Tufts

Class #18: Back-Propagation; Tuning Hyper-Parameters

Machine Learning (COMP 135): M. Allen, 04 Nov. 19

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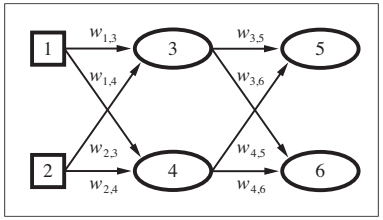
Learning in Neural Networks



- A neural network can learn a classification function by adjusting its weights to compute different responses
- This process is another version of gradient descent: the algorithm moves through a complex space of partial solutions, always seeking to ***minimize*** overall error

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Back-Propagation (Hinton, et al.)

Source: Russel & Norvig, *AI: A Modern Approach* (Prentice Hal, 2010)

function BACK-PROP-LEARNING(*examples*, *network*) **returns** a neural network
inputs: *examples*, a set of examples, each with input vector **x** and output vector **y**
network, a multilayer network with L layers, weights $w_{i,j}$, activation function g
local variables: Δ, a vector of errors, indexed by network node

repeat
for each weight $w_{i,j}$ in *network* **do**
$w_{i,j} \leftarrow$ a small random number
for each example $(\mathbf{x}, \mathbf{y})$ **in** *examples* **do**
/* *Propagate the inputs forward to compute the outputs* */
for each node i in the input layer **do**
$a_i \leftarrow x_i$
for $\ell = 2$ **to** L **do**
for each node j in layer ℓ **do**
$in_j \leftarrow \sum_i w_{i,j} a_i$
$a_j \leftarrow g(in_j)$
/* *Propagate deltas backward from output layer to input layer* */
for each node j in the output layer **do**
$\Delta[j] \leftarrow g'(in_j) \times (y_j - a_j)$
for $\ell = L - 1$ **to** 1 **do**
for each node i in layer ℓ **do**
$\Delta[i] \leftarrow g'(in_i) \sum_j w_{i,j} \Delta[j]$
/* *Update every weight in network using deltas* */
for each weight $w_{i,j}$ in *network* **do**
$w_{i,j} \leftarrow w_{i,j} + \alpha \times a_i \times \Delta[j]$
until some stopping criterion is satisfied
return *network*

Initial random weights

Loop over all training examples, generating the output, and then updating weights based on error

Stop when weights converge or error is minimized

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Propagating Output Values Forward

/* *Propagate the inputs forward to compute the outputs* */
for each node i in the input layer **do**
$a_i \leftarrow x_i$
for $\ell = 2$ **to** L **do**
for each node j in layer ℓ **do**
$in_j \leftarrow \sum_i w_{i,j} a_i$
$a_j \leftarrow g(in_j)$

At first ("top") layer, each neuron input is set to the corresponding feature value

Go down layer-by-layer, calculating weighted input sums for each neuron, and computing output function g

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Propagating Error Backward

/* *Propagate deltas backward from output layer to input layer* */
for each node j in the output layer **do**
  $\Delta[j] \leftarrow g'(in_j) \times (y_j - a_j)$
for $\ell = L - 1$ **to** 1 **do**
  for each node i in layer ℓ **do**
    $\Delta[i] \leftarrow g'(in_i) \sum_j w_{i,j} \Delta[j]$
/* *Update every weight in network using deltas* */
for each weight $w_{i,j}$ in *network* **do**
  $w_{i,j} \leftarrow w_{i,j} + \alpha \times a_i \times \Delta[j]$

At output ("bottom") layer, each delta-value is set to the error on that neuron, multiplied by the derivative of function g

Go bottom-up and set delta to derivative value multiplied by sum of deltas at the next layer down (weighting each such value appropriately)

After all the delta values are computed, update weights on every node in the network

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Hyperparameters for Neural Networks

- Multi-layer (deep) neural networks involve a number of different possible design choices, each of which can affect classifier accuracy:
  - Number of hidden layers
  - Size of each hidden layer
  - Activation function employed
  - Regularization term (controls over-fitting)
- This is not unique to neural networks
  - Logistic regression: regularization (`C` parameter in `sklearn`), class weights, etc.
  - SVM: kernel type, kernel parameters (like polynomial degree), error penalty (`C` again), etc.
- Question is often how we can tune these model control parameters effectively to find best combinations

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Heldout Cross-Validation

- We can use k-fold cross-validation techniques to estimate the real effectiveness of various parameter settings:

1. Divide labeled data into k folds, each of size $1/k$
2. Repeat k times:
   a. Hold aside one of the folds; train on the remaining $(k-1)$; test on the heldout data
   b. Record classification error for both training and heldout data
3. Average over the k trials

