

*Prof. J. M. Buhmann***Final Exam**

January 29th, 2011

First and Last name: _____

ETH number: _____

Signature: _____

	Topic	Max. Points	Points Achieved	Visum
1	Bayesian Inference	25		
2	Regression	25		
3	Bagging and Boosting	25		
4	SVM	25		
5	Mixture Models	25		
Total		125		

Grade:

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Question 1: Bayesian Inference (25 pts.)

Consider the task of estimating mean μ and variance σ^2 of a Gaussian density from n i.i.d. observations $\mathcal{X} = \{x_1, \dots, x_n\}$, $x \in \mathbb{R}$.

- a) Write the maximum likelihood estimator for the mean $\hat{\mu}_{\text{ML}}(\mathcal{X})$ as an explicit function of the i.i.d. observations $\mathcal{X} = \{x_1, \dots, x_n\}$:
(please write the direct closed-form solution)

1. $\hat{\mu}_{\text{ML}}(\mathcal{X}) = \arg \max p(\mathcal{X}|\mu) =$ **1 pts.**

2. Is this a biased estimator? YES\NO **1 pts.**

- b) Write the maximum likelihood estimator for the variance $\hat{\sigma}_{\text{ML}}^2(\mathcal{X})$ as an explicit function of the i.i.d. observations $\mathcal{X} = \{x_1, \dots, x_n\}$:
(please write the direct closed-form solution)

1. $\hat{\sigma}_{\text{ML}}^2(\mathcal{X}) = \arg \max p(\mathcal{X}|\sigma^2) =$ **1 pts.**

2. Is this a biased estimator? YES\NO **1 pts.**

Now, assume that the variance σ^2 is known.

- c) Given a Gaussian prior over the mean (prior with zero mean and variance one), write the posterior density $p(\mu|\mathcal{X})$ as an explicit function of the single observation $\mathcal{X} = \{x_1\}$:
(please write the direct closed-form solution)

1. $p(\mu|\mathcal{X}) = \frac{p(\mathcal{X}|\mu)p(\mu)}{p(\mathcal{X})} =$ **2 pts.**

2. Is the posterior a Gaussian density? YES\NO **1 pts.**

3. Is the posterior a Gaussian density for all priors? YES\NO **1 pts.**

- d) Given a Gaussian prior over the mean (prior with zero mean and variance one), write the maximum a posteriori estimator $\hat{\mu}_{\text{MAP}}(\mathcal{X})$ as an explicit function of the i.i.d. observations $\mathcal{X} = \{x_1, \dots, x_n\}$ (recall that $\int e^{-(\alpha^2)} d\alpha = \sqrt{\pi}$):
 (please write the direct closed-form solution)

1. $\hat{\mu}_{\text{MAP}}(\mathcal{X}) = \arg \max p(\mu | \mathcal{X}) =$ **2 pts.**

2. Does the maximum a posteriori estimate equal the mean of the posterior?
 YES\NO **1 pts.**

Now consider a binary classification task from observations $\mathcal{X} = \{x_1, \dots, x_n\}$, with $x \in \mathbb{R}^D$. Assume that the likelihood of both classes is Gaussian (assume class prior π_i , mean μ_i , and covariance matrix Σ_i for class y_i , with $i = 1, 2$).

- e) Write the discriminant $g_{y_1}(x) = p(y_1|x)$ as an explicit function of class prior, mean and covariance:
 (please write the direct closed-form solution)

$g_{y_1}(x) =$ **3 pts.**

- f) Assume that $\Sigma_1 = \Sigma_2 = \sigma^2 \mathbb{I}$, where \mathbb{I} denotes the identity matrix. Write the equation satisfied by the separating decision surface. The equation must be an explicit function of x_1 (the single observation), of class prior, means, and covariance:
 (please write the direct closed-form solution)

1. $0 = g_{y_1}(x) - g_{y_2}(x) =$ **2 pts.**

2. In this case, is the decision surface constant, linear, quadratic, cubic, or something else? constant\linear\quadratic\cubic\other **2 pts.**

3. Would it be possible to obtain a cylindrical decision surface? YES\NO **1 pts.**

- g) In the two dimensional case subject to uniform class prior, write means (μ_1, μ_2) and covariances (Σ_1, Σ_2) such that the decision surface is a hyperplane:
(any numerical instantiation which satisfies this constraint is acceptable)

$$\mu_1 =$$

$$\mu_2 =$$

$$\Sigma_1 =$$

$$\Sigma_2 =$$

3 pts.

