

Machine Learning

Lecture 4: Linear Classification

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Reading material

Reading material

- Bishop: chapters 4, 4.1.1, 4.1.2, 4.1.7, 4.2, 4.3.0 - 4.3.4

Acknowledgements

- Slides are based on an older version by G. Jensen and J. Bayer
- Some figures are from C. Bishop: "Pattern Recognition and Machine Learning"

Notation

Symbol	Meaning
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s	scalar is lowercase and not bold
\mathbf{s}	vector is lowercase and bold
\mathbf{S}	matrix is uppercase and bold
\hat{y}	predicted class label
y	actual class label
$\mathbb{I}(a)$	Indicator function; $\mathbb{I}(a) = 1$ if a is true, else 0

Section 1

Introduction to linear classification

Classification vs regression

Regression

Output y is continuous (i.e. $y \in \mathbb{R}$).

For example, predict the price of a house given its area.

Classification

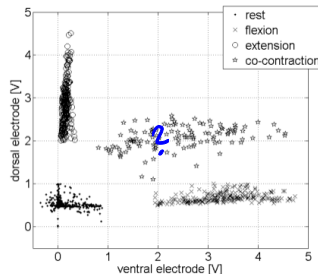
Output y belongs to one of C predetermined classes (i.e. $y \in \{1, \dots, C\}$).

For example, determine whether the picture shows a cat or a dog.

Classification problem

Given

- observations ¹
 $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\}, \mathbf{x}_i \in \mathbb{R}^D$
- set of possible classes.
 $\mathcal{C} = \{1, \dots, C\}$
- labels
 $\mathbf{y} = \{y_1, y_2, \dots, y_N\}, y_i \in \mathcal{C}$



Find

- function $f: \mathbb{R}^D \rightarrow \mathcal{C}$ that maps observations \mathbf{x}_i to class labels y_i

$$y_i = f(\mathbf{x}_i) \quad \text{for } i \in \{1, \dots, N\}$$

¹Like before, we represent samples as a **data matrix** $\mathbf{X} \in \mathbb{R}^{N \times D}$.

Zero-one loss

dog: 5
cat: 1
bird: 2

$$\text{REGRESSION: } \sum_i (\omega^T \tilde{x}_i - \underbrace{y_i}_{\hat{y}_i})^2$$

How do we measure quality of a prediction $\hat{\mathbf{y}} := f(\mathbf{X})$? ²

Zero-one loss denotes the number of misclassified samples.

$$\ell_{01}(\mathbf{y}, \hat{\mathbf{y}}) = \sum_{i=1}^N \mathbb{I}(\hat{y}_i \neq y_i).$$

How do we choose a good $f(\cdot)$?

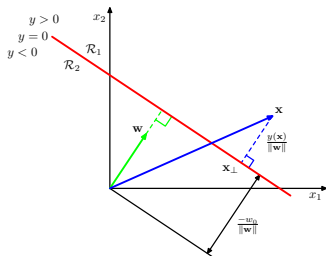
²For brevity, we denote the generated prediction $f(\mathbf{x}_i)$ as \hat{y}_i ,
i.e. $\hat{\mathbf{y}}$ is the vector of predictions for entire \mathbf{X}

Hyperplane as a decision boundary

For a 2 class problem ($\mathcal{C} = \{0, 1\}$) we can try to separate points from the two classes by a **hyperplane**.

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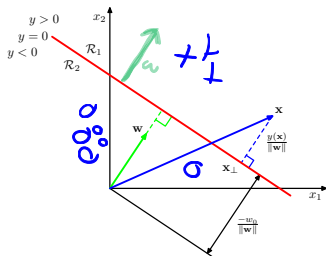
A hyperplane be defined by a normal vector \mathbf{w} and an offset w_0 .

$$\mathbf{w}^T \mathbf{x} + w_0 \begin{cases} = 0 & \text{if } \mathbf{x} \text{ on the plane} \\ > 0 & \text{if } \mathbf{x} \text{ on normal's side} \\ < 0 & \text{else} \end{cases}$$

Hyperplanes are computationally very convenient: easy to evaluate.

Hyperplane as a decision boundary

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Hyperplanes are computationally very convenient: easy to evaluate.

A data set $\mathcal{D} = \{(x_i, y_i)\}$ is **linearly separable** if there exists a hyperplane for which all x_i with $y_i = 0$ are on one and all x_i with $y_i = 1$ on the other side.

