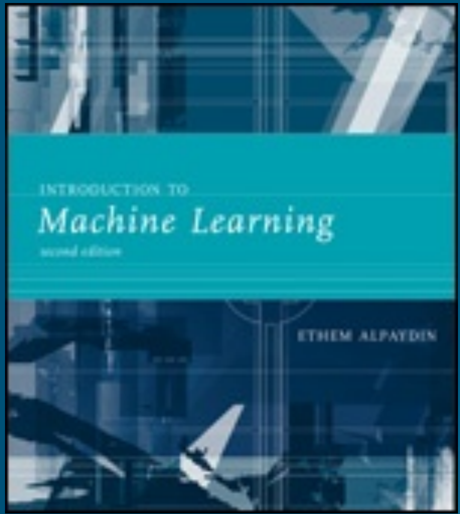

Lecture Slides for

INTRODUCTION TO

Machine Learning

2nd Edition

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CHAPTER 10:

Linear Discrimination

Likelihood- vs. Discriminant-based Classification

- Likelihood-based: Assume a model for $p(\boldsymbol{x}|C_i)$, use Bayes' rule to calculate $P(C_i|\boldsymbol{x})$

$$g_i(\boldsymbol{x}) = \log P(C_i|\boldsymbol{x})$$

- Discriminant-based: Assume a model for $g_i(\boldsymbol{x}|\Phi_i)$; no density estimation
- Estimating the boundaries is enough; no need to accurately estimate the densities inside the boundaries

Linear Discriminant

- Linear discriminant:

$$g_i(\mathbf{x} \mid \mathbf{w}_i, w_{i0}) = \mathbf{w}_i^T \mathbf{x} + w_{i0} = \sum_{j=1}^{d} w_{ij} x_j + w_{i0}$$

- Advantages:
  - Simple: O(d) space/computation
  - Knowledge extraction: Weighted sum of attributes; positive/negative weights, magnitudes (credit scoring)
  - Optimal when $p(\boldsymbol{x}|C_i)$ are Gaussian with shared cov matrix; useful when classes are (almost) linearly separable

Generalized Linear Model

- Quadratic discriminant:

$$g_i(\mathbf{x} \mid \mathbf{W}_i, \mathbf{w}_i, w_{i0}) = \mathbf{x}^T \mathbf{W}_i \mathbf{x} + \mathbf{w}_i^T \mathbf{x} + w_{i0}$$

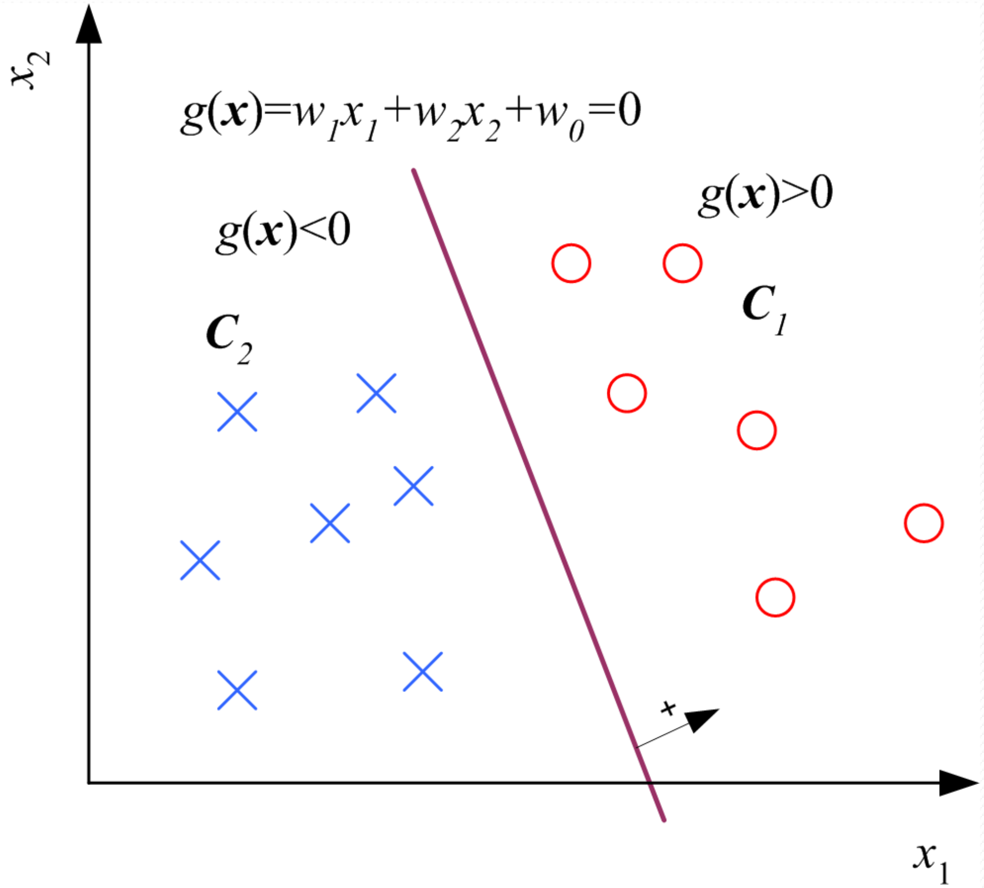
- Higher-order (product) terms:

$$z_1 = x_1,\ z_2 = x_2,\ z_3 = x_1^2,\ z_4 = x_2^2,\ z_5 = x_1 x_2$$

Map from ***x*** to ***z*** using nonlinear basis functions and use a linear discriminant in ***z***-space

$$g_i(\mathbf{x}) = \sum_{j=1}^{k} w_{ij} \phi_j(\mathbf{x})$$

Two Classes



$$
\begin{aligned}
g(\mathbf{x}) &= g_1(\mathbf{x}) - g_2(\mathbf{x}) \\
&= \left(\mathbf{w}_1^T\mathbf{x} + w_{10}\right) - \left(\mathbf{w}_2^T\mathbf{x} + w_{20}\right) \\
&= \left(\mathbf{w}_1 - \mathbf{w}_2\right)^T \mathbf{x} + \left(w_{10} - w_{20}\right) \\
&= \mathbf{w}^T\mathbf{x} + w_0
\end{aligned}
$$

$$
\text{choose } \begin{cases} C_1 & \text{if } g(\mathbf{x}) > 0 \\ C_2 & \text{otherwise} \end{cases}
$$

