

Machine Learning Exercise Sheet 05

Linear Classification



Exercise sheets consist of out-of-class and in-class exercises. You solve the homework exercises on your own or with your group and upload it to Moodle for a possible grade bonus. The in-class exercises will be solved during the tutorial. You do not have to upload any solutions of the in-class exercises.

In-class Exercises

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Multi-Class Classification

Problem 1: Consider a generative classification model for C classes defined by class probabilities $p(y = c) = \pi_c$ and general class-conditional densities $p(\mathbf{x} | y = c, \boldsymbol{\theta}_c)$ where $\mathbf{x} \in \mathbb{R}^D$ is the input feature vector and $\boldsymbol{\theta} = \{\boldsymbol{\theta}_c\}_{c=1}^C$ are further model parameters. Suppose we are given a training set $\mathcal{D} = \{(\mathbf{x}^{(n)}, \mathbf{y}^{(n)})\}_{n=1}^N$ where $\mathbf{y}^{(n)}$ is a binary target vector of length C that uses the 1-of- C (one-hot) encoding scheme, so that it has components $y_c^{(n)} = \delta_{c, a}$ if pattern n is from class $a = a$. Assuming that the data points are i.i.d., show that the maximum-likelihood solution for the class probabilities $\boldsymbol{\pi}$ is given by

$$\pi_c = \frac{N_c}{N}$$

where N_c is the number of data points assigned to class c .

The data likelihood given the parameters $\{\pi_c, \boldsymbol{\theta}_c\}_{c=1}^C$ is

$$p(\mathcal{D} | \{\pi_c, \boldsymbol{\theta}_c\}_{c=1}^C) = \prod_{n=1}^N \prod_{c=1}^C (p(\mathbf{x}^{(n)} | \boldsymbol{\theta}_c) \pi_c)^{y_c^{(n)}}$$

and so the data log-likelihood is given by

$$\log p(\mathcal{D} | \{\pi_c, \boldsymbol{\theta}_c\}_{c=1}^C) = \sum_{n=1}^N \sum_{c=1}^C y_c^{(n)} \log \pi_c + \text{const w.r.t. } \pi_c.$$

In order to maximize the log likelihood with respect to π_c we need to preserve the constraint $\sum_c \pi_c = 1$. For this we use the method of Lagrange multipliers where we introduce λ as an unconstrained additional parameter and find a local extremum of the unconstrained function

$$\sum_{n=1}^N \sum_{c=1}^C y_c^{(n)} \log \pi_c - \lambda \left(\sum_{c=1}^C \pi_c - 1 \right).$$

instead. See wikipedia article on Lagrange multipliers for an intuition of why this works. This function is a sum of concave terms in π_c as well as λ and is therefore itself concave in these variables.

Upload a single PDF file with your homework solution to Moodle by 09.12.2020, 23:59 CET. We recommend to typeset your solution (using L^AT_EX or Word), but handwritten solutions are also accepted. If your handwritten solution is illegible, it won't be graded and you waive your right to dispute that.

We can find the extremum by finding the root of the derivatives. Setting the derivative with respect to π_c equal to zero, we obtain

$$\frac{1}{\lambda} \sum_{n=1}^N y_c^{(n)} = \frac{N_c}{\lambda}.$$

Setting the derivative equal to zero, we obtain the original constraint

$$\sum_{c=1}^C \pi_c = 1$$

where we can now plug in the previous result $\pi_c = \frac{N_c}{\lambda}$ and obtain $\lambda = \sum_c N_c = N$. Plugging this in turn into the expression for π_c we obtain

$$\pi_c = \frac{N_c}{N}$$

which we wanted to show.

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Linear Discriminant Analysis

Problem 2: Using the same classification model as in the previous question, now suppose that the class-conditional densities are given by Gaussian distributions with a *shared* covariance matrix, so that

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

Show that the maximum likelihood estimate for the mean of the Gaussian distribution for class c is given by

$$\mu_c = \frac{1}{N_c} \sum_{\substack{n=1 \\ y^{(n)}=c}}^N \mathbf{x}^{(n)}$$

which represents the mean of the observations assigned to class c .

