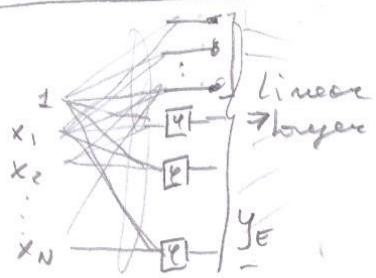


## OTHER TWO-LAYER ARCHITECTURES

The examples seen in the previous section are only some of the possible architectures that can be built. The representation theorem suggests that there exist many other options to build the first layer. We will try to discuss a few of them in the following sections.

### SKIP-CONNECTION ARCHITECTURE



$$y_E = \begin{bmatrix} C_1^T x + b_1 \\ C_2^T x + b_2 \end{bmatrix} = \begin{bmatrix} y_{E1} \\ y_{E2} \end{bmatrix}$$

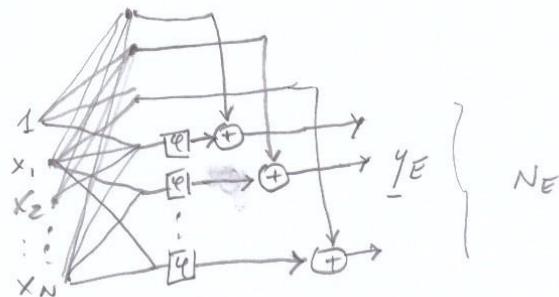
In this architecture, the embedding space is augmented with skip-connections, i.e. with a strictly linear part. The activation functions can be sigmoids, RELUs, or any other function. The idea here is to provide also a strictly linear part into the embedding space. Training of this architecture will ensure that classifiers and regressors are at least linear.

The nonlinear part would be used by the output layer if necessary. Note that the linear and the nonlinear parts can have different sizes.

## RESIDUAL ARCHITECTURE

The residual architecture also builds on the idea of generalizing the linear layer.

In this case the output of the linear part is added to the output of the nonlinear part.



$$\underline{y}_E = \left( \underline{C}_1 \underline{x} + \underline{b}_1 \right) + \mathcal{Q} \left( \underline{C}_2 \underline{x} + \underline{b}_2 \right)$$

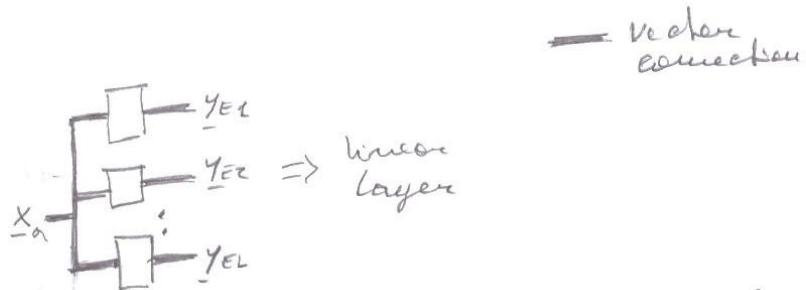
Clearly here the sizes of the linear and nonlinear parts have to be the same ( $N_E$ ). The terminology "residual" comes from the fact that  $\underline{y}_E$  may be considered the difference between a linear (and (differences or may can be learned)) and nonlinear mappings. Clearly this architecture is to be regarded a bit less powerful than the skip connection parallel structure. Usually residual layers are used mostly on multi-layer architectures. A word of caution should be said about using structures with more less constrained parameters: learning has to determine these

TWO.26

parameters and generalization should be checked.  
Therefore any choice of neural network structure  
should be done with careful attention to overfitting.  
The real challenge is therefore in finding  
the proper parameterization for the problem to  
be solved.

## PARALLEL ARCHITECTURES

The SKIP-CONNECTION architecture is a special case of parallel structures



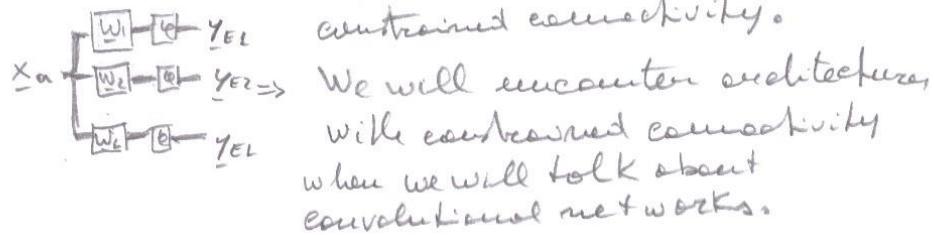
Each element of the parallel may be linear or nonlinear.

The embedding space  $\underline{Y}_E = \begin{bmatrix} Y_{E1} \\ Y_{E2} \\ \vdots \\ Y_{EL} \end{bmatrix}$  is composed by the

concatenation of the various vector-outputs that may specialize on different features.

When all the parallel structures are of the same type, for example linear + activation functions, the network is equivalent to a single network with

constrained connectivity.



We will encounter architecture with constrained connectivity when we will talk about convolutional networks.

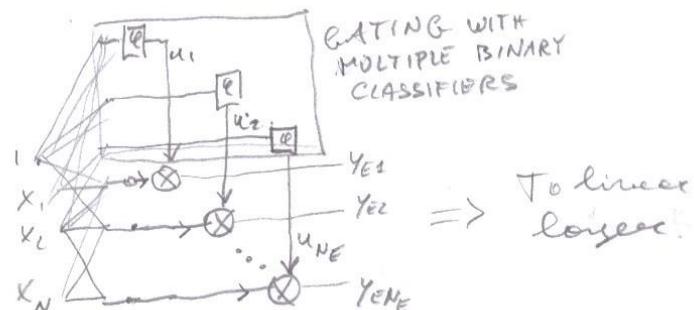
SUM-PRODUCT ARCHITECTURES

Until now we have considered only neural network architectures that use linear combinations and regular nonlinearities. Larger functional capabilities can be obtained if we include also product units, i.e. nodes where the inputs are multiplied.

$$x \rightarrow \otimes \rightarrow c = xy$$

It may be argued that multiplication could be implemented miming the loops and their expensivity. However there are some architectures where the product nodes may be very useful and act as "gates".

It should be pointed out that these structures are not the non-product architectures used to model random variable distributions. They simply indicate the inclusion of product nodes.

GATED ARCHITECTURES

The embedding vector is obtained as

$$Y_E = \ell(G^T \underline{x} + d) \odot (C^T \underline{x} + b)$$

$$\underline{c} = [c_1, c_2, \dots, c_{N_E}]$$

$$\underline{C} = [C_1, C_2, \dots, C_{N_E}]$$

Here each binary classifier "activates" a linear output. If the classifier works in its range  $\approx 1 \text{ or } \approx 0$ , it turns on and off the connected linear filter at the bottom. If instead the specific classifier works in its quasi-linear range, it implements a quadratic transformation.

More specifically if the  $j$ th classifier gives (at a specific  $x$ )  $u_j \approx 1$ ,  $y_{Ej} \approx c_j^T x + b_j$ , otherwise if  $u_j \approx 0$   $y_{Ej} \approx 0$ .

Viceversa if the  $j$ th classifier works in its linear range, we have

$$u_j \approx g_j^T x + d_j$$

and

$$y_{Ej} \approx (g_j^T x + d_j)(c_j^T x + b_j)$$

$$= g_j^T x c_j^T x + d_j c_j^T x + b_j g_j^T x + d_j b_j$$

which is a quadratic function of  $x$ .