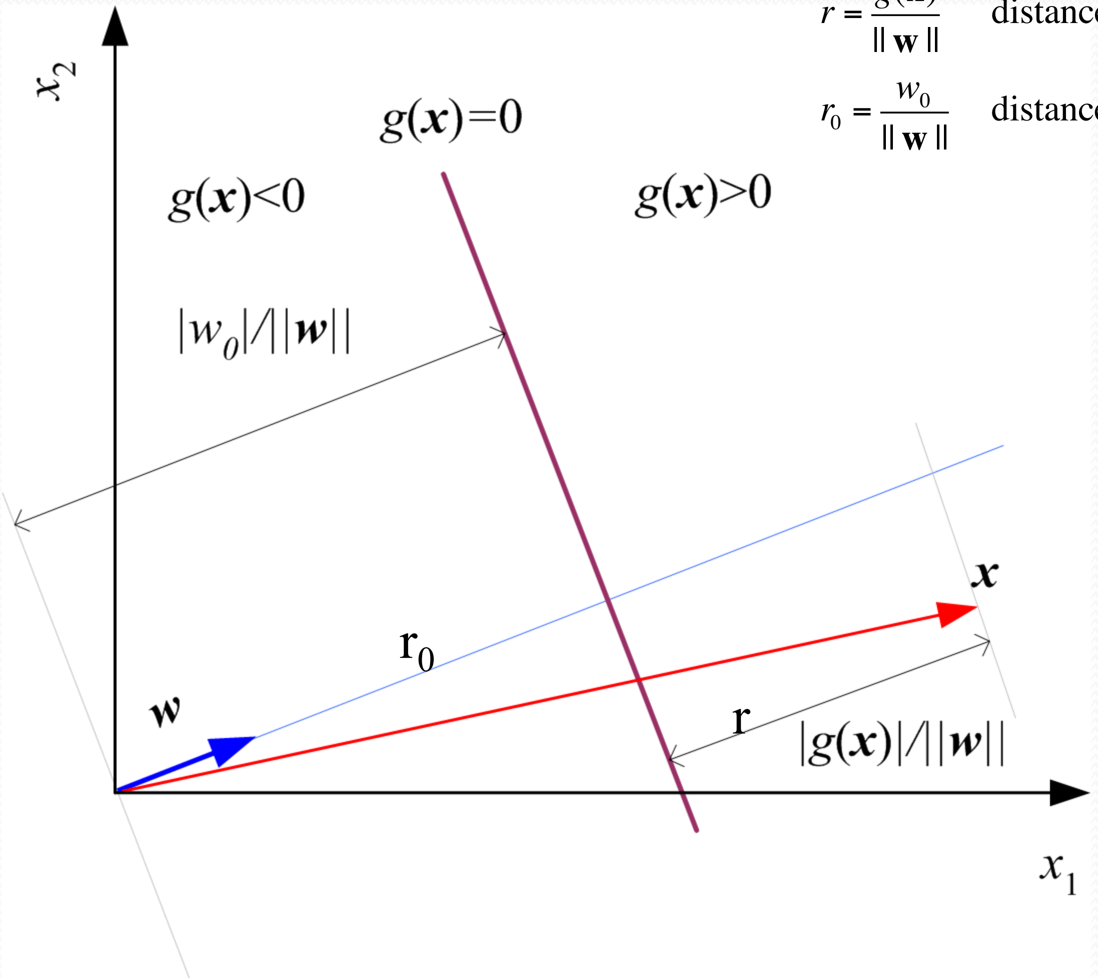
Geometry

$$g(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0$$

$$\mathbf{x} = \mathbf{x}_p + r\frac{\mathbf{w}}{\|\mathbf{w}\|}$$

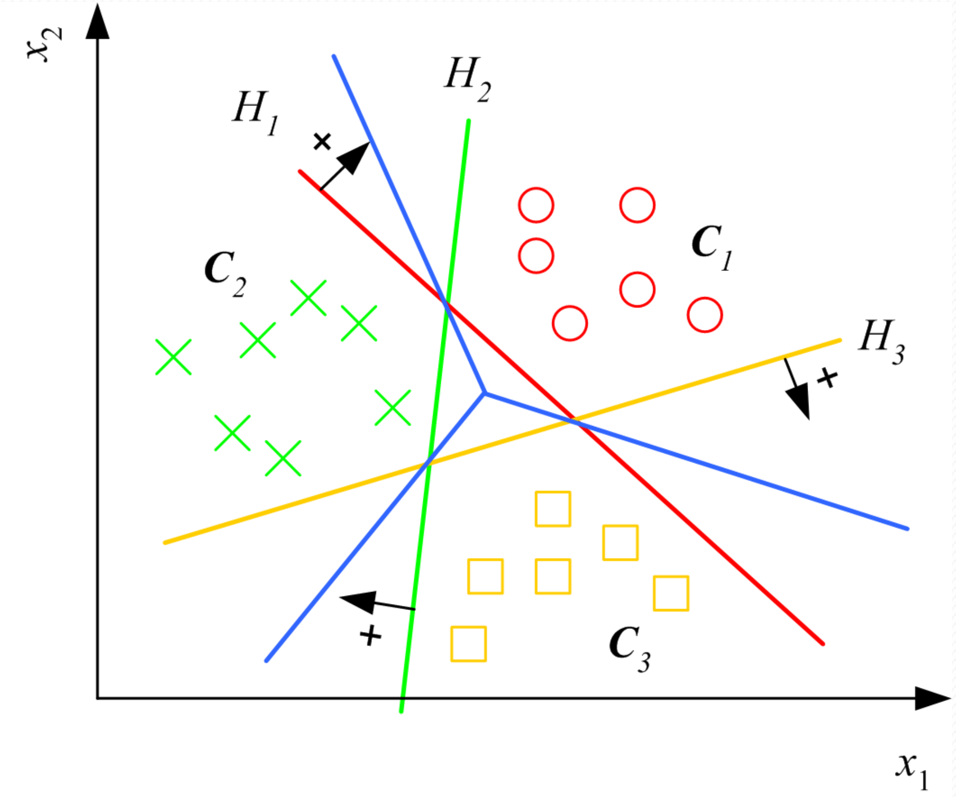
$$r = \frac{g(\mathbf{x})}{\|\mathbf{w}\|}$$ distance of any point x to hyperplane

$$r_0 = \frac{w_0}{\|\mathbf{w}\|}$$ distance of hyperplane to origin



