

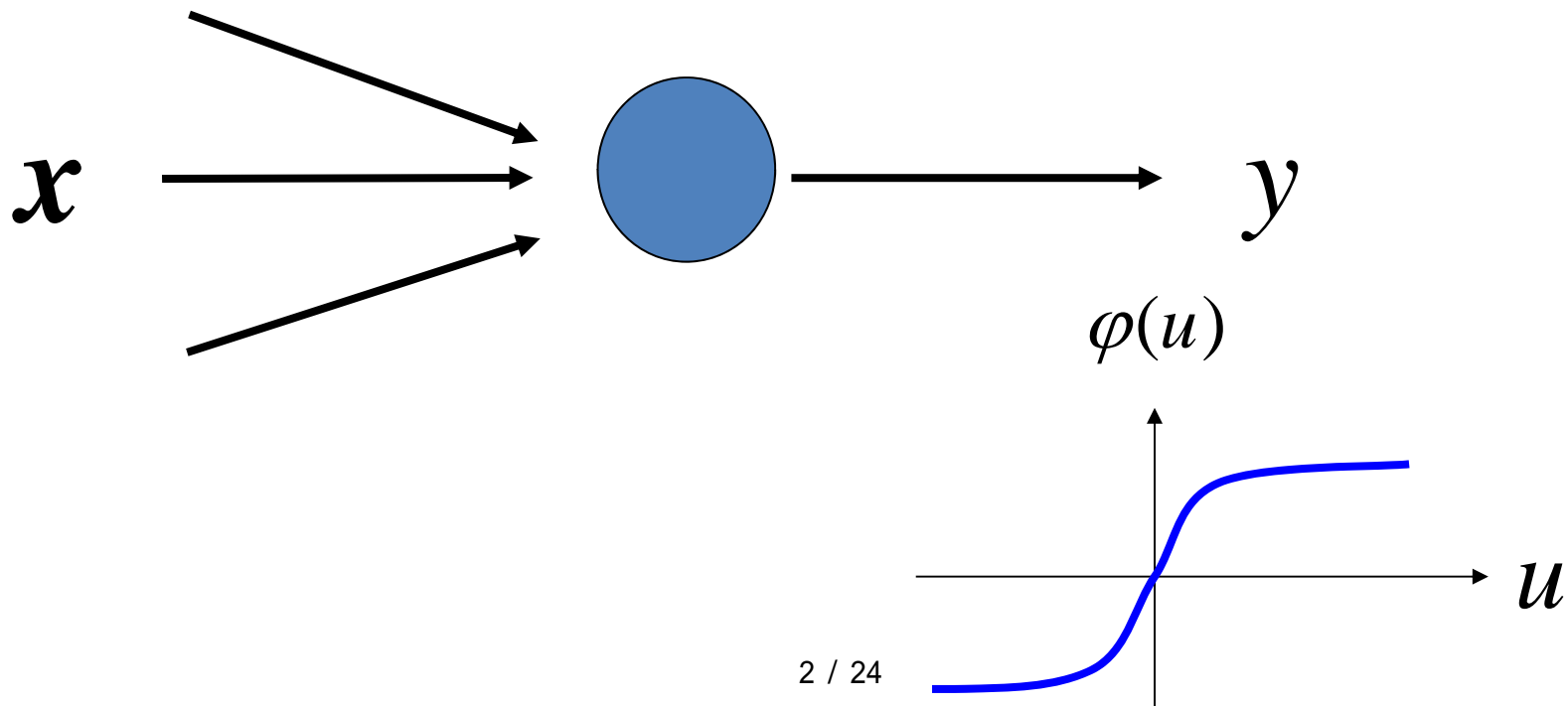
特異モデルと 学習のダイナミックス

甘利俊一 理研脳科学総合研究センター

尾関智子、Florent Cousseau, Hyeyoung Park

Mathematical Neurons

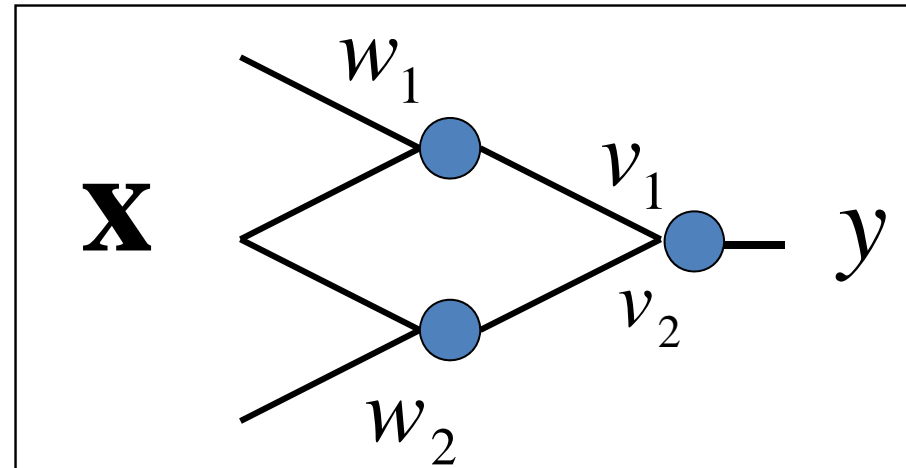
$$y = \varphi\left(\sum w_i x_i - h\right) = \varphi(\mathbf{w} \cdot \mathbf{x})$$