Once we have set  $N_E$ , the learning algorithm will provide the parameters  $C, d, C_i, b_i$  that will characterize the embedding space needed for the final regressor or classifier. (\*)

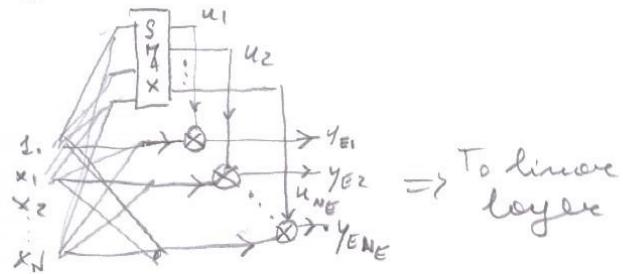
This is a very powerful architecture due to its capabilities of handling linear and non-linear embeddings.

This gating unit is utilized in the LSTM (LONG-SHORT TIME MEMORY) architectures, which is a very powerful recurrent network. The LSTM will be discussed in one of the following chapters.

(\*) Recall the gaussian classifier in the model-based chapter of his book that requires quadratic log-likelihoods. Therefore this architecture may be suitable to build a classifier with clusters that have different covariance matrices. ... (?)

Mr

Another gated architecture is the following see TWO.30



$$y_E = \text{S}_{\max} \left( \underline{c}_x^T \underline{x} + \underline{d} \right) \odot \left( \underline{c}_x^T \underline{x} + \underline{b} \right)$$

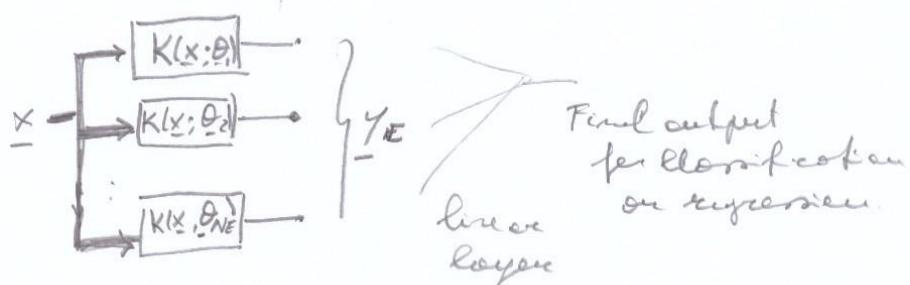
Here the gating is done by all  $N_E$ -class linear classifier.  
The difference with the previous architecture is that here  
the target is one class out of  $N_E$ . (Recall that  $\sum_{i=1}^{N_E} u_i = 1$ )  
Therefore if  $x$  is such that  $u_j \approx 1$  and the others are  
 $\approx 0$ ,  $y_{Ej} \approx c_j^T x + b_j$ . Essentially in every decision  
region of the linear classifier, one output of  $y_E$   
will be active and as a linear function of  $x$ .

Note that both in this and the previous gated architectures,  
 $N_E$  can be made very large giving to the system  
the opportunity of building many useful basis  
functions  $\{y_{Ei}(x), i=1, \dots, N_E\}$ .

## KERNEL-BASED ARCHITECTURES

The representation theorem focuses on finding the proper embedding space with basis functions that can be linearly combined to produce the system output.

One of the early ideas about building such space, is to postulate a number of parametric "Kernels". The following figure shows such an architecture.



Each embedding function is a Kernel function

$$y_i = K(x; \theta_i)$$

that depends on a number of parameters  $\theta_i$ .

A scalar output would be the regression

$$y(x) = \sum_{i=1}^{N_o} c_i K(x; \theta_i) + b$$

or similarly multiple outputs for classification

multiple  
classification  
RADIAL-BASIS FUNCTIONS

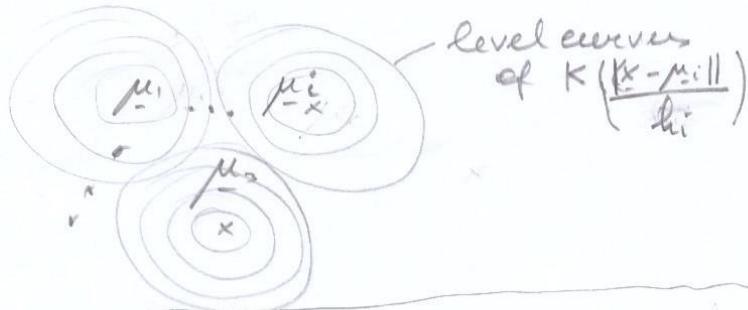
The choice of the Kernel functions  $K(x; \theta_i)$  is done essentially to "cover" the input space with functions that are usually assumed to have

Two.32

a radial symmetry

$$K(\underline{x}; \theta_i) = K\left(\frac{\|\underline{x} - \mu_i\|}{b_i}\right)$$

where  $\|\underline{x} - \mu_i\|$  is the square of the euclidean distance between  $\underline{x}$  and a "cluster point"  $\mu_i$ , and  $b_i$  controls the spread.



NOTA:

The idea of using radial functions has come from the traditional problem of density estimation in statistics. More specifically if we are given a set of samples  $\underline{x}_1, \underline{x}_2, \dots, \underline{x}_L$  we could build density function of  $\underline{x}$  by placing a function around each point  $\underline{x}_i$  and multiplying up.

$$\hat{p}(\underline{x}) = \sum_{i=1}^L x_i K\left(\frac{\|\underline{x} - \underline{x}_i\|}{b_i}\right)$$

To be a valid pdf we have to impose

$$\int_{\mathcal{X}} \hat{p}(\underline{x}) d\underline{x} = 1 \Rightarrow \sum_{i=1}^L x_i \int_{\mathcal{X}} K\left(\frac{\|\underline{x} - \underline{x}_i\|}{b_i}\right) d\underline{x} = 1$$

Kernel functions can be normalized and the coefficients  $x_i$  regulate the height of each function.

The most common choice for  $K(\cdot)$  is the Gaussian function

$$K\left(\frac{\|\underline{x} - \mu\|}{h^2}\right) = e^{-\frac{(\|\underline{x} - \mu\|)^2}{2h^2}}$$

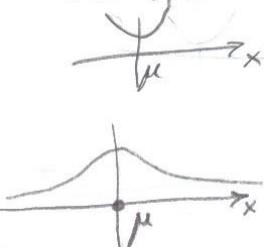
even if other choices are possible, such as the multiquadrate,

$$K(\|\underline{x} - \mu\|^2, \beta) = \sqrt{\|\underline{x} - \mu\|^2 + \beta^2}$$

or the inverse multiquadrate

$$K(\|\underline{x} - \mu\|^2, \beta) = \frac{1}{\sqrt{\|\underline{x} - \mu\|^2 + \beta^2}}$$

$\mu$  is the center  
and  $\beta$  controls  
the spread



These are often called spherical functions...

In any case more generally the  $\mu_i$  are the cluster points and  $h_i$  controls the size of each the spherical region around  $\mu_i$ .

The properties of these spherical functions can build the necessary likelihoods or log-likelihoods for regression or classification.

Usually the determination of the cluster points  $\mu_i$  and the size  $h_i$  is the result of one "unsupervised" phase. We have not talked about unsupervised learning yet as the topic will be more specifically addressed in one of the following chapters.

Essentially we can assume that the clusters will be determined only from  $\{X^{[u]}, u=1, \dots, U_2\}$  in the training set, with an algorithm such as K-means or similar (we will address this <sup>one will follow</sup>) The supervised learning phase determines them the best linear combination for classification or regression.

Usually the size of the embedding space  $H_E$  is kept much smaller than the number of examples and the size of the clusters  $b_i$  is chosen to make the overall function sufficiently smooth. Centres  $b = \frac{\text{d}_{\text{max}}}{\sqrt{2N_E}}$  <sup>max distance between clusters</sup>

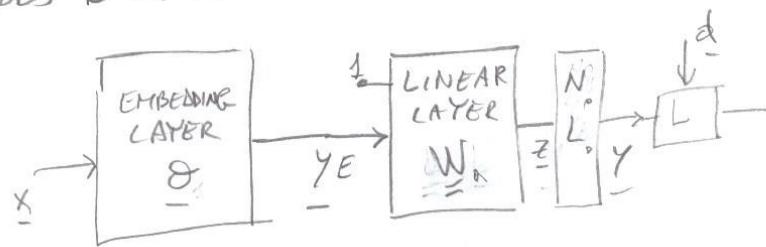
... more ... <sup># of clusters.</sup>  
... example ...

