Machine Learning - Lecture 5

Linear Discriminant Functions

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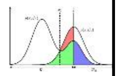
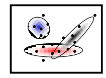
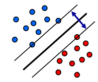
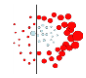
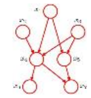
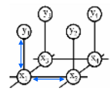
Many slides adapted from B. Schiele

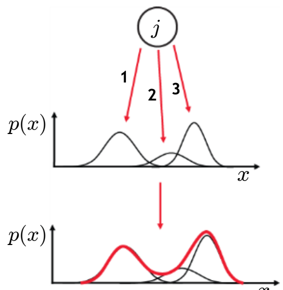
Course Outline

- Fundamentals (2 weeks)
  - Bayes Decision Theory
  - Probability Density Estimation
- Discriminative Approaches (5 weeks)
  - Linear Discriminant Functions
  - Support Vector Machines
  - Ensemble Methods & Boosting
  - Randomized Trees, Forests & Ferns
- Generative Models (4 weeks)
  - Bayesian Networks
  - Markov Random Fields

Recap: Mixture of Gaussians (MoG)

- "Generative model"



$p(j) = \pi_j$ "Weight" of mixture component

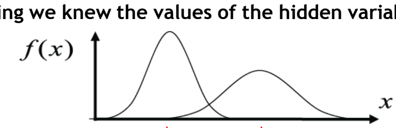
$p(x|\theta_j)$ Mixture component

Mixture density

$$p(x|\theta) = \sum_{j=1}^{M} p(x|\theta_j)p(j)$$

Recap: Estimating MoGs - Iterative Strategy

- Assuming we knew the values of the hidden variable…



ML for Gaussian #1 ML for Gaussian #2

assumed known → 1 111 22 2 2 j

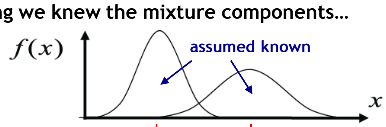
$h(j=1|x_n) =$ 1 111 00 0 0

$h(j=2|x_n) =$ 0 000 11 1 1

$$\mu_1 = \frac{\sum_{n=1}^{N} h(j=1|x_n)x_n}{\sum_{i=1}^{N} h(j=1|x_n)} \qquad \mu_2 = \frac{\sum_{n=1}^{N} h(j=2|x_n)x_n}{\sum_{i=1}^{N} h(j=2|x_n)}$$

Recap: Estimating MoGs - Iterative Strategy

- Assuming we knew the mixture components…



$p(j=1|x)$ $p(j=2|x)$

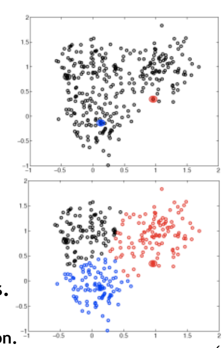
1 111 22 2 2 j

- Bayes decision rule: Decide $j = 1$ if

$$p(j=1|x_n) > p(j=2|x_n)$$

Recap: K-Means Clustering

- Iterative procedure
  1. Initialization: pick K arbitrary centroids (cluster means)
  2. Assign each sample to the closest centroid.
  3. Adjust the centroids to be the means of the samples assigned to them.
  4. Go to step 2 (until no change)
- Algorithm is guaranteed to converge after finite #iterations.
  - Local optimum
  - Final result depends on initialization.



