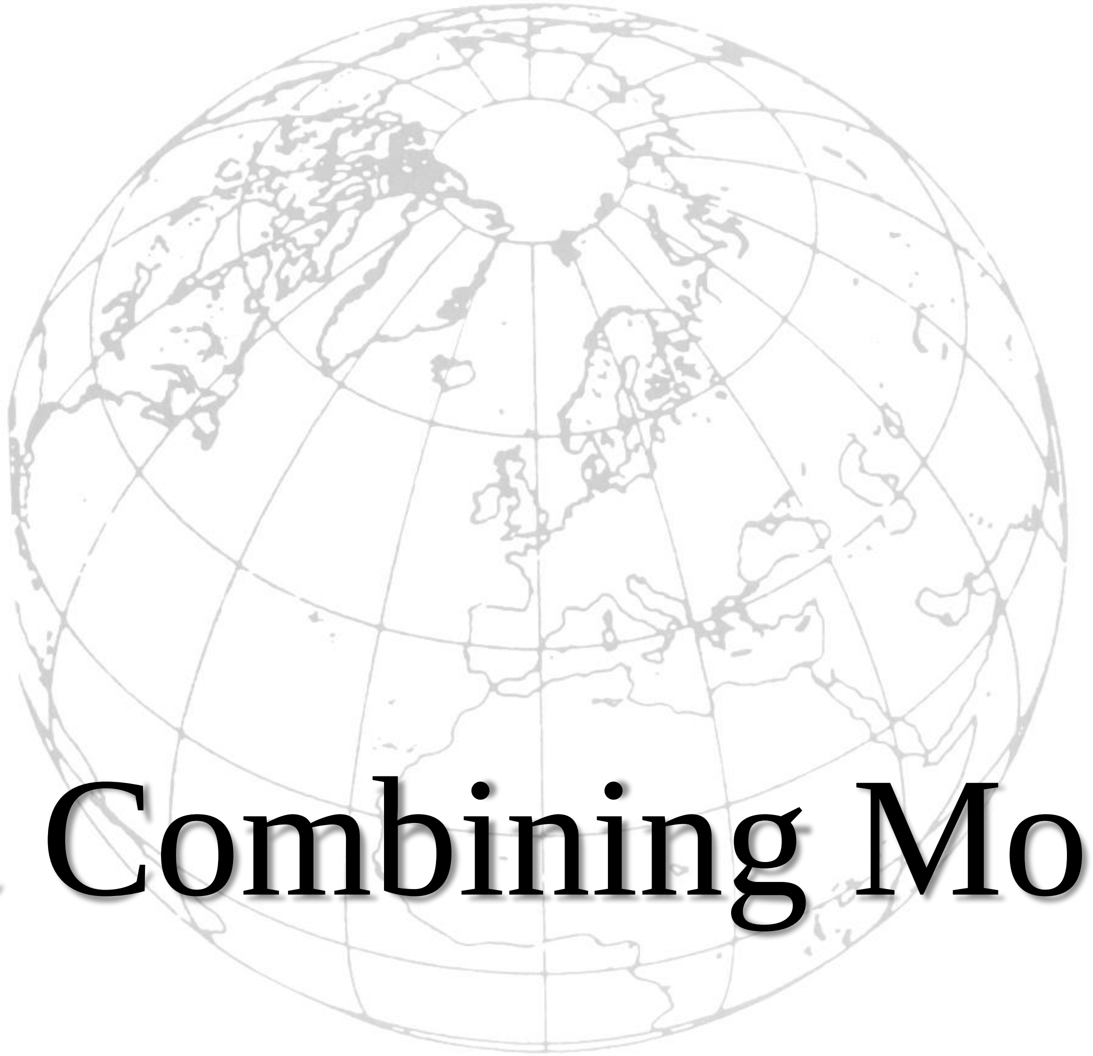


Data Combining Models

Dr. Cahit Karakuş

Motivation

- Many models can be trained on the same data
- Typically none is strictly better than others
  - Recall “no free lunch theorem”
- Can we “combine” predictions from multiple models?