Note that the clusters can be built to have different ellipsoidal shapes & obviously there would be many more parameters to be learned.

- - ~~ANSWER~~ -

## LEARNING IN TWO-LAYER ARCHITECTURE

The general two-layer architecture of Figure (\*), repeated here for convenience, contains all parameters to be learned in both layers



The N.L. block is not present in regression and  
It is made up of ~~non-linearities~~ in the multi-class  
classifier and a softmax in the multi-class  
classifier.

The cost function to be minimized is

$$\mathcal{E}(\theta, W) = \frac{1}{m} \sum_{n=1}^m L(y^{(n)}, d^{(n)})$$

As explained in one of the previous chapters  
we need to compute the gradients

$$\nabla_{W_a} \mathcal{E}(\theta, W) \text{ and } \nabla_{\theta_a} \mathcal{E}(\theta, W)$$

for making the updates

$$W[k] = W[k-1] - \mu \nabla_{W_a} \mathcal{E}(\theta[k-1], W[k-1])$$

$$\theta[k] = \theta[k-1] - \mu \nabla_{\theta_a} \mathcal{E}(\theta[k-1], W[k-1])$$

To simplify notation let us drop the example index  
 $n$  and concentrate on forward propagation and  
gradients on a single example

## THE OUTPUT LAYER

Recall the structure of the linear layer

TWO.36

$$z = \underline{W}^T \underline{y}_E = \begin{bmatrix} b_1 & \underline{w}_1^T \\ b_2 & \underline{w}_2^T \\ \vdots & \vdots \\ b_M & \underline{w}_M^T \end{bmatrix} \begin{bmatrix} 1 \\ \underline{y}_E \end{bmatrix} = \begin{bmatrix} b & \underline{w}_1^T \\ & \underline{w}_2^T \\ & \vdots \\ & \underline{w}_M^T \end{bmatrix} \begin{bmatrix} 1 \\ \underline{y}_E \end{bmatrix}$$

with the augmented matrix

$$\underline{W} = (\underline{w}_1 \ \underline{w}_2 \ \dots \ \underline{w}_M) = \begin{bmatrix} b_1 & b_2 & \dots & b_M \\ \underline{w}_1 & \underline{w}_2 & \dots & \underline{w}_M \end{bmatrix} = \begin{bmatrix} b^T \\ \underline{w}^T \end{bmatrix}$$

that contains in the first row the biases.

Alternatively to the augmented notation we could explicitly name the bias to the output

$$z = \underline{W}^T \underline{y}_E + b$$

This is totally equivalent to the augmented notation but it will allow easier analysis of the gradient propagation.

Now the loss  $L(\underline{y}, \underline{d})$  has to be differentiated with respect to  $\underline{W}$ ,  $b$  and  $\underline{\theta}$ .

For the second layer we need the gradients

$$\frac{\partial L}{\partial \underline{w}_j} = \frac{\partial L}{\partial z_j} \frac{\partial z_j}{\partial \underline{w}_j} \quad ; \quad \frac{\partial L}{\partial b_j} = \frac{\partial L}{\partial z_j} \frac{\partial z_j}{\partial b_j} \quad j = 1, \dots, M$$

since  $\frac{\partial z_j}{\partial b_j} = 1$  for the bias  $\frac{\partial L}{\partial b} = \frac{\partial L}{\partial z}$ ,

Similarly since  $\frac{\partial z_j}{\partial \underline{w}_j} = \underline{y}_E$ ,  $\frac{\partial L}{\partial \underline{w}_j} = \frac{\partial L}{\partial z_j} \underline{y}_E$ .

Now we need the gradient of  $L$  w.r.t.  $\underline{z}$ . For a generic  $z_j$ , using total gradient, we have,

$$\frac{\partial L}{\partial z_j} = \sum_{i=1}^M \frac{\partial L}{\partial y_i} \frac{\partial y_i}{\partial z_j} = \left( \frac{\partial L}{\partial y_1} \frac{\partial L}{\partial y_2} \dots \frac{\partial L}{\partial y_M} \right) \begin{pmatrix} \frac{\partial y_1}{\partial z_j} \\ \frac{\partial y_2}{\partial z_j} \\ \vdots \\ \frac{\partial y_M}{\partial z_j} \end{pmatrix} = \left( \frac{\partial L}{\partial y} \right)^T \frac{\partial y}{\partial z_j}$$

In a comprehensive matrix form (gradient matrix flow) for  $\underline{w}$  we have

$$\frac{\partial L}{\partial \underline{w}} = \left( \frac{\partial L}{\partial w_1} \frac{\partial L}{\partial w_2} \dots \frac{\partial L}{\partial w_M} \right) = \left[ \left( \frac{\partial L}{\partial \underline{y}} \right)^T \frac{\partial \underline{y}}{\partial \underline{z}} \underline{y}_E \left( \frac{\partial \underline{L}}{\partial \underline{y}} \right)^T \frac{\partial \underline{y}}{\partial \underline{z}} \underline{y}_E \right] \cdot \left( \frac{\partial \underline{L}}{\partial \underline{y}} \right)^T \frac{\partial \underline{y}}{\partial \underline{z}} \underline{y}_E$$

$$= \left( \frac{\partial \underline{L}}{\partial \underline{y}} \right)^T \left( \frac{\partial \underline{y}}{\partial \underline{z}} \right) \otimes \underline{y}_E$$

where  $\frac{\partial \underline{y}}{\partial \underline{z}}$  is the Jacobian matrix

$$\left( \frac{\partial \underline{y}}{\partial \underline{z}} \right) = \begin{bmatrix} \left( \frac{\partial y_1}{\partial \underline{z}} \right)^T \\ \left( \frac{\partial y_2}{\partial \underline{z}} \right)^T \\ \vdots \\ \left( \frac{\partial y_M}{\partial \underline{z}} \right)^T \end{bmatrix} = \begin{bmatrix} \frac{\partial y_1}{\partial z_1} & \frac{\partial y_1}{\partial z_2} & \dots & \frac{\partial y_1}{\partial z_N} \\ \frac{\partial y_2}{\partial z_1} & \frac{\partial y_2}{\partial z_2} & & \frac{\partial y_2}{\partial z_N} \\ \vdots & \vdots & & \vdots \\ \frac{\partial y_M}{\partial z_1} & \frac{\partial y_M}{\partial z_2} & \dots & \frac{\partial y_M}{\partial z_N} \end{bmatrix}$$

For the losses

$$\frac{\partial L}{\partial \underline{z}} = \frac{\partial L}{\partial \underline{z}} = \begin{pmatrix} \frac{\partial L}{\partial z_1} \\ \frac{\partial L}{\partial z_2} \\ \vdots \\ \frac{\partial L}{\partial z_N} \end{pmatrix} = \begin{pmatrix} \frac{\partial \underline{y}^T}{\partial \underline{z}} \frac{\partial L}{\partial \underline{y}} \\ \frac{\partial \underline{y}^T}{\partial \underline{z}} \frac{\partial L}{\partial \underline{y}} \\ \vdots \\ \frac{\partial \underline{y}^T}{\partial \underline{z}} \frac{\partial L}{\partial \underline{y}} \end{pmatrix} = \begin{pmatrix} \frac{\partial y_1}{\partial z_1} \frac{\partial y_2}{\partial z_1} \dots \frac{\partial y_M}{\partial z_1} \\ \frac{\partial y_1}{\partial z_2} \frac{\partial y_2}{\partial z_2} \dots \frac{\partial y_M}{\partial z_2} \\ \vdots \\ \frac{\partial y_1}{\partial z_N} \frac{\partial y_2}{\partial z_N} \dots \frac{\partial y_M}{\partial z_N} \end{pmatrix} \begin{pmatrix} \frac{\partial L}{\partial y_1} \\ \frac{\partial L}{\partial y_2} \\ \vdots \\ \frac{\partial L}{\partial y_M} \end{pmatrix}$$

$$= \left( \frac{\partial \underline{y}}{\partial \underline{z}} \right)^T \left( \frac{\partial L}{\partial \underline{y}} \right)$$

