Backpropagation: The Good, the Bad and the Ugly

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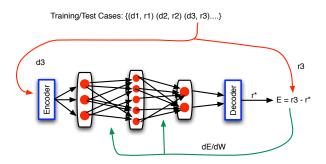


Supervised Learning

- Constant feedback from an instructor, indicating not only right/wrong, but also the correct answer for each training case.
- Many cases (i.e., input-output pairs) to be learned.
- Weights are modified by a complex procedure (back-propagation) based on output error.
- Feed-forward networks with back-propagation learning are the standard implementation.
- 99% of neural network applications use this.
- Typical usage: problems with a) lots of input-output training data, and b) goal of a mapping (function) from inputs to outputs.
- Not biologically plausible, although the cerebellum appears to exhibit some aspects.
- But, the result of backprop, a trained ANN to perform some function, can be very useful to neuroscientists as a sufficiency proof.

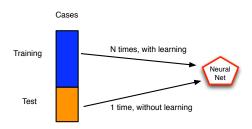


Backpropagation Overview



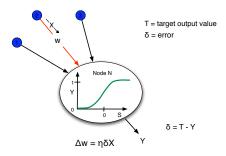
- Feed-Forward Phase Inputs sent through the ANN to compute outputs.
- Feedback Phase Error passed back from output to input layers and used to update weights along the way.

Training -vs- Testing



- Generalization correctly handling test cases (that ANN has not been trained on).
- Over-Training weights become so fine-tuned to the training cases that generalization suffers: failure on many test cases.

Widrow-Hoff (a.k.a. Delta) Rule

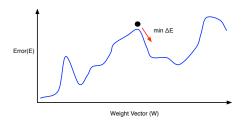


- Delta (δ) = error; Eta (η) = learning rate
- Goal: change w so as to reduce $|\delta|$.
- Intuitive: If $\delta > 0$, then we want to decrease it, so we must increase Y. Thus, we must increase the sum of weighted inputs to N, and we do that by increasing (decreasing) w if X is positive (negative).
- Similar for $\delta < 0$
- Assumes derivative of N's transfer function is everywhere non-negative.



Gradient Descent

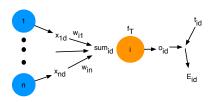
- Goal = minimize total error across all output nodes
- Method = modify weights throughout the network (i.e., at all levels) to follow the route of steepest descent in error space.



$$\Delta w_{ij} = -\eta \frac{\partial E_i}{\partial w_{ij}}$$



Computing $\frac{\partial E_i}{\partial w_{ij}}$



Sum of Squared Errors (SSE)

$$E_i = \frac{1}{2} \sum_{d \in D} (t_{id} - o_{id})^2$$

$$\frac{\partial E}{\partial w_{ij}} = \frac{1}{2} \sum_{d \in D} 2(t_{id} - o_{id}) \frac{\partial (t_{id} - o_{id})}{\partial w_{ij}} = \sum_{d \in D} (t_{id} - o_{id}) \frac{\partial (-o_{id})}{\partial w_{ij}}$$

Computing $\frac{\partial (-o_{id})}{\partial w_{ii}}$



Since output = f(sum weighted inputs)

$$\frac{\partial E}{\partial w_{ij}} = \sum_{d \in D} (t_{id} - o_{id}) \frac{\partial (-f_{\mathcal{T}}(sum_{id}))}{\partial w_{ij}}$$

where

$$sum_{id} = \sum_{k=1}^{n} w_{ik} x_{kd}$$

Using Chain Rule:
$$\frac{\partial f(g(x))}{\partial x} = \frac{\partial f}{\partial g(x)} \times \frac{\partial g(x)}{\partial x}$$

$$\frac{\partial (f_T(sum_{id}))}{\partial w_{ij}} = \frac{\partial f_T(sum_{id})}{\partial sum_{id}} \times \frac{\partial sum_{id}}{\partial w_{ij}} = \frac{\partial f_T(sum_{id})}{\partial sum_{id}} \times x_{jd}$$



Computing $\frac{\partial sum_{id}}{\partial w_{ii}}$ - Easy!!

$$\frac{\partial sum_{id}}{\partial w_{ij}} = \frac{\partial \left(\sum_{k=1}^{n} w_{ik} x_{kd}\right)}{\partial w_{ij}} = \frac{\partial \left(w_{i1} x_{1d} + w_{i2} x_{2d} + \dots + w_{ij} x_{jd} + \dots + w_{in} x_{nd}\right)}{\partial w_{ij}}$$

$$= \frac{\partial \left(w_{i1} x_{1d}\right)}{\partial w_{ij}} + \frac{\partial \left(w_{i2} x_{2d}\right)}{\partial w_{ij}} + \dots + \frac{\partial \left(w_{ij} x_{jd}\right)}{\partial w_{ij}} + \dots + \frac{\partial \left(w_{in} x_{nd}\right)}{\partial w_{ij}}$$

$$= 0 + 0 + \dots + x_{jd} + \dots + 0 = x_{jd}$$

Computing $\frac{\partial f_T(sum_{id})}{\partial sum_{id}}$ - Harder for some f_T

 f_T = Identity function: $f_T(sum_{id}) = sum_{id}$

$$\frac{\partial f_T(sum_{id})}{\partial sum_{id}} = 1$$

Thus:

$$\frac{\partial (f_T(sum_{id}))}{\partial w_{ij}} = \frac{\partial f_T(sum_{id})}{\partial sum_{id}} \times \frac{\partial sum_{id}}{\partial w_{ij}} = 1 \times x_{jd} = x_{jd}$$

$$f_T$$
 = Sigmoid: $f_T(sum_{id}) = \frac{1}{1 + e^{-sum_{id}}}$

$$\frac{\partial f_T(sum_{id})}{\partial sum_{id}} = o_{id}(1 - o_{id})$$

Thus:

$$\frac{\partial (f_T(sum_{id}))}{\partial w_{ij}} = \frac{\partial f_T(sum_{id})}{\partial sum_{id}} \times \frac{\partial sum_{id}}{\partial w_{ij}} = o_{id}(1 - o_{id}) \times x_{jd} = o_{id}(1 - o_{id})x_{jd}$$



The only non-trivial calculation

$$\begin{split} \frac{\partial f_{T}(sum_{id})}{\partial sum_{id}} &= \frac{\partial \left((1 + e^{-sum_{id}})^{-1} \right)}{\partial sum_{id}} = (-1) \frac{\partial (1 + e^{-sum_{id}})}{\partial sum_{id}} (1 + e^{-sum_{id}})^{-2} \\ &= (-1)(-1) e^{-sum_{id}} (1 + e^{-sum_{id}})^{-2} = \frac{e^{-sum_{id}}}{(1 + e^{-sum_{id}})^{2}} \end{split}$$