Similarly, show that the maximum likelihood estimate for the shared covariance matrix is given by

$$\Sigma = \sum_{c=1}^C \frac{N_c}{N} S_c \quad \text{where} \quad S_c = \frac{1}{N_c} \sum_{\substack{n=1 \\ y^{(n)}=c}}^N (\mathbf{x}^{(n)} - \mu_c)(\mathbf{x}^{(n)} - \mu_c)^T.$$

Thus Σ is given by a weighted average of the sample covariances of the data associated with each class, in which the weighting coefficients N_c/N are the prior probabilities of the classes.

We begin by writing out the data log-likelihood.

$$\begin{aligned} & \log p(\mathcal{D} | \{\pi_c, \theta_c\}_{c=1}^C) \\ &= \sum_{n=1}^N \sum_{c=1}^C y_c^{(n)} \log \pi_c \cdot p(\mathbf{x}^{(n)} | \mu_c, \Sigma) \end{aligned}$$

Then we plug in the definition of the multivariate Gaussian

$$= \sum_{n=1}^N \sum_{c=1}^C y_c^{(n)} \log \left((2\pi)^{-\frac{D}{2}} \det(\Sigma)^{-\frac{1}{2}} \exp \left(-\frac{1}{2} (x^{(n)} - \mu_c)^T \Sigma^{-1} (x^{(n)} - \mu_c) \right) \right) + y^{(n)} \log \pi_c$$

and simplify.

$$= -\frac{1}{2} \sum_{n=1}^N \sum_{c=1}^C y_c^{(n)} \left(\log \det \Sigma + (x^{(n)} - \mu_c)^T \Sigma^{-1} (x^{(n)} - \mu_c) - 2 \log \pi_c \right)$$

This expression is concave. To obtain the maximizer by finding the root of the derivative. With the help of the matrix cookbook, we identify the derivative with respect to μ_c as

$$\sum_{n=1}^N y_c^{(n)} \Sigma^{-1} (x^{(n)} - \mu_c)$$

which we can set to 0 and solve for μ_c to obtain

$$\mu_c = \frac{1}{\sum_{n=1}^N y_c^{(n)}} \sum_{n=1}^N y_c^{(n)} x^{(n)} = \frac{1}{\sum_{n=1}^N y^{(n)} = c} \sum_{n=1}^N x^{(n)}$$

To find the optimal Σ , we need the trace trick

$$a = \text{Tr}(a) \text{ for all } a \in \mathbb{R} \quad \text{and} \quad \text{Tr}(ABC) = \text{Tr}(BCA).$$

With this we can rewrite

$$(x^{(n)} - \mu_c)^T \Sigma^{-1} (x^{(n)} - \mu_c) = \text{Tr} \left(\Sigma^{-1} (x^{(n)} - \mu_c) (x^{(n)} - \mu_c)^T \right)$$

and use the matrix-trace derivative rule $\frac{\partial}{\partial A} \text{Tr}(AB) = B^T$ to find the derivative of the data log-likelihood with respect to Σ . Because the log-likelihood contains both Σ and Σ^{-1} , we convert one into the other with $\log \det A = -\log \det A^{-1}$ to obtain

$$-\frac{1}{2} \sum_{n=1}^N \sum_{c=1}^C y_c^{(n)} \left(-\log \det \Sigma^{-1} + \text{Tr} \left(\Sigma^{-1} (x^{(n)} - \mu_c) (x^{(n)} - \mu_c)^T \right) \right) + \text{const w.r.t. } \Sigma.$$

Finally, we use rule (57) from the matrix cookbook $\frac{\partial \log |\det X|}{\partial X} = (X^{-1})^T$ and compute the derivative of the log-likelihood with respect to Σ^{-1} as

$$-\frac{1}{2} \sum_{n=1}^N \sum_{c=1}^C y_c^{(n)} \left(-\Sigma^T + (x^{(n)} - \mu_c) (x^{(n)} - \mu_c)^T \right).$$

We find the root with respect to Σ and find

$$\Sigma = \frac{1}{\sum_{n=1}^N \sum_{c=1}^C y_c^{(n)}} \left(\sum_{n=1}^N \sum_{c=1}^C y_c^{(n)} (x^{(n)} - \mu_c) (x^{(n)} - \mu_c)^T \right)^T = \frac{1}{N} \sum_{c=1}^C \sum_{n=1}^N y^{(n)=c} (x^{(n)} - \mu_c) (x^{(n)} - \mu_c)^T$$

which we can immediately break apart into the representation in the instructions.