Multilayer Perceptrons

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

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



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

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

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

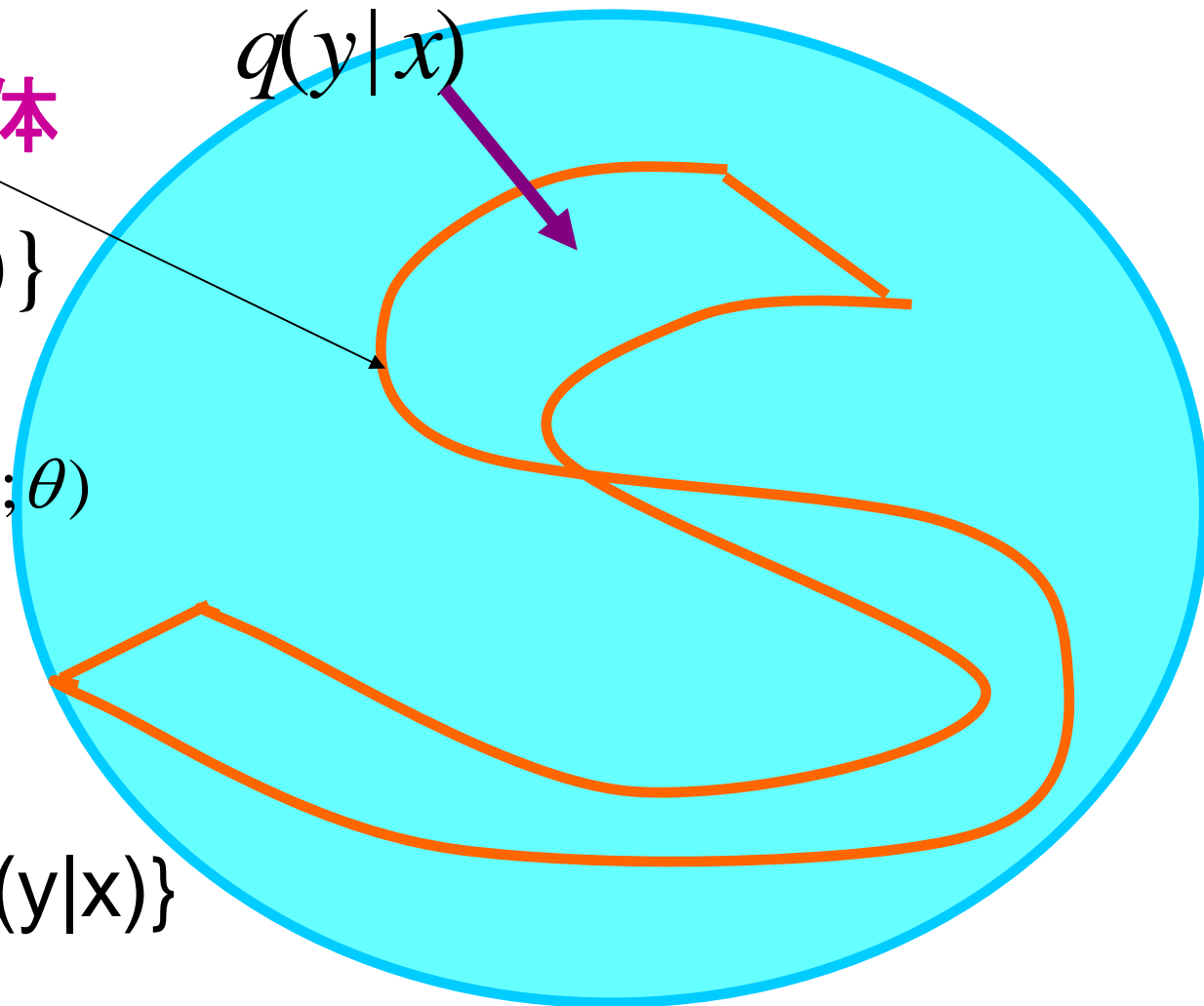
Multilayer Perceptron

神経多様体

$$M = \{p(y | x; \theta)\}$$

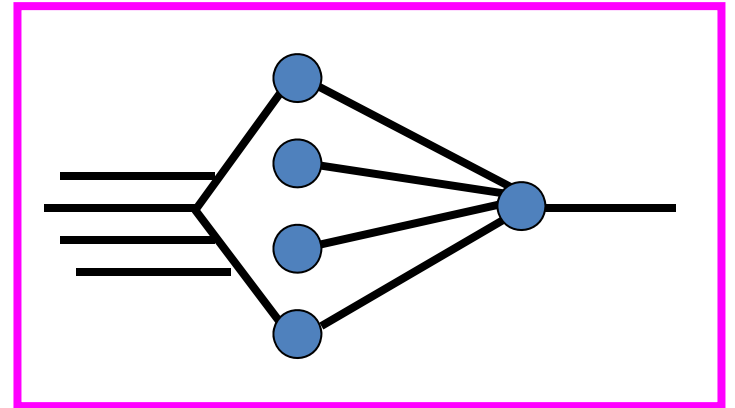
$$p(y, x; \theta) = q(x) p(y | x; \theta)$$