- This can give us a more robust estimate of real effectiveness
- It can also allow us to better detect over-fitting: when average heldout error is significantly worse than average training error, model has grown too complex or otherwise problematic

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Modifying Model Parameters

- Using heldout validation techniques, we can begin to explore various parts of the hyperparameter-space
  - In each case, we try to maximize average performance on the heldout validation data
- For example: ***number*** of layers in a neural network can be explored iteratively, starting with one layer, and increasing one at a time (up to some reasonable) limit until over-fitting is detected
- Similarly, we can explore a range of layer ***sizes***, starting with hidden layers of size equal to the number of input features, and increasing in some logarithmic manner until over-fitting occurs, or some practical limits reach

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Using Grid Search for Tuning

- One basic technique is to list out the different values of each parameter that we want to test, and systematically try different combinations of those values
  - For P distinct tuning parameters, defines a P-dimensional space (or "grid"), that we can explore, one combination at a time
- In many cases, since building, training, and testing the models for each combination all take some time, we may find that there are far too many such combinations to try
  - One possibility: many such models can be explored in ***parallel***, allowing large numbers of combinations to be compared at the same time, given sufficient resources

Costs of Grid Search

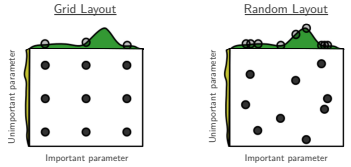
- When we have large numbers of combinations of possible parameters, we may decide to limit the range of some of the parts of our "grid" for feasibility
- For example, we might try:
  1. # Hidden layers: 1, 2, …, 10
  2. Layer size: N, 2N, 5N, 10N, 20N (N: # input features)
  3. Activation: Sigmoid, ReLU, tanh
  4. Regularization (`alpha`): 10^{-5}, 10^{-3}, 10^{-1}, 10^{1}, 10^{3}
- Produces (10 x 5 x 3 x 5) = 750 different models
  - If we are doing 10-fold validation, need to run 7,500 total tests
  - Still only a small fragment of the possible parameter-space

Random Search

- Instead of limiting our grid even further, or trying to spend even more time on more combinations, we might try to randomize the process
- Instead of limiting values, we choose randomly from any of a (larger) range of values:
  1. # Hidden layers: [1, 20]
  2. Layer size: [8, 1024]
  3. Activation: [Sigmoid, ReLU, tanh]
  4. Regularization (`alpha`): [10^{-7}, 10^{7}]
- For each of these, we assign a probability distribution over its values (uniform or otherwise)
  - We may presume these distributions are independent of one another
- For T tests, we sample each of the ranges for one possible value, giving us T different combinations of those values

Performance of Random Search

From: J. Bergstra & Y. Bengio, "Random search for hyper-parameter optimization," *Journal of Machine Learning Research* 13 (2012).

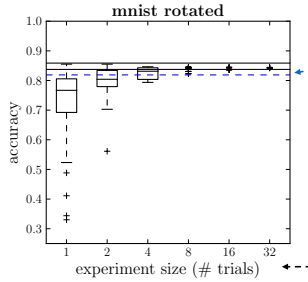


Grid and random search of nine trials for optimizing a function $f(x,y) = g(x) + h(y) \approx g(x)$ with low effective dimensionality. Above each square $g(x)$ is shown in green, and left of each square $h(y)$ is shown in yellow. With grid search, nine trials only test $g(x)$ in three distinct places. With random search, all nine trials explore distinct values of g. This failure of grid search is the rule rather than the exception in high dimensional hyper-parameter optimization.

- This technique can sometimes out-perform grid search
- When using a grid, it is sometimes possible that we just ***miss*** some intermediate, and important, value completely
- The random approach can often hit upon the better combinations with the same (or far less) testing involved

Performance of Random Search

From: J. Bergstra & Y. Bengio, "Random search for hyper-parameter optimization," *Journal of Machine Learning Research* 13 (2012).



Performance for grid search over 100 different neural network parameter combinations

Statistically significant improvement for as few as 8 randomly chosen combination models

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This Week

- **Topics**: Neural Networks
- **Project 01**: due Monday, 04 November, 4:15 PM
  - Can be handed in without penalty until Wed., 06 Nov., 4:15 PM
- **Homework 04**: due Wednesday, 06 November, 9:00 AM
- **Office Hours**: 237 Halligan, Tuesday, 11:00 AM – 1:00 PM
  - TA hours can be found on class website as well

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