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Homework

Linear classification

Problem 3: We want the binary classification model for classifying *non-negative* one-dimensional data. The labels are binary ($y \in \{0, 1\}$) and the samples are $x \in [0, \infty)$.

We assume uniform class



$$p(y = 0) = p(y = 1) = \frac{1}{2}.$$

As our samples x are non-negative, we use exponential distributions (and not Gaussians) as class conditionals:

$$p(x | y = 0) = \text{Expo}(x | \lambda_0) \quad \text{and} \quad p(x | y = 1) = \text{Expo}(x | \lambda_1),$$

where $\lambda_0 \neq \lambda_1$. Assume, that the parameters λ_0 and λ_1 are known and fixed.

- a) Suppose you are given an observation x . What is the name of the posterior distribution $p(y | x)$? You only need to provide the name of the distribution (e.g. “normal”, “gamma” etc.) and estimate its parameters.

Bernoulli.

Remark: y can only take values in $\{0, 1\}$, so obviously Bernoulli is the only possible answer.

- b) What values of x are classified as class 1? (As usual, we assume that the classification decision is $\hat{y} = \arg \max_k p(y = k | x)$.)

Sample x is classified as class 1 if $p(y = 1 | x) > p(y = 0 | x)$. This is the same as saying

$$\frac{p(y = 1 | x)}{p(y = 0 | x)} > 1 \quad \text{or equivalently} \quad \log \frac{p(y = 1 | x)}{p(y = 0 | x)} > 0.$$

We begin by simplifying the left hand side.

$$\begin{aligned} \log \frac{p(y = 1 | x)}{p(y = 0 | x)} &= \log \frac{p(x | y = 1) p(y = 1)}{p(x | y = 0) p(y = 0)} \\ &= \log \frac{p(x | y = 1)}{p(x | y = 0)} \\ &= \log \frac{\lambda_1 \exp(-\lambda_1 x)}{\lambda_0 \exp(-\lambda_0 x)} \\ &= \log \frac{\lambda_1}{\lambda_0} + \lambda_0 x - \lambda_1 x = \log \frac{\lambda_1}{\lambda_0} + (\lambda_0 - \lambda_1)x \end{aligned}$$

To figure out which x are classified as class 1, we need to solve for x .

$$\log \frac{\lambda_1}{\lambda_0} + (\lambda_0 - \lambda_1)x > \log 1 \quad \Leftrightarrow \quad (\lambda_0 - \lambda_1)x > -\log \frac{\lambda_1}{\lambda_0} = \log \lambda_0 - \log \lambda_1$$

We have to be careful, because if $(\lambda_0 - \lambda_1) < 0$, dividing by it will flip the inequality sign. Hence the answer is

$$\begin{cases} \left(\frac{\log \lambda_0 - \log \lambda_1}{-\lambda_1}, \infty \right) & \text{if } \lambda_0 > \lambda_1 \\ \left(\frac{\lambda_0 - \log \lambda_1}{\lambda_0 - \lambda_1} \right) & \text{otherwise.} \end{cases}$$



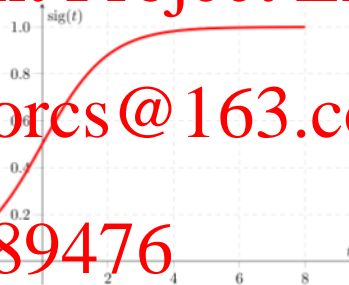
Problem 4: Let $\mathcal{D} = \{x_i, y_i\}_{i=1}^N$ be a linearly separable dataset for 2-class classification, i.e. there exists a vector w such that $\text{sign}(w^T x_i) = y_i$ for all i . Show that the maximum likelihood parameter w of a logistic regression model has $\|w\| \rightarrow \infty$. Assume that w contains the bias term.

How can we modify the training process to prefer a w of finite magnitude?