space of $\{q(y|x)\}$

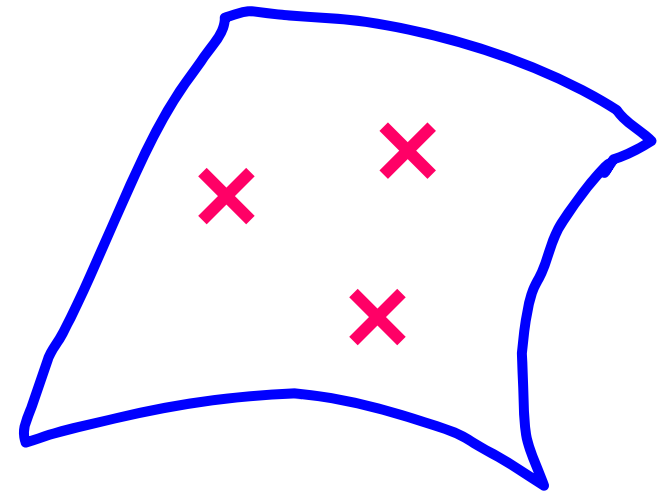
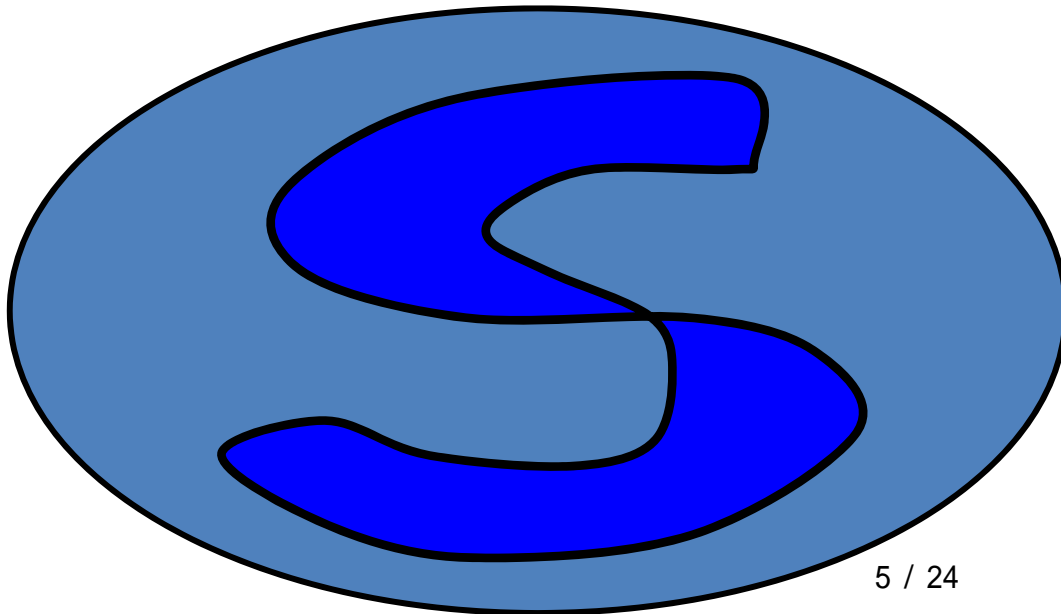


神經多樣體

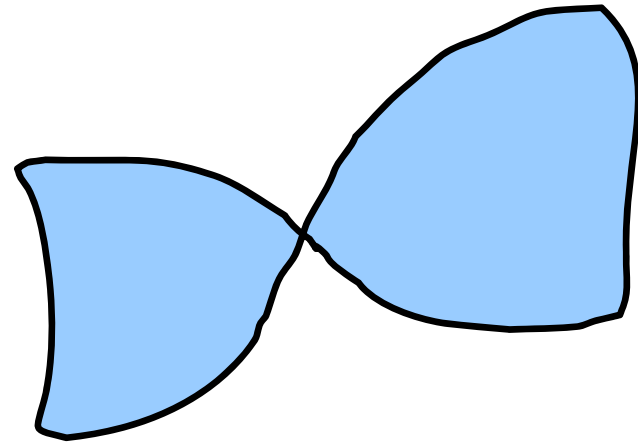
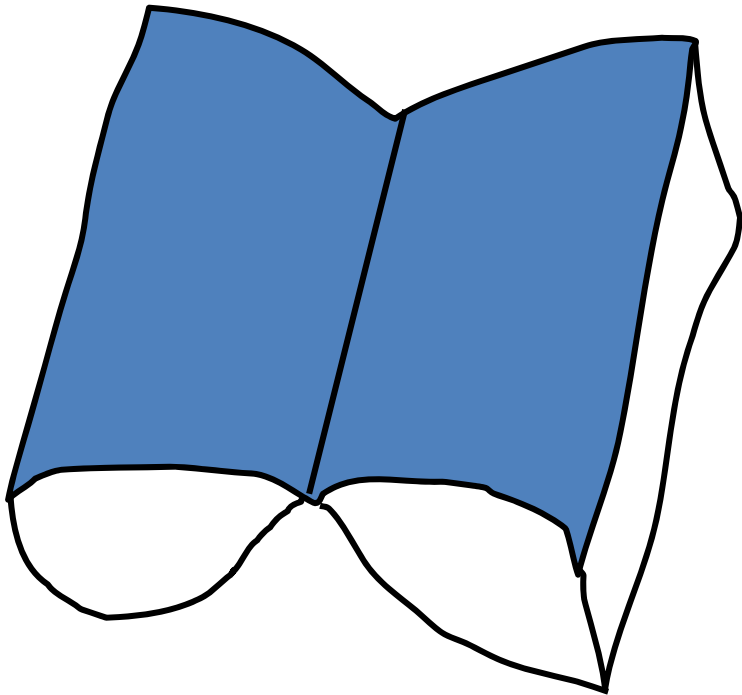
- 計量構造
- 位相構造