- Yes, typically with significant reduction of error!

Motivation

- Combined prediction using Adaptive Basis Functions

$$f(x) = \sum_{i=1}^{M} w_m \phi_m(x; v_m)$$

- M basis functions with own parameters
- Weight / confidence of each basis function
- Parameters including M trained using data

- Another interpretation: automatically learning best representation of data for the task at hand

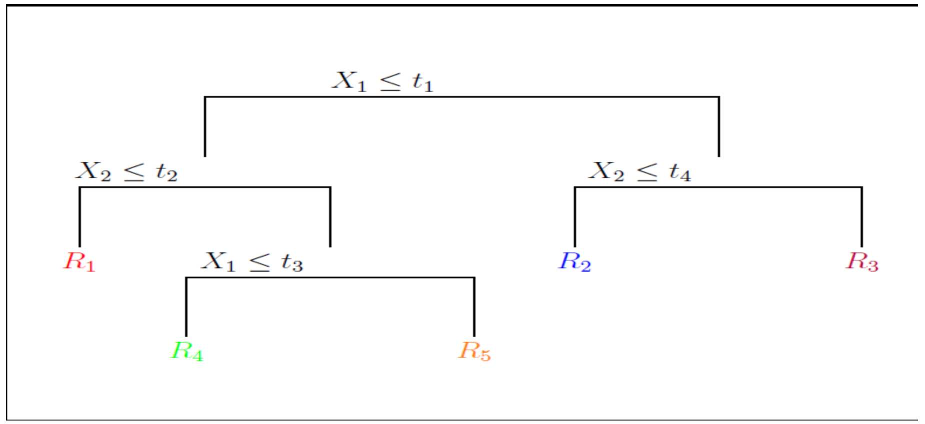
- Difference with mixture models?

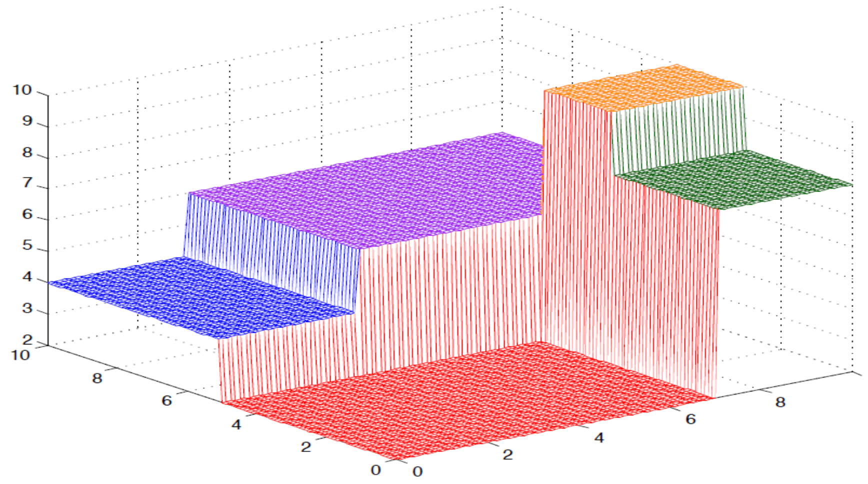
Examples of Model Combinations

- Also called Ensemble Learning
- Decision Trees
- Bagging
- Boosting
- Committee / Mixture of Experts
- Feed forward neural nets / Multi-layer perceptrons
- …

Decision Trees

- Partition input space into cuboid regions
- Simple model for each region
  - Classification: Single label; Regression: Constant real value
- Sequential process to choose model per instance
  – Decision tree





Learning Decision Trees

- Decision for each region
  - Regression: Average of training data for the region
  - Classification: Most likely label in the region
- Learning tree structure and splitting values
  - Learning optimal tree intractable
- Greedy algorithm
  - Find (node, dim., value) w/ largest reduction of “error”
    - Regression error: residual sum of squares
    - Classification: Misclassification error, entropy, …
  - Stopping condition
- Preventing overfitting: Pruning using cross validation