But notice that:

$$\frac{e^{-sum_{id}}}{(1+e^{-sum_{id}})^2} = f_T(sum_{id})(1-f_T(sum_{id})) = o_{id}(1-o_{id})$$

Putting it all together

$$\frac{\partial E_i}{\partial w_{ij}} = \sum_{d \in D} (t_{id} - o_{id}) \frac{\partial (-f_T(sum_{id}))}{\partial w_{ij}} = -\sum_{d \in D} \left((t_{id} - o_{id}) \frac{\partial f_T(sum_{id})}{\partial sum_{id}} \times \frac{\partial sum_{id}}{\partial w_{ij}} \right)$$

So for f_T = Identity:

$$\frac{\partial E_i}{\partial w_{ij}} = -\sum_{d \in D} (t_{id} - o_{id}) x_{jd}$$

and for f_T = Sigmoid:

$$\frac{\partial E_i}{\partial w_{ij}} = -\sum_{d \in D} (t_{id} - o_{id}) o_{id} (1 - o_{id}) x_{jd}$$



Weight Updates (f_T = Sigmoid)

Batch: update weights after each training epoch

$$\Delta w_{ij} = -\eta \frac{\partial E_i}{\partial w_{ij}} = \eta \sum_{d \in D} (t_{id} - o_{id}) o_{id} (1 - o_{id}) x_{jd}$$

The weight changes are actually computed after each training case, but w_{ij} is not updated until the epoch's end.

Incremental: update weights after each training case

$$\Delta w_{ij} = -\eta \frac{\partial E_i}{\partial w_{ij}} = \eta (t_{id} - o_{id}) o_{id} (1 - o_{id}) x_{jd}$$

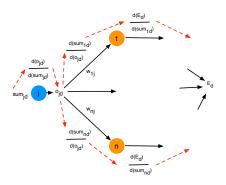
- A lower learning rate (η) recommended here than for Batch method.
- Can be dependent upon case-presentation order. So randomly sort the cases after each epoch.

Stochastic Gradient Descent (SGD)

Similar to Batch, but processing (feed forward + gradient calculations) a subset (minibatch) of D between each weight update.



Backpropagation in Multi-Layered Neural Networks



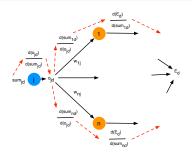
For each node (j) and each training case (d), backpropagation computes an error term:

 $\delta_{jd} = \frac{\partial E_d}{\partial sum_{jd}}$

by calculating the influence of sum_{jd} along each connection from node j to the next downstream layer.



Computing δ_{jd}



Along the upper path, the contribution to $\frac{\partial E_d}{\partial sum_{jd}}$ is:

$$\frac{\partial o_{jd}}{\partial sum_{jd}} \times \frac{\partial sum_{1d}}{\partial o_{jd}} \times \frac{\partial E_d}{\partial sum_{1d}}$$

So summing along all paths:

$$\frac{\partial E_d}{\partial sum_{jd}} = \frac{\partial o_{jd}}{\partial sum_{jd}} \sum_{k=1}^{n} \frac{\partial sum_{kd}}{\partial o_{jd}} \frac{\partial E_d}{\partial sum_{kd}}$$



Computing δ_{jd}

Just as before, most terms are 0 in the derivative of the sum, so:

$$\frac{\partial sum_{kd}}{\partial o_{jd}} = w_{kj}$$

Assuming f_T = a sigmoid:

$$\frac{\partial o_{jd}}{\partial sum_{jd}} = \frac{\partial f_T(sum_{jd})}{\partial sum_{jd}} = o_{jd}(1 - o_{jd})$$

Thus:

$$\delta_{jd} = \frac{\partial E_d}{\partial sum_{jd}} = \frac{\partial o_{jd}}{\partial sum_{jd}} \sum_{k=1}^{n} \frac{\partial sum_{kd}}{\partial o_{jd}} \frac{\partial E_d}{\partial sum_{kd}}$$
$$= o_{jd}(1 - o_{jd}) \sum_{k=1}^{n} w_{kj} \delta_{kd}$$

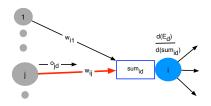
Computing δ_{id}

Note that δ_{jd} is defined recursively in terms of the δ values in the next downstream layer:

$$\delta_{jd} = o_{jd}(1 - o_{jd}) \sum_{k=1}^{n} w_{kj} \delta_{kd}$$

So all δ values in the network can be computed by moving backwards, one layer at a time.

Computing $\frac{\partial E_d}{\partial w_{ii}}$ from δ_{jd} - Easy!!



The only effect of w_{ij} upon the error is via its effect upon sum_{id} , which is:

$$\frac{\partial \mathit{sum}_{\mathit{id}}}{\partial \mathit{w}_{\mathit{ij}}} = \mathit{o}_{\mathit{jd}}$$

So:

$$\frac{\partial \textit{E}_{\textit{d}}}{\partial \textit{w}_{\textit{ij}}} = \frac{\partial \textit{sum}_{\textit{id}}}{\partial \textit{w}_{\textit{ij}}} \times \frac{\partial \textit{E}_{\textit{d}}}{\partial \textit{sum}_{\textit{id}}} = \frac{\partial \textit{sum}_{\textit{id}}}{\partial \textit{w}_{\textit{ij}}} \times (\delta_{\textit{id}}) = o_{\textit{jd}} \delta_{\textit{id}}$$

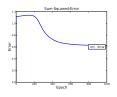
Computing Δw_{ij}

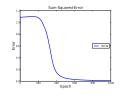
Given an error term, δ_{id} (for node i on training case d), the update of w_{ij} for all nodes j that feed into i is:

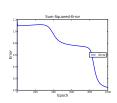
$$\Delta w_{ij} = -\eta \frac{\partial E_d}{\partial w_{ij}} = -\eta (o_{jd}\delta_{id}) = -\eta \delta_{id}o_{jd}$$

So given δ_{id} , you can easily calculate Δw_{ij} for all incoming arcs.