θ



singularities—特異点

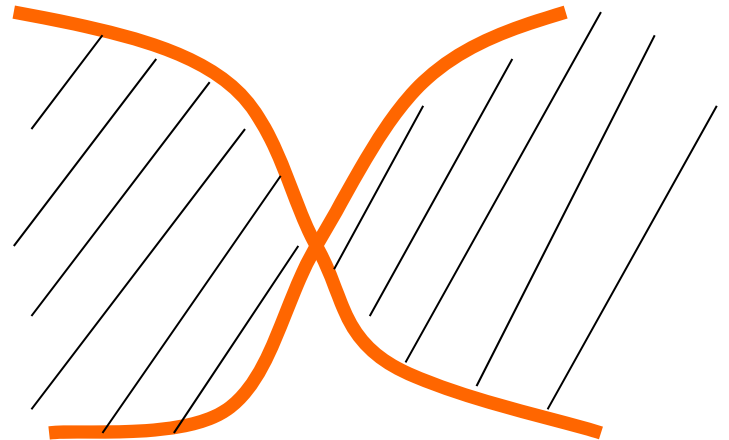
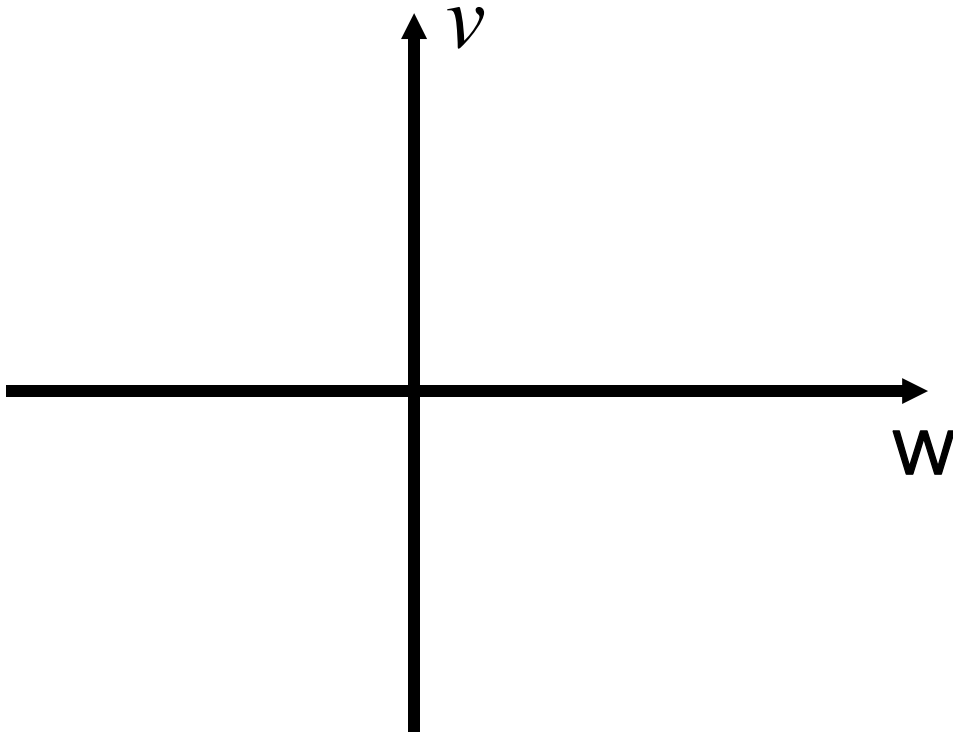


微分幾何—代数幾何

Geometry of singular model

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

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

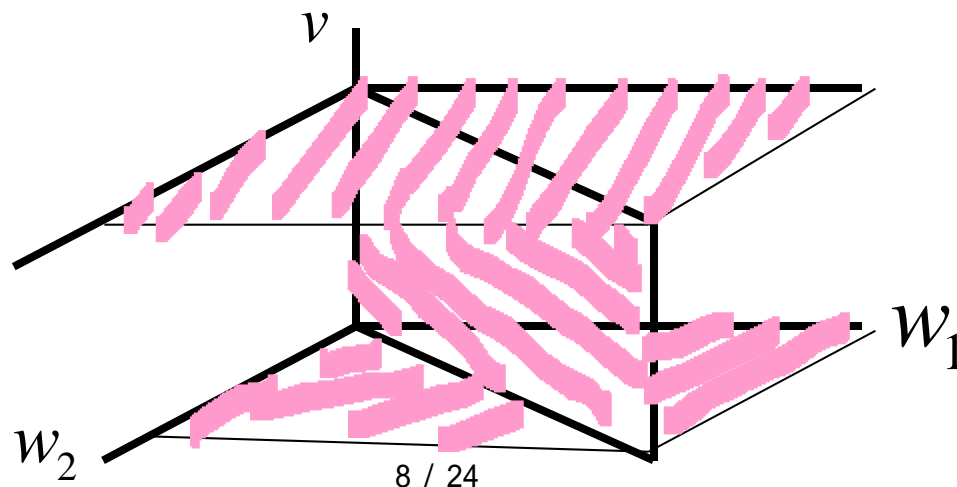


Gaussian mixture

$$p(x; v, w_1, w_2) = (1-v)\varphi(x-w_1) + v\varphi(x-w_2)$$

$$\varphi(x) = \frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{1}{2}x^2\right\}$$

singular: $w_1 = w_2$, $v(1-v) = 0$



特異モデルの解析

1. 真の分布が特異点にあるとき
2. 真の分布がそれ以外するとき

1. 推論—尤度比の奇妙な振舞い—福水
2. 推定量の振舞い
3. Bayes 推定量—渡辺ら
4. 学習ダイナミックス

Regular statistical model

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

G : Fisher information

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

$$\begin{aligned} E\left[KL\left[p(x, \theta_0) : p(x, \hat{\theta})\right]\right] &\approx \frac{1}{2n}G \cdot E[\Delta\theta\Delta\theta] \\ &\approx \frac{d}{2n} \end{aligned}$$

