

# Pattern Recognition

### **Neural Networks**

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Some slides are modified from S.-J. Wang, H.-T. Chen, V. Khalidov, and M. Hansard

### Linear model for regression or classification

A linear model for regression or classification

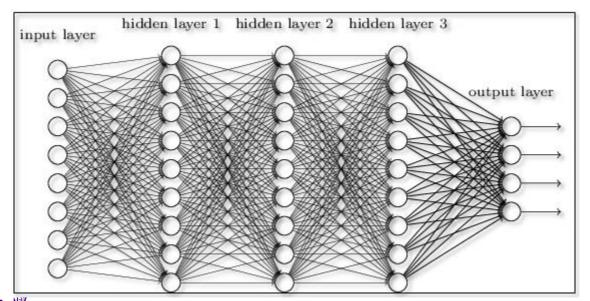
$$y(\mathbf{x}, \mathbf{w}) = f\left(\sum_{j=1}^{M} w_j \phi_j(\mathbf{x})\right)$$

- Decision based on a linear combination of fixed nonlinear basis functions
- $\triangleright f$  is an identity function for regression
- $\triangleright f$  is a nonlinear activation function for classification
  - Logistic sigmoid or softmax function



#### Linear model and neural networks

- Our goal is to extend the linear model by making
  - > 1. The basis functions depend on parameters
    - Parametric basis functions
  - ➤ 2. Their parameters learnable during training
- The goal leads to the basic neural network model





### **Activations**

$$y(\mathbf{x}, \mathbf{w}) = f\left(\sum_{j=1}^{M} w_j \overline{\phi_j}(\mathbf{x})\right)$$

#### **Examples of basis functions**

• Polynomial basis function: taking the form of powers of x

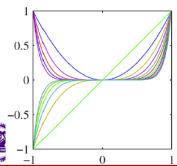
$$\phi_j(x) = \mathbf{v}^j$$

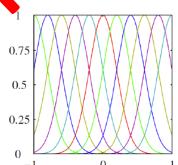
- Gaussian basis function: governed by  $\mu_j$  and s
  - $\triangleright \mu_j$  governs the location while s give his the scale

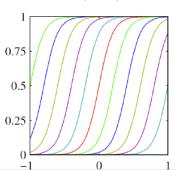
$$\phi_j(x) = \exp\left\{-\frac{(y - \mu_j)^2}{2s^2}\right\}$$

• Sigmoidal basis function: governed by  $\mu_j$  and s

$$\phi_j(x) = \sigma(x) - \lambda$$
 where  $\sigma(a) = \frac{1}{1 + \exp(-a)}$ 









### **Activations**

$$y(\mathbf{x}, \mathbf{w}) = f\left(\sum_{j=1}^{M} w_j \overline{\phi_j}(\mathbf{x})\right)$$

• Construct M linear combinations of the inputs  $x_1, \ldots, x_D$ 

$$a_j = \sum_{i=1}^{D} w_{ji}^{(1)} x_i + w_{j0}^{(1)}$$

- $\triangleright$  where  $a_i$  is the activation for j=1,2,...,M
- >  $\{w_{ji}^{(1)}\}_{i=1}^{D}$  are the weights. Superscript (1) indicates that these parameters are in the first layer of neural networks
- $> w_{j0}^{(1)}$  is the bias
- $\triangleright$  Each activation is nonlinearly transformed by using a differentiable, nonlinear activation function h, i.e.,

$$z_i = h(a_i)$$

•  $\{z_j = h(a_j)\}_{j=1}^M$  are called hidden units



# **Output unit activation**

$$y(\mathbf{x}, \mathbf{w}) = f\left(\sum_{j=1}^{M} w_j \phi_j(\mathbf{x})\right)$$

- The hidden units  $\{z_j = h(a_j)\}_{j=1}^M$  are linearly combined in the second layer of neural networks
- Suppose there are K outputs in the neural networks. We have

$$a_k = \sum_{j=1}^{M} w_{kj}^{(2)} z_j + w_{k0}^{(2)}$$

- $\triangleright$  where  $a_k$  is the output activation for k=1,2,...,K
- $\gt \{w_{kj}^{(2)}\}_{j=1}^M$  are the weights. Superscript (2) indicates that these parameters are in the second layer of neural networks
- $> w_{k0}^{(2)}$  is the bias
- $a_k$  is further transformed by output activation function



$$y_k = \sigma(a_k)$$

# Neural networks for regression and classification

• Output activation  $a_k$  is further transformed by output activation function

$$y_k = \sigma(a_k)$$

- $\{y_k\}_{k=1}^K$  are the final outputs of the neural networks
- For regression,  $\sigma(\cdot)$  is the identity function
- For two-class classification,  $\sigma(\cdot)$  is the logistic sigmoid function

