Linear Classification

Machine Learning

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References

- This slides are based on material of prof. Marcello Restelli
- *Pattern Recognition and Machine Learning*, Bishop
  - Chapter 4 (4.1.1 - 4.1.3, 4.1.7, 4.3.1, 4.3.2)

Outline

- Linear Classification Models
- Direct Approaches
  - Least Squares for Classification
  - The Perceptron Algorithm
- Probabilistic Discriminative Approach
  - Logistic Regression

A quick recap

What is classification?

- Learn, from a dataset $\mathcal{D}$, an **approximation** of function $f(x)$ that maps input x to a discrete class C_k (with $k = 1, \dots, K$)

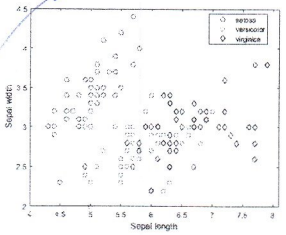
$$\mathcal{D} = \{\langle x, C_k \rangle\} \Rightarrow C_k = f(x)$$

  - How do we model f?
  - How do we encode C_k?
  - How do we evaluate our approximation? (loss function)
  - How do we optimize our approximation? (closed-form optimization? Stochastic Gradient Descent?)

In regression we had a continuous target, here it's a discrete one (class). Problems/questions:

This is equivalent to: how to find our hypothesis space H?

How we encode mathematically the classes?



Classification approaches

- Discriminant function
  - Model a parametric function that maps input to classes (least squares, perceptron)
  - Learn parameters from data
- Probablistic discriminative approach (logistic regression → it models the conditional probability of the class given the input)
  - Design a parametric model of $p(C_k|\mathbf{x})$
  - Learn model parameters from data
- Probabilistic generative approach (more sofisticated: it tries to model generative model for the data for every possible class, the class priors, ... This allows us also to generate the data)
  - Model $p(\mathbf{x}|C_k)$ and class priors $p(C_k)$
  - Fit models to data
  - Infer **posterior** with Bayes' rule: $p(C_k|\mathbf{x}) = p(\mathbf{x}|C_k)p(C_k)/p(\mathbf{x})$

we won't focus on this

Classification approaches

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Discriminant Function

→ linear approach for classification

In classification we cannot have something like:
$f(x,w) = w_0 + \mathbf{x}^T\mathbf{w}$.
This is because the output is no longer a continuous value. That's why we introduce **GENERALIZED LINEAR MODELS**. This model consider $f(\cdot)$ as a function (nonlinear) of a linear combination of the input (/features (we can still use the basis functions)).

Generalized Linear Models for classification

- In linear classification, we will use **generalized linear models**:

$$f(\mathbf{x}, \mathbf{w}) = f\left(w_0 + \sum_{j=1}^{D-1} w_j x_j\right) = f(\mathbf{x}^T\mathbf{w} + w_0)$$

  - $f(\cdot)$ is **not** linear in $\mathbf{w}$ due to the (non linear) **activation function** f, because its output is either a discrete label or a probability value
  - $f(\cdot)$ partitions the input space into **decision regions** whose boundaries are called **decision boundaries** or **decision surfaces**
  - these decision surfaces are linear function of $\mathbf{x}$ and $\mathbf{w}$, as they correspond to $\mathbf{x}^T\mathbf{w} + w_0 = \text{const}$
  - generalized linear models are more complex to use with respect to linear models (both from a computational and analytical perspective)

Label Encoding

- A common encoding for two-class problems is a binary encoding: $t \in \{0,1\}$
  - $t = 1$ encodes **positive** class and $t = 0$ encodes **negative** one
  - with this encoding, t and $f(\cdot)$ represent the **probability** of positive class
- A possible alternative encoding for two-class problems is $t \in \{-1,1\}$
  - this encoding is convenient for some algorithms
- When the problem has K classes, a typical choice is **1-of-K** encoding
  - t is a vector of length K, with a 1 in the position corresponding to the encoded class
  - with this encoding, t and $f(\cdot)$ represent the probability density over the classes
  - as an example, a data sample that belongs to class 4 of a problem with K=5, is encoded as $t = (0,0,0,1,0)^T$

with this we have a concrete interpretation of $f(\cdot)$, which is the probability of belonging to the positive class

convenient because it makes the math compact but we're loosing the interpretation

