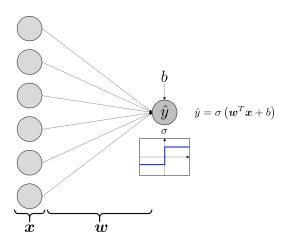
Introduction to Machine Learning Lecture 9 - Feed Forward Networks

1 Introduction to (Feed-forward) Neural Nets

1.1 Introduction

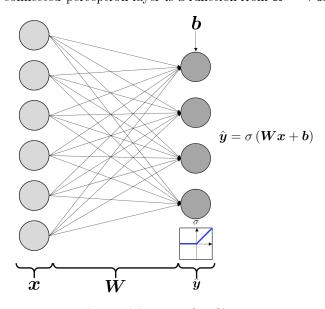
Reminder: Single perceptron



where σ is a non-linear activation function. (For binary classification we set $\sigma(\cdot) = \text{sign}(\cdot)$).

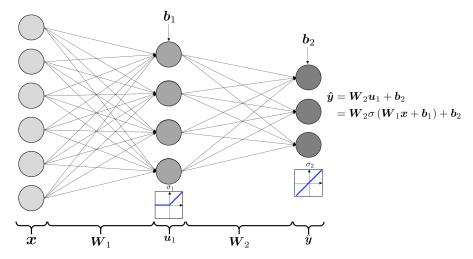
A single perceptron is a function from $\mathbb{R}^d \longrightarrow \mathbb{R}$ (where $\boldsymbol{x} \in \mathbb{R}^d$).

Multiple perceptron: The fully connected perceptron layer is a function from $\mathbb{R}^d \longrightarrow \mathbb{R}^{d_2}$ (where $\hat{y} \in \mathbb{R}^{d_2}$):



Note that in this figure, σ is the ReLU activation (ReLU $(x) = \max\{0, x\}$)

1 hidden layer (Fully connected) To obtain a (complex) non linear function we add additional (hidden) layer:



Remarks:

- 1. By setting different values to $\{W_i\}$ and $\{b_i\}$ we can represent different functions.
- 2. There are several common non-linear activations: tanh, sigmoid, ReLU and more...
- 3. Notice that usually the activation in the output layer is dependent on the network task. For example a linear activation (the identity) for regression, or softmax activation for classification.
- 4. Deep feed-forward neural nets can have more then 1 hidden layer (much more).
- 5. There are more advanced layers: convolution, LSTM and more...

1.2Representation example

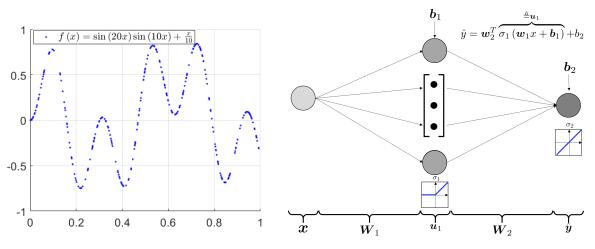
The following example shows the ability of a single hidden layer network to represent some continuous function. Consider the following function:

$$f(x) = \sin(20x)\sin(10x) + \frac{x}{10}$$

We generated a training set (N = 300):

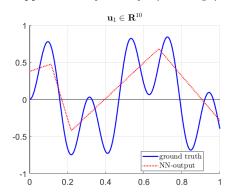
$$y_i = f(x_i), \quad i \in \{1, 2, \dots, N\}$$

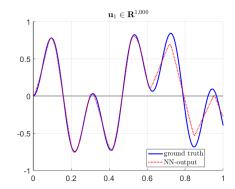
Below are the training set (left) and a simple architecture $\hat{y} = \hat{f}(x)$ with one hidden layer (right).

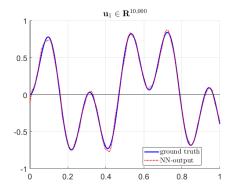


In each experiment, we changed the size of the hidden layer: (1) $\boldsymbol{u}_1 \in \mathbb{R}^{10}$, (2) $\boldsymbol{u}_1 \in \mathbb{R}^{1,000}$ and (3) $\boldsymbol{u}_1 \in \mathbb{R}^{10,000}$.