Recap: EM Algorithm

- Expectation-Maximization (EM) Algorithm
  - E-Step: softly assign samples to mixture components

$$\gamma_j(\mathbf{x}_n) \leftarrow \frac{\pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}{\sum_{k=1}^N \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)} \quad \forall j = 1,\ldots,K, \quad n = 1,\ldots,N$$

  - M-Step: re-estimate the parameters (separately for each mixture component) based on the soft assignments

$$\hat{N}_j \leftarrow \sum_{n=1}^N \gamma_j(\mathbf{x}_n) = \text{soft number of samples labeled } j$$

$$\hat{\pi}_j^{\text{new}} \leftarrow \frac{\hat{N}_j}{N}$$

$$\hat{\boldsymbol{\mu}}_j^{\text{new}} \leftarrow \frac{1}{\hat{N}_j} \sum_{n=1}^N \gamma_j(\mathbf{x}_n)\mathbf{x}_n$$

$$\hat{\boldsymbol{\Sigma}}_j^{\text{new}} \leftarrow \frac{1}{\hat{N}_j} \sum_{n=1}^N \gamma_j(\mathbf{x}_n)(\mathbf{x}_n - \hat{\boldsymbol{\mu}}_j^{\text{new}})(\mathbf{x}_n - \hat{\boldsymbol{\mu}}_j^{\text{new}})^{\text{T}}$$

Slide adapted from Bernt Schiele

Topics of This Lecture

- Linear discriminant functions
  - Definition
  - Extension to multiple classes
- Least-squares classification
  - Derivation
  - Shortcomings
- Generalized linear models
  - Connection to neural networks
  - Generalized linear discriminants & gradient descent

Discriminant Functions

- Bayesian Decision Theory $\quad p(\mathcal{C}_k|x) = \frac{p(x|\mathcal{C}_k)p(\mathcal{C}_k)}{p(x)}$
  - Model conditional probability densities $p(x|\mathcal{C}_k)$ and priors $p(\mathcal{C}_k)$
  - Compute posteriors $p(\mathcal{C}_k|x)$ (using Bayes' rule)
  - Minimize probability of misclassification by maximizing $p(\mathcal{C}|x)$.
- New approach
  - Directly encode decision boundary
  - Without explicit modeling of probability densities
  - Minimize misclassification probability directly.

Slide credit: Bernt Schiele

Recap: Discriminant Functions

- Formulate classification in terms of comparisons
  - Discriminant functions

$$y_1(x), \ldots, y_K(x)$$

  - Classify x as class C_k if

$$y_k(x) > y_j(x) \quad \forall j \neq k$$

- Examples (Bayes Decision Theory)

$$y_k(x) = p(\mathcal{C}_k|x)$$
$$y_k(x) = p(x|\mathcal{C}_k)p(\mathcal{C}_k)$$
$$y_k(x) = \log p(x|\mathcal{C}_k) + \log p(\mathcal{C}_k)$$

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Discriminant Functions

- Example: 2 classes

$$y_1(x) > y_2(x)$$
$$\Leftrightarrow \quad y_1(x) - y_2(x) > 0$$
$$\Leftrightarrow \quad \mathbf{y}(x) > 0$$

- Decision functions (from Bayes Decision Theory)

$$y(x) = p(\mathcal{C}_1|x) - p(\mathcal{C}_2|x)$$

$$y(x) = \ln \frac{p(x|\mathcal{C}_1)}{p(x|\mathcal{C}_2)} + \ln \frac{p(\mathcal{C}_1)}{p(\mathcal{C}_2)}$$

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Learning Discriminant Functions

- General classification problem
  - Goal: take a new input $\mathbf{x}$ and assign it to one of K classes C_k.
  - Given: training set $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ with target values $\mathbf{T} = \{\mathbf{t}_1, \ldots, \mathbf{t}_N\}$.