"ONE-HOT-ENCODING" we have again a probabilistic interpretation (if out of 5 classes we have : [0, 0.1, 0.9, 0, 0] then the probability of being in the 3rd class is 0.9)

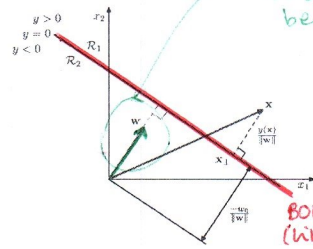
Note: the fact that we interpret the output as a probability does not mean that we're modelling probabilities. Only later, with LOGISTIC REGRESSION, we'll model probabilities!

Discriminant linear function for a two-class problem

$$f(\mathbf{x}, \mathbf{w}) = \begin{cases} C_1, & \text{if } \mathbf{x}^T\mathbf{w} + w_0 \geq 0 \\ C_2, & \text{otherwise} \end{cases}$$

- Properties
  - DS is $y(\cdot) = \mathbf{x}^T\mathbf{w} + w_0 = 0$
  - DS is orthogonal to $\mathbf{w}$
  - distance of DS from origin is $-\frac{w_0}{\|\mathbf{w}\|_2}$
  - distance of $\mathbf{x}$ from DS is $\frac{y(\mathbf{x})}{\|\mathbf{w}\|_2}$

Decision Surface

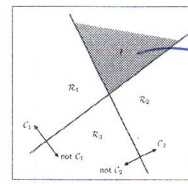


this vector is responsible for the orientation of the DECISION SURFACE (DS) because DS is ⊥ to this vector

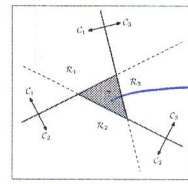
BOUNDARY (linear)

How to deal with multiple classes problems?

- In a multi-class problem we have K classes
- **One-versus-the-rest** approach uses K-1 **binary cassifiers** (i.e., that solve a two-class problem)
  - each classifier discriminates C_i and not C_i regions
  - **ambiguity:** region mapped to several classes
- **One-versus-one** approach uses K(K-1)/2 class binary classifiers
  - each classifier discriminates between C_i and C_j
  - similary ambiguity of previous approach



(*) ambiguity



again ambiguity when more than one classifier is competing for that sample

For example: we have 3 classes: C_1, C_2, C_3. We perform two binary classification problems: C_1 vs. C_2, C_3 and C_2 vs. C_1, C_3. If the first problem and the second has as output 0 then the sample is of class 3.

C_1, C_2, C_3: C_1 vs. C_2, C_3 → 1 0 (C_1); C_2 vs. C_1, C_3 → 1 0 (C_2); C_3

Problem: ambiguity. What if we obtain two "1"? (*)

We compute much more classifiers. If we have 3 classes we have to do C_1 vs. C_2, C_2 vs. C_3 and C_1 vs. C_3. (the number of comparisons increases in a quadratic way)

To avoid **ambiguities** →

A simple solution for multiple classes

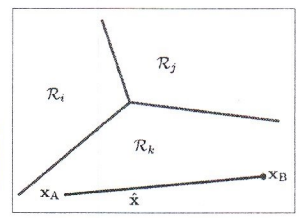
- A possible solutions is to use K linear discriminant functions:

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

  - Map $\mathbf{x}$ to class C_k if $y_k > y_j \quad \forall j \neq k$
  - No ambiguity
  - DS are **singly connected** and **convex**

Let $\mathbf{x}_A, \mathbf{x}_B \in \mathcal{R}_k$
Thus, $y_k(\mathbf{x}_A) > y_j(\mathbf{x}_A)$ and $y_k(\mathbf{x}_B) > y_j(\mathbf{x}_B)$

