Lecture 6:

Regression II:
Adaptive Basis Networks & Supervised Mixtures

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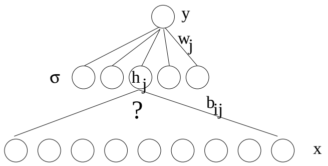
Artificial Neural Networks

- We saw neural nets for classification. Same idea for regression. ANNs are just adaptive basis regression machines of the form:
$$y_k = \sum_j w_{kj}\sigma(\mathbf{b}_j^\top \mathbf{x}) = \mathbf{w}_k\mathbf{h}$$
where $h_j = \sigma(\mathbf{b}_j^\top \mathbf{x})$ are known as the *hidden unit activations*; y_k are the output units and x_i are the input units.
- The nonlinear scalar function σ is called an *activation function*. We usually use *invertible* and *differentiable* activation functions.
- Neural network models with these activations are often called *multi-layer perceptrons* (MLPs), in analogy with the classic perceptron that used a hard-threshold activation.
- In general we want a saturating activation function.
- Sometimes we put an activation on the outputs also: $y_k = \sigma(\mathbf{w}_k\mathbf{h})$.

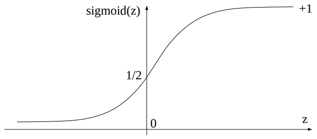
Adaptive Basis Regression

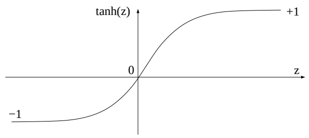
- Previously we considered the generalized linear model
$$y = \sum_j w_j h_j(\mathbf{x})$$
- Originally, the $h_j(\cdot)$ were fixed and we were finding w_j. Now we want to learn *both* the basis functions h_j and weights w_j.
- Today we consider a fixed number of *adaptive* basis functions. (Another way to learn is to select from a large set of candidates h_j.)
- Of course, for a single output we could just absorb w_j into h_j but for multiple outputs this is not possible.



Common Activation Functions

- If the activation function is *linear*, the whole network reduces* to a linear network: equivalent to linear regression. [Only if there are at least as many hiddens as inputs and outputs.]
- Two nonlinear activation functions: *sigmoid* and *hyperbolic tangent*
$$\text{sigmoid(z)} = \frac{1}{1+\exp(-z)} \qquad \text{tanh(z)} = \frac{\exp(z)-\exp(-z)}{\exp(z)+\exp(-z)}$$

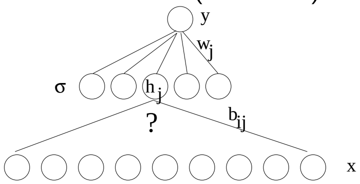




- For small weights, these functions operate near zero and behave almost linearly so the whole network is essentially linear.
- It is often a good idea to add "skip weights" directly connecting inputs to outputs to take care of this linear component directly.

Credit Assignment Problem

- Assume the basis functions are of the form $h_j(\mathbf{x}) = \sigma(\mathbf{b}_j^\top \mathbf{x})$.
- If we knew the desired values h_j^* of $h_j(\mathbf{x})$ we could find $\mathbf{b}_j$ by doing linear regression from $\mathbf{x}$ to $\sigma^{-1}(h_j^*)$.
- Problem: these values are unknown ("hidden"). Must find them.



- Basic idea: try changing the basis functions' values and see how the final output y (and thus the error) is affected.
- If we change several basis functions and the output gets better, which one was responsible? This is the *credit assignment problem*.
- Solution: only change one at a time!

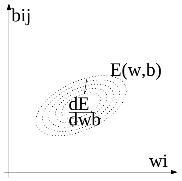
Backpropagation: error gradient in ANNs

- In layered networks (even with more than two layers), there is an elegant, efficient recursive algorithm for computing the gradients of any differentiable error function with respect to each of the weights using message passing up and down the network.
- The calculations depend on which error function is used at output (e.g. squared error or classification loss) and on which nonlinear activation function is used at the hidden units (e.g. tanh/sigmoid).
- Once we have the gradient, we can update the weights using

1. Batch training: sum gradients over all data cases (examples) in the training set, then update weights, then repeat.
2. Mini-batch: sum gradients over next n_{batch} cases, update.
3. Online training: update based on gradient for one case at a time.

