Due: Nov.4, 2pm at the **START** of class Worth: 18% Late assignments not accepted.

1 Pseudo-Bayesian Linear Regression (3%)

In this question you will dabble in Bayesian statistics and extend the probabilistic model formulation to include not only the data but also the weights.

Consider the following conditional model of a scalar output y given some inputs \mathbf{x} :

$$\begin{split} p(y|\mathbf{x}) &= \int_{\mathbf{w}} p(y|\mathbf{x}, \mathbf{w}) p(\mathbf{w}) d\mathbf{w} \\ p(y|\mathbf{x}, \mathbf{w}) &= \mathcal{N}(y; \mathbf{w}^{\top} \mathbf{x}, b) \\ p(\mathbf{w}) &= \mathcal{N}(\mathbf{w}; \mathbf{0}, a\mathbf{I}) \end{split}$$

Here the weight prior $p(\mathbf{w})$ is a Gaussian with mean zero and covariance $a\mathbf{I}$ (\mathbf{I} is the identity matrix) and the data model is a conditional linear-Gaussian with mean $\mathbf{w}^{\mathsf{T}}\mathbf{x}$ and variance b.

- Find the posterior distribution over weights $p(\mathbf{w}|\{\mathbf{x}_n, y_n\}, a, b)$ given a finite training set $\{\mathbf{x}_n, y_n\}$ and the variances a, b. To do this, you will need to form the joint Gaussian $p(y, \mathbf{w}|\mathbf{x})$, marginalize out the weights to form $p(y|\mathbf{x})$ and then use Bayes rule to find $p(\mathbf{w}|\mathbf{x}, y)$.
- Show that the ridge regression weights, which minimize the cost $\lambda \mathbf{w}^{\mathsf{T}} \mathbf{w} + \sum_{n} (y_n \mathbf{w}^{\mathsf{T}} \mathbf{x}_n)^2$ are equal to the mean (and mode) of the posterior above.
- Give the ridge regression penalty λ in terms of the variances a, b above.

2 Regularizing Linear Mixtures of Experts (2%)

In class I did not tell you anything about how to regularlize mixtures of experts models. This question asks you to work out the details for one method and to suggest one more. Recall that the linear mixture of experts model uses a gate to compute $p(j|\mathbf{x}_n)$ and then stochastically selects an expert according to these probabilities. The experts outputs are given by $p(\mathbf{y}|j,\mathbf{x}_n) = \mathcal{N}(\mathbf{y};\mathbf{U}_j\mathbf{x}_n,\Sigma)$. Assume the gate is fixed, so that the quantities $p(j|\mathbf{x}_n)$ are known and do not change. Assume also that the output covariance Σ is known and fixed.

One obvious way to regularlize a *linear* mixtures of experts model using squared error is to do *ridge regression* at the experts instead of maximum likelihood regression. This means the likelihood function would become:

$$\ell^{new} = \sum_{n} \log \sum_{j} p(j|\mathbf{x}_{n}) \mathcal{N}(\mathbf{y}_{n}; \mathbf{U}_{j}\mathbf{x}_{n}, \Sigma) + \lambda \sum_{ijk} U_{ijk}^{2}$$

where U_{ijk} is the weight from input i to output k in expert j.

Recall that the gradient with respect to an expert's weights \mathbf{U}_j in the original linear MOE was:

$$\partial \ell^{old}/\partial \mathbf{U}_j = \sum_n p(j|\mathbf{x}_n,\mathbf{y}_n) \left(\mathbf{y}_n - \mathbf{U}_j \mathbf{x}_n\right) \mathbf{x}_n^{\top}$$

which uses the *posterior* probability of each expert:

$$p(j|\mathbf{x}_n, \mathbf{y}_n) = \frac{p(j|\mathbf{x}_n)p(\mathbf{y}_n|j, \mathbf{x}_n)}{\sum_k p(k|\mathbf{x}_n)p(\mathbf{y}_n|k, \mathbf{x}_n)}$$

- When we use ridge regression, the new likelihood function will, of course, have different gradients with respect to the expert weights. Derive the new gradient $\partial \ell^{new}/\partial \mathbf{U}_j$ with respect to an expert's weights \mathbf{U}_J under the ridge regression likelihood above.
- Suggest one other, different way of regularizing a linear mixture of experts architecture to prevent overfitting.

3 Adapting Centres in Radial Basis Networks (3%)

In this question you will find the derivatives which would allow you to adapt the centres in a radial basis network. Recall that a radial basis network is a generalized linear model of the form

$$y = \sum_{j} w_{j} h_{j}(\mathbf{x})$$
$$h_{j}(\mathbf{x}) = \exp\left[-(\mathbf{x} - \mathbf{z}_{j})^{\top}(\mathbf{x} - \mathbf{z}_{j})/\alpha\right]$$

Assume we are using a Gaussian noise model so that the likelihood becomes squared error:

$$E = \sum_{n} (y_n - \sum_{j} w_j h_j(\mathbf{x}_n))^2$$

As you know, for fixed α and fixed \mathbf{z}_j , the maximum likelihood weights under this Gaussian noise can be found by linear regression. But if \mathbf{z}_j are unknown we would like to adapt them.