For the first layer, we have compacted all the free parameters in a vector  $\underline{\theta}$  and we need the gradient vector.

$$\frac{\partial L}{\partial \underline{\theta}} = \begin{bmatrix} \frac{\partial L}{\partial \theta_1} \\ \frac{\partial L}{\partial \theta_2} \\ \vdots \\ \frac{\partial L}{\partial \theta_{N_\theta}} \end{bmatrix} = \begin{bmatrix} \left( \frac{\partial L}{\partial y_E} \right)^T \frac{\partial y_E}{\partial \theta_1} \\ \left( \frac{\partial L}{\partial y_E} \right)^T \frac{\partial y_E}{\partial \theta_2} \\ \vdots \\ \left( \frac{\partial L}{\partial y_E} \right)^T \frac{\partial y_E}{\partial \theta_{N_\theta}} \end{bmatrix}$$

$$\left( \frac{\partial L}{\partial y_E} \right)^T = \left( \frac{\partial L}{\partial y_{E1}} \frac{\partial L}{\partial y_{E2}} \cdots \frac{\partial L}{\partial y_{EN_E}} \right)$$

$$= \left[ \sum_{i=1}^M \frac{\partial L}{\partial z_i} \frac{\partial z_i}{\partial y_{E1}}, \sum_{i=1}^M \frac{\partial L}{\partial z_i} \frac{\partial z_i}{\partial y_{E2}}, \dots, \sum_{i=1}^M \frac{\partial L}{\partial z_i} \frac{\partial z_i}{\partial y_{EN_E}} \right]$$

$$= \left( \frac{\partial L}{\partial z_1} \frac{\partial L}{\partial z_2} \cdots \frac{\partial L}{\partial z_M} \right) \begin{pmatrix} \frac{\partial z_1}{\partial y_{E1}} & \frac{\partial z_1}{\partial y_{E2}} & \cdots & \frac{\partial z_1}{\partial y_{EN_E}} \\ \frac{\partial z_2}{\partial y_{E1}} & \frac{\partial z_2}{\partial y_{E2}} & \cdots & \frac{\partial z_2}{\partial y_{EN_E}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial z_M}{\partial y_{E1}} & \frac{\partial z_M}{\partial y_{E2}} & \cdots & \frac{\partial z_M}{\partial y_{EN_E}} \end{pmatrix}$$

$$= \left[ \left( \frac{\partial L}{\partial y} \right)^T \frac{\partial y}{\partial z_1}, \left( \frac{\partial L}{\partial y} \right)^T \frac{\partial y}{\partial z_2}, \dots, \left( \frac{\partial L}{\partial y} \right)^T \frac{\partial y}{\partial z_M} \right] \begin{pmatrix} \frac{\partial z_1}{\partial y_{E1}} & \frac{\partial z_1}{\partial y_{E2}} & \cdots & \frac{\partial z_1}{\partial y_{EN_E}} \\ \frac{\partial z_2}{\partial y_{E1}} & \frac{\partial z_2}{\partial y_{E2}} & \cdots & \frac{\partial z_2}{\partial y_{EN_E}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial z_M}{\partial y_{E1}} & \frac{\partial z_M}{\partial y_{E2}} & \cdots & \frac{\partial z_M}{\partial y_{EN_E}} \end{pmatrix}$$

TWD.33

$$\begin{aligned}
 & \left[ \left( \frac{\partial L}{\partial Y} \right)^T \begin{bmatrix} \frac{\partial Y_1}{\partial Z_1} \\ \frac{\partial Y_1}{\partial Z_2} \\ \frac{\partial Y_2}{\partial Z_1} \\ \frac{\partial Y_2}{\partial Z_2} \\ \vdots \\ \frac{\partial Y_H}{\partial Z_1} \\ \frac{\partial Y_H}{\partial Z_2} \end{bmatrix} \right] - \left( \frac{\partial L}{\partial Y} \right)^T \begin{bmatrix} \frac{\partial Y_1}{\partial Z_H} \\ \frac{\partial Y_2}{\partial Z_H} \\ \vdots \\ \frac{\partial Y_H}{\partial Z_H} \end{bmatrix} \\
 & \quad \left[ \begin{bmatrix} \frac{\partial z_1}{\partial y_{E1}} & \frac{\partial z_1}{\partial y_{E2}} \\ \frac{\partial z_2}{\partial y_{E1}} & \frac{\partial z_2}{\partial y_{E2}} \\ \vdots & \vdots \\ \frac{\partial z_H}{\partial y_{E1}} & \frac{\partial z_H}{\partial y_{E2}} \end{bmatrix} \begin{bmatrix} \frac{\partial z_1}{\partial y_{E1}} \\ \frac{\partial z_2}{\partial y_{E1}} \\ \vdots \\ \frac{\partial z_H}{\partial y_{E1}} \end{bmatrix} \right] = \begin{bmatrix} \frac{\partial z_1}{\partial y_{E1}} \\ \frac{\partial z_2}{\partial y_{E1}} \\ \vdots \\ \frac{\partial z_H}{\partial y_{E1}} \end{bmatrix}
 \end{aligned}$$

$$= \left( \frac{\partial L}{\partial Y} \right)^T \left( \frac{\partial Y}{\partial Z} \right) \left( \frac{\partial Z}{\partial Y_E} \right) \quad (\text{row vector})$$

Defining the Seconder

$$\frac{\partial Y_E}{\partial \underline{\theta}} = \begin{bmatrix} \frac{\partial Y_{E1}}{\partial \theta_1} & \frac{\partial Y_{E1}}{\partial \theta_2} & \frac{\partial Y_{E1}}{\partial \theta_N} \\ \frac{\partial Y_{E2}}{\partial \theta_1} & \frac{\partial Y_{E2}}{\partial \theta_2} & \frac{\partial Y_{E2}}{\partial \theta_N} \\ \vdots & \vdots & \vdots \\ \frac{\partial Y_{EN}}{\partial \theta_1} & \frac{\partial Y_{EN}}{\partial \theta_2} & \frac{\partial Y_{EN}}{\partial \theta_N} \end{bmatrix}$$

We have

$$\frac{\partial L}{\partial \underline{\theta}} = \left[ \left( \frac{\partial L}{\partial Y} \right)^T \left( \frac{\partial Y}{\partial Z} \right) \left( \frac{\partial Z}{\partial Y_E} \right) \left( \frac{\partial Y_E}{\partial \underline{\theta}} \right) \right]^T$$

$$= \left( \frac{\partial Y_E}{\partial \underline{\theta}} \right)^T \left( \frac{\partial Z}{\partial Y_E} \right)^T \left( \frac{\partial Y}{\partial Z} \right)^T \frac{\partial L}{\partial Y}$$

$$N_\theta = N_B \begin{bmatrix} N_E \\ N_E \\ M \\ M \end{bmatrix} \begin{bmatrix} M \end{bmatrix} = M$$