Multiple Classes

$$g_i(\mathbf{x} \mid \mathbf{w}_i, w_{i0}) = \mathbf{w}_i^T \mathbf{x} + w_{i0}$$



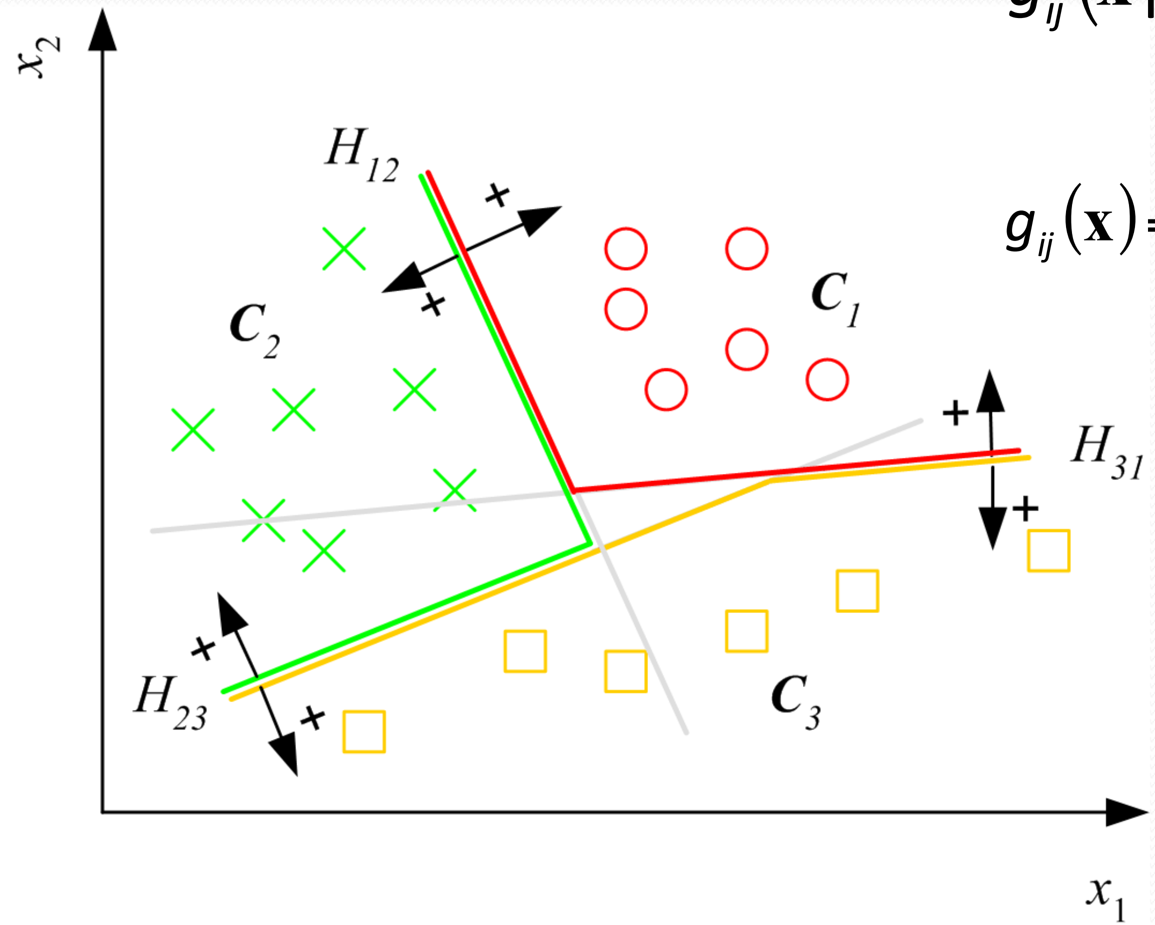
Choose C_i if

$$g_i(\mathbf{x}) = \max_{j=1}^{K} g_j(\mathbf{x})$$

Classes are
linearly separable

Pairwise Separation

$$g_{ij}\left(\mathbf{x} \mid \mathbf{w}_{ij}, w_{ij0}\right) = \mathbf{w}_{ij}^{T}\mathbf{x} + w_{ij0}$$