Perceptron

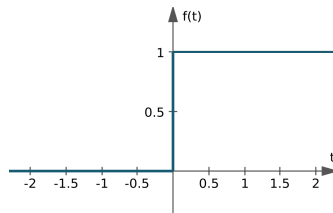
Perceptron algorithm is one of the oldest methods for binary classification.

Decision rule

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

where f is the step function defined as:

$$f(t) = \begin{cases} 1 & \text{if } t > 0, \\ 0 & \text{else.} \end{cases}$$



Learning rule for the perceptron

Initialize parameters to any value, e.g., a zero vector: $\mathbf{w}, w_0 \leftarrow \mathbf{0}$.

³However, there is no way to determine the number of required iterations in advance.

Learning rule for the perceptron

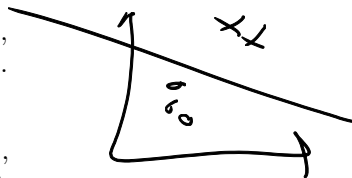
$$\hat{x}_i = [x_i, 1]$$

Initialize parameters to any value, e.g., a zero vector: $w, w_0 \leftarrow 0$.

For each misclassified sample x_i in the training set update

$$w \leftarrow \begin{cases} w + x_i & \text{if } y_i = 1, \\ w - x_i & \text{if } y_i = 0. \end{cases}$$

$$w_0 \leftarrow \begin{cases} w_0 + 1 & \text{if } y_i = 1, \\ w_0 - 1 & \text{if } y_i = 0. \end{cases}$$



until all samples are classified correctly.

This method takes a finite number of steps to converge to a (w, w_0) discriminating between two classes [if it exists](#).³

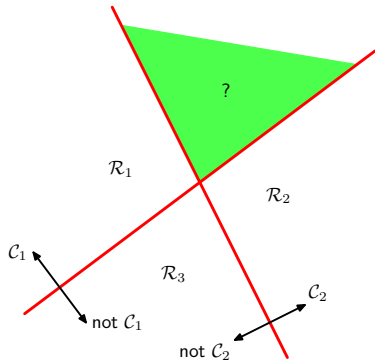
³However, there is no way to determine the number of required iterations in advance.

Does this scale up to multiple classes?

One-versus-rest classifier

Each hyperplane \mathcal{H}_i makes a decision

class $\mathcal{C}_i \leftrightarrow$ not class \mathcal{C}_i

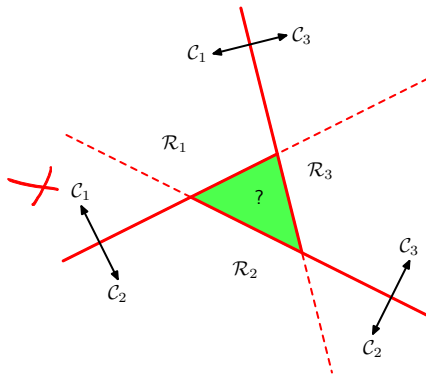


One-versus-one classifier

Hyperplane \mathcal{H}_{ij} makes a decision for each pair of classes

class $\mathcal{C}_i \leftrightarrow$ class \mathcal{C}_j

Use majority vote to classify.



