6.867 Machine learning

Final exam

December 3, 2004

Your name and MIT ID:

(Optional) **The grade you would give to yourself + a brief justification.**

Problem 1

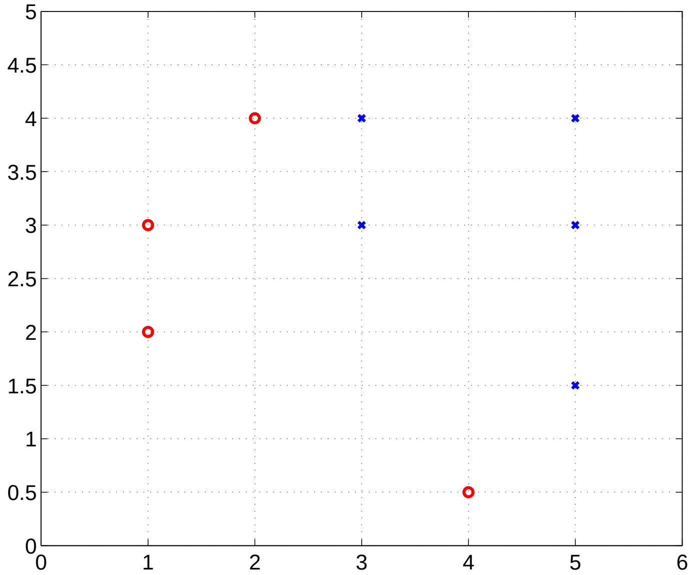


Figure 1: Labeled training points for problem 1.

Consider the labeled training points in Figure 1, where 'x' and 'o' denote positive and negative labels, respectively. We wish to apply AdaBoost with decision stumps to solve the classification problem. In each boosting iteration, we select the stump that minimizes the weighted training error, breaking ties arbitrarily.

1. **(3 points)** In figure 1, draw the decision boundary corresponding to the first decision stump that the boosting algorithm would choose. Label this boundary (1), and also indicate +/- side of the decision boundary.

2. **(2 points)** In the same figure 1 also circle the point(s) that have the highest weight after the first boosting iteration.

3. **(2 points)** What is the weighted error of the first decision stump after the first boosting iteration, i.e., after the points have been reweighted? □

4. **(3 points)** Draw the decision boundary corresponding to the second decision stump, again in Figure 1, and label it with (2), also indicating the +/- side of the boundary.

5. **(3 points)** Would some of the points be misclassified by the combined classifier after the two boosting iterations? Provide a brief justification. (the points will be awarded for the justification, not whether your y/n answer is correct)

Problem 2

1. **(2 points)** Consider a linear SVM trained with n labeled points in $\mathcal{R}^2$ without slack penalties and resulting in $k = 2$ support vectors ($k < n$). By adding one additional labeled training point and retraining the SVM classifier, what is the maximum number of support vectors in the resulting solution?

   ( ) k
   ( ) $k + 1$
   ( ) $k + 2$
   ( ) $n + 1$

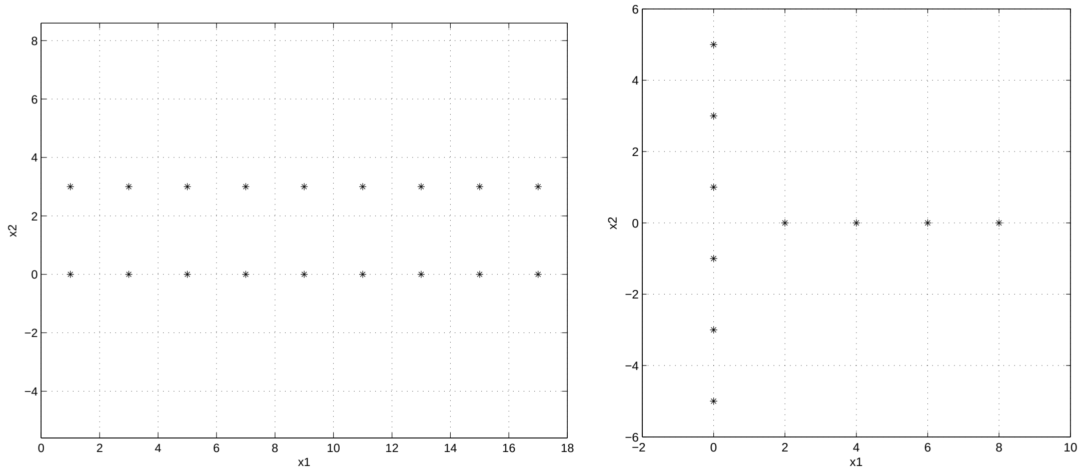
2. We train two SVM classifiers to separate points in $\mathcal{R}^2$. The classifiers differ only in terms of the kernel function. Classifier 1 uses the linear kernel $K_1(\mathbf{x}, \mathbf{x}') = \mathbf{x}^T\mathbf{x}'$, and classifier 2 uses $K_2(\mathbf{x}, \mathbf{x}') = p(\mathbf{x})p(\mathbf{x}')$, where $p(\mathbf{x})$ is a 3-component Gaussian mixture density, estimated on the basis of related other problems.

   (a) **(3 points)** What is the VC-dimension of the second SVM classifier that uses kernel $K_2(\mathbf{x}, \mathbf{x}')$? □

   (b) **(T/F – 2 points)** The second SVM classifier can only separate points that are likely according to $p(\mathbf{x})$ from those that have low probability under $p(\mathbf{x})$. □

   (c) **(4 points)** If both SVM classifiers achieve zero training error on n labeled points, which classifier would have a better generalization guarantee? Provide a brief justification.

Problem 3



(a) (b)

Figure 2: Data sets for clustering. Points are located at integer coordinates.

1. **(4 points)** First consider the data plotted in Figure 2a, which consist of two rows of equally spaced points. If k-means clustering ($k = 2$) is initialised with the two points whose coordinates are $(9, 3)$ and $(11, 3)$, indicate the final clusters obtained (after the algorithm converges) on Figure 2a.

2. **(4 points)** Now consider the data in Figure 2b. We will use spectral clustering to divide these points into two clusters. Our version of spectral clustering uses a neighbourhood graph obtained by connecting each point to its two nearest neighbors (breaking ties randomly), and by weighting the resulting edges between points $\mathbf{x}_i$ and $\mathbf{x}_j$ by $W_{ij} = \exp(-||\mathbf{x}_i - \mathbf{x}_j||)$. Indicate on Figure 2b the clusters that we will obtain from spectral clustering. Provide a brief justification.

3. **(4 points)** Can the solution obtained in the previous part for the data in Figure 2b also be obtained by k-means clustering ($k = 2$)? Justify your answer.

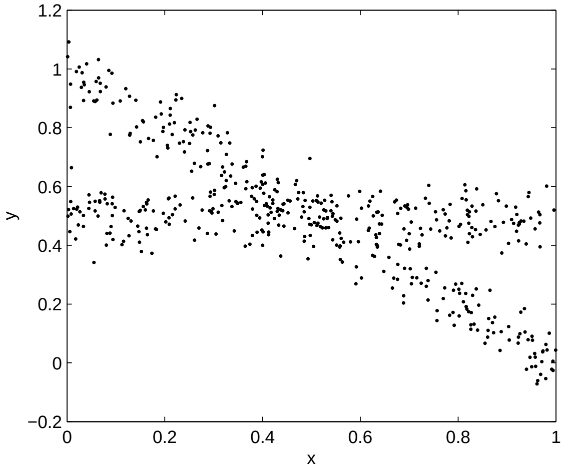


Figure 3: Training sample from a mixture of two linear models

Problem 4

The data in Figure 3 comes from a mixture of two linear regression models with Gaussian noise:

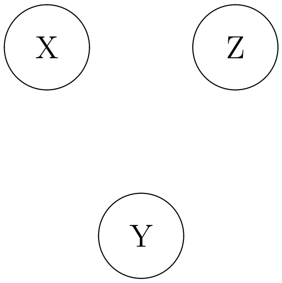
$$P(y|x;\theta) = p_1\mathcal{N}(y\,;\,w_{10}+w_{11}x,\ \sigma_1^2) + p_2\mathcal{N}(y\,;\,w_{20}+w_{21}x,\ \sigma_2^2)$$

where $p_1 + p_2 = 1$ and $\theta = (p_1, p_2, w_{10}, w_{11}, w_{20}, w_{21}, \sigma_1, \sigma_2)$. We hope to estimate θ from such data via the EM algorithm.

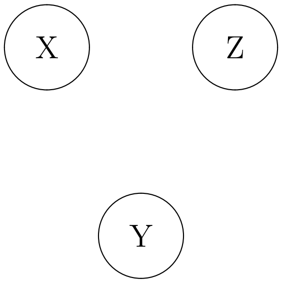
To this end, let $z \in \{1, 2\}$ be the mixture index, variable indicating which of the regression models is used to generate y given x.

1. **(6 points)** Connect the random variables X, Y, and Z with directed edges so that the graphical model on the left represents the mixture of linear regression models described above, and the one on the right represents a mixture-of-experts model. For both models, Y denotes the output variable, X the input, and Z is the choice of the linear regression model or expert.

mixture of linear regressions



mixture of experts

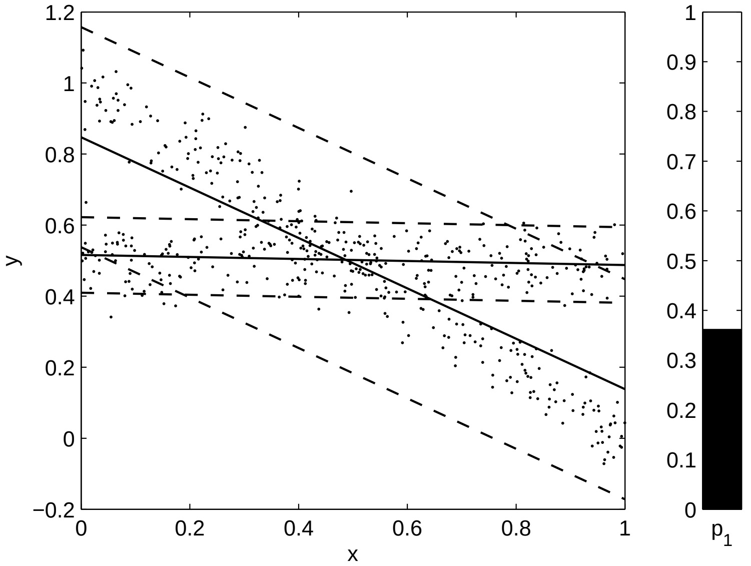


We use a single plot to represent the model parameters (see the figure below). Each linear regression model appears as a solid line ($y = w_{i0} + w_{i1}x$) in between two parallel dotted lines at vertical distance $2\sigma_i$ to the solid line. Thus each regression model "covers" the data that falls between the dotted lines. When $w_{10} = w_{20}$ and $w_{11} = w_{21}$ you would only see a single solid line in the figure; you may still see two different sets of dotted lines corresponding to different values of σ_1 and σ_2. The solid bar to the right represents p_1 (and $p_2 = 1 - p_1$).

For example, if

$$\begin{aligned} \theta &= (\quad p_1, \quad p_2, \quad w_{10}, \quad w_{11}, \quad w_{20}, \quad w_{21}, \quad \sigma_1, \quad \sigma_2) \\ &= (\quad 0.35, \quad 0.65, \quad 0.5, \quad 0, \quad 0.85, \quad -0.7, \quad 0.05, \quad 0.15) \end{aligned}$$

the plot is

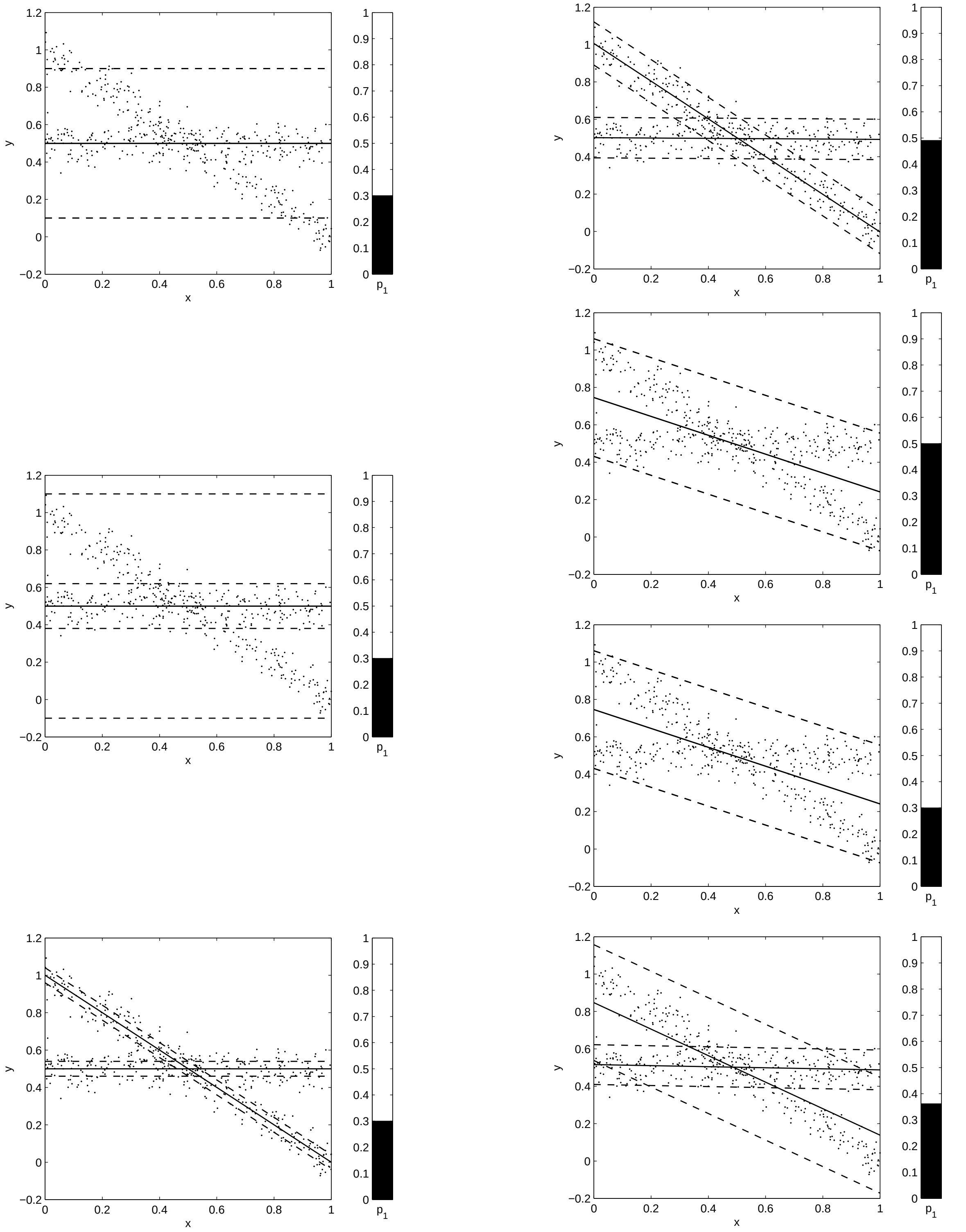


2. **(6 points)** We are now ready to estimate the parameters θ via EM. There are, however, many ways to initialize the parameters for the algorithm.

   On the next page you are asked to connect 3 different initializations (left column) with the parameters that would result after one EM iteration (right column). Different initializations may lead to the same set of parameters. Your answer should consist of 3 arrows, one from each initialization.

Initialization

Next Iteration



Problem 5

Assume that the following sequences are very long and the pattern highlighted with spaces is repeated:

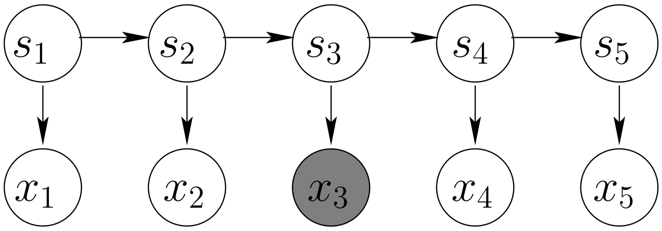
Sequence 1: `1 0 0   1 0 0   1 0 0   1 0 0  ...  1 0 0`

Sequence 2: `1   1 0 0   1 0 0   1 0 0  ...  1 0 0`

1. **(4 points)** If we model each sequence with a different first-order HMM, what is the number of hidden states that a reasonable model selection method would report?

	HMM for Sequence 1	HMM for Sequence 2
No. of hidden states		

2. **(2 points)** The following Bayesian network depicts a sequence of 5 observations from an HMM, where s_1, s_2, s_3, s_4, s_5 is the hidden state sequence.



Are x_1 and x_5 independent given x_3? Briefly justify your answer.

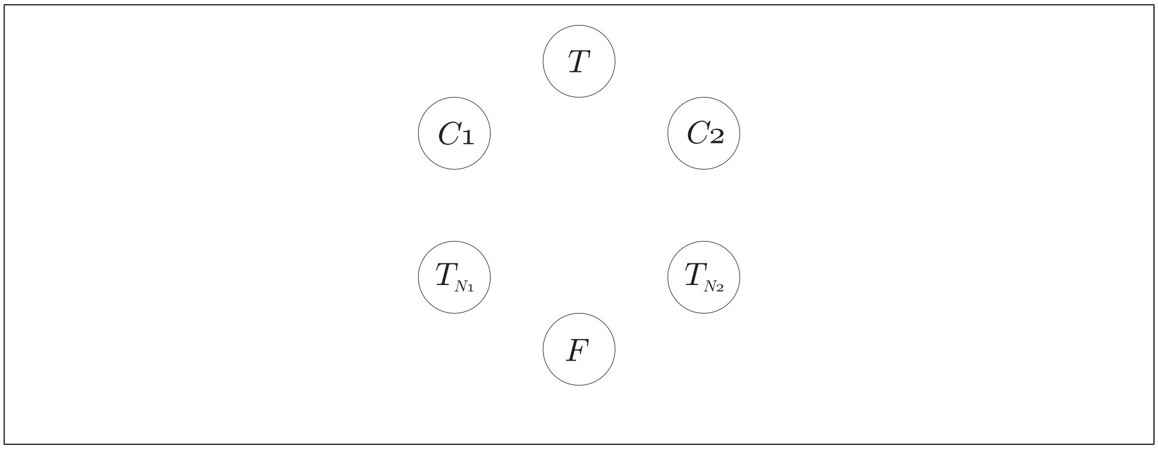
3. **(3 points)** Does the order of Markov dependencies in the observed sequence always determine the number of hidden states of the HMM that generated the sequence? Provide a brief justification.

Problem 6

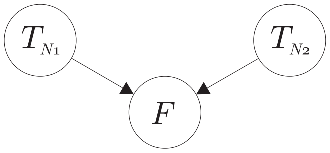
We wish to develop a graphical model for the following transportation problem. A transport company is trying to choose between two alternative routes for commuting between Boston and New York. In an experiment, two identical busses leave Boston at the same but otherwise random time, T_B. The busses take different routes, arriving at their (common) destination at times T_{N1} and T_{N2}.

Transit time for each route depends on the congestion along the route, and the two congestions are unrelated. Let us represent the random delays introduced along the routes by variables $C1$ and $C2$. Finally, let F represent the identity of the bus which reaches New York first. We view F as a random variable that takes values 1 or 2.

1. **(6 points)** Complete the following directed graph (Bayesian network) with edges so that it captures the relationships between the variables in this transportation problem.