$$g_{ij}(\mathbf{x}) = \begin{cases} > 0 & \text{if } \mathbf{x} \in C_i \\ \leq 0 & \text{if } \mathbf{x} \in C_j \\ \text{don't care} & \text{otherwise} \end{cases}$$

choose C_i if

$$\forall j \neq i, g_{ij}(\mathbf{x}) > 0$$

From Discriminants to Posteriors

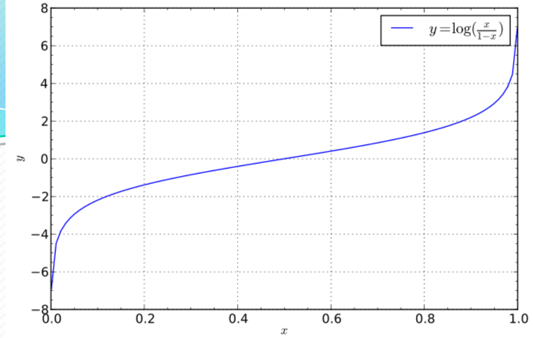
When $p\ (\boldsymbol{x} \mid C_i) \sim N\ (\boldsymbol{\mu}_i\ ,\ \boldsymbol{\Sigma})$

$$g_i(\mathbf{x} \mid \mathbf{w}_i, w_{i0}) = \mathbf{w}_i^T \mathbf{x} + w_{i0}$$

$$\mathbf{w}_i = \Sigma^{-1}\mu_i \quad w_{i0} = -\frac{1}{2}\mu_i^T \Sigma^{-1}\mu_i + \log P(C_i)$$

$$y \equiv P(C_1 \mid \mathbf{x}) \text{ and } P(C_2 \mid \mathbf{x}) = 1 - y$$

$$\text{choose } C_1 \text{ if} \begin{cases} y > 0.5 \\ y/(1-y) > 1 \\ \log\left[y/(1-y)\right] > 0 \end{cases} \text{ and } C_2 \text{ otherwise}$$



$$\operatorname{logit}(P(C_1|\mathbf{x})) = \log\frac{P(C_1|\mathbf{x})}{1-P(C_1|\mathbf{x})} = \log\frac{P(C_1|\mathbf{x})}{P(C_2|\mathbf{x})}$$

$$= \log\frac{p(\mathbf{x}|C_1)}{p(\mathbf{x}|C_2)} + \log\frac{P(C_1)}{P(C_2)}$$

$$= \log\frac{(2\pi)^{-d/2}|\Sigma|^{-1/2}\exp\left[-(1/2)(\mathbf{x}-\mu_1)^T\Sigma^{-1}(\mathbf{x}-\mu_1)\right]}{(2\pi)^{-d/2}|\Sigma|^{-1/2}\exp\left[-(1/2)(\mathbf{x}-\mu_2)^T\Sigma^{-1}(\mathbf{x}-\mu_2)\right]} + \log\frac{P(C_1)}{P(C_2)}$$

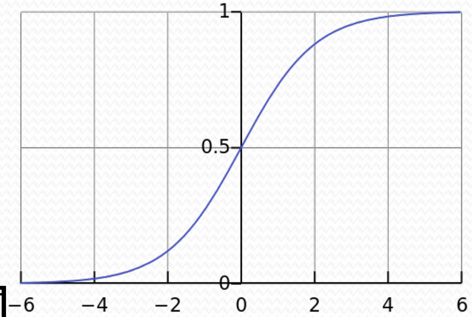
$$= \mathbf{w}^T\mathbf{x} + w_0$$

where $\mathbf{w} = \Sigma^{-1}(\mu_1 - \mu_2)$ $\quad w_0 = -\frac{1}{2}(\mu_1+\mu_2)^T\Sigma^{-1}(\mu_1-\mu_2) + \log\frac{P(C_1)}{P(C_2)}$

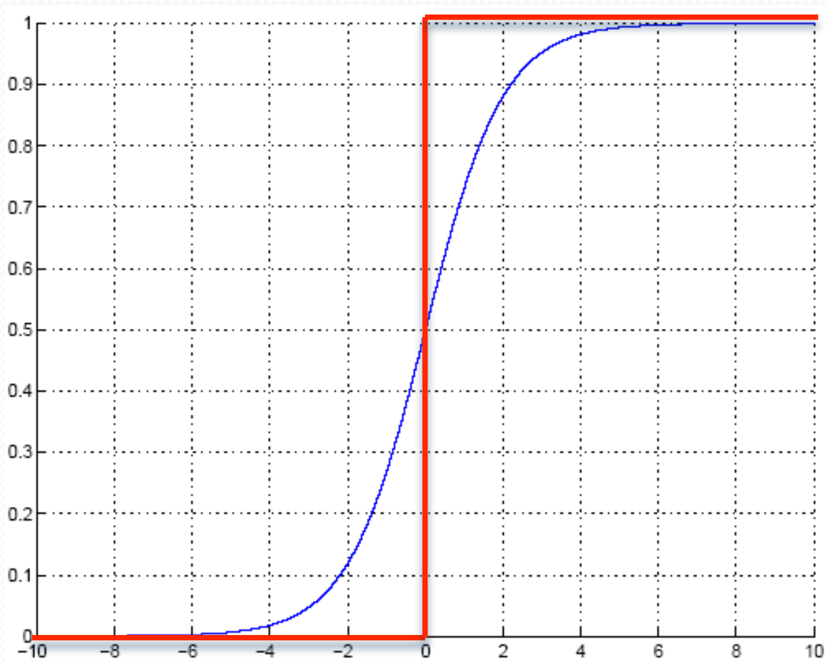
The inverse of logit

$$\log\frac{P(C_1|\mathbf{x})}{1-P(C_1|\mathbf{x})} = \mathbf{w}^T\mathbf{x} + w_0$$

$$P(C_1|\mathbf{x}) = \operatorname{sigmoid}(\mathbf{w}^T\mathbf{x}+w_0) = \frac{1}{1+\exp\left[-(\mathbf{w}^T\mathbf{x}+w_0)\right]}$$