AIC, BIC, MDL

$$\lambda = 2 \sum \log \frac{p(y_i, \mathbf{x}_i, \hat{\boldsymbol{\theta}})}{p(y_i, \mathbf{x}_i, \boldsymbol{\theta}_0)}$$

$$\lambda = n(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}_0)^T G^{-1}(\boldsymbol{\theta}_0)(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}_0)$$

$$E[\lambda] = c(n)k$$

$$c(n) = \log n$$

$$c(n) = \sqrt{\log \log n}$$

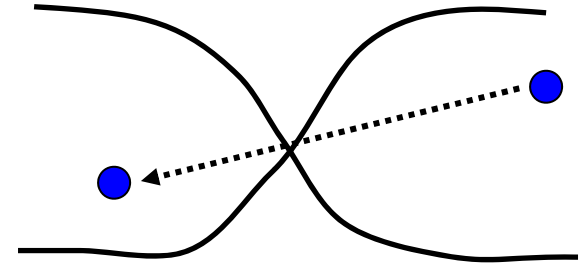
Learning, Estimation, and Model Selection

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

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

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

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



Learning from examples

$$\psi(\mathbf{x}) \approx f(x, \hat{\theta}) = \sum v_i \phi(\mathbf{w}_i \bullet \mathbf{x}_i)$$

Training set T

examples $\cdots (\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_n, y_n)$

learning ; estimation

Backpropagation ---gradient learning

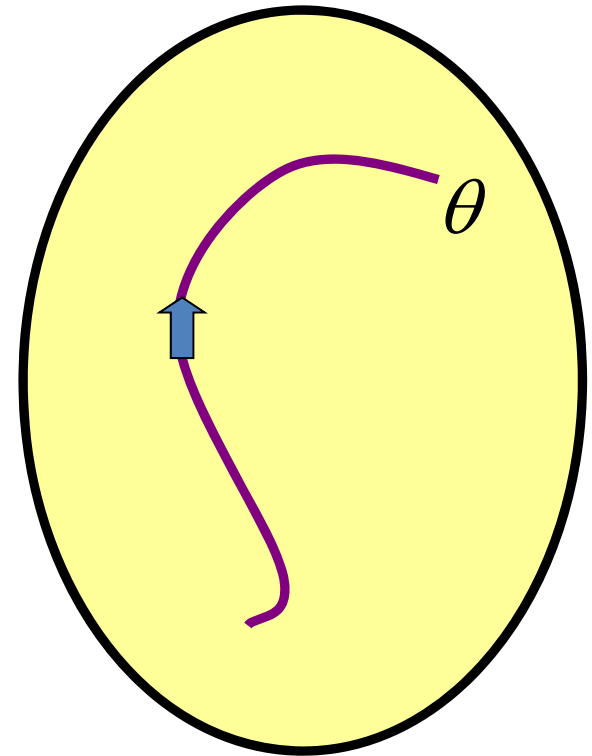
examples : $(y_1, \mathbf{x}_1), \dots, (y_t, \mathbf{x}_t)$ -- training set

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

$$= -\log p(y, \mathbf{x}; \theta)$$

$$\Delta \theta_t = -\eta_t \frac{\partial l}{\partial \theta}$$

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



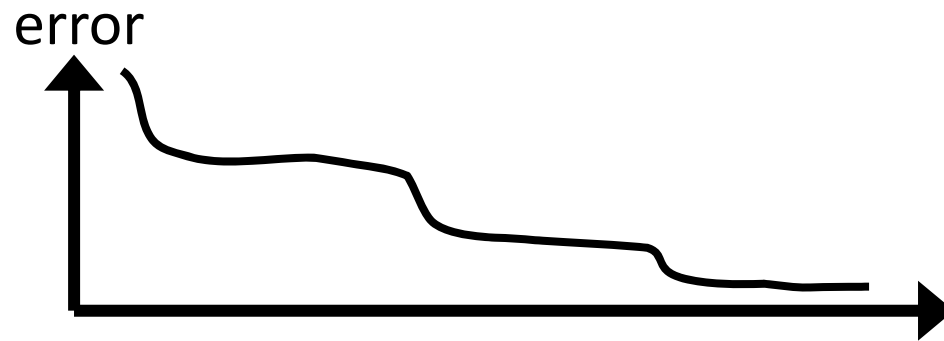
Problem of Backprop

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

$$\Delta \theta_t = -\eta_t \nabla l(x_t, y_t; \theta_t)$$

Flaws of MLP

slow convergence : Plateau



local minima



➔ Boosting and Bagging

Natural Gradient

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

$$|d\boldsymbol{\theta}|^2 = \varepsilon$$

$$\tilde{\nabla}l = G^{-1}(\boldsymbol{\theta}) \nabla l$$

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

Information Geometry of MLP

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

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

$$\mathbf{G}_{t+1}^{-1} = (1 + \varepsilon) \mathbf{G}_t^{-1} - \varepsilon \mathbf{G}_t^{-1} \nabla f \nabla f^T \mathbf{G}_t^{-1}$$

