Applications of Information Geometry

Clustering based on Divergence: Cluster Center Stochastic Reasoning: Belief Propagation in Graphical Model Support Vector Machine Bayesian Framework and Restricted Boltzmann Machine Natural Gradient in Multilayer Perceptron Learning Independent Component Analysis Sparse Signal Analysis and Minkovskian Gradient Convex Optimization

Clustering of Points $D = \{\theta_1, \theta_2, \theta_3, \dots, \theta_N\}$ C2 X

Clustering : center of a cluster of points $C = \{\theta_1, \dots, \theta_m\}$

$$\theta^* = \arg\min_{\theta} \sum_i D[\theta, \theta_i]$$



η^* is simply the arithmetic average in the dual coordinate system

$$D[\theta:\theta_i] = \psi(\theta) + \varphi(\eta_i) - \theta \cdot \eta_i$$
$$\partial_{\theta} D[\theta:\theta_i] = \eta - \eta_i$$
$$\sum (\eta - \eta_i) = 0$$
$$\eta^* = \frac{1}{m} \sum \eta_i$$

k-means: clustering algorithm



k-means: clustering algorithm

- **1. Choose k cluster centers**
- 2. Classify patterns of D into clusters
- 3. Calculate new cluster centers



Voronoi Diagram: Boundaries of Clusters





Total Bregman divergence (Vemuri)

 $tBD(p:q) = \frac{\psi(p) + \varphi(q) - \theta_p \cdot \eta_q}{\sqrt{1 + |\nabla \psi(q)|^2}}$



t-center of C η^*

$$\eta^* = \frac{\sum w_i \eta_i}{\sum w_i}$$

$$w_{i} = \frac{1}{\sqrt{1 + \left\|\nabla \psi\left(\eta_{i}\right)\right\|^{2}}}$$

Conformal change of divergence

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

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

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

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

t-center is robust

$$E^* = \big\{ \boldsymbol{\eta}_1, \cdots, \boldsymbol{\eta}_n; \boldsymbol{y} \big\}$$

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

influence function
$$z(\eta^*; y)$$

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

minimize
$$\frac{1}{N+1} \left(\sum \frac{D[\eta : \eta_i]}{w_i} + \frac{D[\eta : \mathbf{y}]}{w_{N+1}} \right)$$

$$\boldsymbol{z}(\boldsymbol{\eta}^*,\boldsymbol{y}) = \boldsymbol{G}^{-1} \frac{\nabla \boldsymbol{\psi}(\boldsymbol{\theta}_{\boldsymbol{y}}) - \nabla \boldsymbol{\psi}(\boldsymbol{\eta}^*)}{\boldsymbol{w}(\boldsymbol{y})}$$

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

Robust: *z* is bounded

$$\frac{\nabla \psi(\theta_{y})}{w(y)} = \frac{\nabla \psi(\theta_{y})}{\sqrt{1 + \left\|\nabla \psi(\theta_{y})\right\|^{2}}} < \infty$$
$$w(y) > 1$$

$$z(\eta^*, y) = y$$

Euclidean case
$$f = \frac{1}{2} |\mathbf{x}|^2$$

MPEG7 database

• Great intraclass variability, and small interclass dissimilarity.



Shape representation

A shape is represented using a mixture of Gaussians from the aligned boundary points.



First clustering then retrieval

Retrieval in the whole MPEG-7 database

First clustering and then retrieval.



Figure: *k*-Tree diagram. G-M: mixture of Gaussians. Every key is a mixture of Gaussians. Each key in the inner nodes is the *t*-center of all keys in its children nodes. The key of a leaf is a mixture of Gaussians corresponding to an individual shape.

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

Information Geometry of Stochastic Reasing

Belief Propagation in Graphical Model

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

Stochastic Reasoning: Graphical Model

$$p(x, y, z, r, s) = 1, -1$$

Stochastic Reasonin

q(x₁,x₂,x₃,...| observation)

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

X Z S R

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

X_i = sgn E[x_i] least bit error rate estimator

Mean Value

Marginalization: projection to independent distributions



$$\Pi_0 q(\mathbf{x}) = q_1(x_1) q_2(x_2) \dots q_n(x_n) = q_0(\mathbf{x})$$
$$q_i(x_i) = \int q(x_{1,1}, \dots, x_n) dx_1 \dots d\tilde{x}_i \dots dx_n$$

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

cliques



$$q(\mathbf{x}) = \exp\left\{\sum_{i=1}^{L} k_{i} \cdot x_{i} + \sum_{r=1}^{L} c_{r}(\mathbf{x}) - \psi_{q}\right\}$$
$$c_{r}(\mathbf{x}) = c_{r} x_{i_{1}} \cdots x_{i_{s}}, \quad r = (i_{1} \cdots i_{s})$$
$$x_{i} = \{1, -1\} \quad r = (i_{1}, i_{2})$$