$\Rightarrow \forall \alpha\ (0 < \alpha < 1)$
$y_k(\alpha\mathbf{x}_A + (1-\alpha)\mathbf{x}_B) > y_j(\alpha\mathbf{x}_A + (1-\alpha)\mathbf{x}_B)$



This means that if $\underline{x}_A$ and $\underline{x}_B$ belong to a region then all the points in the middle necessarily need to belong to the same region (**singly connected**: there is at most one path from any point to any other point)

For a new point $\underline{x}$ we compute the linear discriminant function for all the classes ($y_k = \underline{x}^T\underline{w}_k + w_{k0}$) and the linear discriminant function with the heigher value will determine the class of the point.

Notice: the decision boundaries are still **linear**!

$y_1(\underline{x}) = \underline{x}^T\underline{w}_1 + w_{01}$
$y_2(\underline{x}) = \underline{x}^T\underline{w}_2 + w_{02}$
we choose y_1 if $y_1 > y_2$ and so:
$(y_1 - y_2) > 0$
$y_1 - y_2 = \underline{x}^T(\underline{w}_1 - \underline{w}_2) + (w_{01} - w_{02})$

this is again a linear discriminant function (linear boundary)

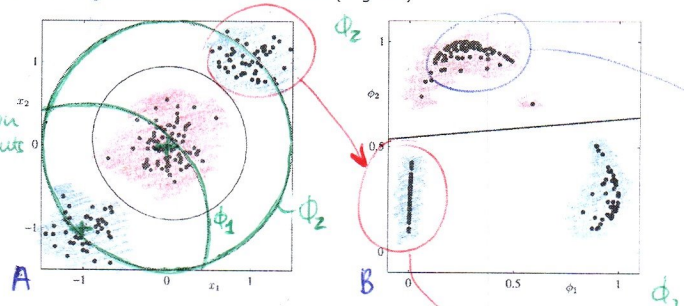
$\underline{x}$ point in the middle of $\underline{x}_A$ and $\underline{x}_B$ then:
$\underline{x} = \lambda\underline{x}_A + (1-\lambda)\underline{x}_B$, so:
$y_k(\underline{x}) = \lambda y_k(\underline{x}_A) + (1-\lambda)y_k(\underline{x}_B)$
and given that $y_k(\underline{x}_A)$ and $y_k(\underline{x}_B)$ are the longest ones then also the combination will be the longest one w.r.t. the others.

Linear Basis Function Models

- So far we considered models that work in the **input space** (i.e., with $\mathbf{x}$)
- However, we can still extend models by using a fixed set of basis function $\phi(\mathbf{x})$
- Basically, we apply a non-linear transformation to map the **input space** into a **feature space**
- As a result, decision boundaries that are **linear** in the **feature space** would correspond to **nonlinear** boundaries in the **input space**
- This allows to apply linear classification models also to problem where samples are not **linearly separable**

Linear Basis Function Models: an example

- Assuming two Gaussian basis functions (in green)



The "+" represents the center of the gaussian basis function and the circle represents the variance.

The **idea** is: in A points are not linearly separable, can we map the points into a new features space, B, where we can find a linear decision boundary between classes?

We can see in A that these points have high values of Φ_2 and low values of Φ_1 (having a high value for Φ_2 kind of means "it fits fine Φ_2")

This set of points has low values for both Φ_1 and Φ_2, it kind of means that it doesn't fit either Φ_1 and Φ_2 (and from the image A we can clearly see why)

Least Squares for Classification

- Let consider a K-class problem and use a 1-of-K encoding for target
- Each class is modeled with a linear function:

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

Using the 1-of-K we'll be able to learn a linear function that will have values close to 1 near to the points that are of class k and 0 elsewhere.