2. **(3 points)** Consider the following directed graph as a possible representation of the independences between the variables T_{N1}, T_{N2}, and F only:



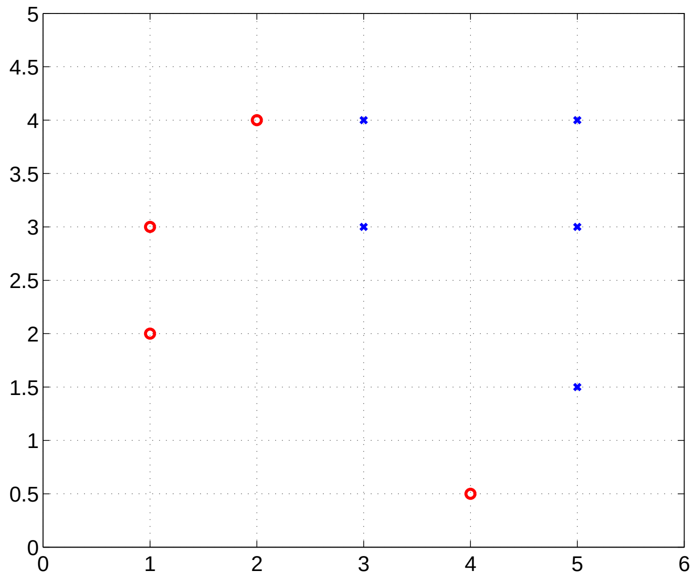
Which of the following factorizations of the joint are consistent with the graph?

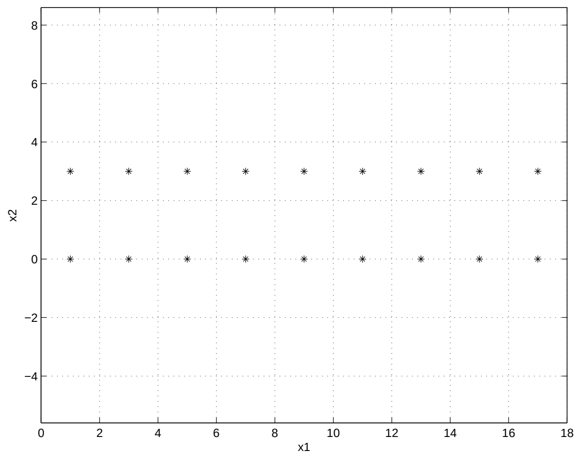
$P(T_{N1})P(T_{N2})P(F|T_{N1}, T_{N2})$ □

$P(T_{N1})P(T_{N2})P(F|T_{N1})$ □

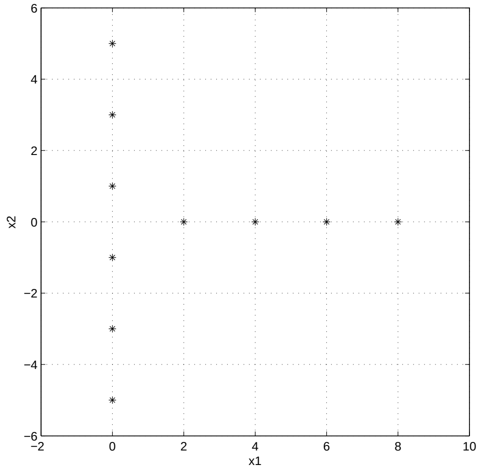
$P(T_{N1})P(T_{N2})P(F)$ □

Additional set of figures



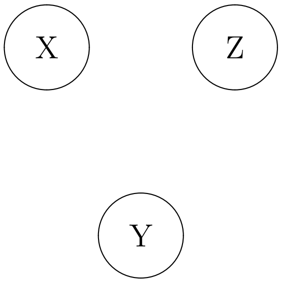


(a)

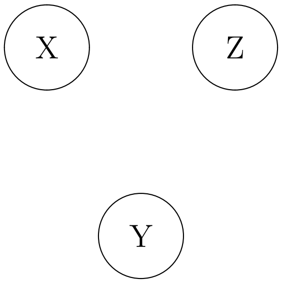


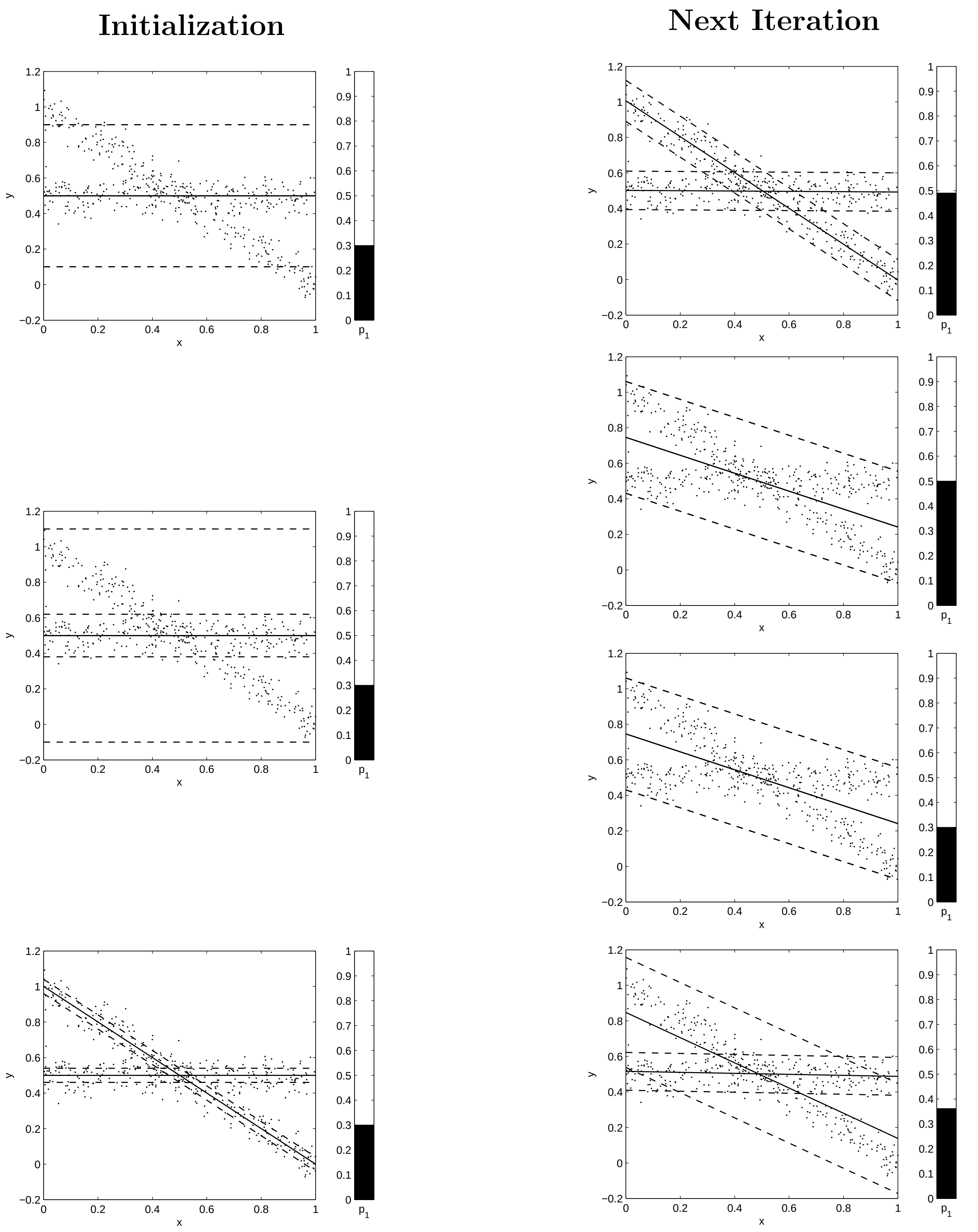
(b)

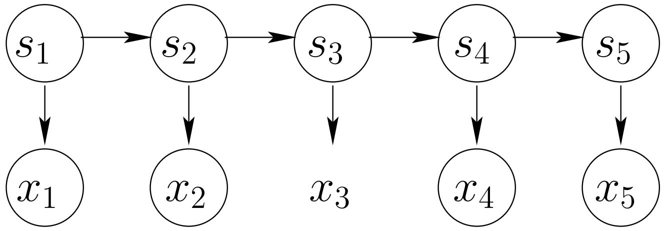
mixture of linear regressions

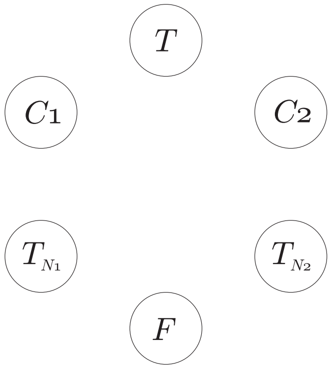


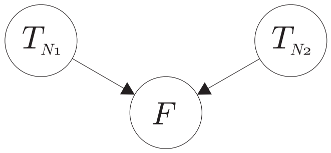
mixture of experts




Initialization
Next Iteration
y
x
p_1
1.2
1
0.8
0.6
0.4
0.2
0
−0.2
0.9
0.7
0.5
0.3
0.1


s_1
s_2
s_3
s_4
s_5
x_1
x_2
x_3
x_4
x_5


T
C_1
C_2
T_{N_1}
T_{N_2}
F


T_{N_1}
T_{N_2}
F

6.867 Machine learning

Final exam (Fall 2003)

December 10, 2003

Problem 1: your information

1.1. Your name and MIT ID:

1.2. The grade you would give to yourself + brief justification (if you feel that there's no question your grade should be an A, then just say A):

Problem 2

2.1. **(3 points)** Let $\mathcal{F}$ be a set of classifiers whose VC-dimension is 5. Suppose we have four training examples and labels, $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_4, y_4)\}$, and select a classifier $\hat{f}$ from $\mathcal{F}$ by minimizing classification error on the training set. In the absence of any other information about the set of classifiers $\mathcal{F}$, can we say that the prediction $\hat{f}(\mathbf{x}_5)$ for a new example $\mathbf{x}_5$ has any relation to the training set? Briefly justify your answer.

2.2. **(T/F – 2 points)** Consider a set of classifiers that includes all linear classifiers that use different choices of strict subsets of the components of the input vectors $\mathbf{x} \in \mathcal{R}^d$. Claim: the VC-dimension of this combined set cannot be more than $d + 1$. □

2.3. **(T/F – 2 points)** Structural risk minimization is based on comparing upper bounds on the generalization error, where the bounds hold with probability $1 - \delta$ over the choice of the training set. Claim: the value of the confidence parameter δ cannot affect model selection decisions. □

2.4. **(6 points)** Suppose we use class-conditional Gaussians to solve a binary classification task. The covariance matrices of the two Gaussians are constrained to be $\sigma^2 I$, where the value of σ^2 is fixed and I is the identity matrix. The only adjustable parameters are therefore the means of the class conditional Gaussians, and the prior class frequencies. We use the maximum likelihood criterion to train the model. Check all that apply.

( ) For any three distinct training points and sufficiently small σ^2, the classifier would have zero classification error on the training set

( ) For any three training points and sufficiently large σ^2, the classifier would always make one classification error on the training set

( ) The classification error of this classifier on the training set is always at least that of a linear SVM, whether the points are linearly separable or not

Problem 3

3.1. (T/F – 2 points) In the AdaBoost algorithm, the weights on all the misclassified points will go up by the same multiplicative factor. □

3.2. (3 points) Provide a brief rationale for the following observation about AdaBoost. The weighted error of the k^{th} weak classifier (measured relative to the weights at the beginning of the k^{th} iteration) tends to increase as a function of the iteration k.

Consider a text classification problem, where documents are represented by binary (0/1) feature vectors $\phi = [\phi_1, \ldots, \phi_m]^T$; here ϕ_i indicates whether word i appears in the document. We define a set of weak classifiers, $h(\phi; \theta) = y\phi_i$, parameterized by $\theta = \{i, y\}$ (the choice of the component, $i \in \{1, \ldots, m\}$, and the class label, $y \in \{-1, 1\}$, that the component should be associated with). There are exactly $2m$ possible weak learners of this type.

We use this boosting algorithm for feature selection. The idea is to simply run the boosting algorithm and select the features or components in the order in which they were identified by the weak learners. We assume that the boosting algorithm finds the best available weak classifier at each iteration.

3.3. (T/F – 2 points) The boosting algorithm described here can select the exact same weak classifier more than once. □

3.4. (4 points) Is the ranking of features generated by the boosting algorithm likely to be more useful for a linear classifier than the ranking from simple mutual information calculations (estimates $\hat{I}(y; \phi_i)$). Briefly justify your answer.

Problem 4

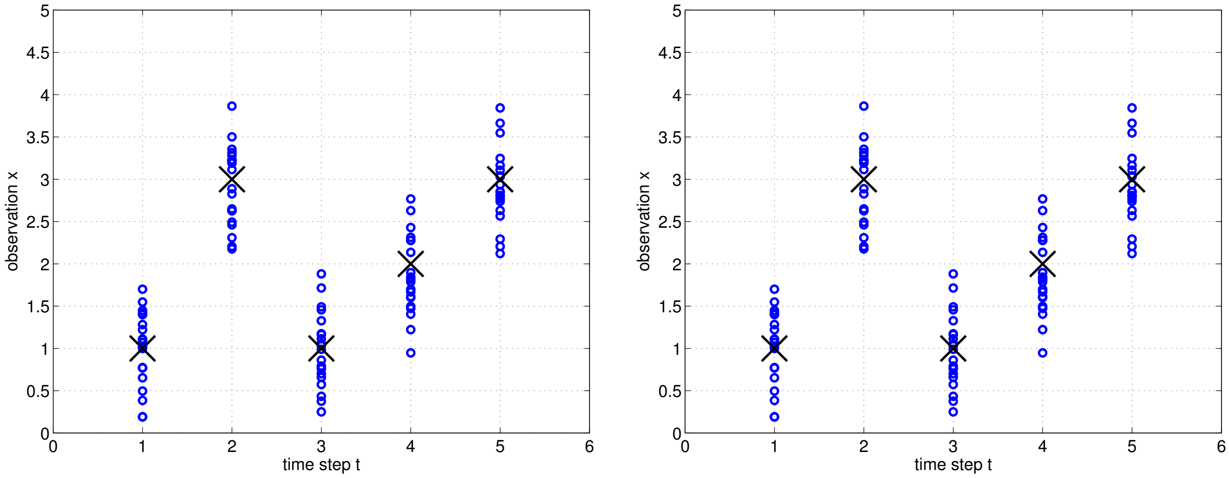


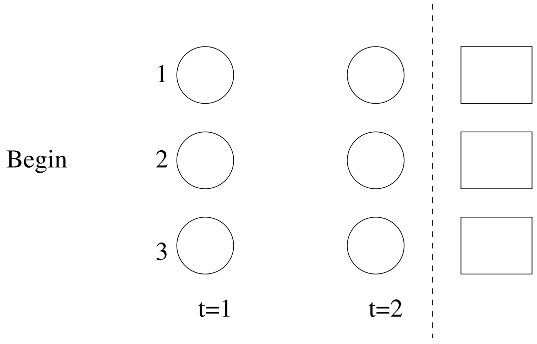
Figure 1a)

Figure 1b)

Figure 1: Time dependent observations. The data points in the figure are generated as sets of five consecutive time dependent observations, $x_1, \ldots, x_5$. The clusters come from repeatedly generating five consecutive samples. Each visible cluster consists of 20 points, and has approximately the same variance. The mean of each cluster is shown with a large X.

Consider the data in Figure 1 (see the caption for details). We begin by modeling this data with a three state HMM, where each state has a Gaussian output distribution with some mean and variance (means and variances can be set independently for each state).

4.1. (4 points) Draw the state transition diagram and the initial state distribution for a three state HMM that models the data in Figure 1 in the maximum likelihood sense. Indicate the possible transitions and their probabilities in the figure below (whether or not the state is reachable after the first two steps). In order words, your drawing should characterize the 1st order homogeneous Markov chain govering the evolution of the states. Also indicate the means of the corresponding Gaussian output distributions (please use the boxes).



4.2. **(4 points)** In Figure 1a draw as ovals the clusters of outputs that would form if we repeatedly generated samples from your HMM over time steps $t = 1, \ldots, 5$. The height of the ovals should reflect the variance of the clusters.

4.3. **(4 points)** Suppose at time $t = 2$ we observe $x_2 = 1.5$ but don't see the observations for other time points. What is the most likely state at $t = 2$ according to the marginal posterior probability $\gamma_2(s)$ defined as $P(s_2 = s|x_2 = 1.5)$.

4.4. **(2 points)** What would be the most likely state at $t = 2$ if we also saw $x_3 = 0$ at $t = 3$? In this case $\gamma_2(s) = P(s_2 = s|x_2 = 1.5, x_3 = 0)$.

4.5. **(4 points)** We can also try to model the data with conditional mixtures (mixtures of experts), where the conditioning is based on the time step. Suppose we only use two experts which are linear regression models with additive Gaussian noise, i.e.,

$$P(x|t, \theta_i) = \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left\{ -\frac{1}{2\sigma_i^2}(x - \theta_{i0} - \theta_{i1}t)^2 \right\}$$

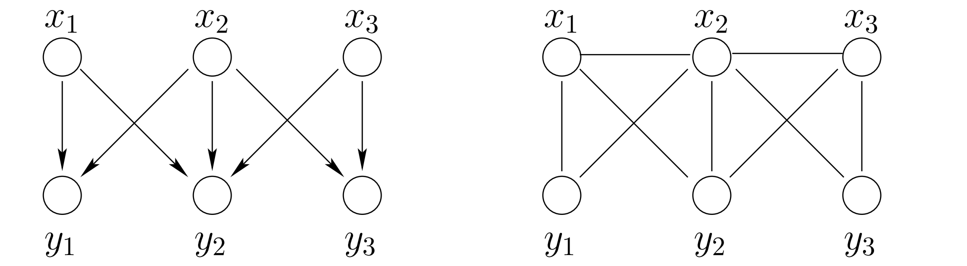
for $i = 1, 2$. The gating network is a logistic regression model from t to binary selection of the experts. Assuming your estimation of the conditional mixture model is successfully in the maximum likelihood sense, draw the resulting mean predictions of the two linear regression models as a function of time t in Figure 1b). Also, with a vertical line, indicate where the gating network would change it's preference from one expert to the other.

4.6. **(T/F – 2 points)** Claim: by repeatedly sampling from your conditional mixture model at successive time points $t = 1, 2, 3, 4, 5$, the resulting samples would resemble the data in Figure 1

.

4.7. **(4 points)** Having two competing models for the same data, the HMM and the mixture of experts model, we'd like to select the better one. We think that any reasonable model selection criterion would be able to select the better model in this case. Which model would we choose? Provide a brief justification.

Problem 5



a) Bayesian network (directed) b) Markov random field (undirected)

Figure 2: Graphical models

5.1. (2 points) List two different types of independence properties satisfied by the Bayesian network model in Figure 2a.

5.2. (2 points) Write the factorization of the joint distribution implied by the directed graph in Figure 2a.

5.3. (2 points) Provide an alternative factorization of the joint distribution, different from the previous one. Your factorization should be consistent with all the properties of the directed graph in Figure 2a. Consistency here means: whatever is implied by the graph should hold for the associated distribution.

5.4. (4 points) Provide an independence statement that holds for the undirected model in Figure 2b but does NOT hold for the Bayesian network. Which edge(s) should we add to the undirected model so that it would be consistent with (wouldn't imply anything that is not true for) the Bayesian network?

5.5. (2 points) Is your resulting undirected graph triangulated (Y/N)?

5.6. (4 points) Provide two directed graphs representing 1) a mixture of two experts model for classification, and 2) a mixture of Gaussians classifiers with two mixture components per class. Please use the following notation: $\mathbf{x}$ for the input observation, y for the class, and i for any selection of components.