We approximate f with \hat{f} by setting (training) the values of $\mathbf{w}_1, \mathbf{w}_2, b_1$ and b_2 .







As one can see, the approximation ability is improving as the number of neurons increases.

Universal approximation theorem

Let σ be a non-constant, bounded, and monotonically-increasing continuous function.

Let $f: \mathbb{R}^d \to \mathbb{R}$ be a continuous on the d-dimensional unit hypercube $[0,1]^d$.

Then, given any $\varepsilon > 0$, there exist an integer D, constants vectors $\boldsymbol{b}, \boldsymbol{w}_2 \in \mathbb{R}^D$ and a matrix $\boldsymbol{W}_1 \in \mathbb{R}^{D \times d}$ such that we may define:

$$\hat{f}\left(\boldsymbol{x}\right) = \boldsymbol{w}_{2}^{T} \sigma \left(\boldsymbol{W}_{1} \boldsymbol{x} + \boldsymbol{b}\right)$$

as an approximate realization of the function f where f is independent of σ ; that is,

$$\left|\hat{f}\left(\boldsymbol{x}\right) - f\left(\boldsymbol{x}\right)\right| < \varepsilon, \quad \forall \boldsymbol{x} \in \left[0, 1\right]^{d}$$

In other words, functions of the form F(x) are dense in $C([0,1]^d)$.

This still holds when replacing $[0,1]^d$ with any compact subset of \mathbb{R}^d .

2 Training the network

We can train the network, that is, finding the weights $\{\boldsymbol{W}_i\}$ and biases $\{b_i\}$, by using a training set $\mathcal{D} = \{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}_{i=1}^N$ of size N. This can be done both for regression and classification tasks.

2.1 Loss functions

2.1.1 Regression

• L_2 loss (MSE):

$$L_2 = \frac{1}{2N} \sum_{i=1}^{N} \|\hat{\boldsymbol{y}}_i - \boldsymbol{y}\|_2^2$$

• L_1 loss:

$$L_1 = \frac{1}{N} \sum_{i=1}^{N} \|\hat{\boldsymbol{y}}_i - \boldsymbol{y}\|_1$$

In regression, the MSE loss function is a common choice. However, other types of losses can be used (such as the L_1 loss: Mean Absolute Error (MAE)).

2.1.2 Classification

• One-hot encoding.

In classification tasks, it is common to set the target vector \boldsymbol{y} as a delta function (one-hot encoding):

$$\boldsymbol{y}_i = \begin{bmatrix} 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \end{bmatrix}^T \in \mathbb{R}^{|\mathcal{Y}|}$$

where \mathcal{Y} is the set of all classes, and the value 1 location is associate with the class number. For example, if x_i belongs to the second class, then:

$$\boldsymbol{y}_i = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \end{bmatrix}^T$$

• Softmax layer:

$$oldsymbol{z} = \phi_{ ext{softmax}}\left(\hat{oldsymbol{y}}
ight) = rac{\exp\left(\hat{oldsymbol{y}}
ight)}{\mathbf{1}^T \exp\left(\hat{oldsymbol{y}}
ight)}$$

The output vector z, of the softmax function $\phi_{\text{softmax}} : \mathbb{R}^d \to \mathbb{R}^d$ is a probability vector. Namely, $z[i] \geq 0$ and $\sum_i z[i] = 1$.

For example:

$$\hat{m{y}} = \begin{bmatrix} 3 \\ 1 \\ -1 \end{bmatrix} \Longrightarrow m{z} = \phi_{ ext{softmax}} \left(\hat{m{y}} \right) = \begin{bmatrix} 0.87 \\ 0.12 \\ 0.01 \end{bmatrix}$$

• Cross entropy loss.

In classification tasks, a common loss function is the cross-entropy (together with a softmax layer):

$$L = -\frac{1}{N} \sum_{i=1}^{N} \boldsymbol{y}_{i}^{T} \log \left(\boldsymbol{z}_{i}\right)$$

2.2 Training

We train the network by minimizing the loss function L:

$$\min_{\{\boldsymbol{W}_i\},\{b_i\}} L$$

This is done by optimization algorithms, such as the gradient descent (or some more advanced algorithms). In most cases, the number of samples N is extremely large so stochastic optimization methods are used.