- In matrix notation:

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

  - $\tilde{\mathbf{W}}$ has size (D+1)xK
  - k-th column of $\tilde{\mathbf{W}}$ is $\tilde{\mathbf{w}}_k = (w_{k0}, \mathbf{w}_k^T)^T$
  - $\tilde{\mathbf{x}} = (1, \mathbf{x}^T)^T$

Least Squares for Classification (2)

- Given a dataset $\mathcal{D} = \{\mathbf{x}_i, \mathbf{t}_i\}$, where i=1,…,N
- We can apply Least Squares to find the optimal value of $\tilde{\mathbf{W}}$

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

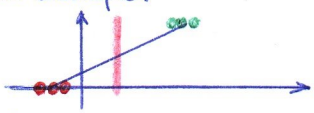
  - $\tilde{\mathbf{X}}$ is a Nx(D+1) matrix whose i-th is $\tilde{\mathbf{x}}_i^T$
  - $\mathbf{T}$ is a NxK matrix whose i-th row is $\mathbf{t}_i^T$

- Any new sample $\tilde{\mathbf{x}}_{new}^T$ is mapped to class C_k if $t_k > t_j \ \forall j$, where t_k is the k-th component of the model output, computed as $t_k = \tilde{\mathbf{x}}^T \tilde{\mathbf{w}}_k$

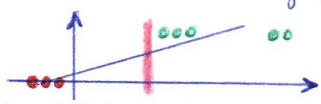
Problems:
- this solution is extremely sensitive to **outliers**
- for ordinary least squares we assume that the model is the best choice if we expect the target to be computed by a linear function + gaussian noise, however in this case we don't have gaussian noise (we have classes 0/1, is no noise in the targets)

Problems with Least Squares: Outliers and Output Distribution

In this case we would like to have the green line but we end up having the red instead. Why? Because we're performing least squares, which tries to minimize the errors squared. The group * strongly influences. For example:

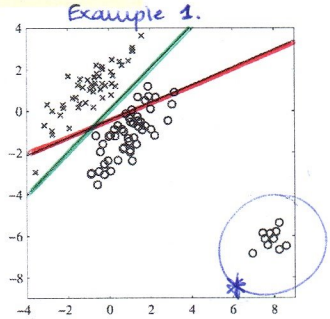


The blue one it the function that we learn to classify green points. (the one for the reds will be opposite). In this way the class separator will be: instead if we add some outliers we get:

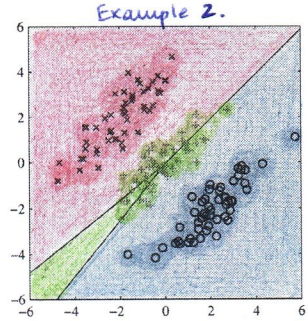


The class separator moves. (The blue line is *)

Example 1.



Example 2.



This is what happened assuming gaussian noise. There is no noise in labeling

Perceptron

- The **perceptron** is a linear discriminant model proposed by Rosenblatt in 1958 along with a **sequential learning** algorithm
- Perceptron is devised for a two-class problem, where classes encoding is {-1,1}

$$f(\mathbf{x}, \mathbf{w}) = \begin{cases} +1, & \text{if } \mathbf{w}^T \phi(\mathbf{x}) \geq 0 \\ -1, & \text{otherwise} \end{cases}$$

(we already using the notation of the features space, so $\phi(\cdot)$)

- The **perceptron algorithm** aims at finding a **decision surface** (also called **separating hyperplane**) by minimizing the distance of **misclassified samples** to the boundary
- Minimization of this loss function can be performed using **stochastic gradient descent**
- Despite a simpler loss function could be used in principle (e.g., number of misclassified samples), this are more complex to minimize.

Why we minimize the distance of the missclassified points instead of, for example, the number of misclassified points? The distance is a continuous function and it's easier to minimize.

