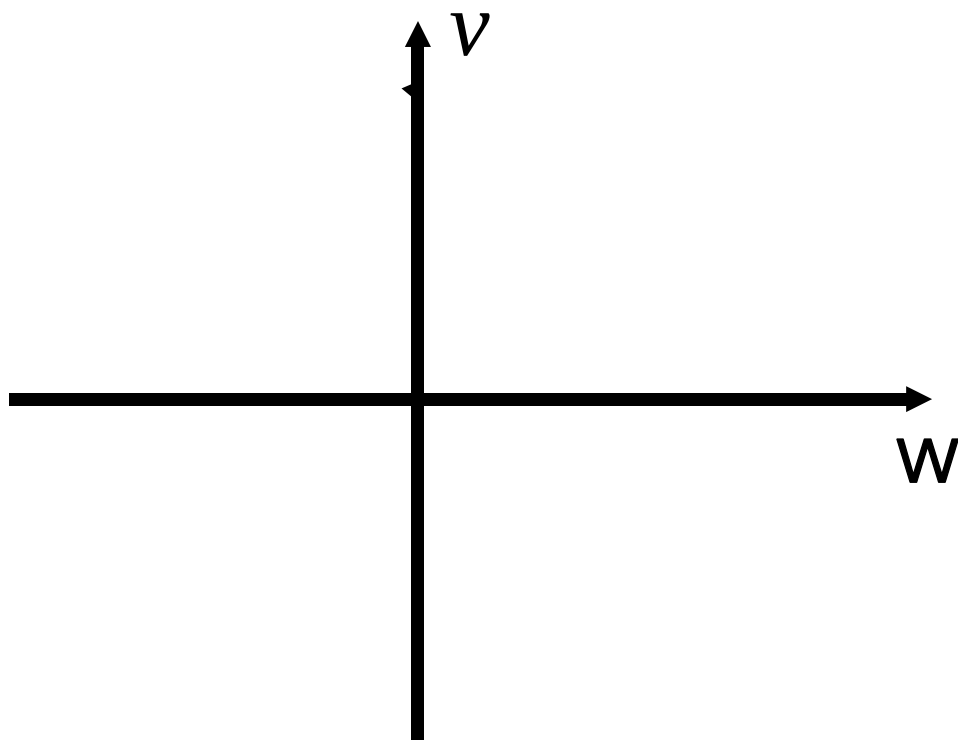
# singularities



# Geometry of singular model

$$y = v\varphi(\mathbf{w} \cdot \mathbf{x}) + n$$

$$v \mid \mathbf{w} \models 0$$



# Backpropagation ---gradient learning

---

examples :  $(y_1, \mathbf{x}_1), \dots (y_t, \mathbf{x}_t)$

$$E = \frac{1}{2} |y - f(\mathbf{x}, \boldsymbol{\theta})|^2 = -\log p(y, \mathbf{x}; \boldsymbol{\theta})$$

natural gradient (Riemannian)

$$\tilde{\nabla} E = G^{-1} \nabla E \text{ --steepest descent}$$

$$\Delta \boldsymbol{\theta}_t = -\eta_t \frac{\partial E}{\partial \boldsymbol{\theta}}$$

$$f(\mathbf{x}, \boldsymbol{\theta}) = \sum v_i \varphi(\mathbf{w}_i \cdot \mathbf{x})$$

