

Radford Neal's Entries for the NIPS*2004 Predictive Uncertainty Challenge

I entered predictions for the CATALYSIS and GATINEAU classification tasks. Both entries used Bayesian neural networks, with computation using Markov chain Monte Carlo. I used my flexible Bayesian modeling software, which is available at <http://www.cs.toronto.edu/~radford/fbm.software.html>

Some characteristics of these entries:

- I used multilayer perceptron networks with two hidden layers (with 16 units and 8 units), with connections only from each layer to the next (eg, no direct input-output connections).
- I used all features (617 for CATALYSIS, 1092 for GATINEAU), but I used an Automatic Relevance Determination (ARD) prior, which allows the model to discover that some features are more relevant than others.
- Two MCMC runs were done for each data set, each taking about four days. I averaged the predictions found with all iterations from both runs, except that the first few “burn-in” iterations from each run were discarded.
- Two entries were made — one using only the training data, the other both training data and validation data (after validation labels were released).

Some More Details

- I used slightly different ARD priors for the two data sets — the GATINEAU prior allowed greater differences in relevance than the CATALYSIS prior. This was based on the distribution of ARD hyperparameters in preliminary runs. This is a manual approximation to what would result from making this parameter of the prior be a variable hyperparameter (which my software doesn't support at present).
- I let the MCMC runs go for four days, since running a long time may improve results a bit. But similar results are obtained using only one tenth this much time (eg, the predictions differ for only 9% of CATALYSIS test cases, in all of which the predictive probabilities were near 0.5).
- All predictions for GATINEAU gave probability less than 0.5 to class 1. The highest probability of class 1 in any test case was 0.329.

The command scripts used will shortly be posted on my web page.