Partial Derivatives and Weight Space Again

- Question: if we wiggle $h_j(\mathbf{x})$ *and keep everything else the same*, does the error get better or worse?
- Luckily, calculus has an answer to exactly this question: $\frac{\partial E}{\partial h_j}$.
- Plan: use a differentiable cost function E on the outputs and inside the basis functions $h_j(\mathbf{x})$. Now compute the *partial derivative* of each parameter with respect to the error: $\frac{\partial E}{\partial h_j}$.
- Use the *chain rule* to compute gradient components $\frac{\partial E}{\partial b_{ij}} = \frac{\partial E}{\partial h_j}\frac{\partial h_j}{\partial b_{ij}}$

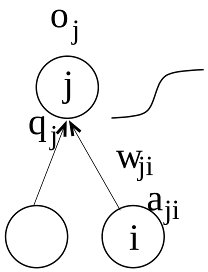


Adaptive basis regularization is all about descending the error surface in (w,b) weight space by following the gradient.

- The trick becomes computing these derivatives efficiently.

Backpropagation: some notation

- a_{ji} → i^{th} input to unit j.
  w_{ji} → weight associated with i^{th} input to j.
  $q_j = \sum_i w_{ji} a_{ji}$ → net input to unit j.
  o_j → output of unit j.
- For hidden units j, $o_j = \sigma(q_j)$.
- For input units i, $o_i = x_i$ (and $q_i, a_{i\cdot}, w_{i\cdot}$ are undefined).
- For output units k, $o_k = \sigma(q_k)$ or $o_k = q_k$.



Derivative of Output Error

- Assuming the error is additive across examples:

$$E = \sum_n E_n$$

$$\frac{\partial E_n}{\partial w_{ji}} = \frac{\partial E_n}{\partial q_j}\frac{\partial q_j}{\partial w_{ji}}$$
$$= \frac{\partial E_n}{\partial q_j} a_{ji}$$

- So the real question is how to efficiently compute the derivative of the output error with respect to the net input of each unit: $\frac{\partial E_n}{\partial q_j}$.
- To do this we need to compute the derivative of a unit's output with respect to its net input, i.e. the derivative of the activation function.

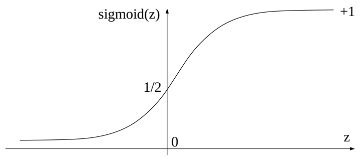
Derivative of Activation Function

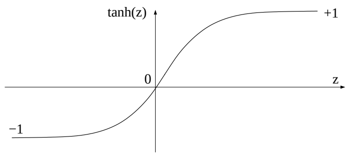
- For a sigmoid activation, $o_j = \sigma(q_j) = \frac{1}{1+\exp(-q_j)}$ and

$$\frac{\partial o_j}{\partial q_j} = o_j(1 - o_j)$$

- For a tanh activation, $o_j = \sigma(q_j) = \frac{\exp(q_j)-\exp(-q_j)}{\exp(q_j)+\exp(-q_j)}$ and

$$\frac{\partial o_j}{\partial q_j} = (1 - o_j^2)$$





Output Units

- For output unit(s) o_k, $\frac{\partial E_n}{\partial q_k} = \frac{\partial E_n}{\partial o_k}$.
- Let's assume squared error and sigmoid activations:

$$E_n = \sum_k (y_{nk} - o_{nk})^2$$

$$\frac{\partial E_n}{\partial o_k} = -2(y_k - o_k)\frac{\partial o_k}{\partial q_k}$$
$$= -2(y_k - o_k)o_k(1 - o_k)$$

- Putting it all together, the final derivative is:

$$\frac{\partial E_n}{\partial w_{kj}} = -2(y_k - o_k)o_k(1 - o_k)a_{kj}$$

(This assumed activations on outputs.)
(We dropped the n from y_k and o_k for ease.)