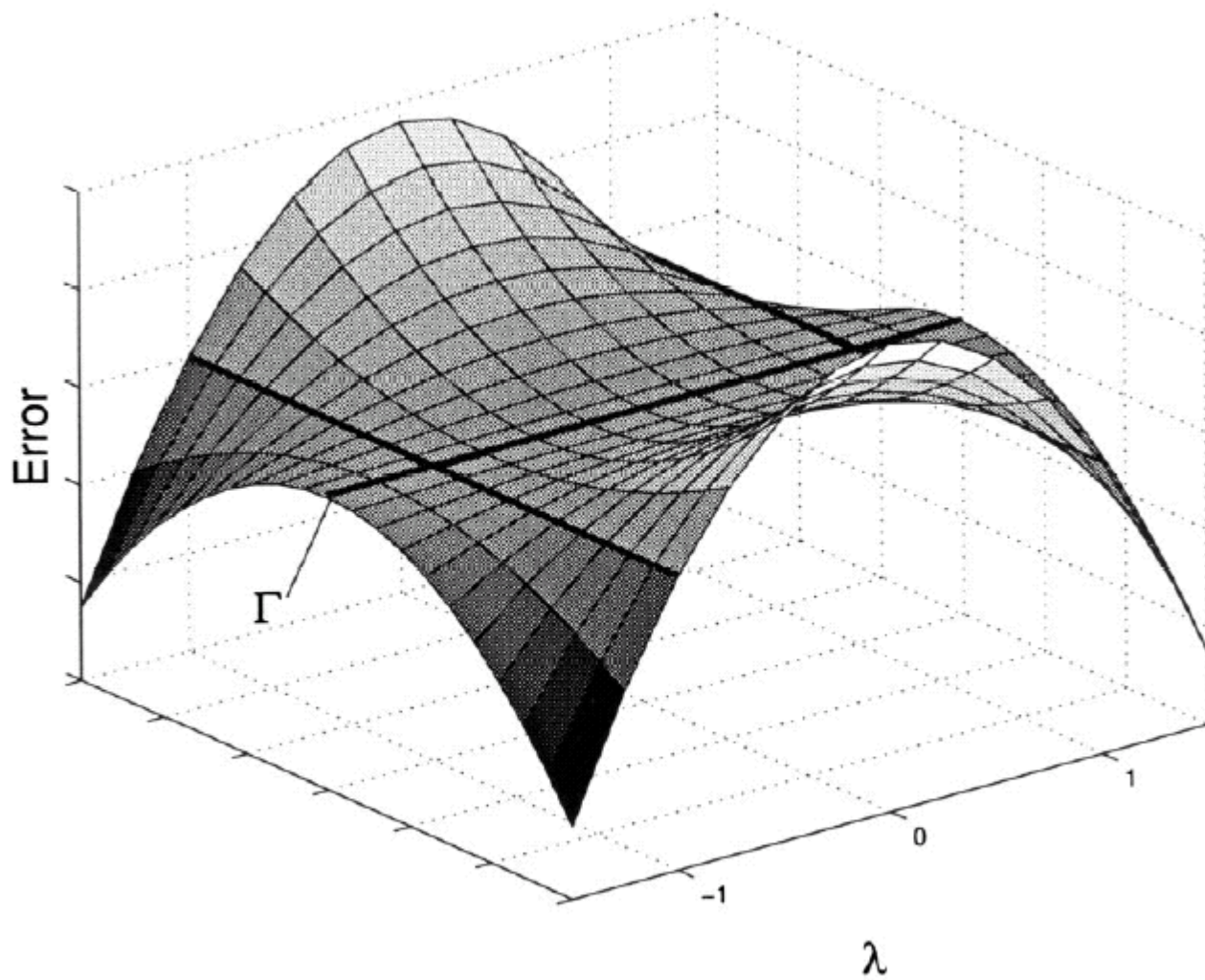
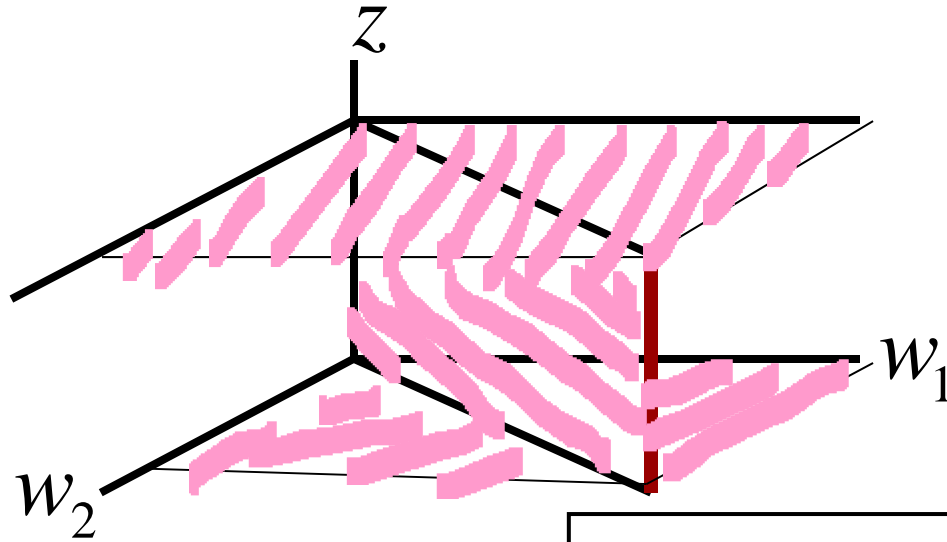


