CSC 411: Lecture 07: Multiclass Classification

Class based on Raquel Urtasun & Rich Zemel's lectures

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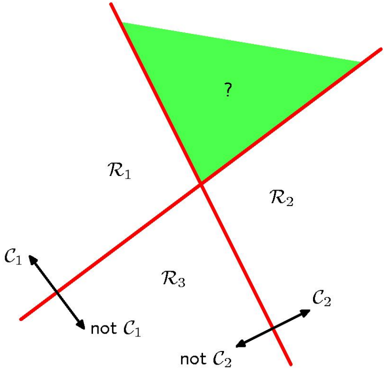
Today

Multi-class classification with:

- Least-squares regression
- Logistic Regression
- K-NN
- Decision trees

Discriminant Functions for $K > 2$ classes

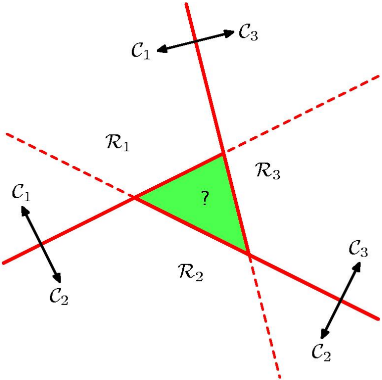
- First idea: Use $K - 1$ classifiers, each solving a two class problem of separating point in a class C_k from points not in the class.
- Known as **1 vs all** or **1 vs the rest** classifier



- PROBLEM: More than one good answer for green region!

Discriminant Functions for $K > 2$ classes

- Another simple idea: Introduce $K(K-1)/2$ two-way classifiers, one for each possible pair of classes
- Each point is classified according to majority vote amongst the disc. func.
- Known as the **1 vs 1 classifier**



- PROBLEM: Two-way preferences need not be transitive

K-Class Discriminant

- We can avoid these problems by considering a single K-class discriminant comprising K functions of the form

$$y_k(\mathbf{x}) = \mathbf{w}_k^T \mathbf{x} + w_{k,0}$$

and then assigning a point $\mathbf{x}$ to class C_k if

$$\forall j \neq k \qquad y_k(\mathbf{x}) > y_j(\mathbf{x})$$

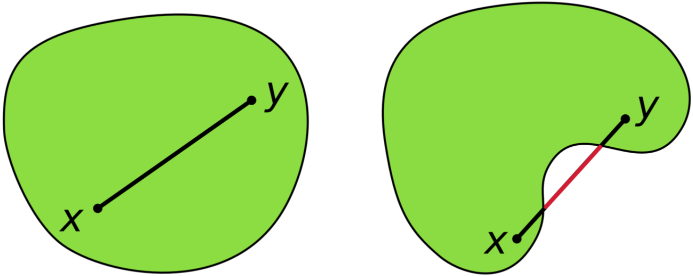
- Note that $\mathbf{w}_k^T$ is now a vector, not the k-th coordinate
- The decision boundary between class C_j and class C_k is given by $y_j(\mathbf{x}) = y_k(\mathbf{x})$, and thus it's a $(D-1)$ dimensional hyperplane defined as

$$(\mathbf{w}_k - \mathbf{w}_j)^T \mathbf{x} + (w_{k0} - w_{j0}) = 0$$

- What about the binary case? Is this different?
- What is the shape of the overall decision boundary?

K-Class Discriminant

- The decision regions of such a discriminant are always **singly connected** and **convex**
- In Euclidean space, an object is **convex** if for every pair of points within the object, every point on the straight line segment that joins the pair of points is also within the object

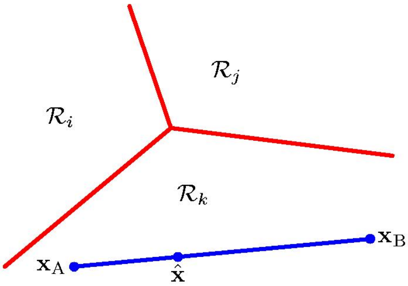


- Which object is convex?