Hidden Units

- Let $\delta_j = \frac{\partial E_n}{\partial q_j}$ for all units.
- F_j are the units which j feeds into (undefined if j is an output).

$$\delta_j = \frac{\partial E_n}{\partial q_j} = \sum_{i \in F_j} \frac{\partial E_n}{\partial q_i}\frac{\partial q_i}{\partial q_j} = \sum_{i \in F_j} \delta_i \frac{\partial q_i}{\partial q_j}$$
$$= \sum_{i \in F_j} \delta_i \frac{\partial q_i}{\partial o_j}\frac{\partial o_j}{\partial q_j}$$
$$= \frac{\partial o_j}{\partial q_j} \sum_{i \in F_j} \delta_i w_{ij}$$

(assume sigmoid activation)

$$= o_j(1 - o_j) \sum_{i \in F_j} \delta_i w_{ij}$$

Recursion for Hidden Units

- The previous equations lead to a recursion for computing δs:

$$\delta_j = o_j(1 - o_j) \sum_{i \in F_j} \delta_i w_{ij}$$

- This recursive runs downwards, from the top of the network back towards the inputs. We initialize it at the output units k using:

$$\delta_k = \frac{\partial E_n}{\partial q_k} = \frac{\partial E_n}{\partial o_k} = -2(y_k - o_k)o_k(1 - o_k)$$

- Given the δs we can compute the final gradients:

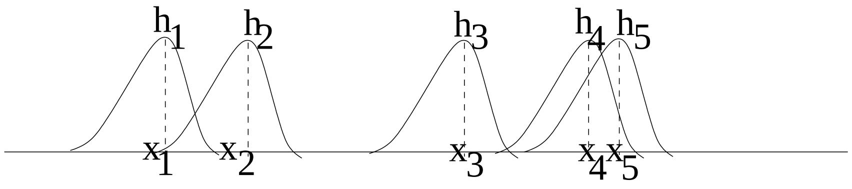
$$\frac{\partial E_n}{\partial w_{ji}} = \delta_j a_{ji}$$

Radial Basis Networks

- Instead of sigmoidal hidden units, we can use Gaussian shaped "bumps" as our basis functions:

$$h_j(\mathbf{x}) = \exp\left[-\frac{1}{2\sigma^2}\|\mathbf{x} - \mathbf{z}_j\|^2\right]$$

- The goal now is to *learn* the bump centres $\mathbf{z}_j$.
(Of course, we also have to set σ^2 somehow.)
- How? You got it! Take the derivative using backprop.
- Now, the activation function derivatives will be different, but the basic algorithm is exactly the same.



Backprop Algoritm

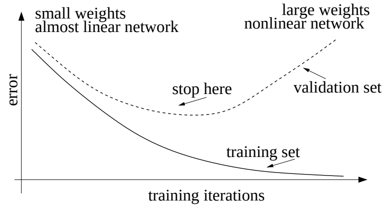
- The final backprop procedure does this for each training case:
  1. Propagate the inputs forward through the network:
  inputs: $o_i \leftarrow x_i$
  hiddens & outputs: $o_j \leftarrow \sigma(\sum_i w_{ji} x_j)$
  2. Compute the output error $E_n = \sum_k (y_k - o_k)^2$ for this case.
  3. Propagate the deltas backwards through the network:
  outputs: $\delta_k \leftarrow -2(y_k - o_k)o_k(1 - o_k)$
  hiddens: $\delta_j \leftarrow o_j(1 - o_j) \sum_{i \in F_j} \delta_i w_{ij}$
  4. Compute the gradients: $\frac{\partial E_n}{\partial w_{ji}} = \delta_j a_{ji}$
- Batch: sum errors and gradients over all training cases.
Mini-batch: sum errors and gradients over next n_{batch} cases.
Online: return gradient and error for this one case.

