2015 Workshop on High-Dimensional Statistical Analysis
DEC.11 (Friday) ~ DEC. 15 (Tuesday)
Humanities and Social Sciences Center, Academia Sinica, Taiwan

Information Geometry
and
Spontaneous Data Learning

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Spontaneous learning?

We focus on a collapse of consistency for estimation

Model assumes unimodality;

the true distribution may be multimodal.

There is a wide class of consistent estimators

Select the optimal estimator under a fixed model

to get the information for the true distribution

Cf. Model selection

Power divergence

β-cross entropy $$C_\beta(g,f) = -\frac{1}{\beta}\int f^\beta g \mathrm{d}\mu + \frac{1}{\beta+1}\int f^{\beta+1}\mathrm{d}\mu$$

β-diagonal entropy $$H_\beta(f) = C_\beta(f,f)$$

β-divergence $$D_\beta(g,f) = C_\beta(g,f) - H_\beta(g)$$

Hill (1971), Tsallis (1988) Basu et al (1998) Minami-Eguchi (2002)

$$U(s) = \frac{1}{1+\beta}(1+\beta s)^{\frac{1+\beta}{\beta}},\ \phi(t) = \frac{t^\beta - 1}{\beta},\ C_U(f,g) = \int \{-\phi(g)f + U(\phi(g))\}\mathrm{d}\mu$$
$$= C_\beta(f,g)$$

Projective power divergence

γ-cross entropy $$C_\gamma(g,f) = -\frac{1}{\gamma(\gamma+1)}\int \left\{\frac{f(x)}{\| f \|}\right\}^\gamma g(x)\mathrm{d}\mu(x)$$

$$\| f \| = \left\{\int f(x)^{\gamma+1}\mathrm{d}\mu(x)\right\}^{\frac{1}{1+\gamma}} \quad (\text{Lebesgue } \mathrm{L}_p \text{ norm}, p = \gamma+1)$$

γ-diagonal entropy $$H_\gamma(f) = C_\gamma(f,f)$$

γ-divergence $$D_\gamma(g,f) = C_\gamma(g,f) - H_\gamma(g)$$

Fujisawa-Eguchi (2008), Eguchi-Kato (2010)

Three properties

$$C_\gamma(g,f) = -\int \left(\frac{f}{\|f\|}\right)^\gamma g \, \mathrm{d}\mu$$

1. linearity $\quad C_\gamma(\alpha g+\beta h, f) = \alpha C_\gamma(g,f) + \beta C_\gamma(h,f)$

2. scale invariance $\quad C_\gamma(g,\lambda f) = C_\gamma(g,f) \quad (\forall \lambda > 0)$

3. lower bound $\quad C_\gamma(g,f) \geq H_\gamma(g)$ or $D_\gamma(g,f) \geq 0$

Characterization

Thm: Let $F(g,f) = \Phi\left(\int \rho(f)\right) \int \psi(f) g$

If F satisfies

(i) $F(g, \lambda f) = F(g,f) \quad (\forall \lambda > 0)$

(ii) $F(g,f) \geq F(g,g)$

then there is a constant γ suct that $F(g,f) = C_\gamma(g,f)$

Remark: If $(\Phi(Y), \rho(f), \psi(f)) = (Y^{-\frac{\gamma}{1+\gamma}}, f^{1+\gamma}, f^\gamma)$,

then $F(g,f) = \left(\int f(x)^{1+\gamma} dx\right)^{-\frac{\gamma}{1+\gamma}} \int f^\gamma g = C_\gamma(g,f)$

γ-power divergence geometry

For a model $M = \{f_\theta(x) : \theta \in \Theta\}$

γ -**power metric**

$$G_{ij}^{(\gamma)}(\theta) = \frac{1}{\gamma}\int \frac{\partial f_\theta}{\partial \theta_i}\frac{\partial}{\partial \theta_j}\left(\frac{f_\theta}{\| f_\theta \|}\right)^\gamma \mathrm{d}\mu$$

γ -**power connection pair**

$$\Gamma_{ij,k}^{(\gamma)}(\theta) = \frac{1}{\gamma}\int \frac{\partial^2 f_\theta}{\partial \theta_i \partial \theta_j}\frac{\partial}{\partial \theta_k}\left(\frac{f_\theta}{\| f_\theta \|}\right)^\gamma \mathrm{d}\mu$$

$$^*\Gamma_{ij,k}^{(\gamma)}(\theta) = \frac{1}{\gamma}\int \frac{\partial f_\theta}{\partial \theta_k}\frac{\partial^2}{\partial \theta_j \partial \theta_j}\left(\frac{f_\theta}{\| f_\theta \|}\right)^\gamma \mathrm{d}\mu$$

β-**power metric**

$$G_{ij}^{(\beta)}(\theta) = \frac{1}{\beta}\int \frac{\partial f_\theta}{\partial \theta_i}\frac{\partial f_\theta^{\beta}}{\partial \theta_j} \mathrm{d}\mu$$

β -**power connection pair**

$$\Gamma_{ij,k}^{(\beta)}(\theta) = \frac{1}{\beta}\int \frac{\partial^2 f_\theta}{\partial \theta_i \partial \theta_j}\frac{\partial f_\theta^{\beta}}{\partial \theta} \mathrm{d}\mu$$

$$^*\Gamma_{ij,k}^{(\beta)}(\theta) = \frac{1}{\beta}\int \frac{\partial f_\theta}{\partial \theta_k}\frac{\partial^2 f_\theta^{\beta}}{\partial \theta_j \partial \theta_j} \mathrm{d}\mu$$

γ-estimation

Parametric model $M = \{ f_\theta(x) : \theta \in \Theta \}$

γ-power loss function $L_\gamma(\theta) = -\frac{1}{n}\frac{1}{\gamma(\gamma+1)}\sum_{i=1}^{n}\left(\frac{f_\theta(x_i)}{\| f_\theta \|}\right)^\gamma$

γ-estimator $\hat{\theta}_\gamma = \arg\min_{\theta \in \Theta} L_\gamma(\theta)$

β-power loss function $L_\beta(\theta) = -\frac{1}{n\beta}\sum_{i=1}^{n} f(x_i,\theta)^\beta + \frac{1}{\beta+1}\| f(\cdot,\theta) \|^{\beta+1}$

β-estimator $\hat{\theta}_\beta = \arg\min_{\theta \in \Theta} L_\beta(\theta)$

Consistency

$$\text{If } x_1,\ldots,x_n \underset{\text{iid}}{\sim} g(x), \text{ then } \hat{\theta}_\gamma \underset{\text{as}}{\to} \theta_g$$

$$\text{where } \theta_g = \arg\min_{\theta \in \Theta} C_\gamma(g, f(\cdot,\theta))$$

$$\text{If } g(x) = f(x,\theta), \text{ then } \quad \theta_g = \theta$$

$$\text{because } C_\gamma(f(\cdot,\theta), f(\cdot,\theta^*)) \geq H_\gamma(f(\cdot,\theta))$$

$$\boxed{\text{If } x_1,\ldots,x_n \underset{\text{iid}}{\sim} f(x,\theta), \text{ then } \hat{\theta}_\gamma \underset{\text{as}}{\to} \theta}$$

Cf. Wald (1947), White (1982)

γ-estimating function

γ-estimating function

$$\mathrm{e}_{\gamma}(x,\theta) = f_{\theta}(x)^{\gamma} S_{\theta}(x) - \boxed{\frac{f_{\theta}(x)^{\gamma}}{\| f_{\theta} \|^{\gamma+1}}} \mathrm{E}_{f_{\theta}}(f_{\theta}{}^{\gamma} S_{\theta})$$

β-estimating function

$$\mathrm{e}_{\beta}(x,\theta) = f_{\theta}(x)^{\beta} S_{\theta}(x) - \mathrm{E}(f_{\theta}{}^{\beta} S_{\theta})$$

Asymptotic variance

$$\mathrm{var}_{\mathrm{A}}(\hat{\theta}_{\gamma}) = \frac{1}{n}\left\{\mathrm{E}\left(\frac{\partial \mathrm{e}_{\gamma}}{\partial \theta^{\mathrm{T}}}\right)\right\}^{-1} \mathrm{Var}(\mathrm{e}_{\gamma}) \left\{\mathrm{E}\left(\frac{\partial \mathrm{e}_{\gamma}{}^{\mathrm{T}}}{\partial \theta}\right)\right\}^{-1}$$

Note: $\beta = 0 \quad \Rightarrow \quad \mathrm{e}_{\beta}(x,\theta) = S_{\theta}(x)$; $\gamma = 0 \quad \Rightarrow \quad \mathrm{e}_{\gamma}(x,\theta) = S_{\theta}(x)$

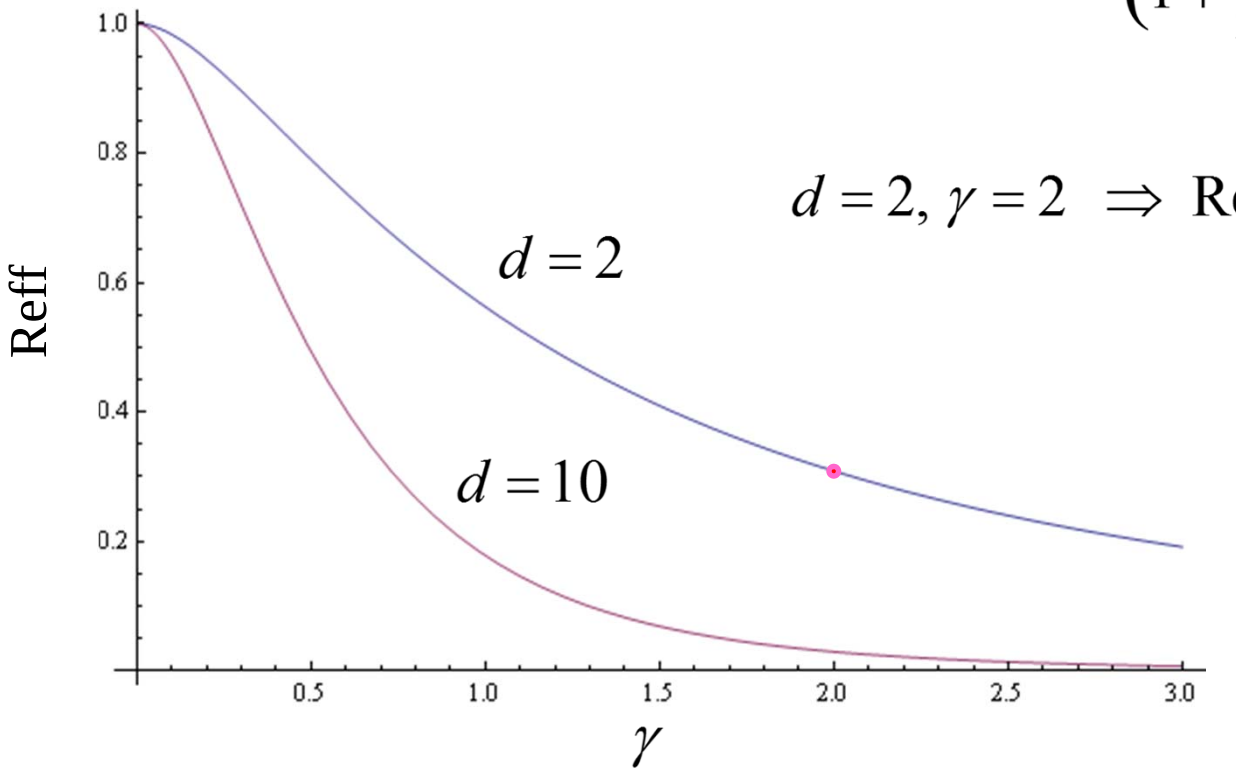
For any $\gamma \neq 0$, $\hat{\theta}_{\gamma}$ is ineffecient relative to MLE (Also $\hat{\theta}_{\beta}$)

Relative efficiency for γ-estimator

Normal mean model $f(\boldsymbol{x},\boldsymbol{\theta}) = (2\pi)^{-d/2} \exp\{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\theta})^{\mathrm{T}}(\boldsymbol{x}-\boldsymbol{\theta})\}, \quad \boldsymbol{x} \in \mathbb{R}^d$

Relative efficiency $$\mathrm{Reff} = \frac{\det(\mathrm{var}_{\mathrm{A}}(\hat{\boldsymbol{\theta}}_{\mathrm{ML}}))}{\det(\mathrm{var}_{\mathrm{A}}(\hat{\boldsymbol{\theta}}_{\gamma}))} = \frac{1}{\left(1+\frac{\gamma^2}{2\gamma+1}\right)^{-\frac{d+2}{2}}} < 1$$

$$d = 2,\ \gamma = 2 \ \Rightarrow\ \mathrm{Reff} = 0.309$$



γ-estimator for normal mean

γ-loss function $L_\gamma(\boldsymbol{\theta}) \propto -\sum_{i=1}^{n} f(\boldsymbol{x}_i, \boldsymbol{\theta})^\gamma$ for normal mean model

$$\frac{\partial}{\partial \boldsymbol{\theta}} L_\gamma(\boldsymbol{\theta}) \propto -\sum_{i=1}^{n} f(\boldsymbol{x}_i, \boldsymbol{\theta})^\gamma (\boldsymbol{x}_i - \boldsymbol{\theta}) = 0$$

$\hat{\boldsymbol{\theta}}_\gamma$ is a weighted mean: $\hat{\boldsymbol{\theta}}_\gamma = \dfrac{\sum \{f(\boldsymbol{x}_i, \hat{\boldsymbol{\theta}}_\gamma)\}^\gamma \boldsymbol{x}_i}{\sum \{f(\boldsymbol{x}_i, \hat{\boldsymbol{\theta}}_\gamma)\}^\gamma}$

Iteratively reweighted mean

$$\boldsymbol{\theta}_{t+1} \leftarrow \frac{\sum \{f(\boldsymbol{x}_i, \boldsymbol{\theta}_t)\}^\gamma \boldsymbol{x}_i}{\sum \{f(\boldsymbol{x}_i, \boldsymbol{\theta}_t)\}^\gamma} \quad \text{starting from } \hat{\boldsymbol{\theta}}_0 = \hat{\boldsymbol{\theta}}_{\mathrm{MLE}}$$

Note: β-estimator $\hat{\boldsymbol{\theta}}_\beta$ is the same as γ-estimator $\hat{\boldsymbol{\theta}}_\gamma$

γ-estimator for normal mean and variance

Normal model $$M = \{ \; f(\boldsymbol{x},\theta,V) = \det(2\pi V)^{-\frac{1}{2}} \exp\{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\theta})^{\mathrm{T}} V^{-1}(\boldsymbol{x}-\boldsymbol{\theta})\}$$

γ-loss function $$L_\gamma(\boldsymbol{\theta},\boldsymbol{V}) = -\frac{1}{n}\frac{(2\pi)^d}{\gamma(\gamma+1)^{d+1}}\sum_{i=1}^{n}\det(V)^{-\frac{1}{2}\frac{\gamma}{\gamma+1}} f(\boldsymbol{x}_i,\boldsymbol{\theta},\boldsymbol{V})^\gamma$$

γ-estimator $$\hat{\boldsymbol{\theta}}_\gamma = \frac{\sum\{f(\boldsymbol{x}_i,\hat{\boldsymbol{\theta}}_\gamma,\hat{\boldsymbol{V}}_\gamma)\}^\gamma \boldsymbol{x}_i}{\sum\{f(\boldsymbol{x}_i,\hat{\boldsymbol{\theta}}_\gamma,\hat{\boldsymbol{V}}_\gamma)\}^\gamma}$$

$$\hat{\boldsymbol{V}}_\gamma = \frac{(\gamma+1)\sum\{f(\boldsymbol{x}_i,\hat{\boldsymbol{\theta}}_\gamma,\hat{\boldsymbol{V}}_\gamma)\}^\gamma(\boldsymbol{x}_i-\hat{\boldsymbol{\theta}}_\gamma)(\boldsymbol{x}_i-\hat{\boldsymbol{\theta}}_\gamma)^{\mathrm{T}}}{\sum\{f(\boldsymbol{x}_i,\hat{\boldsymbol{\theta}}_\gamma,\hat{\boldsymbol{V}}_\gamma)\}^\gamma}$$