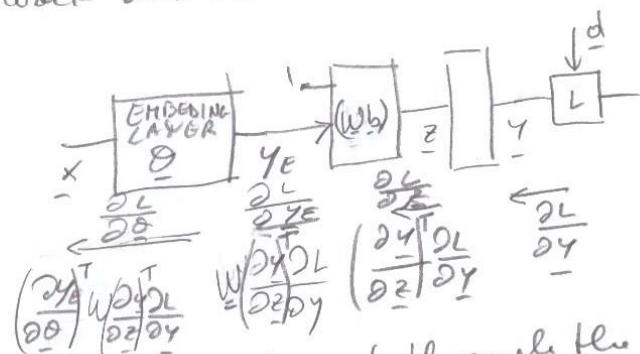
Since the linearity of the next layer

$$\left( \frac{\partial Z}{\partial Y_E} \right)^T = \left( \begin{bmatrix} \frac{\partial z_1}{\partial y_{E1}} & \frac{\partial z_1}{\partial y_{E2}} \\ \frac{\partial z_2}{\partial y_{E1}} & \frac{\partial z_2}{\partial y_{E2}} \\ \vdots & \vdots \\ \frac{\partial z_H}{\partial y_{E1}} & \frac{\partial z_H}{\partial y_{E2}} \end{bmatrix} \begin{bmatrix} \frac{\partial z_1}{\partial y_{E1}} \\ \frac{\partial z_2}{\partial y_{E1}} \\ \vdots \\ \frac{\partial z_H}{\partial y_{E1}} \end{bmatrix} \right)^T = \begin{bmatrix} w_1^+ \\ w_2^+ \\ \vdots \\ w_H^+ \end{bmatrix} = W$$

therefore

$$\frac{\partial L}{\partial \underline{o}} = \left( \frac{\partial \underline{y}_e}{\partial \underline{o}} \right)^T W \left( \frac{\partial \underline{y}}{\partial \underline{z}} \right)^T \frac{\partial L}{\partial \underline{y}}$$

Note how the backward flow evolves over the network architecture



Note that going backward through the linear block the bias  $b$  carries no gradient.  
This is the essence of the back propagation

algorithm, that will be extended to multi-layer architectures, that essentially consists in propagating in the backward direction the gradient flow.

~~BACKWARD FLOW ON THE OUTPUT LAYER~~

Now we examine the three different kinds of layers: binary architecture for regression; multiple binary classification and multi-class classification.

Regression In regression the loss function is

$$L(\underline{y}, \underline{d}) = \sum_{i=1}^n \psi(d_i - y_i) = \sum_{i=1}^n \psi(\epsilon_i)$$

and  $\underline{y} = \underline{\epsilon}$ . Therefore

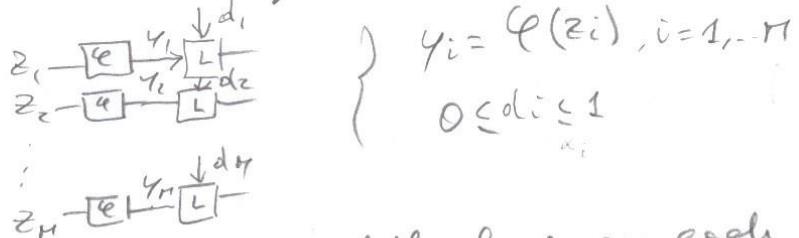
$$\frac{\partial L}{\partial \underline{y}} = \begin{bmatrix} \frac{\partial \psi(\epsilon_1)}{\partial y_1} \\ \vdots \\ \frac{\partial \psi(\epsilon_n)}{\partial y_n} \end{bmatrix} = - \begin{bmatrix} \psi'(\epsilon_1) \\ \psi'(\epsilon_2) \\ \vdots \\ \psi'(\epsilon_n) \end{bmatrix} = -\psi'(\underline{\epsilon}) \quad \text{and} \quad \frac{\partial \underline{y}}{\partial \underline{z}} = I^n$$

The derivatives<sup>(4.1)</sup> of the loss functions have been discussed in previous chapters. For example for the quadratic loss  $\Phi(\epsilon_i) = \epsilon_i^2$  we have namely

$$\frac{\partial L}{\partial \epsilon} = -2\epsilon$$

### MULTIPLE BINARY CLASSIFIER

In the multiple binary classifier we have



The total loss is the sum of the losses on each output

$$L(y, d) = \sum_{i=1}^n L(y_i, d_i)$$

We could use standard loss functions just like in regression

$$L(y, d) = \sum_{i=1}^n \Phi(d_i - y_i) = \sum_{i=1}^n \Phi(\epsilon_i)$$

so that

$$\frac{\partial L}{\partial y} = -\Phi'(\epsilon)$$

Plot for the quadratic loss is  $\frac{\partial L}{\partial y} = -2\epsilon$ .

More appropriately, using the binary crossentropy

$$L(y, d) = \sum_{i=1}^n H(d_i, y_i) = \sum_{i=1}^n \left( d_i \log \frac{1}{y_i} + (1-d_i) \log \frac{1}{1-y_i} \right)$$

already discussed in the chapter on linear binary classifiers. The gradient is easily computed (see Appendix)

Two. 4d

$$\frac{\partial L}{\partial \underline{y}} = \begin{bmatrix} \frac{y_1 - d_1}{y_1(1-y_1)} \\ \frac{y_2 - d_2}{y_2(1-y_2)} \\ \vdots \\ \frac{y_n - d_n}{y_n(1-y_n)} \end{bmatrix}$$

The gradient ~~matrix~~ <sup>matrix</sup> across the nonlinearities  
is diagonal and is

$$\frac{\partial \underline{y}}{\partial \underline{z}} = \text{diag}\left(\frac{\partial y_1}{\partial z_1}, \frac{\partial y_2}{\partial z_2}, \dots, \frac{\partial y_n}{\partial z_n}\right) = \text{diag}\left(\varphi'(z_1), \varphi'(z_2), \dots, \varphi'(z_n)\right)$$

A table of sigmoidal functions is reported in  
Appendix X. For the popular logistic function

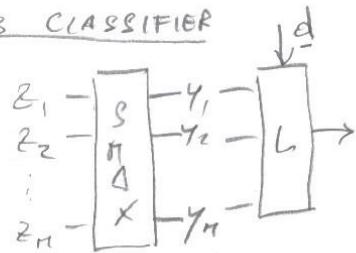
$$\varphi'(z_i) = \varphi(z_i)(1-\varphi(z_i)), \text{ and}$$

$$\frac{\partial \underline{y}}{\partial \underline{z}} = \text{diag}(y_1(1-y_1), y_2(1-y_2), \dots, y_n(1-y_n))$$

Note that using the cross entropy the denominators  
in  $\frac{\partial L}{\partial \underline{y}}$  cancel out and we have simply

$$\frac{\partial L}{\partial \underline{z}} = \left[ \frac{\partial \underline{y}}{\partial \underline{z}} \right]^T \frac{\partial L}{\partial \underline{y}} = \underline{y} - \underline{d}$$

TWO.43

MULTI-CLASS CLASSIFIER

(Recall that  $\underline{d}$  may be  
the one-hot coded class  
or a smooth desired  
distribution.)