Additional set of figures

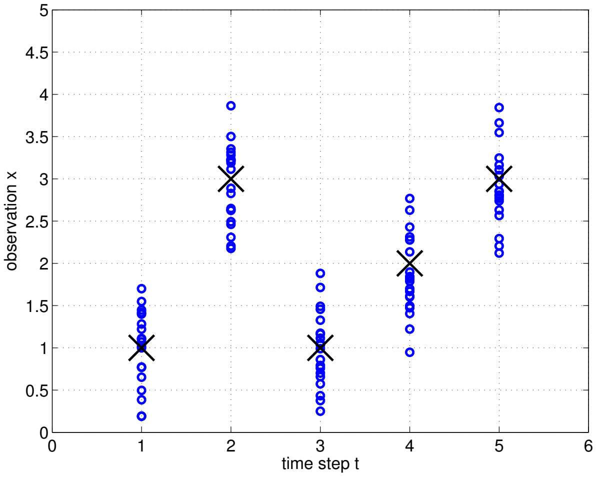


Figure 1a)

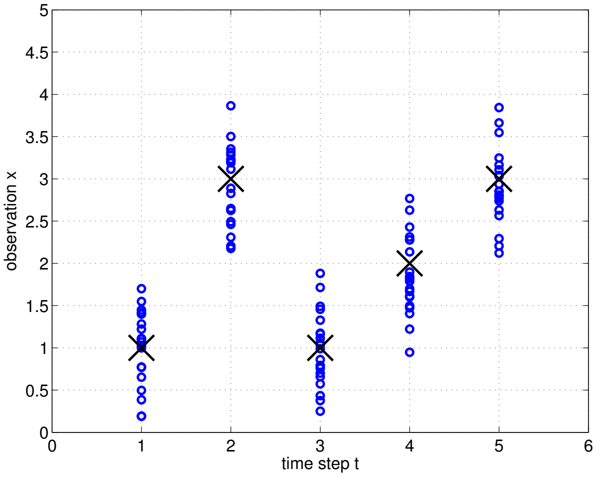
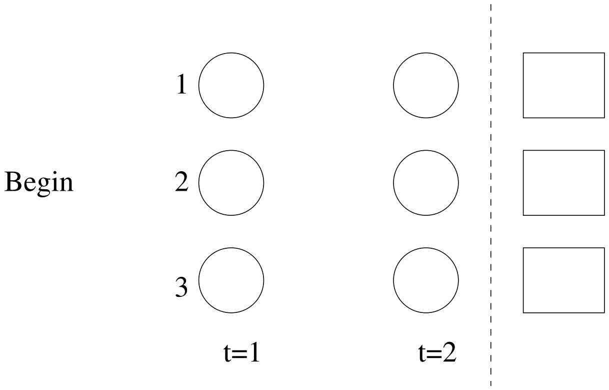
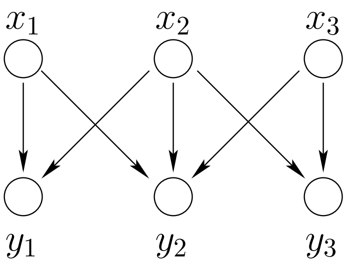
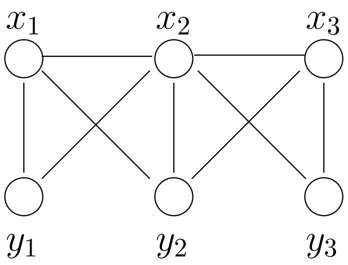


Figure 1b)





a) Bayesian network (directed)



b) Markov random field (undirected)

6.867 Machine learning

Final exam

December 5, 2002

(2 points) Your name and MIT ID:

(4 points) The grade you would give to yourself + a brief justification:

Problem 1

We wish to estimate a mixture of two experts model for the data displayed in Figure 1. The experts we can use here are linear regression models of the form

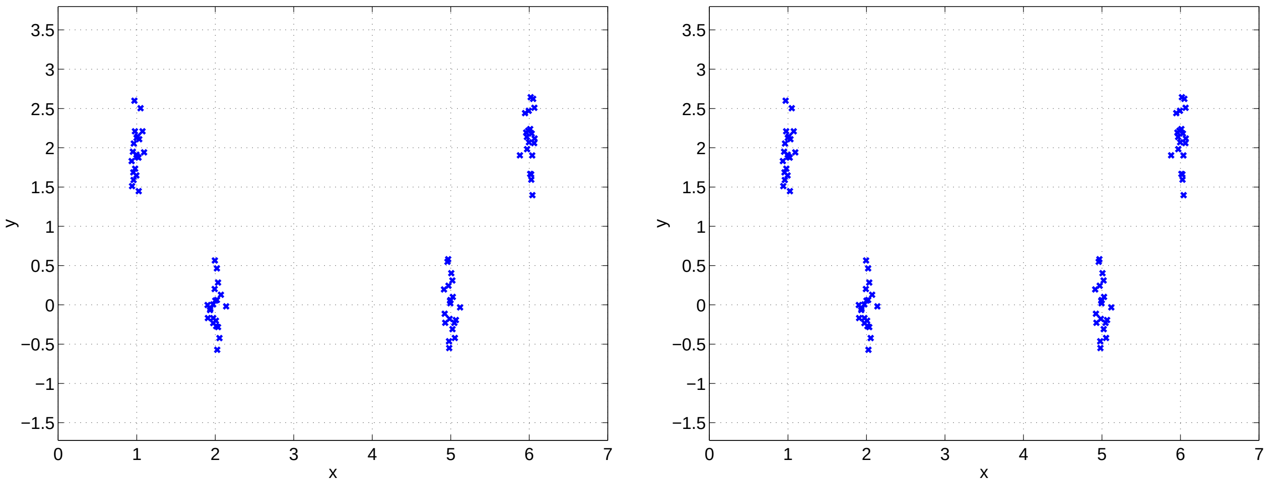
$$p(y|x, \mathbf{w}) = N(\,y;\, w_1 x + w_0,\, \sigma^2\,)$$

where $N(y; \mu, \sigma^2)$ denotes a Gaussian distribution over y with mean μ and variance σ^2. Each expert i can choose its parameters $\mathbf{w}_i = [w_{i0}, w_{i1}]^T$ and σ_i^2 independently from other experts. Note that the first subindex i in w_{ij} refers to the expert.

The gating network in the case of two experts is given by a logistic regression model

$$P(\text{expert} = 1|x, \mathbf{v}) = g(\,v_1 x + v_0\,)$$

where $g(z) = (1 + \exp(-z))^{-1}$ and $\mathbf{v} = [v_0, v_1]^T$.



a) unregularized case

b) regularized case

Figure 1: Data for mixtures of experts

1. **(4 points)** Suppose we estimate a mixture of two experts model based on the data in Figure 1. You can assume that the estimation is successful in the sense that we will find a setting of the parameters that maximizes the log-likelihood of the data. Please indicate (approximately) in Figure 1a) the mean predictions from the two experts as well as the decision boundary for the gating network. Label the mean predictions – functions of x – with "(1)" and "(2)" corresponding to the two experts, and the decision boundary with "gate".

2. **(4 points)** We now switch to a regularized maximum likelihood objective by incorporating the following regularization penalty

$$-\frac{c}{2}(w_{11}^2 + w_{21}^2)$$

into the log-likelihood objective. Note that the penalty includes only one parameter from each of the experts. By increasing c, we impose a stronger penalty. Similarly to the previous question, please indicate in Figure 1b) the optimal regularized solution for the mixture of two experts model when the regularization parameter c is set to a very large value.

3. **(3 points)** Are the variances in the predictive Gaussian distributions of the experts

( ) larger,

( ) smaller,

( ) about the same

after the regularization?

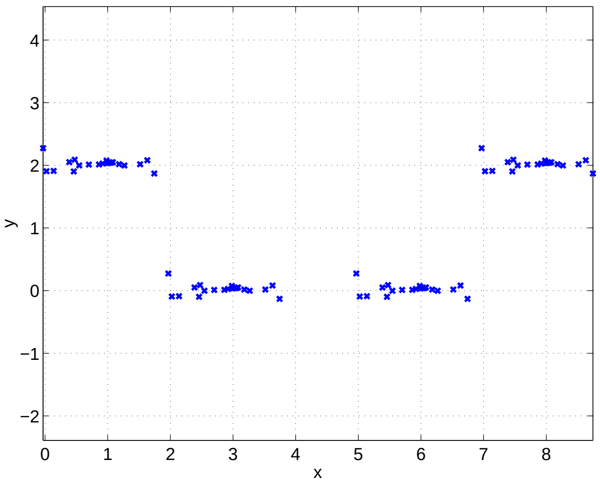


Figure 2: Different data for mixtures of experts

4. **(4 points)** Consider again the unregularized mixture of two experts. If we tried to estimate this model on the basis of the data in figure 2, what would the solution look like in this case? As before, indicate the solution in the figure. Briefly justify your answer.

s	1	2
P(x=1)	0	0.1
P(x=2)	0.199	0
P(x=3)	0.8	0.7
P(x=4)	0.001	0.2

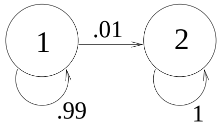


Figure 3: A two-state HMM for Problem 2

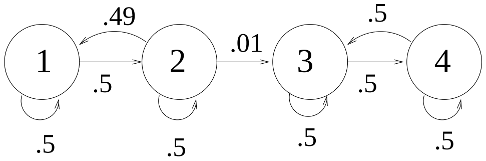


Figure 4: An alternative, four-state HMM for Problem 2

Problem 2

Figure 3 shows a two-state HMM. The transition probabilities of the Markov chain are given in the transition diagram. The output distribution corresponding to each state is defined over $\{1, 2, 3, 4\}$ and is given in the table next to the diagram. The HMM is equally likely to start from either of the two states.

1. **(3 points)** Give an example of an output sequence of length 2 which can not be generated by the HMM in Figure 3.
2. **(2 points)** We generated a sequence of $6,867^{2002}$ observations from the HMM, and found that the last observation in the sequence was 3. What is the most likely hidden state corresponding to that last observation?
3. **(2 points)** Consider an output sequence 3 3. What is the most likely sequence of hidden states corresponding to these observations?
4. **(2 points)** Now, consider an output sequence 3 3 4. What are *the first two states* of the most likely hidden state sequence?

5. **(4 points)** We can try to increase the modeling capacity of the HMM a bit by breaking each state into two states. Following this idea, we created the diagram in Figure 4. Can we set the initial state distribution and the output distributions so that this 4-state model, with the transition probabilities indicated in the diagram, would be equivalent to the original 2-state model? If yes, how? If no, why not?

6. **(T/F – 2 points)** The Markov chain in Figure 4 is ergodic □

Problem 3

Figure 5 shows a graphical model over four binary valued variables, $x_1, \ldots, x_4$. We do not know the parameters of the probability distribution associated with the graph.

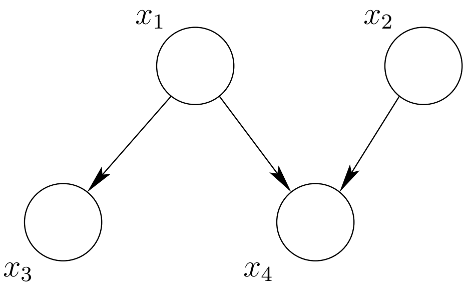


Figure 5: A graphical model

1. **(2 points)** Would it typically help to know the value of x_3 so as to gain more information about x_2? (please answer **yes** or **no**) □

2. **(2 points)** Assume we already know the value of x_4. Would it help in this case to know the value of x_3 to gain more information about x_2? (please answer **yes** or **no**) □

3. **(3 points)** List three different conditional independence statements between the four variables that can be inferred from the graph. You can include marginal independence by saying "given nothing".

   (a) ( ) is independent of ( ) given ( )

   (b) ( ) is independent of ( ) given ( )

   (c) ( ) is independent of ( ) given ( )

4. **(2 points)** The following table gives a possible partial specification of the conditional probability $P(x_4|x_1, x_2)$ associated with the graph. Fill in the missing values so that we could omit the arrow $x_1 \rightarrow x_4$ in the graph and the graph would still adequately represent the probability distribution.

$P(x_4 = 1 \mid x_1 = 0, x_2 = 0)$	0.8
$P(x_4 = 1 \mid x_1 = 0, x_2 = 1)$	0.4
$P(x_4 = 1 \mid x_1 = 1, x_2 = 0)$	
$P(x_4 = 1 \mid x_1 = 1, x_2 = 1)$	

5. **(4 points)** Let's again focus on the original graph in Figure 5. Since we don't know the underlying probability distribution, we need to estimate it from observed data. Unfortunately, the dataset we have is incomplete and contains only observations for x_2 and x_3. In other words, the dataset is $D = \{(x_2^t, x_3^t), t = 1, \ldots, n\}$. In the joint distribution

$$P(x_1, x_2, x_3, x_4) = P(x_1)P(x_2)P(x_3|x_1)P(x_4|x_1, x_2)$$

we have a number of components (smaller probability tables) that need to be estimated. Please indicate which components we can hope to estimate (adjust) on the basis of the available data?

( ) $P(x_1)$

( ) $P(x_2)$

( ) $P(x_3|x_1)$

( ) $P(x_4|x_1, x_2)$

6. **(4 points)** If we use the EM algorithm to carry out the estimation task, what posterior probabilities do we have to evaluate in the E-step? Please provide the necessary posterior probabilities in the form $P(\cdots|x_1^t, x_2^t)$.

Problem 4

We try to select here between two models. Both models are logistic regression models but differ in terms of the type of features that are used in making the predictions. More specifically, the models have the common squashed additive form

$$P(y=1|x,\mathbf{w}) = g(\, w_0 + w_1\phi_1(x) + \ldots + \phi_m(x)\,)$$

where the input is a real number $x \in \mathcal{R}$. The models differ in terms of the number and the type of basis functions used:

$$\begin{aligned} \text{model 1} &\;:\; m=1,\ \phi_1(x)=x \\ \text{model 2} &\;:\; m=2,\ \phi_1(x)=x,\ \phi_2(x)=\sin(x) \end{aligned}$$

1. **(1 points)** The VC-dimension of the set of classifiers corresponding to model 1 is □

2. **(1 points)** The VC-dimension of the set of classifiers corresponding to model 2 is □

3. **(4 points)** Suppose we have n training examples (x^t, y^t), $t = 1, \ldots, n$, and we evaluate structural risk minimization scores (bounds on the generalization error) for the two classifiers. Which of the following statements are valid in general for our two models:

   ( ) Score for model 1 $\geq$ Score for model 2

   ( ) Score for model 1 $\leq$ Score for model 2

   ( ) Score for model 1 $=$ Score for model 2

   ( ) Each of the above three cases may be correct depending on the data

   ( ) None of the above

4. **(4 points)** We will now switch to the Bayesian information criterion (BIC) for selecting among the two models. Let $L_1(n)$ be the log-probability of the labels that model 1 assigns to n training labels, where the probabilities are evaluated at the maximum likelihood setting of the parameters. Let $L_2(n)$ be the corresponding log-probability for model 2. We imagine here that $L_1(n)$ and $L_2(n)$ are evaluated on the basis of the first n training examples from a much larger set.

   Now, in our empirical studies, we found that these log-probabilities are related in a simple way:

   $$L_2(n) - L_1(n) \approx 0.01 \cdot n$$

   How will we end up selecting between the two models as a function of the number of training examples? Please choose one of the following cases.

   ( ) Always select 1

   ( ) Always select 2

   ( ) First select 1, then 2 for larger n

   ( ) First select 2, then 1 for larger n

5. **(4 points)** Provide a brief justification for your answer to the previous question.

Problem 5

Consider a simple two-class document (text) classification problem. Each document is represented by a binary feature vector $[\phi_1^i, \ldots, \phi_N^i]$, where $\phi_k^i = 1$ if keyword k is present in the document, and zero otherwise. N is the number of keywords we have chosen to include.

We use a Naive Bayes model for this classification task. The joint distribution of the features and the binary labels $y \in \{0, 1\}$ is in this case given by

$$P(\phi_1, \ldots, \phi_N, y) = P(y) \prod_{k=1}^{N} P(\phi_k | y)$$

where, for example,

$$P(\phi_k = 1 | y = 0) = \theta_{k,0}, \;\; P(\phi_k = 1 | y = 1) = \theta_{k,1}$$

1. **(2 points)** In the space below, draw the graphical model corresponding to Naive Bayes generative model described above. Assume that $N = 3$ (three keywords).

2. **(4 points)** To be able to make use of training examples with possibly missing labels, we will have to resort to the EM algorithm. In the EM algorithm we need to evaluate the posterior probability of the label y given the document. We will use a message passing algorithm (belief propagation) to get this posterior probability. The problem here is that we relied on a rather careless friend to evaluate whether a document contains any of the keywords. In other words, we do not fully trust the "observed" values of the features. Let $\hat{\phi}_k$ be the "observed" value for the k^{th} feature in a given document. The evidence we now have about the actual value of ϕ_k is given by $P(\hat{\phi}_k | \phi_k)$, which is a table that models how we expect the friend to respond.

   Given that we observe $\hat{\phi}_k = 1$, what is the message that ϕ_k needs to send to y?

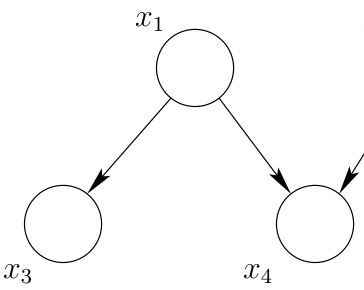
3. **(3 points)** We know that the EM algorithm is in some sense monotonic. Let $\hat{\theta}_{k,y}^{(t)}$ be the estimate of the parameters $\theta_{k,y}$ in the beginning of iteration t of the EM algorithm, and $\theta^{(t)}$ be the vector of all parameter estimates in that iteration, $[\hat{\theta}_{1,0}^{(t)}, \hat{\theta}_{1,1}^{(t)}, \ldots, \hat{\theta}_{N,y=1}^{(t)}]$. Which of the following quantities increases monotonically with t?

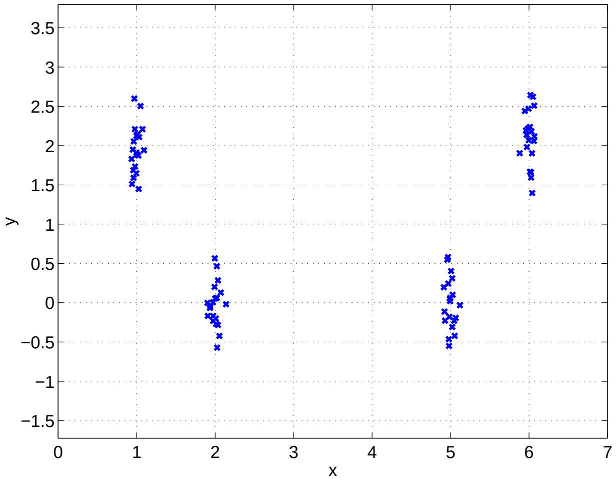
( ) $P(\phi_k = 1|y, \theta_{k,y}^{(t)})$ for all k
( ) $\prod_{i=1}^{N} P(\phi_1^i, \ldots, \phi_N^i|\theta^{(t)})$
( ) $\prod_{i=1}^{N} P(y_i = 1|\phi_1^i, \ldots, \phi_N^i, \theta^{(t)})$

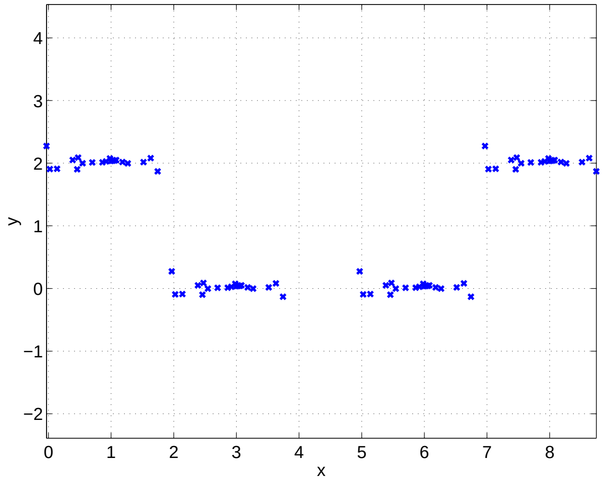
4. **(4 points)** The class labels actually correspond to "relevant" and "irrelevant" documents. In classifying any document as relevant or irrelevant, we have to take into account that we might prefer to miss a few relevant documents if we can avoid misclassifying a large number of irrelevant documents as relevant. To express such a preference we define a utility $U(y, \hat{y})$, where y is the correct label and $\hat{y}$ is how we classify the document. Draw an influence diagram that incorporates the Naive Bayes model, our decisions, and the utility. Mark each node in the graph according to the variables (or utility) that they represent.