K-Class Discriminant

- The decision regions of such a discriminant are always **singly connected** and **convex**
- Consider 2 points $\mathbf{x}_A$ and $\mathbf{x}_B$ that lie inside decision region R_k
- Any convex combination $\hat{\mathbf{x}}$ of those points also will be in R_k

$$\hat{\mathbf{x}} = \lambda \mathbf{x}_A + (1 - \lambda)\mathbf{x}_B$$



Proof

- A convex combination point, i.e., $\lambda \in [0, 1]$

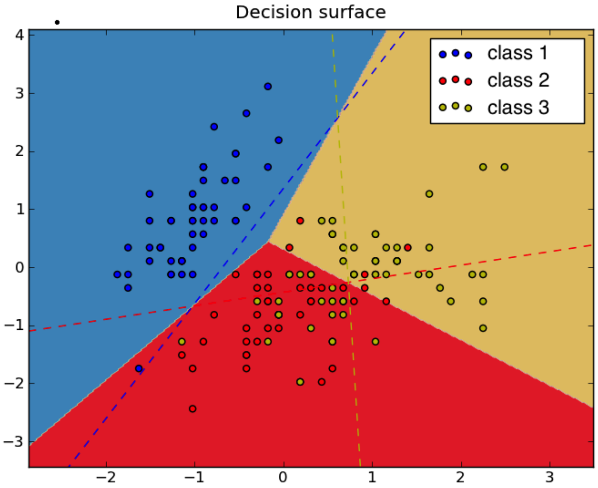
$$\hat{\mathbf{x}} = \lambda \mathbf{x}_A + (1 - \lambda)\mathbf{x}_B$$

- From the linearity of the classifier $y(\mathbf{x})$

$$y_k(\hat{\mathbf{x}}) = \lambda y_k(\mathbf{x}_A) + (1 - \lambda) y_k(\mathbf{x}_B)$$

- Since $\mathbf{x}_A$ and $\mathbf{x}_B$ are in R_k, it follows that $y_k(\mathbf{x}_A) > y_j(\mathbf{x}_A)$, $y_k(\mathbf{x}_B) > y_j(\mathbf{x}_B)$, $\forall j \neq k$
- Since λ and $1 - \lambda$ are positive, then $\hat{\mathbf{x}}$ is inside R_k
- Thus R_k is singly connected and convex

Example



Multi-class Classification with Linear Regression

- From before we have:
$$y_k(\mathbf{x}) = \mathbf{w}_k^T \mathbf{x} + w_{k,0}$$
which can be rewritten as:
$$\mathbf{y}(\mathbf{x}) = \tilde{\mathbf{W}}^T \tilde{\mathbf{x}}$$
where the k-th column of $\tilde{\mathbf{W}}$ is $[w_{k,0}, \mathbf{w}_k^T]^T$, and $\tilde{\mathbf{x}}$ is $[1, \mathbf{x}^T]^T$
- **Training:** How can I find the weights $\tilde{\mathbf{W}}$ with the standard sum-of-squares regression loss?

1-of-K encoding:

For multi-class problems (with K classes), instead of using $t = k$ (target has label k) we often use a **1-of-K encoding**, i.e., a vector of K target values containing a single 1 for the correct class and zeros elsewhere

Example: For a 4-class problem, we would write a target with class label 2 as:
$$\mathbf{t} = [0, 1, 0, 0]^T$$

Multi-class Classification with Linear Regression

- Sum-of-least-squares loss:

$$\begin{aligned}\ell(\tilde{\mathbf{W}}) &= \sum_{n=1}^{N} ||\tilde{\mathbf{W}}^T \tilde{\mathbf{x}}^{(n)} - \mathbf{t}^{(n)}||^2 \\ &= ||\tilde{\mathbf{X}}\,\tilde{\mathbf{W}} - \mathbf{T}||_F^2\end{aligned}$$

  where the n-th row of $\tilde{\mathbf{X}}$ is $[\tilde{\mathbf{x}}^{(n)}]^T$, and n-th row of $\mathbf{T}$ is $[\mathbf{t}^{(n)}]^T$

- Setting derivative wrt $\tilde{\mathbf{W}}$ to 0, we get:

$$\tilde{\mathbf{W}} = (\tilde{\mathbf{X}}^T \tilde{\mathbf{X}})^{-1} \tilde{\mathbf{X}}^T \mathbf{T}$$

Multi-class Logistic Regression

- Associate a set of weights with each class, then use a normalized exponential output

$$p(C_k|\mathbf{x}) = y_k(\mathbf{x}) = \frac{\exp(z_k)}{\sum_j \exp(z_j)}$$

where the **activations** are given by

$$z_k = \mathbf{w}_k^T \mathbf{x}$$

- The function $\frac{\exp(z_k)}{\sum_j \exp(z_j)}$ is called a **softmax function**