  ⇒ Learn a discriminant function $y(\mathbf{x})$ to perform the classification.
- 2-class problem
  - Binary target values: $\quad t_n \in \{0, 1\}$
- K-class problem
  - 1-of-K coding scheme, e.g. $\quad \mathbf{t}_n = (0, 1, 0, 0, 0)^{\mathrm{T}}$

Linear Discriminant Functions

- 2-class problem
  - $y(x) > 0$: Decide for class C_1, else for class C_2
- In the following, we focus on linear discriminant functions

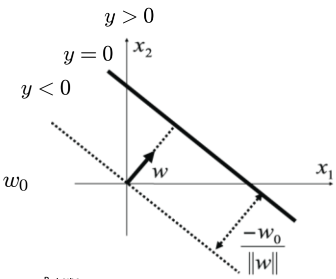
$$y(\mathbf{x}) = \underbrace{\mathbf{w}^{\mathrm{T}}}_{\text{weight vector}}\mathbf{x} + \underbrace{w_0}_{\text{"bias" (= threshold)}}$$

  - If a data set can be perfectly classified by a linear discriminant, then we call it linearly separable.

Linear Discriminant Functions

- Decision boundary $y(\mathbf{x}) = 0$ defines a hyperplane
  - Normal vector: $\mathbf{w}$
  - Offset: $\frac{-w_0}{\|\mathbf{w}\|}$

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



Linear Discriminant Functions

- Notation
  - D : Number of dimensions

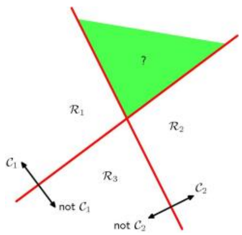
$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_D \end{bmatrix} \quad \mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_D \end{bmatrix}$$

$$\begin{aligned} y(\mathbf{x}) &= \mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0 \\ &= \sum_{i=1}^{D} w_i x_i + w_0 \\ &= \sum_{i=0}^{D} w_i x_i \quad \text{with } x_0 = 1 \text{ constant} \end{aligned}$$

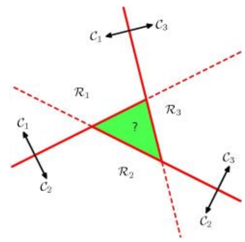
Extension to Multiple Classes

- Two simple strategies

One-vs-all classifiers



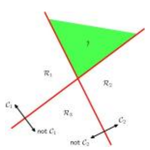
One-vs-one classifiers

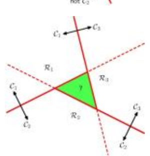


  - How many classifiers do we need in both cases?
  - What difficulties do you see for those strategies?

Extension to Multiple Classes

- Problem
  - Both strategies result in regions for which the pure classification result ($y_k > 0$) is ambiguous.
  - In the *one-vs-all* case, it is still possible to classify those inputs based on the continuous classifier outputs $y_k > y_j \; \forall j \neq k$.

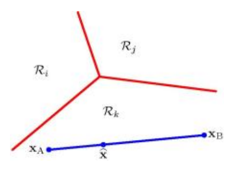




- Solution
  - We can avoid those difficulties by taking K linear functions of the form
    $$y_k(\mathbf{x}) = \mathbf{w}_k^{\mathrm{T}}\mathbf{x} + w_{k0}$$
    and defining the decision boundaries directly by deciding for C_k iff $y_k > y_j \; \forall j \neq k$.
  - This corresponds to a 1-of-K coding scheme
    $$\mathbf{t}_n = (0, 1, 0, \ldots, 0, 0)^{\mathrm{T}}$$

Extension to Multiple Classes

- K-class discriminant
  - Combination of K linear functions
    $$y_k(\mathbf{x}) = \mathbf{w}_k^{\mathrm{T}}\mathbf{x} + w_{k0}$$
  - Resulting decision hyperplanes:
    $$(\mathbf{w}_k - \mathbf{w}_j)^{\mathrm{T}}\mathbf{x} + (w_{k0} - w_{j0}) = 0$$



  - It can be shown that the decision regions of such a discriminant are always singly connected and convex.
  - This makes linear discriminant models particularly suitable for problems for which the conditional densities $p(\mathbf{x}|w_i)$ are unimodal.