Sigmoid (Logistic) Function



1. Calculate $g(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0$ and choose C_1 if $g(\mathbf{x}) > 0$, or

2. Calculate $y = \text{sigmoid}\left(\mathbf{w}^T\mathbf{x} + w_0\right)$ and choose C_1 if $y > 0.5$

Gradient-Descent

- $E(\boldsymbol{w}|X)$ is error with parameters $\boldsymbol{w}$ on sample X

$$\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} E(\boldsymbol{w} \mid X)$$

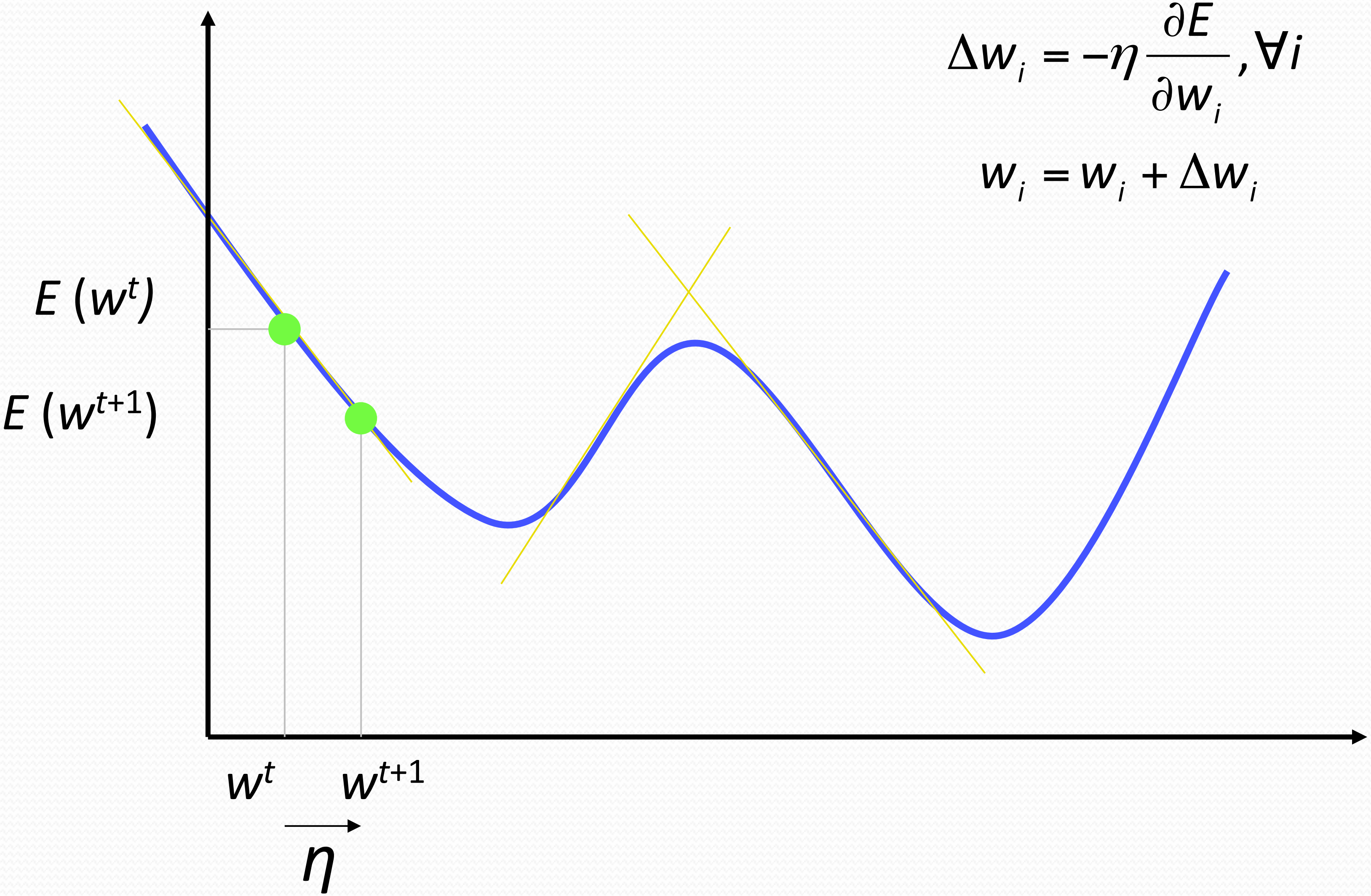
- Gradient

$$\nabla_w E = \left[\frac{\partial E}{\partial w_1}, \frac{\partial E}{\partial w_2}, \ldots, \frac{\partial E}{\partial w_d}\right]^T$$

- Gradient-descent:

  Starts from random $\boldsymbol{w}$ and updates $\boldsymbol{w}$ iteratively in the negative direction of gradient