Pros and Cons of Decision Trees

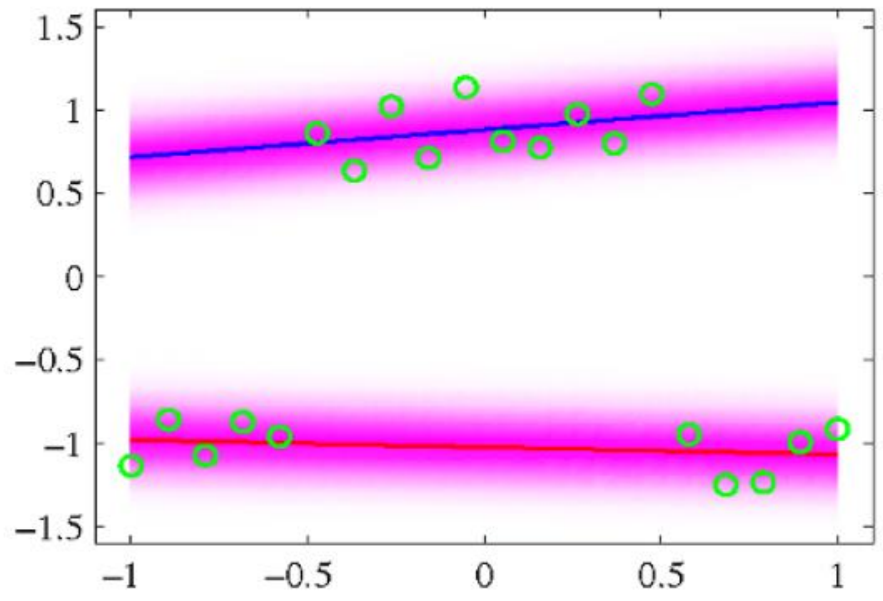
- Easily interpretable decision process
  - Widely used in practice, e.g. medical diagnosis

- Not very good performance
  - Restricted partition of space
  - Restricted to choose one model per instance
  - Unstable