- h) In the two dimensional case subject to uniform class prior, write means (μ_1, μ_2) and covariances (Σ_1, Σ_2) such that the decision surface is spherical:
(any numerical instantiation which satisfies this constraint is acceptable)

$$\mu_1 =$$

$$\mu_2 =$$

$$\Sigma_1 =$$

$$\Sigma_2 =$$

3 pts.

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Question 2: Regression (25 pts.)

Consider the linear regression model expressed in the homogeneous coordinates:

$$y = \beta_{(0)} + \sum_{i=1}^D \mathbf{x}_{(i)} \beta_{(i)} = \mathbf{x}^\top \boldsymbol{\beta},$$

where $\mathbf{x} = (1, \mathbf{x}_{(1)}, \dots, \mathbf{x}_{(D)}) \in \mathbb{R}^{D+1}$ is the input variable and y is the corresponding target variable.

Assume that the input dataset is given by the matrix $\mathbf{X} \in \mathbb{R}^{N \times (D+1)}$ whose first column is $\mathbf{1}$. Then the linear regression model for all the observations is written as $\mathbf{y} = \mathbf{X}\boldsymbol{\beta}$. Consider this linear regression model and answer the following questions:

- a) For this problem, formally define the Residual Sum of Squares (RSS) cost function and write it down in matrix notation.

Answer:

2 pts.

- b) Briefly motivate the connection between minimizing the Residual Sum of Squares and maximizing the likelihood of \mathbf{y} given \mathbf{X} .

Answer:

2 pts.

- c) We minimize the RSS function and infer the model parameters as $\hat{\beta} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$. Considering the matrix inverse operation, mathematically describe why in practice we are interested in regularized models such as *ridge* regression models rather than the given unregularized model.

Answer:

3 pts.

- d) Formally define ridge and LASSO regression models. By depicting appropriate plots, demonstrate the difference between these two models in inferring the model parameters $\hat{\beta}$.

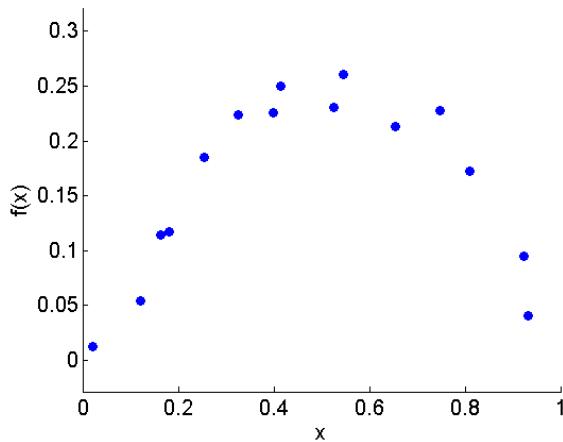
Answer:

5 pts.

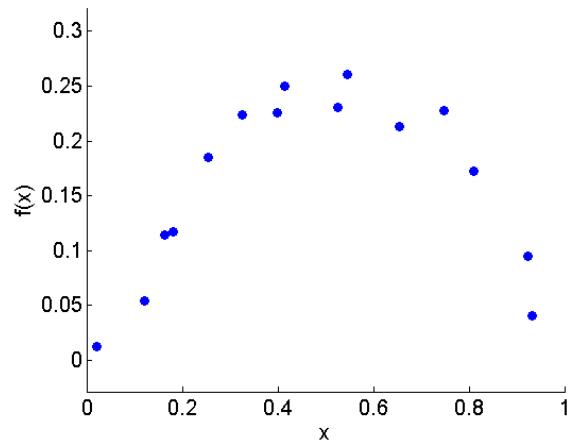
Now, we consider a general form of the problem where the set of observation $\{(\mathbf{x}_i, y_i)\}_{i=1}^n, \mathbf{x}_i \in \mathbb{R}^D, y_i \in \mathbb{R}$ are drawn i.i.d. from the joint distribution $P(X, Y)$. The goal is to find the regression function $f \in \mathcal{F}$ such that the mean squared error $\mathbb{E}_{XY}[(Y - f(X))^2]$ is minimal. Where the hypothesis class \mathcal{F} contains the set of all polynomial functions.