3 The Gradient and the Chain Rule

Consider a network with two hidden layers and activation functions ϕ_i :

$$\hat{y} = W_3 \phi_2 (W_2 \phi_1 (W_1 x + b_1) + b_2) + b_3$$

we denote:

$$egin{aligned} oldsymbol{v}_1 & extstyle & oldsymbol{w}_1 oldsymbol{x} + oldsymbol{b}_1, & oldsymbol{u}_1 & extstyle & oldsymbol{\phi}_1 \left(oldsymbol{v}_1
ight) \ oldsymbol{v}_2 & extstyle & oldsymbol{\psi}_2 oldsymbol{u}_1 + oldsymbol{b}_2, & oldsymbol{u}_2 & extstyle & oldsymbol{\phi}_2 \left(oldsymbol{v}_2
ight) \ & extstyle &$$

Consider the MSE loss function (given some training set):

$$L = \frac{1}{2N} \sum_{i=1}^{N} \|\hat{\boldsymbol{y}}_i - \boldsymbol{y}\|_2^2$$

To apply gradient descent and update the weights $\{W_i\}$ and $\{b_i\}$, we need to compute the gradient of L with respect to $\{W_i\}$ and $\{b_i\}$. For simplicity we will focus only on a single example (N=1):

$$L = \frac{1}{2} \left\| \hat{\boldsymbol{y}} - \boldsymbol{y} \right\|_2^2$$

3.1 Warm-up

Exercise 1 Find the gradient (with respect to x) of:

$$f(\mathbf{x}) = \frac{1}{2} \|\mathbf{x} - \mathbf{a}\|_2^2$$
$$\nabla_{\mathbf{x}} f = ?$$

Solution:

$$f = \frac{1}{2} (\mathbf{x} - \mathbf{a})^T (\mathbf{x} - \mathbf{a})$$

$$\Rightarrow df = \frac{1}{2} \left(d\mathbf{x}^T (\mathbf{x} - \mathbf{a}) + (\mathbf{x} - \mathbf{a})^T d\mathbf{x} \right) = \frac{1}{2} \left((\mathbf{x} - \mathbf{a})^T d\mathbf{x} + (\mathbf{x} - \mathbf{a})^T d\mathbf{x} \right) = (\mathbf{x} - \mathbf{a})^T d\mathbf{x}$$

$$\Rightarrow \overline{\nabla_x f = \mathbf{x} - \mathbf{a}}$$

Exercise 2 Find the gradient of:

$$f\left(oldsymbol{x}
ight) = egin{bmatrix} \phi\left(oldsymbol{x}\left[1
ight]
ight) \ \phi\left(oldsymbol{x}\left[2
ight]
ight) \ \vdots \ \phi\left(oldsymbol{x}\left[d
ight]
ight) \end{bmatrix}, \qquad oldsymbol{x} \in \mathbb{R}^{d}$$

for some differential scalar function $\phi: \mathbb{R} \to \mathbb{R}$.

Solution:

$$f(\boldsymbol{x}) = \begin{bmatrix} \phi(\boldsymbol{x}[1]) \\ \vdots \\ \phi(\boldsymbol{x}[d]) \end{bmatrix}$$

$$\Rightarrow df = \begin{bmatrix} d\phi(\boldsymbol{x}[1]) \\ \vdots \\ d\phi(\boldsymbol{x}[d]) \end{bmatrix} = \begin{bmatrix} \phi'(\boldsymbol{x}[1]) d\boldsymbol{x}[1] \\ \vdots \\ \phi'(\boldsymbol{x}[d]) d\boldsymbol{x}[d] \end{bmatrix} = \underbrace{\begin{bmatrix} \phi'(\boldsymbol{x}[1]) & 0 & 0 \\ 0 & \vdots & 0 \\ 0 & 0 & \phi'(\boldsymbol{x}[d]) \end{bmatrix}}_{\triangleq \boldsymbol{\Phi}'(\boldsymbol{x})} d\boldsymbol{x}$$

$$\Rightarrow \boxed{\nabla f = (\boldsymbol{\Phi}'(\boldsymbol{x}))^T = \boldsymbol{\Phi}'(\boldsymbol{x})}$$