In logistic regression, we model the posterior distribution as

$$y_i | x \sim \text{Bernoulli}(\sigma(w^T x_i)) \text{ where } \sigma(a) = \frac{1}{1 + \exp(-a)}.$$

$$\text{sig}(t) = \frac{1}{1 + e^{-t}}$$



We fit the logistic regression model by choosing the parameter w that maximizes the data log-likelihood or alternatively minimizes the negative log-likelihood which expands to

$$E(w) = -\log p(y | w, X) = -\sum_{i=1}^N y_i \log \sigma(w^T x_i) + (1 - y_i) \log(1 - \sigma(w^T x_i)).$$

We assumed that the data-set is linearly separable, so by definition there is a \tilde{w} such that

$$\tilde{w}^T x_i > 0 \text{ if } y_i = 1 \text{ and } \tilde{w}^T x_i < 0 \text{ if } y_i = 0.$$

Scaling this separator \tilde{w} by a factor $\lambda \gg 0$ makes the negative log-likelihood smaller and smaller. To see this, we compute the limit

$$\lim_{\lambda \rightarrow \infty} E(\lambda \tilde{w}) = -\left(\sum_{\substack{i=1 \\ y_i=1}}^N \log \lim_{\lambda \rightarrow \infty} \sigma(\lambda \tilde{w}^T x_i) + \sum_{\substack{i=1 \\ y_i=0}}^N \log \left(1 - \lim_{\lambda \rightarrow \infty} \sigma(\lambda \tilde{w}^T x_i) \right) \right) = 0$$

which equals the smallest achievable value (E is the negative log of a probability, so $E(w) \in [0, \infty)$ and thus $E(w) \geq 0$).

We can see that E is a convex function because \log is concave and $\log \sigma(a)$ is concave if $a > 0$ and $\log(1 - \sigma(a))$ is concave if $a < 0$. It follows that E is a convex function because E is the negative sum of concave functions.

A convex function has a unique minimum if it attains its minimum value. We know that E tends towards its minimum but does not have a finite minimizer and all its minima are only achieved in the limit. In other words, the loss minimization problem has infinite norm.

Because E is convex and has a limit of 0 in some directions, we can move the minimum into the space of finite weights by adding a convex term that achieves its minimum such as $w^T w$ or similar forms of weight regularization.



Problem 5: Show that the softmax function is equivalent to a sigmoid in the 2-class case.

$$\begin{aligned} \frac{\exp(w_1^T x)}{\exp(w_1^T x) + \exp(w_0^T x)} &= \frac{1}{1 + \exp(w_0^T x) / \exp(w_1^T x)} \\ &= \frac{1}{1 + \exp(w_0^T x - w_1^T x)} \\ &= \frac{1}{1 + \exp((w_0 - w_1)^T x)} \\ &= \sigma(w^T x) \end{aligned}$$

where $\hat{w} = w_1 - w_0$.

One conclusion we can draw from this is that if we have C parameter vectors w_c for C classes, the logistic regression model is unidentifiable. This means that adding a constant $\tau \in \mathbb{R}^D$ to each vector $w_c := w_c + \tau$ would lead to the same logistic regression model. We can fix this issue by adding a constraint $w_1 = 0$, which is what is done implicitly when we use sigmoid (instead of 2-class softmax) in binary classification.

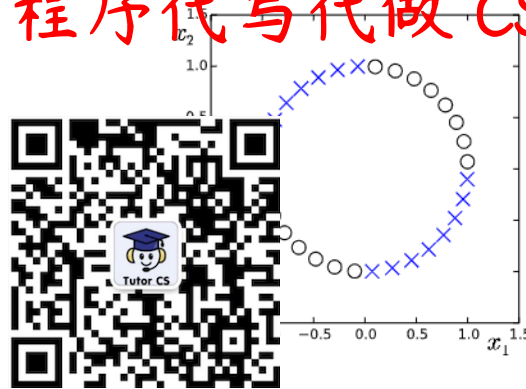
Problem 6: Show that the derivative of the sigmoid function $\sigma(a) = (1 + e^{-a})^{-1}$ can be written as

$$\frac{\partial \sigma(a)}{\partial a} = \sigma(a) (1 - \sigma(a)).$$

$$\frac{\partial \sigma(a)}{\partial a} = -\frac{1}{(1 + e^{-a})^2} \cdot e^{-a} \cdot (-1) = \frac{1}{1 + e^{-a}} \frac{e^{-a}}{1 + e^{-a}} = \sigma(a) \frac{1 + e^{-a} - 1}{1 + e^{-a}} = \sigma(a) (1 - \sigma(a))$$

Problem 7: Give a basis function $\phi(x_1, x_2)$ that makes the data in the example below linearly separable (crosses in one class, circles in the other).