5. **(2 points)** Let's modify the Naive Bayes model a bit, to account for some of the possible dependencies between the keywords. For example, suppose we order the keywords so that it would be useful to model the dependency of ϕ_k on ϕ_{k-1}, $k = 2, \ldots, N$ (the keywords may, for example, represent nested categories). We expect these dependencies to be the same for each class, but the parameters can be affected by the class label. Draw the graphical model for this – call it *Sophisticated Bayes* – model. Please assume again that $N = 3$.

Additional set of figures







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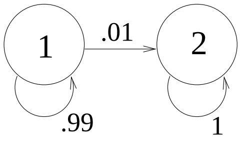
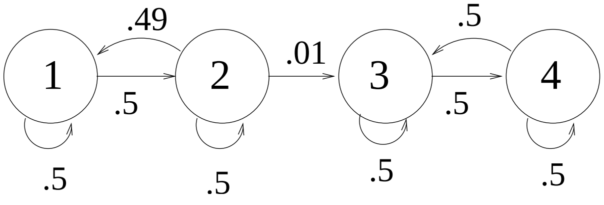




6.867 Machine learning and neural networks

FALL 2001 – Final exam

December 11, 2001

(2 points) Your name and MIT ID #:

(4 points) The grade you would give to yourself + brief justification. If you feel that there's no question that your grade should be A (and you feel we agree with you) then just write "A".

Problem 1

1. **(T/F – 2 points)** The sequence of output symbols sampled from a hidden Markov model satisfies the first order Markov property □

2. **(T/F – 2 points)** Increasing the number of values for the the hidden states in an HMM has much greater effect on the computational cost of forward-backward algorithm than increasing the length of the observation sequence. □

3. **(T/F – 2 points)** In HMMs, if there are at least two distinct most likely hidden state sequences and the two state sequences cross in the middle (share a single state at an intermediate time point), then there are at least four most likely state sequences. □

4. **(T/F – 2 points)** One advantage of Boosting is that it does not overfit. □

5. **(T/F – 2 points)** Support vector machines are resistant to outliers, i.e., very noisy examples drawn from a different distribution. □

6. **(T/F – 2 points)** Active learning can substantially reduce the number of training examples that we need. □

Problem 2

Consider two classifiers: 1) an SVM with a quadratic (second order polynomial) kernel function and 2) an unconstrained mixture of two Gaussians model, one Gaussian per class label. These classifiers try to map examples in $\mathcal{R}^2$ to binary labels. We assume that the problem is separable, no slack penalties are added to the SVM classifier, and that we have sufficiently many training examples to estimate the covariance matrices of the two Gaussian components.

1. **(T/F – 2 points)** The two classifiers have the same VC-dimension. □

2. **(4 points)** Suppose we evaluated the structural risk minimization score for the two classifiers. The score is the bound on the expected loss of the classifier, when the classifier is estimated on the basis of n training examples. Which of the two classifiers might yield the better (lower) score? Provide a brief justification.

3. **(4 points)** Suppose now that we regularize the estimation of the covariance matrices for the mixture of two Gaussians. In other words, we would estimate each class conditional covariance matrix according to

$$\hat{\Sigma}_{reg} = \frac{n}{n+n'}\hat{\Sigma} + \frac{n'}{n+n'}S \tag{1}$$

where n is the number of training examples, $\hat{\Sigma}$ is the unregularized estimate of the covariance matrix (sample covariance matrix of the examples in one class), S is our prior covariance matrix (same for both classes), and n' the equivalent sample size that we can use to balance between the prior and the data.

In computing the VC-dimension of a classifier, we can choose the set of points that we try to "shatter". In particular, we can scale any k points by a large factor and use the resulting set of points for shattering. In light of this, would you expect our regularization to change the VC-dimension? Why or why not?

4. **(T/F – 2 points)** Regularization in the above sense would improve the structural risk minimization score for the mixture of two Gaussians. □

Problem 3

The problem here is to predict the identity of a person based on a single handwritten character. The observed characters (one of 'a', 'b', or 'c') are transformed into binary 8 by 8 pixel images. There are four different people we need to identify on the basis of such characters. To do this, we have a training set of about 200 examples, where each example consists of a binary 8x8 image and the identity of the person it belongs to. You can assume that the overall number of occurences of each person and each character in the training set is roughly balanced.

We would like to use a mixture of experts architecture to solve this problem.

1. **(2 points)** How might the experts be useful ? Suggest what task each expert might solve.

2. **(4 points)** Draw a graphical model that describes the mixture of experts architecture in this context. Indicate what the variables are and the number of values that they can take. Shade any nodes corresponding to variables that are always observed.

3. **(4 points)** Before implementing the mixture of experts architecture, we need to know the parametric form of the conditional probabilities in your graphical model. Provide a *reasonable* specification of the relevant conditional probabilities to the extent that you could ask your class-mate to implement the classifier.

4. **(4 points)** So we implemented your method, ran the estimation algorithm once, and measured the test performance. The method was unfortunately performing at a chance level. Provide *two* possible explanations for this. (there may be multiple correct answers here)

5. **(3 points)** Would we get anything reasonable out of the estimation if, initially, all the experts were identical while the parameters of the gating network would be chosen randomly? By reasonable we mean training performance. Provide a brief justification.

6. **(3 points)** Would we get anything reasonable out the estimation if now the gating network is initially set so that it assigns each training example uniformly to all experts but the experts themselves are initialized with random parameter values? Again, reasonable refers to the training error. Provide a brief justification.

Problem 4

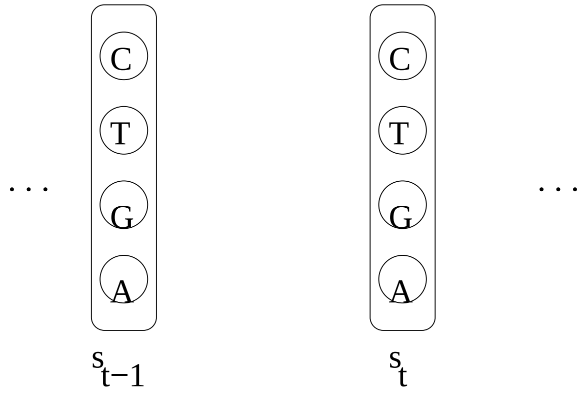
Consider the following pair of observed sequences:

Sequence 1 (s_t): `A A T T G G C C  A A T T G G C C  ...`
Sequence 2 (x_t): `1 1 2 2 1 1 2 2  1 1 2 2 1 1 2 2  ...`

Position t: `0 1 2 3 4 ...`

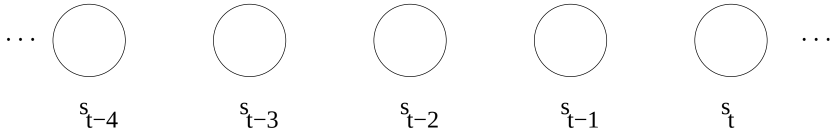
where we assume that the pattern (highlighted with the spaces) will continue forever. Let $s_t \in \{A, G, T, C\}$, $t = 0, 1, 2, \ldots$ denote the variables associated with the first sequence, and $x_t \in \{1, 2\}$, $t = 0, 1, 2, \ldots$ the variables characterizing the second sequence. So, for example, given the sequences above, the observed values for these variables are $s_0 = A, s_1 = A, s_2 = C, \ldots$, and, similarly, $x_0 = 1, x_1 = 1, x_2 = 2, \ldots$.

1. **(4 points)** If we use a simple first order homogeneous markov model to predict the first sequence (values for s_t only), what is the maximum likelihood solution that we would find? In the *transition diagram* below, please draw the relevant transitions and the associated probabilities (this should not require much calculation)

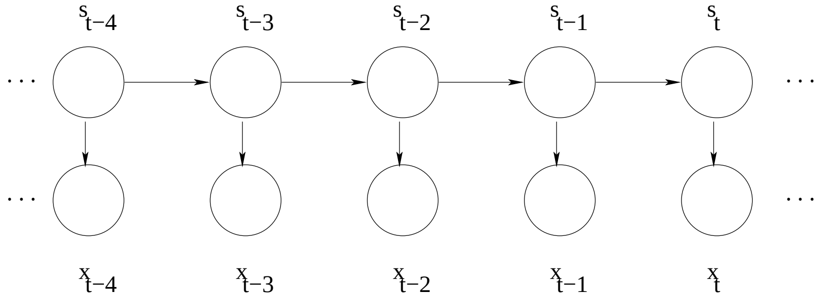


2. **(T/F – 2 points)** The resulting first order Markov model is *ergodic* □

3. **(4 points)** To improve the Markov model a bit we would like to define a graphical model that predicts the value of s_t on the basis of the previous observed values $s_{t-1}, s_{t-2}, \ldots$ (looking as far back as needed). The model parameters/structure are assumed to remain the same if we shift the model one step. In other words, it is the same graphical model that predicts s_t on the basis of $s_{t-1}, s_{t-2}, \ldots$ as the model that predicts s_{t-1} on the basis of $s_{t-2}, s_{t-3}, \ldots$. In the graph below, draw the *minimum number of arrows* that are needed to predict the first observed sequence perfectly (disregarding the first few symbols in the sequence). Since we slide the model along the sequence, you can draw the arrows only for s_t.



4. Now, to incorporate the second observation sequence, we will use a standard hidden Markov model:



where again $s_t \in \{A, G, T, C\}$ and $x_t \in \{1, 2\}$. We will estimate the parameters of this HMM in two different ways.

(I) Treat the pair of observed sequences (s_t, x_t) (given above) as complete observations of the variables in the model and estimate the parameters in the maximum likelihood sense. The initial state distribution $P_0(s_0)$ is set according to the overall frequency of symbols in the first observed sequence (uniform).

(II) Use only the second observed sequence (x_t) in estimating the parameters, again in the maximum likelihood sense. The initial state distribution is again uniform across the four symbols.

We assume that both estimation processes will be successfull relative to their criteria.

a) **(3 points)** What are the observation probabilities $P(x|s)$ ($x \in \{1,2\}$, $s \in \{A,G,T,C\}$) resulting from the first estimation approach? (should not require much calculation)

b) **(3 points)** Which estimation approach is likely to yield a more accurate model over the second observed sequence (x_t)? Briefly explain why.

5. Consider now the two HMMs resulting from using each of the estimation approaches (approaches I and II above). These HMMs are estimated on the basis of the pair of observed sequences given above. We'd like to evaluate the probability that these two models assign to a new (different) observation sequence `1 2 1 2`, i.e., $x_0 = 1, x_1 = 2, x_2 = 1, x_3 = 2$. For the first model, for which we have some idea about what the s_t variables will capture, we also want to know the the associated most likely hidden state sequence. (these should not require much calculation)

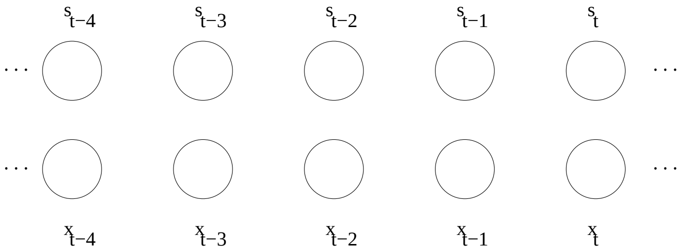
   a) **(2 points)** What is the probability that the first model (approach I) assigns to this new sequence of observations?

   b) **(2 points)** What is the probability that the second model (approach II) gives to the new sequence of observations?

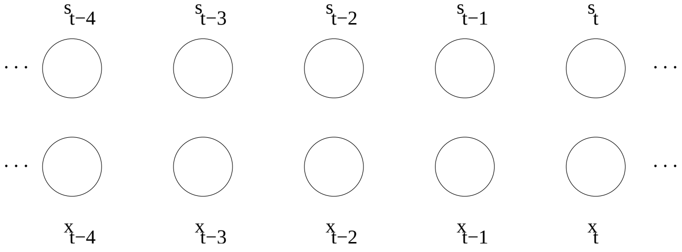
c) **(2 points)** What is the most likely hidden state sequence in the first model (from approach I) associated with the new observed sequence?

6. **(4 points)** Finally, let's assume that we observe only the second sequence (x_t) (the same sequence as given above). In building a graphical model over this sequence we are no longer limiting ourselves to HMMs. However, we only consider models whose structure/parameters remain the same as we slide along the sequence. The variables s_t are included as before as they might come handy as hidden variables in predicting the observed sequence.

a) In the figure below, draw the arrows that any reasonable model selection criterion would find given an unlimited supply of the observed sequence $x_t, x_{t+1}, \ldots$. You only need to draw the arrows for the last pair of variables in the graphs, i.e., (s_t, x_t)).



b) Given only a small number of obervations, the model selection criterion might select a different model. In the figure below, indicate a possible alternate model that any reasonable model selection criterion would find given only a few examples. You only need to draw the arrows for the last pair of variables in the graphs, i.e., (s_t, x_t)).



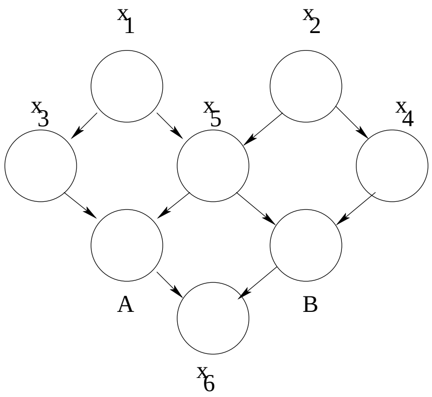


Figure 1: Decision makers A and B and their "context"

Problem 5

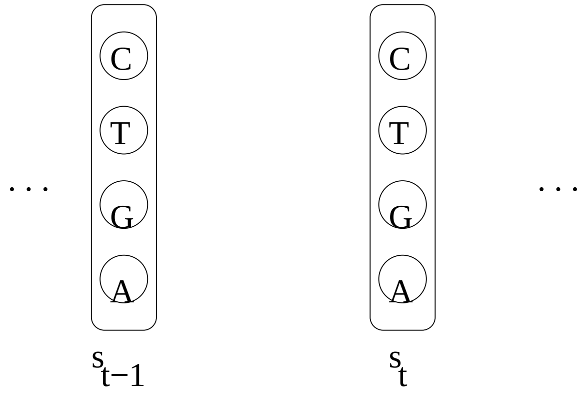
The Bayesian network in figure 1 claims to model how two people, call them A and B, make decisions in different contexts. The context is specified by the setting of the binary context variables $x_1, x_2, \ldots, x_6$. The values of these variables are not known unless we specifically ask for such values.

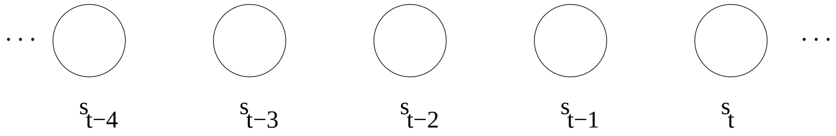
1. **(6 points)** We are interested in finding out what information we'd have to acquire to ensure that A and B will make their decisions independently from one another. Specify the *smallest set of context variables* whose instantiation would render A and B independent. Briefly explain your reasoning (there may be more than one strategy for arriving at the same decision)

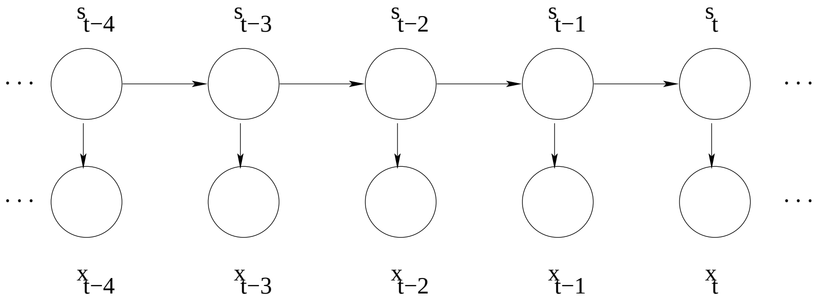
2. **(T/F – 2 points)** We can in general achieve independence with less information, i.e., we don't have to fully instantiate the selected context variables but provide some evidence about their values □

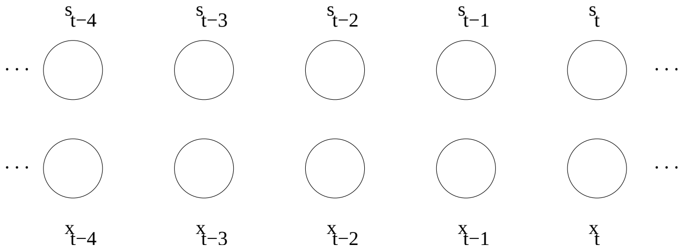
3. **(4 points)** Could your choice of the minimal set of context variables change if we also provided you with the actual probability values associated with the dependencies in the graph? Provide a brief justification.

Additional set of figures








s_{t-4}
s_{t-3}
s_{t-2}
s_{t-1}
s_t
...
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...
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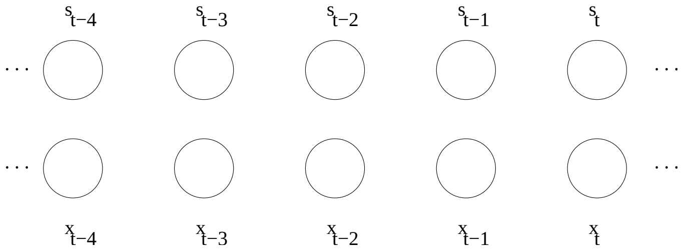
x_{t-4}
x_{t-3}
x_{t-2}
x_{t-1}
x_t


s_{t-4}
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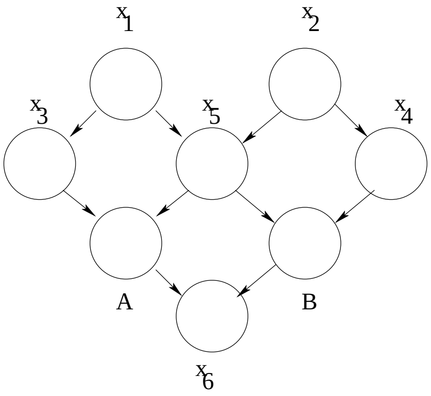

x_1
x_2
x_3
x_5
x_4
A
B
x_6

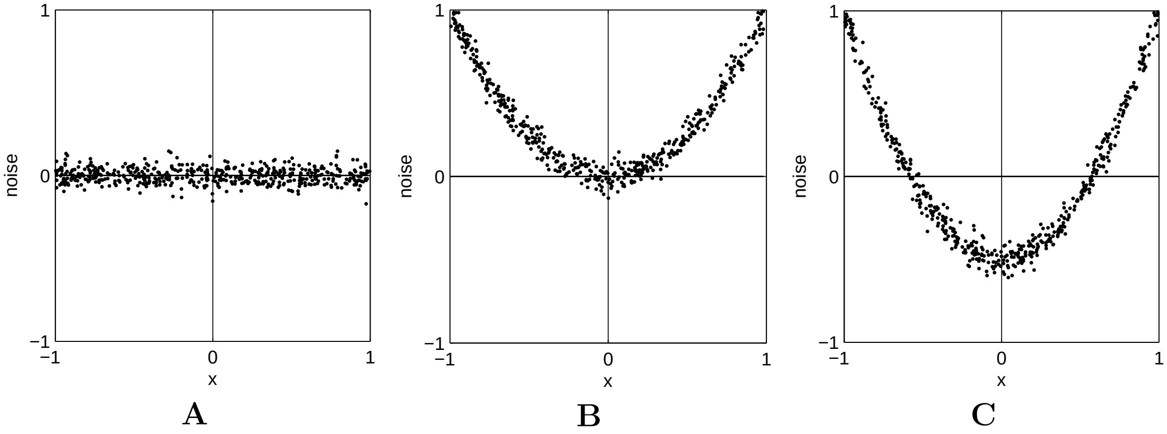
6.867 Machine learning

Mid-term exam

October 13, 2004

(2 points) Your name and MIT ID:

Problem 1



1. **(6 points)** Each plot above claims to represent prediction errors as a function of x for a trained regression model based on some dataset. Some of these plots could potentially be prediction errors for linear or quadratic regression models, while others couldn't. The regression models are trained with the least squares estimation criterion. Please indicate compatible models and plots.