$\mathcal{C}_1 : 2$
 $\mathcal{C}_2 : 1$
 $\mathcal{C}_3 : 0$

Multiclass discriminant

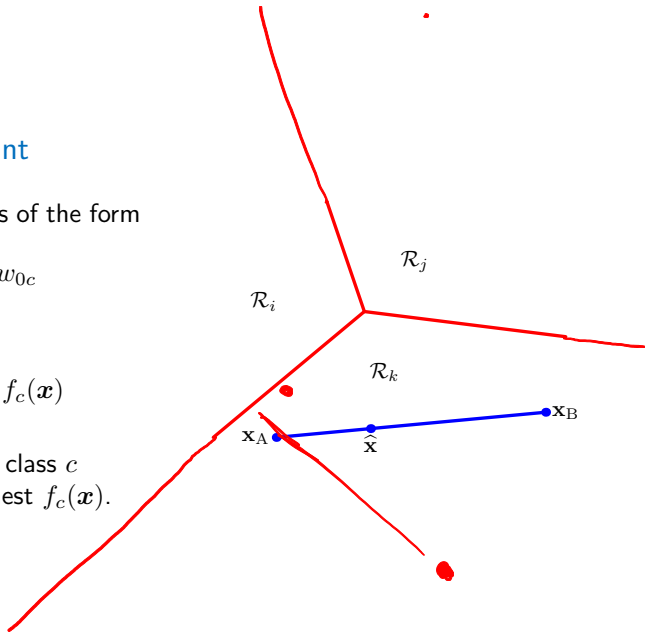
Define C linear functions of the form

$$f_c(\mathbf{x}) = \mathbf{w}_c^T \mathbf{x} + w_{0c}$$

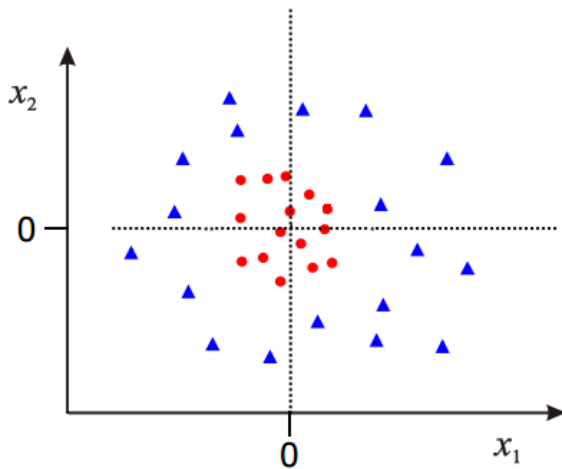
with the decision rule

$$\hat{y} = \arg \max_{c \in \mathcal{C}} f_c(\mathbf{x})$$

That is, assign \mathbf{x} to the class c which produces the highest $f_c(\mathbf{x})$.

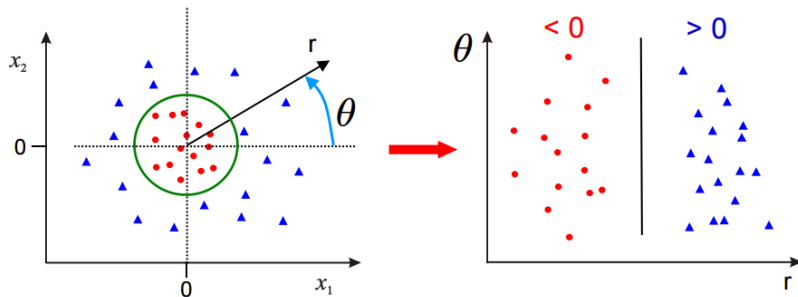


What if the classes are not linearly separable?



Basis functions

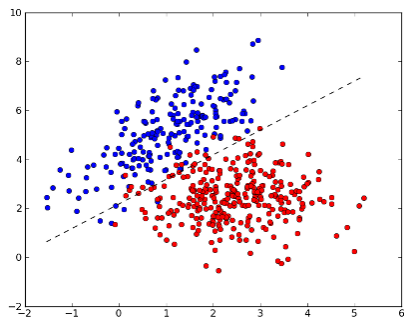
Like in the Linear Regression lecture last week, we can apply a nonlinear transformation $\phi : \mathbb{R}^D \rightarrow \mathbb{R}^M$. We need to choose a ϕ that maps samples to a space where they are linearly separable.



Here, $\phi(x) = (\theta, r) = (\text{angle}(x), \sqrt{x^T x})$.

Limitations of hard-decision based classifiers

- No measure of uncertainty
- Can't handle noisy data
- Poor generalization
- Difficult to optimize



What are the alternatives?

Probabilistic models for classification

Solution: model the distribution of the class label y given the data \mathbf{x} .

$$p(y = c \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid y = c) \cdot p(y = c)}{p(\mathbf{x})}$$

Two types of models:

Generative

- Model the joint distribution $p(\mathbf{x}, y = c) = p(\mathbf{x} \mid y = c) \cdot p(y = c)$

Discriminative

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↑ 006
 c as

- Directly model the posterior $p(y = c \mid \mathbf{x})$

Given $p(y \mid \mathbf{x})$ we can make the prediction \hat{y} based on our problem.

Popular choice is the mode: $\hat{y} = \arg \max_{c \in \mathcal{C}} p(y = c \mid \mathbf{x})$.