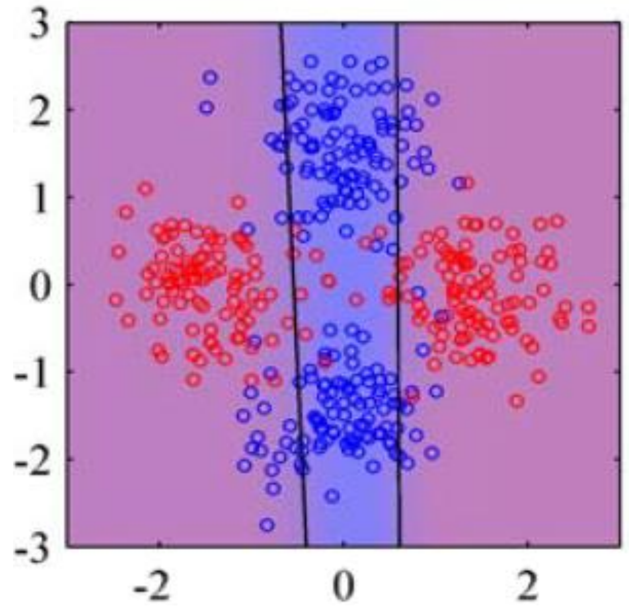
Mixture of Supervised Models

$$f(x) = \sum_i \pi_k \phi_k(x, w)$$

Mixture of linear regression models



Mixture of logistic regression models

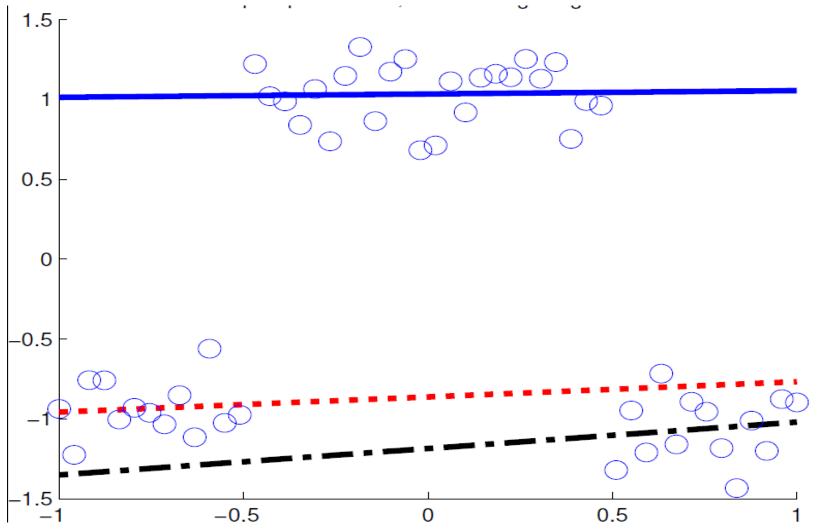


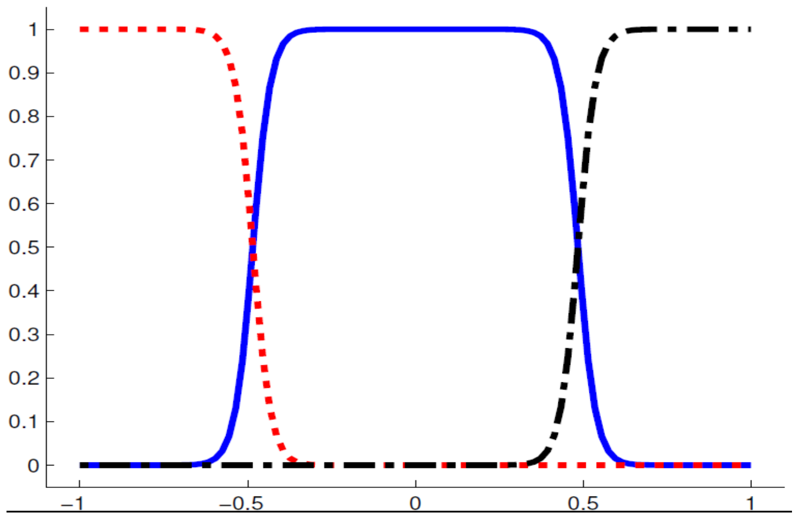
- Training using EM

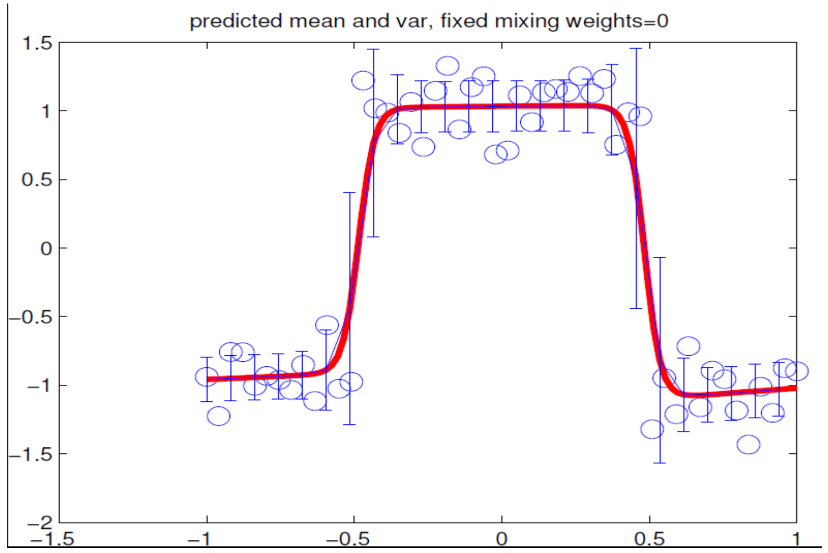
Conditional Mixture of Supervised Models

- Mixture of experts

$$f(x) = \sum_i \pi_k(x)\phi_k(x,w)$$







Bootstrap Aggregation / Bagging

- Individual models (e.g. decision trees) may have high variance along with low bias