- e) Choosing an inappropriate function f might lead to either underfitting or overfitting. For the depicted given data, draw relevant plots to show each of these situations. For the overfitting case, briefly explain what happens if we have more observations.

Answer:



underfitting



overfitting

4 pts.

We can split the mean squared error $\mathbb{E}_{XY}[(Y - f(X))^2]$ into bias and variance, and find the best tradeoff between them.

- f) Write down the mathematical definition of bias and variance.

Answer:

2 pts.

- g) Expand the mean squared error $\mathbb{E}_{XY}[(Y - f(X))^2]$ and write it in the form of variance + squared bias.

Answer:

3 pts.

In this section we study how the averaging changes the bias of a set of unbiased estimators. Assume that we are given a set of B estimators $\hat{f}_1(\mathbf{x}), \hat{f}_2(\mathbf{x}), \dots, \hat{f}_B(\mathbf{x})$. We take the average estimator by $\hat{f}(\mathbf{x}) = \frac{1}{B} \sum_{b=1}^B \hat{f}_b(\mathbf{x})$.

- h) Calculate the bias of the average estimator $\hat{f}(\mathbf{x})$ in terms of the bias of the estimators $\hat{f}_1(\mathbf{x}), \dots, \hat{f}_B(\mathbf{x})$.

Hint: Start with the mathematical definition of the bias for $\hat{f}(\mathbf{x})$.

Answer:

3 pts.

- i) According to the results, briefly explain why unbiased estimators remain unbiased after averaging.

Answer:

1 pts.

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Question 3: Bagging and Boosting (25 pts.)

Bagging and *boosting* are two possible approaches to combine multiple models (classifiers or regressors) to achieve a *composite model* with improved performance. Both methods can be used in both a classification and a regression setting.

- a) State two essential differences between bagging and boosting.

Answer:

2 pts.

- b) Explain in terms of the bias-variance trade-off why the idea of combining models works.

Answer:

2 pts.

c) We now look at the problem of regression and how the combination of individual regression models can give better results. Left-column figures show the individual regression models, right-column figures show the true target function (solid) and the output of averaging the individual models to obtain a composite model (dashed).

1. The individual regression models (in Figure 1 and Figure 3) have been regularized using a regularization parameter λ , i.e. the cost function had the following form

$$RSS_{Ridge}(\boldsymbol{\beta}) = \sum_{i=1}^n (t_i - \boldsymbol{\phi}(\mathbf{x}_i)^\top \boldsymbol{\beta})^2 + \lambda \|\boldsymbol{\beta}\|_2^2$$

The parameters used were $\lambda = 0.09$ and $\lambda = 13.5$.

Associate the regularization parameters to the figures in the left column.

Answer:

Figure 1: $\lambda = \dots$

Figure 3: $\lambda = \dots$

2. Please interpret the figures in terms of the bias-variance trade-off

Answer:

Figure 1 and 2:

Figure 3 and 4:

Figure 1

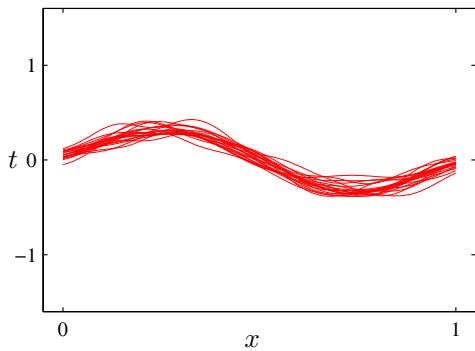


Figure 2

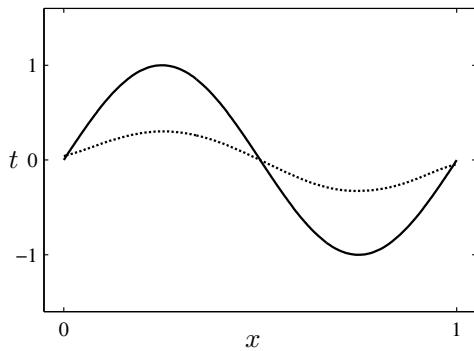


Figure 3

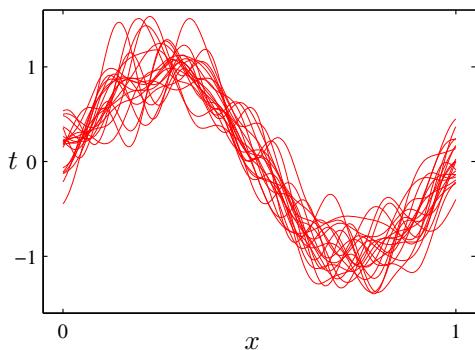
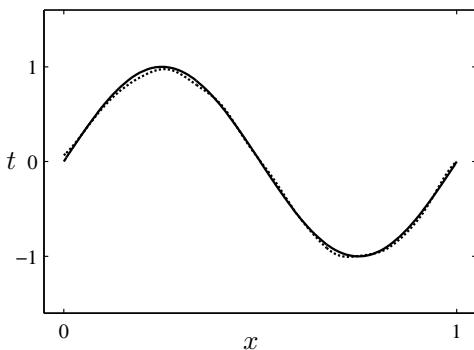


Figure 4



4 pts.

d) We now consider *bagging* in a regression setting. In order to model a *target function* $h(x)$, we combine M *individual models* $y_m(x)$, $m = 1..M$ to obtain a *committee model* $y_{COM}(x)$. We model the *error* of each individual model using $\epsilon_m(x)$, $m = 1..M$. This question's final goal is to show that the error of the committee model is M times smaller than the average error of the individual models.

1. Write down the output of the committee model, which averages the individual model's outputs. Answer:

$$y_{COM}(x) = \dots$$

2. Write down the error $\epsilon_m(x)$ of an individual model in terms of the target function $h(x)$ and the output of the individual model $y_m(x)$. Answer:

$$\epsilon_m(x) = \dots - \dots$$

3. Write down the expected squared error of an individual model. \mathbb{E}_x denotes the expectation value w.r.t. the distribution of x . Answer:

$$E_m = \mathbb{E}_x \left[\dots \right]$$

4. Write down the average of the expected squared errors made by the individual models

Answer:

$$E_{AV} = \dots$$

5. Write down the expected squared error made by the committee model, in terms of the output of the committee model and the target function.

Answer:

$$E_{COM} = \mathbb{E}_x \left[\dots \right]$$

6. Show that $E_{COM} = \frac{1}{M} E_{AV}$.

Hint: Use the assumption that the errors of the individual models are uncorrelated, i.e. $\mathbb{E}_x[\epsilon_m(x)\epsilon_l(x)] = 0$, $m \neq l$, and that the mean error of the individual models is zero, i.e. $\mathbb{E}_x[\epsilon_m(x)] = 0$.

Answer:

10 pts.

We now turn our attention to *boosting* in a classification setting.

- e) Given i.i.d. training data $\{(\mathbf{x}_1, c_1), (\mathbf{x}_2, c_2), \dots, (\mathbf{x}_n, c_n)\}$, $\mathbf{x}_i \in \mathbb{R}^D$, $c_i \in \{-1, 1\}$, and individual classifiers $y_m(\mathbf{x})$, $m = 1 \dots M$, we can define the following additive model

$$f_k(\mathbf{x}) = \frac{1}{2} \sum_{j=1}^k \alpha_j y_j(\mathbf{x})$$

where α_j are weights, $k \leq M$.