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

Computationally Difficult

$$q(\mathbf{x}) \to \eta = E[\mathbf{x}]$$
$$q(\mathbf{x}) = \exp\left\{\sum_{r} c_r(\mathbf{x}) - \psi_q\right\}$$

mean-field approximation

belief propagation

tree propagation, CCCP (convex-concave)

Information Geometry of Mean Field Approximation

- m-projection
- e-projection



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

Z(2C)

m

M

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

m-projection keeps the expectation of x





Belief Prop Algorithm



Belief Propagation $p(x, \mathbf{g}_r) = \exp\{c_r(x) + \mathbf{g}_r \cdot x - \psi_r\}$ $\prod_{n} p_{r}(x, \theta_{r}^{t}) \Longrightarrow p_{r}(x, \theta_{0}^{t})$ $\xi_r^{t+1} = \prod_0 p_r(x, \theta_r^t) - \theta_r^t$: belief for $c_r(x)$ $\theta_r^{t+1} = \sum \xi_{r'}^{t+1}$ $r' \neq r$ $\boldsymbol{\theta}_{0}^{t+1} = \sum_{r} \boldsymbol{\xi}_{r}^{t+1}$ r.



Belief Propagation e-condition OK $(\theta; \xi_1, \xi_2, ..., \xi_L), \quad \theta' = \sum \xi'_r$ $(\theta_1, \theta_2, ..., \theta_L) \rightarrow (\theta'_1, \theta'_2, ..., \theta'_L)$

CCCP m-condition OK $\boldsymbol{\theta}_0 \rightarrow \boldsymbol{\theta}_r : \prod p_0(x, \theta_r) = p_r(x, \theta_r)$

$$\mathbf{\theta}_0' = \sum \boldsymbol{\xi}_r$$

Convex-Concave Computational Procedure (CCCP): A. Yuille

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

Elimination of double loops

Geometry of Support Vector Machine modification of kernel

Simple perceptron: decision surface

$$f(x) = w \cdot x + b$$
$$d = \frac{|w \cdot x + b|}{|w|}$$

nel inface minimize $|w|^2$ constraint $y_i(w \cdot x_i + b) \ge 1$

W.x+b=0

$$L(w,b,\alpha) = \frac{1}{2} |w|^2 - \sum \alpha_i (w \cdot x_i + b)$$

$$\sum \alpha_i y_i = 0: \text{ support vector } x_i: \alpha_i \neq 0$$

$$w = \sum \alpha_i y_i x_i \qquad f(x,w) = \sum \alpha_i y_i x_i + b$$

Embedding in higher-dimensional space

$$x \Longrightarrow z = \varphi(x)$$
$$f(x) = w \cdot \varphi(x) + b$$

z: infinite-dimensional



Kernel trick

$$K(x, x') = \varphi(x) \cdot \varphi(x')$$
$$\int K(x, x') \tilde{\varphi}_i(x') dx' = \lambda_i \tilde{\varphi}_i(x')$$
$$\varphi(x) = \frac{1}{\sqrt{\lambda_i}} \tilde{\varphi}_i(x)$$

$$f(x,w) = \sum \alpha_i y_i K(x_i,x)$$



Conformal Transformation of Kernel

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

$$\tilde{K}(x,x') = \sigma(x)\sigma(x')K(x,x')$$

$$\sigma(x) = \sum \exp\{-\kappa_i ||\mathbf{x} - \mathbf{x}_i^*|^2\}$$

 $g_{ij}(x) = \{\sigma(x)\}^2 g_{ij}(x) + \partial_i \sigma(x) \partial_j \sigma(x)$

Basic Principles of Unsupervised and Supervised Learning Toward Deep Learning

Shun-ichi Amari (RIKEN Brain Science Institute) collaborators: R. Karakida, M. Okada (U. Tokyo)
Self-Organization + Supervised Learning

N h1 hm

Deep Learning

RBM: Restricted Boltzmann Machine Auto-Encoder, Recurrent Net

tricks !! ideas !