Note: β-estimator $\hat{\boldsymbol{V}}_\beta$ has not such a weighted expression

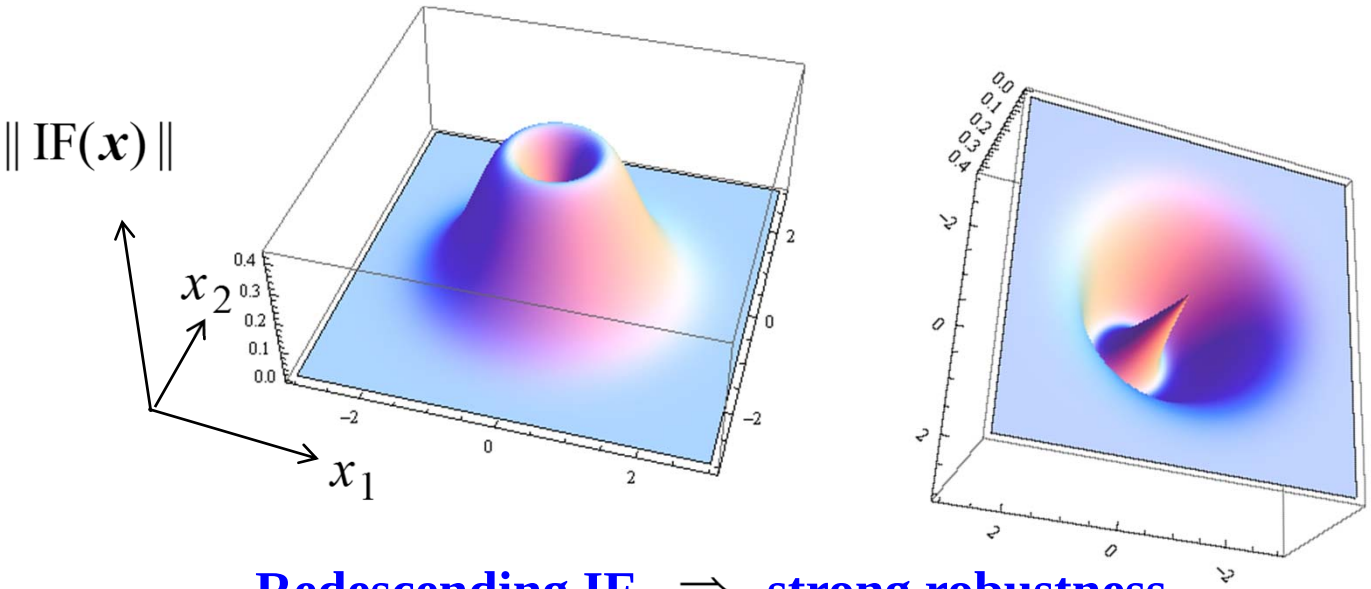
Influence function of γ-estimator

γ-estimator functional $$\hat{\boldsymbol{\theta}}_\gamma(g) = \arg\min_{\boldsymbol{\theta}\in\Theta} C_\gamma(g, f_{\boldsymbol{\theta}})$$

ε-contamination model $$g_\varepsilon(\boldsymbol{x}) = (1-\varepsilon) f(\boldsymbol{x},\boldsymbol{\theta}) + \varepsilon\delta(\boldsymbol{x})$$

$\delta(\boldsymbol{x})$ is Dirac delta function

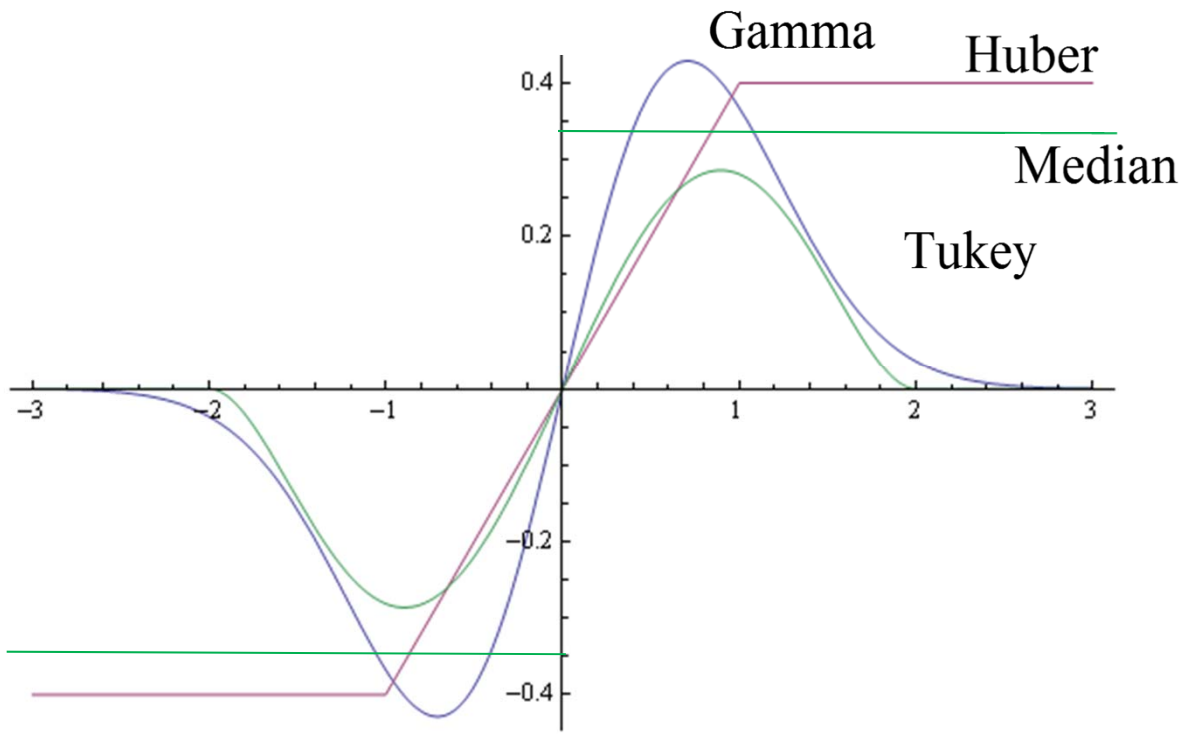
Influence function $$\mathrm{IF}(\boldsymbol{x}) = \frac{\partial}{\partial\varepsilon}\hat{\boldsymbol{\theta}}_\gamma(g_\varepsilon)|_{\varepsilon=0} = f(\boldsymbol{x},\boldsymbol{\theta})^\gamma(\boldsymbol{x}-\boldsymbol{\theta})$$



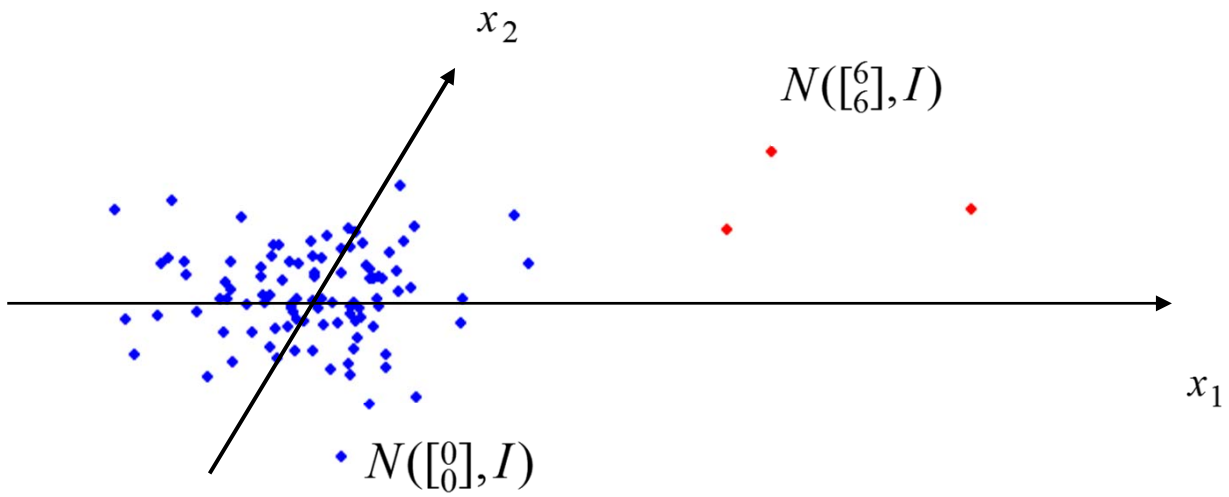
Redescending IF $\Rightarrow$ **strong robustness**

Influence functions

γ-weight	$xe^{-\frac{\gamma}{2}x^2}$
Median weight	$\mathrm{sgn}(x)$
Huber's weight	$xI_{[-c,c]}(x)+cI_{(c,\infty)}(x)-cI_{(-\infty,-c)}(x)$
Tukey's biweight	$x(1-x^2/c^2)^2 I_{[-c,c]}(x)$

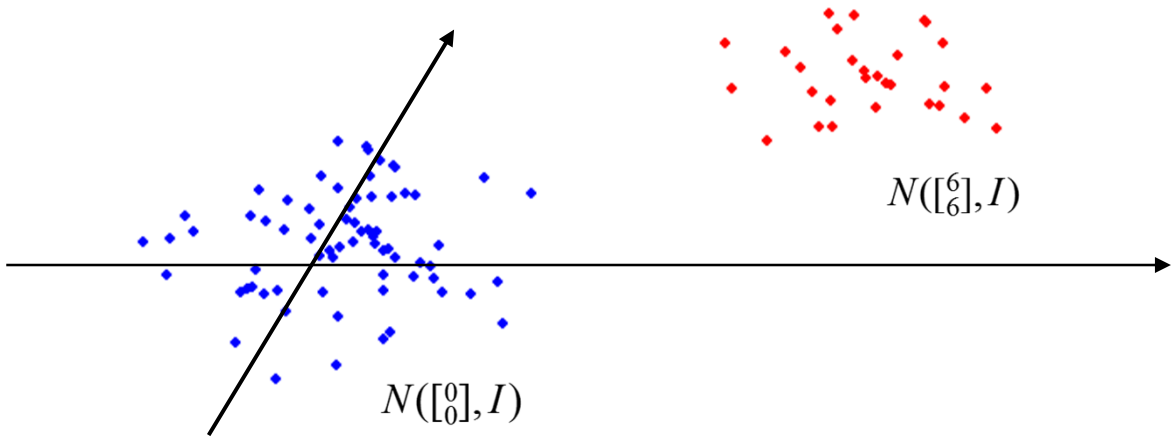


Robustness



true value	(0, 0)	(0, 0) + **outlying (6,6)**
maximum likelihood	(–0.0738, 0.0065)	(–0.1082, 0.1612)
median	(0.0260,-0.0606)	(0.0166,–0.0241)
γ–estimator (γ=1)	(–0.0192, 0.0279)	(–0.0192, 0.0279)

Super robustness



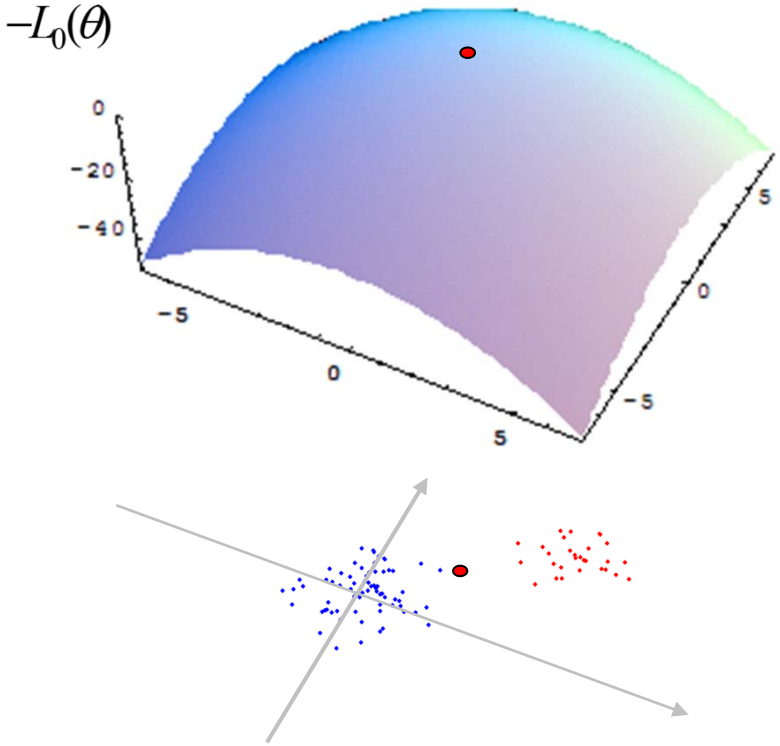
true value	(0, 0)	(0, 0) + **more outlying (6,6)**
maximum likelihood	(0.0067, –0.0196)	(1.93068, 1.76655)
median	(-0.06663, 0.0429)	(0.56484, 0.399286)
γ-estimator (γ=1)	(0.01069, 0.01595)	(0.01069, 0.01595)

Convex Learning

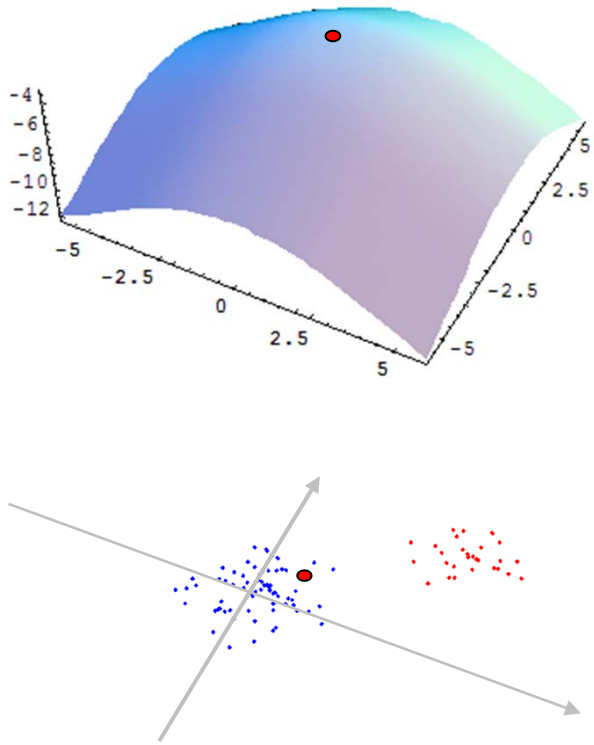
$$L_0(\mu) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^{\mathrm{T}}(x_i - \mu)$$