- Construct M bootstrap datasets
- Train separate copy of predictive model on each
- Average prediction over copies

$$f(x) = \frac{1}{M} \sum_{i} f_m(x)$$

- If the errors are uncorrelated, then bagged error reduces linearly with M

Random Forests

- Training same algorithm on bootstraps creates correlated errors

- Randomly choose (a) subset of variables and (b) subset of training data

- Good predictive accuracy
- Loss in interpretability

Boosting

- Combining weak learners, ϵ-better than random
  - E.g. Decision stumps

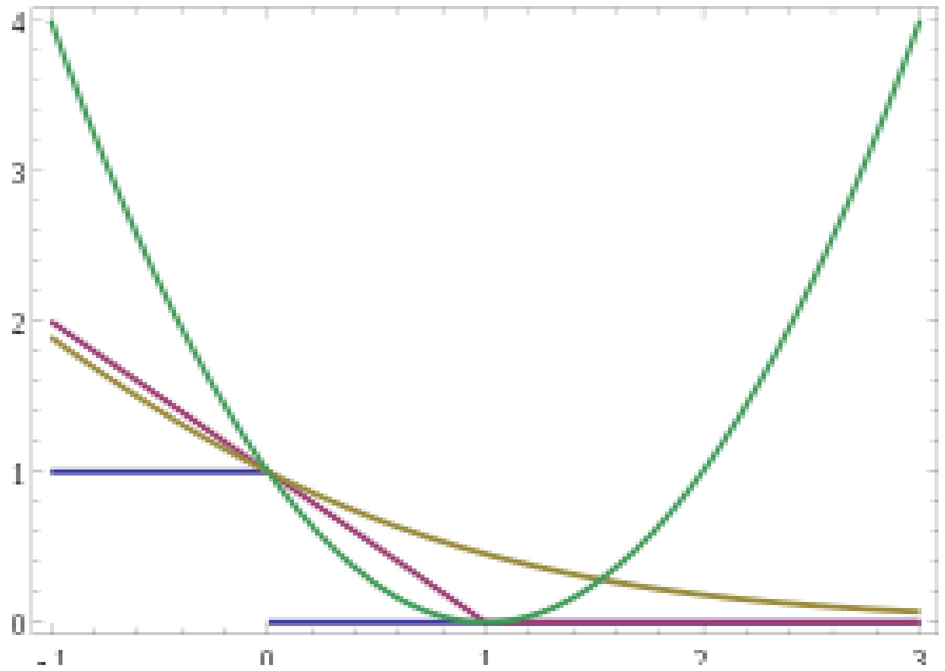
- Sequence of weighted datasets
- Weight of data point in each iteration proportional to no of misclassifications in earlier iterations

- Specific weighting scheme depends on loss function
- Theoretical bounds on error

Example loss functions and algorithms

- Squared error $(y_i - f(x_i))^2$
- Absolute error $|y_i - f(x_i)|$

- Squared loss $(1 - \tilde{y}_i f(x_i))^2$
- 0-1 loss $I(\tilde{y}_i \neq f(x_i))$
- Exponential loss $\exp(-\tilde{y}_i f(x_i))$
- Logloss $\frac{1}{\log 2}\log(1 + e^{-\tilde{y}_i f(x_i)})$
- Hinge loss $|1 - \tilde{y}_i f(x_i)|_+$



Example: AdaBoost

- Binary classification problem + Exponential loss

1. Initialize $w_n^{(1)} = \frac{1}{N}$
2. Train classifier $y_m(x)$ minimizing $\sum_n w_n^{(m)} I(y_m(x_n) \neq y_n)$
3. Evaluate $\epsilon_m = \frac{\sum_n w_n^{(m)} I(y_m(x_n) \neq y_n)}{\sum_n w_n^{(m)}}$ and $\alpha_m = \log \frac{1-\epsilon_m}{\epsilon_m}$
4. Update wts $w_n^{(m+1)} = w_n^{(m)} \exp\{\alpha_m I(y_m(x_n) \neq y_n)\}$
5. Predict $f_M(x) = sgn(\sum_{i=1}^{M} \alpha_m y_m(x))$