Think of $f_k(\mathbf{x})$ as the *additive model* which uses the first $1..k$ individual classifiers.

1. Define the sum-of-squares error of $f_k(\mathbf{x})$ on the training dataset.

Answer:

$$Err_k = \dots$$

2. Assume that the first $1..(k-1)$ classifiers $y_j(\mathbf{x})$ and weights α_j , $j = 1..(k-1)$ have already been determined, i.e. fixed.

Show that finding the optimal k -th classifier $y_k(\mathbf{x})$ and its weight α_k involves fitting the k -th classifier to the residual errors $f_{k-1}(\mathbf{x}_i) - c_i$ made by the $(k-1)$ -th additive model.

(*Hint: Start from the expression Err_k and recognize the terms $f_{k-1}(\mathbf{x}_i) - c_i$*)

7 pts.

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Question 4: SVM (25 pts.)

In the following questions choose one answer only.

a) Why does a Support Vector Machine generalizes better than a Perceptron?

1. The selected support vectors tend to be very typical samples.
2. By supporting vectors it is not restricted to scalar input.
3. The requirement of maximal margins reduces the arbitrariness.
4. The support vector machine will have access to more training data.

2 pts.

b) What is the advantage of using kernels in support vector machines?

1. They tend to maximize the margins.
2. They enable non-linear separations.
3. They will increase the number of support vectors.
4. They reduce the risk of getting stuck in local minima.

2 pts.

Explain your answer to the following questions in 1-2 sentences.

c) Suppose that you have a binary SVM classifier with a linear kernel. Consider a vector \mathbf{x}_i for which $y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + w_0) > 1$ ($\mathbf{x}_i \in \mathbb{R}^D$, $y_i \in \{-1, +1\}$)

1. Is \mathbf{x}_i correctly classified? YES\NO
2. If we remove \mathbf{x}_i from the training set and re-train the classifier, will the decision boundary change or stay the same?

Answer:

3 pts.

- d) We would like to build a binary SVM classifier for histograms. Let H denote the class of histograms, for each $\mathbf{h} \in H$ the following properties hold:

1. $\mathbf{h} = \{h_1, \dots, h_m\}, \quad \forall j : h_j \geq 0$

2. $\sum_{j=1}^m h_j = L \quad \text{for some } L \in \mathbb{N}.$

Consider using the following kernel function:

$$K(\mathbf{h}, \tilde{\mathbf{h}}) = \sum_{j=1}^m \min(h_j, \tilde{h}_j) \quad \mathbf{h}, \tilde{\mathbf{h}} \in H$$

What kind of separation is imposed by this kernel? (which points in the space will become close/far using this kernel).

Answer:

3 pts.

- e) Let \mathcal{X} be a finite set and consider the following function. For $\mathbf{x}, \bar{\mathbf{x}} \in \mathcal{X}$:

$$K(\mathbf{x}, \bar{\mathbf{x}}) = \begin{cases} 1 & \text{if } \mathbf{x} = \bar{\mathbf{x}} \\ 0 & \text{else} \end{cases}$$

Prove that $K(\mathbf{x}, \bar{\mathbf{x}})$ is a legitimate kernel function.

Hint: One possible way to prove it is to find a feature mapping $\phi(\mathbf{x})$, such that

$$K(\mathbf{x}, \bar{\mathbf{x}}) = \langle \phi(\mathbf{x}), \phi(\bar{\mathbf{x}}) \rangle.$$

Answer:

3 pts.

L2-SVM use the square sum of the slack variables ξ_i in the objective function instead of the linear sum of the slack variables (squaring the hinge loss). Let $S = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$ be a training set of examples and binary labels $y_i \in \{-1, +1\}$. The primal formulation of the *L2-SVM* is as follows

$$\min_{\mathbf{w}, w_0, \xi} \frac{1}{2} \|\mathbf{w}\|^2 + \frac{C}{2} \sum_{i=1}^n \xi_i^2$$

s.t.

$$\begin{aligned} y_i(\langle \mathbf{w}, \mathbf{x}_i \rangle + w_0) &\geq 1 - \xi_i & i = 1, \dots, n \\ \xi_i &\geq 0 & i = 1, \dots, n \end{aligned}$$

- f) Show that removing the last set of constraints: $\forall i : \xi_i \geq 0$ does not change the optimal solution to the primal problem.