$$L(\mu) = \frac{1}{n}\sum_{i=1}^{n}\| x_i - \mu \|_{L_1}$$

MLE $\begin{bmatrix} 1.93 \\ 1.76 \end{bmatrix}$

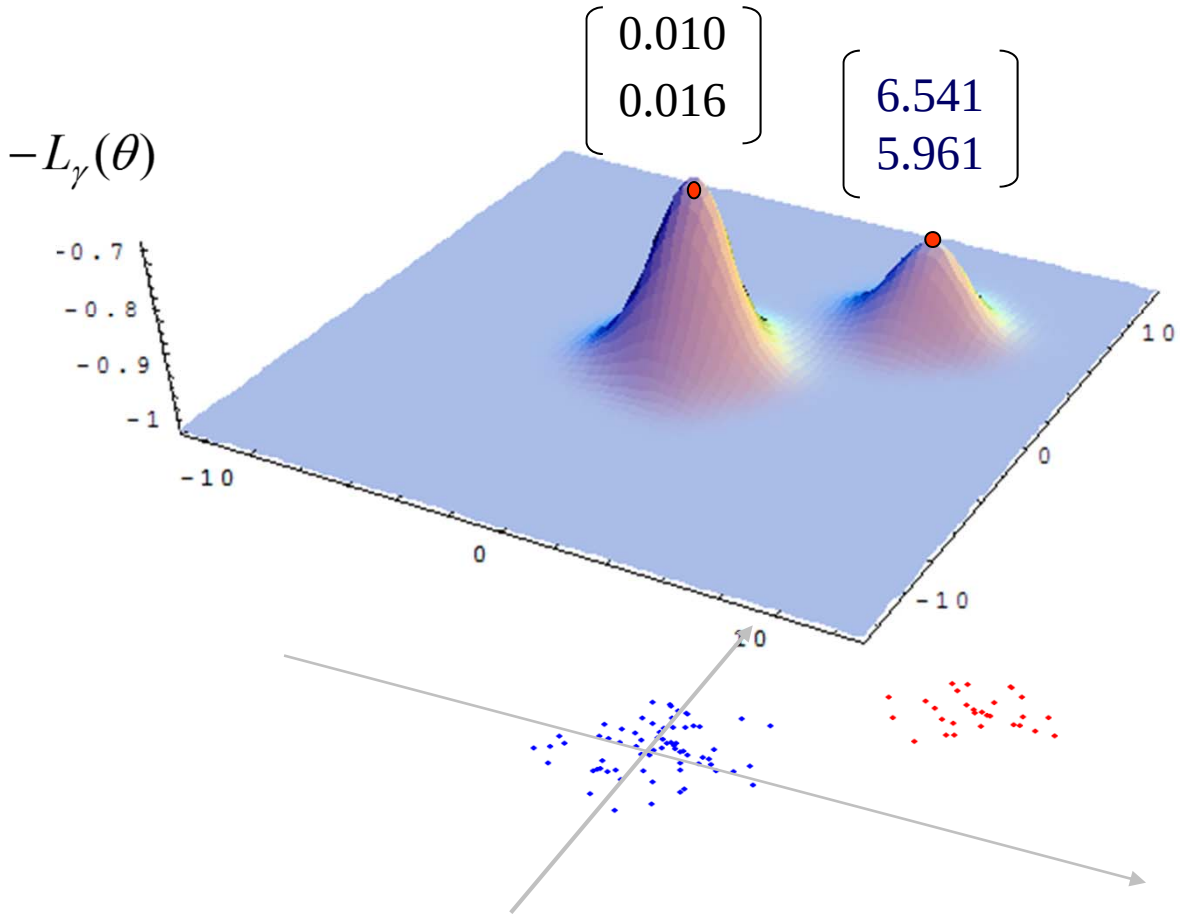


Median $\begin{bmatrix} 0.565 \\ 0.399 \end{bmatrix}$

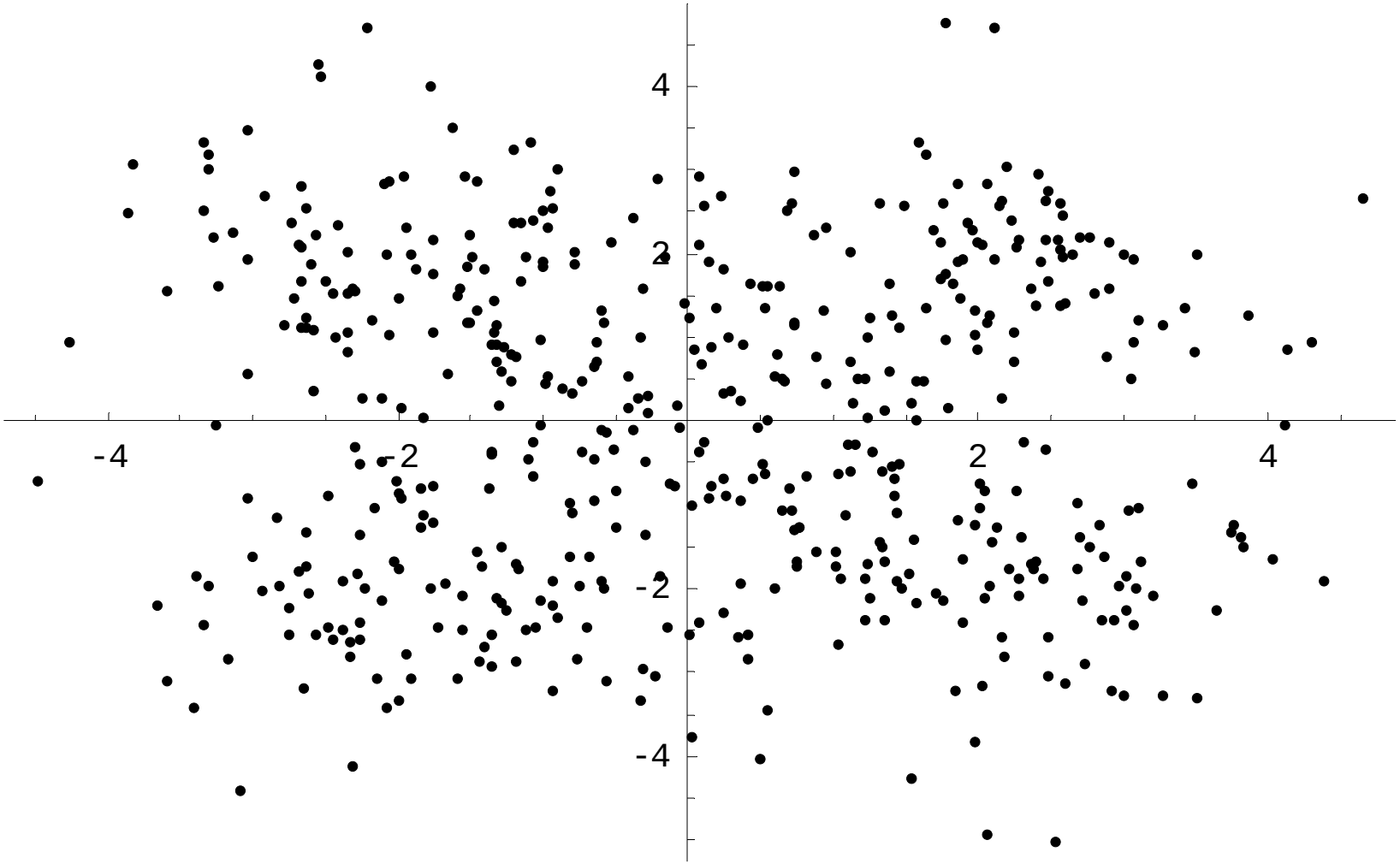


Non-convex learning

$$L_\gamma(\mu) = -\frac{1}{\gamma(\gamma+1)}\frac{1}{n}\sum_{i=1}^{n} e^{-\frac{\gamma}{2}(x_i-\mu)^{\mathrm{T}}(x_i-\mu)}$$



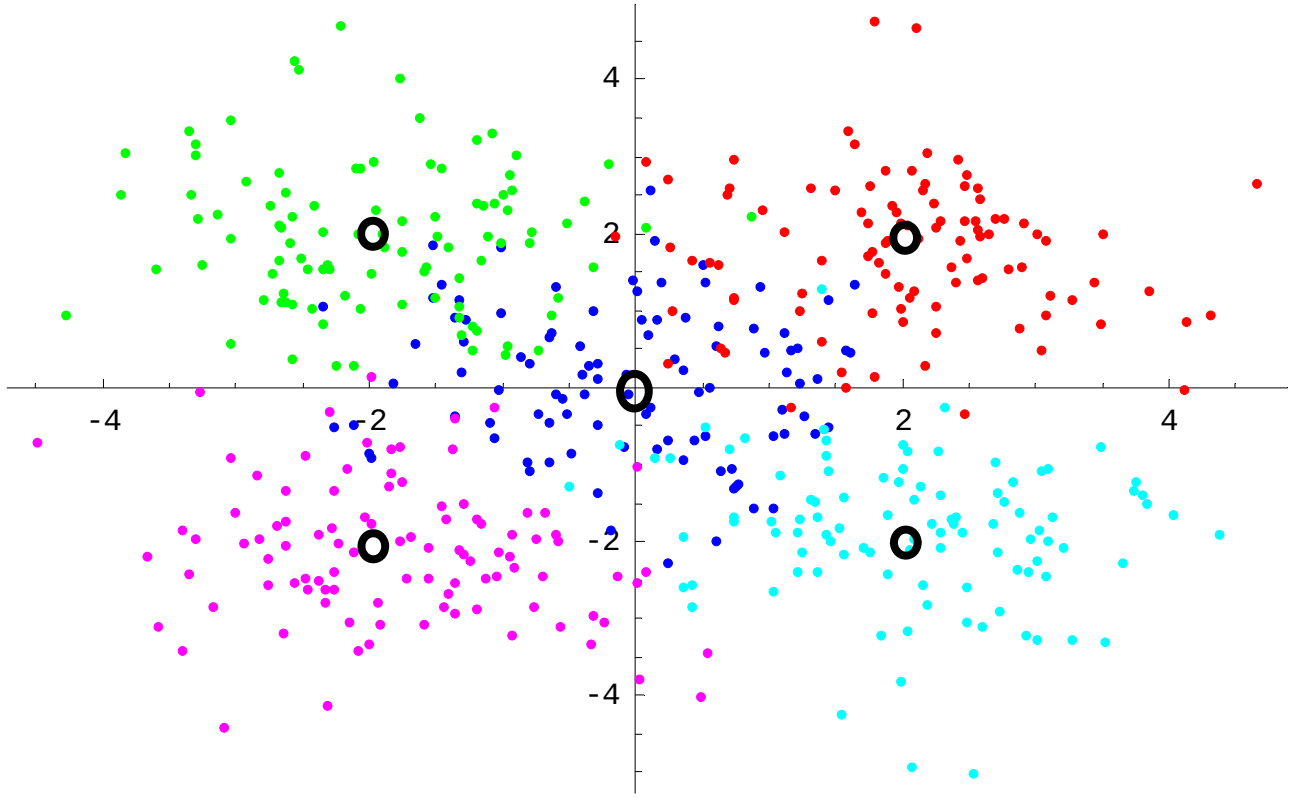
A data plot



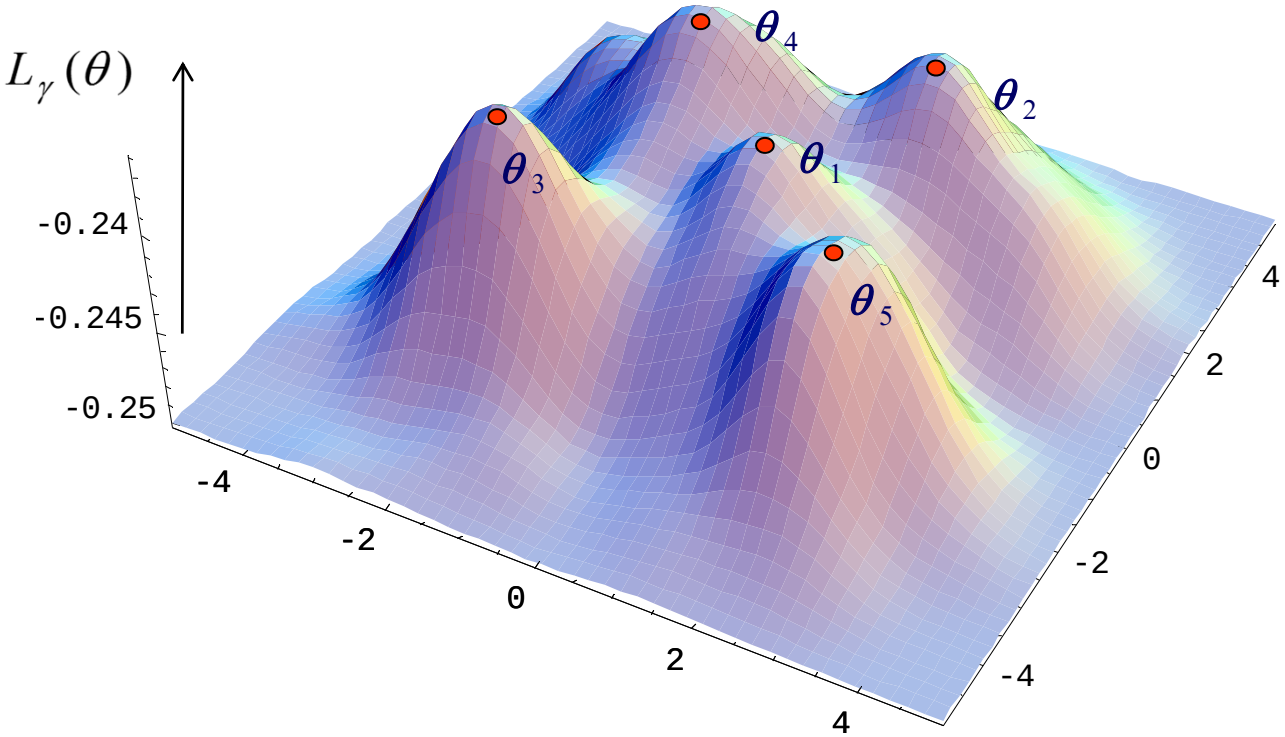
Five-mixture

Deta set $\{\boldsymbol{x}_i\}_{i=1}^n$ follows a data density

$$p(\boldsymbol{x}) = \frac{1}{5}\phi(\boldsymbol{x}, \begin{bmatrix} 0 \\ 0 \end{bmatrix}) + \frac{1}{5}\phi(\boldsymbol{x}, \begin{bmatrix} 2 \\ 2 \end{bmatrix}) + \frac{1}{5}\phi(\boldsymbol{x}, \begin{bmatrix} 2 \\ -2 \end{bmatrix}) + \frac{1}{5}\phi(\boldsymbol{x}, \begin{bmatrix} -2 \\ 2 \end{bmatrix}) + \frac{1}{5}\phi(\boldsymbol{x}, \begin{bmatrix} -2 \\ -2 \end{bmatrix})$$



Plot of γ-loss



$\theta_1 = \{-0.6040, 0.4878\}$, Loss = -0.4576

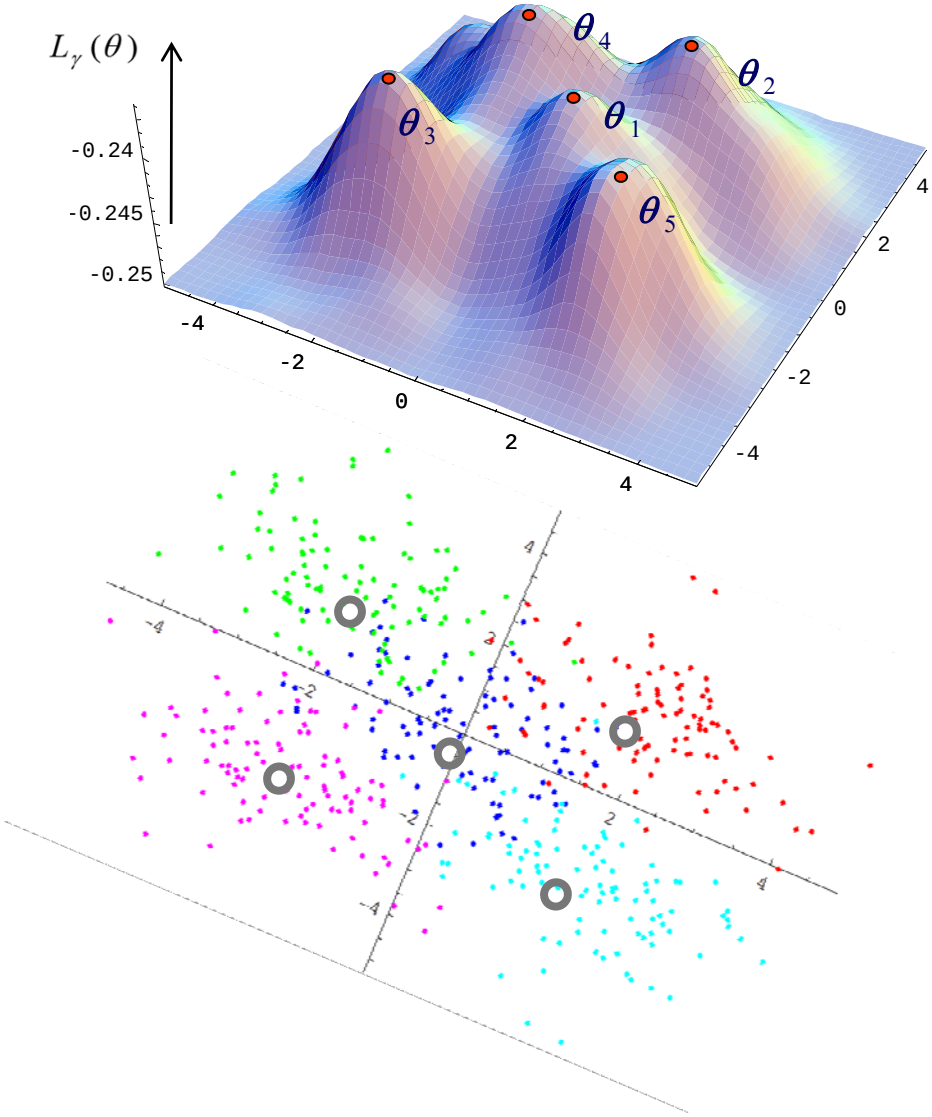
$\theta_2 = \{2.095, 1.846\}$, Loss = -0.4584