Fig. 5. Critical set with $\frac{19}{24}$ minima and plateaus.

$$y = v_1 \varphi(w_1 x) + v_2 \varphi(w_2 x) + n$$

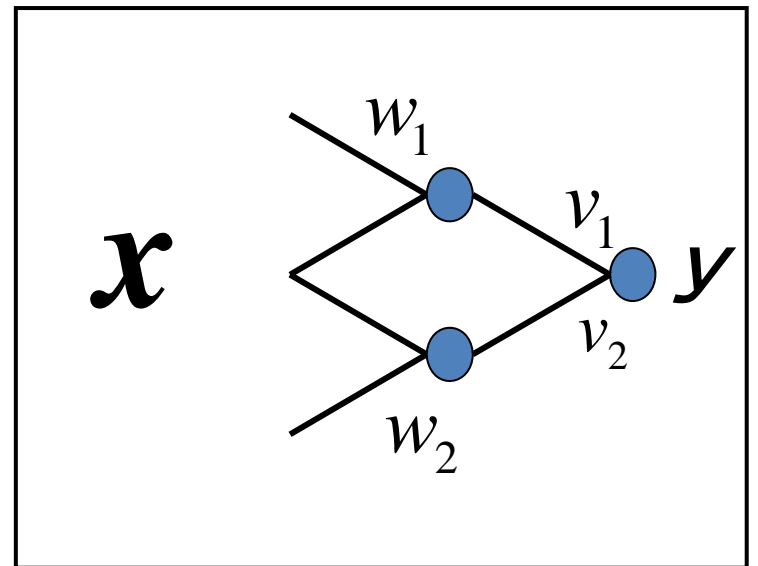
$$w_1 = w_2 = w$$

$$v_1 + v_2 = v$$



$$u = w_2 - w_1$$

$$z = v_2 - v_1$$



Coordinate Transformation

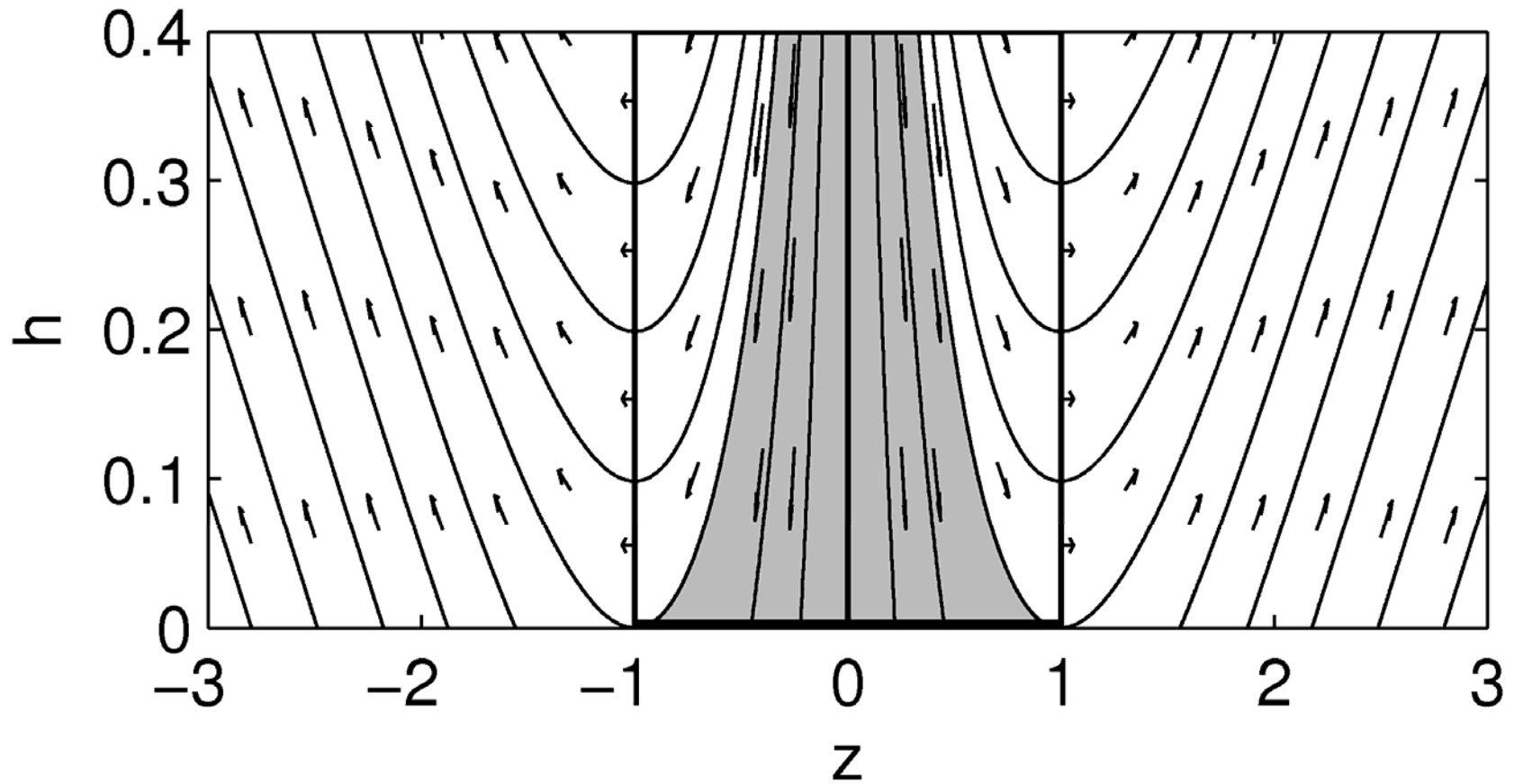
$$\left\{ \begin{array}{l} \mathbf{u} = \mathbf{w}_2 - \mathbf{w}_1 \\ \mathbf{w} = \frac{v_1 \mathbf{w}_1 + v_2 \mathbf{w}_2}{v} \\ v = v_1 + v_2 \\ z = \frac{v_2 - v_1}{v} \end{array} \right. \quad \begin{array}{l} : \mathbf{u} = 0 \\ \mathbf{w} = \mathbf{w}^* \\ v = v^* \\ z = \pm 1 \end{array} \quad \begin{array}{l} \mathcal{R}_1 \\ \\ \\ \mathcal{R}_2 \end{array}$$