Topics of This Lecture

- Linear discriminant functions
  - Definition
  - Extension to multiple classes
- Least-squares classification
  - Derivation
  - Shortcomings
- Generalized linear models
  - Connection to neural networks
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General Classification Problem

- Classification problem
  - Let's consider K classes described by linear models

$$y_k(\mathbf{x}) = \mathbf{w}_k^{\mathrm{T}}\mathbf{x} + w_{k0}, \qquad k = 1, \ldots, K$$

  - We can group those together using vector notation

$$\mathbf{y}(\mathbf{x}) = \widetilde{\mathbf{W}}^{\mathrm{T}}\widetilde{\mathbf{x}}$$

where

$$\widetilde{\mathbf{W}} = [\widetilde{\mathbf{w}}_1, \ldots, \widetilde{\mathbf{w}}_K] = \begin{bmatrix} w_{10} & \ldots & w_{K0} \\ w_{11} & \ldots & w_{K1} \\ \vdots & \ddots & \vdots \\ w_{1D} & \ldots & w_{KD} \end{bmatrix}$$

  - The output will again be in 1-of-K notation.

⇒ We can directly compare it to the target value $\mathbf{t} = [t_1, \ldots, t_k]^{\mathrm{T}}$.

General Classification Problem

- Classification problem
  - For the entire dataset, we can write

$$\mathbf{Y}(\widetilde{\mathbf{X}}) = \widetilde{\mathbf{X}}\widetilde{\mathbf{W}}$$

and compare this to the target matrix $\mathbf{T}$ where

$$\widetilde{\mathbf{W}} = [\widetilde{\mathbf{w}}_1, \ldots, \widetilde{\mathbf{w}}_K]$$

$$\widetilde{\mathbf{X}} = \begin{bmatrix} \mathbf{x}_1^{\mathrm{T}} \\ \vdots \\ \mathbf{x}_N^{\mathrm{T}} \end{bmatrix} \qquad \mathbf{T} = \begin{bmatrix} \mathbf{t}_1^{\mathrm{T}} \\ \vdots \\ \mathbf{t}_N^{\mathrm{T}} \end{bmatrix}$$

  - Result of the comparison:

$$\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T}$$

Goal: Choose $\widetilde{\mathbf{W}}$ such that this is minimal!

Least-Squares Classification

- Simplest approach
  - Directly try to minimize the sum-of-squares error
  - We could write this as

$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K}\left(y_k(\mathbf{x}_n;\mathbf{w}) - t_{kn}\right)^2 = \frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K}\left(\mathbf{w}_k^T\mathbf{x}_n - t_{kn}\right)^2$$

  - But let's stick with the matrix notation for now...
  - (The result will be simpler to express and we'll learn some nice matrix algebra rules along the way...)

Least-Squares Classification

using: $\sum_{i,j} a_{ij}^2 = \mathrm{Tr}\{\mathbf{A}^{\mathrm{T}}\mathbf{A}\}$

- Multi-class case
  - Let's formulate the sum-of-squares error in matrix notation

$$E_D(\widetilde{\mathbf{W}}) = \frac{1}{2}\mathrm{Tr}\left\{(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})^{\mathrm{T}}(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})\right\}$$

  - Taking the derivative yields

chain rule: $\frac{\partial \mathbf{Z}}{\partial \mathbf{X}} = \frac{\partial \mathbf{Z}}{\partial \mathbf{Y}}\frac{\partial \mathbf{Y}}{\partial \mathbf{X}}$

$$\begin{aligned} \frac{\partial}{\partial \widetilde{\mathbf{W}}}E_D(\widetilde{\mathbf{W}}) &= \frac{1}{2}\frac{\partial}{\partial \widetilde{\mathbf{W}}}\mathrm{Tr}\left\{(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})^{\mathrm{T}}(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})\right\} \\ &= \frac{1}{2}\frac{\partial}{\partial(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})^{\mathrm{T}}(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})}\mathrm{Tr}\left\{(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})^{\mathrm{T}}(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})\right\} \\ &\quad \cdot \frac{\partial}{\partial \widetilde{\mathbf{W}}}(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})^{\mathrm{T}}(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T}) \\ &= \widetilde{\mathbf{X}}^{\mathrm{T}}(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T}) \end{aligned}$$

using: $\frac{\partial}{\partial \mathbf{A}}\mathrm{Tr}\{\mathbf{A}\} = \mathbf{I}$