	A	**B**	**C**
linear regression	( )	( )	( )
quadratic regression	( )	( )	( )

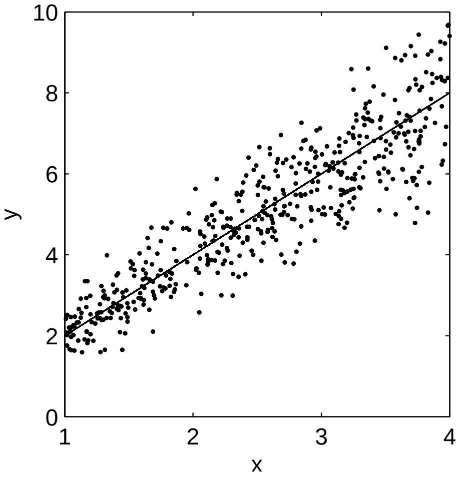
Problem 2

Here we explore a regression model where the noise variance is a function of the input (variance increases as a function of input). Specifically

$$y = wx + \epsilon$$

where the noise ϵ is normally distributed with mean 0 and standard deviation σx. The value of σ is assumed known and the input x is restricted to the interval $[1, 4]$. We can write the model more compactly as $y \sim N(wx, \sigma^2 x^2)$.

If we let x vary within $[1, 4]$ and sample outputs y from this model with some w, the regression plot might look like



1. **(2 points)** How is the ratio y/x distributed for a fixed (constant) x?

2. Suppose we now have n training points and targets $\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$, where each x_i is chosen at random from $[1, 4]$ and the corresponding y_i is subsequently sampled from $y_i \sim N(w^* x_i, \sigma^2 x_i^2)$ with some true underlying parameter value w^*; the value of σ^2 is the same as in our model.

(a) **(3 points)** What is the maximum-likelihood estimate of w as a function of the training data?

(b) **(3 points)** What is the variance of this estimator due to the noise in the target outputs as a function of n and σ^2 for fixed inputs $x_1, \ldots, x_n$? For later utility (if you omit this answer) you can denote the answer as $V(n, \sigma^2)$.

Some potentially useful relations: if $z \sim N(\mu, \sigma^2)$, then $az \sim N(a\mu, \sigma^2 a^2)$ for a fixed a. If $z_1 \sim N(\mu_1, \sigma_1^2)$ and $z_2 \sim N(\mu_2, \sigma_2^2)$ and they are independent, then $\text{Var}(z_1 + z_2) = \sigma_1^2 + \sigma_2^2$.

3. In sequential active learning we are free to choose the next training input x_{n+1}, here within $[1, 4]$, for which we will then receive the corresponding noisy target y_{n+1}, sampled from the underlying model. Suppose we already have $\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$ and are trying to figure out which x_{n+1} to select. The goal is to choose x_{n+1} so as to help minimize the variance of the predictions $f(x; \hat{w}_n) = \hat{w}_n x$, where $\hat{w}_n$ is the maximum likelihood estimate of the parameter w based on the first n training examples.

(a) **(2 points)** What is the variance of $f(x; \hat{w}_n)$ due to the noise in the training outputs as a function of x, n, and σ^2 given fixed (already chosen) inputs $x_1, \ldots, x_n$?

(b) **(2 points)** Which x_{n+1} would we choose (within $[1, 4]$) if we were to next select x with the maximum variance of $f(x; \hat{w}_n)$?

(c) **(T/F – 2 points)** Since the variance of $f(x; \hat{w}_n)$ only depends on x, n, and σ^2, we could equally well select the next point at random from $[1, 4]$ and obtain the same reduction in the maximum variance. □

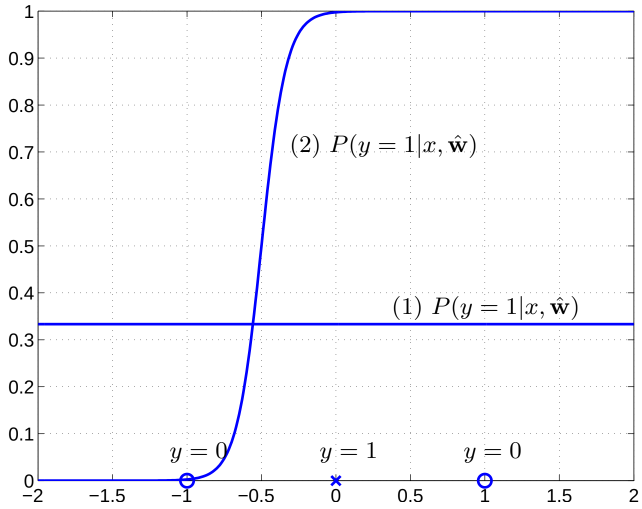


Figure 1: Two possible logistic regression solutions for the three labeled points.

Problem 3

Consider a simple one dimensional logistic regression model

$$P(y = 1|x, \mathbf{w}) = g(w_0 + w_1 x)$$

where $g(z) = (1 + \exp(-z))^{-1}$ is the logistic function.

1. Figure 3 shows two possible conditional distributions $P(y = 1|x, \mathbf{w})$, viewed as a function of x, that we can get by changing the parameters $\mathbf{w}$.

   (a) **(2 points)** Please indicate the number of classification errors for each conditional given the labeled examples in the same figure

   Conditional (1) makes (   ) classification errors
   Conditional (2) makes (   ) classification errors

   (b) **(3 points)** One of the conditionals in Figure 3 corresponds to the maximum likelihood setting of the parameters $\hat{\mathbf{w}}$ based on the labeled data in the figure. Which one is the ML solution (1 or 2)? □

   (c) **(2 points)** Would adding a regularization penalty $|w_1|^2/2$ to the log-likelihood estimation criterion affect your choice of solution (Y/N)? □

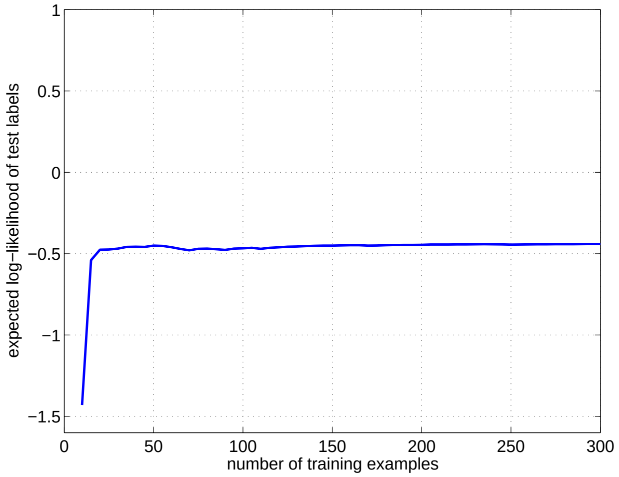


Figure 2: The expected log-likelihood of test labels as a function of the number of training examples.

2. **(4 points)** We can estimate the logistic regression parameters more accurately with more training data. Figure 2 shows the expected log-likelihood of test labels for a simple logistic regression model as a function of the number of training examples and labels. *Mark in the figure* the structural error (SE) and approximation error (AE), where "error" is measured in terms of log-likelihood.

3. **(T/F – 2 points)** In general for small training sets, we are likely to reduce the approximation error by adding a regularization penalty $|w_1|^2/2$ to the log-likelihood criterion. □

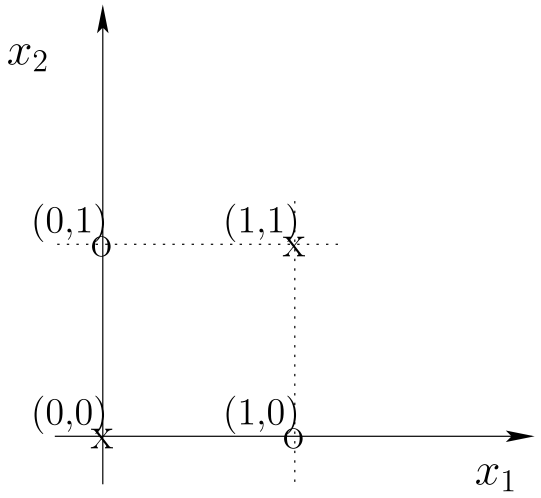


Figure 3: Equally likely input configurations in the training set

Problem 4

Here we will look at methods for selecting input features for a logistic regression model

$$P(y = 1|\mathbf{x}, \mathbf{w}) = g(w_0 + w_1x_1 + w_2x_2)$$

The available training examples are very simple, involving only binary valued inputs:

Number of copies	x_1	x_2	y
10	1	1	1
10	0	1	0
10	1	0	0
10	0	0	1

So, for example, there are 10 copies of $\mathbf{x} = [1, 1]^T$ in the training set, all labeled $y = 1$. The correct label is actually a deterministic function of the two features: $y = 1$ if $x_1 = x_2$ and zero otherwise.

We define greedy selection in this context as follows: we start with no features (train only with w_0) and successively try to add new features provided that each addition strictly improves the training log-likelihood. We use no other stopping criterion.

1. **(2 points)** Could greedy selection add either x_1 or x_2 in this case? Answer Y or N. □

2. **(2 points)** What is the classification error of the training examples that we could achieve by including both x_1 and x_2 in the logistic regression model? □

3. **(3 points)** Suppose we define another possible feature to include, a function of x_1 and x_2. Which of the following features, if any, would permit us to correctly classify all the training examples when used in combination with x_1 and x_2 in the logistic regression model:

( ) $x_1 - x_2$
( ) $x_1 x_2$
( ) x_2^2

4. **(2 points)** Could the greedy selection method choose this feature as the first feature to add when the available features are x_1, x_2 and your choice of the new feature? Answer Y or N. □

Problem 5

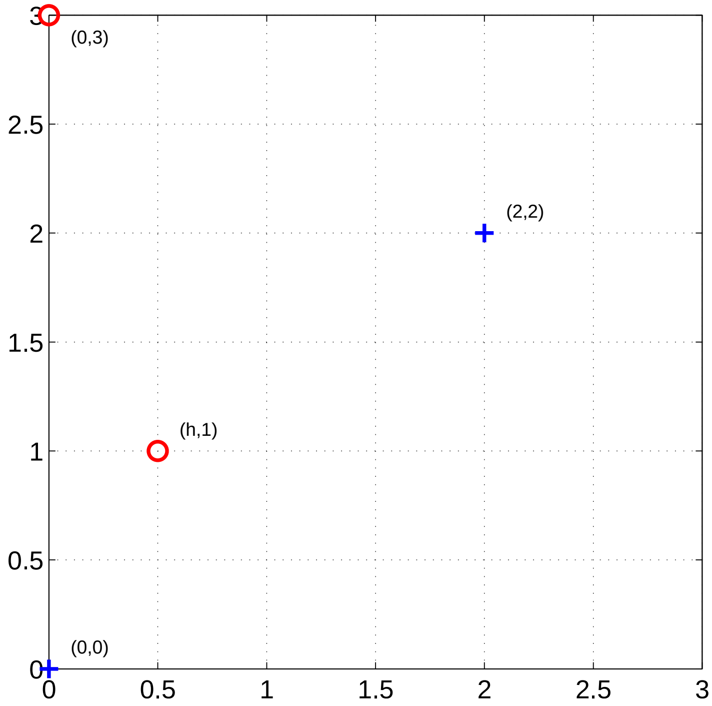


Figure 4: Labeled training examples

Suppose we only have four training examples in two dimensions (see Figure 4):

positive examples at $\mathbf{x}_1 = [0,0]^T, \mathbf{x}_2 = [2,2]^T$ and
negative examples at $\mathbf{x}_3 = [h,1]^T, \mathbf{x}_4 = [0,3]^T$.

where we treat $h \geq 0$ as a parameter.

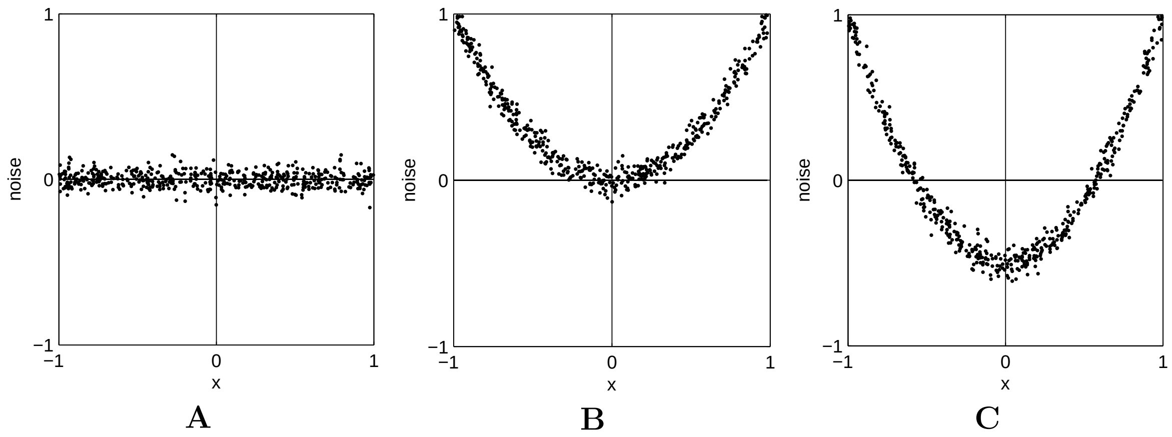
1. **(2 points)** How large can $h \geq 0$ be so that the training points are still linearly separable? □

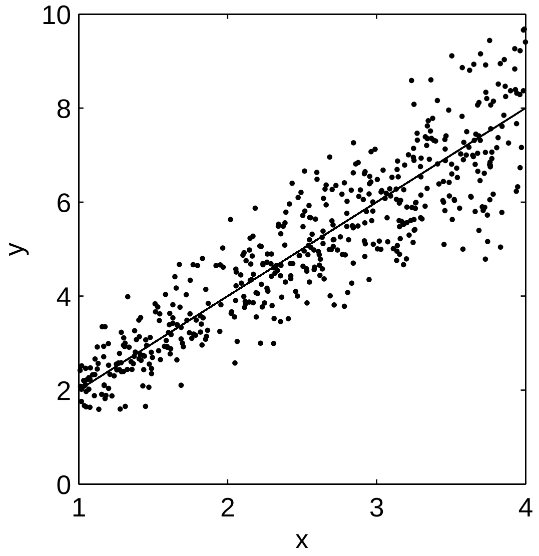
2. **(2 points)** Does the orientation of the maximum margin decision boundary change as a function of h when the points are separable? Answer Y or N. □

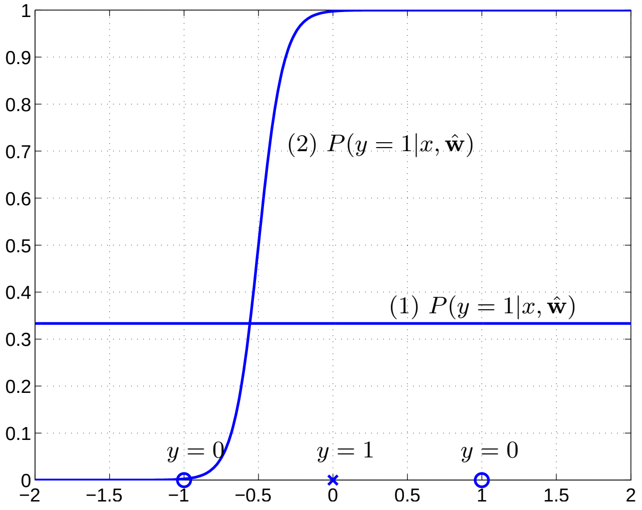
3. **(4 points)**What is the margin achieved by the maximum margin boundary as a function of h?

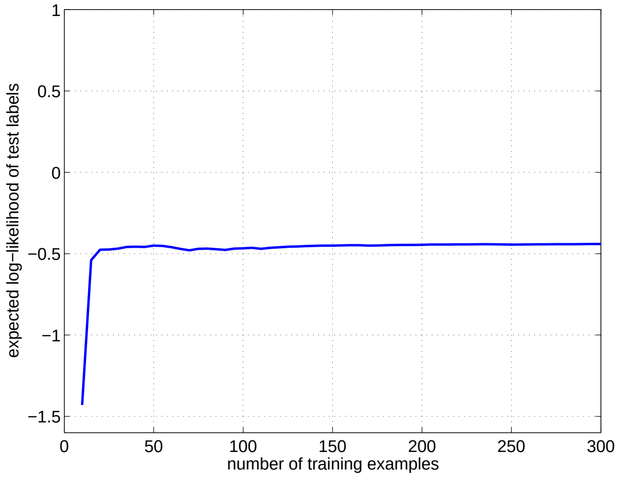
4. **(3 points)** Assume that $h = 1/2$ (as in the figure) and that we can only observe the x_2-component of the input vectors. Without the other component, the labeled training points reduce to $(0, y = 1)$, $(2, y = 1)$, $(1, y = -1)$, and $(3, y = -1)$. What is the lowest order p of polynomial kernel that would allow us to correctly classify these points?

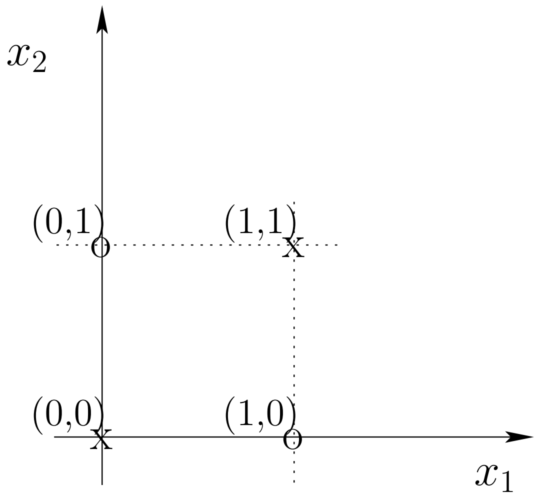
Additional set of figures

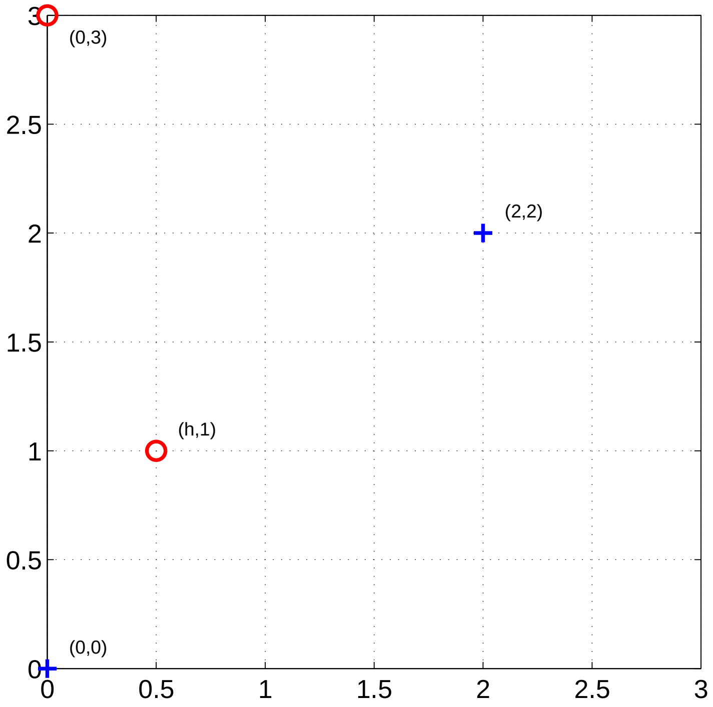







expected log−likelihood of test labels
1
0.5
0
−0.5
−1
−1.5
0
50
100
150
200
250
300
number of training examples


x_2
(0,1)
o
(1,1)
x
(0,0)
x
(1,0)
o
x_1


(0,3)
(2,2)
(h,1)
(0,0)
3
2.5
2
1.5
1
0.5
0
0
0.5
1
1.5
2
2.5
3

6.867 Machine learning

Mid-term exam

October 13, 2006

(2 points) Your name and MIT ID:

Problem 1

Suppose we are trying to solve an active learning problem, where the possible inputs you can select form a discrete set. Specifically, we have a set of N unlabeled documents, $\Phi_1, \ldots, \Phi_N$, where each document is represented as a binary feature fector

$$\Phi = [\phi_1, \ldots, \phi_m]^T$$

and $\phi_i = 1$ if word i appears in the document and zero otherwise. Our goal is to quickly label these N documents with 0/1 labels. We can request a label for any of the N documents, preferably as few as possible. We also have a small set of n already labeled documents to get us started.