The total loss can be computed just as in regression, using the sum of individual losses, as

$$L(\underline{y}, \underline{d}) = \sum_{i=1}^n \Psi(d_i - y_i) = \sum_{i=1}^n \Psi(\epsilon_i)$$

that for the quadratic loss function gives

$$L(\underline{y}, \underline{d}) = -\frac{1}{2} \sum$$

More appropriately using the cross entropy loss or

$$L(\underline{y}, \underline{d}) = H(\underline{d}, \underline{y}) = \sum_{i=1}^n d_i \log \frac{d_i}{y_i}$$

and the gradient is (see Appendix)

$$\frac{\partial L}{\partial \underline{y}} = - \begin{bmatrix} \frac{d_1}{y_1} \\ \frac{d_2}{y_2} \\ \vdots \\ \frac{d_M}{y_M} \end{bmatrix} = - \frac{\underline{d}}{\underline{y}} \quad / \text{divided element by element.}$$

The Jacobian over the softmax function is  
(see Appendix)

$$\frac{\partial \underline{y}}{\partial \underline{z}} = \text{diag}(\underline{y}) - \underline{y}\underline{y}^T.$$

Recall that both  $\underline{d}$  and  $\underline{y}$  are distributions, i.e.  
 $\sum_{i=1}^M d_i = 1$  and  $\sum_{i=1}^M y_i = 1$ . Therefore when we use  
the cross-entropy

Two.44

$$\frac{\partial L}{\partial \underline{z}} = \left( \frac{\partial \underline{y}}{\partial \underline{z}} \right)^T \frac{\partial L}{\partial \underline{y}} = -\text{diag}(\underline{y}) \frac{\underline{d}}{\underline{y}} + \underline{y} \underline{y}^T \frac{\underline{d}}{\underline{I}}$$

$$= -\underline{d} + \begin{pmatrix} y_1^2 & y_1 y_2 & \dots & y_1 y_M \\ y_2 y_1 & y_2^2 & \dots & y_2 y_M \\ \vdots & \vdots & \ddots & \vdots \\ y_M y_1 & y_M y_2 & \dots & y_M^2 \end{pmatrix} \begin{pmatrix} \frac{d_1}{y_1} \\ \frac{d_2}{y_2} \\ \vdots \\ \frac{d_M}{y_M} \end{pmatrix}$$

$$= -\underline{d} + \begin{pmatrix} y_1 d_1 + y_2 d_2 + \dots + y_M d_M \\ y_2 d_1 + y_3 d_2 + \dots + y_M d_{M-1} \\ \vdots \\ y_M d_1 + y_1 d_2 + \dots + y_{M-1} d_M \end{pmatrix}$$

$$= -\underline{d} + \underline{y} = \underline{y} - \underline{d}$$

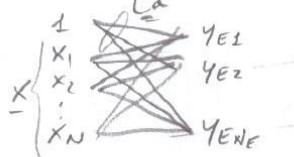
It simplifies  
just as we  
the multiple  
binary classifier.

## GRADIENTS FOR THE FIRST LAYER

Two.45

clearly the gradient  $\frac{\partial y_E}{\partial \underline{x}}$  depends on the type of embedding layer. Let us look at few options.

### LINEAR LAYER



$$y_E = \underline{c}_a^T \underline{x}_a = \begin{bmatrix} c_{1a} & c_{2a} & \dots & c_{Na} \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix} = \begin{bmatrix} c_{1a} & c_{2a} & \dots & c_{Na} \end{bmatrix} = \begin{bmatrix} c_{1a}^T \\ c_{2a}^T \\ \vdots \\ c_{Na}^T \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix}$$

Since the following layer is linear

$$\underline{z} = \underline{W}_a^T \underline{y}_E = \underline{W}_a^T \begin{bmatrix} 1 \\ c_{1a}^T x_a \\ c_{2a}^T x_a \\ \vdots \\ c_{Na}^T x_a \end{bmatrix}$$

The entire mapping from  $\underline{x}$  to  $\underline{z}$  will be linear, and it may be useful to consider this option because  $c_a$  could be absorbed into the next layer matrix  $W_a$ .

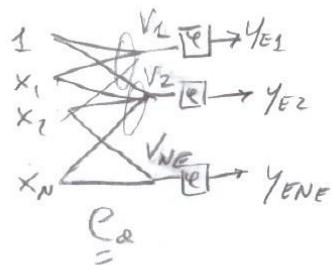
A possibility that could be interesting is to use the first layer as a compression layer, i.e. with  $N_E \ll N$  as in principal component analysis. In this case looking at the connectivity

$$\frac{\partial L}{\partial c_j^a} = \frac{\partial L}{\partial y_E} \frac{\partial y_E}{\partial c_j^a} = \frac{\partial L}{\partial y_E} x_a \quad j = 1, \dots, N_E$$

$$\frac{\partial L}{\partial c_i^a} = \left[ \frac{\partial L}{\partial c_1^a} \frac{\partial L}{\partial c_2^a} \dots \frac{\partial L}{\partial c_{N_E}^a} \right] = \left[ \frac{\partial L}{\partial y_{E1}} x_a \frac{\partial L}{\partial y_{E2}} x_a \dots \frac{\partial L}{\partial y_{EN_E}} x_a \right]^T \otimes x_a$$

TWO0.46

### LINEAR LAYER WITH NON-LINEARITIES



$\varphi(\cdot)$  could be RELU  
Sigmoid

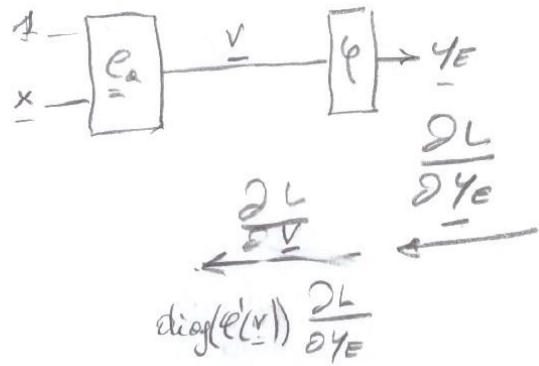
$$\underline{C}_a = \begin{bmatrix} c_{11} & c_{21} & \dots & c_{N1} \\ c_{12} & c_{22} & \dots & c_{N2} \\ \vdots & \vdots & \ddots & \vdots \\ c_{1N} & c_{2N} & \dots & c_{NN} \end{bmatrix} = \begin{bmatrix} c_1^a & c_2^a & \dots & c_N^a \end{bmatrix}$$

$$\underline{y}_E = \begin{bmatrix} \varphi(v_1) \\ \varphi(v_2) \\ \vdots \\ \varphi(v_{NE}) \end{bmatrix} = \varphi(\underline{v}) = \varphi(\underline{c}_a^T \underline{x}_a)$$

$$\begin{aligned} \frac{\partial L}{\partial c_j^a} &= \frac{\partial L}{\partial y_{Ej}} \frac{\partial y_{Ej}}{\partial c_j^a} = \frac{\partial L}{\partial y_{Ej}} \frac{\partial y_{Ej}}{\partial v_j} \frac{\partial v_j}{\partial c_j^a} \\ &= \frac{\partial L}{\partial y_{Ej}} \varphi'(v_j) x_a \end{aligned}$$

$$\begin{aligned} \frac{\partial L}{\partial \underline{c}_a} &= \left[ \frac{\partial L}{\partial c_1^a} \frac{\partial L}{\partial c_2^a} \dots \frac{\partial L}{\partial c_{NE}^a} \right] = \left[ \frac{\partial L}{\partial y_{E1}} \frac{\partial y_{E1}}{\partial v_1} x_a, \frac{\partial L}{\partial y_{E2}} \frac{\partial y_{E2}}{\partial v_2} x_a, \dots, \frac{\partial L}{\partial y_{EN}} \frac{\partial y_{EN}}{\partial v_{NE}} x_a \right] \\ &= \left[ \frac{\partial L}{\partial y_{E1}} \varphi'(v_1) x_a, \frac{\partial L}{\partial y_{E2}} \varphi'(v_2) x_a, \dots, \frac{\partial L}{\partial y_{EN}} \varphi'(v_{NE}) x_a \right] \\ &= \left[ \frac{\partial L}{\partial v_1} x_a, \frac{\partial L}{\partial v_2} x_a, \dots, \frac{\partial L}{\partial v_{NE}} x_a \right] \\ &= \left( \frac{\partial L}{\partial v} \right)^T \otimes x_a - \left( \left( \frac{\partial L}{\partial y_E} \right)^T \text{diag}(\varphi'(v)) \right) \otimes x_a \end{aligned}$$

Two.47



The rule is here: Once reached the linear layer output  $\underline{v}$  with  $\frac{\partial L}{\partial \underline{v}}$ ,

$$\frac{\partial L}{\partial x_a} = \left( \frac{\partial L}{\partial \underline{v}} \right)^T \otimes x_a$$

In going through a block multiply by the Jacobian transposed.