Multi-class Logistic Regression

- The likelihood

$$p(\mathbf{T}|\mathbf{w}_1, \cdots, \mathbf{w}_k) = \prod_{n=1}^{N} \prod_{k=1}^{K} p(C_k|\mathbf{x}^{(n)})^{t_k^{(n)}} = \prod_{n=1}^{N} \prod_{k=1}^{K} y_k^{(n)}(\mathbf{x}^{(n)})^{t_k^{(n)}}$$

  with

$$p(C_k|\mathbf{x}) = y_k(\mathbf{x}) = \frac{\exp(z_k)}{\sum_j \exp(z_j)}$$

  where n-th row of $\mathbf{T}$ is 1-of-K encoding of example n and

$$z_k = \mathbf{w}_k^T \mathbf{x} + w_{k0}$$

- What assumptions have I used to derive the likelihood?
- Derive the loss by computing the negative log-likelihood:

$$E(\mathbf{w}_1, \cdots, \mathbf{w}_K) = -\log p(\mathbf{T}|\mathbf{w}_1, \cdots, \mathbf{w}_K) = -\sum_{n=1}^{N} \sum_{k=1}^{K} t_k^{(n)} \log[y_k^{(n)}(\mathbf{x}^{(n)})]$$

This is known as the **cross-entropy** error for multiclass classification

- How do we obtain the weights?

Training Multi-class Logistic Regression

- How do we obtain the weights?

$$E(\mathbf{w}_1, \cdots, \mathbf{w}_K) = -\log p(\mathbf{T}|\mathbf{w}_1, \cdots, \mathbf{w}_K) = -\sum_{n=1}^{N} \sum_{k=1}^{K} t_k^{(n)} \log[y_k^{(n)}(\mathbf{x}^{(n)})]$$

- Do gradient descent, where the derivatives are

$$\frac{\partial y_j^{(n)}}{\partial z_k^{(n)}} = \delta(k,j) y_j^{(n)} - y_j^{(n)} y_k^{(n)}$$

and

$$\frac{\partial E}{\partial z_k^{(n)}} = \sum_{j=1}^{K} \frac{\partial E}{\partial y_j^{(n)}} \cdot \frac{\partial y_j^{(n)}}{\partial z_k^{(n)}} = y_k^{(n)} - t_k^{(n)}$$

$$\frac{\partial E}{\partial w_{k,j}} = \sum_{n=1}^{N} \sum_{j=1}^{K} \frac{\partial E}{\partial y_j^{(n)}} \cdot \frac{\partial y_j^{(n)}}{\partial z_k^{(n)}} \cdot \frac{\partial z_k^{(n)}}{\partial w_{k,j}} = \sum_{n=1}^{N} (y_k^{(n)} - t_k^{(n)}) \cdot x_j^{(n)}$$

- The derivative is the error times the input

Softmax for 2 Classes

- Let's write the probability of one of the classes

$$p(C_1|\mathbf{x}) = y_1(\mathbf{x}) = \frac{\exp(z_1)}{\sum_j \exp(z_j)} = \frac{\exp(z_1)}{\exp(z_1) + \exp(z_2)}$$

- I can equivalently write this as

$$p(C_1|\mathbf{x}) = y_1(\mathbf{x}) = \frac{\exp(z_1)}{\exp(z_1) + \exp(z_2)} = \frac{1}{1 + \exp\left(-(z_1 - z_2)\right)}$$

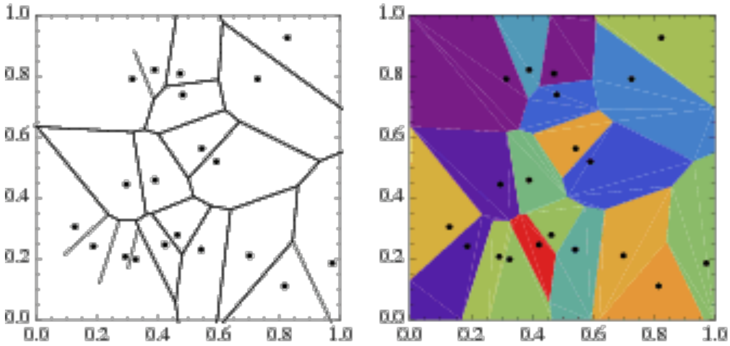
- So the logistic is just a special case that avoids using redundant parameters
- Rather than having two separate set of weights for the two classes, combine into one

$$z' = z_1 - z_2 = \mathbf{w}_1^T\mathbf{x} - \mathbf{w}_2^T\mathbf{x} = \mathbf{w}^T\mathbf{x}$$

- The over-parameterization of the softmax is because the probabilities must add to 1.

Multi-class K-NN

- Can directly handle multi class problems



Multi-class Decision Trees

- Can directly handle multi class problems
- How is this decision tree constructed?