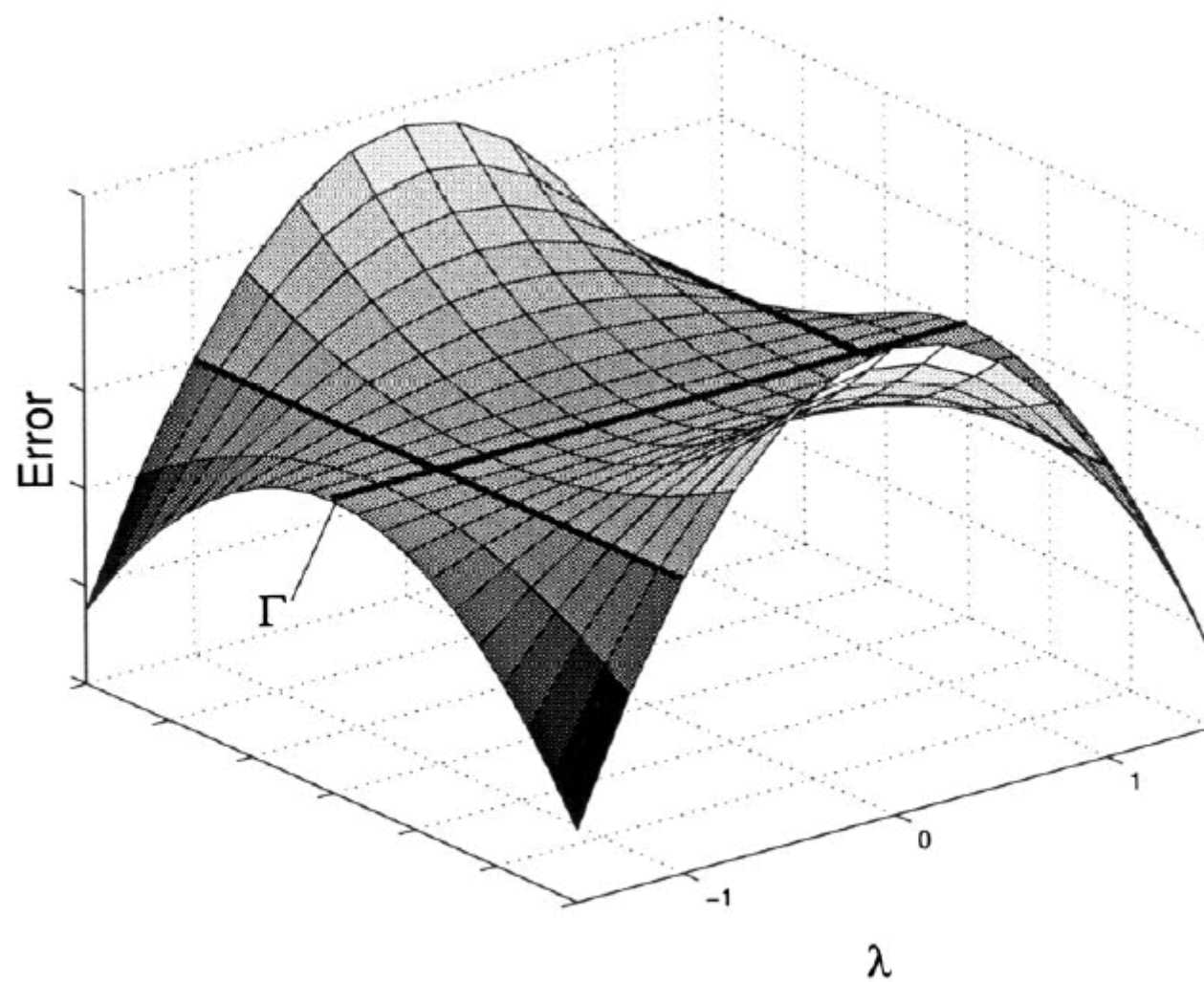
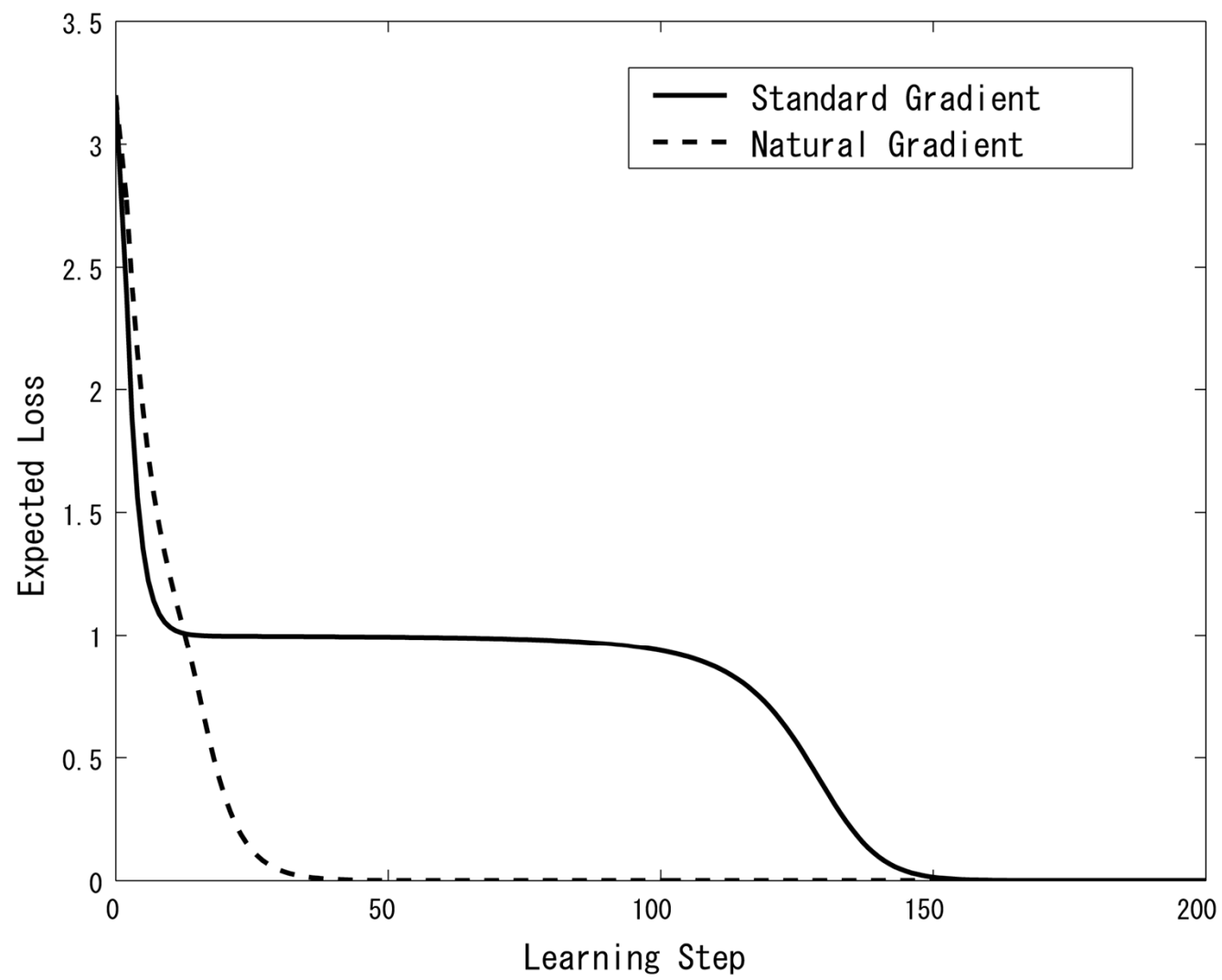