Dropout **Contrastive divergence**

bi-directional

→ Z

Boltzmann Machine Markov chain $P(\mathbb{Z}_{+} | \mathbb{Z}_{+})$

$$P(z=1) = f(u) , u_i = \sum v_{ij} z_j - b_i$$
 $w_{ij} =$

stable distr.
$$P(Z) = exp\{\Sigma_{i}, z_{i} + \frac{1}{2}\Sigma_{i}, z_{j} - 4\}$$

RBM: Restricted Boltzmann Machine

 $P(w, h) = \exp \{ b \cdot v + c \cdot h$ $+ h W w - \psi - \frac{1}{2} |w|^2 - \frac{1}{2} |h|^2 \}$ T $F_h w_{ij} v_{j}$ $E \cdot v_{ij} v_{j}$

RBM

$$\mathcal{E}(\mathcal{W}, \mathbb{h}) = \exp \{\mathbb{h}^{*} \mathcal{W} \mathcal{V} - \mathcal{V}\}$$

 \mathcal{M}
 \mathcal

Simple Hebbian Self-Organization

$$h = f(w \cdot w - \tau)$$

$$receptive field$$

$$R(w) = \{v \mid w \cdot w - v_0 > 0\}$$

$$|w|^2 = const$$

$$R(w)$$

•



•



Self-Organization
minimize
$$KL [f(w) : f_{w}(w; W)]$$

 $W = \int f(w) \int_{\mathcal{F}_{w}(w; W)} \int_{\mathcal{F}_{w}(w; W)}$

Bayesian Duality in Exponential Family

Data x Parameter (higher-order concepts) () $P(\mathbf{x} \mid \mathbf{0}) = \exp \{ \mathbf{0} \cdot \mathbf{x} - \overline{\mathbf{k}}(\mathbf{x}) - \Psi(\mathbf{0}) \}$ $P(\mathbf{x}, \mathbf{0}) = \exp \{ \mathbf{0} \cdot \mathbf{x} - \overline{\mathbf{k}}(\mathbf{x}) - \overline{\Psi}(\mathbf{0}) \}$ $\Psi(\mathbf{0} \mid \mathbf{x}) = \exp \{ \mathbf{0} \cdot \mathbf{x} - \mathbf{k}(\mathbf{x}) - \overline{\Psi}(\mathbf{0}) \}$

 $\mathcal{X}(\mathcal{W}), \mathcal{O}(\mathcal{U}) : = \exp\{\mathcal{O}(\mathcal{U}) \cdot \mathcal{X}(\mathcal{V}) - \overline{\mathcal{R}} - \overline{\mathcal{V}}\}$

Curved exponential family

RBM : currored exp. family

Gaussian Boltzmann Machine

$$\begin{aligned} & \left\{ \left(\frac{1}{2} \right) \right\} = \exp \left\{ -\frac{1}{2} \left| \frac{1}{2} \right|^{2} - \frac{1}{2} \left| \frac{1}{2} \right|^{2} + \frac{1}{2} \frac{1}{2} \frac{1}{2} - \frac{1}{2} \frac{1}{2} \frac{1}{2} \frac{1}{2} \frac{1}{2} + \frac{1}{2} \frac{1}{2}$$

Equilibrium Solution

$$WC = (I - WW^{r})^{-'}W \qquad W = \begin{pmatrix} w_{i} \\ \vdots \\ w_{k} \end{pmatrix}$$
solution:

$$m_{i} \cdot m_{j} = 0 \quad (i \neq j > 1) \quad W_{i} \rangle^{2} = m_{i}$$

$$m_{i} C' = (1 - m_{i})^{-'} \quad W_{i} \qquad W_{i} C' = \lambda_{i} \cdot W_{i}$$

$$m_{i} = 1 - \frac{1}{\lambda_{i}}$$

$$PCA!$$

Equilibrium Solution $WC = (I - WW^{T'})^{-1}W$ General Solution $W = U \operatorname{diag} \left(\sqrt{1 - \frac{1}{\lambda_1}}, ..., \sqrt{1 - \frac{1}{\lambda_m}}, 0, ..., 0 \right) V$

- othogonal matrix : *U*, *V*
- C diagonalized by V $C = V^T \operatorname{diag}(\lambda_1, ..., \lambda_n) V$

You can choose m(\leq k) eigen values form $\lambda_1, ..., \lambda_k > 1$

Contrastive Divergence

- RBM
 - 2-layered probabilistic neural network
 - No connections within layers

$$q(\mathbf{h}, \mathbf{v}; W) = \exp\left(-\mathbf{h}^T W \mathbf{v}\right) / \sum_{\mathbf{h}, \mathbf{v}} \exp\left(-\mathbf{h}^T W \mathbf{v}\right)$$

