Big Data and AI Strategies

Neural Network Explained Part VI: Preventing Overfitting

In the previous note, we started the discussion around the numerical aspects for training neural nets. The main pitfall with training any model is overfitting, and neural nets are no exception. The overfitting issue is in many ways more acute for neural nets, due to the exponentially greater number of parameters. Thoughtful architectural design is clearly the most preferred solution. In addition, there are numerical techniques which reduce the likelihood of overfitting. This is a vast area of active research and we only briefly touch on a small number of topics below.

Regularization

Regularization in neural network works similarly to the classical regularization in regression. Specifically, we add to the loss function a penalty term, which is either the L1 (sum of absolute values) or the L2 (sum of squares) norm of the parameters. Doing so will have a shrinkage effect on the parameters and prevent them from becoming too large. It is well known in statistics that shrinking parameters towards 0 broadly enhances the model performance. To see why, consider any model where we start out with a null hypothesis that all parameters are 0. If we find the model producing parameters with extreme values, is it likely to be a representation of the true underlying relationship, or a product of overfitting? Given our null hypothesis, the probability of the former is quite low. In the much more likely latter case, model performance will be improved if we shrink the parameters towards 0.

Ensemble Learning

As its name suggests, ensemble learning involves combining a portfolio of models. Statisticians have long observed that averaging a large number of independent model predictions is likely to have better out of sample performance than any single model. Ensemble learning has found extensive uses in machine learning, and serves as the foundation of some of the most popular techniques such random forest.

When it comes to neural network specifically, ensemble learning refers to averaging the predictions of a number of networks with different architectures (i.e. different number of neurons, layers, and/or connections). However, compared to tree based methods, ensemble learning in neural network has received less attention. This is because it is highly computationally intensive to train multiple neural nets. At any rate, given the large number of combinations in a deep neural net, it is impossible to train all possible architectures. Therefore, the portfolio of models should be chosen to have as much diversity as possible, in order to maximize the effectiveness. In addition, some less expensive alternatives such as dropout has been developed.

Dropout

When training a neural net, instead of taking the structure as deterministic, we assume any neuron and its connections may be removed from the network at random, e.g. with a probability of 50%. In effect, we are fitting a large number of different networks on the same data, and averaging them. This approach is computationally less expensive than ensemble learning. The lower computational cost comes from the fact that dropout works well with stochastic gradient descent, and can be implemented jointly. In contrast to the ensemble learning where a large number of architectures are all trained fully, each model 'thinned' by dropout is trained only for one iteration during the stochastic gradient descent process.

Dropout has a regularization interpretation. This is because during testing, the parameters obtained from training will be scaled by the dropout retain ratio (which is always less than 1), in order to approximate the averaging effect on the test set.

Compatibility issue with batch normalization
Previously, we discussed the importance of normalizing the inputs into the neural net, i.e. converting the inputs into zero mean and unit variance. In deep neural network, the inputs are transformed through many layers, and there is no guarantee that the layer inputs will stay well behaved throughout. The practice of batch normalization refers to normalizing the hidden layer inputs in every batch of the random samples during the stochastic gradient descent process. Empirically we have

observed that batch normalization is effective in improving the performance of deep neural nets. Interestingly, the original authors of the technique note that batch normalization seems to reduce the effectiveness of dropout[1].

The reason for the incompatibility was not immediately obvious but was later discovered by Li et al. (2018)[2]. They observe that batch normalization attempts to maintain a constant input variance throughout the training process. On the other hand, the dropout method inherently makes the distribution of the inputs unstable. Fortunately, this conflict can be remedied. Given the dropout ratio, we can compute its effect on the input variance and compensate by adding white noise.

Noise Addition

Both ensemble learning and dropout attempt to perturb the model in order to achieve better out of sample performance. An alternative and more direct way is to simply add white noise to the inputs. The noisier inputs will force the neural net to produce more robust estimates[3]. What's more, the implementation of noise addition is straight forward and therefore amenable to being combined with other techniques. This contrasts with more complex techniques like dropout, which as we saw above can sometimes cause compatibility issues that are difficult to diagnose. In addition, unlike some methods with hyperparameters which themselves require expensive tuning, the noise level can be calibrated to a number of observable and economically meaningful variables. For instance, we can align the level of noise in training set to match the test set or the most recent data.

Just like dropout, noise addition also has an interpretation from the regularization angle. In this paper[4], the author shows that that noise addition is equivalent to L2 regularization when the loss function is sum of squares.

An Evolutionary Perspective

As we saw in a number of cases in this note, out of sample model performance seems to benefit from random resampling and averaging. This is true not only for neural nets but for statistical models in general. The original authors of the dropout paper draw comparison to biological evolution[5]: in sexual reproduction, the genes of an offspring are the average results of its parents (50% from each parent), plus a small amount of random mutation. This seems to offer evolutionary advantages since most advanced organisms evolved in such a way. On a related note, numerical methods inspired by biological behaviours, known as evolutionary algorithms, have made significant progress in the field of machine learning. Some other examples include particle swarm and genetic optimization algorithm.

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