3.2 Back-propagation (the chain rule)

The architecture is given by:

$$\hat{\boldsymbol{y}} = \boldsymbol{W}_{3}\phi_{2}\left(\boldsymbol{W}_{2}\phi_{1}\left(\boldsymbol{W}_{1}\boldsymbol{x} + \boldsymbol{b}_{1}\right) + \boldsymbol{b}_{2}\right) + \boldsymbol{b}_{3}$$

The MSE loss is given by:

$$L = \frac{1}{2} \left\| \hat{\boldsymbol{y}} - \boldsymbol{y} \right\|_2^2$$

3.2.1 Step I:

Note that:

$$\Rightarrow \nabla_{\hat{y}} L = \hat{y} - y$$

3.2.2 Step II:

Let us calculate $\nabla_{b_3}L$.

Using the chain rule we have:

$$\Rightarrow d_{b_3}L = \nabla_{\hat{y}}^T L \cdot d_{b_3} \hat{y}$$

$$= (\hat{y} - y)^T \cdot d_{b_3} \hat{y}, \qquad \hat{y} = W_3 u_2 + b_3$$

$$= (\hat{y} - y)^T db_3$$

$$\Rightarrow \nabla_{b_3} L = \hat{y} - y$$

3.2.3 Step III:

Let us calculate $\nabla_{b_2} L$.

Using the previous result, we have:

$$\Rightarrow \mathbf{d}_{b_2} L = \nabla_{b_3}^T L \cdot \mathbf{d}_{b_2} \hat{\boldsymbol{y}}, \qquad \hat{\boldsymbol{y}} = \boldsymbol{W}_3 \boldsymbol{u}_2 + \boldsymbol{b}_3$$

$$= \nabla_{b_3}^T L \cdot \boldsymbol{W}_3 \mathbf{d}_{b_2} \boldsymbol{u}_2, \qquad \boldsymbol{u}_2 = \phi_2 \left(\boldsymbol{v}_2 \right)$$

$$= \nabla_{b_3}^T L \cdot \boldsymbol{W}_3 \boldsymbol{\Phi}_2' \left(\boldsymbol{u}_2 \right) \mathbf{d}_{b_2} \boldsymbol{v}_2, \qquad \boldsymbol{v}_2 = \boldsymbol{W}_2 \boldsymbol{u}_1 + \boldsymbol{b}_2$$

$$= \nabla_{b_3}^T L \cdot \boldsymbol{W}_3 \boldsymbol{\Phi}_2' \left(\boldsymbol{u}_2 \right) \mathbf{d} \boldsymbol{b}_2$$

$$\Rightarrow \left[\nabla_{b_2} L = \boldsymbol{\Phi}_2' \left(\boldsymbol{u}_2 \right) \boldsymbol{W}_3^T \nabla_{b_3} L \right] = \boldsymbol{\Phi}_2' \left(\boldsymbol{u}_2 \right) \boldsymbol{W}_3^T \left(\hat{\boldsymbol{y}} - \boldsymbol{y} \right)$$

3.2.4 Step IV:

Let us calculate $\nabla_{b_1} L$.

Using the previous result, we have:

$$\Rightarrow \mathbf{d}_{b_1} L = \nabla_{b_2}^T L \cdot \mathbf{d}_{b_1} \boldsymbol{v}_2, \qquad \boldsymbol{v}_2 = \boldsymbol{W}_2 \boldsymbol{u}_1 + \boldsymbol{b}_2$$

$$= \nabla_{b_2}^T L \cdot \boldsymbol{W}_2 \mathbf{d}_{b_1} \boldsymbol{u}_1, \qquad \boldsymbol{u}_1 = \phi_1 \left(\boldsymbol{v}_1 \right)$$

$$= \nabla_{b_2}^T L \cdot \boldsymbol{W}_2 \Phi_1' \left(\boldsymbol{u}_1 \right) \mathbf{d}_{b_1} \boldsymbol{v}_1, \qquad \boldsymbol{v}_1 = \boldsymbol{v}_1 = \boldsymbol{W}_1 \boldsymbol{x} + \boldsymbol{b}_1$$