Neural networks: Multilayer Perceptrons

- Multiple layers of logistic regression models
- Parameters of each optimized by training

- Motivated by models of the brain
- Powerful learning model regardless

LR and R remembered …

- Linear models wi tions

$$y(x,w) = f(\sum_i w_i \phi_i(x))$$

- Fixed basis functions
- Non-linear transformation
- ϕ_i linear $\hat{y}(x; w, v) = h(\sum_{j=1\ to\ M} w_{kj}\ g(\sum_{i=1\ to\ D} v_{ji} x_i))$ tion

Feed-forward network functions

- M linear combinations of input variables

$$a_j = \sum_{i=1 \ to \ D} v_{ji} x_i$$

- Apply non-linear activation function

$$z_j = g(a_j)$$

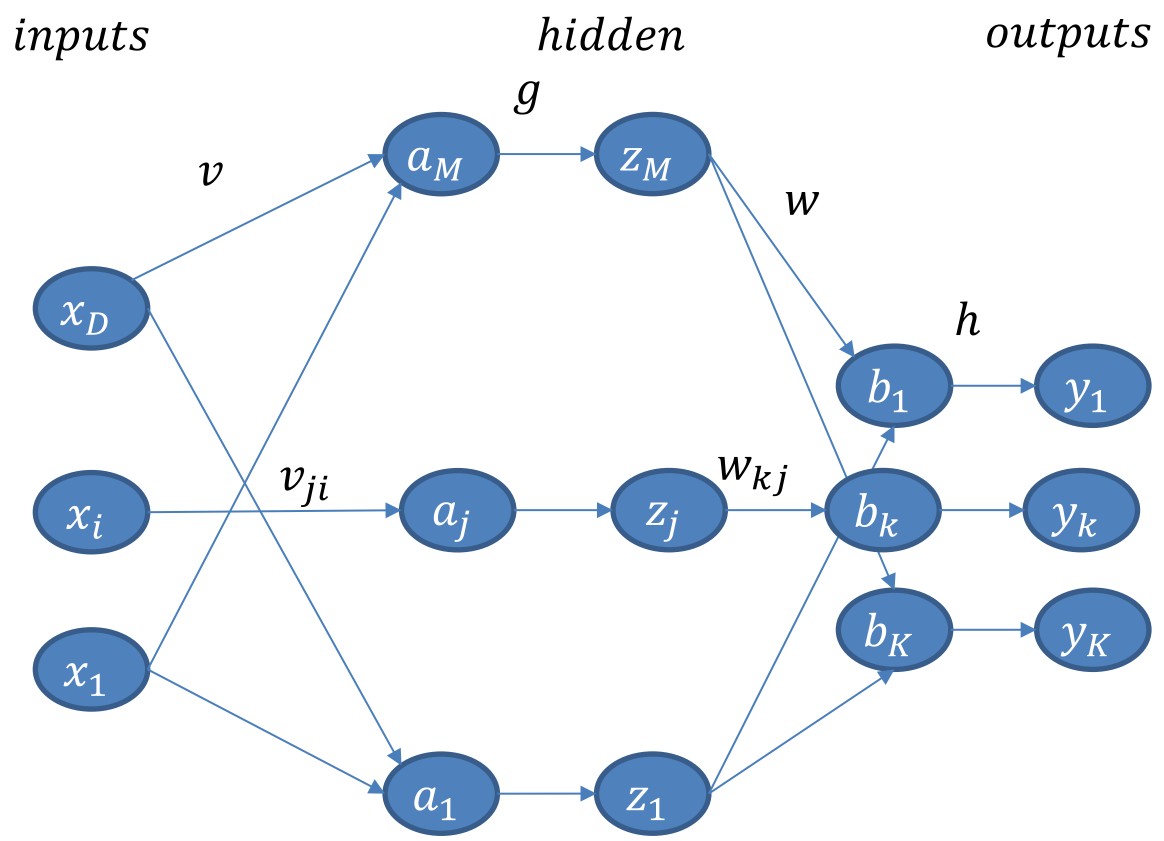
- Linear combinations to get output activations

$$b_k = \sum_{j=1 \ to \ M} w_{kj} z_j$$

- Apply output activation function to get outputs

$$y_k = h(b_k)$$

Network Representation



Easy to generalize to multiple layers

Power of feed-forward networks

- Universal approximators

  A 2 layer network with linear outputs can uniformly approximate any smooth continuous function with arbitrary accuracy given sufficient number of nodes in hidden layer

- Why are >2 layers needed?