$\theta_3 = \{-1.595, -2.028\}$, Loss = -0.4575

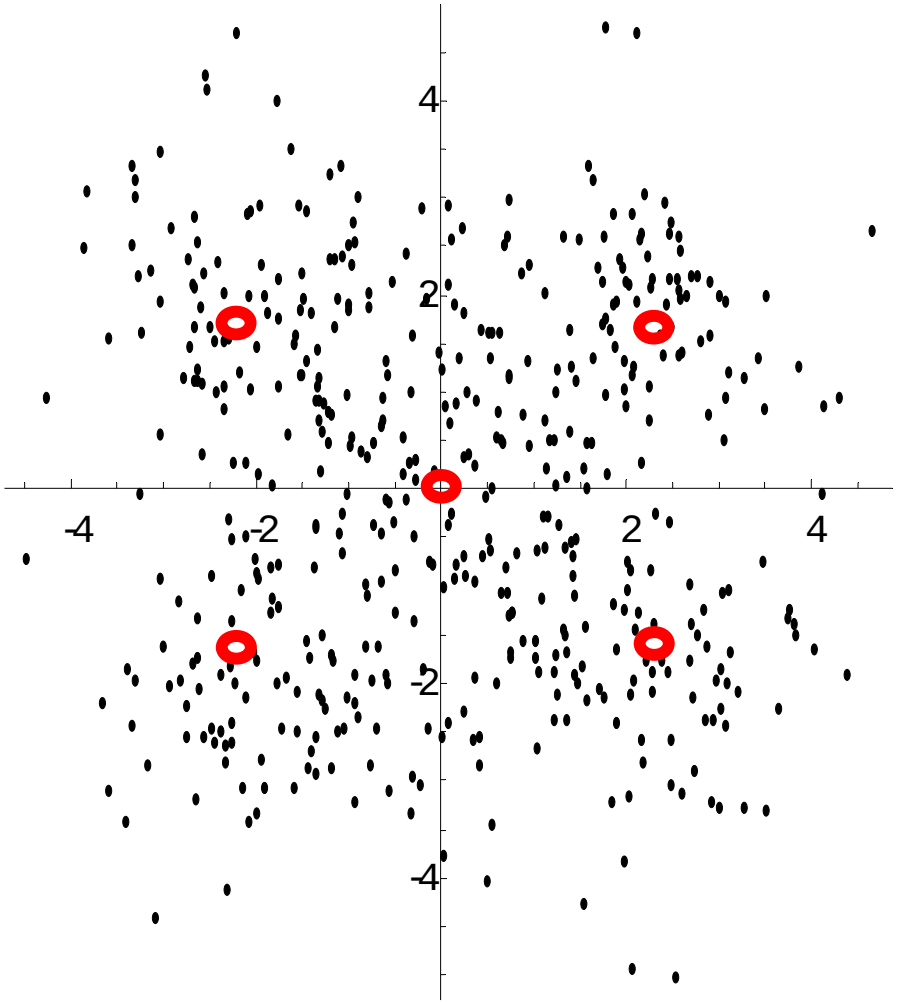
$\theta_4 = \{-1.437, 1.287\}$, Loss = -0.4576

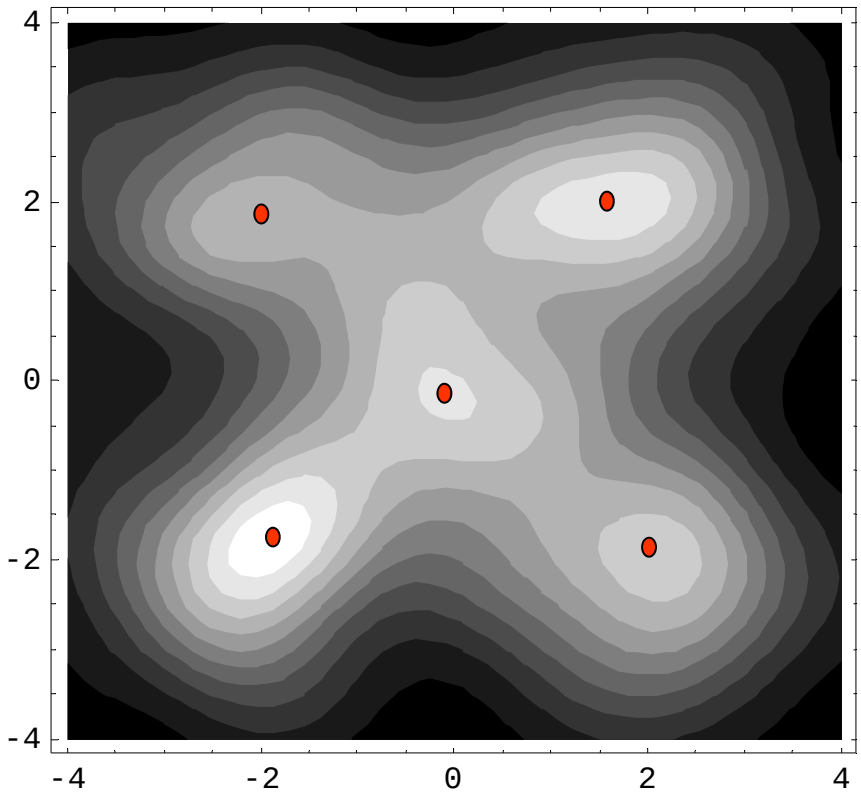
$\theta_5 = \{1.268, -1.277\}$, Loss = -0.4584

Detecting hidden structure!



Cluster Number = 5





Clustering algorithm

$$\text{IRM}: \quad \boldsymbol{\mu} \leftarrow \sum_{i=1}^{n} w_i(\boldsymbol{\mu})\boldsymbol{x}_i, \qquad w_i(\boldsymbol{\mu}) = \frac{\{f(\boldsymbol{x}_i, \boldsymbol{\mu})\}^{\gamma}}{\sum \{f(\boldsymbol{x}_i, \boldsymbol{\mu})\}^{\gamma}}$$

Step 1. Find $\boldsymbol{\mu}_1 \xleftarrow{\text{IRM}} \boldsymbol{\mu}_{\text{ML}}$

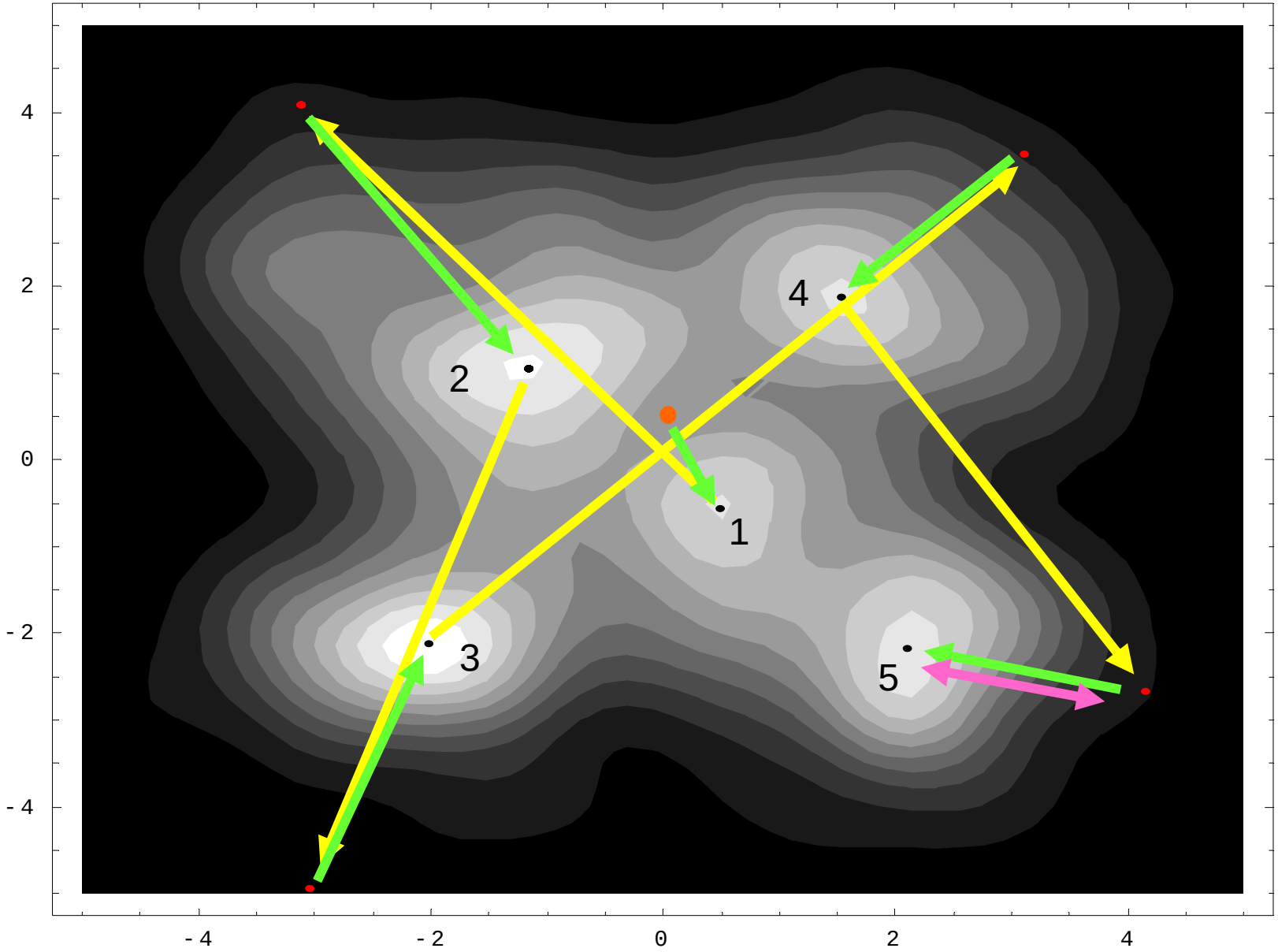
Step 2. Find $\boldsymbol{\mu}_{t+1} \xleftarrow{\text{IRM}} \boldsymbol{\mu}_{0t}$ for $t \geq 1$

where $\boldsymbol{\mu}_{0t} = \arg\max \{ \min_{1 \leq s \leq t} \| \boldsymbol{\mu} - \boldsymbol{\mu}_s \| : \boldsymbol{\mu} \in \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\} \}$

Repeat until $\boldsymbol{\mu}_{k+1} \in \{\boldsymbol{\mu}_1, \cdots, \boldsymbol{\mu}_k\}$.

Cf. k-means, model-based

Starting from MLE



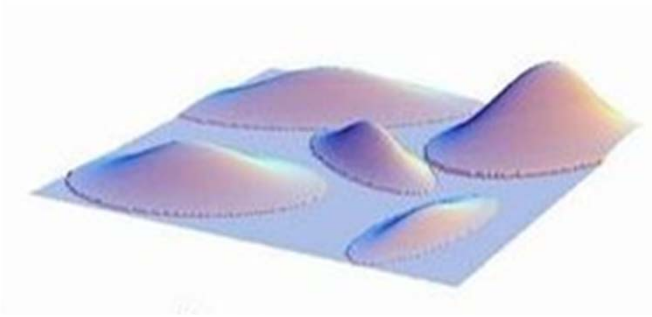
Variance adapt

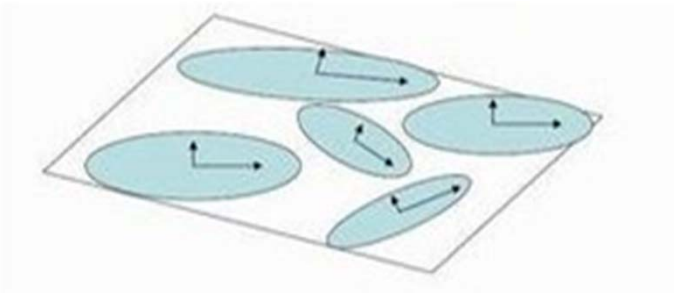
γ-loss function

$$L_\gamma(\mu\ ,\Sigma) = -\frac{1}{n}\det(\Sigma)^{-\frac{\gamma}{1+\gamma}}\sum_{i=1}^{n}\exp\{-\tfrac{\gamma}{2}(x_i-\mu)^{\mathrm{T}}\Sigma^{-1}(x_i-\mu)\}$$

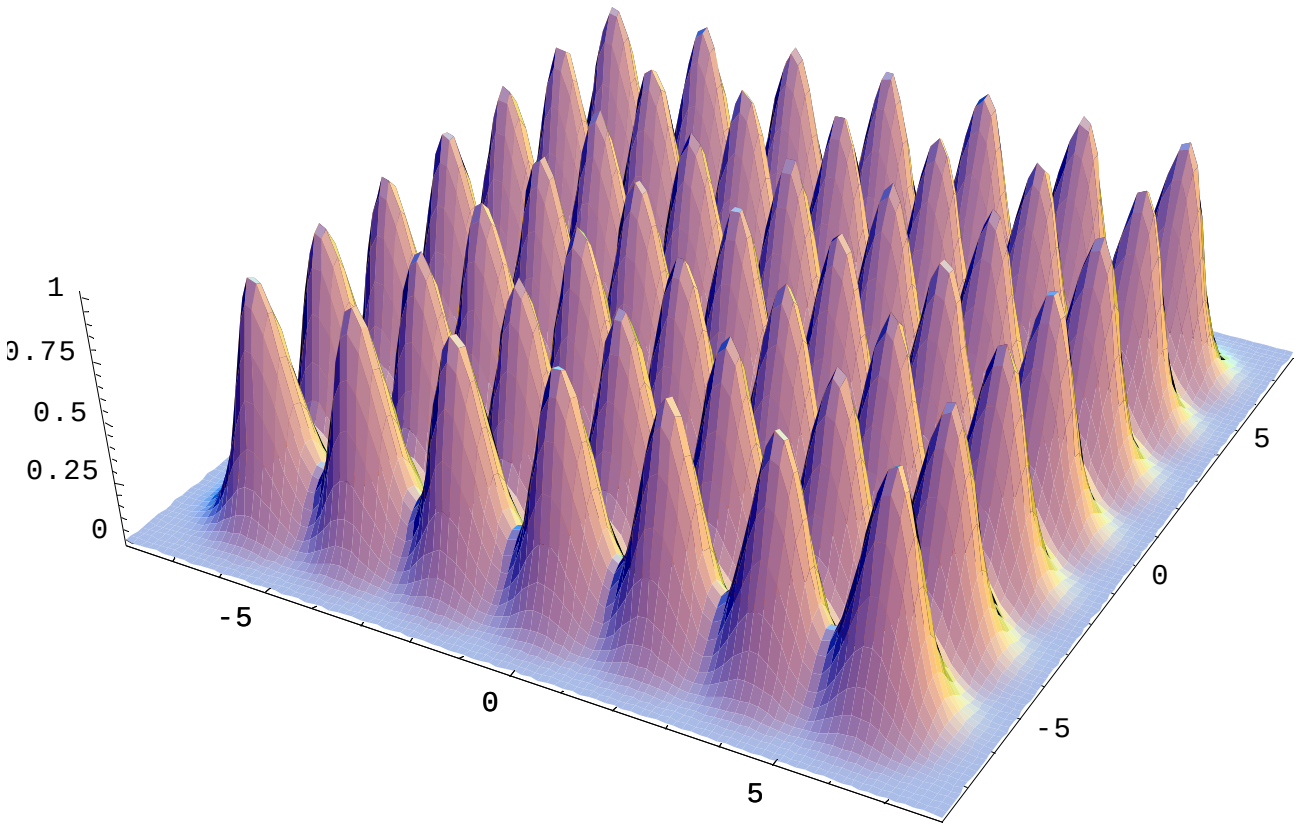
$$\text{IRV} \quad (**) \quad \boldsymbol{\Sigma} \quad \leftarrow \quad (1+\gamma)\sum_{i=1}^{n} w_i(\boldsymbol{\mu},\boldsymbol{\Sigma})(\boldsymbol{x}_i-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}_i-\boldsymbol{\mu})$$

$$\text{with weights} \quad w_i(\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{f(\boldsymbol{x}_i,\boldsymbol{\mu},\boldsymbol{\Sigma})^\gamma}{\sum f(\boldsymbol{x}_i,\boldsymbol{\mu},\boldsymbol{\Sigma})^\gamma}$$