Fig. 5. Critical set with local minima and plateaus.



# conformal transformation

## $q$ -Fisher information

$$g_{ij}^{(q)}(p) = \frac{q}{h_q(p)} g_{ij}^F(p)$$

## $q$ -divergence

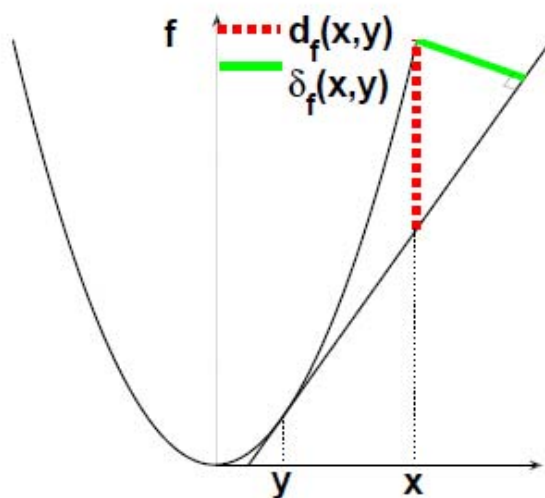
$$D_q[p(x) : r(x)] = \frac{1}{(1-q)h_q(p)} \left(1 - \int p(x)^q r(x)^{1-q} dx\right)$$