Learning XOR



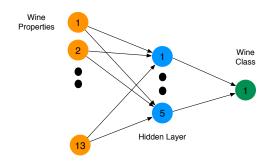




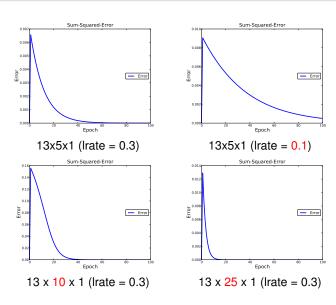
- Epoch = All 4 entries of the XOR truth table.
- 2 (inputs) X 2 (hidden) X 1 (output) network
- Random init of all weights in [-1 1].
- Not linearly separable, so it takes awhile!
- Each run is different due to random weight init.

Learning to Classify Wines

Class	Properties							
1	14.23	1.71	2.43	15.6	127	2.8		
1	13.2	1.78	2.14	11.2	100	2.65		
2	13.11	1.01	1.7	15	78	2.98		
3	13.17	2.59	2.37	20	120	1.65		
				:				



Wine Runs



Backwards in high heels

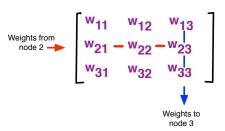
I did everything he did, but backwards and in high heels

.... Ginger Rogers describing her career as Fred Astaire's dance partner.

Now we'll go through similar backpropagation derivations, but with matrices: backwards in high heels.

Matrix Notation

- In the literature, the notation w_{ij} may EITHER denote the weight on the connection from node j to node i OR the connection from node i to node j. This varies; there is no standard.
- When working with matrices, it is often easier when w_{ij} := weight on connection i → j This is the case in the remainder of this slide series.
- Then, the normal syntax for matrix row-column indices implies that:
 - The values in row i are written as w_{i?} and denote the weights on the outputs of node i.
 - The values in column j are written as w_{?j} and denote the weights on the inputs to node j.





Tensor Operations (Notation, Rules)

- Tensors = arrays of 1 or more dimensions. They will be represented by CAPITAL letters. Scalers will be in small letters, often with subscripts.
- W X = dot product of vectors OR the multiplication of a matrix with another matrix or vector, depending upon the situation. This is similar to the semantics of the (very versatile) numpy.dot function.
- The Product Rule for tensors (A, B, X):

$$\frac{\partial (A \bullet B)}{\partial X} = A \bullet \frac{\partial B}{\partial X} + \frac{\partial A}{\partial X} \bullet B$$

 The Chain Rule for tensor X and functions F and G, which take tensors as input and produce tensors as output.

$$\frac{\partial F(G(X))}{\partial X} = \frac{\partial F(.)}{\partial G(.)} \bullet \frac{\partial G(X)}{\partial X}$$

• If tensors A and B have dimensions m and n, respectively, then the Jacobian $J = \frac{\partial A}{\partial B}$ has dimensions m x n.



Tensor Tension

In the numerator layout for Jacobians:

$$J_{i,\dots q,r,\dots z} = \frac{\partial A_{i,\dots q}}{\partial B_{r,\dots z}}$$

In the denominator layout for Jacobians:

$$J_{i,\dots q,r\dots z} = \frac{\partial A_{r,\dots z}}{\partial B_{i,\dots q}}$$

- The numerator layout is more common but is not a hard standard.
- These slides will use the numerator layout as much as possible. Any
 usage of denominator layout will be noted.
- Tensor calculus is the combination of linear algebra and multivariate calculus. It is very useful for mathematically describing the operations of deep-learning systems, but occasionally the link between theory and implementation gets twisted a bit.
- I try to minimize these twists, and I mark these twists/hacks.
- For more on tensor calculus, go to: explained.ai/matrix-calculus/



Numerator -vs- Denominator Layout

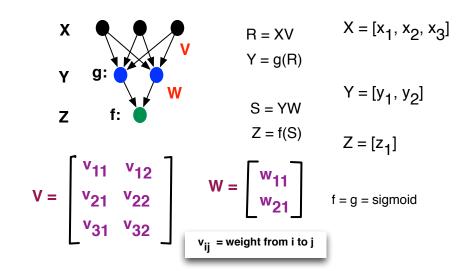
 Numerator Layout (A's index remains constant across each row; the first dimension of J pertains to A.)

$$J_{B}^{A} = \begin{bmatrix} \frac{\partial \mathbf{a}_{1}}{\partial b_{1}} & \frac{\partial \mathbf{a}_{1}}{\partial b_{2}} & \frac{\partial \mathbf{a}_{1}}{\partial b_{3}} \\ \frac{\partial \mathbf{a}_{2}}{\partial b_{1}} & \frac{\partial \mathbf{a}_{2}}{\partial b_{2}} & \frac{\partial \mathbf{a}_{2}}{\partial b_{3}} \\ \frac{\partial \mathbf{a}_{3}}{\partial b_{1}} & \frac{\partial \mathbf{a}_{3}}{\partial b_{2}} & \frac{\partial \mathbf{a}_{3}}{\partial b_{3}} \end{bmatrix}$$
(1)

 Denominator Layout (B's index remains constant across each row; the first dimension of J pertains to B.)

$$J_{B}^{A} = \begin{bmatrix} \frac{\partial a_{1}}{\partial b_{1}} & \frac{\partial a_{2}}{\partial b_{1}} & \frac{\partial a_{3}}{\partial b_{1}} \\ \frac{\partial a_{1}}{\partial b_{2}} & \frac{\partial a_{2}}{\partial b_{2}} & \frac{\partial a_{3}}{\partial b_{2}} \\ \frac{\partial a_{1}}{\partial b_{3}} & \frac{\partial a_{2}}{\partial b_{3}} & \frac{\partial a_{3}}{\partial b_{3}} \end{bmatrix}$$
 (2)

Backpropagation using Tensors



Goal: Compute $\frac{\partial Z}{\partial W}$

Using the Chain Rule of Tensor Calculus:

$$\frac{\partial Z}{\partial W} = \frac{\partial f(S)}{\partial W} = \frac{\partial f(S)}{\partial S} \bullet \frac{\partial S}{\partial W} = \frac{\partial f(S)}{\partial S} \bullet \frac{\partial (Y \bullet W)}{\partial W}$$

• f(S) is sigmoid, so $\frac{\partial f(S)}{\partial S} = f(S)(1 - f(S)) = z_1(1 - z_1)$, a scalar:

$$z_1(1-z_1)\frac{\partial (Y \bullet W)}{\partial W}$$

Using the product rule:

$$z_1(1-z_1)\frac{\partial (Y \bullet W)}{\partial W} = z_1(1-z_1)\left[\frac{\partial Y}{\partial W} \bullet W + Y \bullet \frac{\partial W}{\partial W}\right]$$