• How to train RBM



Maximum Likelihood (ML) learning is hard



Many iterations of Gibbs Sampling demand too much computational time

Contrastive Divergence Solution

$$\langle h v \rangle_{\tilde{q}} = W C W^{T} W + W$$

 $W C = W C W^{T} W + W$
 $w_{i} C = \frac{1}{1-m_{i}} w_{i}$ PCA





Bernoulli-Gaussian RBM

ICA

R. Karakida



P(v): v = 0D5

 $W = A^{-1}$

Simulation

The number of Neurons: N = M = 2, $\sigma = 1/2$



Independent sources are extracted in G-B RBM

Information Geometry of Neuromanifolds

Natural Gradient and Singularities

Multilayer Perceptron

Shun-ichi Amari RIKEN Brain Science Institute

Mathematical Neurons

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





$$y = \sum v_i \varphi(w_i \cdot x) + n$$
$$x = (x_1, x_2, ..., x_n)$$



$$p(y|\mathbf{x};\boldsymbol{\theta}) = c \exp\left\{-\frac{1}{2}(y - f(\mathbf{x},\boldsymbol{\theta}))^{2}\right\}$$
$$f(\mathbf{x},\boldsymbol{\theta}) = \sum v_{i}\varphi(\mathbf{w}_{i}\cdot\mathbf{x})$$
$$\boldsymbol{\theta} = (w_{1},...,w_{m};v_{1},...,v_{m})$$

Multilayer Perceptron: Neuromanifold



Universal Function Approximator

$$\psi(\mathbf{x}) \approx \sum_{i=1}^{N} \mathrm{v}_{i} a_{i}(\mathbf{x})$$

_ _

$$\psi(\mathbf{x}) \approx \sum_{i=1}^{m} v_i \varphi_i(\mathbf{x})$$
$$\varphi_i(\mathbf{x}) = \varphi(\mathbf{w}_i \cdot \mathbf{x})$$

Learning from examples

$$\psi(\mathbf{x}) \approx f(\mathbf{x}, \hat{\theta})$$

examples
$$\cdots D = \{ (x_1, y_1), \dots, (x_n, y_n) \}$$

learning; estimation

Backpropagation ---gradient learning

examples :
$$(y_1, \mathbf{x}_1), \dots (y_t, \mathbf{x}_t)$$
 - -training set $y = f(x, \theta) + n$
 $E(y, x; \theta) = \frac{1}{2} |y - f(\mathbf{x}, \theta)|^2$
 $= -\log p(y, \mathbf{x}; \theta)$
 $\Delta \theta_t = -\eta_t \frac{\partial E}{\partial \theta}$
 $f(\mathbf{x}, \theta) = \sum v_i \varphi(\mathbf{w}_i \cdot \mathbf{x})$



Metric: Riemannian manifold



Topology: Neuromanifold

- Metrical structure
- Topological structure











Geometry of singular model



Parameter Space
$$S$$

 $S = \{ \boldsymbol{\theta} \}$ $y = \sum v_i \varphi(\boldsymbol{w}_i \cdot \boldsymbol{x}) + n$
Equivalence
1) $v_i \boldsymbol{w}_i = 0$
2) $\boldsymbol{w}_i = \boldsymbol{w}_j \Rightarrow v_i + v_j$
 $M = S / \approx$



2 hidden-units

$$y = v_1 \varphi(\mathbf{w}_1 \cdot \mathbf{x}) + v_2 \varphi(\mathbf{w}_2 \cdot \mathbf{x}) + n$$

$$\mathbf{w}_2$$

$$S: v_1 v_2 |\mathbf{w}_1 - \mathbf{w}_2| |\mathbf{w}_1 + \mathbf{w}_2| = 0$$

$$(1-v)\varphi(x-w_1)+v\varphi(x-w_2)$$

Gaussian mixtures

$$p(x) = \sum v_i \exp\left\{-\frac{1}{2}(x - w_i)^2\right\}$$

Gaussian mixture

$$p(x;v,w_1,w_2) = (1-v)\varphi(x-w_1) + v\varphi(x-w_2)$$
$$\varphi(x) = \frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{1}{2}x^2\right\}$$
singular: $w_1 = w_2$, $v(1-v) = 0$

 W_2

 W_1
Learning, Estimation, and Model Selection

$$E_{\text{gen}} = D\left[p_0(y|\boldsymbol{x}): p(y|\boldsymbol{x};\hat{\boldsymbol{\theta}})\right]$$
$$E_{\text{train}} = D\left[p_{\text{emp}}(y|\boldsymbol{x};\hat{\boldsymbol{\theta}})\right]$$



$$E_{\text{gen}} = \frac{d}{2n}$$
 d : dimension
 $E_{\text{gen}} = E_{\text{train}} + \frac{d}{n}$



Problem of Backprop

$$\Delta \boldsymbol{\theta}_t = -\eta_t \nabla l(\boldsymbol{x}_t, \boldsymbol{y}_t; \boldsymbol{\theta}_t)$$