# Total Bregman Divergence and its Applications to Shape Retrieval

•Baba C. Vemuri, Meizhu Liu, Shun-ichi Amari,  
Frank Nielsen

IEEE Conference on Computer Vision and Pattern Recognition (CVPR),  
2010

# Total Bregman Divergence



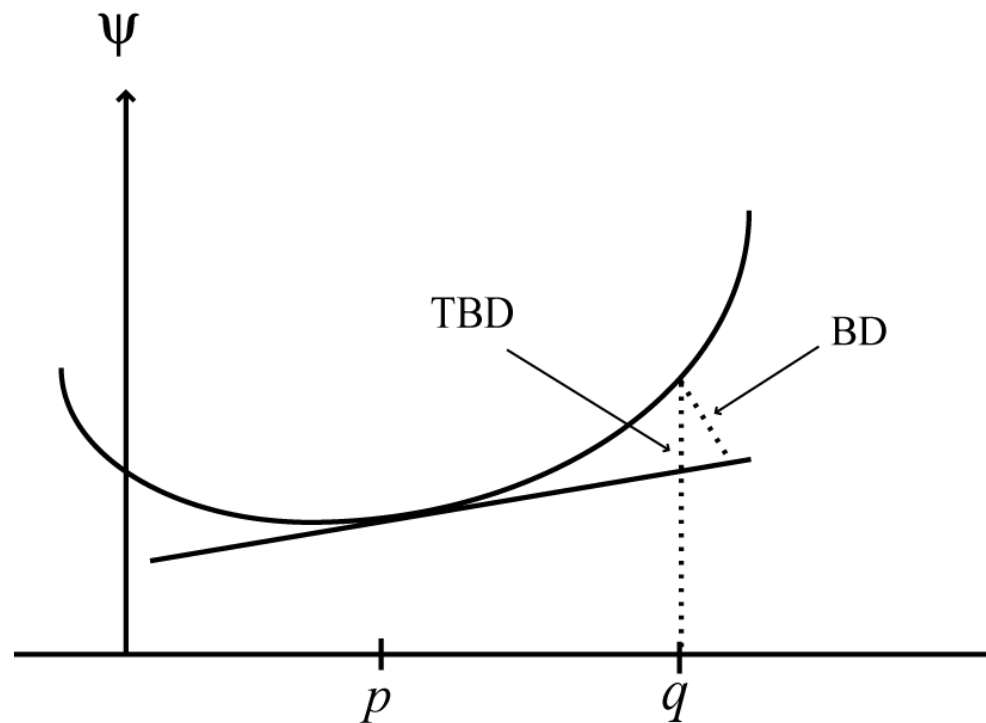
$$TD[x : y] = \frac{D[x : y]}{\sqrt{1 + \|\nabla f\|^2}}$$

- rotational invariance
- conformal geometry

Figure:  $d_f(x, y)$  (dotted red line) is BD,  $\delta_f(x, y)$  (bold green line) is TBD, and the two arrows indicate the coordinate system. Note that  $d_f(x, y)$  changes with rotation unlike  $\delta_f(x, y)$  which is invariant to rotation.

# Total Bregman divergence (Vemuri)

$$\text{TBD}(p : q) = \frac{\varphi(p) - \varphi(q) - \nabla \varphi(q) \cdot (p - q)}{\sqrt{1 + |\nabla \varphi(q)|^2}}$$