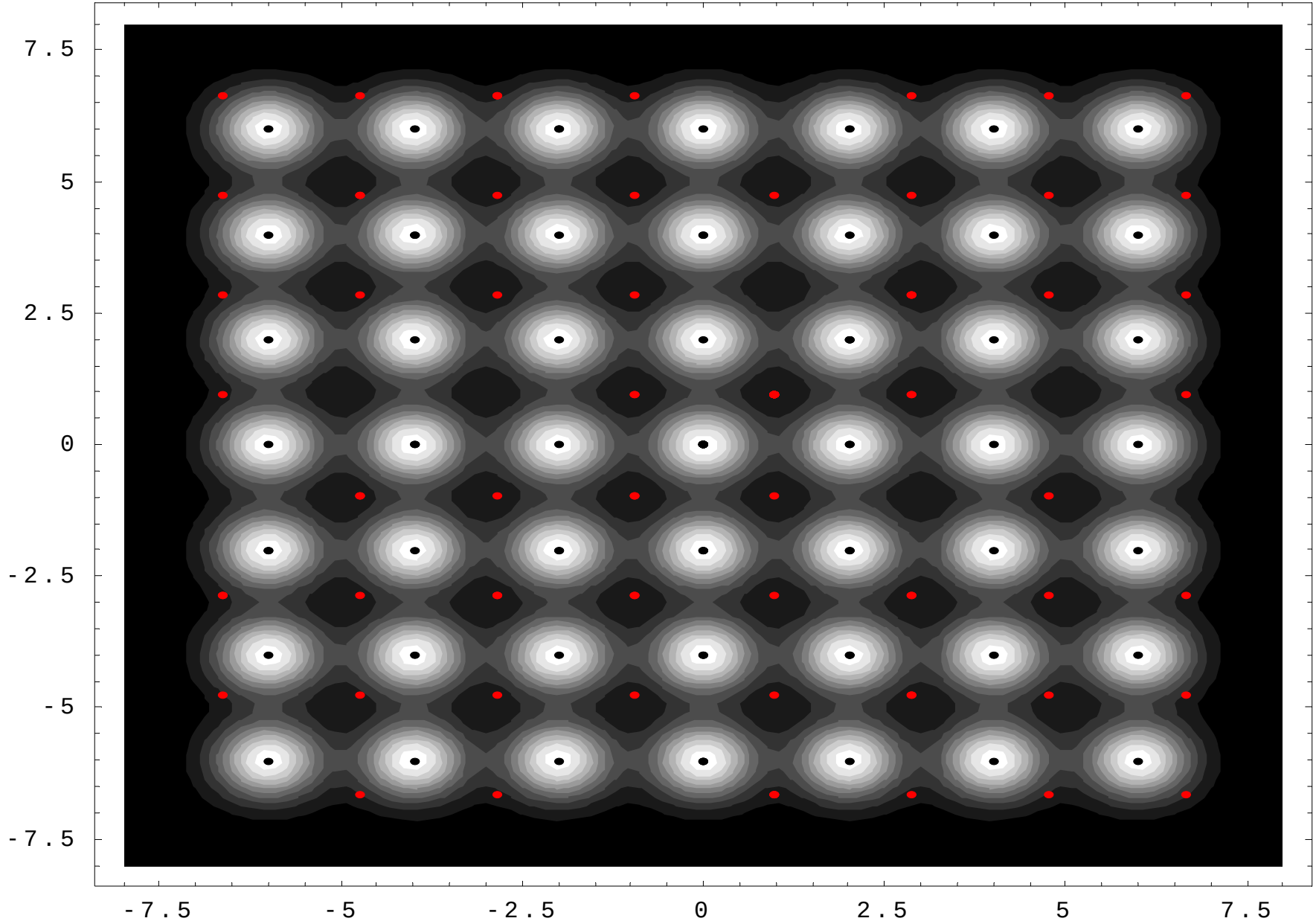


7 x 7 modes

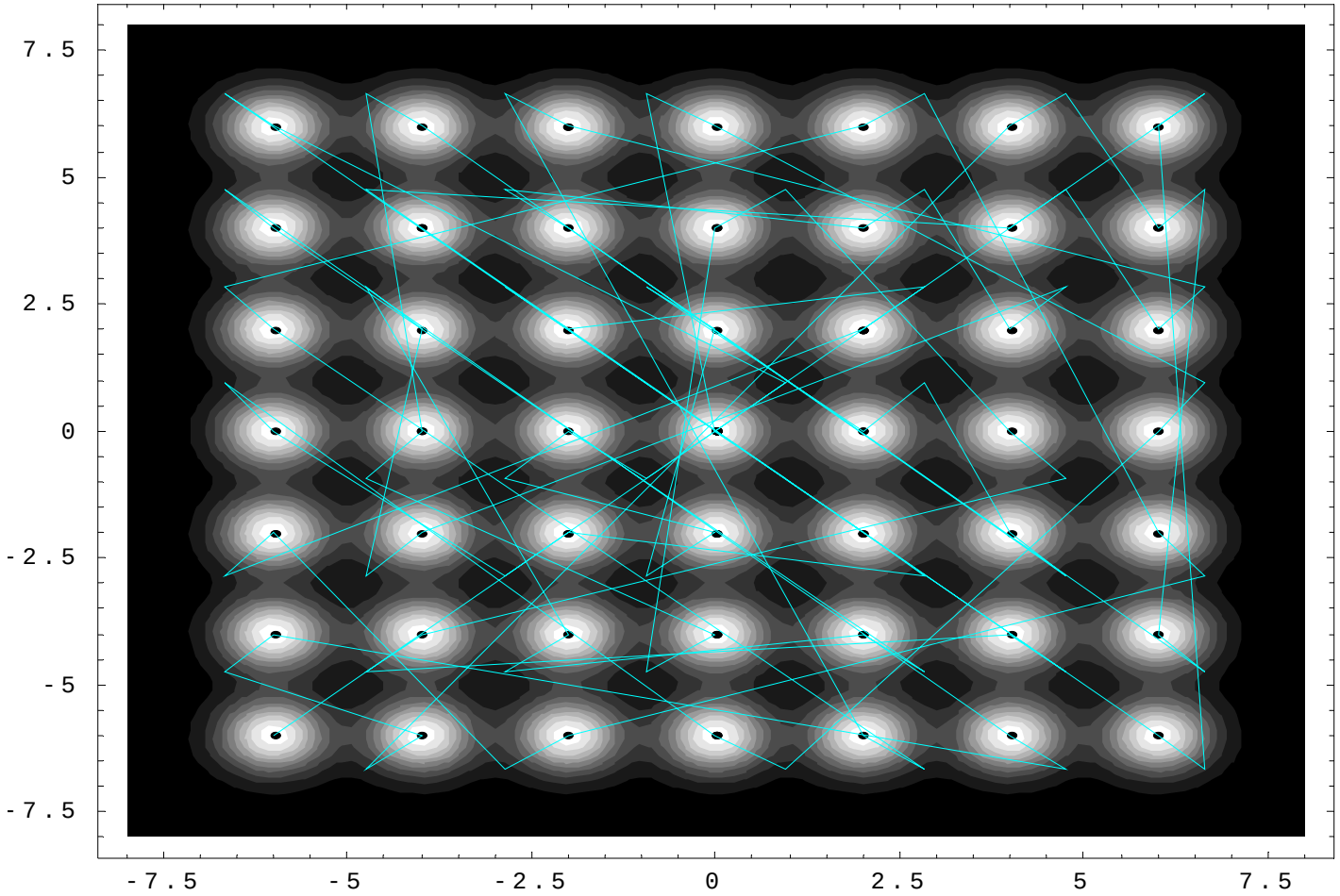


$$g(\boldsymbol{x}) = \sum_{j=1}^{7}\sum_{i=1}^{7}\frac{1}{2\pi}\exp\{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_{ij})^{\mathrm{T}}((\boldsymbol{x}-\boldsymbol{\mu}_{ij})\}$$

Expected case



Trace of IRM



Scalable !

Why spontaneous data learning?

- We just estimate a normal mean adopting γ-estimator
- The γ-loss function becomes nonconvex if data distribution is multimodal, and γ is selected between 1 and 3.
- Local minima correspond to cluster centers if γ is adaptively selected, for example K-fold cross validation, information criterion.

Difference of convex functions

γ–loss function

$$\log\{-L_\gamma(\boldsymbol{\mu})\} = \log\sum_{i=1}^{n}\exp\{-\tfrac{\gamma}{2}(\boldsymbol{x}_i-\boldsymbol{\mu})^{\mathrm{T}}(\boldsymbol{x}_i-\boldsymbol{\mu})\} + \mathrm{const}$$

$$= \log\Big(\sum_{i=1}^{n} e^{\gamma\,\boldsymbol{x}_i^{\mathrm{T}}\boldsymbol{\mu}-\frac{\gamma}{2}\boldsymbol{x}_i^{\mathrm{T}}\boldsymbol{x}_i}\Big) - \tfrac{\gamma}{2}\boldsymbol{\mu}^{\mathrm{T}}\boldsymbol{\mu}$$

Hessian

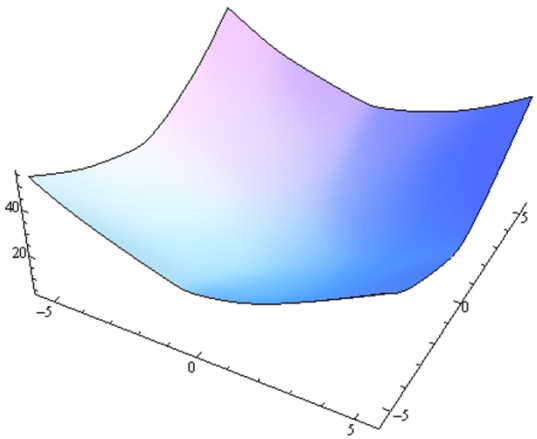
$$\frac{\partial}{\partial\boldsymbol{\mu}\partial\boldsymbol{\mu}^{\mathrm{T}}}\log\Big\{\sum_{i=1}^{n} e^{\gamma\,\boldsymbol{x}_i^{\mathrm{T}}\boldsymbol{\mu}-\frac{\gamma}{2}\boldsymbol{x}_i^{\mathrm{T}}\boldsymbol{x}_i}\Big\} = \sum_{i=1}^{n} w_i(\boldsymbol{\mu})(\boldsymbol{x}_i-\overline{\boldsymbol{\mu}})(\boldsymbol{x}_i-\overline{\boldsymbol{\mu}})^{\mathrm{T}}$$

$$\text{where}\quad w_i(\boldsymbol{\mu}) = \frac{f(\boldsymbol{x}_i,\boldsymbol{\mu})^{\gamma}}{\sum f(\boldsymbol{x}_j,\boldsymbol{\mu})^{\gamma}},\ \overline{\boldsymbol{\mu}} = \sum w_i(\boldsymbol{\mu})\boldsymbol{x}_i$$

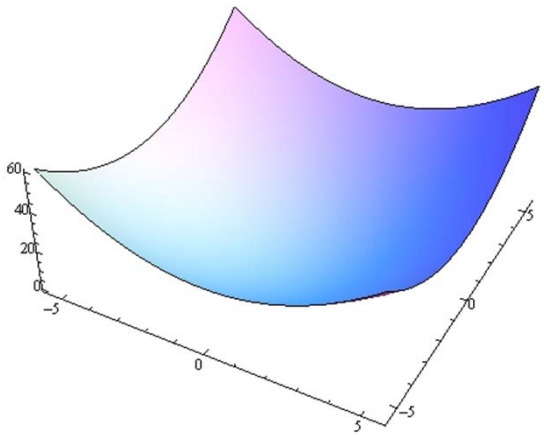
Cf. CCCP, Yuille & Rangarajan (2002), An & Tao (2005)

Difference of convex functions

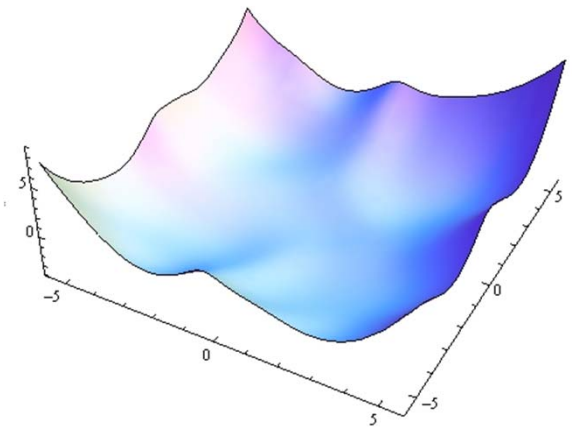
$$\log\{\sum_{i=1}^{n} e^{\gamma \boldsymbol{x}_i^{\mathrm{T}}\boldsymbol{\theta} - \frac{\gamma}{2}\boldsymbol{x}_i^{\mathrm{T}}\boldsymbol{x}_i}\}$$



$$\frac{\gamma}{2}\boldsymbol{\theta}^{\mathrm{T}}\boldsymbol{\theta}$$



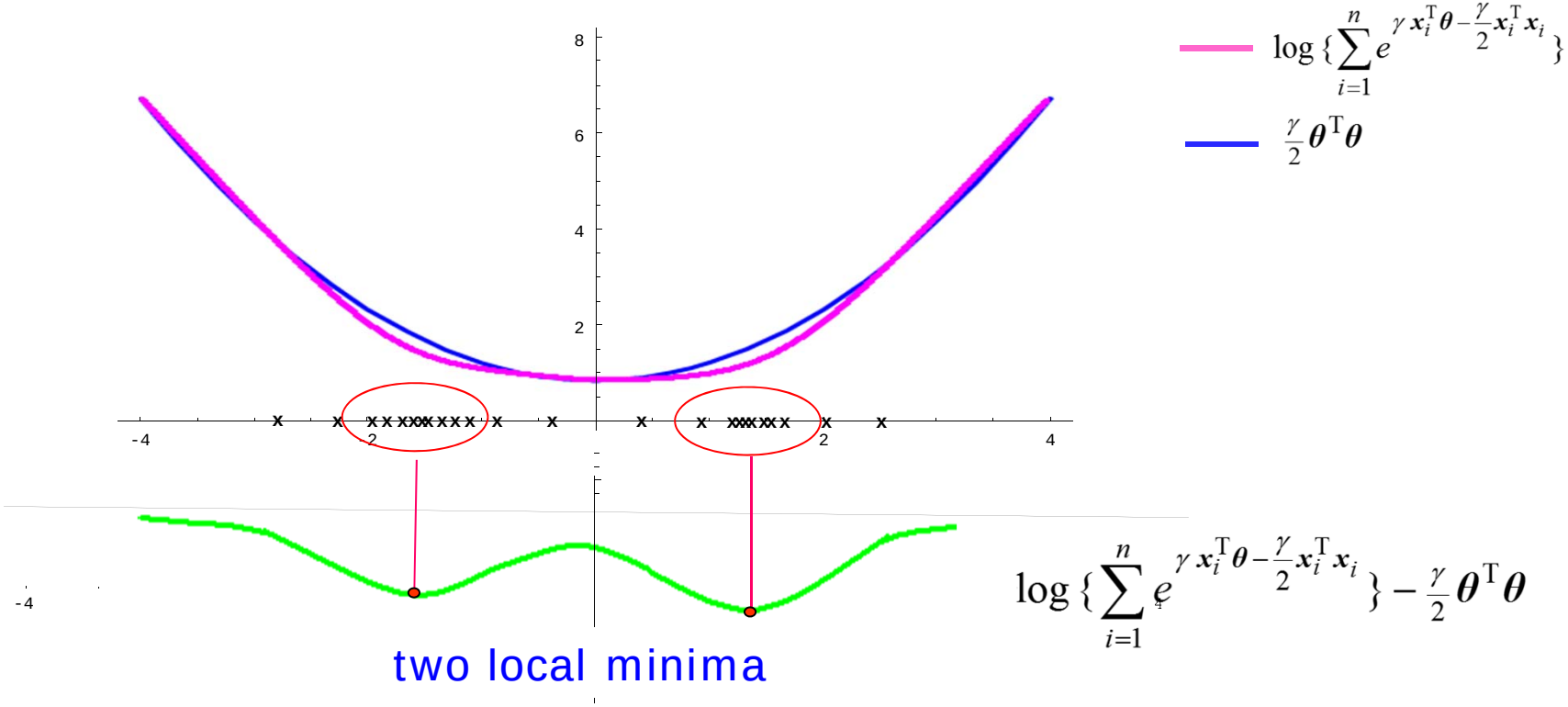
difference



Rem If $\{\boldsymbol{x}_i\} \sim \sum_{k=1}^{K} \pi_k N(\boldsymbol{\theta}_k, I)$, then $L_\gamma(\boldsymbol{\theta}) \xrightarrow{\text{a.s.}} \sum_{k=1}^{K} \pi_k e^{-\frac{1}{2}\frac{\gamma}{\gamma+1}(\boldsymbol{\theta}-\boldsymbol{\theta}_k)^{\mathrm{T}}(\boldsymbol{\theta}-\boldsymbol{\theta}_k)}$

If $\{\boldsymbol{x}_i\} \sim N(\boldsymbol{\theta}_0, I)$, then $L_\gamma(\boldsymbol{\theta}) \xrightarrow{\text{a.s.}} e^{-\frac{1}{2}\frac{\gamma}{\gamma+1}(\boldsymbol{\theta}-\boldsymbol{\theta}_0)^{\mathrm{T}}(\boldsymbol{\theta}-\boldsymbol{\theta}_0)}$

Convexity depending on data



γ–loss function suggests local minima as centers of clusters

Why spontaneous data learning?