Section 2

Probabilistic generative models for linear
classification

Generative model

The idea is to obtain the class posterior using the Bayes formula

$$p(y = c \mid \mathbf{x}) \propto \underbrace{p(\mathbf{x} \mid y = c)}_{\text{class conditional}} \cdot \underbrace{p(y = c)}_{\text{class prior}} \quad (1)$$

The model consists of

- **class prior** - a priori probability of a point belonging to a class c
- **class conditional** - probability of generating a point \mathbf{x} , given that it belongs to class c

Applying a generative model

$$y_i \sim \mathcal{N}(f_w(x_i), \beta)$$

Applying a generative model typically works as following

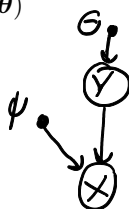
- Choose a parametric model for the class conditional $p(\mathbf{x} \mid y = c, \psi)$ and the class prior $p(y = c \mid \theta)$.
- Estimate the parameters of our model $\{\psi, \theta\}$ from the data \mathcal{D} (e.g., using maximum likelihood - obtain estimates $\{\hat{\psi}, \hat{\theta}\}$).
This step is called **learning**.

Once fitted, we can perform **inference** - classify a new \mathbf{x} using Bayes rule

$$p(y = c \mid \mathbf{x}, \hat{\psi}, \hat{\theta}) \propto p(\mathbf{x} \mid y = c, \hat{\psi})p(y = c \mid \hat{\theta}) \quad (2)$$

Additionally, we can **generate** new data - hence the name.

- sample a class label $y_{new} \sim p(y \mid \hat{\theta})$
- sample a feature vector $\mathbf{x}_{new} \sim p(\mathbf{x} \mid y = y_{new}, \hat{\psi})$



Choosing class prior

How do we choose the class prior $p(y = c)$?

The label y can take one of C discrete values.

\Rightarrow Use categorical distribution!

$$y \sim \text{Categorical}(\boldsymbol{\theta})$$

The parameter $\boldsymbol{\theta} \in \mathbb{R}^C$ specifies the probability of each class

$$p(y = c) = \theta_c \quad \text{or equivalently} \quad p(y) = \prod_{c=1}^C \theta_c^{\mathbb{I}(y=c)}$$

and is subject to the constraints $0 \leq \theta_c \leq 1$ and $\sum_{c=1}^C \theta_c = 1$.

The maximum likelihood estimate for $\boldsymbol{\theta}$ given the data $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}$ is

$$\theta_c^{MLE} = \frac{1}{N} \sum_{i=1}^N \mathbb{I}(y_i = c)$$

Class conditionals

How do we choose the class conditionals $p(x | y = c)$?

The feature vector $x \in \mathbb{R}^D$ is continuous.

\Rightarrow Use a multivariate normal for each class!

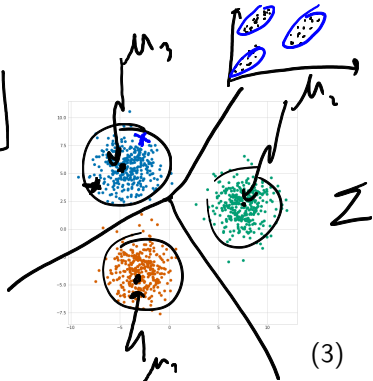
$$p(x | y = c) = \mathcal{N}(x | \mu_c, \Sigma)$$

$$x \sim \mathcal{N}(\mu_c, \Sigma) = \frac{1}{(2\pi)^{D/2} |\Sigma|^{1/2}} \exp \left\{ -\frac{1}{2} (x - \mu_c)^T \Sigma^{-1} (x - \mu_c) \right\} \quad (4)$$

We use the same Σ for each class, as estimating all Σ_c 's behaves badly numerically, unless we have **lots** of data.

The MLE estimates for $\{\mu_1, \dots, \mu_C, \Sigma\}$ will be derived in the tutorial (or see Bishop 4.2.2).

HOW MANY PARAMETERS TO LEARN: $\frac{(D+1)^2}{2} + C \cdot D$



Posterior distribution

Now that we have chosen $p(\mathbf{x} | y)$ and $p(y)$, and have estimated their parameters from the training data ⁴, how do we perform classification?