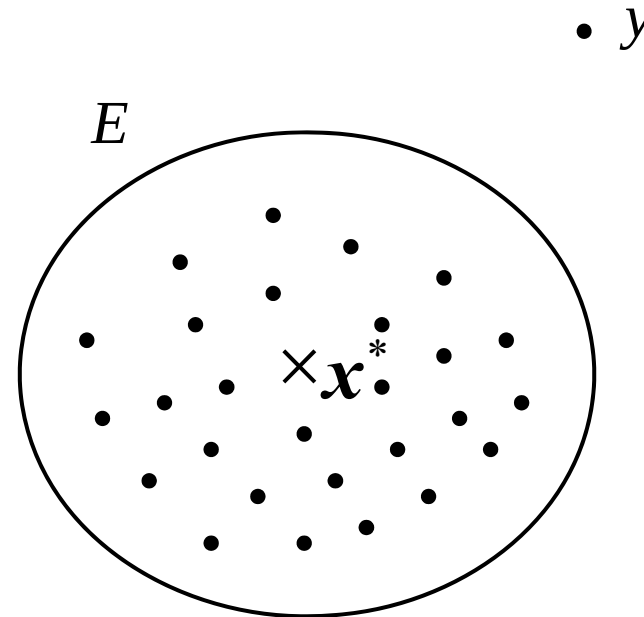


# Clustering : *t*-center

$$E = \{x_1, \dots, x_m\}$$

**T-center of  
E**

$$x^* = \arg \min \sum_i TD[x, x_i]$$



**$t$ -center $\mathbf{x}^*$**

$$\nabla f(\mathbf{x}^*) = \frac{\sum w_i \nabla f(\mathbf{x}_i)}{\sum w_i}$$

$$w_i = \frac{1}{\sqrt{1 + \|\nabla f(\mathbf{x}_i)\|^2}}$$

## $q$ -super-robust estimator (Eguchi)

$$\max \hat{p}(x, \xi) \rightarrow \max \frac{p(x, \xi)}{h_{q+1}}$$

bias-corrected  $q$ -estimating function

$$s_q(x, \xi) = \hat{p}(x, \xi) \{ \partial_i \log p - c_{q+1}(\xi) \}$$

$$c_{q+1} = \frac{1}{q+1} \partial \log h_{q+1}(\xi)$$

$$\sum_{i=0}^N s_q(x_i, \xi) = 0 \quad \Leftrightarrow \max \frac{1}{h_{q+1}} \sum \hat{p}(x_i, \xi)$$

## Conformal change of divergence

$$\tilde{D}(p : q) = \sigma(p) D[p : q]$$

$$\tilde{g}_{ij} = \sigma(p) g_{ij}$$

$$\tilde{T}_{ijk} = \sigma(T_{ijk} + s_k g_{ij} + s_j g_{ik} + s_i g_{jk})$$

$$s_i = \partial_i \log \sigma$$

# *t*-center is robust

$$E^* = \{\mathbf{x}_1, \dots, \mathbf{x}_n; \mathbf{y}\}$$

$$\tilde{\mathbf{x}}^* = \mathbf{x}^* + \varepsilon \mathbf{z}(\mathbf{x}^*; \mathbf{y}), \quad \varepsilon = \frac{1}{n}$$

influence function  $\mathbf{z}(\mathbf{x}^*; \mathbf{y})$

$|\mathbf{z}| < c$  as  $|\mathbf{y}| \rightarrow \infty$  : robust

$$\mathbf{z}(\mathbf{x}^*, \mathbf{y}) = G^{-1} \frac{\nabla f(\mathbf{y}) - \nabla f(\mathbf{x}^*)}{w(\mathbf{y})}$$

$$G = \frac{1}{n} \sum w(\mathbf{x}_i) \nabla \nabla f(\mathbf{x}_i)$$

Robust:  $\mathbf{z}$  is bounded

$$\mathbf{z}(\mathbf{x}^*, \mathbf{y}) = G^{-1} \frac{\mathbf{y}}{\sqrt{1 + \|\mathbf{y}\|^2}}$$

$$\frac{\nabla f(\mathbf{y})}{w(\mathbf{y})} = \frac{\nabla f(\mathbf{y})}{\sqrt{1 + \|\nabla f(\mathbf{y})\|^2}} < \infty$$

$$\mathbf{z}(\mathbf{x}^*, \mathbf{y}) = \mathbf{y} \quad \text{Euclidean case} \quad f = \frac{1}{2} \|\mathbf{x}\|^2$$

$$w(\mathbf{y}) > 1$$

# MPEG7 database

- Great intraclass variability, and small interclass dissimilarity.



# Other TBD applications

## Diffusion tensor imaging (DTI) analysis [Vemuri]

- Interpolation
- Segmentation

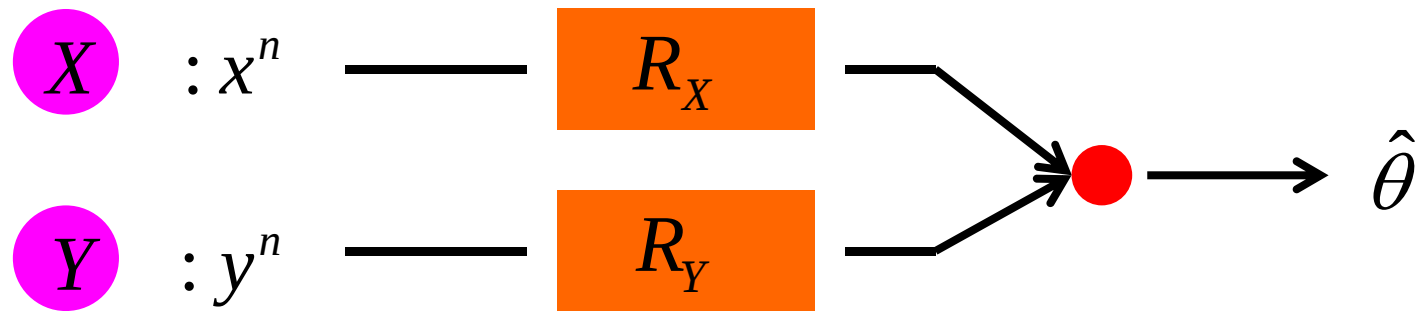
Baba C. Vemuri, Meizhu Liu, Shun-ichi Amari and Frank Nielsen, *Total Bregman Divergence and its Applications to DTI Analysis*, IEEE TMI, to appear