Perceptron Criterion

- We aim at finding $\mathbf{w}$ such that $\mathbf{w}^T \phi(\mathbf{x}_i) \geq 0$ for $\mathbf{x}_i \in C_1$ and $\mathbf{w}^T \phi(\mathbf{x}_i) < 0$ otherwise
- The **Perceptron Criterion** is defined as:

$$L_P(\mathbf{w}) = -\sum_{n \in \mathcal{M}} \mathbf{w}^T \phi(\mathbf{x}_n) t_n$$

  - samples clssified correctly do not contribute to L
  - each misclassified sample $\mathbf{x}_i \in \mathcal{M}$ contributes as $\mathbf{w}^T \phi(\mathbf{x}_i) t_i$

- L_P can be minimized using **stochastic gradient descent**:

$$\mathbf{w}^{(k+1)} = \mathbf{w}^{(k)} - \alpha \nabla L_P(\mathbf{w}) = \mathbf{w}^{(k)} + \alpha \phi(\mathbf{x}_n) t_n$$

  - Since the scale of $\mathbf{w}$ does not change the perceptron function, usually the **learning rate** α is set to 1

(the scale does not change because $\mathbf{w}^T \Phi(\underline{x}) = 0$ is equal to (for example) $4\,\mathbf{w}^T \Phi(\underline{x}) = 0$)

$\mathcal{M}$ is the set of missclassified points. For each missclassified point we compute (something proportional to) the distance to the boundary. The distance of $\mathbf{w}^T \phi(\mathbf{x}_n)$. We multiply by the target to have always $\mathbf{w}^T \phi(\mathbf{x}_n) t_n < 0$ (because of the missclassification) and then we add a "−" to have something overall positive.

Why "stochastic"? Because it's not computing the gradient along the complete loss function. It's computing the gradient taking into account just one point. At each step the correction is not (probably) the best for the overall loss. Keeping correcting we converge to the solution. There is a theorem that guarantees convergence if the points are linearly separable.

Perceptron Algorithm

Given $\mathcal{D} = \{\mathbf{x}_i, \mathbf{t}_i\}$, where i=1,...,N

Initialize $\mathbf{w}_0$
k ← 0
repeat
  k ← k+1
  n ← k mod N
  if $\hat{t}_n \neq t_n$ **then**
    $\mathbf{w}_{k+1} \leftarrow \mathbf{w}_k + \phi(x_n)t_n$
  endif
until convergence

we keep iterating on the dataset: if the points are misclassified we adjust the weights. We keep repeating until convergence.

This is simply to say that when k becomes n then we start from 0 again (k becomes 0 again)

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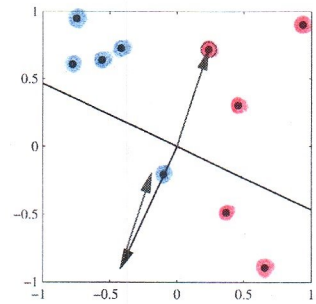

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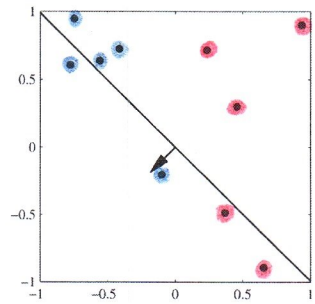

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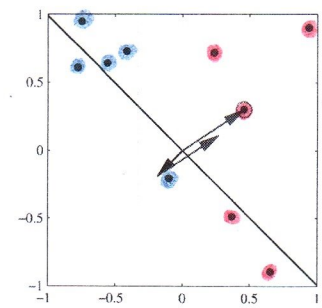

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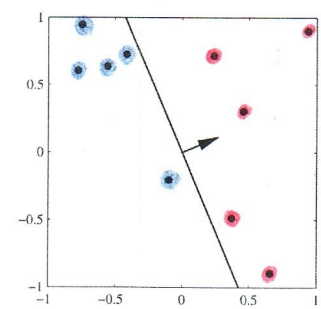


At this point we stop since we have no longer misclassified points.