We use a logistic regression model to solve the classification task:

$$P(y = 1|\Phi, \mathbf{w}) = g(\,\mathbf{w}^T\Phi\,)$$

where $g(\cdot)$ is the logistic function. Note that we do not include the bias term.

1. **(T/F – 2 points)** Any word that appears in all the N documents would effectively provide a bias term for the logistic regression model. □

2. **(T/F – 2 points)** Any word that appears only in the available n labeled documents used for initially training the logistic regression model, would serve equally well as a bias term. □

3. Having trained the logistic regression model on the basis of the n labeled documents, obtaining $\hat{\mathbf{w}}_n$, we'd like to request additional labeled documents. For this, we will use the following measure of uncertainty in our predictions:

$$E_{y\sim p_t}|y - p_t| = p_t|1 - p_t| + (1 - p_t)|0 - p_t| = 2p_t(1 - p_t)$$

where $p_t = P(y = 1|\Phi_t, \hat{\mathbf{w}}_n)$, our current prediction of the probability that $y = 1$ for the t^{th} unlabeled document Φ_t.

a) **(4 points)** We would request the label for the document/query point Φ_t that has

( ) the smallest value of $2p_t(1 - p_t)$
( ) the largest value of $2p_t(1 - p_t)$
( ) an intermediate value of $2p_t(1 - p_t)$

Briefly explain the rationale behind the selection criterion that you chose.

b) **(2 points)** Sketch $\hat{\mathbf{w}}_n$ in Figure 1.1. Write down the equation, expressed solely in terms of Φ and $\hat{\mathbf{w}}_n$, that Φ has to satisfy for it to lie exactly on the decision boundary:

c) **(4 points)** In figure 1.2, circle the next point we would select according to the criterion. Draw two decision boundaries that would result from incorporating the new point in the training set, labeling the boundaries as $y = 1$ and $y = 0$, depending on the outcome of the query.

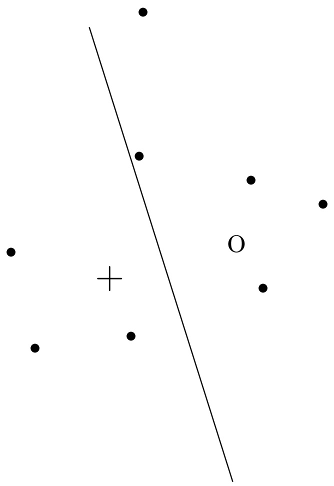


Figure 1.1. Two labeled points, unlabeled points, and the decision boundary. The point "+" corresponds to $y = 1$.

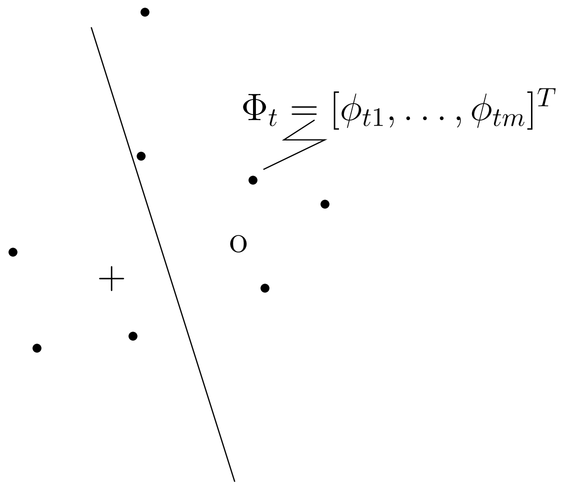


Figure 1.2. Two labeled points, unlabeled points, and the decision boundary. The point "+" corresponds to $y = 1$.

4. **(T/F – 2 points)** The criterion we have used here for active learning guarantees that the measure of uncertainty about the labels of the unlabeled points will decrease monotonically for each point after each query. □

Problem 2

Consider a regression problem where the two dimensional input points $\mathbf{x} = [x_1, x_2]^T$ are constrained to lie within the unit square: $x_i \in [-1, 1]$, $i = 1, 2$. The training and test input points $\mathbf{x}$ are sampled uniformly at random within the unit square. The target outputs y are governed by the following model

$$y \sim N(x_1^3 x_2^5 - 10x_1x_2 + 7x_1^2 + 5x_2 - 3,\ 1)$$

In other words, the outputs are normally distributed with mean given by

$$x_1^3 x_2^5 - 10x_1x_2 + 7x_1^2 + 5x_2 - 3$$

and variance 1.

We learn to predict y given $\mathbf{x}$ using linear regression models with 1st through 10th order polynomial features. The models are nested in the sense that the higher order models will include all the lower order features. The estimation criterion is the mean squared error.

We first train a 1st, 2nd, 8th, and 10th order model using $n = 20$ training points, and then test the predictions on a large number of independently sampled points.

1. **(6 points)** Select all the appropriate model(s) for each column. If you think the highest, or lowest, error would be shared among several models, be sure to list all models.

	Lowest training error	Highest training error	Lowest test error (typically)
1st order	( )	( )	
2nd order	( )	( )	( )
8th order	( )	( )	
10th order	( )	( )	( )

Briefly explain your selection in the last column, i.e., the model you would expect to have the lowest test error:

2. **(6 points)** We now train the polynomial regression models using $n = 10^6$ (one million) training points. Again select the appropriate model(s) for each column. If you think the highest, or lowest, error would be shared among several models, be sure to list all models.

	Lowest structural error	Highest approx. error	Lowest test error
1st order	( )	( )	( )
2nd order	( )	( )	( )
8th order	( )	( )	( )
10th order	( )	( )	( )

3. **(T/F – 2 points)** The approximation error of a polynomial regression model depends on the number of training points. □

4. **(T/F – 2 points)** The structural error of a polynomial regression model depends on the number of training points. □

Problem 3

We consider here linear and non-linear support vector machines (SVM) of the form:

$$\begin{aligned} \min\ w_1^2/2 \quad &\text{subject to} \quad y_i(w_1 x_i + w_0) - 1 \geq 0, \quad i = 1, \ldots, n, \quad \text{or} \\ \min\ \mathbf{w}^T\mathbf{w}/2 \quad &\text{subject to} \quad y_i(\mathbf{w}^T \Phi_i + w_0) - 1 \geq 0, \quad i = 1, \ldots, n \end{aligned}$$

where Φ_i is a feature vector constructed from the corresponding real valued input x_i. We wish to compare the simple linear SVM classifier $(w_1 x + w_0)$ and the non-linear classifier $(\mathbf{w}^T\Phi + w_0)$, where $\Phi = [x, x^2]^T$.

1. **(3 points)** Provide three input points x_1, x_2, and x_3 and their associated ± 1 labels such that they cannot be separated with the simple linear classifier, but are separable by the non-linear classifer with $\Phi = [x, x^2]^T$. You may find Figure 3.1. helpful in answering this question.

2. **(3 points)** In the figure below (Figure 3.1), mark your three points x_1, x_2, and x_3 as points in the feature space with their associated labels. Draw the *decision boundary* of the non-linear SVM classifier with $\Phi = [x, x^2]^T$ that separates the points.

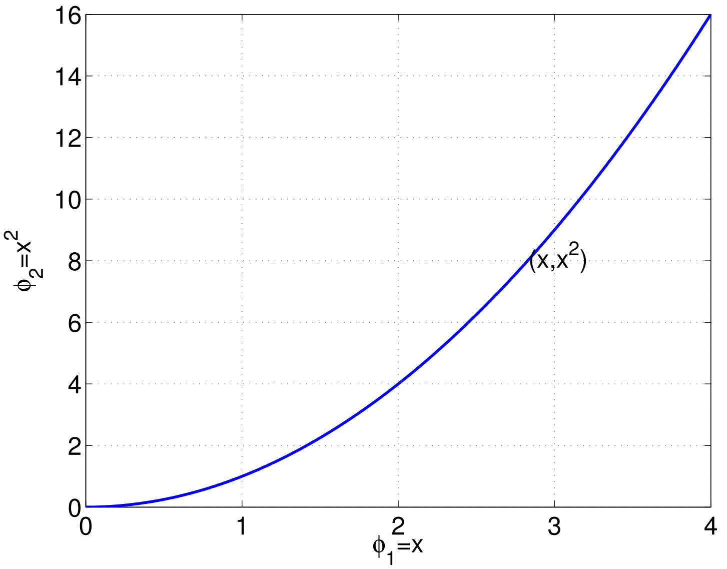


Figure 3.1. Feature space.

3. **(3 points)** Consider two labeled points $(x = 1, y = 1)$ and $(x = 3, y = -1)$. Is the margin we attain using feature vectors $\Phi = [x, x^2]^T$

   ( ) greater

   ( ) equal

   ( ) smaller

   than the margin resulting from using the input x directly?

4. **(2 points)** In general, is the margin we would attain using scaled feature vectors $\Phi = [2x, 2x^2]^T$

   ( ) greater

   ( ) equal

   ( ) smaller

   ( ) any of the above

   in comparison to the margin resulting from using $\Phi = [x, x^2]^T$?

5. **(T/F – 2 points)** The values of the margins obtained by two different kernels $K(x, x')$ and $\tilde{K}(x, x')$ on the same training set do not tells us which classifier will perform better on the test set. □

Problem 4

We consider here generative and discriminative approaches for solving the classification problem illustrated in Figure 4.1. Specifically, we will use a mixture of Gaussians model and regularized logistic regression models.

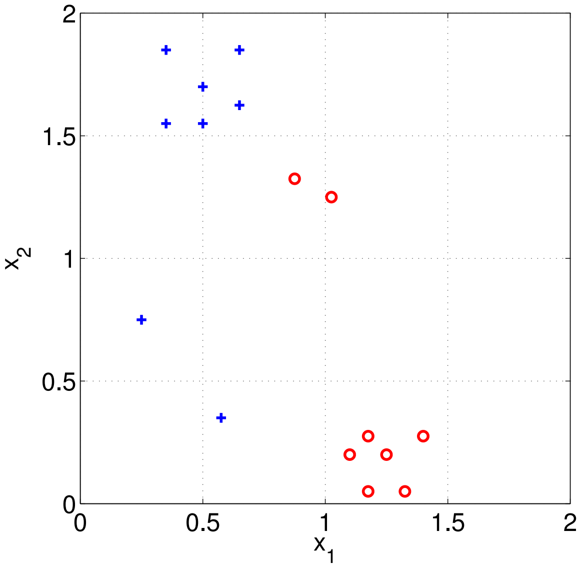


Figure 4.1. Labeled training set, where "+" corresponds to class $y = 1$.

1. We will first estimate a mixture of Gaussians model, one Gaussian per class, with the constraint that the covariance matrices are identity matrices. The mixing proportions (class frequencies) and the means of the two Gaussians are free parameters.

   a) **(3 points)** Plot the maximum likelihood estimates of the means of the two class conditional Gaussians in Figure 4.1. Mark the means as points "x" and label them "0" and "1" according to the class.

   b) **(2 points)** Draw the decision boundary in the same figure.

2. We have also trained regularized linear logistic regression models

$$P(y = 1|\mathbf{x}, \mathbf{w}) = g(w_0 + w_1 x_1 + w_2 x_2)$$

for the same data. The regularization penalties, used in penalized conditional log-likelihood estimation, were $-Cw_i^2$, where $i = 0, 1, 2$. In other words, only one of the parameters were regularized in each case. Based on the data in Figure 4.1, we generated three plots, one for each regularized parameter, of the number of misclassified training points as a function of C (Figure 4.2). The three plots are not identified with the corresponding parameters, however. Please assign the "top", "middle", and "bottom" plots to the correct parameter, w_0, w_1, or w_2, the parameter that was regularized in the plot. Provide a brief justification for each assignment.

- **(3 points)** "top" = ( )

- **(3 points)** "middle" = ( )

- **(3 points)** "bottom" = ( )

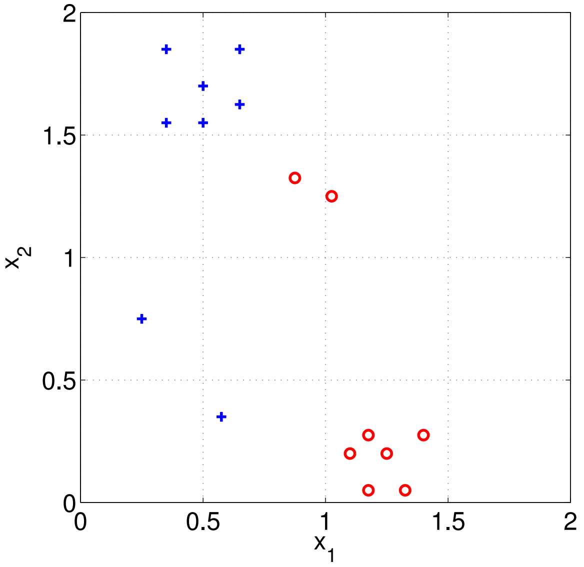


Figure 4.1 Labeled training set (reproduced here for clarity)

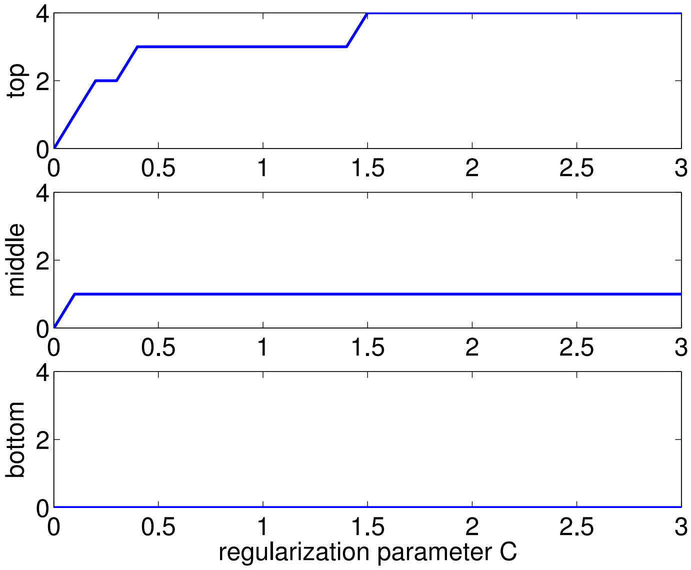


Figure 4.2. Training errors as a function of regularization penalty

Additional set of figures

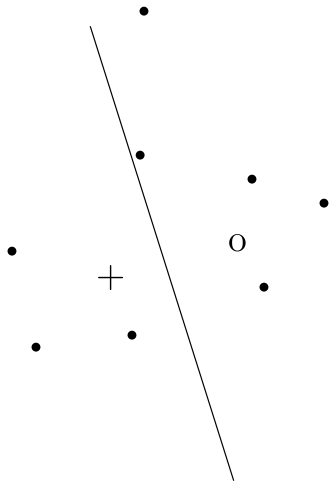


Figure 1.1. Two labeled points, unlabeled points, and the decision boundary. The point "+" corresponds to $y = 1$.

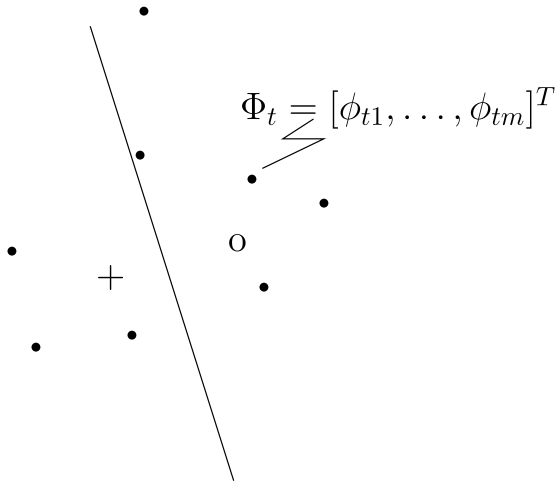


Figure 1.2. Two labeled points, unlabeled points, and the decision boundary. The point "+" corresponds to $y = 1$.

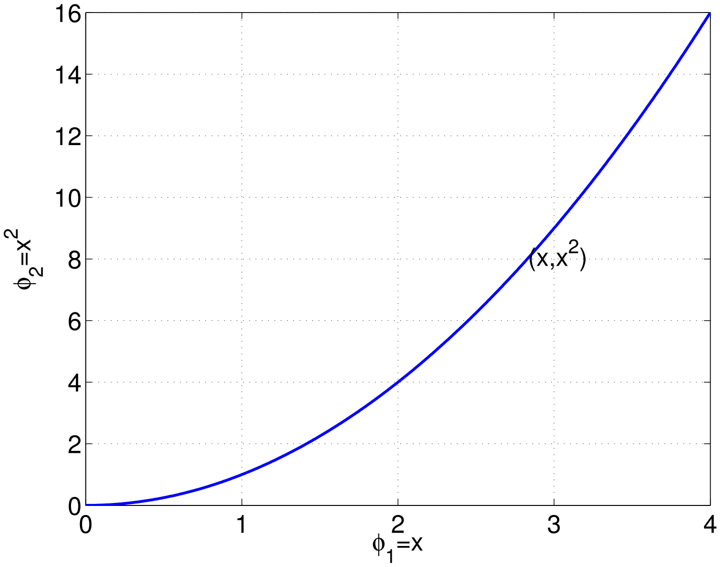


Figure 3.1. Feature space.

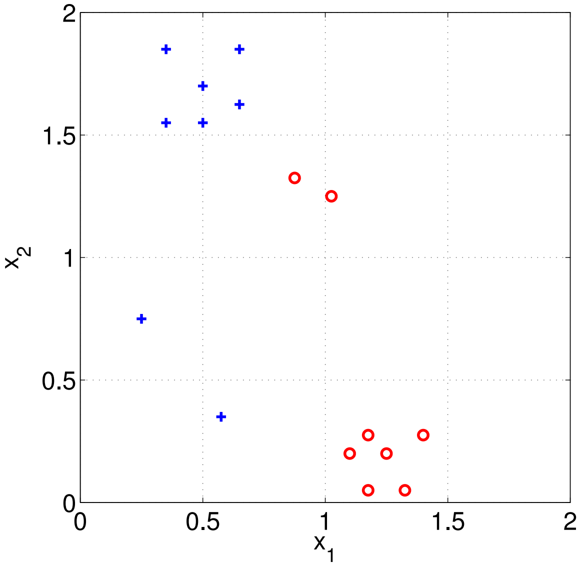


Figure 4.1. Labeled training set, where "+" corresponds to class $y = 1$.