# **TBD application-shape retrieval**

- **Using MPEG7 database;**
- **70 classes, with 20 shapes each class  
(Meizhu Liu)**

# Multiterminal Information & Statistical Inference

---

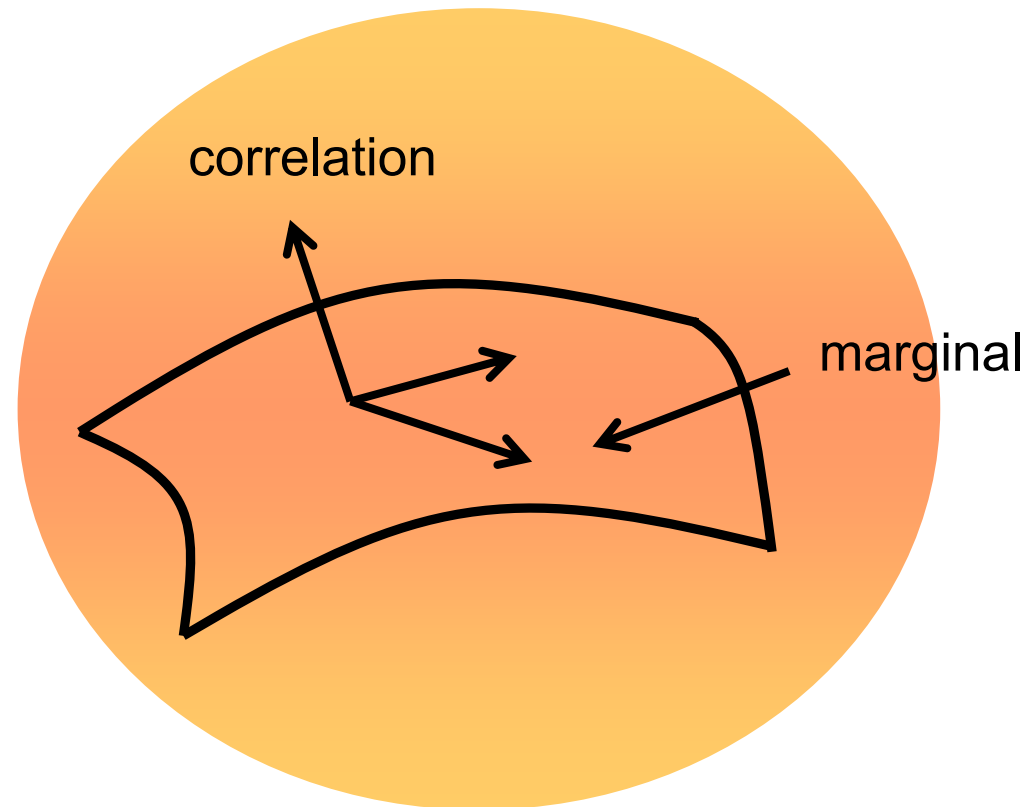


$$p(x, y; \theta)$$

$$|M_X| = 2^{R_X n} \quad |M_r| = 2^{R_Y n}$$

$p(x,y)$

$p(x,y,z)$



$$G = G_M + G_C$$

0-rate

Slepian-Wolf

# Linear Systems



## ARMA

$$x_{t+1} = \frac{1 + b_1 z^{-1} + \dots + b_q z^{-q}}{1 + a_1 z^{-1} + \dots + a_p z^{-p}} u_t$$

$$\theta = (a_1, \dots, a_p : b_1, \dots, b_q)$$

$$x_{t+1} = f(\theta, z^{-1}, u_t)$$

**AR---e-flat**

**MA---m-flat**

# Machine Learning

**Boosting : combination of weak learners**

$$D = \left\{ (\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \dots, (\mathbf{x}_N, y_N) \right\}$$

$$y_i = \pm 1$$

$$f(\mathbf{x}, \mathbf{u}) : y = h(\mathbf{x}, \mathbf{u}) = \text{sgn } f(\mathbf{x}, \mathbf{u})$$