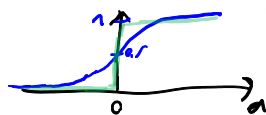
Let's assume for simplicity that we have two classes $\mathcal{C} = \{0, 1\}$.

$$p(y = 1 | \mathbf{x}) = \frac{p(\mathbf{x} | y = 1) p(y = 1)}{p(\mathbf{x} | y = 1) p(y = 1) + p(\mathbf{x} | y = 0) p(y = 0)} \quad (5)$$

$$= \frac{1}{1 + \exp(-a)} =: \sigma(a) \quad (6)$$

where we defined

$$a = \ln \frac{p(\mathbf{x} | y = 1) p(y = 1)}{p(\mathbf{x} | y = 0) p(y = 0)} \quad (7)$$



and σ is the **sigmoid function**.

⁴To avoid clutter, we implicitly condition the distributions on their respective parameters (θ, μ_c, Σ)

Linear discriminant analysis (LDA)



Let's look at how this function looks for Gaussian class-conditional with the same covariance Σ

$$a = \ln \frac{p(\mathbf{x} \mid y = 1)p(y = 1)}{p(\mathbf{x} \mid y = 0)p(y = 0)} \quad (8)$$

$$= -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_1)^T \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}_1) + \ln p(y = 1) \quad (9)$$

$$+ \frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_0)^T \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu}_0) - \ln p(y = 0) \quad (10)$$

$$= \mathbf{w}^T \mathbf{x} + w_0 \quad (11)$$

where we define

$$\mathbf{w} = \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0) \quad (12)$$

$$w_0 = -\frac{1}{2}\boldsymbol{\mu}_1^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_1 + \frac{1}{2}\boldsymbol{\mu}_0^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_0 + \ln \frac{p(y = 1)}{p(y = 0)} \quad (13)$$

LDA for $C = 2$ classes

$$(X, y) \sim \mu_c, \Sigma \sim \omega$$

This means, that the posterior distribution is a sigmoid of a linear function of \mathbf{x}

$$p(y = 1 \mid \mathbf{x}) = \frac{1}{1 + \exp(-(\mathbf{w}^T \mathbf{x} + w_0))} \quad (14)$$

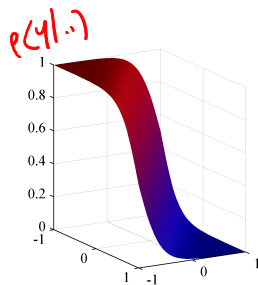
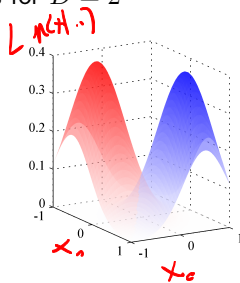
$$= \sigma(\mathbf{w}^T \mathbf{x} + w_0) \quad (15)$$

or equivalently

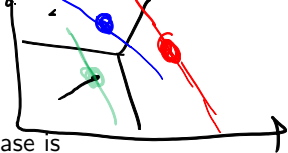
$$y \mid \mathbf{x} \sim \text{Bernoulli}(\sigma(\mathbf{w}^T \mathbf{x} + w_0)) \quad (16)$$

This is how this function looks for $D = 2$

- Right:
 $p(\mathbf{x} \mid y = 1)$ - red
 $p(\mathbf{x} \mid y = 0)$ - blue
- Left:
 $p(y = 1 \mid \mathbf{x})$



LDA for $C > 2$ classes



Using Bayes formula, the posterior for the $C > 2$ case is

$$p(y = c \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid y = c)p(y = c)}{\sum_{c'=1}^C p(\mathbf{x} \mid y = c')p(y = c')} \quad (17)$$

working out through some math we get

$$= \frac{\exp(\mathbf{w}_c^T \mathbf{x} + w_{c0})}{\sum_{c'=1}^C \exp(\mathbf{w}_{c'}^T \mathbf{x} + w_{c'0})} \quad (18)$$

where

$$\mathbf{w}_c = \Sigma^{-1} \boldsymbol{\mu}_c \quad (19)$$

$$w_{c0} = -\frac{1}{2} \boldsymbol{\mu}_c^T \Sigma^{-1} \boldsymbol{\mu}_c + \ln p(y = c) \quad (20)$$

Softmax function

In the slide above we made use of the [softmax function](#).