Least-Squares Classification

- Minimizing the sum-of-squares error

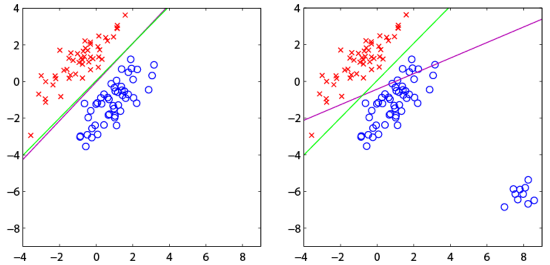
$$\begin{aligned} \frac{\partial}{\partial \widetilde{\mathbf{W}}}E_D(\widetilde{\mathbf{W}}) = \widetilde{\mathbf{X}}^{\mathrm{T}}(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T}) &\overset{!}{=} 0 \\ \widetilde{\mathbf{X}}\widetilde{\mathbf{W}} &= \mathbf{T} \\ \widetilde{\mathbf{W}} &= (\widetilde{\mathbf{X}}^{\mathrm{T}}\widetilde{\mathbf{X}})^{-1}\widetilde{\mathbf{X}}^{\mathrm{T}}\mathbf{T} \\ &= \widetilde{\mathbf{X}}^{\dagger}\mathbf{T} \qquad \text{“pseudo-inverse”} \end{aligned}$$

  - We then obtain the discriminant function as

$$\mathbf{y}(\mathbf{x}) = \widetilde{\mathbf{W}}^{\mathrm{T}}\widetilde{\mathbf{x}} = \mathbf{T}^{\mathrm{T}}\left(\widetilde{\mathbf{X}}^{\dagger}\right)^{\mathrm{T}}\widetilde{\mathbf{x}}$$

⇒ Exact, closed-form solution for the discriminant function parameters.

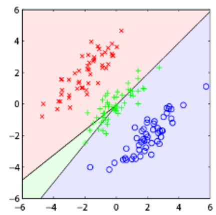
Problems with Least Squares



- **Least-squares is very sensitive to outliers!**
  - The error function penalizes predictions that are "too correct".

Problems with Least-Squares

- **Another example:**
  - 3 classes (red, green, blue)
  - Linearly separable problem
  - Least-squares solution:
    Most green points are misclassified!



- **Deeper reason for the failure**
  - Least-squares corresponds to Maximum Likelihood under the assumption of a Gaussian conditional distribution.
  - However, our binary target vectors have a distribution that is clearly non-Gaussian!

  $\Rightarrow$ Least-squares is the wrong probabilistic tool in this case!

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- Linear discriminant functions
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- Least-squares classification
  - Derivation
  - Shortcomings
- **Generalized linear models**
  - Connection to neural networks
  - Generalized linear discriminants & gradient descent

Generalized Linear Models

- **Linear model**

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

- **Generalized linear model**

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

  - $g(\cdot)$ is called an activation function and may be nonlinear.
  - The decision surfaces correspond to

$$y(\mathbf{x}) = const. \quad \Leftrightarrow \quad \mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0 = const.$$

  - If g is monotonous (which is typically the case), the resulting decision boundaries are still linear functions of $\mathbf{x}$.