$$= \nabla_{b_2}^T L \cdot \boldsymbol{W}_2 \Phi_1' \left(\boldsymbol{u}_1 \right) \mathbf{d}_{b_1} \boldsymbol{b}_1$$

$$\Rightarrow \left[\nabla_{b_1} L = \Phi_1' \left(\boldsymbol{u}_1 \right) \boldsymbol{W}_2^T \nabla_{b_2} L \right] = \Phi_1' \left(\boldsymbol{u}_1 \right) \boldsymbol{W}_2^T \Phi_2' \left(\boldsymbol{u}_2 \right) \boldsymbol{W}_3^T \left(\hat{\boldsymbol{y}} - \boldsymbol{y} \right)$$

Summary (derivatives of $\{b_i\}$):

Derivative	Chain Rule
$\boldsymbol{g}_3 \triangleq \nabla_{b_3} L$	$oldsymbol{g}_3 = \hat{oldsymbol{y}} - oldsymbol{y}$
$oldsymbol{g}_2 \triangleq abla_{b_2} L$	$oldsymbol{g}_2 = oldsymbol{\Phi}_2'\left(oldsymbol{u}_2 ight) oldsymbol{W}_3^T oldsymbol{g}_3$
$oldsymbol{g}_1 \triangleq abla_{b_1} L$	$oldsymbol{g}_1 = oldsymbol{\Phi}_1'\left(oldsymbol{u}_1 ight)oldsymbol{W}_2^Toldsymbol{g}_2$

For a general network with L layers, we can compute the gradients $g_i \triangleq \nabla_{b_i} L$ using the back-propagation rule by:

$$\begin{cases} \boldsymbol{g}_L = \hat{\boldsymbol{y}} - \boldsymbol{y} & i = L \\ \boldsymbol{g}_i = \boldsymbol{\Phi}_i'\left(\boldsymbol{u}_i\right) \boldsymbol{W}_{i+1}^T \boldsymbol{g}_{i+1} & i < L \end{cases}$$

In a vary similar way (see appendix) we obtain the derivatives of $\{W_i\}$:

Derivative	Chain Rule	Notations
$\nabla_{W_3}L$	$ abla_{W_3} L = oldsymbol{g}_3 oldsymbol{u}_2^T$	$\boldsymbol{g}_3 \triangleq \nabla_{b_3} L$
$\nabla_{W_2}L$	$ abla_{W_2} L = oldsymbol{g}_2 oldsymbol{u}_1^T$	$m{g}_2 \triangleq abla_{b_2} L$
$\nabla_{W_1}L$	$ abla_{W_1} L = oldsymbol{g}_1 oldsymbol{x}^T$	$m{g}_1 \triangleq abla_{b_1} L$

This process of calculating the gradient of each layer using the later layer's gradient is called back-propagation.

The gradient of the ReLU activation is simply:

$$\operatorname{ReLU}(x) = \begin{cases} x & x \ge 0 \\ 0 & \text{else} \end{cases}$$
$$\Rightarrow \frac{\mathrm{d}}{\mathrm{d}x} \operatorname{ReLU}(x) = \begin{cases} 1 & x \ge 0 \\ 0 & \text{else} \end{cases}$$

For other activation functions, one just needs to compute their respective derivative.

4 Softmax and Cross-entropy Loss:

• The softmax layer:

$$oldsymbol{z} riangleq rac{\exp{(\hat{oldsymbol{y}})}}{\mathbf{1}^T \exp{(\hat{oldsymbol{y}})}}$$

• Cross entropy loss:

$$\begin{split} L &= -\boldsymbol{y}^T \log \left(\boldsymbol{z} \right) \\ &= -\boldsymbol{y}^T \log \left(\frac{\exp \left(\hat{\boldsymbol{y}} \right)}{\boldsymbol{1}^T \exp \left(\hat{\boldsymbol{y}} \right)} \right) \\ &= -\boldsymbol{y}^T \left(\hat{\boldsymbol{y}} - \boldsymbol{1} \cdot \log \left(\boldsymbol{1}^T \exp \left(\hat{\boldsymbol{y}} \right) \right) \right) \\ &= -\boldsymbol{y}^T \hat{\boldsymbol{y}} + \boldsymbol{y}^T \boldsymbol{1} \log \left(\boldsymbol{1}^T \exp \left(\hat{\boldsymbol{y}} \right) \right) \end{split}$$