Backprop is efficient

- What's so deep about the backprop algorithm?
Isn't is just the chain rule applied to the ANN model? Yes, but...
- It does all gradient computations in $O(|W|)$ rather than $O(|W|^2)$.
[If you just write down the derivatives, each one contains some forward activation terms. It takes $O(|W|)$ to compute these terms, and there are $|W|$ weights so the naive procedure is $O(|W|^2)$.]
- Backprop uses messages and caching to share forward and backward calculations across the network and so is roughly $O(3|W|)$.
This is the same time complexity as to make a single forward pass!
- The original backprop paper is:
Learning representation by backpropagating errors,
Rumelhart, Hinton and Williams; (Nature, 1986)

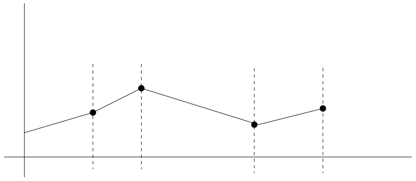
Network Regularlization

- We have to regularize ANNs and RBFs just like all other models.
- Shrinkage is the standard approach: here it is called *weight decay*: Add a term $\lambda \sum_{ij} w_{ij}^2$ to the cost function.
- This adds $-2\lambda w_{ij}$ to the gradient of each weight. Makes large weights get smaller (hence the name).
- Set λ by (cross-)validation.
- Can also start with small weights (and thus a linear network) and stop training when the (cross-)validation error starts to increase. This is called *early stopping*, and effectively keeps weights small.



Divide and Conquer

- One important idea in regression, similar to that in decision trees for classification, is to divide the problem into many regions so that within each region a simple model (e.g. linear) will suffice.
- If we divide into fixed regions, we have a general basis model (e.g. splines, CART). But what if we want to adjust the boundaries also?



- Problem: since the cost function is *piecewise constant* with respect to these boundaries, taking derivatives will not work.
- Solution: use "soft" splits of the data space, rather than hard splits. Radial Basis Networks (RBFs) are a simple example of this.

Multi-layer nets and representational capacity

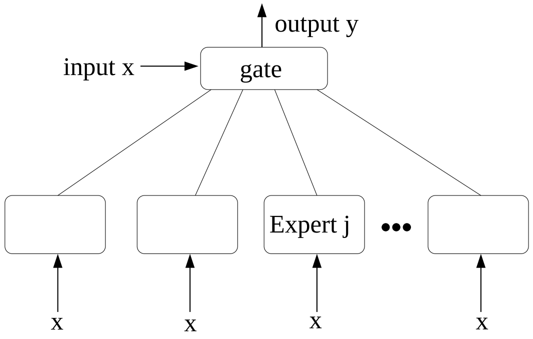
- We have considered only one hidden layer but we can have more.
- However, there is a deep result, (Kolmogorov's theorem) which tells us that *any* real valued function of K real inputs can be created by composing addition and single input functions.
  [This answered Hilbert's 13th problem in the affirmative, which asked if specific 3-variable functions could be written as compositions of continuous functions of two or less variables.]
- In other words, there are *no* true functions of two variables. e.g. $xy = \exp(\log x + \log y) \quad \log xy = \log x + \log y \quad \ldots$
- This tells us that a one-hidden layer net will always do the job, in theory. But it may take *a lot* of hidden units.
- Want to know more?

F. Girosi and T. Poggio. Kolmogorov's theorem is irrelevant. Neural Computation, 1(4):465–469, 1989.

V. Kurkova, "Kolmogorov's Theorem Is Relevant", Neural Computation, 1991, Vol. 3, pp. 617–622.

Mixtures of Experts

- Basic idea: there are a collection of "experts", each of which can produce sensible outputs $\mathbf{y}$ for a small region of the input space $\mathbf{x}$.
- There is also a "manager" or "gate"which decides which expert should be called upon for a particular set of inputs.
- We must train *both* the gate and the experts.