- slow convergence----plateau---saddle
- local minima



slow convergence : plateau



Steepest Direction --- Natural Gradient



$$\nabla l = \left(\frac{\partial l}{\partial \theta_1}, \cdots, \frac{\partial l}{\partial \theta_n}\right) \qquad \Delta \theta_t = -\eta_t \nabla l(x_t, y_t; \theta_t)$$
$$\widetilde{\nabla} l = G^{-1}(\theta) \nabla l$$
$$|d\theta|^2 = d\theta^T G d\theta = \sum G_{ij} d\theta^i d\theta^j$$

Natural Gradient

max
$$dl = l(\boldsymbol{\theta} + d\boldsymbol{\theta}) - l(\boldsymbol{\theta}) = \nabla l \cdot d\boldsymbol{\theta}$$

under $|d\boldsymbol{\theta}|^2 = \sum g_{ij} d\theta_i d\theta_j = \varepsilon^2$
 $d\theta \approx \widetilde{\nabla}l = G^{-1}(\boldsymbol{\theta})\nabla l$

$$\Delta \boldsymbol{\theta}_t = -\eta_t \tilde{\nabla} l(\boldsymbol{x}_t, \boldsymbol{y}_t; \boldsymbol{\theta}_t)$$

Information Geometry of MLP

Natural Gradient Learning : S. Amari ; H.Y. Park

$$\Delta \boldsymbol{\theta} = -\eta G^{-1} \left(\boldsymbol{\theta} \right) \frac{\partial l}{\partial \boldsymbol{\theta}}$$

Adaptive natural gradient learning

$$G_{t+1}^{-1} = (1 + \varepsilon)G_t^{-1} - \varepsilon G_t^{-1}\nabla f \nabla f^T G_t^{-1}$$

Regular statistical model

$$M = \left\{ p(x, \theta) \right\}$$

G: Fisher information

$$E\left[\Delta \theta \Delta \theta^{T}\right] = \frac{1}{n}G^{-1}$$

$$E\left[KL\left[p\left(x,\theta_{0}\right):p\left(x,\hat{\theta}\right)\right]\right] \approx \frac{1}{2n}G \cdot E\left[\Delta\theta\Delta\theta\right]$$
AIC, MDL
$$\approx \frac{d}{2n}$$

Landscape of error at singularity



Milner attractor



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

Dynamics of Learning

$$\frac{d\theta}{dt} = -\eta \nabla l, \qquad \frac{d\theta}{dt} = -\eta G^{-1} \nabla l$$

$$\frac{du}{dt} = f(u, z), \quad \frac{dz}{dt} = k(u, z)$$

$$\frac{du}{dz} = \frac{f(u,z)}{k(u,z)}, \qquad u^2 = z^2 - \frac{1}{2}\log|z| + c$$

Coordinate Transformation

$$\begin{cases} \boldsymbol{u} = \boldsymbol{w}_{2} - \boldsymbol{w}_{1} & : \boldsymbol{u} = 0 \quad \mathcal{R}_{1} \\ \boldsymbol{w} = \frac{v_{1}\boldsymbol{w}_{1} + v_{2}\boldsymbol{w}_{2}}{v} & \boldsymbol{w} = \boldsymbol{w}^{*} \\ v = v_{1} + v_{2} & v = v^{*} \\ z = \frac{v_{2} - v_{2}}{v} & z = \pm 1 \quad \mathcal{R}_{2} \end{cases}$$

Dynamics of Learning: Natural gradient works!!

$$\frac{d\theta}{dt} = -\eta \nabla l, \qquad \frac{d\theta}{dt} = -\eta G^{-1} \nabla l$$

$$\frac{du}{dt} = f(u, z), \quad \frac{dz}{dt} = k(u, z)$$

$$\frac{du}{dz} = \frac{f(u,z)}{k(u,z)}, \qquad u^2 = z^2 - \frac{1}{2}\log|z| + c$$



Dynamic vector fields: General case (|z|<1 part stable)



Dynamic vector fields: General case (|z|>1 part stable)

Adaptive Natural Gradient works well



Signal Processing

ICA : Independent Component Analysis

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



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

$$\boldsymbol{x} = A\boldsymbol{s}$$
 $x_i = \sum A_{ij} s_j$
 $\boldsymbol{y} = W\boldsymbol{x}$ $W = A^{-1}$

observations: x(1), x(2), ..., x(t) recover: s(1), s(2), ..., s(t)



Cocktail party experiment



• 5 microphones (sensors) and only 3 speakers

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1. Motivation

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

Semiparametric Statistical Model

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

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

x(1), x(2), ..., x(t)