(Note that for classification tasks we can assume: $y^T \mathbf{1} = 1$):

$$\Rightarrow L = -\mathbf{y}^T \hat{\mathbf{y}} + \log \left(\mathbf{1}^T \exp \left(\hat{\mathbf{y}} \right) \right)$$

• Gradient with respect to \hat{y} :

$$d_{\hat{\boldsymbol{y}}}L = -\boldsymbol{y}^T d\hat{\boldsymbol{y}} + \frac{1}{\left(\mathbf{1}^T \exp\left(\hat{\boldsymbol{y}}\right)\right)} \exp\left(\hat{\boldsymbol{y}}^T\right) d\hat{\boldsymbol{y}}$$

$$= \left(\frac{\exp\left(\hat{\boldsymbol{y}}^T\right)}{\left(\mathbf{1}^T \exp\left(\hat{\boldsymbol{y}}\right)\right)} - \boldsymbol{y}^T\right) d\hat{\boldsymbol{y}}$$

$$= \left(\boldsymbol{z}^T - \boldsymbol{y}^T\right) d\hat{\boldsymbol{y}}$$

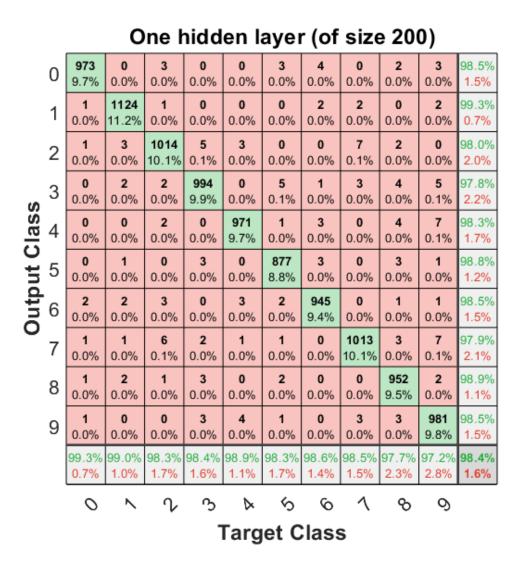
$$\Rightarrow \left[\nabla_{\hat{\boldsymbol{y}}}L = \boldsymbol{z} - \boldsymbol{y}\right]$$

In the general case where $y^T \mathbf{1} \neq 1$ we have:

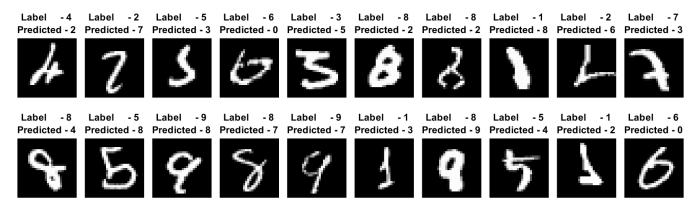
$$abla_{\hat{m{y}}} L = \left(m{y}^T \mathbf{1}\right) m{z} - m{y}$$

5 MNIST Example

We trained a NN with one hidden layer architecture ($u_1 \in \mathbb{R}^{200}$) on the MNIST training set. This is the classification result on the test set:

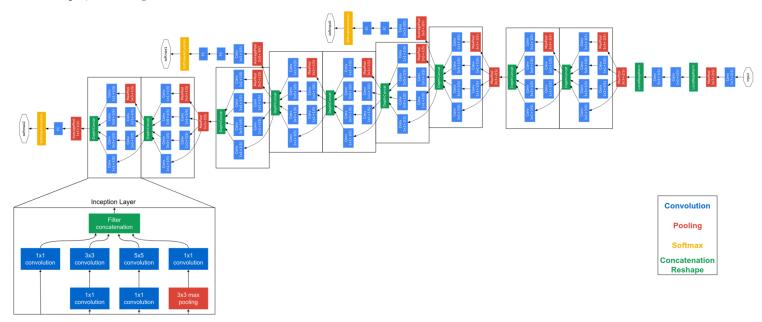


Some errors:



6 Deep Networks

In deep networks, there are usually millions of parameters to optimize. For example, the GoogLeNet network:

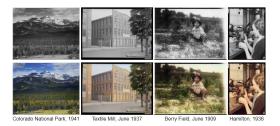


Tasks Deep learning can be useful in many practical task such as:

• Face detection + recognition



 \bullet Gray to Color



- ullet Text translation
- Language recognition
- Autonomous vehicles
- Deep-learning robots
- and much much more

7 Appendix

7.1 The gradient with respect to W_i

$$\Rightarrow \hat{y} = \phi_3 \left(W_3 \left(\phi_2 \left(W_2 \left(\phi_1 \left(W_1 x + b_1 \right) \right) + b_2 \right) \right) + b_3 \right)
L = \frac{1}{2} \| \hat{y} - y \|_2^2
d \hat{y} = d u_3 = d \phi_3 \left(v_3 \right)
= \Phi_3' \left(v_3 \right) d v_3
= \Phi_3' \left(v_3 \right) W_3 d u_2
= \Phi_3' \left(v_3 \right) W_3 \Phi_2' \left(v_2 \right) d v_2
= \Phi_3' \left(v_3 \right) W_3 \Phi_2' \left(v_2 \right) W_2 d u_2
= \Phi_3' \left(v_3 \right) W_3 \Phi_2' \left(v_2 \right) W_2 \Phi_1' \left(v_1 \right) d v_1
= \Phi_3' \left(v_3 \right) W_3 \Phi_2' \left(v_2 \right) W_2 \Phi_1' \left(v_1 \right) d W_1 x$$

$$\begin{aligned} \mathbf{d}_{W_3} L &= (\hat{\boldsymbol{y}} - \boldsymbol{y})^T \, \mathbf{d}_{W_3} \hat{\boldsymbol{y}} \\ &= (\hat{\boldsymbol{y}} - \boldsymbol{y})^T \, \boldsymbol{\Phi}_3' \, (\boldsymbol{v}_3) \, \mathbf{d} \boldsymbol{W}_3 \boldsymbol{u}_2 \\ &= \mathrm{Tr} \left\{ (\hat{\boldsymbol{y}} - \boldsymbol{y})^T \, \boldsymbol{\Phi}_3' \, (\boldsymbol{v}_3) \, \mathbf{d} \boldsymbol{W}_3 \boldsymbol{u}_2 \right\} \\ &= \mathrm{Tr} \left\{ \boldsymbol{u}_2 \, (\hat{\boldsymbol{y}} - \boldsymbol{y})^T \, \boldsymbol{\Phi}_3' \, (\boldsymbol{v}_3) \, \mathbf{d} \boldsymbol{W}_3 \right\} \end{aligned}$$

$$\begin{aligned} \mathbf{d}_{W_2} L &= \left(\hat{\boldsymbol{y}} - \boldsymbol{y}\right)^T \mathbf{d}_{W_2} \hat{\boldsymbol{y}} \\ &= \left(\hat{\boldsymbol{y}} - \boldsymbol{y}\right)^T \boldsymbol{\Phi}_3' \left(\boldsymbol{v}_3\right) \boldsymbol{W}_3 \boldsymbol{\Phi}_2' \left(\boldsymbol{v}_2\right) \mathbf{d} \boldsymbol{W}_2 \boldsymbol{u}_1 \\ &= \mathrm{Tr} \left\{ \left(\hat{\boldsymbol{y}} - \boldsymbol{y}\right)^T \boldsymbol{\Phi}_3' \left(\boldsymbol{v}_3\right) \boldsymbol{W}_3 \boldsymbol{\Phi}_2' \left(\boldsymbol{v}_2\right) \mathbf{d} \boldsymbol{W}_2 \boldsymbol{u}_1 \right\} \\ &= \mathrm{Tr} \left\{ \boldsymbol{u}_1 \left(\hat{\boldsymbol{y}} - \boldsymbol{y}\right)^T \boldsymbol{\Phi}_3' \left(\boldsymbol{v}_3\right) \boldsymbol{W}_3 \boldsymbol{\Phi}_2' \left(\boldsymbol{v}_2\right) \mathbf{d} \boldsymbol{W}_2 \right\} \end{aligned}$$