Answer:

4 pts.

Now we would like to derive the dual form of the *L2-SVM*.

- g) Write down the Lagrangian of the *L2-SVM*.

Answer:

$$L(\quad) =$$

2 pts.

- h) Compute the derivatives of the Lagrangian with respect to the appropriate variables.

Answer:

3 pts.

We decided not to bother you with the remaining computation, instead we finished the derivation ourselves.

i) Below are 4 optimization problems, only 1 of which is the dual L_2 -SVM.
Circle the optimization problem corresponding to the dual L_2 -SVM.

Explain your choice by either shortly falsifying the other options or by showing the full derivation.

Hint: The full derivation is more time consuming.

$$\max_{\alpha} \quad \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j - \frac{1}{2C} \sum_{i=1}^n \alpha_i^2 \quad \max_{\alpha} \quad \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

s.t.:

$$\sum_{i=1}^n \alpha_i y_i = 0$$

$$\forall i : \alpha_i \geq 0$$

(a)

s.t.:

$$\sum_{i=1}^n \alpha_i y_i = 0$$

$$\forall i : 0 \leq \alpha_i \leq \frac{\xi_i}{C}$$

(b)

$$\min_{\alpha} \quad \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j \mathbf{x}_i^T \mathbf{x}_j - \frac{1}{2C} \sum_{i=1}^n \alpha_i^2$$

$$\max_{\alpha, \xi} \quad \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j + C \sum_{i=1}^n \xi_i$$

s.t.:

$$\sum_{i=1}^n \alpha_i y_i = 0$$

$$\forall i : \alpha_i \geq 0$$

s.t.:

$$\sum_{i=1}^n \alpha_i y_i = 0$$

$$\forall i : \alpha_i \geq 0$$

(c)

(d)

Answer:

3 pts.

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Question 5: Mixture of Bernoulli models (25 pts.)

Let $\mathbf{x} = (x_1, \dots, x_D)^T \in \{0, 1\}^D$ be a D -dimensional random binary vector. We assume that every x_i is Bernoulli distributed with parameter μ_i , i.e.

$$\begin{aligned} p(x_i = 1; \mu_i) &= \mu_i \\ p(x_i = 0; \mu_i) &= 1 - \mu_i, \end{aligned}$$

which can be also written as

$$p(x_i; \mu_i) = \mu_i^{x_i} (1 - \mu_i)^{1-x_i}.$$

Under the assumption of the x_i 's being independent, the distribution of the random vector $\mathbf{x} = (x_1, \dots, x_D)^T$ is

$$p(\mathbf{x}; \boldsymbol{\mu}) = \prod_{i=1}^D \mu_i^{x_i} (1 - \mu_i)^{1-x_i},$$

with $\boldsymbol{\mu} = (\mu_1, \dots, \mu_D)^T$.

- a) What is $\mathbb{E}(\mathbf{x})$ and $\text{Cov}(\mathbf{x})$ in this setting?

Answer:

3 pts.

- b) Consider a Bernoulli mixture model for binary random vectors with K mixture components, i.e.

$$p(\mathbf{x}; (\boldsymbol{\mu}_k)_k, \mathbf{w}) = \sum_{k=1}^K w_k p(\mathbf{x}; \boldsymbol{\mu}_k)$$

with weights $\mathbf{w} = (w_1, \dots, w_K)^T$ and Bernoulli parameters $(\boldsymbol{\mu}_k)_k = (\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_K)$.

(Side remark, which is not relevant to solve the question: The number of mixture components K cannot be larger than the dimension D of the random vector to ensure identifiability.)

What are natural constraints on \mathbf{w} to obtain a proper probability distribution $p(\mathbf{x}; (\boldsymbol{\mu}_k)_k, \mathbf{w})$?