• Y is independent of W, so red term = 0. But $\frac{\partial W}{\partial W}$ is not simply 1, but:

$$\left(\begin{array}{c|c} 1 \\ 0 \\ 0 \\ 0 \\ 1 \end{array}\right)$$



$$Y \bullet \frac{\partial W}{\partial W} = (y_1, y_2) \bullet \begin{pmatrix} \begin{vmatrix} 1 \\ 0 \end{vmatrix} \\ \begin{vmatrix} 0 \\ 1 \end{vmatrix} \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$$

Putting it all together:

$$\frac{\partial Z}{\partial W} = z_1(1 - z_1) \times Y \bullet \frac{\partial W}{\partial W} = \begin{pmatrix} z_1(1 - z_1)y_1 \\ z_1(1 - z_1)y_2 \end{pmatrix} = \begin{pmatrix} \frac{\partial Z}{\partial W_{1,1}} \\ \frac{\partial Z}{\partial W_{2,1}} \end{pmatrix}$$

• For each case, c_k , in a minibatch, the forward pass will produce values for X, Y, and Z. Those values will be used to compute actual numeric gradients by filling in these symbolic gradients:

$$\frac{\partial Z}{\partial W}|_{c_k} = \begin{pmatrix} z_1(1-z_1)y_1 \\ z_1(1-z_1)y_2 \end{pmatrix}|_{c_k}$$

Tensor Calculations across Several Layers

Goal: Compute $\frac{\partial Z}{\partial V}$

• Expanding using the Chain Rule (with $\frac{\partial f(S)}{\partial S} = z_1(1-z_1)$, a scalar):

$$\frac{\partial Z}{\partial V} = \frac{\partial f(S)}{\partial V} = \frac{\partial f(S)}{\partial S} \bullet \frac{\partial S}{\partial V} = z_1(1 - z_1) \frac{\partial (Y \bullet W)}{\partial V}$$

Using the Product Rule:

$$\frac{\partial (Y \bullet W)}{\partial V} = \frac{\partial Y}{\partial V} \bullet W + Y \bullet \frac{\partial W}{\partial V} = \frac{\partial (g(R))}{\partial V} \bullet W$$

• W is indep. of V, so red term = 0; and Y = g(R). Using Chain Rule:

$$\frac{\partial (g(R))}{\partial V} \bullet W = \left[\frac{\partial g(R)}{\partial R} \bullet \frac{\partial R}{\partial V}\right] \bullet W$$

g(R) is sigmoid, and R is a vector (size 2), so:

$$\frac{\partial g(R)}{\partial R} = \begin{bmatrix} \frac{\partial g(r_1)}{\partial r_1} & \frac{\partial g(r_1)}{\partial r_2} \\ \frac{\partial g(r_2)}{\partial r_1} & \frac{\partial g(r_2)}{\partial r_2} \end{bmatrix} = \begin{bmatrix} y_1(1-y_1) & 0 \\ 0 & y_2(1-y_2) \end{bmatrix}$$



• Since $R = X \bullet V$, and using the Product Rule:

$$\frac{\partial R}{\partial V} = \frac{\partial (X \bullet V)}{\partial V} = X \bullet \frac{\partial V}{\partial V} + \frac{\partial X}{\partial V} \bullet V$$

• X is indep. of V, so red term = 0; $\frac{\partial V}{\partial V}$ is 4-dimensional:

• Take dot product of X = $[x_1, x_2, x_3]$ with each internal maxtrix of $\frac{\partial V}{\partial V}$:

$$X \bullet \frac{\partial V}{\partial V} = [x_1, x_2, x_3] \bullet \begin{pmatrix} \begin{vmatrix} 1 & 0 & | & 0 & 1 \\ 0 & 0 & | & 0 & 0 \\ 0 & 0 & | & 0 & 0 \end{vmatrix} \\ \begin{vmatrix} 0 & 0 & | & 0 & 0 \\ 1 & 0 & | & 0 & 0 \\ 0 & 0 & | & 0 & 0 \end{vmatrix} \\ \begin{vmatrix} 0 & 0 & | & 0 & 0 \\ 0 & 0 & | & 0 & 0 \\ 0 & 0 & | & 0 & 1 \end{vmatrix} \end{pmatrix}$$
$$= \begin{pmatrix} \begin{vmatrix} x_1 & 0 & | & | & 0 & x_1 & | \\ | & x_2 & 0 & | & | & 0 & x_2 & | \\ | & x_3 & 0 & | & | & 0 & x_3 & | \end{pmatrix}$$

Putting the pieces back together for $\frac{\partial Y}{\partial V} = \frac{\partial g(R)}{\partial R} \bullet \frac{\partial R}{\partial V}$:

$$\frac{\partial g(R)}{\partial R} \bullet \frac{\partial R}{\partial V} = \begin{bmatrix} y_1(1-y_1) & 0 \\ 0 & y_2(1-y_2) \end{bmatrix} \bullet \begin{pmatrix} | x_1 & 0 | | 0 & x_1 | \\ | x_2 & 0 | | 0 & x_2 | \\ | x_3 & 0 | | 0 & x_3 | \end{pmatrix}$$

$$\frac{\partial Y}{\partial V} = \begin{pmatrix} | x_1 y_1(1-y_1) & 0 | & | 0 & x_1 y_2(1-y_2) | \\ | x_2 y_1(1-y_1) & 0 | & | 0 & x_2 y_2(1-y_2) | \\ | x_3 y_1(1-y_1) & 0 | & | 0 & x_3 y_2(1-y_2) | \end{pmatrix}$$

Note: Row vectors of $\frac{\partial R}{\partial V}$ need to be treated as column vectors for the internal matrix multiplication. The results of each multiplication are then transposed (to get row vectors). Twist/Hack.



$$\frac{\partial(g(R))}{\partial V} \bullet W = \left[\frac{\partial g(R)}{\partial R} \bullet \frac{\partial R}{\partial V}\right] \bullet W$$

$$= \begin{pmatrix} | x_1 y_1 (1 - y_1) & 0 & | & | & 0 & x_1 y_2 (1 - y_2) & | \\ | x_2 y_1 (1 - y_1) & 0 & | & | & 0 & x_2 y_2 (1 - y_2) & | \\ | x_3 y_1 (1 - y_1) & 0 & | & | & 0 & x_3 y_2 (1 - y_2) & | \end{pmatrix} \bullet \begin{pmatrix} w_{11} \\ w_{21} \end{pmatrix}$$

$$= \begin{pmatrix} x_1 y_1 (1 - y_1) w_{11} & x_1 y_2 (1 - y_2) w_{21} \\ x_2 y_1 (1 - y_1) w_{11} & x_2 y_2 (1 - y_2) w_{21} \\ x_3 y_1 (1 - y_1) w_{11} & x_3 y_2 (1 - y_2) w_{21} \end{pmatrix} = \frac{\partial (Y \bullet W)}{\partial V}$$

Each of the 6 inner vectors is dotted with W. This is compatible with numpy.dot but may be a theoretical twist/hack.