Why difference of convex functions?

I like to elucidate the reason why SDL occur

in information geometric understandings

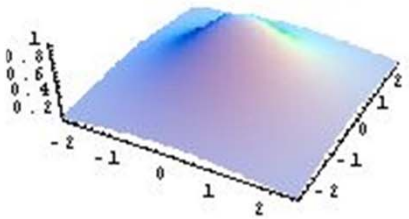
Max γ-entropy

γ-diagonal entropy $$H_\gamma(g) = \left(\int g(\boldsymbol{x})^{\gamma+1} \mathrm{d}\boldsymbol{x}\right)^{\frac{1}{\gamma+1}}$$

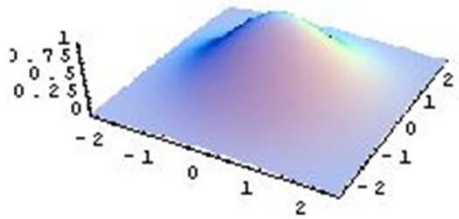
Equal mean space $$F(\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \{ f(\boldsymbol{x}) : \mathrm{E}_f(\boldsymbol{X}) = \boldsymbol{\mu}, \mathrm{V}_f(\boldsymbol{X}) = \boldsymbol{\Sigma} \}$$

Max γ-entropy $$f_\gamma(\cdot, \mu, \Sigma) = \underset{f \in F(\mu,\Sigma)}{\arg\max} \; H_\gamma(f)$$

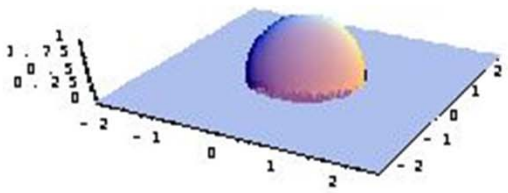
γ-model $$f_\gamma(\boldsymbol{x}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = c_\gamma \det(2\pi\boldsymbol{\Sigma})^{-\frac{1}{2}} \{ 1 - \tfrac{1}{2}\gamma(\boldsymbol{x}-\boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}) \}_+^{\frac{1}{\gamma}}$$



$\gamma = -0.3$ (t-distribution)



$\gamma = 0$ (normal)



$\gamma = 2$ (Wigner)

γ-estimator on γ-model

Let $(x_1,\ldots,x_n)$ be iid from $f_\gamma(\cdot,\mu,\Sigma)$

γ-loss function $$L_\gamma(\mu,\Sigma)=\frac{1}{n}\sum_{i=1}^{n}\det(\Sigma)^{-\frac{1}{2}\frac{\gamma}{\gamma+1}}\{1-\frac{1}{2}\gamma(x_i-\mu)^{\mathrm{T}}\Sigma^{-1}(x_i-\mu)\}$$

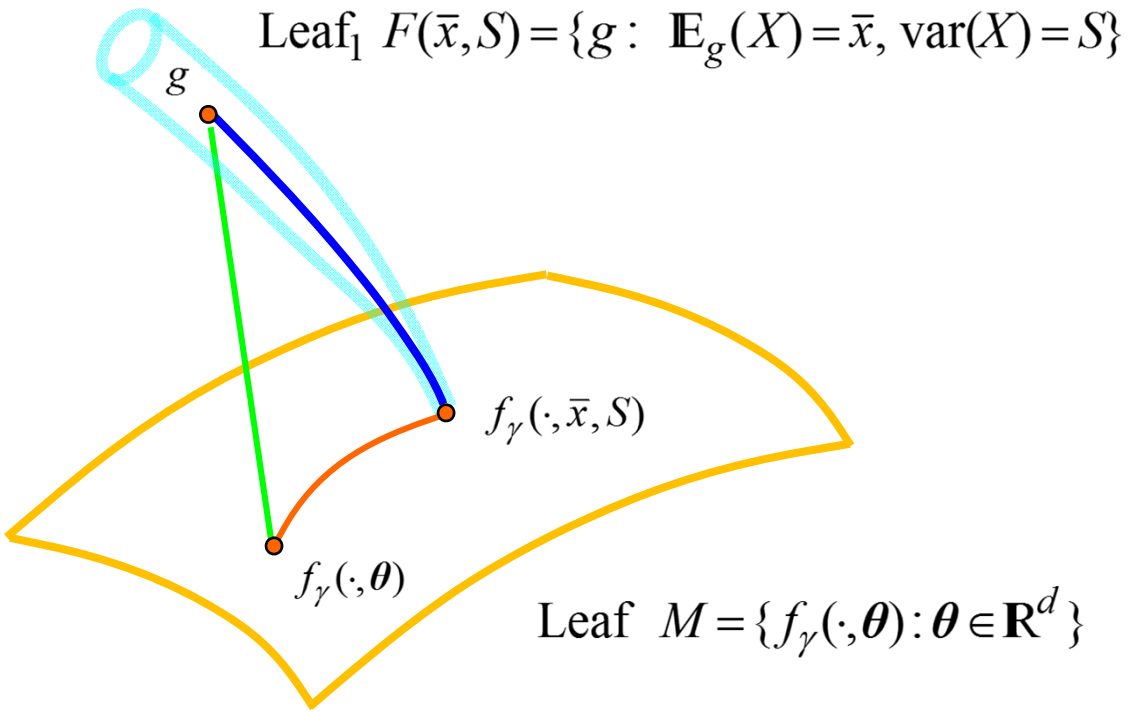
$$(\bar{x},S)=\arg\min_{(\mu,\Sigma)} L_\gamma(\mu,\Sigma) \quad \forall\gamma>\frac{2}{d+2}$$

$$L_\gamma(\mu,\Sigma)-L_\gamma(\bar{x},S)=D_\gamma(f_{\bar{x},S},f_{\mu,\Sigma})\geq 0$$

Let $g_{\mu,\Sigma}$ be a location-scale family.
The γ-estimator for (μ,Σ) is the sample mean and sample variance if and only if $g_{\mu,\Sigma}$ is the γ-model.

Cf. Teicher (1961)

Pythagoras foliation



Loss decomposition $L_\gamma(\boldsymbol{\theta})-L_\gamma(\bar{\boldsymbol{x}},\boldsymbol{S})=D_\gamma(f_\gamma(\cdot,\bar{\boldsymbol{x}},\boldsymbol{S}),f_\gamma(\cdot,\boldsymbol{\theta}))$

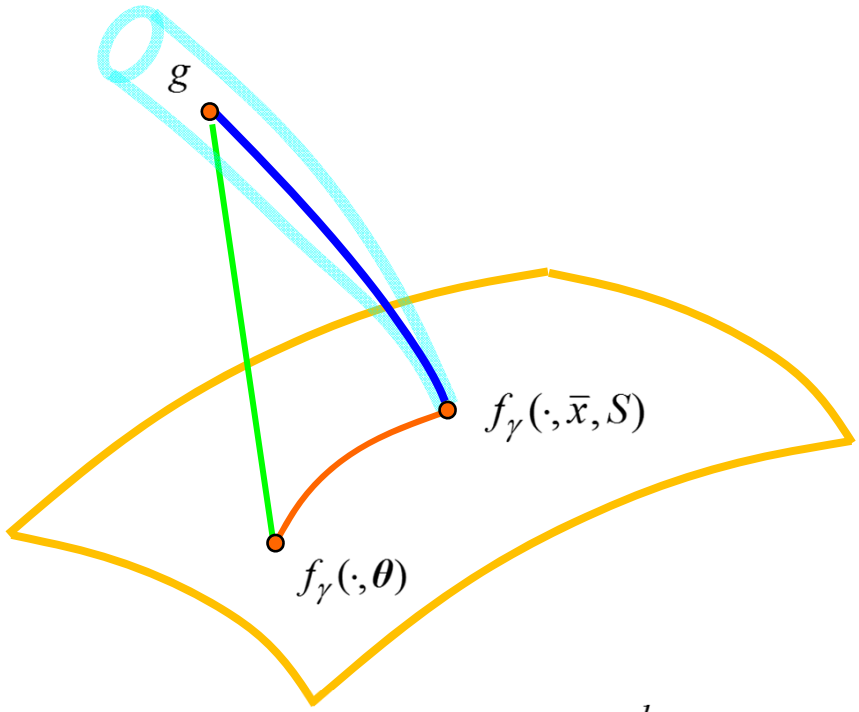
{Pythagorian triangle} $\bigcup_{\boldsymbol{\theta}\in\mathbf{R}^d} F(\boldsymbol{\theta})$

(γ-estimator , γ'-model)

model / loss function	0-model	γ-model
0-loss	$(\bar{x}, S)$ MLE	M-estimator
γ-loss	**Spontaneous Data learning**	$(\bar{x}, S)$ γ-estimator

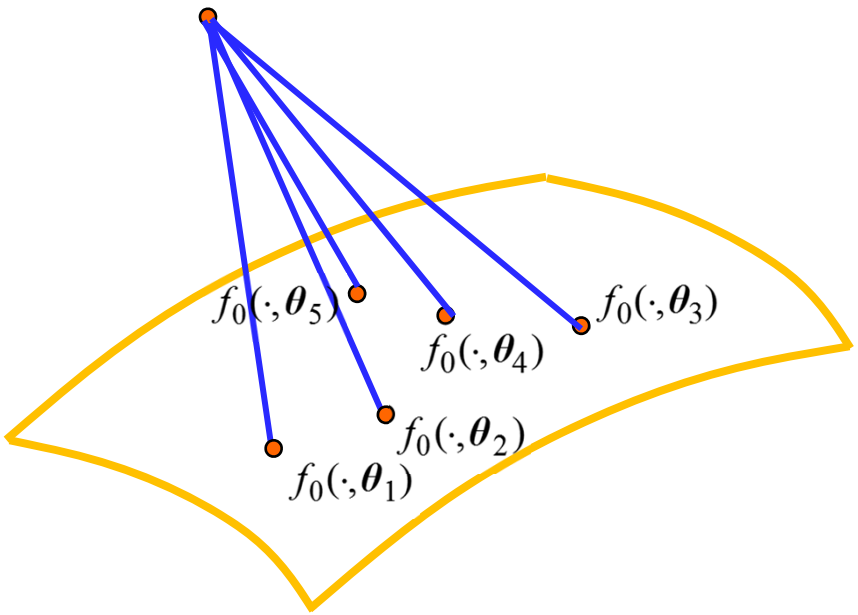
Break for Pythagoras foliation arises SDL

$\text{Leaf}_1 \;\; F(\bar{x}, S) = \{g : \; \mathbb{E}_g(X) = \bar{x}, \; \text{var}(X) = S\}$



$\text{Leaf} \;\; M = \{f_\gamma(\cdot, \boldsymbol{\theta}) : \boldsymbol{\theta} \in \mathbf{R}^d\}$

$g = \sum_{k=1}^{K} \pi_k f(\cdot, \theta_k)$



$M_0 = \{f_0(\boldsymbol{x}, \boldsymbol{\theta}) := (2\pi)^{-d/2} \exp\{-(\boldsymbol{x} - \boldsymbol{\theta})^{\mathrm{T}} (\boldsymbol{x} - \boldsymbol{\theta})/2\} : \boldsymbol{\theta} \in \mathbb{R}^d\}$

Five local minima of $L_\gamma(\boldsymbol{\theta})$

What justification for SDL?

- **SDL is a result from nonconvex learning,**

  cf. CCCP, Yuille & Rangarajan (2002), An & Tao (2005)

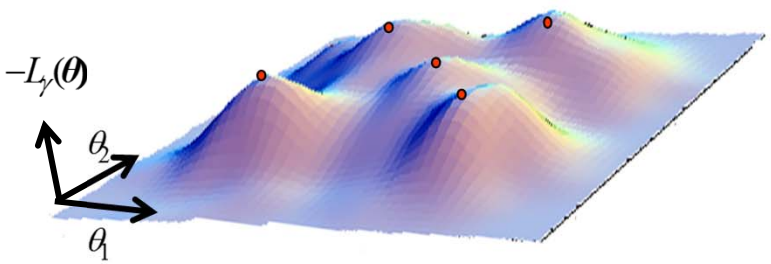
- **SDL is led to by a break of canonical duality between statistical model and estimation**

I like to elucidate a statistical justification for SDL

The break reveals the true distribution?

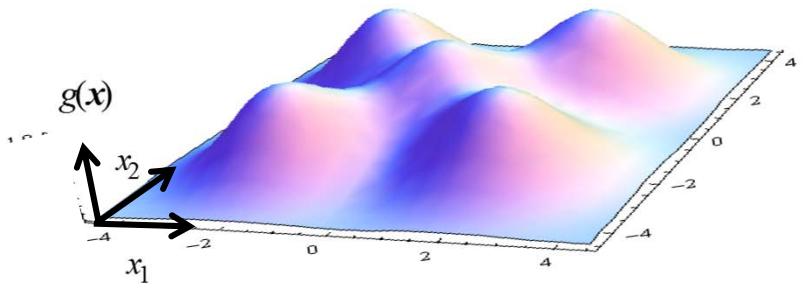
Let $\boldsymbol{X}_1,\ldots,\boldsymbol{X}_1 \sim g(\boldsymbol{x}) = \sum_{j=1}^{K} \pi_j \phi(\boldsymbol{x}, \boldsymbol{\theta}_j, I)$ (normal mixture)

Then $$-L_\gamma(\boldsymbol{\theta}) \xrightarrow[n\to\infty]{} \mathrm{E}\{-L_\gamma(\boldsymbol{\theta})\} = \sum_{j=1}^{K} \pi_j \phi(\boldsymbol{\theta}, \boldsymbol{\theta}_j, \frac{\gamma+1}{\gamma} I)$$



$n = 500,\ \gamma = 2$

$\cong$



In general $n \to \infty, \gamma \to \infty \Rightarrow -L_\gamma(\boldsymbol{\theta}) \xrightarrow{\text{a.s.}} g(\boldsymbol{\theta})$?