Answer:

2 pts.

c) Show that

$$\mathbb{E}(\mathbf{x}) = \sum_k w_k \boldsymbol{\mu}_k \quad \text{and}$$

$$(\mathbf{Cov}(\mathbf{x}))_{i,j} = \begin{cases} \sum_k w_k \mu_{ki} - \mathbb{E}(\mathbf{x}_i)^2 & \text{if } i = j \\ \sum_k w_k \mu_{ki} \mu_{kj} - \mathbb{E}(\mathbf{x}_i) \mathbb{E}(\mathbf{x}_j) & \text{if } i \neq j \end{cases}$$

(the elements of the covariance matrix)

where μ_{ki} is the i -th component of $\boldsymbol{\mu}_k$.

Hints:

1. You do not need to include the last terms, $-\mathbb{E}(\mathbf{x}_i)^2$ and $-\mathbb{E}(\mathbf{x}_i) \mathbb{E}(\mathbf{x}_j)$, in your derivation, since these follow from the relation

$$\mathbf{Cov}(\mathbf{x}) = \mathbb{E}(\mathbf{x}\mathbf{x}^T) - \mathbb{E}(\mathbf{x})\mathbb{E}(\mathbf{x})^T.$$

Thus, you need to focus only on $\mathbb{E}(\mathbf{x}\mathbf{x}^T)$.

2. Consider $\mathbb{E}(\mathbf{x}_i \mathbf{x}_j)$ separately for the cases $i = j$ and $i \neq j$. Use the fact that $\mathbb{E}(\mathbf{x}_i \mathbf{x}_j) = P(\mathbf{x}_i = 1 \wedge \mathbf{x}_j = 1)$, since \mathbf{x} is a binary vector.

What is the main (qualitative) difference between the covariance derived in a) and the one for the mixture model?

Answer:

5 pts.

- d) In order to derive an EM-method to determine the mixture of Bernoulli parameters, we introduce a latent binary vector $\mathbf{z} = (z_1, \dots, z_K)^T \in \{0, 1\}^K$ linked with \mathbf{x} , such that $\sum_k z_k = 1$ and $z_k = 1$ if \mathbf{x} is generated by the k -th mixture component. Hence, we have

$$p(\mathbf{x} | \mathbf{z}) = \prod_{k=1}^K p(\mathbf{x}; \boldsymbol{\mu}_k)^{z_k} \quad \text{and} \quad p(\mathbf{z}) = \prod_{k=1}^K w_k^{z_k}.$$

Derive $p(\mathbf{x})$ by marginalizing over \mathbf{z} . Answer:

3 pts.

- e) M-step: let $\mathbf{X} := (\mathbf{x}_n)_n \in \mathbb{R}^{D \times N}$ be a sequence of N i.i.d. samples drawn from the mixture of Bernoulli distribution. We have a corresponding matrix of the latent variables $\mathbf{Z} := (\mathbf{z}_n)_n \in \mathbb{R}^{K \times N}$.

Write down the joint log-likelihood function $\ln p(\mathbf{X}, \mathbf{Z}; (\boldsymbol{\mu}_k)_k, \mathbf{w})$ and derive the M-step by maximizing the joint log-likelihood over the unknown parameters $(\boldsymbol{\mu}_k)_k$ and \mathbf{w} . Hint: don't forget to introduce a Lagrange multiplier for the constraint on \mathbf{w} .

Answer:

6 pts.

f) E-step: derive the expectation of the joint log-likelihood function with respect to \mathbf{Z} . Hints:

1. Derive $p(\mathbf{Z} | \mathbf{X})$ first via $p(\mathbf{z})$ and $p(\mathbf{x} | \mathbf{z})$ given above.
2. Consider $\mathbb{E}(z_{nk}) = p(z_{nk} = 1)$, since $z_{nk} \in \{0, 1\}$.
3. Observe that z_{nk} appears only linearly in the joint log-likelihood function.

Answer:

6 pts.

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Supplementary Sheet

Supplementary Sheet