Softmax σ is a generalization of sigmoid to multiple dimensions

$$\sigma : \mathbb{R}^K \rightarrow \Delta^{K-1} \quad (21)$$

where

$$\Delta^{K-1} = \left\{ \mathbf{x} \in \mathbb{R}^K \mid \sum_{k=1}^K x_k = 1 \text{ and } x_k \geq 0, k = 1, \dots, K \right\} \quad (22)$$

is the standard [probability simplex](#).

Softmax is defined as

$$\sigma(\mathbf{x})_i = \frac{\exp(x_i)}{\sum_{k=1}^K \exp(x_k)} \quad (23)$$

Section 3

Probabilistic discriminative models for linear
classification

Probabilistic discriminative model

An alternative approach to generative modeling is to model the posterior distribution $p(y | \mathbf{x})$ directly. Such models are called **discriminative**.

We saw in the previous section that a generative approach with Gaussian class-conditional distributions with same covariance matrix Σ produces the following decision rule

$$p(y = 1 | \mathbf{x}) = \sigma(\mathbf{x}^T \mathbf{w} + w_0), \quad (24)$$

$$p(y = 0 | \mathbf{x}) = 1 - \sigma(\mathbf{x}^T \mathbf{w} + w_0) \quad (25)$$

where \mathbf{w}, w_0 depend on the parameters of class-conditionals μ_0, μ_1, Σ .

Why not just let \mathbf{w} and w_0 be free parameters and choose them directly?

Logistic regression

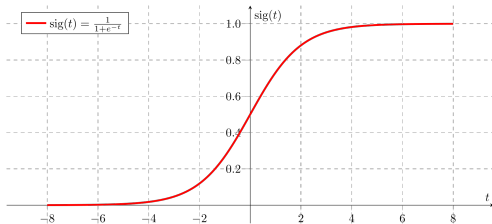
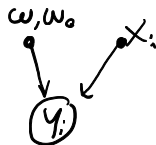
We model the posterior distribution as

$$y \mid x \sim \text{Bernoulli}(\sigma(\mathbf{w}^T \mathbf{x} + w_0)) \quad (26)$$

where

$$\sigma(a) = \frac{1}{1 + \exp(-a)}$$

and \mathbf{w}, w_0 are the free model parameters.



This model is called **logistic regression**.

$$\begin{aligned} & (x_i, y_i) \\ & (\tilde{x}, 0) = (x_i, 0) \\ & (\tilde{x}, 1) \\ & (\tilde{x}, 0) \end{aligned}$$

$$\begin{aligned} & \mathcal{L}(\mathbf{w}, w_0) \\ & p(y \mid x, \mathbf{w}, w_0) \quad (27) \\ & = \prod_{i=1}^n p(y_i \mid x_i, \mathbf{w}, w_0) \end{aligned}$$

Absorbing the bias term

Like in the previous lecture, we again absorb the bias term by overloading the notation and defining

$$\mathbf{w}^T \mathbf{x} := w_0 + w_1 x_1 + \dots + w_D x_D \quad (28)$$

Which is equivalent to defining $x_0 = 1$.

Likelihood of logistic regression

Learning logistic regression comes down to finding a “good” setting of parameters \mathbf{w} that “explain” the training set $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^N$.

Assuming that all samples (\mathbf{x}_i, y_i) are drawn i.i.d., we can write the likelihood as

$$p(\mathbf{y} \mid \mathbf{w}, \mathbf{X}) = \prod_{i=1}^N p(y_i \mid \mathbf{x}_i, \mathbf{w}) \quad (29)$$

$$= \prod_{i=1}^N \underbrace{p(y=1 \mid \mathbf{x}_i, \mathbf{w})^{y_i}}_{=1 \text{ if } y_i=0} \underbrace{(1 - p(y=1 \mid \mathbf{x}_i, \mathbf{w}))^{1-y_i}}_{=1 \text{ if } y_i=1} \quad (30)$$

$$= \prod_{i=1}^N \sigma(\mathbf{w}^T \mathbf{x}_i)^{y_i} (1 - \sigma(\mathbf{w}^T \mathbf{x}_i))^{1-y_i} \quad (31)$$

Negative log-likelihood

$$\sum [y_i \cdot \ln p_i + (1 - y_i) \cdot \ln(1 - p_i)]$$

Similarly to the linear regression case, we can define an error function as **negative log-likelihood**

$$E(\mathbf{w}) = -\ln p(\mathbf{y} \mid \mathbf{w}, \mathbf{X}) \quad \text{predictions } p_i \quad (32)$$

$$= -\sum_{i=1}^N (\underbrace{y_i}_{\text{GIVEN/TRUE TARGETS}} \ln \sigma(\mathbf{w}^T \mathbf{x}_i) + (1 - y_i) \ln(1 - \sigma(\mathbf{w}^T \mathbf{x}_i))) \quad (33)$$

This loss function is called **binary cross entropy**.