Perceptron Convergence Theorem

- A single update **reduce the error** on the **single** misclassifed sample:

$$-\mathbf{w}^{(k+1)^T}\phi(\mathbf{x}_n)t_n = -\mathbf{w}^{(k)^T}\phi(\mathbf{x}_n)t_n - (\phi(\mathbf{x}_n)t_n)^T\phi(\mathbf{x}_n)t_n < -\mathbf{w}^{(k)^T}\phi(\mathbf{x}_n)t_n$$

  - This does **not** imply that the entire loss is reduced after each update
- Perceptron Convergence Theorem

  *If the training data set is **linearly separable** in the feature space Φ, then the perceptron learning algorithm is guaranteed to find an **exact solution** in a **finite number of steps***

  - How many steps? Several steps might be necessary, thus it might be difficult to distinguish between **nonseparable** problems and **slowly converging** ones
  - Which solution? If **multiple solutions** exist, the one found by the algorithms depends from **initialization** of parameters and the **order** of updates

Probabilistic Discriminative Approaches

Two-Class Logistic Regression

we model the conditional probability of the class given the input and to do this we use a sigmoidal function (it's an assumption)

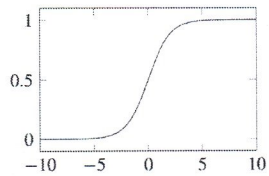
probability of a point (ϕ) to be of class C_1

- In a discriminative approach we model directly the conditioned class probability:

$$p(C_1|\phi) = \frac{1}{1+\exp(-\mathbf{w}^T\phi)} = \sigma(\mathbf{w}^T\phi)$$

  - where $\sigma(a) = 1/(1+\exp(-a))$ is the sigmoidal function
  - $p(C_2|\phi) = 1 - p(C_1|\phi)$
  - this model is knonw as **logistic regression**

The goal is to optimize $\mathbf{w}$ in order to make this probability distribution fit as good as possible the observed data



in order to do this we have to go through the likelihood function

Maximum Likelihood for Logistic Regression

- Given dataset $\mathcal{D} = \{\mathbf{x}_i, t_i\}$, where i=1,...,N and $t_i \in \{0,1\}$ we want to maximize the likelihood, i.e., the probability to observe the targets given the inputs: $p(\mathbf{t}|\mathbf{X},\mathbf{w})$
- We model the likelihood of the single sample using a Bernoulli distribution, using the logistic regression model for conditioned class probability:

$$p(t_n|\mathbf{x}_n,\mathbf{w}) = y_n^{t_n}(1-y_n)^{1-t_n} \quad \text{where} \quad y_n = p(t_n=1|\mathbf{x}_n,\mathbf{w}) = \sigma(\mathbf{w}^T\phi_n)$$

- Assuming that data in $\mathcal{D}$ have been independently sampled we get:

$$p(\mathbf{t}|\mathbf{X},\mathbf{w}) = \prod_{n=1}^{N} y_n^{t_n}(1-y_n)^{1-t_n}, \quad y_n = \sigma(\mathbf{w}^T\phi_n)$$

(total) likelihood

once again, given this form, it's easier for us to use the log-likelihood and instead of maximize the log-likelihood we'll minimize the - log-likelihood

Maximum Likelihood for Logistic Regression (2)

- A convenient loss function to **minimize** is the negative log-likelihood (also **known as cross-entropy error function**)

$$L(\mathbf{w}) = -\ln p(\mathbf{t}|\mathbf{X},\mathbf{w}) = -\sum_{n=1}^{N}(t_n \ln y_n + (1-t_n)\ln(1-y_n)) = \sum_{n=1}^{N} L_n$$

- Now we have to compute the derivative of $L(\mathbf{w})$:

$$\frac{\partial L_n}{\partial y_n} = \frac{y_n - t_n}{y_n(1-y_n)}, \quad \frac{\partial y_n}{\partial \mathbf{w}} = y_n(1-y_n)\phi_n; \Rightarrow \frac{\partial L_n}{\partial \mathbf{w}} = \frac{\partial L_n}{\partial y_n}\frac{\partial y_n}{\partial \mathbf{w}} = (y_n - t_n)\phi_n$$

Maximum Likelihood for Logistic Regression (3)