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

Space of Matrices : Lie group



dX: **non-holonomic basis**

Information Geometry of ICA



Estimating Functions

$$\Delta W = -\eta F(y, W)$$
$$E_{W,r} \begin{bmatrix} F(y, W') \end{bmatrix} \begin{cases} = 0, & W' = W \\ \neq 0, & W' \neq W \end{cases}$$

estimating equation

$$\sum_{t} F(y_{t}, W) = 0 \qquad y_{t} = W x_{t}$$

learning
$$\Delta W_{t} = -\eta F(W_{t} x_{t})$$

Admissible class

$$F(y,W) = \{I - \varphi(y)y^T\}W$$

$$\tilde{F} = R(W)F(y,W) \qquad \{ o \varphi(y_i)y_j - \varphi(y_j)y_i\}W$$

$$\sum R(W)F(Wx_t) = 0: \text{ estimating equation}$$

on-line learning : $\Delta W_t = -\eta R(W_t)F(W_tx_t)$
canonical estimating function: $\frac{\partial \tilde{F}}{\partial W} = I$

Basis Given: overcomplete case Sparse Solution

$$x = As = \sum s_i a_i$$

many solutions
many $s_i \rightarrow 0$
 $x_t = \hat{A}s_t$





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).

Minkovskian Gradient

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

typical case:
$$\psi(\boldsymbol{\beta}) = \frac{1}{2} |\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}|^2 = \frac{1}{2} (\boldsymbol{\beta} - \boldsymbol{\beta}^*)^T G(\boldsymbol{\beta} - \boldsymbol{\beta}^*)$$

 $F(\boldsymbol{\beta}) = \frac{1}{p} \sum |\boldsymbol{\beta}_i|^p$; $p = 2, p = 1, p = 1/2$

Optimization under Sparsity Condition:

$$y = X \beta \quad (+n)$$

 $\boldsymbol{\beta}$: k-sparse



$$m > 2k \log n$$



Linear regression

$$y_t = \sum_{i=1}^k x_i^t \beta_i + n_t, \quad t = 1, 2, ... N$$

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{n} \qquad \boldsymbol{X} = \begin{bmatrix} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \\ \boldsymbol{x}_N \end{bmatrix}$$

Overcomplete: N < k under-determined → infinitely many solutions

Sparsity constraint solves the problem

Maximum likelihood estimator

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \sum_{t} \psi \left(y_{t} - \boldsymbol{\beta} \cdot \boldsymbol{x}_{t} \right), \quad \psi(u) = \frac{1}{2}u^{2}$$
$$\sum_{t} \psi' \left(y_{t} - \boldsymbol{\beta} \cdot \boldsymbol{x}_{t} \right) \boldsymbol{x}_{t} = 0$$

Euclidean case (Gaussian noise):

$$G = \nabla \nabla \psi = X^T X, \quad G \hat{\beta} = X^T y$$
$$\hat{\beta} = (X^T X)^{-1} X^T y = X^{\dagger} y \quad \text{Not sparse}$$

Sparse Solution $\min \psi(\boldsymbol{\beta}) = \min D[\boldsymbol{\beta} : \boldsymbol{\beta}^*] = \psi(\boldsymbol{\beta}) - \psi(\boldsymbol{\beta}^*) - \nabla \psi(\boldsymbol{\beta}^*)(\boldsymbol{\beta} - \boldsymbol{\beta}^*)$ $\nabla \psi(\boldsymbol{\beta}^*) = 0$ penalty $F_p(\boldsymbol{\beta}) = \sum |\boldsymbol{\beta}_i|^p = c$ $F_0(\boldsymbol{\beta}) = \#1[\boldsymbol{\beta}_i \neq 0]$: sparsest solution $F_1(\boldsymbol{\beta}) = \sum |\beta_i| : L_1$ solution $F_p(\beta): 0 \le p \le 1$ Sparse solution: overcomplete case $F_2(\boldsymbol{\beta}) = \sum |\beta_i|^2$: generalized inverse solution

orthogonal projection, dual projection

min $\Psi(\beta) = D[\beta:\beta^*]$, $F(\beta) = c$: dual geodesic projection





Fig. 1

L1-constrained optimization

- $\mathbf{P}_{\lambda} \quad \mathbf{Problem} \qquad \begin{array}{l} \min \ \psi(\boldsymbol{\beta}) + \lambda F(\boldsymbol{\beta}) & \mathbf{LARS} \\ \text{solution} \ \boldsymbol{\beta}^{*}(\lambda) & \lambda = \infty \to 0 \\ \boldsymbol{\beta}_{\lambda}^{*} = 0 \to \boldsymbol{\beta}^{*} \end{array} \\ \text{solutions} \quad \boldsymbol{\beta}_{\mathbf{c}}^{*} \text{ and } \boldsymbol{\beta}_{\lambda}^{*} : \text{ coincide, } \lambda = \lambda(\mathbf{c}), \quad \mathbf{p} \ge 1 \\ \mathbf{p} < 1: \ \lambda = \lambda(\mathbf{c}) \text{ multiple, noncontinuous} \\ \text{stability different} \end{array}$