Finding the maximum likelihood estimate for \mathbf{w} is equivalent to solving

$$\mathbf{w}^* = \arg \min E(\mathbf{w}) \quad (34)$$

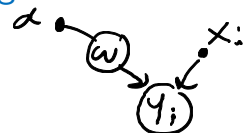
Solving the minimization problem

There doesn't exist a **closed form** solution for logistic regression. This means, we cannot compute the optimal w^* using standard mathematical operations, such as multiplication, matrix inversion, etc.

However, there is still hope! We can use **optimization** to numerically solve our problem. We will cover this in the next lecture (19.11.2018).

For now, just assume that we can find w^* .

Logistic regression + weights regularization

$$w \sim \mathcal{N}(0, \alpha^{-1} \cdot I)$$


As we already well know, maximum likelihood estimation may often lead to overfitting. Just like in case of linear regression, we can control this by penalizing large weights.

$$E(w) = -\ln p(y \mid w, X) + \lambda \|w\|_q^2 \quad (35)$$

Like before, for $q = 2$ this corresponds to MAP estimation with a Gaussian prior on w .

Again, there is no closed form solution available.

Multiclass logistic regression

$$\text{softmax}\left(\begin{bmatrix} 3 \\ -5 \\ 15 \end{bmatrix}\right) = \begin{bmatrix} \pi_1 \\ \pi_2 \\ \pi_3 \end{bmatrix}$$

$$\sum \pi_i = 1 \quad \pi_i \geq 0$$

For the binary classification we used the sigmoid function to "squeeze" the unnormalized probability $w^T x$ into the range $(0, 1)$.

The same can be done for multiple classes using the **softmax** function.

$$p(y = c \mid \mathbf{x}) = \frac{\exp(\mathbf{w}_c^T \mathbf{x})}{\sum_{c'} \exp(\mathbf{w}_{c'}^T \mathbf{x})}$$

How does this relate to multiclass LDA?

Loss for multiclass logistic regression

The negative log-likelihood for multiclass LR can be written as

$$E(\mathbf{w}) = -\ln p(\mathbf{Y} \mid \mathbf{w}, \mathbf{X}) \quad (36)$$

$$= -\sum_{i=1}^N \sum_{c=1}^C y_{ic} \ln p(y_i = c \mid \mathbf{x}_i, \mathbf{w}) \quad (37)$$

$$= -\sum_{i=1}^N \sum_{c=1}^C y_{ic} \ln \frac{\exp(\mathbf{w}_c^T \mathbf{x})}{\sum_{c'} \exp(\mathbf{w}_{c'}^T \mathbf{x})} \quad (38)$$

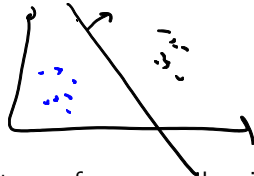
and is called cross entropy.


TRUE TARGETS PREDICTION p_i

Here we use **one-hot encoding**: vector of categorical variables $\mathbf{y} \in \mathcal{C}^N$ is encoded as a binary matrix $\mathbf{Y} \in \{0, 1\}^{N \times C}$, where

$$y_{ic} = \begin{cases} 1 & \text{if sample } i \text{ belongs to class } c \\ 0 & \text{else} \end{cases} \quad (39)$$

Generative vs. discriminative models



- In general, discriminative models achieve better performance when it comes to pure classification tasks.
- While generative models work reasonably well when their assumptions hold, they are quite fragile when these assumptions are violated.
- Generative modeling for high-dimensional / strongly correlated data like images or graphs is still an open research challenge.
- Nevertheless, generative models provide the added benefits of better handling missing data, detecting outliers, generating new data and being more appropriate in the semi-supervised setting.