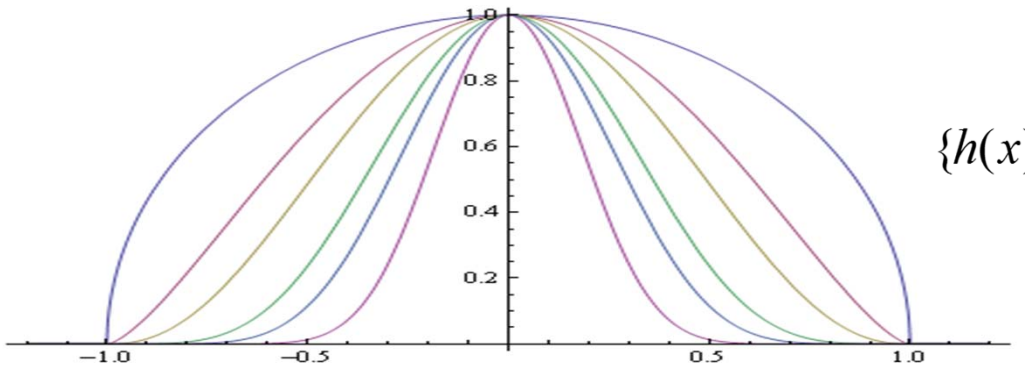
γ-loss for location model

A location model $M = \{ h(\boldsymbol{x} - \boldsymbol{\theta}) : \boldsymbol{\theta} \in \mathbb{R}^d \}$

γ-loss function $$\widetilde{L}_\gamma(\boldsymbol{\theta}) = -\frac{1}{n} \sum_{i=1}^{n} \frac{h(\boldsymbol{x}_i - \boldsymbol{\theta})^\gamma}{\int h(\boldsymbol{y})^\gamma \, d\boldsymbol{y}}$$

Note that $-\widetilde{L}_\gamma(\boldsymbol{\theta})$ can be viewed as a density since $\int -\widetilde{L}_\gamma(\boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{\theta} = 1$

Semi-circle distribution $h(x) = I(x^2 < 1)\,(1 - x^2)$



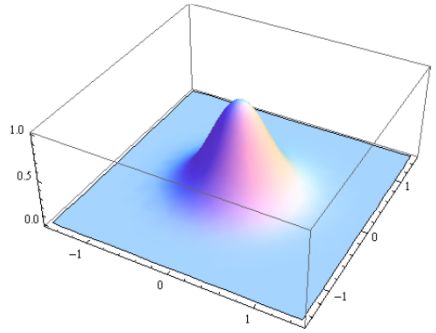
$\{ h(x)^\gamma : \ \gamma = 1, 3, 10, 15, 30 \}$

power

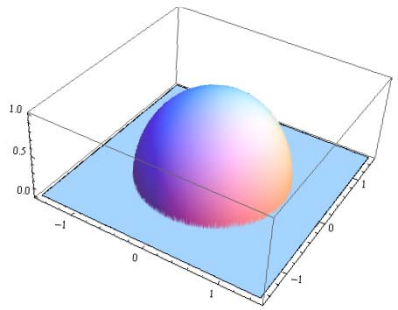
γ-loss as a density estimator

$h(\boldsymbol{x})$

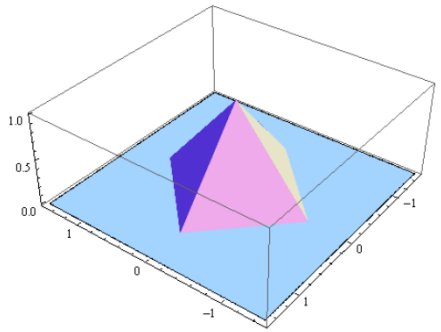
Normal



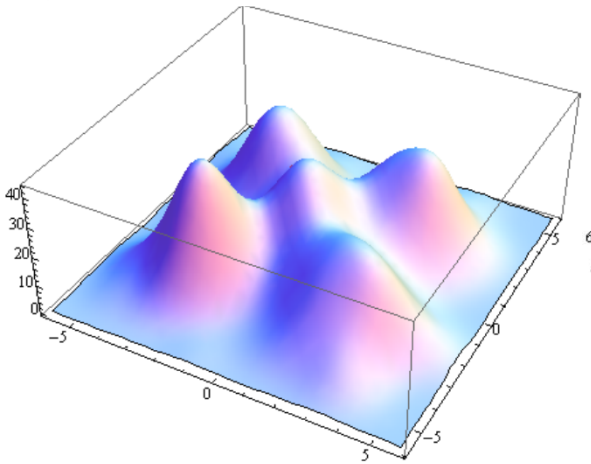
Semi-L_2circle

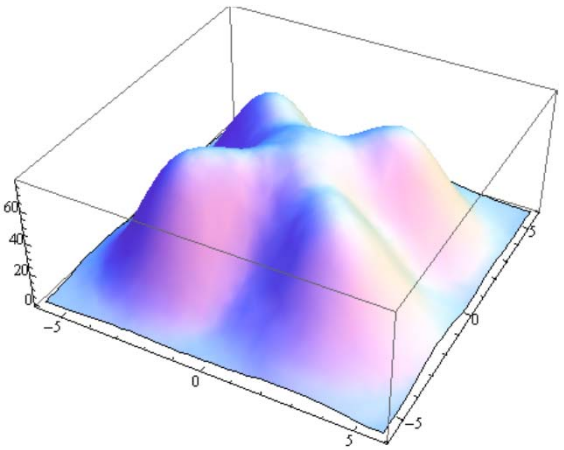


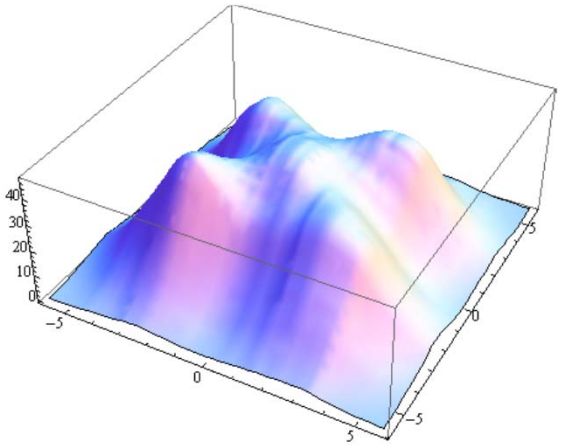
Semi-L_1circle



$-\widetilde{L}_{\gamma}(\boldsymbol{\theta})$







Nonparametric consistency

Theorem Let $g(\boldsymbol{x})$ be a true density function.

We assume : $h(\boldsymbol{x}) < h(0)$ if $x \neq 0$

Then $\lim_{\gamma \to \infty} \mathbb{E}\{\tilde{L}_\gamma(\boldsymbol{\theta})\} = -g(\boldsymbol{\theta})$

Proof.

$$\mathbb{E}\{L_\gamma(\boldsymbol{\theta})\} = -\int \psi_\gamma(\boldsymbol{\theta} - \boldsymbol{y}) g(\boldsymbol{y}) d\boldsymbol{y}, \text{ where } \psi_\gamma(\boldsymbol{x}) = \frac{h(\boldsymbol{x})^\gamma}{\int h(\boldsymbol{y})^\gamma d\boldsymbol{y}}$$

$$\int \psi_\gamma(\boldsymbol{\theta} - \boldsymbol{y}) g(\boldsymbol{y}) d\boldsymbol{y} \xrightarrow[\gamma \to \infty]{} \int \delta(\boldsymbol{\theta} - \boldsymbol{y}) g(\boldsymbol{y}) d\boldsymbol{y} = g(\boldsymbol{\theta})$$

(Dirac's delta function δ).

Mean Integrated Square Error

Theorem. We assume: $\exists$ a strictly decreasing function $\eta(s)$ for $s > 0$ such that $h(\boldsymbol{x}) = \eta(\| \boldsymbol{x} \|)$.

Then
$$\mathrm{MISE}_\gamma = \frac{1}{4}\int \left\{V_\gamma \mathrm{tr}\left(\frac{\partial^2 g(\boldsymbol{y})}{\partial \boldsymbol{y}\partial \boldsymbol{y}^{\mathrm{T}}}\right)\right\}^2 + \frac{1}{n}\frac{\int h(y)^{2\gamma}\,dy}{\left(\int h(y)^{\gamma}\,dy\right)^2}$$

where
$$V_\gamma = \int \boldsymbol{y}\boldsymbol{y}^{\mathrm{T}} \frac{h(\boldsymbol{y})^{\gamma}}{\int h(\boldsymbol{z})^{\gamma}\,d\boldsymbol{z}}\,d\boldsymbol{y}$$

Kernel density estimator
$$\tilde{g}_h(\boldsymbol{x}) = \frac{1}{nh}\sum_{i=1}^{n} K((\boldsymbol{x}-\boldsymbol{x}_i)/h)$$

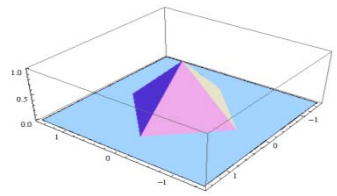
If $h(\boldsymbol{x})$ and $K(\boldsymbol{x})$ are normal, then $L_\gamma(\boldsymbol{x}) = -\tilde{g}_h(\boldsymbol{x})$ with $h = \gamma^{-\frac{1}{2}}$

In general $h_{\mathrm{opt}} = n^{-1/(d+4)}$ cf. Parzen (1962), Li - Racine (2004)

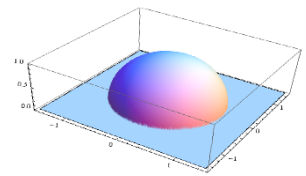
Semicircle distributions

A location model $M = \{ h(\boldsymbol{x} - \boldsymbol{\theta}) : \boldsymbol{\theta} \in \mathbb{R}^d \}$

L_1 semicircle distribution $h^{(1)}(\boldsymbol{x}) = \begin{cases} c_d^{(1)} \{1 - \| \boldsymbol{x} \|_{L_1}\} & \text{if} \quad \| \boldsymbol{x} \|_{L_1} \le 1 \\ 0 & \text{otherwise} \end{cases}$



L_2 semicircle distribution $h^{(2)}(\boldsymbol{x}) = \begin{cases} c_d^{(2)} (1 - \boldsymbol{x}^{\mathrm{T}} \boldsymbol{x}) & \text{if} \quad \boldsymbol{x}^{\mathrm{T}} \boldsymbol{x} \le 1, \\ 0 & \text{otherwise.} \end{cases}$



where $c_d^{(1)}$ and $c_d^{(2)}$ are normalizing constants.

Rem.

The support of $h^{(2)}$ is a d - dimesional hypershere S_d;

the support of $h^{(1)}$ is a d - dimensional hypercube C_d.

$$\mathrm{S}_d \subseteq \mathrm{C}_d$$

$$r_d = \frac{\mathrm{vol}(\mathrm{C}_d)}{\mathrm{vol}(\mathrm{S}_d)} = \frac{d 2^{d-1} \Gamma(d/2)}{\pi^{d/2}} \xrightarrow{d \to \infty} \infty$$

$d = 10, 15 \Rightarrow r_d = 401, 8.5905$ Cf. curse of dimensionality

Mean Integrated Square Error

Theorem.

Let $\mathrm{MISE}_\gamma(h)$ be the mean integrated square error of $L_\gamma(\boldsymbol{x})$ with $h(\boldsymbol{x})$.

Then

$$\mathrm{MISE}_\gamma(h^{(2)}) = \frac{d^2 e^2}{4\gamma^2} \int \left\{ \mathrm{tr}\left(\frac{\partial^2 g(\boldsymbol{y})}{\partial \boldsymbol{y} \partial \boldsymbol{y}^{\mathrm{T}}} \right) \right\}^2 d\boldsymbol{y} + \frac{1}{n} \left(\frac{\gamma}{4e\pi} \right)^{\frac{d}{2}}$$

$$\mathrm{MISE}_\gamma(h^{(1)}) = \frac{1}{4\gamma^4} \left(\sum_{k=1}^{d} \frac{1}{k^2} \right) \int \left\{ \mathrm{tr}\left(\frac{\partial^2 g(\boldsymbol{y})}{\partial \boldsymbol{y} \partial \boldsymbol{y}^{\mathrm{T}}} \right) \right\}^2 d\boldsymbol{y} + \frac{1}{n} \left(\frac{\gamma}{4} \right)^d$$

Kernel density estimator

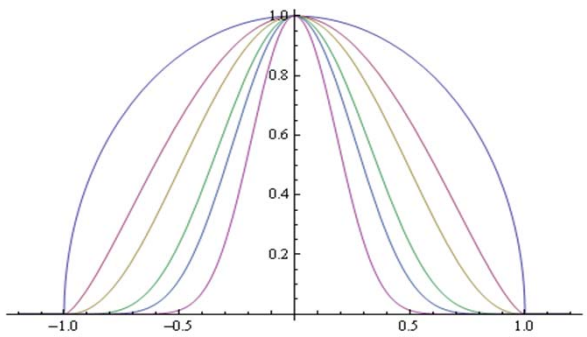
A location model $M = \{ h(\boldsymbol{x} - \boldsymbol{\theta}) : \boldsymbol{\theta} \in \mathbb{R}^d \}$

γ-loss function $$\widetilde{L}_\gamma(\boldsymbol{\theta}) = -\frac{1}{n} \sum_{i=1}^{n} \frac{h(\boldsymbol{x}_i - \boldsymbol{\theta})^\gamma}{\int h(\boldsymbol{y})^\gamma \, d\boldsymbol{y}}$$

kernel density estimator $$\hat{g}_b(\boldsymbol{x}) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{b^d} h\left(\frac{\boldsymbol{x} - \boldsymbol{x}_i}{b} \right)$$

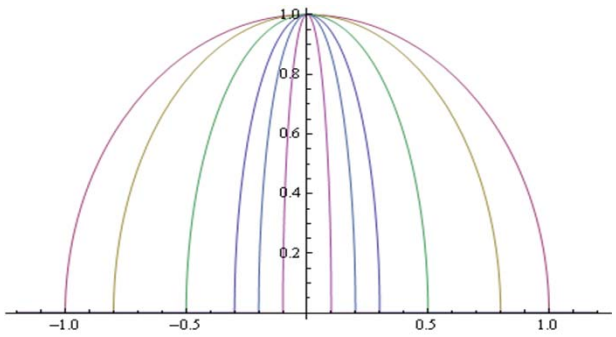
Semi-circle distribution $h(x) = I(x^2 < 1)\,(1 - x^2)$

$\{ h(x)^\gamma : \ \gamma = 1, 3, 10, 15, 30 \}$



power

$\{ h(x/b) : \ b = 1, 0.8, 0.6, 0.3, 0.1 \}$



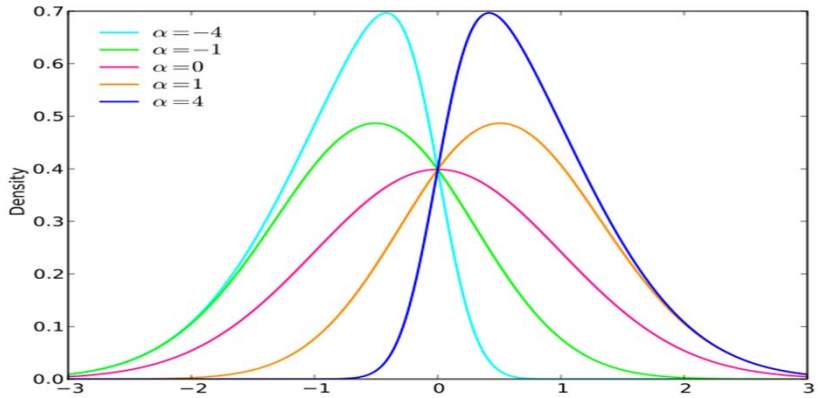
bandwidth

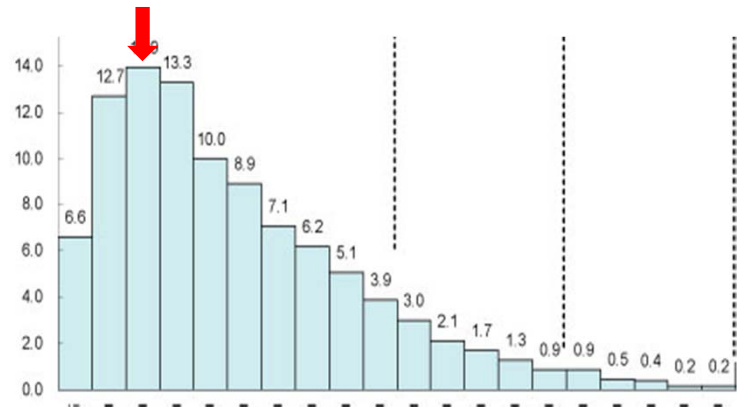
Skew normal distribution

Skew normal distribution $$f(x,\tau,\omega,\alpha)=\frac{2}{\omega}\phi(\frac{x-\tau}{\omega})\Phi(\alpha\frac{x-\tau}{\omega})$$