Gradient-Descent



$$\Delta w_i = -\eta \frac{\partial E}{\partial w_i}, \forall i$$

$$w_i = w_i + \Delta w_i$$

Logistic Discrimination

- Two classes: Assume log likelihood ratio is linear

$$\log \frac{p(\mathbf{x} \mid C_1)}{p(\mathbf{x} \mid C_2)} = \mathbf{w}^T \mathbf{x} + w_0^o$$

$$\operatorname{logit}(P(C_1 \mid \mathbf{x})) = \log \frac{P(C_1 \mid \mathbf{x})}{1 - P(C_1 \mid \mathbf{x})} = \log \frac{p(\mathbf{x} \mid C_1)}{p(\mathbf{x} \mid C_2)} + \log \frac{P(C_1)}{P(C_2)}$$

$$= \mathbf{w}^T \mathbf{x} + w_0$$

$$\text{where } w_0 = w_0^o + \log \frac{P(C_1)}{P(C_2)}$$

$$y = \hat{P}(C_1 \mid \mathbf{x}) = \frac{1}{1 + \exp\left[-\left(\mathbf{w}^T \mathbf{x} + w_0\right)\right]}$$

Training: Two Classes

$$\mathcal{X} = \{\mathbf{x}^t, r^t\}_t \quad r^t \mid \mathbf{x}^t \sim \text{Bernoulli}\left(y^t\right)$$

$$y = P(C_1 \mid \mathbf{x}) = \frac{1}{1 + \exp\left[-\left(\mathbf{w}^T \mathbf{x} + w_0\right)\right]}$$

$$l(\mathbf{w}, w_0 \mid \mathcal{X}) = \prod_t \left(y^t\right)^{\left(r^t\right)} \left(1 - y^t\right)^{\left(1 - r^t\right)}$$

$$E = -\log l$$

$$E(\mathbf{w}, w_0 \mid \mathcal{X}) = -\sum_t r^t \log y^t + \left(1 - r^t\right) \log\left(1 - y^t\right)$$

Cross Entropy

Training: Gradient-Descent

$$E(\mathbf{w}, w_0 \mid \mathcal{X}) = -\sum_t r^t \log y^t + (1 - r^t) \log (1 - y^t)$$

$$\text{If } y = \text{sigmoid}(a) \quad \frac{dy}{da} = y(1 - y)$$

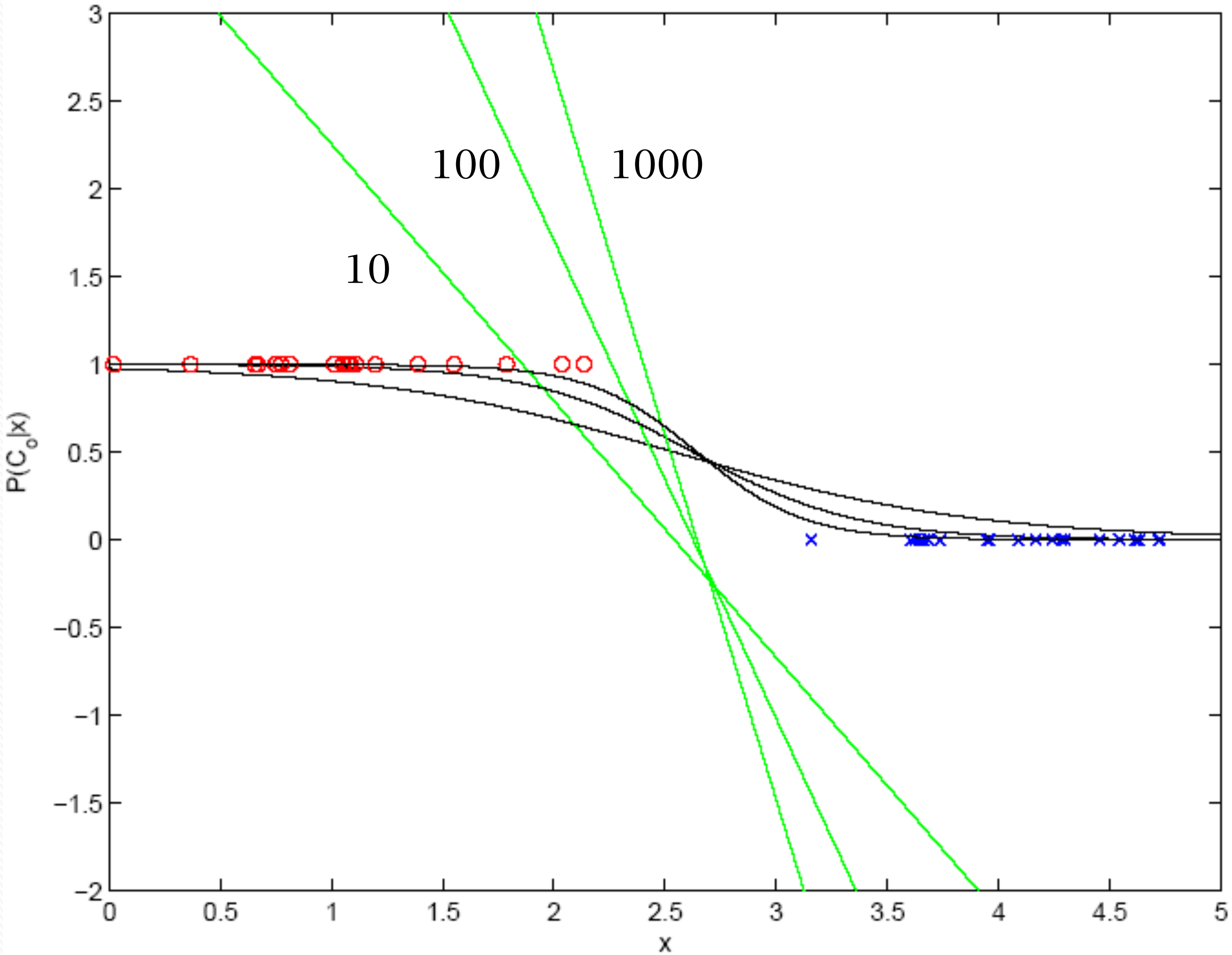
$$\Delta w_j = -\eta \frac{\partial E}{\partial w_j} = \eta \sum_t \left(\frac{r^t}{y^t} - \frac{1 - r^t}{1 - y^t} \right) y^t (1 - y^t) x_j^t$$