...and finally...

$$\frac{\partial Z}{\partial V} = \frac{\partial f(S)}{\partial V} = z_1 (1 - z_1) \frac{\partial (Y \bullet W)}{\partial V}$$

$$= z_1 (1 - z_1) \times \begin{pmatrix} x_1 y_1 (1 - y_1) w_{11} & x_1 y_2 (1 - y_2) w_{21} \\ x_2 y_1 (1 - y_1) w_{11} & x_2 y_2 (1 - y_2) w_{21} \\ x_3 y_1 (1 - y_1) w_{11} & x_3 y_2 (1 - y_2) w_{21} \end{pmatrix}$$

$$= \begin{pmatrix} z_1 (1 - z_1) x_1 y_1 (1 - y_1) w_{11} & z_1 (1 - z_1) x_1 y_2 (1 - y_2) w_{21} \\ z_1 (1 - z_1) x_2 y_1 (1 - y_1) w_{11} & z_1 (1 - z_1) x_2 y_2 (1 - y_2) w_{21} \\ z_1 (1 - z_1) x_3 y_1 (1 - y_1) w_{11} & z_1 (1 - z_1) x_3 y_2 (1 - y_2) w_{21} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{\partial Z}{\partial v_{11}} & \frac{\partial Z}{\partial v_{12}} \\ \frac{\partial Z}{\partial v_{21}} & \frac{\partial Z}{\partial v_{22}} \\ \frac{\partial Z}{\partial v_{31}} & \frac{\partial Z}{\partial v_{32}} \end{pmatrix}$$

Gradients and the Minibatch

• For every case c_k in a minibatch, the values of X, Y and Z are computed during the forward pass. The symbolic gradients in $\frac{\partial Z}{\partial V}$ are filled in using these values in X,Y and Z (along with W), producing one numeric, 3 x 2 matrix **per case**:

$$\left(\frac{\partial Z}{\partial V}\right)_{|_{\mathcal{C}_{k}}} = \begin{pmatrix} \frac{\partial Z}{\partial V_{11}} & \frac{\partial Z}{\partial V_{12}} \\ \frac{\partial Z}{\partial V_{21}} & \frac{\partial Z}{\partial V_{22}} \\ \frac{\partial Z}{\partial V_{31}} & \frac{\partial Z}{\partial V_{32}} \end{pmatrix}_{|_{\mathcal{C}_{k}}}$$

$$= \left(\begin{array}{ccc} z_1(1-z_1)x_1y_1(1-y_1)w_{11} & z_1(1-z_1)x_1y_2(1-y_2)w_{21} \\ z_1(1-z_1)x_2y_1(1-y_1)w_{11} & z_1(1-z_1)x_2y_2(1-y_2)w_{21} \\ z_1(1-z_1)x_3y_1(1-y_1)w_{11} & z_1(1-z_1)x_3y_2(1-y_2)w_{21} \end{array}\right)_{|c_k|}$$

Gradients and the Minibatch

- In most Deep Learning situations, the gradients will be based on a loss function, L, not simply the output of the final layer. But that's just one more level of derivative calculations (see below).
- At the completion of a minibatch, the numeric gradient matrices are added together to yield the complete gradient, which is then used to update the weights.
- For any weight matrix U in the network, and minibatch M, update weight $u_{i,j}$ as follows:

$$(\frac{\partial L}{\partial u_{i,j}})_{|_{M}} = \sum_{c_{k} \in M} (\frac{\partial L}{\partial u_{i,j}})_{|_{c_{k}}}$$

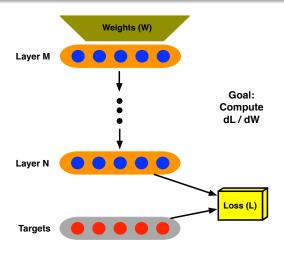
 η = learning rate

$$\triangle u_{i,j} = -\eta \left(\frac{\partial L}{\partial u_{i,j}}\right)_{|_{\mathbf{M}}}$$

- Tensorflow and PyTorch do all of this for you.
- Everytime you write Deep Learning code, be grateful!!



The Jacobian Product Chain



$$\frac{\partial L}{\partial W} = \frac{\partial L}{\partial N} \bullet \frac{\partial N}{\partial N - 1} \bullet \cdots \bullet \frac{\partial M + 1}{\partial M} \bullet \frac{\partial M}{\partial W}$$



Jacobian Matrix Linking Neighboring Layers: $Y \rightarrow Z$

$$\mathbf{J}_{Y}^{Z} = \begin{pmatrix} \frac{\partial z_{1}}{\partial y_{1}} & \frac{\partial z_{1}}{\partial y_{2}} & \cdots & \frac{\partial z_{1}}{\partial y_{n}} \\ \frac{\partial z_{2}}{\partial y_{1}} & \frac{\partial z_{2}}{\partial y_{2}} & \cdots & \frac{\partial z_{2}}{\partial y_{n}} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial z_{m}}{\partial y_{1}} & \frac{\partial z_{m}}{\partial y_{2}} & \cdots & \frac{\partial z_{m}}{\partial y_{n}} \end{pmatrix}$$

Note: This Jacobian is in numerator format.

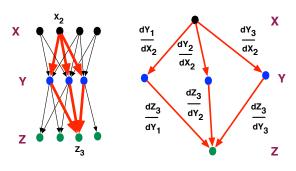


Jacobian Linking Outputs(Z) to Incoming Weights (W)

$$\mathbf{J}_{W}^{Z} = \begin{pmatrix} \frac{\partial Z}{\partial w_{11}} & \frac{\partial Z}{\partial w_{12}} & \cdots & \frac{\partial Z}{\partial w_{1m}} \\ \frac{\partial Z}{\partial w_{21}} & \frac{\partial Z}{\partial w_{22}} & \cdots & \frac{\partial Z}{\partial w_{2m}} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial Z}{\partial w_{n1}} & \frac{\partial Z}{\partial w_{n2}} & \cdots & \frac{\partial Z}{\partial w_{nm}} \end{pmatrix}$$

Note: This Jacobian is in **denominator** format (since the high-level form, i.e. the first 2 dimensions, are that of the denominator tensor), which is most convenient (readable) for weight-to-layer derivatives.