# Weak Learners

$$H(\mathbf{x}) = \text{sgn}\left(\sum \alpha_t h_t(\mathbf{x})\right)$$

$$\varepsilon_t : \text{Prob} \{h_t(\mathbf{x}_i) \neq y_i\} \quad |W_t$$

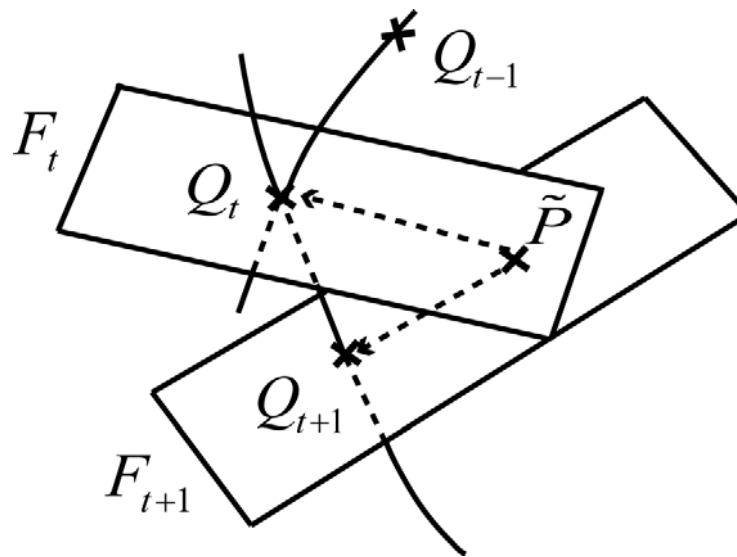
$$W_{t+1}(i) = cW_t(i) \exp\{-\alpha_t y_i h_t(\mathbf{x}_i)\}$$

**weight distribution**

# Boosting —generalization

$$Q_t = \left\{ Q_t(y|x) = Q_{t-1}(y|x) \exp \left\{ \alpha_t y h_t(x) - \tilde{f} \right\} \right\}$$

$$F_t = \left\{ P(y, x) E y h_t(x) = \text{const} \right\}$$



$$\alpha_t : \min D[\tilde{P} : Q_t]$$

$$D(\tilde{P}, Q_{t+1}) < D(\tilde{P}, Q_t)$$

# Integration of evidences:

$$X_1, X_2, \dots, X_m$$

arithmetic mean

geometric mean

harmonic mean

$\alpha$  -mean

# Various Means

$$\frac{a+b}{2}$$

arithmetic

:

$$\sqrt{ab}$$

geometric

:

$$\frac{2}{\frac{1}{a} + \frac{1}{b}}$$

harmonic

Any other mean?

# Generalized mean: f-mean

**f(u): monotone; f-representation of u**

$$m_f(a, b) = f^{-1}\left\{\frac{f(a) + f(b)}{2}\right\}$$

**scale free**

$$m_f(ca, cb) = cm_f(a, b)$$

**$\alpha$ -representation**

$$f_\alpha(u) = u^{\frac{1-\alpha}{2}}, \quad \alpha \neq 1$$
$$\log u, \quad \alpha = 1$$

**$\alpha$ -mean** :  $m_{\alpha}(p_1(s), p_2(s))$

$$\alpha = 1 : \sqrt{ab}$$

$$\alpha = -1 : \frac{a+b}{2}$$

$$\alpha = 0 : (\sqrt{a} + \sqrt{b})^2 = \frac{a+b}{4} + \frac{1}{2}\sqrt{ab}$$

$$\alpha = \infty \quad m_{\alpha} = \min(a, b)$$

$$\alpha = -\infty \quad m_{\alpha} = \max(a, b)$$

# $\alpha$ — Family of Distributions

$$\{p_1(s), \dots, p_k(s)\} \quad p(x; \theta) = f_\alpha^{-1} \left\{ \sum \theta_i f_\alpha(p_i(x)) \right\}$$

**mixture family :**

$$p_{\text{mix}}(s) = \sum_{i=1}^k t_i p_i(s), \quad \sum t_i = 1$$

**exponential family :**

$$\log p_{\text{exp}}(s) = \sum t_i \log p_i(s) - \psi$$