Fig. 5 subgradient

LASSO path and LARS path (stagewise solution)

min $\psi(\boldsymbol{\beta})$: $F(\boldsymbol{\beta}) = c$ min $\psi(\boldsymbol{\beta}) + \lambda F(\boldsymbol{\beta})$

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

Active set and gradient

 $A(\boldsymbol{\beta}) = \left\{ i | \beta_i \neq 0 \right\}$ $\nabla F_p(\boldsymbol{\beta}) = \begin{cases} \operatorname{sgn}(\beta_i) | \beta_i|^{-(1-p)}, & i \in A \\ (-\infty, \infty), & i \notin A \\ [-1,1] \end{cases}$

Solution path

$$\nabla_{A}\varphi\left(\boldsymbol{\beta}_{c}^{*}\right) + \lambda_{c}\nabla_{A}F\left(\boldsymbol{\beta}_{c}^{*}\right) = 0, \quad \boldsymbol{\beta}_{c}^{*}$$

$$\left\{\nabla_{A}\nabla_{A}\varphi\left(\boldsymbol{\beta}_{c}^{*}\right) + \lambda_{c}\nabla_{A}\nabla_{A}F\left(\boldsymbol{\beta}_{c}^{*}\right)\right\} \cdot \dot{\boldsymbol{\beta}}_{c} = -\dot{\lambda}_{c}\nabla_{A}F\left(\boldsymbol{\beta}_{c}^{*}\right)$$

$$\dot{\boldsymbol{\beta}}_{c} = -\dot{\lambda}_{c}K^{-1}\nabla_{A}F\left(\boldsymbol{\beta}_{c}^{*}\right) \quad ; \quad \dot{\boldsymbol{\beta}}_{c} = \frac{d}{dc}\boldsymbol{\beta}_{c}$$

$$K = G\left(\boldsymbol{\beta}_{c}^{*}\right) + \lambda_{c}\nabla\nabla F\left(\boldsymbol{\beta}_{c}^{*}\right)$$

$$\left(\nabla\nabla F_{1} = 0; \quad \nabla F_{1} = (\operatorname{sgn}\boldsymbol{\beta}_{i}): L_{1}\right)$$

Solution path in the subspace of the active set

 $\nabla_{A} \varphi \left(\boldsymbol{\beta}_{\lambda}^{*} \right) + \lambda \nabla_{A} F \left(\boldsymbol{\beta}_{\lambda}^{*} \right) = 0 \qquad \nabla_{A} : \text{active direction}$ $\dot{\boldsymbol{\beta}}_{\lambda}^{*} = -K_{A}^{-1} \nabla_{A} F \left(\boldsymbol{\beta}_{\lambda}^{*} \right)$

turning point $A \rightarrow A'$

Gradient Descent Method $\min L(\beta+a): \quad g_{ij}a^{i}a^{j} = \varepsilon^{2}$ $\nabla L = \{\frac{\partial}{\partial \beta_{i}}L(\beta)\}: \quad \text{covariant}$ $\tilde{\nabla}L = \{\sum g^{ji}\frac{\partial}{\partial \beta_{i}}L(\beta)\}: \quad \text{contravariant}$

$$\beta_{t+1} = \beta_t - c \nabla L(\beta_t)$$

 \sim

Steepest direction of L

 $G(\boldsymbol{a}) = \sum g_{ij}(\boldsymbol{\beta}) a_i a_j$

Riemannian metric

 $G(ta) = |t|^{p} G(a) > 0$ Minkovskian metric

$$G(\boldsymbol{a}) = \sum |a_i|^p$$
. $p > 1$ Lp-norm

$$\frac{\delta}{\delta a} \{ \nabla L \cdot a - \lambda G(a) \} = 0$$

$$\delta G(\boldsymbol{a}) = p(\operatorname{sign} a_i) |a_i|^{p-1}$$

$$f_{i} = \frac{\partial}{\partial \beta_{i}} F\left(\boldsymbol{\beta}\right)$$

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

$$G(\boldsymbol{a}) = \sum g_{ij} a_i a_j, \quad \tilde{\nabla}F = G^{-1} \nabla f$$
 Natural gradient