Distant Gradients = Sums of Path Products



$$\frac{\partial z_3}{\partial x_2} = \frac{\partial z_3}{\partial y_1} \frac{\partial y_1}{\partial x_2} + \frac{\partial z_3}{\partial y_2} \frac{\partial y_2}{\partial x_2} + \frac{\partial z_3}{\partial y_3} \frac{\partial y_3}{\partial x_2}$$

More generally:

$$\frac{\partial z_i}{\partial x_j} = \sum_{k \in Y} \frac{\partial z_i}{\partial y_k} \frac{\partial y_k}{\partial x_j}$$

This results from the multiplication of two Jacobian matrices.



Multiplying Jacobian Matrices

$$\mathbf{J}_{y}^{\mathbf{Z}} \bullet \mathbf{J}_{x}^{\mathbf{Y}} = \begin{vmatrix}
\vdots & \vdots & \vdots & \vdots \\
\frac{\partial z_{i}}{\partial y_{1}} & \frac{\partial z_{i}}{\partial y_{2}} & \frac{\partial z_{i}}{\partial y_{3}} \\
\vdots & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots \\
\end{bmatrix} \bullet \begin{vmatrix}
\vdots & \vdots & \vdots & \vdots \\
\frac{\partial y_{1}}{\partial x_{i}} & \cdots & \vdots \\
\frac{\partial y_{2}}{\partial x_{i}} & \cdots & \vdots \\
\vdots & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots \\
\end{bmatrix} = \mathbf{J}_{x}^{\mathbf{Z}}$$

We can do this repeatedly to form J_m^p , the Jacobian relating the activation levels of upstream layer m with those of downstream layer n:

- R = Identity Matrix
- For q = n down to m+1 do:

•
$$R \leftarrow R \bullet J_{q-1}^q$$

• $J_m^n \leftarrow R$



Last of the Jacobians

Once we've computed J_m^n , we need one final Jacobian: J_w^m , where w are the weights feeding into layer m. Then we have the standard Jacobian, J_w^n needed for updating all weights in matrix w.

$$J_w^n \leftarrow J_m^n \bullet J_w^m$$

Weights V from layer X to Y (from the earlier example)

$$J_{V}^{Y} = \frac{\partial Y}{\partial V} = \left| \begin{array}{ccc} \left(\begin{array}{cc} \frac{\partial y_{1}}{\partial v_{11}} & \frac{\partial y_{2}}{\partial v_{11}} \\ \frac{\partial y_{1}}{\partial v_{21}} & \frac{\partial y_{2}}{\partial v_{21}} \end{array} \right) & \left(\begin{array}{ccc} \frac{\partial y_{1}}{\partial v_{12}} & \frac{\partial y_{2}}{\partial v_{12}} \\ \cdots & \cdots & \cdots \end{array} \right| \\ \left(\begin{array}{ccc} \frac{\partial y_{1}}{\partial v_{31}} & \frac{\partial y_{2}}{\partial v_{31}} \\ \end{array} \right) & \cdots & \cdots \end{array} \right|$$

• Since a) the act func for Y is sigmoid, and b) $\frac{\partial y_k}{\partial v_{ii}} = 0$ when $j \neq k$:

$$J_{V}^{Y} = \frac{\partial Y}{\partial V} = \begin{vmatrix} (y_{1}(1-y_{1})x_{1} & 0) & (0 & y_{2}(1-y_{2})x_{1}) \\ (y_{1}(1-y_{1})x_{2} & 0) & (0 & y_{2}(1-y_{2})x_{2}) \\ (y_{1}(1-y_{1})x_{3} & 0) & (0 & y_{2}(1-y_{2})x_{3}) \end{vmatrix}$$



Last of the Jacobian Multiplications

From the previous example (the network with layer sizes 3-2-1), once we have J_Y^Z and J_V^Y , we can multiply (taking dot products of J_Y^Z with the inner vectors of J_V^Y) to produce J_V^Z : the matrix of gradients that backprop uses to modify the weights in V.

$$J_V^Z = J_Y^Z \bullet J_V^Y = \begin{vmatrix} \frac{\partial z_1}{\partial y_1} & \frac{\partial z_1}{\partial y_2} \end{vmatrix} \bullet \frac{\partial Y}{\partial V}$$

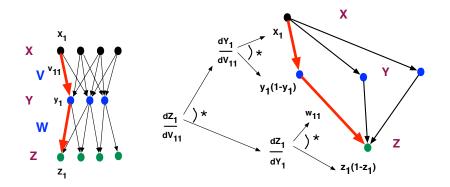
• Since a) the act func for Z is sigmoid, and b) $\frac{\partial sum(z_k)}{\partial y_i} = w_{ik}$ (where $sum(z_k)$ = sum of weighted inputs to node z_k):

$$= | z_1(1-z_1)w_{11} z_1(1-z_1)w_{21} | \bullet \frac{\partial Y}{\partial V}$$

$$J_{V}^{Z} = \begin{pmatrix} z_{1}(1-z_{1})x_{1}y_{1}(1-y_{1})w_{11} & z_{1}(1-z_{1})x_{1}y_{2}(1-y_{2})w_{21} \\ z_{1}(1-z_{1})x_{2}y_{1}(1-y_{1})w_{11} & z_{1}(1-z_{1})x_{2}y_{2}(1-y_{2})w_{21} \\ z_{1}(1-z_{1})x_{3}y_{1}(1-y_{1})w_{11} & z_{1}(1-z_{1})x_{3}y_{2}(1-y_{2})w_{21} \end{pmatrix}$$