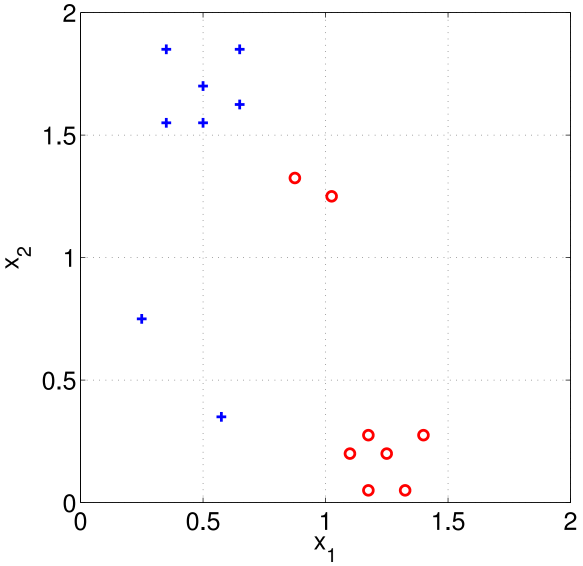


Figure 4.1 Labeled training set (reproduced here for clarity)

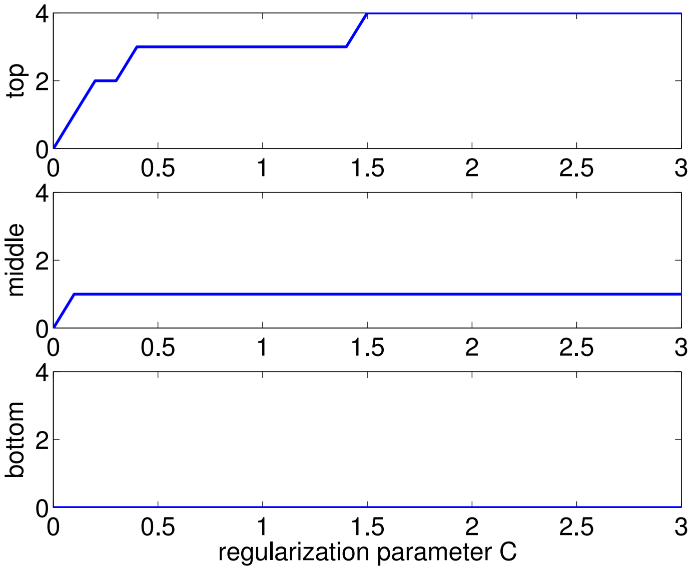


Figure 4.2. Training errors as a function of regularization penalty

6.867 Machine learning

Mid-term exam

October 8, 2003

(2 points) Your name and MIT ID:

Problem 1

We are interested here in a particular 1-dimensional linear regression problem. The dataset corresponding to this problem has n examples $(x_1, y_1), \ldots, (x_n, y_n)$, where x_i and y_i are real numbers for all i. Part of the difficulty here is that we don't have access to the inputs or outputs directly. We don't even know the number of examples in the dataset. We are, however, able to get a few numbers computed from the data.

Let $\mathbf{w}^* = [w_0^*, w_1^*]^T$ be the least squares solution we are after. In other words, $\mathbf{w}^*$ minimizes

$$J(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i)^2$$

You can assume for our purposes here that the solution is unique.

1. **(4 points)** Check each statement that must be true if $\mathbf{w}^* = [w_0^*, w_1^*]^T$ is indeed the least squares solution

   ( ) $(1/n) \sum_{i=1}^{n} (y_i - w_0^* - w_1^* x_i) y_i = 0$
   ( ) $(1/n) \sum_{i=1}^{n} (y_i - w_0^* - w_1^* x_i)(y_i - \bar{y}) = 0$
   ( ) $(1/n) \sum_{i=1}^{n} (y_i - w_0^* - w_1^* x_i)(x_i - \bar{x}) = 0$
   ( ) $(1/n) \sum_{i=1}^{n} (y_i - w_0^* - w_1^* x_i)(w_0^* + w_1^* x_i) = 0$

   where $\bar{x}$ and $\bar{y}$ are the sample means based on the same dataset.

2. **(4 points)** There are several numbers (statistics) computed from the data that we can use to infer $\mathbf{w}^*$. These are

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i, \quad \bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i, \quad C_{xx} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2$$
$$C_{xy} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y}), \quad C_{yy} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \bar{y})^2$$

   Suppose we only care about the value of w_1^*. We'd like to determine w_1^* on the basis of only two numbers (statistics) listed above. Which two numbers do we need for this?

3. Here we change the rules governing our access to the data. Instead of simply getting the statistics we want, we have to reconstruct these from examples that we query. There are two types of queries we can make. We can either request additional randomly chosen examples from the training set, or we can query the output corresponding to a specific input that we specify. (We assume that the dataset is large enough that there is always an example whose input x is close enough to our query).

   The active learning scenario here is somewhat different from the typical one. Normally we would assume that the data is governed by a linear model and choose the input points so as to best recover this assumed model. Here the task is to recover the best fitting linear model to the data but we make no assumptions about whether the linear model is appropriate in the first place.

   (2 points) Suppose in our case the input points are constrained to lie in the interval $[0, 1]$. If we followed the typical active learning approach, where we assume that the true model is linear, what are the input points we would query?

   (3 points) In the new setting, where we try to recover the best fitting linear model or parameters $\mathbf{w}^*$, we should (choose only one):

   ( ) Query inputs as you have answered above

   ( ) Draw inputs and corresponding outputs at random from the dataset

   ( ) Use another strategy since neither of the above choices would yield satisfactory results

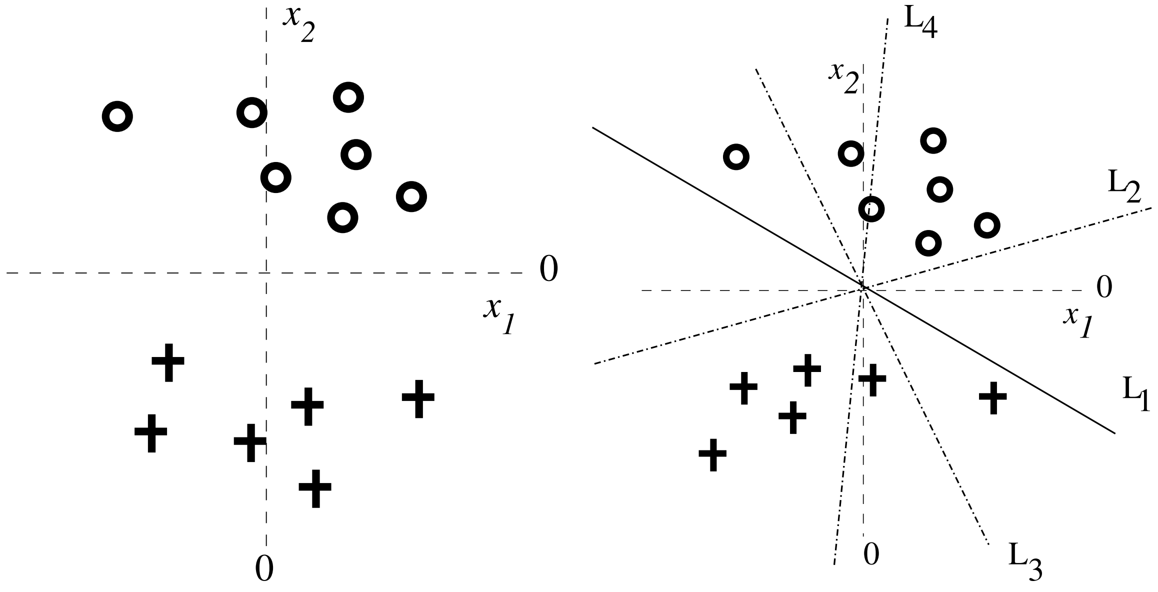
(4 points) Briefly justify your answer to the previous question

Problem 2

In this problem we will refer to the binary classification task depicted in Figure 1(a), which we attempt to solve with the simple linear logistic regression model

$$\hat{P}\left(y=1|\mathbf{x},w_1,w_2\right) = g(w_1x_1+w_2x_2) = \frac{1}{1+\exp(-w_1x_1-w_2x_2)}$$

(for simplicity we do not use the bias parameter w_0). The training data can be separated with zero training error - see line L_1 in Figure 1(b) for instance.



(a) The 2-dimensional data set used in Problem 1

(b) The points can be separated by L_1 (solid line). Possible other decision boundaries are shown by L_2, L_3, L_4.

1. **(6 points)** Consider a regularization approach where we try to maximize

$$\sum_{i=1}^{n} \log p(y_i|\mathbf{x}_i, w_1, w_2) - \frac{C}{2} w_2^2$$

for large C. Note that **only** w_2 is penalized. We'd like to know which of the four lines in Figure 1(b) could arise as a result of such regularization. For each potential line L_2, L_3 or L_4 determine whether it can result from regularizing w_2. If not, explain very briefly why not.

- $L2$

- $L3$

- $L4$

2. **(4 points)**If we change the form of regularization to one-norm (absolute value) and also regularize w_1 we get the following penalized log-likelihood

$$\sum_{i=1}^{n} \log p(y_i|\mathbf{x}_i, w_1, w_2) - \frac{C}{2}\left(|w_1| + |w_2|\right).$$

Consider again the problem in Figure 1(a) and the same linear logistic regression model $\hat{P}(y = 1|\mathbf{x}, w_1, w_2) = g(w_1 x_1 + w_2 x_2)$. As we increase the regularization parameter C which of the following scenarios do you expect to observe (choose only one):

( ) First w_1 will become 0, then w_2.

( ) w_1 and w_2 will become zero simultaneously

( ) First w_2 will become 0, then w_1.

( ) None of the weights will become exactly zero, only smaller as C increases

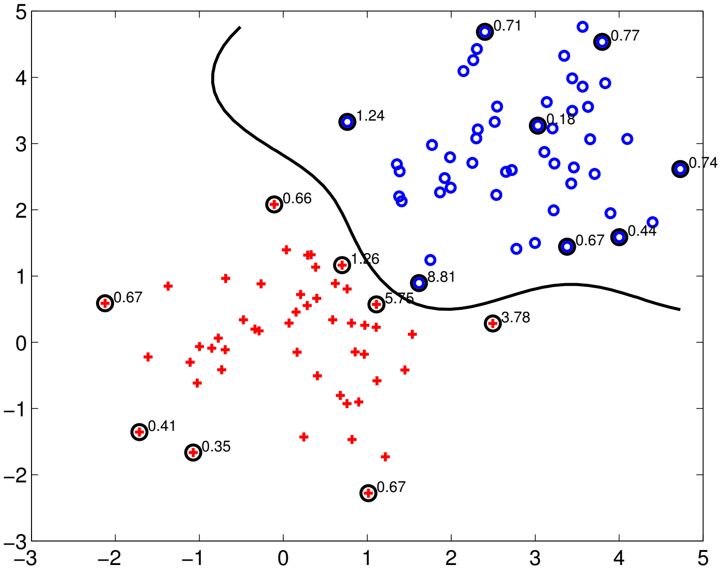


Figure 1: A 2-dim classification problem, the resulting SVM decision boundary with a radial basis kernel, as well as the support vectors (indicated by larger circles around them). The numbers next to the support vectors are the corresponding coefficients $\hat{\alpha}$.

Problem 3

Figure 1 illustrates a binary classification problem along with our solution using support vector machines (SVMs). We have used a radial basis kernel function given by

$$K(\mathbf{x}, \mathbf{x}') = \exp\{\, -\|\mathbf{x} - \mathbf{x}'\|^2/2 \,\}$$

where $\|\cdot\|$ is a Euclidean distance and $\mathbf{x} = [x_1, x_2]^T$. The classification decision for any $\mathbf{x}$ is made on the basis of the sign of

$$\hat{\mathbf{w}}^T \phi(\mathbf{x}) + \hat{w}_0 = \sum_{j \in \mathrm{SV}} y_j \hat{\alpha}_j K(\mathbf{x}_j, \mathbf{x}) + \hat{w}_0 = f(\mathbf{x}; \hat{\alpha}, \hat{w}_0)$$

where $\hat{\mathbf{w}}$, $\hat{w}_0$, $\hat{\alpha}_i$ are all coefficients estimated from the available data displayed in the figure and SV is the set of support vectors. $\phi(\mathbf{x})$ is the feature vector derived from $\mathbf{x}$ corresponding to the radial basis kernel. In other words, $K(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x})^T \phi(\mathbf{x}')$. While technically $\phi(\mathbf{x})$ is an infinite dimensional vector in this case, this fact plays no role in the questions below. You can assume and treat it as a finite dimensional vector if you like.

The support vectors we obtain for this classification problem (indicated with larger circles in the figure) seem a bit curious. Some of the support vectors appear to be far away from the decision boundary and yet be support vectors. Some of our questions below try to resolve this issue.

1. **(3 points)** What happens to our SVM predictions $f(\mathbf{x}; \hat{\alpha}, \hat{w}_0)$ with the radial basis kernel if we choose a test point $\mathbf{x}_{far}$ far away from any of the training points $\mathbf{x}_j$ (distances here measured in the space of the original points)?

2. **(3 points)** Let's assume for simplicity that $\hat{w}_0 = 0$. What equation do all the training points $\mathbf{x}_j$ have to satisfy? Would $\mathbf{x}_{far}$ satisfy the same equation?

3. **(4 points)** If we included $\mathbf{x}_{far}$ in the training set, would it become a support vector? Briefly justify your answer.

4. **(T/F – 2 points)** Leave-one-out cross-validation error is always small for support vector machines. □

5. **(T/F – 2 points)** The maximum margin decision boundaries that support vector machines construct have the lowest generalization error among all linear classifiers □

6. **(T/F – 2 points)** Any decision boundary that we get from a generative model with class-conditional Gaussian distributions could in principle be reproduced with an SVM and a polynomial kernel of degree less than or equal to three □.

7. **(T/F – 2 points)** The decision boundary implied by a generative model (with parameterized class-conditional densities) can be optimal only if the assumed class-conditional densities are correct for the problem at hand □

Problem 4

Consider the following set of 3-dimensional points, sampled from two classes:

	x_1	x_2	x_3
labeled ’1’:	1,	1,	-1
	0,	2,	-2
	0,	-1,	1
	0,	-2,	2

	x_1	x_2	x_3
labeled ’0’:	1,	1,	2
	0,	2,	1
	1,	-1,	-1
	1,	-2,	-2

We have included 2-dimensional plots of pairs of features in the “Additional set of figures” section (figure 3).

1. **(4 points)** Explain briefly why features with higher mutual information with the label are likely to be more useful for classification task (in general, not necessarily in the given example).

2. **(3 points)** In the example above, which feature (x_1, x_2 or x_3) has the highest mutual information with the class label, based on the training set?

3. **(4 points)** Assume that the learning is done with quadratic logistic regression, where

$$P(y = 1|\mathbf{x}, \mathbf{w}) = g(w_0 + w_1 x_i + w_2 x_j + w_3 x_i x_j + w_4 x_i^2 + w_5 x_j^2)$$

for some pair of features (x_i, x_j). Based on the training set given above, which pair of features would result in the lowest training error for the logistic regression model?

4. **(T/F – 2 points)** From the point of view of classification it is always beneficial to remove features that have very high variance in the data

5. **(T/F – 2 points)** A feature which has zero mutual information with the class label might be selected by a greedy selection method, if it happens to improve classifier’s performance on the training set

Problem 5

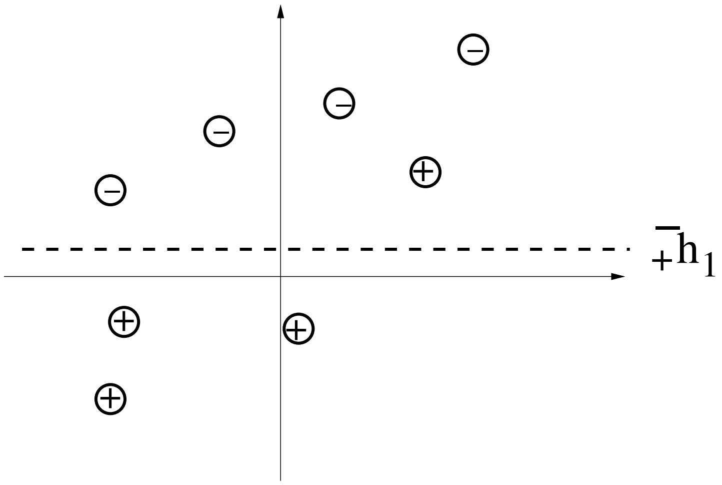


Figure 2: h_1 is chosen at the first iteration of boosting; what is the weight α_1 assigned to it?

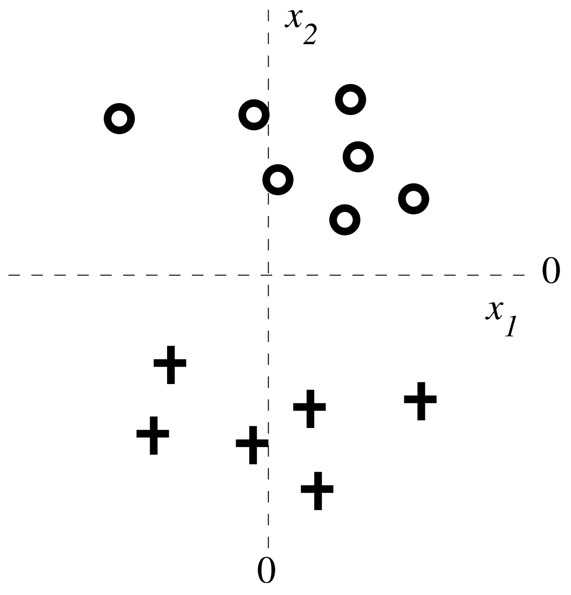
1. **(3 points)** Figure 2 shows a dataset of 8 points, equally divided among the two classes (positive and negative). The figure also shows a particular choice of decision stump h_1 picked by AdaBoost in the first iteration. What is the weight α_1 that will be assigned to h_1 by AdaBoost? (Initial weights of all the data points are equal, or 1/8.) □

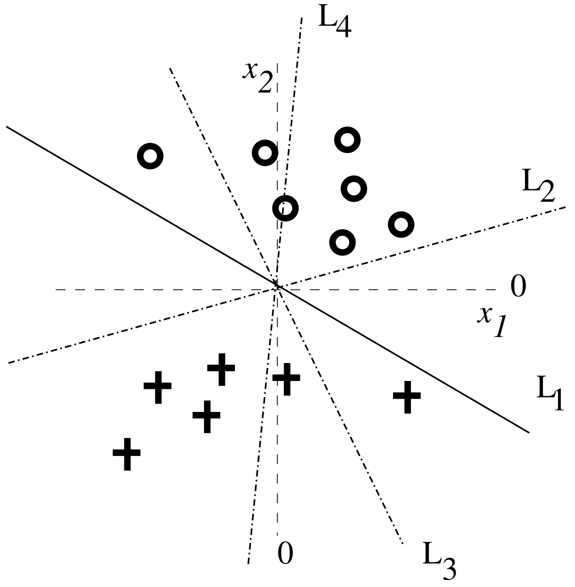
2. **(T/F – 2 points)** AdaBoost will eventually reach zero training error, regardless of the type of weak classifier it uses, provided enough weak classifiers have been combined. □

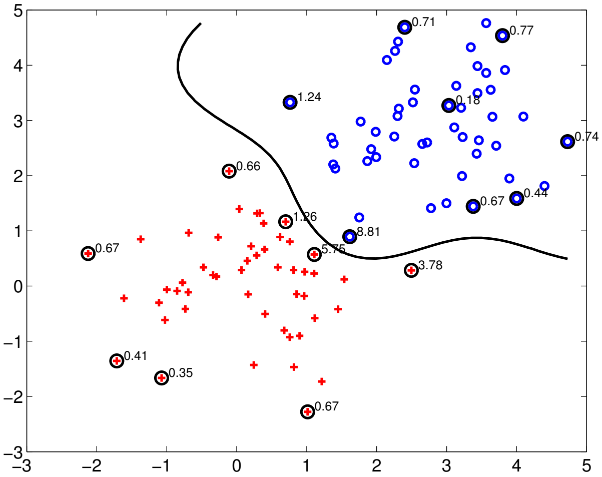
3. **(T/F – 2 points)** The votes α_i assigned to the weak classifiers in boosting generally go down as the algorithm proceeds, because the weighted training error of the weak classifiers tends to go up □

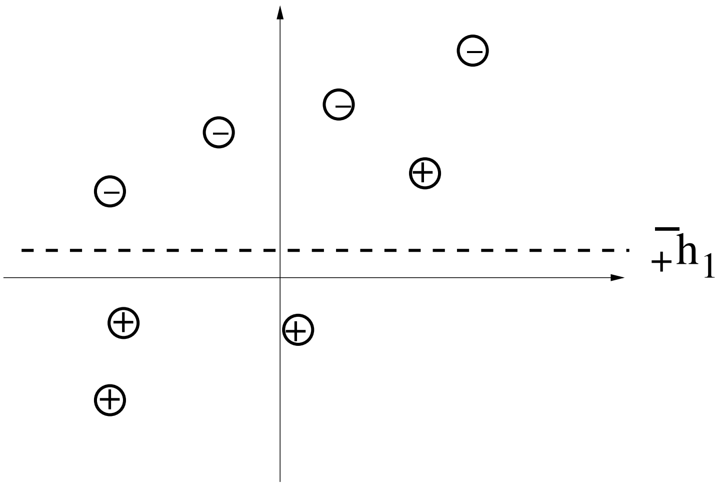
4. **(T/F – 2 points)** The votes α assigned to the classifiers assembled by AdaBoost are always non-negative □

Additional set of figures









there's more ...