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

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

$$i^* = \arg \max |f_i|$$
$$\max |f_i| = |f_{i^*}| = |f_{j^*}|$$
$$\left(\tilde{\nabla}F\right)_i = \begin{cases} 1, & \text{for } i = i^* \text{ and } j^*, \\ 0 & \text{otherwise.} \end{cases}$$

$$\boldsymbol{\beta}_{t+1} = \boldsymbol{\beta}_t - \eta \tilde{\nabla} F$$
 LASSO

Try for various p, p->1 Try for various noise function LASSO and flat geometry

Extended LARS (p = 1) and Minkovskian gradient

norm $\|\boldsymbol{a}\|_{p} = \sum |a_{i}|^{p}$ max $\psi(\boldsymbol{\beta} + \varepsilon \boldsymbol{a})$ under $\|\boldsymbol{a}\|_{p} = 1$ $\psi(\boldsymbol{\beta} + \varepsilon \boldsymbol{a}) - \lambda \|\boldsymbol{a}\|_{p}$ $p = 1^{+}$ $\nabla_{1}\psi(\boldsymbol{\beta}) = \mathbf{1}_{A} \begin{cases} \operatorname{sgn} \eta_{i}, & |\eta_{i}| = \max \{|\eta_{1}|, \dots, |\eta_{N}|\} \\ 0, & \text{otherwise} \end{cases}$ $\eta = \nabla \psi(\boldsymbol{\beta})$

$$i^* = \arg \max |f_i|$$
$$\max |f_i| = |f_{i^*}| = |f_{j^*}|$$
$$\left(\tilde{\nabla}F\right)_i = \begin{cases} 1, & \text{for } i = i^* \text{ and } j^*, \\ 0 & \text{otherwise.} \end{cases}$$

$$\int_{i} \left[0 \quad \text{otherwise.} \right]$$

$$\boldsymbol{\beta}_{t+1} = \boldsymbol{\beta}_t - \eta \tilde{\nabla} F$$
 LARS

L1/2 constraint: non-convex optimization

λ -trajectory and -trajectory

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

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





LASSO and LARS :

$$p > 1$$
 : $\boldsymbol{\beta}_c^*$ is non-sparse
 $p = 1$: sparse



Minkovskian gradient

$$D\left[\boldsymbol{\beta}_{c}:\boldsymbol{\beta}^{*}\right] - \lambda F\left(\boldsymbol{\beta}\right)$$
$$\nabla \varphi\left(\boldsymbol{\beta}_{c}\right) - \nabla \varphi\left(\boldsymbol{\beta}^{*}\right) - \lambda_{c} \nabla F\left(\boldsymbol{\beta}_{c}\right) = 0$$
$$\boldsymbol{\eta}_{c} - \boldsymbol{\eta}^{*} = \lambda_{c} \nabla F\left(\boldsymbol{\beta}_{c}\right)$$





$$\nabla \nabla \varphi (\boldsymbol{\beta}_{c}) \cdot \dot{\boldsymbol{\beta}}_{c} - \lambda_{c} \nabla \nabla F (\boldsymbol{\beta}_{c}) \cdot \dot{\boldsymbol{\beta}}_{c} = \dot{\lambda}_{c} \nabla F (\boldsymbol{\beta}_{c})$$

$$G \qquad H$$

$$\dot{\boldsymbol{\beta}}_{c} = (G - \lambda_{c} H)^{-1} \nabla F (\boldsymbol{\beta}_{c})$$

Solution Path :λ↔c not continuous, not-monotone jump

 $\beta_{\lambda} \Leftrightarrow \beta_{c}$

Linear Programming

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

max $\sum c_i x_i$
 $\psi(\mathbf{x}) = \sum_i \log(\sum A_{ij} x_j - b_i)$



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





Convex Programming — Inner Method

 $LP: Ax \ge b$

min $c \cdot x$

Barrier function

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

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

 I_c



Simplex method ; inner method

Polynomial-Time Algorithm



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

Integration of evidences:

 $X_1, X_2, \dots X_m$

arithmetic mean geometric mean harmonic mean α -mean

Generalized mean: f-mean f(u): monotone; f-representation of u

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

scale free $m_f(ca,cb) = cm_f(a,b)$ α -representation $f_{\alpha}(u) = u^{\frac{1-\alpha}{2}}, \quad \alpha \neq 1$ $\log u, \quad \alpha = 1$



Various Means



Any other mean?

α – Family of Distributions

$$\{p_1(s), \cdots, p_k(s)\} \qquad p(x; \theta) = f_\alpha^{-1}\{\sum \theta_i f_\alpha(p_i(x))\}$$

mixture family :

$$p_{mix}(s) = \sum_{i=1}^{\kappa} t_i p_i(s), \qquad \sum t_i = 1$$

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



 α -geodesic projection



robust estimator