One entry of J_V^Z



$$J_V^Z(1,1) = z_1(1-z_1)x_1y_1(1-y_1)w_{11}$$



First of the Jacobians

- This iterative process is very general, and permits the calculation of J^N_M
 (M < N) for any layers M and N, or J^N_W for an weights (W) upstream of N.
- However, the standard situation in backpropagation is to compute J^L_{W_i} ∀i
 where L is the objective (loss) function and W_i are the weight matrices.
- This follows the same procedure as sketched above, but the series of dot products **begins** with J^L_N: the Jacobian of derivatives of the loss function w.r.t. the activations of the output layer.
- For example, assume L = Mean Squared Error (MSE), Z is an output layer of 3 sigmoid nodes, and t_i are the target values for those 3 nodes for a particular case (c):

$$L(c) = \frac{1}{3} \sum_{i=1}^{3} (z_i - t_i)^2$$

Taking partial derivatives of L(c) w.r.t. the z_i yields:

$$J_{Z}^{L} = \frac{\partial L}{\partial Z} = \begin{vmatrix} \frac{2}{3}(z_1 - t_1) & \frac{2}{3}(z_2 - t_2) & \frac{2}{3}(z_3 - t_3) \end{vmatrix}$$



First of the Jacobian Multiplications

 Continuing the example: Assume that layer Y (of size 2) feeds into layer Z, using weights W, then:

$$J_Y^Z = \begin{vmatrix} z_1(1-z_1)w_{11} & z_1(1-z_1)w_{21} \\ z_2(1-z_2)w_{12} & z_2(1-z_2)w_{22} \\ z_3(1-z_3)w_{13} & z_3(1-z_3)w_{23} \end{vmatrix}$$

• Our first Jacobian multiplication yields J_Y^L , a 1 x 2 row vector (shown transposed to fit on the page):

$$J_Z^L \bullet J_Y^Z = J_Y^L = \left| \begin{array}{cc} \frac{\partial L}{\partial y_1} & & \frac{\partial L}{\partial y_2} \end{array} \right| =$$

$$\left| \begin{array}{c} \frac{2}{3}(z_1-t_1)z_1(1-z_1)w_{11}+\frac{2}{3}(z_2-t_2)z_2(1-z_2)w_{12}+\frac{2}{3}(z_3-t_3)z_3(1-z_3)w_{13} \\ \frac{2}{3}(z_1-t_1)z_1(1-z_1)w_{21}+\frac{2}{3}(z_2-t_2)z_2(1-z_2)w_{22}+\frac{2}{3}(z_3-t_3)z_3(1-z_3)w_{23} \end{array} \right|^T$$



Backpropagation with Tensors: The Big Picture

General Algorithm

- Assume Layer M is upstream of Layer N (the output layer). So M < N.
- Assume V is the tensor of weights feeding into Layer M.
- Assume L is the loss function.
- Goal: Compute $J_V^L = \frac{\partial L}{\partial V}$
- R = J_N^L (the partial derivatives of the loss function w.r.t. the output layer)
- If output layer is Softmax: R ← R J^{soft}
- For q = N down to M + 1 do:

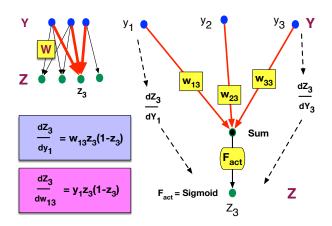
•
$$R \leftarrow R \bullet J_{q-1}^q$$

- Use J_V^L to update the weights in V.

... And now some practical details on implementing this...



Building the J_Y^Z and J_W^Z Jacobians



Detailed Entries of J_Y^Z

$$J_{Y}^{Z} = \begin{cases} w_{11}z_{1}(1-z_{1}) & w_{21}z_{1}(1-z_{1}) & \cdots & w_{n1}z_{1}(1-z_{1}) \\ w_{12}z_{2}(1-z_{2}) & w_{22}z_{2}(1-z_{2}) & \cdots & w_{n2}z_{2}(1-z_{2}) \\ \vdots & \vdots & \vdots & \vdots \\ w_{1m}z_{m}(1-z_{m}) & w_{2m}z_{m}(1-z_{m}) & \cdots & w_{nm}z_{m}(1-z_{m}) \end{cases}$$

More succinctly:

$$J_Y^Z = (W \bullet J_{Sum}^Z)^T = J_{Sum}^Z \bullet W^T$$



Jacobian J_{Sum}^{Z} Linking Z to Summed Inputs

$$J_{Sum}^{Z} = \begin{cases} z_{1}(1-z_{1}) & 0 & \cdots & 0 \\ 0 & z_{2}(1-z_{2}) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & z_{m}(1-z_{m}) \end{cases}$$

Simplifying J_W^Z

In an earlier slide, J_W^Z was presented. Note that it has the same shape as the weight matrix, W:

$$\mathbf{J}_{W}^{Z} = \begin{pmatrix} \frac{\partial Z}{\partial w_{11}} & \frac{\partial Z}{\partial w_{12}} & \cdots & \frac{\partial Z}{\partial w_{1m}} \\ \frac{\partial Z}{\partial w_{21}} & \frac{\partial Z}{\partial w_{22}} & \cdots & \frac{\partial Z}{\partial w_{2m}} \\ \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial Z}{\partial w_{n1}} & \frac{\partial Z}{\partial w_{n2}} & \cdots & \frac{\partial Z}{\partial w_{nm}} \end{pmatrix}$$

- Weight w_{ik} connects y_i to z_k.
- So z_k is the only element of Z that w_{ik} affects.
- Thus, $\frac{\partial Z}{\partial w_{ik}} = [0, \cdots, y_i z_k (1 z_k), \cdots, 0]^T$ (only kth entry is non-zero).
- Make a simpler, more practical, matrix of only these positive values: \hat{J}_W^Z .



The Simplified Jacobian: \hat{J}_W^Z

$$\begin{pmatrix} \frac{\partial z_1}{\partial w_{11}} & \frac{\partial z_2}{\partial w_{12}} & \cdots & \frac{\partial z_m}{\partial w_{1m}} \\ \frac{\partial z_1}{\partial w_{21}} & \frac{\partial z_2}{\partial w_{22}} & \cdots & \frac{\partial z_m}{\partial w_{2m}} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{\partial z_1}{\partial w_{n1}} & \frac{\partial z_2}{\partial w_{n2}} & \cdots & \frac{\partial z_m}{\partial w_{nm}} \end{pmatrix} = \begin{pmatrix} y_1 z_1 (1 - z_1) & y_1 z_2 (1 - z_2) & \cdots & y_1 z_m (1 - z_m) \\ y_2 z_1 (1 - z_1) & y_2 z_2 (1 - z_2) & \cdots & y_2 z_m (1 - z_m) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ y_n z_1 (1 - z_1) & y_n z_2 (1 - z_2) & \cdots & y_n z_m (1 - z_m) \end{pmatrix}$$

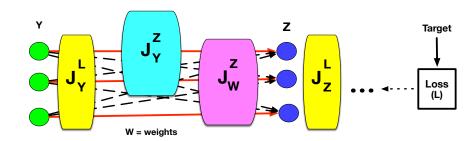
More succinctly:

$$\hat{J}_W^Z = Y \otimes Diag(J_{Sum}^Z)$$

where \otimes = Outer Product and Diag(J_{Sum}^{Z}) = diagonal of J_{Sum}^{Z} .