Generalized Linear Models

- **Consider 2 classes:**

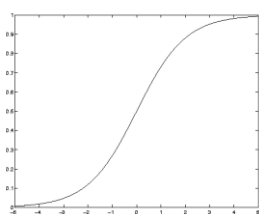
$$\begin{aligned} p(\mathcal{C}_1|\mathbf{x}) &= \frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1) + p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)} \\ &= \frac{1}{1 + \frac{p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)}{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}} \\ &= \frac{1}{1+\exp(-a)} \equiv g(a) \end{aligned}$$

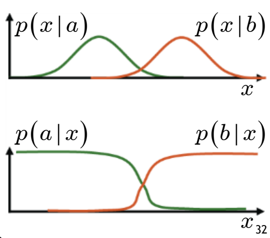
with $\quad a = \ln \dfrac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)}$

Logistic Sigmoid Activation Function

$$g(a) \equiv \frac{1}{1+\exp(-a)}$$

Example: Normal distributions with identical covariance





Normalized Exponential

- General case of $K > 2$ classes:

$$p(\mathcal{C}_k|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{\sum_j p(\mathbf{x}|\mathcal{C}_j)p(\mathcal{C}_j)} = \frac{\exp(a_k)}{\sum_j \exp(a_j)}$$

with $a_k = \ln p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)$

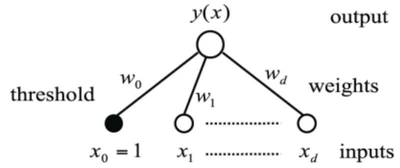
  - This is known as the normalized exponential or softmax function
  - Can be regarded as a multiclass generalization of the logistic sigmoid.

Relationship to Neural Networks

- 2-Class case

$$y(\mathbf{x}) = g\left(\sum_{i=0}^{D} w_i x_i\right) \quad \text{with } x_0 = 1 \text{ constant}$$

- Neural network ("single-layer perceptron")

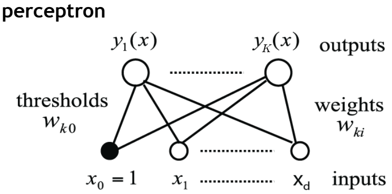


Relationship to Neural Networks

- Multi-class case

$$y_k(\mathbf{x}) = g\left(\sum_{i=0}^{D} w_{ki} x_i\right) \quad \text{with } x_0 = 1 \text{ constant}$$

- Multi-class perceptron

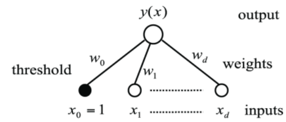


Logistic Discrimination

- If we use the logistic sigmoid activation function…

$$g(a) \equiv \frac{1}{1+\exp(-a)}$$

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



… then we can interpret the $y(x)$ as posterior probabilities!

Other Motivation for Nonlinearity

- Recall least-squares classification
  - One of the problems was that data points that are "too correct" have a strong influence on the decision surface under a squared-error criterion.

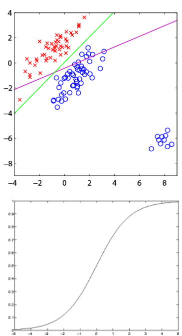
$$E(\mathbf{w}) = \sum_{n=1}^{N} (y(\mathbf{x}_n;\mathbf{w}) - \mathbf{t}_n)^2$$

  - Reason: the output of $y(\mathbf{x}_n;\mathbf{w})$ can grow arbitrarily large for some $\mathbf{x}_n$:

$$y(\mathbf{x};\mathbf{w}) = \mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0$$

  - By choosing a suitable nonlinearity (e.g. a sigmoid), we can limit those influences

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

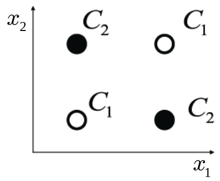


Discussion: Generalized Linear Models

- Advantages
  - The nonlinearity gives us more flexibility.
  - Can be used to limit the effect of outliers.
  - Choice of a sigmoid leads to a nice probabilistic interpretation.
- Disadvantage
  - Least-squares minimization in general no longer leads to a closed-form analytical solution.
  - ⇒ Need to apply iterative methods.
  - ⇒ Gradient descent.