$$= \eta \sum_t (r^t - y^t) x_j^t, \; j = 1, \ldots, d$$

$$\Delta w_0 = -\eta \frac{\partial E}{\partial w_0} = \eta \sum_t (r^t - y^t)$$

```
For j = 0,...,d
    w_j ←rand(-0.01,0.01)
Repeat
    For j = 0,...,d
        Δw_j ← 0
    For t = 1,...,N
        o ← 0
        For j = 0,...,d
            o ← o + w_j x_j^t
        y ← sigmoid(o)
        Δw_j ← Δw_j + (r^t − y) x_j^t
    For j = 0,...,d
        w_j ← w_j + ηΔw_j
Until convergence
```

$$y = \hat{P}(C_1|\mathbf{x}) = \frac{1}{1+\exp\left[-\left(\mathbf{w}^T\mathbf{x}+w_0\right)\right]}$$



K>2 Classes

$$\mathcal{X} = \{\mathbf{x}^t, \mathbf{r}^t\}_t \quad r^t \mid \mathbf{x}^t \sim \text{Mult}_K(1, \mathbf{y}^t)$$

$$\log \frac{p(\mathbf{x} \mid C_i)}{p(\mathbf{x} \mid C_K)} = \mathbf{w}_i^T \mathbf{x} + w_{i0}^o$$

$$y = \hat{P}(C_i \mid \mathbf{x}) = \boxed{\frac{\exp\left[\mathbf{w}_i^T \mathbf{x} + w_{i0}\right]}{\sum_{j=1}^{K} \exp\left[\mathbf{w}_j^T \mathbf{x} + w_{j0}\right]}}, i = 1, \ldots, K$$

softmax

$$l(\{\mathbf{w}_i, w_{i0}\}_i \mid \mathcal{X}) = \prod_t \prod_i \left(y_i^t\right)^{\left(r_i^t\right)}$$

$$E(\{\mathbf{w}_i, w_{i0}\}_i \mid \mathcal{X}) = -\sum_t r_i^t \log y_i^t$$

$$\Delta \mathbf{w}_j = \eta \sum_t \left(r_j^t - y_j^t\right) \mathbf{x}^t \quad \Delta w_{j0} = \eta \sum_t \left(r_j^t - y_j^t\right)$$

For $i = 1, \ldots, K$, For $j = 0, \ldots, d$, $w_{ij} \leftarrow$ rand$(-0.01, 0.01)$