The Backward Pass across a Layer



- Receive J_Z^L from downstream.
- **②** Compute $J_W^L \leftarrow J_Z^L \bullet J_W^Z$ and use it to update W.
- **1** Compute $J_Y^L \leftarrow J_Z^L \bullet J_Y^Z$ and pass it back (upstream).



Details of $J_W^L \leftarrow J_Z^L \bullet J_W^Z$

- Remember that every element of J_W^Z is a vector, so $J_Z^L \bullet J_W^Z$ involves many vector dot products: $J_Z^L \bullet Q$ for each vector (Q) in J_W^Z . This produces a final matrix with the same dimensions as W.
- In numpy, the "dot" function produces the desired result, but it is sensitive to argument order; the proper call is: numpy.dot(J_W^Z , J_Z^L)
- If we use \hat{J}_W^Z instead of J_W^Z , then the dot product is replaced by this:

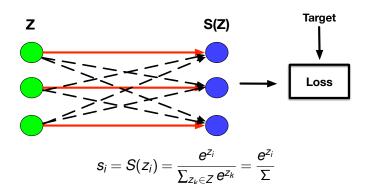
$$J_W^L \leftarrow J_Z^L {\times} \hat{J}_W^Z$$

- The use of "x" means that the ith element of J_Z^L is multiplied by every item in the ith column of \hat{J}_W^Z
- In numpy, the standard multiplication operator, "*" between the vector J_Z^L and the matrix \hat{J}_W^Z will perform the desired operation, as long as $||J_Z^L|| =$ the number of columns in \hat{J}_W^Z .



SoftMax: One More Layer (but without weights)

$$Softmax(Z) = S(Z)$$



Derivatives of Softmax

Effect of z_i on $S(z_i)$

$$\frac{\partial S(z_i)}{\partial z_i} = \frac{\frac{\partial e^{z_i}}{\partial z_i} \sum - \frac{\partial \Sigma}{\partial z_i} e^{z_i}}{\sum^2} = \frac{e^{z_i} \sum - e^{z_i} e^{z_i}}{\sum^2} = \frac{e^{z_i} \sum - e^{z_i} e^{z_i}}{\sum^2} = \frac{e^{z_i}}{\sum^2} - \left(\frac{e^{z_i}}{\sum^2}\right)^2 = S(z_i) - S(z_i)^2 = s_i - s_i^2 = s_i(1 - s_i)$$

Effect of z_i on $S(z_k)$ where $i \neq k$

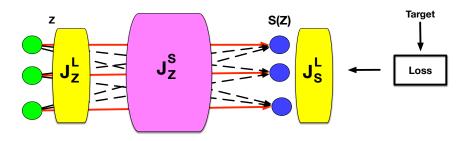
$$\frac{\partial S(z_k)}{\partial z_i} = \frac{\frac{\partial e^{z_k}}{\partial z_i} \sum - \frac{\partial \Sigma}{\partial z_i} e^{z_k}}{\Sigma^2} = \frac{\mathbf{0} - e^{z_i} e^{z_k}}{\Sigma^2} = \frac{\mathbf{0} - e^{z_i} e^{z_k}}{\Sigma^2} = \frac{\mathbf{0} - e^{z_i} e^{z_k}}{\Sigma^2}$$

The Softmax (m x m) Jacobian Matrix

Jsoft

$$\mathbf{J}_{Z}^{S} = \begin{pmatrix} \frac{\partial s_{1}}{\partial z_{1}} & \frac{\partial s_{1}}{\partial z_{2}} & \cdots & \frac{\partial s_{1}}{\partial z_{m}} \\ \frac{\partial s_{2}}{\partial z_{1}} & \frac{\partial s_{2}}{\partial z_{2}} & \cdots & \frac{\partial s_{2}}{\partial z_{m}} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial s_{m}}{\partial z_{1}} & \frac{\partial s_{m}}{\partial z_{2}} & \cdots & \frac{\partial z_{m}}{\partial z_{m}} \end{pmatrix} = \begin{pmatrix} \mathbf{s_{1}} - \mathbf{s_{1}^{2}} & -s_{1}s_{2} & \cdots & -s_{1}s_{m} \\ -s_{2}s_{1} & s_{2} - s_{2}^{2} & \cdots & -s_{2}s_{m} \\ \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ -s_{m}s_{1} & -s_{m}s_{2} & \cdots & s_{m} - s_{m}^{2} \end{pmatrix}$$

Backward Pass Across Softmax



$$J_Z^L = J_S^L \bullet J_Z^S$$

This assumes J_S^L is a row vector. If it's a column vector, then:

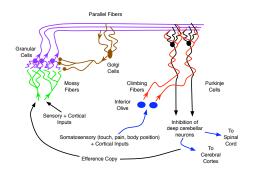
$$J_Z^L = \left(J_S^L\right)^T \bullet J_Z^S$$



Practical Tips

- Only add as many hidden layers and hidden nodes as necessary. Too many → more weights to learn + increased chance of over-specialization.
- Scale all input values to the same range, typically [0 1] or [-1 1].
- Use target values of 0.1 (for zero) and 0.9 (for 1) to avoid saturation effects of sigmoids.
- Beware of tricky encodings of input (and decodings of output) values. Don't combine too much info into a single node's activation value (even though it's fun to try), since this can make proper weights difficult (or impossible) to learn.
- For discrete (e.g. nominal) values, one (input or output) node per value is often most effective. E.g. car model and city of residence -vs- income and education for assessing car-insurance risk.
- All initial weights should be relatively small: [-0.1 0.1]
- Bias nodes can be helpful for complicated data sets.
- Check that all your layer sizes, activation functions, activation ranges, weight ranges, learning rates, etc. make sense in terms of each other and your goals for the ANN. One improper choice can ruin the results.

Supervised Learning in the Cerebellum



- Granular cells detect contexts.
- Parallel fibers and Purkinje cells map contexts to actions
- Climbing fibers from Inferior Olive provide (supervisory) feedback signals for LTD on Parallel-Purkinje synapses