Recall that for REUS  $\ell'(v_i) = u(v_i)$  that sets to zero some components of  $\frac{\partial L}{\partial y_E}$

$$\begin{aligned} \text{For logistic sigmoid } \ell'(v_i) &= \ell(v_i)(1 - \ell(v_i)) \\ &= y_{Ei}(1 - y_{Ei}) \end{aligned}$$

For all other nonlinearities Appendix X gives expressions and derivatives.

TWO.48

### SKIP-CONNECTION LAYER

$$g = \underline{C}_a^T \underline{x}_a$$

$$\underline{z} = \mathcal{L}(\underline{C}_a^T \underline{x}_a)$$

$$\underline{y}_E = \begin{pmatrix} \underline{g} \\ \underline{z} \end{pmatrix}$$

$$\frac{\partial L}{\partial \underline{y}_E} = \begin{pmatrix} \frac{\partial L}{\partial \underline{g}} \\ \frac{\partial L}{\partial \underline{z}} \end{pmatrix}$$

The backward gradient on  $\underline{y}_E$  is split in two parts.

The gradient for the update of  $\underline{C}_a$ , similarly to the above cases becomes

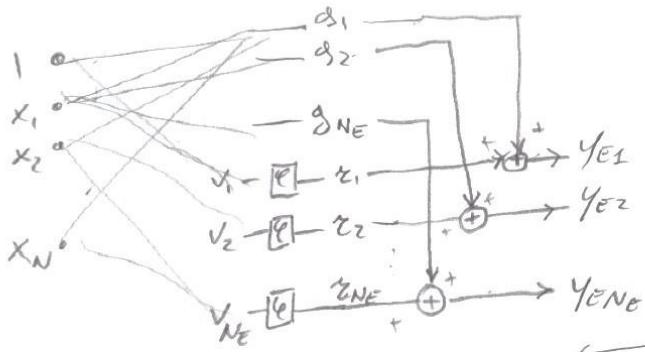
$$\frac{\partial L}{\partial \underline{C}_a} = \left( \frac{\partial L}{\partial \underline{g}} \right)^T \otimes \underline{x}_a$$

The gradient for the update of matrix  $\underline{C}_a$  is

$$\frac{\partial L}{\partial \underline{C}_a} = \left( \left( \frac{\partial L}{\partial \underline{z}} \right)^T \text{diag}(\mathcal{L}'(\underline{z})) \right) \otimes \underline{x}_a$$

## RESIDUAL LAYER

TWO.4B



$$\underline{y}_E = \underline{c}_a^T \underline{x}_a + \ell(\underline{c}_a^T \underline{x}_a) \quad \frac{\partial L}{\partial y_E}$$

The gradient for the update of  $\underline{c}_a$  is

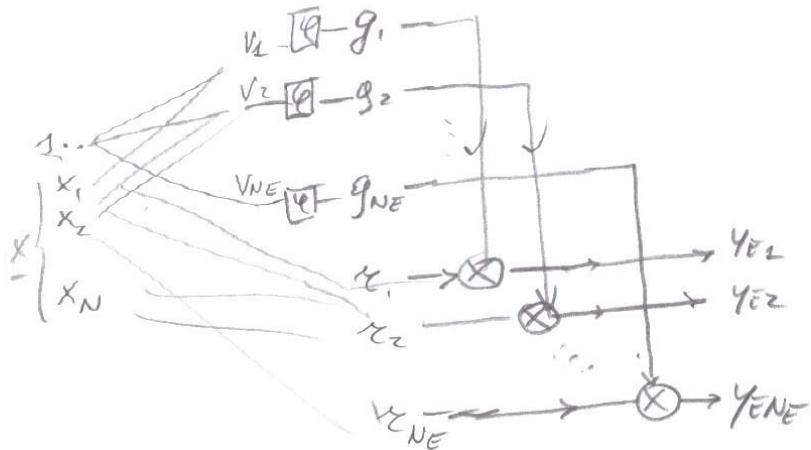
$$\frac{\partial L}{\partial \underline{c}_a} = \left( \frac{\partial L}{\partial y_E} \right)^T \otimes \underline{x}_a$$

and the one for the update of  $\underline{c}_a$

$$\frac{\partial L}{\partial \underline{c}_a} = \left[ \left( \frac{\partial L}{\partial y_E} \right)^T \text{diag}(\ell'(v)) \right] \otimes \underline{x}_a$$

TW0.50.

### GATED LAYER WITH SIGMOIDS



$$y_E = \underbrace{g_1 \odot \dots \odot g_N}_{\|N\|} = \varphi(\underline{G_a^T} \underline{x_a}) \odot \underbrace{\underline{C_a^T} \underline{x_a}}_{\|N_a\|}$$

To go through the multiplier we can consider

$$\frac{\partial L}{\partial \underline{x}} \text{ and } \frac{\partial L}{\partial \underline{g}} \text{ that give}$$

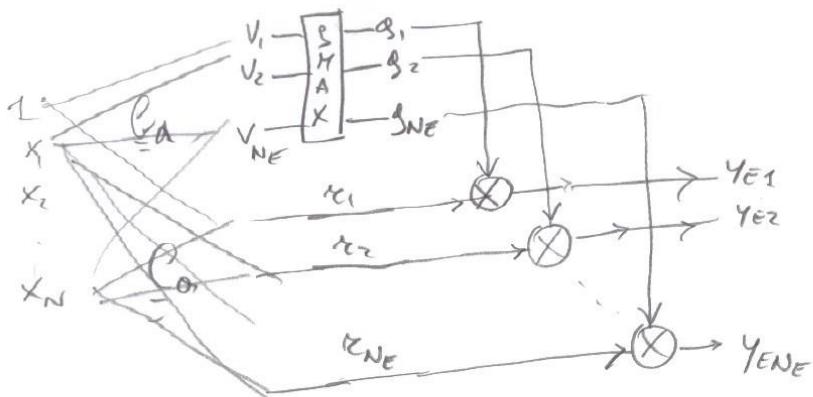
$$\frac{\partial L}{\partial \underline{x}} = \frac{\partial L}{\partial \underline{y}_E} \odot \underline{g}$$

$$\frac{\partial L}{\partial \underline{g}} = \frac{\partial L}{\partial \underline{y}_E} \odot \underline{x}$$

$$\left. \begin{aligned} \frac{\partial L}{\partial \underline{C_a}} &= \left( \frac{\partial L}{\partial \underline{x}} \right)^T \otimes \underline{x_a} = \left( \underline{g}^T \odot \left( \frac{\partial L}{\partial \underline{y}_E} \right)^T \right) \otimes \underline{x_a} \\ \frac{\partial L}{\partial \underline{G_a}} &= \left( \frac{\partial L}{\partial \underline{g}} \right)^T \text{diag}(\varphi'(\underline{v})) \otimes \underline{x_a} = \left[ \underline{z}^T \odot \left( \frac{\partial L}{\partial \underline{y}_E} \right)^T \right] \text{diag}(\varphi'(\underline{v})) \otimes \underline{x_a} \end{aligned} \right\}$$

## GATED LAYER WITH SOFTMAX

TWD. 51



$$y_E = g \odot \underline{x} = \sum_{\text{non-zero}} \left( \underline{\underline{C}}^T \underline{x}_a \right) \odot \left( \underline{\underline{C}}^T \underline{x}_a \right)$$