Training

- Formulate error function in terms of weights

$$E(w, v) = \sum_{i=1\ to\ N} \left|\left|\hat{y}(x_n; w, v) - y_n\right|\right|^2$$

- Optimize weights using gradient descent

$$(w, v)^{(t+1)} = (w, v)^{(t)} - \eta \nabla E((w, v)^{(t)})$$

- Deriving the gradient looks complicated because of feed-forward …

Error Backpropagation

- Full gradient: sequence of local computations and propagations over the network

Output layer

$$\frac{\partial E_n}{\partial w_{kj}} = \frac{\partial E_n}{\partial b_{nk}} \frac{\partial b_{nk}}{\partial w_{kj}} = \delta^w_{nk} z_{nj}$$

$$\delta^w_{nk} = \hat{y}_{nk} - y_{nk}$$

Hidden layer

$$\frac{\partial E_n}{\partial v_{ji}} = \frac{\partial E_n}{\partial a_{nj}} \frac{\partial a_{nj}}{\partial v_{ji}} = \delta^v_{nj} x_{ni}$$

$$\delta^v_{nj} = \sum_k \frac{\partial E_n}{\partial b_{nk}} \frac{\partial b_{nk}}{\partial a_{nj}} = \sum_k \delta^w_{nk} w_{kj} g'(a_{nj})$$

$forward\ function$

$$\begin{tikzcd}
x_i \arrow[r, "v_{ji}"] & a_j \arrow[r, "g"] & z_j \arrow[r, "w_{kj}"] & b_k \arrow[r, "h"] & \hat{y}_k & \\
 & & \delta^v_{nj} & \delta^w_{nk} & & y_k
\end{tikzcd}$$

$backward\ error$

$$\frac{\partial E}{\partial w} = \sum_n \frac{\partial E_n}{\partial w}$$

Backpropagation Algorithm

1. Apply input vector x_n and compute derived variables $a_j, z_j, b_k, \hat{y}_k$
2. Compute δ_{nk}^{w} at all output nodes
3. Back propagate δ_{nk}^{w} to compute δ_{nj}^{v} at all hidden nodes
4. Compute derivatives $\frac{\partial E_n}{\delta w_{kj}}$ and $\frac{\partial E_n}{\delta v_{ji}}$
5. Batch: Sum derivatives over all input vectors

- Vanishing gradient problem

Neural Network Regularization

- Given such a large number of parameters, preventing overfitting is vitally important

- Choosing the number of layers + no of hidden nodes
- Controlling the weights
  - Weight decay
- Early stopping
- Weight sharing
- Structural regularization
  - Convolutional neural networks for invariances in image data

So… Which classifier is the best in practice?

- Low dimensions (9-200)

1. Boosted decision trees
2. Random forests
3. Bagged decision trees
4. SVM
5. Neural nets
6. K nearest neighbors
7. Boosted stumps
8. Decision tree
9. Logistic regression
10. Naïve Bayes

- High dimensions (500-100K)

1. HMC MLP
2. Boosted MLP
3. Bagged MLP
4. Boosted trees
5. Random forests

Usage Notes

- A lot of slides are adopted from the presentations and documents published on internet by experts who know the subject very well.
- I would like to thank who prepared slides and documents.
- Also, these slides are made publicly available on the web for anyone to use
- If you choose to use them, I ask that you alert me of any mistakes which were made and allow me the option of incorporating such changes (with an acknowledgment) in my set of slides.

Sincerely,
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