學習方程式

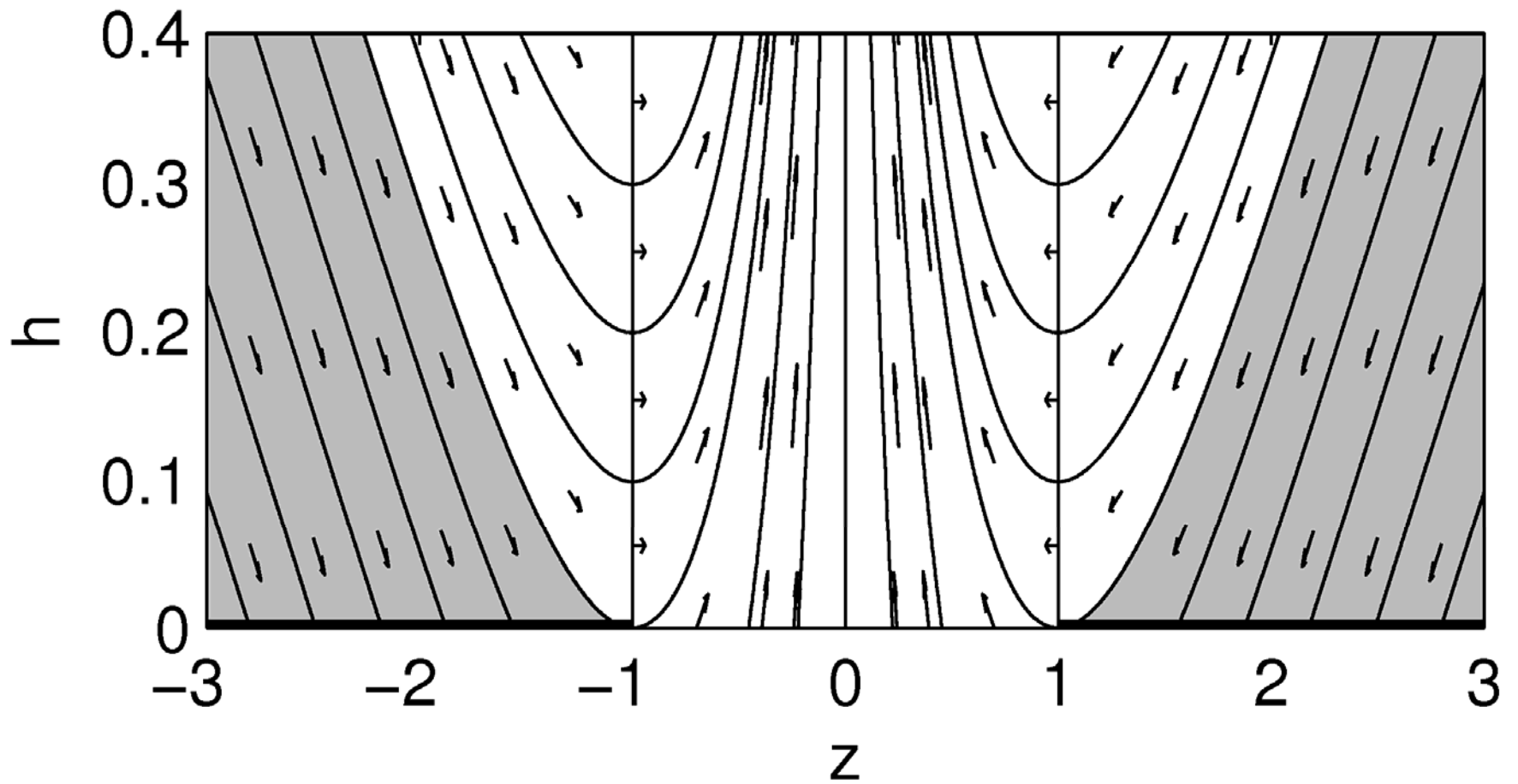
$$\frac{d\theta}{dt} = -\eta \nabla l, \quad \frac{d\theta}{dt} = -\eta G^{-1} \nabla l$$

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

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



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



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