For the lower branch, we have just as per  
the gated layer with sigmoids

$$\frac{\partial L}{\partial \underline{\underline{C}}_a} = \left( \underline{\underline{g}}^T \odot \left( \frac{\partial L}{\partial y_E} \right)^T \right) \otimes \underline{x}_a$$

For the upper branch we need the Jacobian  
over the softmax that we recall is

$$\frac{\partial \underline{\underline{g}}}{\partial \underline{\underline{V}}} = \text{diag}(\underline{\underline{g}}) - \underline{\underline{g}} \underline{\underline{g}}^T$$

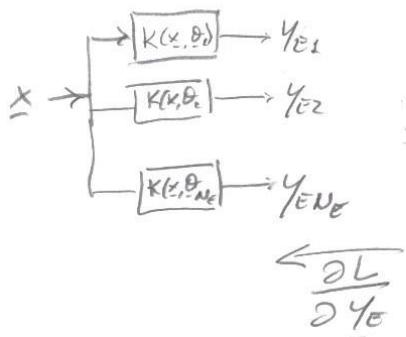
$$\frac{\partial L}{\partial \underline{\underline{C}}_a} = \left( \frac{\partial L}{\partial \underline{\underline{V}}} \right)^T \otimes \underline{x}_a = \left( \left( \frac{\partial \underline{\underline{g}}}{\partial \underline{\underline{V}}} \right)^T \frac{\partial L}{\partial \underline{\underline{g}}} \right)^T \otimes \underline{x}_a$$

$$= \left[ \left( \frac{\partial L}{\partial \underline{\underline{g}}} \right)^T \left( \text{diag}(\underline{\underline{g}}) - \underline{\underline{g}} \underline{\underline{g}}^T \right) \right] \otimes \underline{x}_a$$

$$= \left[ \left( \frac{\partial L}{\partial y_E} \right)^T \odot \underline{\underline{g}} \right] \left( \text{diag}(\underline{\underline{g}}) - \underline{\underline{g}} \underline{\underline{g}}^T \right) \otimes \underline{x}_a$$

## GRADIENT FOR <sup>BORIS</sup> KERNEL-BASED ARCHITECTURES

Kernel-based architectures, such as the radial-basis functions, are usually learned in an unsupervised way, i.e. only on the input sequence  $\{\underline{x}[n]\}$  of the training set. However, their parameters, at least in principle, can be adjusted according to a backwards gradient flow coming from the output.



For each kernel function  $K(\underline{x}, \theta_i)$  we need the gradient for  $\theta_i$ :

$$\frac{\partial L}{\partial \theta_i} = \frac{\partial L}{\partial y_{ei}} \frac{\partial y_{ei}}{\partial \theta_i}$$

$$\frac{\partial y_{ei}}{\partial \theta_i} = \frac{\partial K(\underline{x}, \theta_i)}{\partial \theta_i}$$

For radial functions

$$K(\underline{x}, \theta_i) = K\left(\frac{\|\underline{x} - \mu_i\|^2}{l_i}\right), \quad \theta_i = \begin{pmatrix} \mu_i \\ l_i \end{pmatrix}$$

where  $\mu_i$  is the center centers and  $l_i$  controls the size of the sphere around  $\mu_i$ .

Two.53

For gamma radial functions

$$K(\underline{x}, \underline{\mu}_i) = e^{-\frac{(\underline{x} - \underline{\mu}_i)^T (\underline{x} - \underline{\mu}_i)}{2h_i^2}}$$

$$\begin{aligned} \frac{\partial K}{\partial \underline{\mu}_i} &= -e^{-\frac{(\underline{x} - \underline{\mu}_i)^T (\underline{x} - \underline{\mu}_i)}{2h_i^2}} \frac{\partial}{\underline{\mu}_i} \left[ \frac{(\underline{x} - \underline{\mu}_i)^T (\underline{x} - \underline{\mu}_i)}{2h_i^2} \right] \\ &= -e^{-\frac{(\underline{x} - \underline{\mu}_i)^T (\underline{x} - \underline{\mu}_i)}{2h_i^2}} \frac{\partial}{\underline{\mu}_i} \left[ \frac{\underline{x}^T \underline{x} - 2\underline{\mu}_i^T \underline{x} + \underline{\mu}_i^T \underline{\mu}_i}{2h_i^2} \right] \\ &= -e^{-\frac{(\underline{x} - \underline{\mu}_i)^T (\underline{x} - \underline{\mu}_i)}{2h_i^2}} \frac{\cancel{\underline{x}}}{\cancel{2h_i^2}} \frac{\cancel{(\underline{x} - \underline{\mu}_i)}}{\cancel{2h_i^2}} = Y_{Ei} \left( \frac{\underline{x} - \underline{\mu}_i}{h_i^2} \right) \\ \frac{\partial K}{\partial h_i} &= -e^{-\frac{(\underline{x} - \underline{\mu}_i)^T (\underline{x} - \underline{\mu}_i)}{2h_i^2}} \frac{\partial}{\partial h_i} \left( \frac{(\underline{x} - \underline{\mu}_i)^T (\underline{x} - \underline{\mu}_i)}{2h_i^2} \right) \\ &= -e^{-\frac{(\underline{x} - \underline{\mu}_i)^T (\underline{x} - \underline{\mu}_i)}{2h_i^2}} \frac{1}{2} (\underline{x} - \underline{\mu}_i)^T (\underline{x} - \underline{\mu}_i) \left( \frac{1}{h_i^3} \right) \\ &= Y_{Ei} \frac{\|\underline{x} - \underline{\mu}_i\|^2}{h_i^3} \end{aligned}$$

$$\begin{cases} \frac{\partial K}{\partial \underline{\mu}_i} = Y_{Ei} \frac{\underline{x} - \underline{\mu}_i}{h_i^2} \\ \frac{\partial K}{\partial h_i} = Y_{Ei} \frac{\|\underline{x} - \underline{\mu}_i\|^2}{h_i^3} \end{cases}$$

FOR Multiquadratic functions

Two.54

$$K(\underline{x}, \theta_i) = \sqrt{\|\underline{x} - \mu_i\|^2 + \beta_i^2}$$

$$\frac{\partial K}{\partial \mu_i} = \frac{-(\underline{x} - \mu_i)}{\sqrt{\|\underline{x} - \mu_i\|^2 + \beta_i^2}} = -\gamma_{Ei} (\underline{x} - \mu_i)$$

$$\frac{\partial K}{\partial \beta_i} = \frac{\beta_i}{\sqrt{\|\underline{x} - \mu_i\|^2 + \beta_i^2}} = \gamma_{Ei} \beta_i$$

$$\begin{aligned} \frac{\partial \|\underline{x} - \mu_i\|^2}{\partial \mu_i} &= 2(\underline{x} - \mu_i) \\ &= -2\underline{x} + 2\mu_i = \\ &= 2(\mu_i - \underline{x}) \end{aligned}$$

FOR the INVERSE MULTIQUADRATIC

$$K(\underline{x}, \theta_i) = \frac{1}{\sqrt{\|\underline{x} - \mu_i\|^2 + \beta_i^2}}$$

$$\frac{\partial K}{\partial \mu_i} = +\frac{1}{\sqrt{(\|\underline{x} - \mu_i\|^2 + \beta_i^2)^{3/2}}} \cancel{(\underline{x} - \mu_i)}$$

$$= \gamma_{Ei}^3 (\underline{x} - \mu_i)$$

$$\frac{\partial K}{\partial \beta_i} = -\frac{1}{2} \frac{\cancel{\partial \beta_i}}{\sqrt{(\|\underline{x} - \mu_i\|^2 + \beta_i^2)^{3/2}}} = -\gamma_{Ei}^3 \beta_i$$