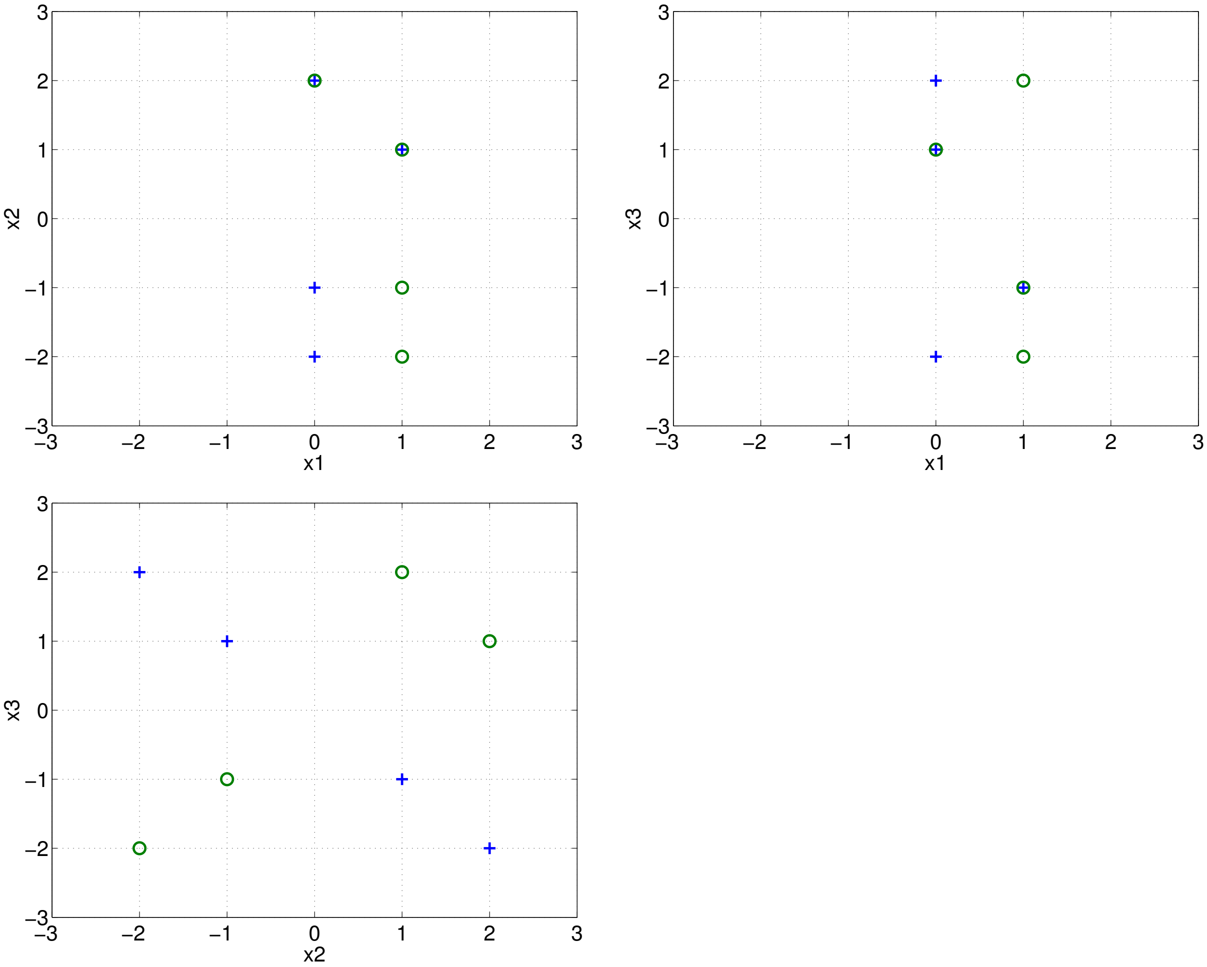


Figure 3: 2-dimensional plots of pairs of features for problem 4. Here '+' corresponds to class label '1' and 'o' to class label '0'.

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6.867 Machine learning

Mid-term exam

October 8, 2003

(2 points) Your name and MIT ID:

Problem 1

In this problem we use sequential active learning to estimate a linear model

$$y = w_1 x + w_0 + \epsilon$$

where the input space (x values) are restricted to be within $[-1, 1]$. The noise term ϵ is assumed to be a zero mean Gaussian with an unknown variance σ^2. Recall that our sequential active learning method selects input points with the highest variance in the predicted outputs. Figure 1 below illustrates what outputs would be returned for each query (the outputs are not available unless specifically queried).

We start the learning algorithm by querying outputs at two input points, $x = -1$ and $x = 1$, and let the sequential active learning algorithm select the remaining query points.

1. **(4 points)** Give the next two inputs that the sequential active learning method would pick. Explain why.

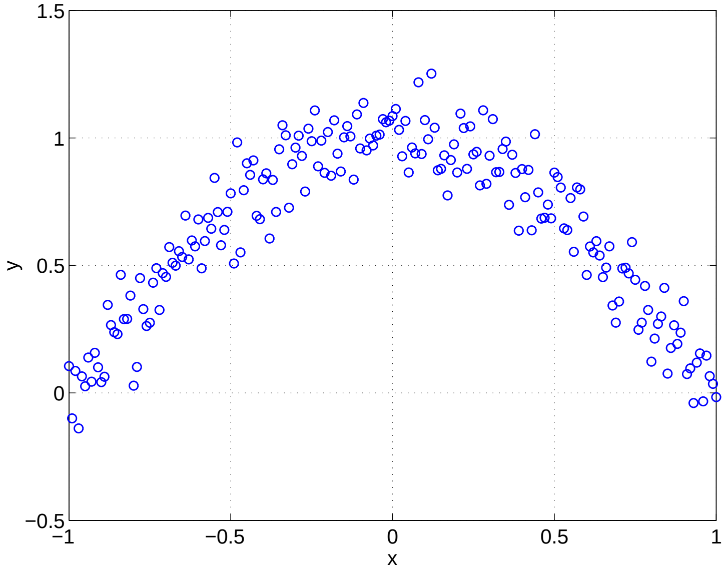

Figure 1: Samples from the underlying relation between the inputs x and outputs y. The outputs are not available to the learning algorithm unless specifically queried.

2. **(4 points)** In the figure 1 above, draw (approximately) the linear relation between the inputs and outputs that the active learning method would find after a large number of iterations.

3. **(6 points)** Would the result be any different if we started with query points $x = 0$ and $x = 1$ and let the sequential active learning algorithm select the remaining query points? Explain why or why not.

Problem 2

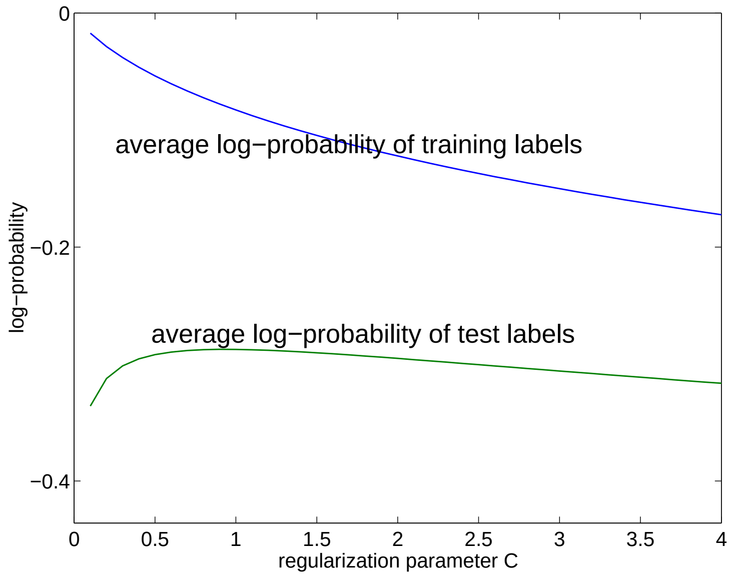

Figure 2: Log-probability of labels as a function of regularization parameter C

Here we use a logistic regression model to solve a classification problem. In Figure 2, we have plotted the mean log-probability of labels in the training and test sets after having trained the classifier with quadratic regularization penalty and different values of the regularization parameter C.

1. **(T/F – 2 points)** In training a logistic regression model by maximizing the likelihood of the labels given the inputs we have multiple locally optimal solutions. □
2. **(T/F – 2 points)** A stochastic gradient algorithm for training logistic regression models with a fixed learning rate will find the optimal setting of the weights exactly. □
3. **(T/F – 2 points)** The average log-probability of training labels as in Figure 2 can never increase as we increase C. □

4. **(4 points)** Explain why in Figure 2 the test log-probability of labels decreases for large values of C.

5. **(T/F – 2 points)** The log-probability of labels in the test set would decrease for large values of C even if we had a large number of training examples.

6. **(T/F – 2 points)** Adding a quadratic regularization penalty for the parameters when estimating a logistic regression model ensures that some of the parameters (weights associated with the components of the input vectors) vanish.

Problem 3

Consider a training set consisting of the following eight examples:

Examples labeled "0"	Examples labeled "1"
3,3,0	2,2,0
3,3,1	1,1,1
3,3,0	1,1,0
2,2,1	1,1,1

The questions below pertain to various feature selection methods that we could use with the logistic regression model.

1. **(2 points)** What is the mutual information between the third feature and the target label based on the training set?

2. **(2 points)** Which feature(s) would a filter feature selection method choose? You can assume here that the mutual information criterion is evaluated between a single feature and the label.

3. **(2 points)** Which two feature(s) would a greedy wrapper process choose?

4. **(4 points)** Which features would a regularization approach with a 1-norm penalty $\sum_{i=1}^{3} |w_i|$ choose? Explain briefly.

Problem 4

1. **(6 points)** Figure 3 shows the first decision stump that the AdaBoost algorithm finds (starting with the uniform weights over the training examples). We claim that the weights associated with the training examples after including this decision stump will be $[1/8, 1/8, 1/8, 5/8]$ (the weights here are enumerated as in the figure). Are these weights correct, why or why not?

   Do not provide an explicit calculation of the weights.

2. **(T/F – 2 points)** The votes that AdaBoost algorithm assigns to the component classifiers are optimal in the sense that they ensure larger "margins" in the training set (higher majority predictions) than any other setting of the votes.

3. **(T/F – 2 points)** In the boosting iterations, the training error of each new decision stump and the training error of the combined classifier vary roughly in concert .

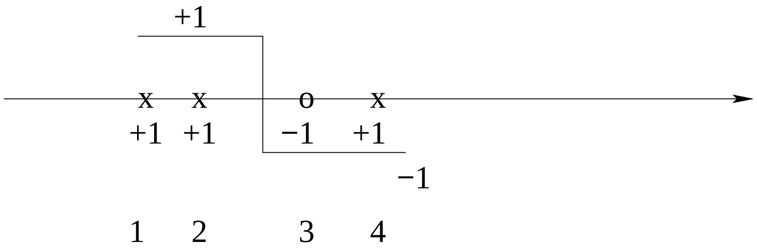

Figure 3: The first decision stump that the boosting algorithm finds.

Problem 5

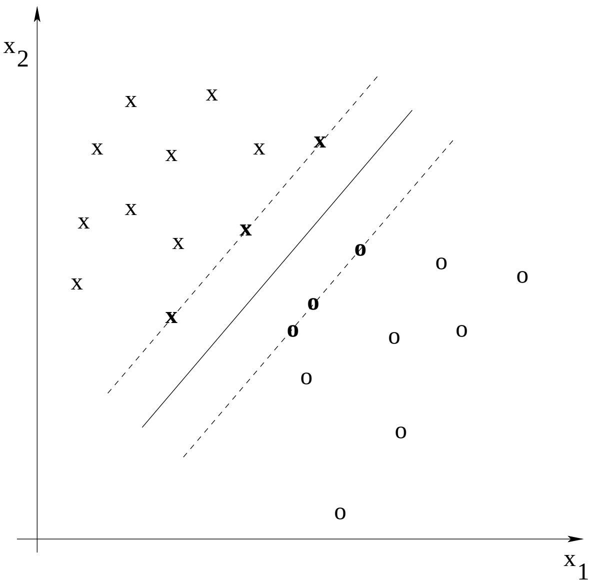

Figure 4: Training set, maximum margin linear separator, and the support vectors (in bold).

1. **(4 points)** What is the leave-one-out cross-validation error estimate for maximum margin separation in figure 4? (we are asking for a number)

2. **(T/F – 2 points)** We would expect the support vectors to remain the same in general as we move from a linear kernel to higher order polynomial kernels.

3. **(T/F – 2 points)** Structural risk minimization is guaranteed to find the model (among those considered) with the lowest expected loss

4. **(6 points)** What is the VC-dimension of a mixture of two Gaussians model in the plane with equal covariance matrices? Why?

Problem 6

Using a set of 100 labeled training examples (two classes), we train the following models:

GaussI A Gaussian mixture model (one Gaussian per class), where the covariance matrices are both set to I (identity matrix).

GaussX A Gaussian mixture model (one Gaussian per class) without any restrictions on the covariance matrices.

LinLog A logistic regression model with linear features.

QuadLog A logistic regression model, using all linear and quadratic features.

1. **(6 points)** After training, we measure for each model *the average log probability of labels given examples in the training set*. Specify all the equalities or inequalities that must *always* hold between the models relative to this performance measure. We are looking for statements like "model 1 $\leq$ model 2" or "model 1 $=$ model 2". If no such statement holds, write "none".

2. **(4 points)** Which equalities and inequalities must *always* hold if we instead use the *mean classification error in the training set* as the performance measure? Again use the format "model 1 $\leq$ model 2" or "model 1 = model 2". Write "none" if no such statement holds.

Another set of figures

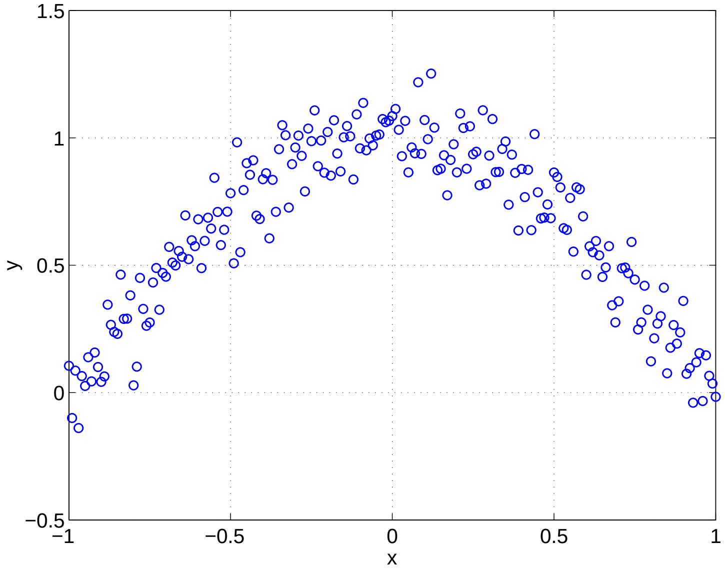

Figure 1. Samples from the underlying relation between the inputs x and outputs y. The outputs are not available to the learning algorithm unless specifically queried

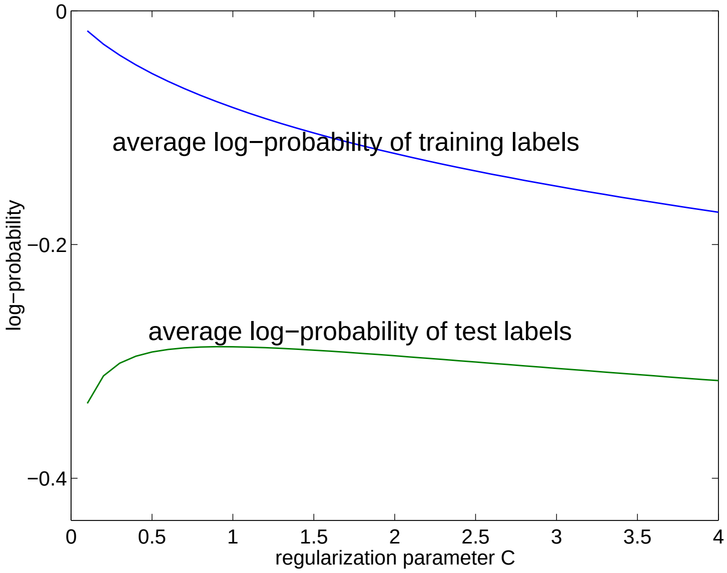

Figure 2. Log-probability of labels as a function of regularization parameter C

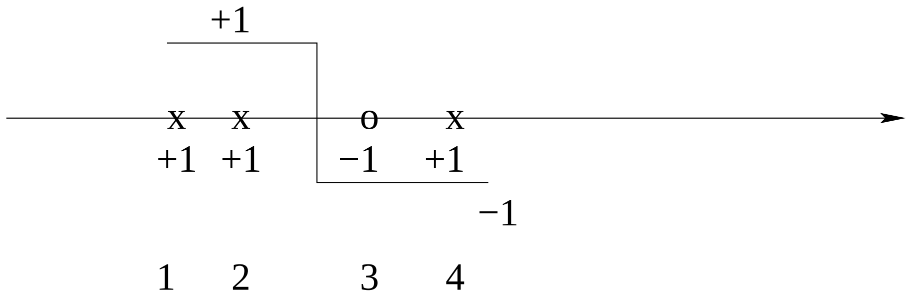

Figure 3. The first decision stump that the boosting algorithm finds.

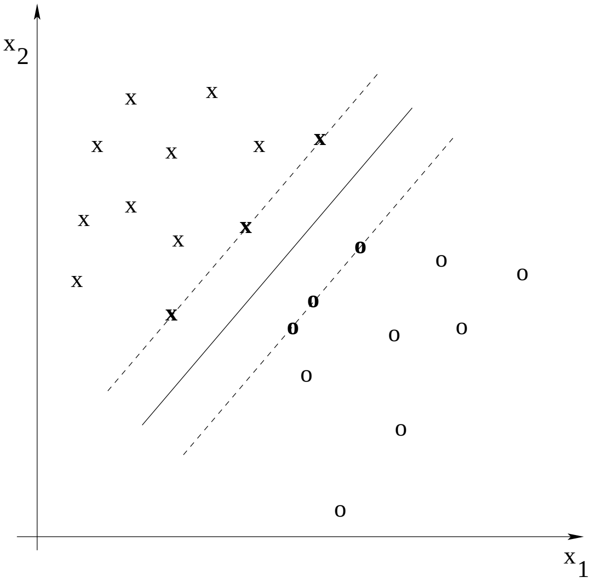

Figure 4. Training set, maximum margin linear separator, and the support vectors (in bold).