- Thus the gradient of the loss function is:

$$\nabla L(\mathbf{w}) = \sum_{n=1}^{N}(y_n - t_n)\boldsymbol{\phi}_n$$

  - due to the nonlinear logistic regression function it is not possible to find a closed-form solution
  - however, the error function is **convex** and **gradient-based optimization** can be applied (also in an **online learning setting**)

Multiclass Logistic Regression

- In multiclass problems, $p(C_k|\boldsymbol{\phi})$ is modeled by a **softmax** tranformation of the output of K linear functions (one for each class):

$$p(C_k|\boldsymbol{\phi}) = y_k(\boldsymbol{\phi}) = \frac{\exp(\mathbf{w}_k{}^T\boldsymbol{\phi})}{\sum_j \exp(\mathbf{w}_j{}^T\boldsymbol{\phi})}$$

- As for the two-class logistic regression and assuming 1-of-K encoding for the target, we can compute **likelihood** as:

$$p(\mathbf{T}|\boldsymbol{\Phi}, \mathbf{w}_1, \ldots, \mathbf{w}_K) = \prod_{n=1}^{N} \underbrace{\left(\prod_{k=1}^{K} p(C_k|\boldsymbol{\phi}_n)^{t_{nk}}\right)}_{\text{Only one term corresponding to correct class}} = \prod_{n=1}^{N}\left(\prod_{k=1}^{K} y_{nk}^{t_{nk}}\right)$$

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- As $y_{nk} = p(C_k|\boldsymbol{\phi}_n) = \frac{\exp(\mathbf{w}_k{}^T\boldsymbol{\phi}_n)}{\sum_j \exp(\mathbf{w}_j{}^T\boldsymbol{\phi}_n)}$ and assuming 1-of-K encoding for the target, we can compute likelihood as:

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Multiclass Logistic Regression (2)

- As for the two-class problem, we can minimize the **cross-entropy error function**:

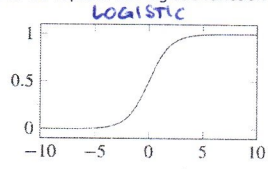
$$L(\mathbf{w}_1, \ldots, \mathbf{w}_K) = -\ln p(\mathbf{T}|\boldsymbol{\Phi}, \mathbf{w}_1, \ldots, \mathbf{w}_K) = -\sum_{n=1}^{N}\left(\sum_{k=1}^{K} t_{nk} \ln y_{nk}\right)$$

- Then, we compute the gradient for each weights vector:

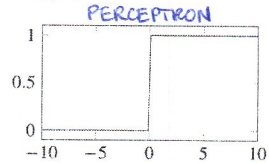
$$\nabla L_{\mathbf{w}_j}(\mathbf{w}_1, \ldots, \mathbf{w}_K) = \sum_{n=1}^{N}(y_{nj} - t_{nj})\boldsymbol{\phi}_n$$

Logistic Regression and Perceptron Algorithm

- If we replace the logistic function with a step function...



$$y(\mathbf{x}, \mathbf{w}) = \frac{1}{1 + e^{-\mathbf{w}\cdot\boldsymbol{\phi}(\mathbf{x})}}$$



$$y(\mathbf{x}, \mathbf{w}) = \begin{cases} 1 & \text{if } \mathbf{w}\cdot\boldsymbol{\phi}(\mathbf{x}) > 0 \\ 0 & \text{otherwise} \end{cases}$$

- ... logisitc regression leads to the same **updating rule** of perceptron algorithm:

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha\,(y(\mathbf{x}_n, \mathbf{w}) - t_n)\,\boldsymbol{\phi}_n$$

Logistic regression and perceptron algorithm have the same update rule. What is the major difference? The structure of updating is the same, what changes is $y(\underline{x}, \underline{w})$: in the perceptron we have a step function, in the logistic regression we have a sigmoid (a continuous function).
⇒ The perceptron algorithm is a logistic regression using as model distribution of the probability a step function.