Repeat

  For $i = 1, \ldots, K$, For $j = 0, \ldots, d$, $\Delta w_{ij} \leftarrow 0$

  For $t = 1, \ldots, N$

    For $i = 1, \ldots, K$

      $o_i \leftarrow 0$

      For $j = 0, \ldots, d$

        $o_i \leftarrow o_i + w_{ij} x_j^t$

    For $i = 1, \ldots, K$

      $y_i \leftarrow \exp(o_i) / \sum_k \exp(o_k)$

    For $i = 1, \ldots, K$

      For $j = 0, \ldots, d$

        $\Delta w_{ij} \leftarrow \Delta w_{ij} + (r_i^t - y_i) x_j^t$

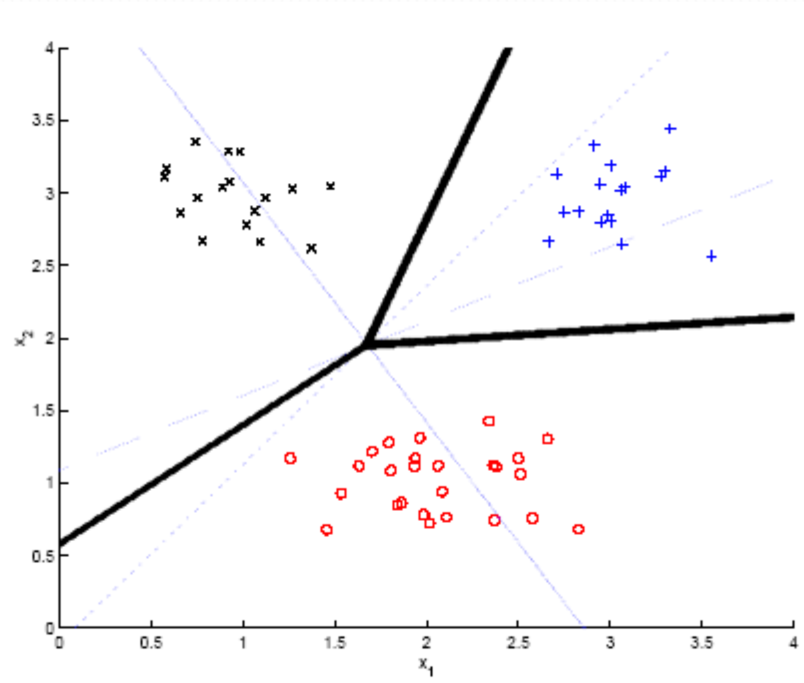
  For $i = 1, \ldots, K$

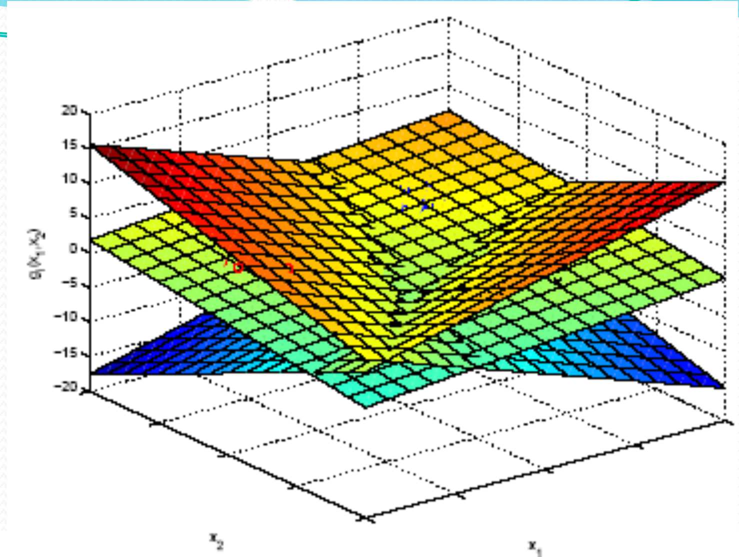
    For $j = 0, \ldots, d$

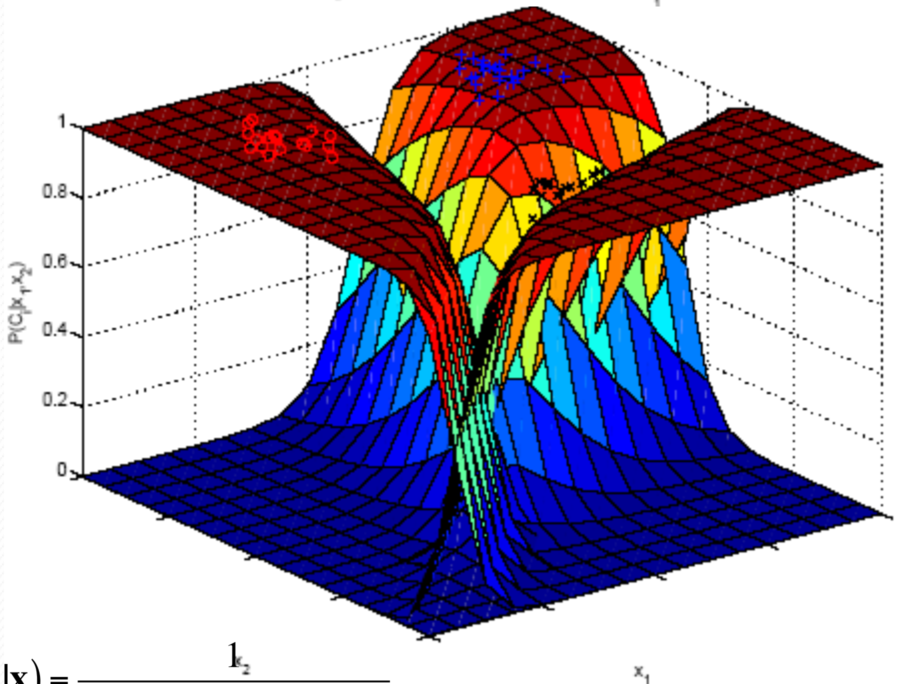
      $w_{ij} \leftarrow w_{ij} + \eta \Delta w_{ij}$

Until convergence

Example







$$y = \hat{P}\left(C_1|\mathbf{x}\right) = \frac{1}{1+\exp\left[-\left(\mathbf{w}^T\mathbf{x}+w_0\right)\right]}$$

Generalizing the Linear Model

- Quadratic:

$$\log \frac{p(\mathbf{x} | C_i)}{p(\mathbf{x} | C_K)} = \mathbf{x}^T \mathbf{W}_i \mathbf{x} + \mathbf{w}_i^T \mathbf{x} + w_{i0}$$

- Sum of basis functions:

$$\log \frac{p(\mathbf{x} | C_i)}{p(\mathbf{x} | C_K)} = \mathbf{w}_i^T \phi(\mathbf{x}) + w_{i0}$$

where $\boldsymbol{\phi}(\boldsymbol{x})$ are basis functions

- Hidden units in neural networks (Chapters 11 and 12)
- Kernels in SVM (Chapter 13)

Discrimination by Regression

- Classes are NOT mutually exclusive and exhaustive

$$r^t = y^t + \varepsilon \text{ where } \varepsilon \sim \mathcal{N}\left(0,\sigma^2\right) \qquad r^t \in \{0,1\}$$

$$y^t = \text{sigmoid}\left(\mathbf{w}^T\mathbf{x}^t + w_0\right) = \frac{1}{1+\exp\left[-\left(\mathbf{w}^T\mathbf{x}^t + w_0\right)\right]}$$

$$l\left(\mathbf{w}, w_0 \mid \mathcal{X}\right) = \prod_t \frac{1}{\sqrt{2\pi\sigma}} \exp\left[-\frac{\left(r^t - y^t\right)^2}{2\sigma^2}\right]$$

$$E\left(\mathbf{w}, w_0 \mid \mathcal{X}\right) = \frac{1}{2}\sum_t \left(r^t - y^t\right)^2$$

$$\Delta \mathbf{w} = \eta \sum_t \left(r^t - y^t\right) y^t \left(1 - y^t\right) \mathbf{x}^t$$