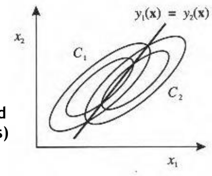
Linear Separability

- Up to now: restrictive assumption
  - Only consider linear decision boundaries
- Classical counterexample: XOR



Linear Separability

- Even if the data is not linearly separable, a linear decision boundary may still be "optimal".
  - Generalization
  - E.g. in the case of Normal distributed data (with equal covariance matrices)



- Choice of the right discriminant function is important and should be based on
  - Prior knowledge (of the general functional form)
  - Empirical comparison of alternative models
  - Linear discriminants are often used as benchmark.

Generalized Linear Discriminants

- Generalization
  - Transform vector $\mathbf{x}$ with M nonlinear basis functions $\phi_j(\mathbf{x})$:

$$y_k(\mathbf{x}) = \sum_{j=1}^{M} w_{kj}\phi_j(\mathbf{x}) + w_{k0}$$

  - Purpose of $\phi_j(\mathbf{x})$: basis functions
  - Allow non-linear decision boundaries.
  - By choosing the right ϕ_j, every continuous function can (in principle) be approximated with arbitrary accuracy.
- Notation

$$y_k(\mathbf{x}) = \sum_{j=0}^{M} w_{kj}\phi_j(\mathbf{x}) \qquad \text{with } \phi_0(\mathbf{x}) = 1$$

Generalized Linear Discriminants

- Model

$$y_k(\mathbf{x}) = \sum_{j=0}^{M} w_{kj}\phi_j(\mathbf{x}) = y_k(\mathbf{x};\mathbf{w})$$

  - K functions (outputs) $y_k(\mathbf{x};\mathbf{w})$
- Learning in Neural Networks
  - Single-layer networks: ϕ_j are fixed, only weights $\mathbf{w}$ are learned.
  - Multi-layer networks: both the $\mathbf{w}$ and the ϕ_j are learned.
  - In the following, we will not go into details about neural networks in particular, but consider generalized linear discriminants in general…

Gradient Descent

- Learning the weights $\mathbf{w}$:
  - N training data points: $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$
  - K outputs of decision functions: $y_k(\mathbf{x}_n;\mathbf{w})$
  - Target vector for each data point: $\mathbf{T} = \{\mathbf{t}_1, \ldots, \mathbf{t}_N\}$
  - Error function (least-squares error) of linear model

$$\begin{aligned} E(\mathbf{w}) &= \frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K}\left(y_k(\mathbf{x}_n;\mathbf{w}) - t_{kn}\right)^2 \\ &= \frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K}\left(\sum_{j=1}^{M} w_{kj}\phi_j(\mathbf{x}_n) - t_{kn}\right)^2 \end{aligned}$$

Gradient Descent

- Problem
  - The error function can in general no longer be minimized in closed form.
- Idea (Gradient Descent)
  - Iterative minimization
  - Start with an initial guess for the parameter values $w_{kj}^{(0)}$.
  - Move towards a (local) minimum by following the gradient.

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left.\frac{\partial E(\mathbf{w})}{\partial w_{kj}}\right|_{\mathbf{w}^{(\tau)}}$$

η: Learning rate

  - This simple scheme corresponds to a 1st-order Taylor expansion (There are more complex procedures available).