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One example is $\phi(x) = x_1 x_2$ which makes the data separable by the hyperplane $w = (1)$ because the circles will be mapped to the positive real numbers while the crosses go to the negative numbers, i.e. $w^T x > 0$ if x is a circle and $w^T x < 0$ otherwise.

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Naive Bayes

Problem 8: In 2-class classification the decision boundary Γ is the set of points where both classes are assigned equal probability,

$$\Gamma = \{x \mid p(y = 1 \mid x) = p(y = 0 \mid x)\}.$$

Show that Naive Bayes with Gaussian class likelihoods produces a quadratic decision boundary in the 2-class case, i.e. that Γ can be written with a quadratic equation of x ,

$$\Gamma = \{x \mid x^T A x + b^T x + c = 0\},$$

for some A , b and c .

As a reminder, in Naive Bayes we assume class prior probabilities

$$p(y = 0) = \pi_0 \quad \text{and} \quad p(y = 1) = \pi_1$$

and class likelihoods

$$p(x \mid y = c) = \mathcal{N}(x \mid \mu_c, \Sigma_c)$$

with per-class means μ_c and *diagonal* (because of the feature independence) covariances Σ_c .

Because $p(y = 1 \mid x) + p(y = 0 \mid x) = 1$ and we want them to be equal, we can assume that $p(y = 0 \mid x) > 0$ and rewrite the defining equation as

$$\frac{p(y = 1 \mid x)}{p(y = 0 \mid x)} = 1.$$

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Now apply the logarithm to both sides and simplify.

$$\begin{aligned} \log \frac{p(y=1|x)}{p(y=0|x)} &= \log \left(\frac{p(x|y=1)p(y=1)}{p(x|y=0)p(y=0)} \cdot \frac{p(x)}{p(x)} \right) \\ &= \log(p(x|y=1)p(y=1)) - \log(p(x|y=0)p(y=0)) \\ &= \log \mathcal{N}(x|\mu_1, S_1) - \log \mathcal{N}(x|\mu_0, S_0) + \log \frac{\pi_1}{\pi_0} \\ &= -\frac{1}{2} \log |S_1| - \frac{1}{2} (x - \mu_1)^T S_1^{-1} (x - \mu_1) \\ &\quad + \frac{1}{2} \log |S_0| + \frac{1}{2} (x - \mu_0)^T S_0^{-1} (x - \mu_0) + \log \frac{\pi_1}{\pi_0} \\ &= -\frac{1}{2} x^T S_1^{-1} x + x^T S_1^{-1} \mu_1 - \frac{1}{2} \mu_1^T S_1^{-1} \mu_1 \\ &\quad + \frac{1}{2} x^T S_0^{-1} x - x^T S_0^{-1} \mu_0 + \frac{1}{2} \mu_0^T S_0^{-1} \mu_0 + \frac{1}{2} \log \frac{|S_0|}{|S_1|} + \log \frac{\pi_1}{\pi_0} \\ &= \frac{1}{2} x^T [S_0^{-1} - S_1^{-1}] x + x^T [S_1^{-1} \mu_1 - S_0^{-1} \mu_0] \\ &\quad - \frac{1}{2} \mu_1^T S_1^{-1} \mu_1 + \frac{1}{2} \mu_0^T S_0^{-1} \mu_0 + \log \frac{\pi_1}{\pi_0} + \frac{1}{2} \log \frac{|S_0|}{|S_1|} \end{aligned}$$

This shows that Γ is quadratic and can alternatively be written as

$$\Gamma = \{x \mid x^T A x + b^T x + c = 0\}$$

where

$$\begin{aligned} A &= \frac{1}{2} (S_0^{-1} - S_1^{-1}) & b &= S_1^{-1} \mu_1 - S_0^{-1} \mu_0 \\ c &= -\frac{1}{2} \mu_1^T S_1^{-1} \mu_1 + \frac{1}{2} \mu_0^T S_0^{-1} \mu_0 + \log \frac{\pi_1}{\pi_0} + \frac{1}{2} \log \frac{|S_0|}{|S_1|}. \end{aligned}$$

If both classes had the same covariance matrix ($S_0 = S_1$), A would be the zero matrix and we would obtain a linear decision boundary as we did in the lecture (also, $\log \frac{|S_0|}{|S_1|} = 0$).