• Compute the gradient $\partial E/\partial \mathbf{z}_f$ of E with respect to \mathbf{z}_f , given α , a finite training set $\{\mathbf{x}_n, y_n\}$ and the current values of \mathbf{z}_j for all j.

4 Fully Observed Trees (10%)

IMPORTANT: please do your computing on CDF or your own machine and not on CSLAB machines since they have limited Matlab licenses.

In this assignment you will train a fully observed tree model on word-document vectors taken from USENET articles.

4.1 What to do

- Using the data provided in a2newsgroups.mat, train a fully observed tree model with the optimal structure. Training the model structure should give you an *undirected* tree. Using this, you can pick a root node arbitrarily and form a *directed tree*.
- The matrix documents contains one column per USENET article.

 Each of the 100 rows is a binary variable indicating whether a certain keyword appears in the posting or not.

 The cell array wordlist has the 100 words corresponding to these rows. The data has 100 (binary) features and 16242 training cases.

4.2 What to hand in

- Any compact, clear and unambiguous representation of the optimal (undirected) tree structure found by your algorithm. For example, you might print out all 99 pairs of words (word_i--word_j) corresponding to edges chosen by the tree learning algorithm. Or you might want to draw a picture of the graph (see below). DO NOT hand in lists of numbers corresponding to the indices of pairs of features chosen convert everything back to words using the wordlist cell array. Since the order of the words is arbitrary, the number of the word index is meaningless, and printing it out tells someone else nothing about your model.
- After finding the optimal tree structure for the 100 variables, you may choose any node you wish as the root and form a directed graph. Different choices of root node will result in different output when you visualize a directed tree, but of course the undirected model structure always remains the same. Chose a root word. Hand in a compact, clear and unambiguous representation of a directed tree structure created by directing all arcs in the optimal structure away from a your chosen root. For example, you might print out a breadth-first list of directed links (word_i->word_j) in the tree. Alternately, you might want to draw a picture (see below).
- A histogram (with at least 100 bins) of the log likelihoods of the training cases under your optimal model.
 Notice that these likelihoods are the same no matter how you chose to convert your undirected tree into a directed tree.

Compute and print out the min, max, mean and median log likelihood.

Which training case (give its number) has the worst (lowest) log likelihood?

Print out the list of keywords appearing in this posting.

4.3 Some hints

- Be careful when computing the mutual information weights for pairs of variables that have zero counts for some
 of their joint settings. In this case the mutual information should be zero, but a careless calculation will lead
 to division by zero or log of zero errors in the code.
- To save you some trouble, I've written the function mwst.m for you, which finds minimum or maximum weight spanning trees given a weight matrix.
- Here is a trick for computing the 2 by 2 joint count table of two binary column vectors v1 and v2: counts12 = reshape(hist(v1+2*v2,0:3),2,2);

but make sure you understand it before using it!

- The data is almost a megabyte in Matlab, stored as a sparse matrix, so be careful about making copies of it in memory. You should be able to do everything you need without making another (sparse or nonsparse) copy of the whole dataset.
- In case you are interested, the array newsgroup tells you the toplevel newsgroup category of each posting, 1=comp.*, 2=rec.*, 3=sci.*, 4=talk.*, although we won't use it in this assignment.

4.4 Reminders

Amongst other things, your code will need to:

- Compute the marginal count for every feature being on or off summed across all documents.
- Compute the joint counts for every pair of features being on together, off together, on-off or off-on, summed across all documents.
- Convert these counts into mutual information weights.

 Be careful to do this properly for joint counts which are zero!
- Find the best spanning tree over the features given these weights. Depending on how you compute the weights, you will either need a minimum or maximum weight spanning tree.

 (This will in turn affect how you call mwst.m if you choose to use it.)
- Select a root for the tree and direct all edges away from it to get a directed graph.

4.5 Automatic Graph Layout

- If you want to be really fancy, you can try using the function dottree.m and the automatic graph layout programs dot and neato to draw pictures of your final structures. It is very cool looking, but you will not get any more or any fewer marks for using this method or a simpler method to display your results. Caution: do not waste too much time trying to get this to work, since it doesn't get you any more marks. It is just for fun. Get the rest of the assignment finished first.
- Call dottree(tree, 'fname', wordlist) and it will write out two files, fname.u and fname.d. Now call the neato and dot programs to convert these files into pictures.
- Information and downloads for dot and neato are available at http://www.graphviz.org/. The programs are already installed in /local/bin/ on CDF (and in /pkgs/graphvis/linux/bin/ on CSLAB if you want to use them in your own research later).