How the Experts and Gate Interact

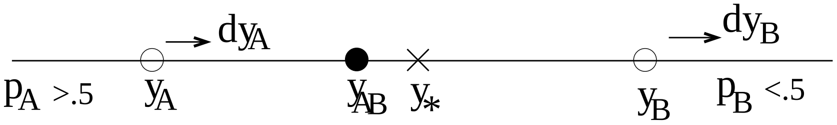
- The gate must look at the input and the proposed outputs of each expert to come up with an overall output.
  (Remember that the true output is unknown at test time!)
- The gate gives each expert a score, representing how well it thinks the expert can predict the output on this input vector.
- How should the gate be used to combine the experts?
  - Select the best expert (max score) and report its output?
  - Linearly combine the expert outputs based on the expert scores?
  - Stochastically select an expert based on the scores?

Linear Combination

- Let the score assigned by the gate to expert j be $\eta_j(\mathbf{x})$.
  Let the associated probabilities be $g_j = \exp \eta_j / \sum_k \exp \eta_k$.
  Let the output of each expert be $\mathbf{y}_j$.
- Linear combination of the experts' outputs:

$$p(\mathbf{y}|\mathbf{x}) = \mathcal{N}(\mathbf{y}; \textstyle\sum_j g_j \mathbf{y}_j, \Sigma)$$

- Seems like an obvious solution, but it actually encourages co-operation instead of specialization.
- This can lead to crazy gradients.

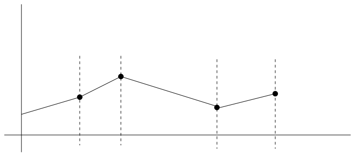


Hard Selection

- Let the score assigned by the gate to expert j be $\eta_j(\mathbf{x})$.
  Let the output of each expert be $\mathbf{y}_j$.
  Assume there is Gaussian noise with covar Σ on the outputs.
- If the gate selects the best expert, it is just doing a hard partitioning of the input space:

$$p(\mathbf{y}|\mathbf{x}) = \mathcal{N}(\mathbf{y}; \mathbf{y}_k, \Sigma) \qquad \text{iff } g_k = \max \ \{g_j\}$$

- As we have seen, this makes the cost function piecewise constant with respect to gate parameters, so training the gate using gradients becomes very difficult.

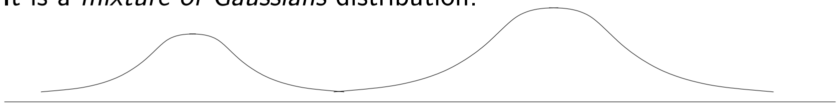


Stochastic Selection

- Gate picks a single expert, with probabilities dictated by scores:

$$p(\mathbf{y}|\mathbf{x}) = \sum_j g_j \mathcal{N}(\mathbf{y}; \mathbf{y}_j, \Sigma)$$

- The output distribution is no longer unimodal!
  It is a *mixture of Gaussians* distribution.



- Now, there is no co-operation. Each expert tries to get the answer right on their own, but the size of their learning signal depends on how likely the gate is to select them.
- Your first exposure to a very important idea: the difference between linearly combining means and linearly combining distributions.

MOE Components

- We typically use a *linear logistic regression* model for the gate:

$$p(j|\mathbf{x}) = g_j = \frac{\exp(\eta_j)}{\sum_k \exp(\eta_k)} = \frac{\exp(\mathbf{v}_j^\top \mathbf{x})}{\sum_k \exp(\mathbf{v}_k^\top \mathbf{x})}$$

- We can use a linear model for each expert, or a linear model with a nonlinearity, or a neural network or anything else:

$$\begin{aligned} p(\mathbf{y}|\mathbf{x}, j) &= \mathcal{N}(\mathbf{y}; \mathbf{U}_j\mathbf{x}, \Sigma) \qquad && \text{or} \\ p(\mathbf{y}|\mathbf{x}, j) &= \mathcal{N}(\mathbf{y}; f(\mathbf{U}_j\mathbf{x}), \Sigma) \qquad && \text{or } \ldots \end{aligned}$$

- In fact, radial basis networks and multilayer perceptrons/neural networks can be thought of as very simple mixtures of experts which use linear combination to fuse the experts and have a gate which is a constant function (represented by the last layer of weights).