Normal distribution $$f(x,\tau,\omega,0)=\frac{1}{\omega}\phi(\frac{x-\tau}{\omega})$$

Parameter of interests $$\theta(\tau,\omega,\alpha)=\arg\max_{x\in\mathbb{R}} f(x,\tau,\omega,\alpha)$$





Japanese income data

Estimation for a mode θ

MLE under skew normal

$$\hat{\theta}_{\mathrm{ML}} = \theta(\hat{\tau}, \hat{\omega}, \hat{\alpha}), \text{where } \hat{\tau}, \hat{\omega}, \hat{\alpha} \text{ are MLEs for } \tau, \omega, \alpha.$$

γ-estimator under normal

$$\hat{\theta}_{\gamma} = \arg\min_{\theta \in \Theta} L_{\gamma}(\theta) \quad \text{where} \quad L_{\gamma}(\theta) = -\sum_{i=1}^{n} \exp\{-\frac{\gamma}{2}(x_i - \theta)^2\}$$

MSE

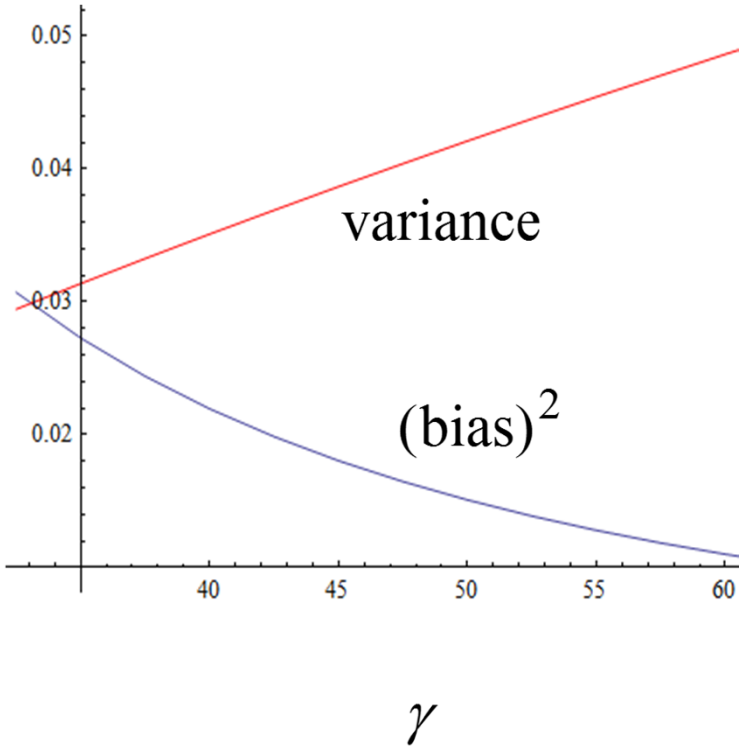
$$\mathrm{MSE}(\theta_{\mathrm{ML}}, \theta) = \frac{1}{n} I(\theta)^{-1} + o(n^{-1}) \quad \text{where} \quad I(\theta) = (\frac{\partial\theta}{\partial\tau}, \frac{\partial\theta}{\partial\omega}, \frac{\partial\theta}{\partial\alpha}) I(\tau, \omega, \alpha) (\frac{\partial\theta}{\partial\tau}, \frac{\partial\theta}{\partial\omega}, \frac{\partial\theta}{\partial\alpha})^{\mathrm{T}}$$

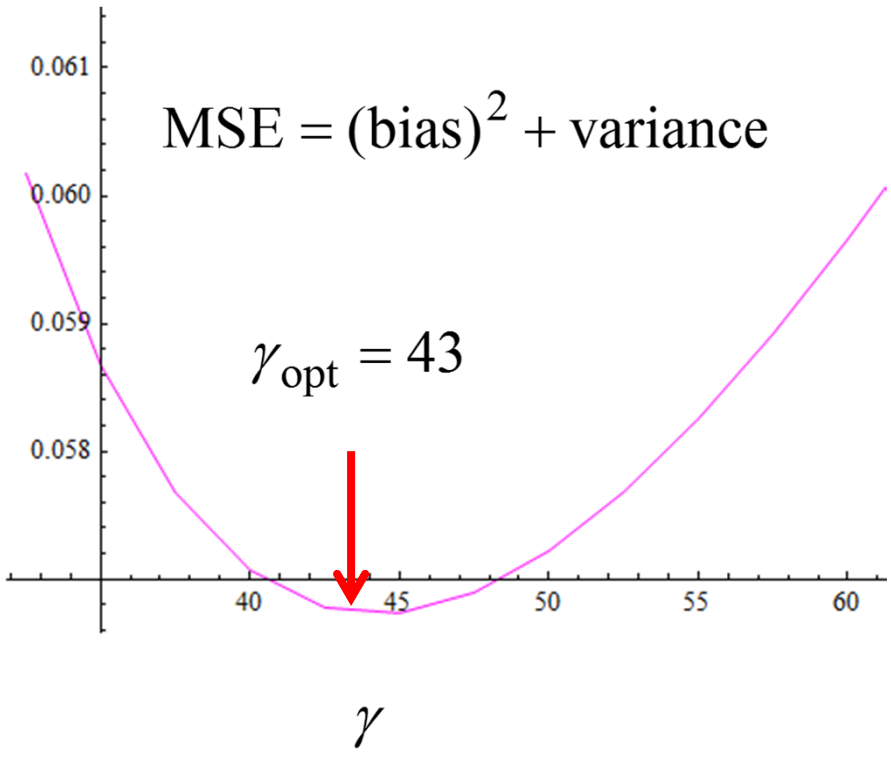
$$\mathrm{MSE}(\theta_{\gamma}, \theta) = \left\{\mathrm{E}(\phi(\theta - X)^{\gamma}) - f(\theta, \tau, \omega, \alpha)\right\}^2 + \frac{1}{n} \mathrm{Var}\left(\frac{\phi(\theta - X)^{\gamma}}{\mathrm{E}\{\phi(\theta - X)^{\gamma}\}}\right)$$

$$\mathrm{MSE}(\hat{\theta}_{\mathrm{ML}}, \theta) < \mathrm{MSE}(\hat{\theta}_{\gamma}, \theta) \text{ for sufficiently large } n$$

Trade between bias and variance

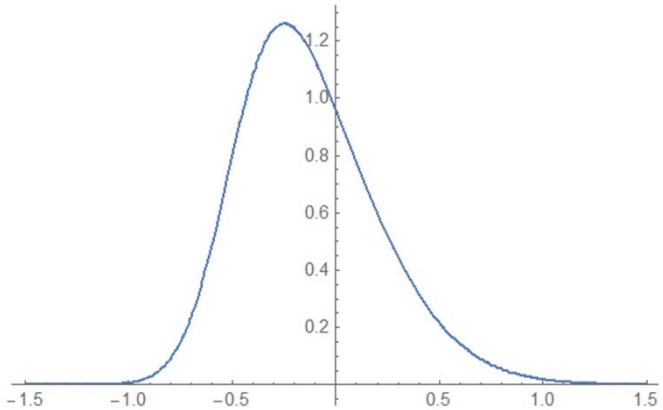
True values $(\tau, \omega, \alpha) = (0.5,\ 0.5,\ 2.5)$ $\theta = -0.248$, $n = 20$





Simulation study

True distribution



$$f(x,\tau_0,\omega_0,\alpha_0) = \frac{2}{\omega_0}\phi\left(\frac{x-\tau_0}{\omega_0}\right)\Phi\left(\alpha_0\frac{x-\tau_0}{\omega_0}\right)$$

$$(\tau_0,\omega_0,\alpha_0) = (0.5,\ 0.5,\ 2.5) \quad \theta_0 = -0.248$$

sample size	$\hat{\theta}_{\mathrm{ML}}$	$\hat{\theta}_{\gamma}$	$\bar{x}$
$n = 20$	2.35514	1.32099	2.02219
$n = 50$	1.41589	0.896704	1.67111
$n = 200$	0.248097	0.459803	1.48877

ML has also SDL?

loss \ model	0-model	γ-model
0-loss	$(\bar{x}, S)$	M-estimator
γ-loss	SDL	$(\bar{x}, S)$

γ-model

$$f_\gamma(\boldsymbol{x},\boldsymbol{\theta},I) = c_\gamma \{ 1 - \tfrac{1}{2}\gamma(\boldsymbol{x}-\boldsymbol{\theta})^{\mathrm{T}}(\boldsymbol{x}-\boldsymbol{\theta}) \}_+^{\frac{1}{\gamma}}$$

log likelihood

$$L_0(\boldsymbol{\theta}) = \sum_{i=1}^{n} \log f_\gamma(\boldsymbol{x}_i,\boldsymbol{\theta},I)$$

$$\frac{\partial}{\partial\boldsymbol{\theta}} L_0(\boldsymbol{\theta}) = \sum_{i=1}^{n} f_\gamma(\boldsymbol{x}_i,\boldsymbol{\theta},I)^{-\gamma}(\boldsymbol{x}_i-\boldsymbol{\theta})$$

Rem **If we assume normality, take $\gamma < 0$, then the log likelihood for γ–model has (weak) SDL.**

MLE for Cauchy location model

Cauchy location model

$$f(x,\theta) = \frac{1}{\pi}\frac{1}{1+(x-\theta)^2} \qquad (-\infty < x < \infty)$$

Log-likelihood function

$$L(\theta) = -\sum_{i=1}^{n} \log\{1+(x_i-\theta)^2\} \text{ if } \{x_i\}_{i=1}^{n} \underset{\text{iid}}{\sim} f(x,\theta)$$

Likelihood equation

$$\frac{\partial}{\partial\theta} L(\theta) = \sum_{i=1}^{n} f(x_i,\theta)(\theta - x_i) = 0$$

Maximum likelihood

$$\hat{\theta}_{\mathrm{ML}} = \frac{\sum f(x_i,\hat{\theta}_{\mathrm{ML}})x_i}{\sum f(x_i,\hat{\theta}_{\mathrm{ML}})}$$

Fixed-point iteration

$$\hat{\theta}_{t+1} = \frac{\sum f(x_i,\hat{\theta}_t)x_i}{\sum f(x_i,\hat{\theta}_t)}$$

Reeds, Asymptotic number of roots of Cauchy location likelihood equations. Ann. Statist. (1985), 775-784.

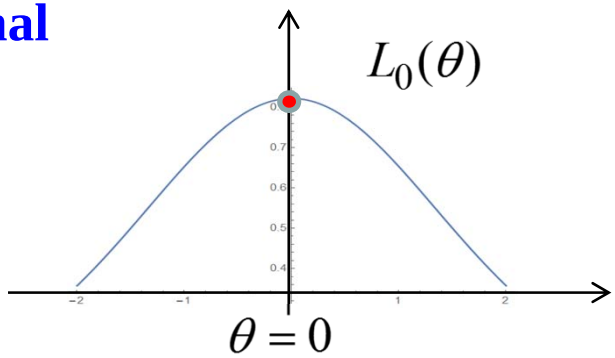
Weak SDL

Expected log-likelihood function

$$L_0(\theta) = -\mathbb{E}(\log\{1+(X-\theta)^2\}) = -\int_{-\infty}^{\infty} \log\{1+(x-\theta)^2\} g(x)\mathrm{d}x \quad \text{if} \quad X \sim g(x)$$

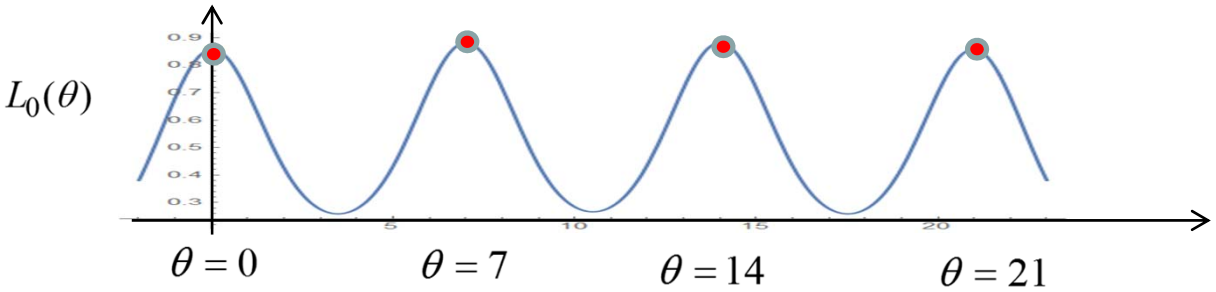
Case 1: true distribution is a normal

$$g(x) \sim N(0,1)$$



Case 2: true distribution is a normal mixture

$$g(x) \sim \tfrac{1}{4}N(0,1) + \tfrac{1}{4}N(7,1) + \tfrac{1}{4}N(14,1) + \tfrac{1}{4}N(21,1)$$



SDL is from the break of max-entropy

loss \ model	0-model	γ-model
0-loss	$(\bar{x}, S)$	M-estimator
γ-loss	γ-estimator	$(\bar{x}, S)$

(γ–model, γ–estimator) leads to a canonical statistics

(0 –model, γ–estimator) leads to strong SDL if $\gamma > 0$

(γ–model, MLE) leads to weak SDL if $\gamma < 0$

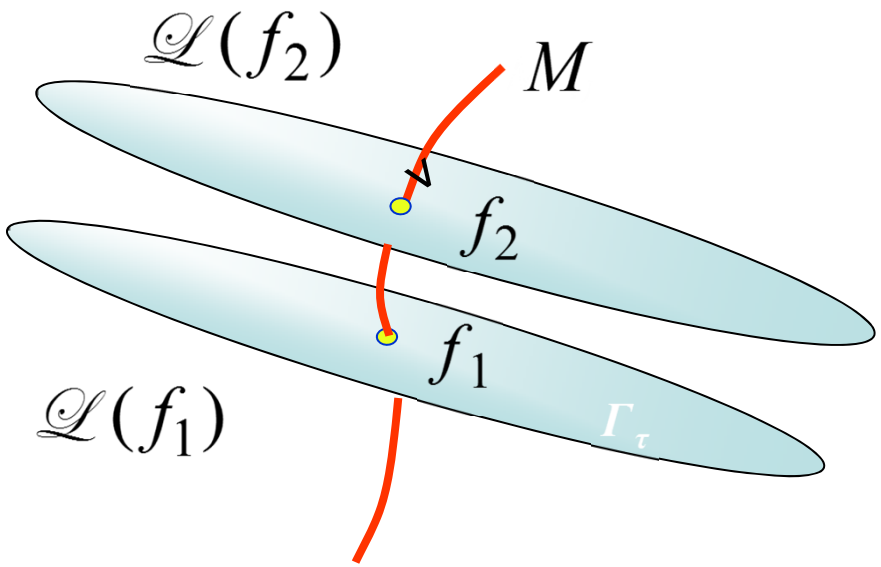
(γ–model, MLE) leads to non-robustness if $\gamma > 0$

(0 –model, γ–estimator) leads to unstable if $\gamma < 0$

Estimator selection vs model selection

Fix a model $M = \{f_\theta : \theta \in \Theta\}$, find a good estimator in $\{\hat{\theta}_\omega : \omega \in \Omega\}$

Fix a loglikelihood $L(M) = \sum \log f_\theta(x_i)$, find a good model in $\{M_k\}_k$



$$\mathscr{L}(f) = \{\, g \in \mathscr{F}_\mu : \hat{\theta}(g) = \hat{\theta}(f) \,\}$$

Future work

- Kernel density estimator vs. power entropy density estimator

  The curse of dimensionality? cf. Huber (1985)

- Informative incomplete data

  The MLE has a fragile property under selective samples.

  What about the γ-estimator ? Any robustness selection bias?

Τηανκ ψου!