Gradient Descent - Basic Strategies

- "Batch learning"

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left.\frac{\partial E(\mathbf{w})}{\partial w_{kj}}\right|_{\mathbf{w}^{(\tau)}}$$

η: Learning rate

- Compute the gradient based on all training data:

$$\frac{\partial E(\mathbf{w})}{\partial w_{kj}}$$

Gradient Descent - Basic Strategies

- "Sequential updating"

$$E(\mathbf{w}) = \sum_{n=1}^{N} E_n(\mathbf{w})$$

$$w_{kj}^{(\tau+1)} = w_{kj}^{(\tau)} - \eta \left.\frac{\partial E_n(\mathbf{w})}{\partial w_{kj}}\right|_{\mathbf{w}^{(\tau)}}$$

η: Learning rate

- Compute the gradient based on a single data point at a time:

$$\frac{\partial E_n(\mathbf{w})}{\partial w_{kj}}$$

Gradient Descent

- Error function

$$\begin{aligned}
E(\mathbf{w}) = \sum_{n=1}^{N} E_n(\mathbf{w}) &= \frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K}\left(\sum_{j=1}^{M} w_{kj}\phi_j(\mathbf{x}_n) - t_{kn}\right)^2 \\
E_n(\mathbf{w}) &= \frac{1}{2}\sum_{k=1}^{K}\left(\sum_{j=1}^{M} w_{kj}\phi_j(\mathbf{x}_n) - t_{kn}\right)^2 \\
\frac{\partial E_n(\mathbf{w})}{\partial w_{kj}} &= \left(\sum_{\tilde{j}=1}^{M} w_{k\tilde{j}}\phi_{\tilde{j}}(\mathbf{x}_n) - t_{kn}\right)\phi_j(\mathbf{x}_n) \\
&= \left(y_k(\mathbf{x}_n;\mathbf{w}) - t_{kn}\right)\phi_j(\mathbf{x}_n)
\end{aligned}$$

Gradient Descent

- Delta rule (=LMS rule)

$$\begin{aligned}
w_{kj}^{(\tau+1)} &= w_{kj}^{(\tau)} - \eta\left(y_k(\mathbf{x}_n;\mathbf{w}) - t_{kn}\right)\phi_j(\mathbf{x}_n) \\
&= w_{kj}^{(\tau)} - \eta\delta_{kn}\phi_j(\mathbf{x}_n)
\end{aligned}$$

- where

$$\delta_{kn} = y_k(\mathbf{x}_n;\mathbf{w}) - t_{kn}$$

⇒ Simply feed back the input data point, weighted by the classification error.

Gradient Descent

- Cases with differentiable, non-linear activation function

$$y_k(\mathbf{x}) = g(a_k) = g\left(\sum_{j=0}^{M} w_{ki}\phi_j(\mathbf{x}_n)\right)$$

- Gradient descent

$$\begin{aligned}
\frac{\partial E_n(\mathbf{w})}{\partial w_{kj}} &= \frac{\partial g(a_k)}{\partial w_{kj}}\left(y_k(\mathbf{x}_n;\mathbf{w}) - t_{kn}\right)\phi_j(\mathbf{x}_n) \\
w_{kj}^{(\tau+1)} &= w_{kj}^{(\tau)} - \eta\delta_{kn}\phi_j(\mathbf{x}_n) \\
\delta_{kn} &= \frac{\partial g(a_k)}{\partial w_{kj}}\left(y_k(\mathbf{x}_n;\mathbf{w}) - t_{kn}\right)
\end{aligned}$$

Summary: Generalized Linear Discriminants

- Properties
  - General class of decision functions.
  - Nonlinearity $g(\cdot)$ and basis functions ϕ_j allow us to address linearly non-separable problems.
  - Shown simple sequential learning approach for parameter estimation using gradient descent.
  - Better 2nd order gradient descent approaches available (e.g. Newton-Raphson).
- Limitations / Caveats
  - Flexibility of model is limited by curse of dimensionality
    - $g(\cdot)$ and ϕ_j often introduce additional parameters.
    - Models are either limited to lower-dimensional input space or need to share parameters.
  - Linearly separable case often leads to overfitting.
    - Several possible parameter choices minimize training error.

References and Further Reading

- More information on Linear Discriminant Functions can be found in Chapter 4 of Bishop's book (in particular Chapter 4.1).

Christopher M. Bishop
Pattern Recognition and Machine Learning
Springer, 2006