Gradients for a Mixture of Experts

- The gradients include the *posterior* probability of each expert:

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

- Think of a *latent* or *hidden* unobserved random variable associated with each data case indicating which expert was responsible for generating its output given the input.
- There is a fundamental idea here: *sum over all possible ways in which the model could have produced the data*.
- The gradient for each expert is like that of a normal regression problem but with the data weighted by the expert posterior.
- The gradient of the gate parameters depends on the difference between the prior probability of an expert (as predicted by the gate) and the posterior (as predicted by how well they predict the true output). This is like logistic regression with soft targets.

Objective Function for MOEs

- Consider the log likelihood function for the linear MOE architecture:

$$\begin{aligned} \ell(\mathbf{v}, \mathbf{U}) &= \sum_n \log p(\mathbf{y}_n|\mathbf{x}_n) \\ &= \sum_n \log \sum_j \frac{\exp(\mathbf{v}_j^\top \mathbf{x}_n)}{\sum_k \exp(\mathbf{v}_k^\top \mathbf{x}_n)} \mathcal{N}(\mathbf{y}_n; \mathbf{U}_j\mathbf{x}_n, \Sigma) \end{aligned}$$

- For maximum likelihood learning, we want to take derivatives of this objective function with respect to the parameters.
- This looks hard! The objective function is a log of a sum.
- Actually the gradients come out quite nicely:

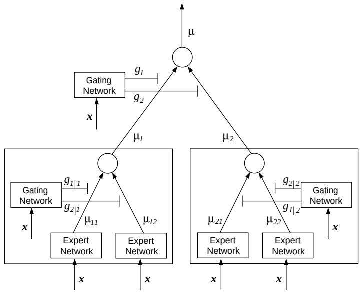
$$\begin{aligned} \partial\ell/\partial\mathbf{U}_j &= \sum_n p(j|\mathbf{x}_n, \mathbf{y}_n) \left(\mathbf{y}_n - \mathbf{U}_j\mathbf{x}_n\right) \mathbf{x}_n^\top \\ \partial\ell/\partial\mathbf{v}_j &= \sum_n \left(p(j|\mathbf{x}_n, \mathbf{y}_n) - p(j|\mathbf{x}_n)\right) \mathbf{x}_n \end{aligned}$$

MOE at Test Time

- Assume we have trained a MOE. How do we use it at test time?
- The correct thing to do is to get the test inputs $\mathbf{x}_{test}$, probabilistically select an expert using the gate, report that expert's output, *and repeat the process many times*.
- This gives you a whole distribution $p(\mathbf{y}|\mathbf{x}_{test})$ over outputs given the single test input.
- However, we might want to *summarize* this distribution.
- We can choose the *mode* of this distribution, corresponding to the output of the most likely expert.
- Or we can choose the *mean* of this distribution, corresponding to the weighted sum of the expert outputs.
- Notice: even though we might use these tricks to summarize the outputs, the underlying model is still one of stochastic selection, and so our training will not be messed up.

Hierarchical Mixtures of Experts

- The simple MOE idea can be extended to a hierarchical architecture in which each expert is itself a MOE, until the last layer in which the experts actually make output predictions.



- Very similar to a decision tree for regression but trained using maximum likelihood rather than greedy minimization of impurity.

An Idea...

- What if instead of using the gradient to adjust MOE parameters, we just used the posterior weightings and solved a weighted least-squares problem for each expert and a soft-target logistic-regression problem for the gate.
- Both of these problems are convex, so we can solve them exactly without needing to do any gradient descent.
- Then we could alternate: find the "optimum" parameters given the current posterior weightings and then recalculate the weights given the new parameters, and repeat.
- We will explore this idea more soon. It is called *Expectation Maximization* or EM, and is a form of bound optimization as opposed to gradient methods.