$$\sigma(a) = \frac{1}{1 + \exp(-a)}$$

• For multiclass classification,  $\sigma(\cdot)$  is the softmax function

$$\frac{\exp(a_k)}{\sum_j \exp(a_j)}$$



# Two-layer neural networks

The two-layer neural network model

$$y_{k}(\mathbf{x}, \mathbf{w}) = \sigma \left( \sum_{j=1}^{M} w_{kj}^{(2)} h \left( \sum_{i=1}^{D} w_{ji}^{(1)} x_{i} + w_{j0}^{(1)} \right) + w_{k0}^{(2)} \right)$$

$$z_{j} \underline{a_{j}}$$

$$y_{k} \underline{a_{k}}$$

- $\triangleright$  where  ${f w}$  is the set of all weight and bias parameters
- The bias parameters can be absorbed into weight parameters by using one additional input  $x_0=1$

$$y_k(\mathbf{x}, \mathbf{w}) = \sigma \left( \sum_{j=0}^M w_{kj}^{(2)} h \left( \sum_{i=0}^D w_{ji}^{(1)} x_i \right) \right)$$



#### Feed-forward neural networks

Evaluating the following equation is called forward propagation

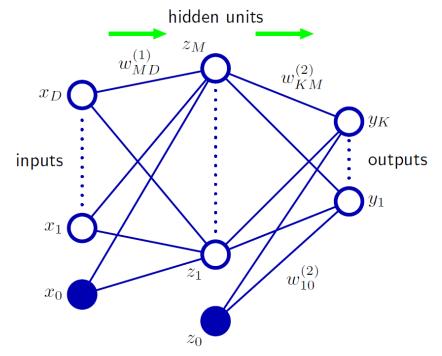
$$y_k(\mathbf{x}, \mathbf{w}) = \sigma \left( \sum_{j=0}^M w_{kj}^{(2)} h \left( \sum_{i=0}^D w_{ji}^{(1)} x_i \right) \right)$$

Network Diagram

Nodes: Input, hidden, and output variables

Links: Weights and biases

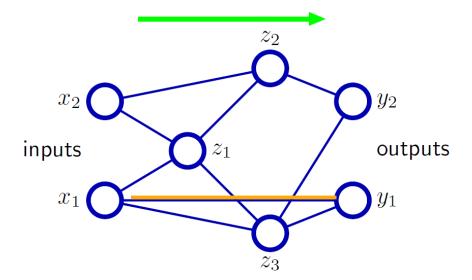
**Arrows**: Propagation direction





#### Generalizations

- There may be more than one layer of hidden units
  - Deep learning
- Individual units need not be fully connected to the next layer
  - Convolutional neural networks
- Individual links may skip over one or more subsequent layers
  - Skip connections





# Neural networks as universal approximators

Points: training data

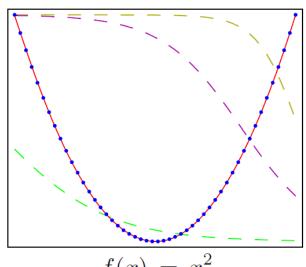
#### Dashed curves:

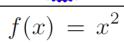
Outputs of three hidden units

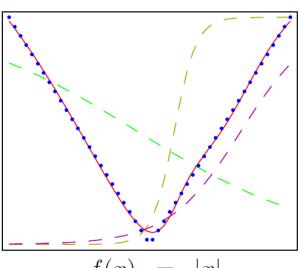
#### Curve:

Prediction by the NN

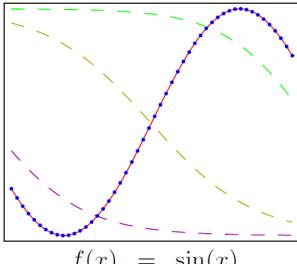




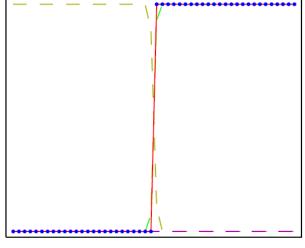




$$f(x) = |x|$$



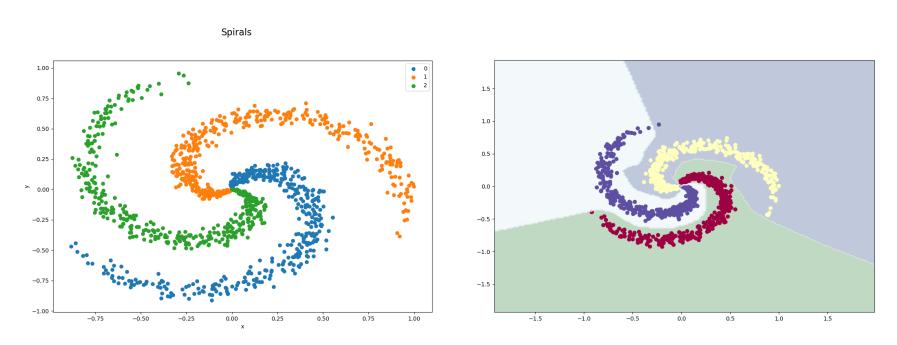
f(x) $\sin(x)$ 



Heaviside step function

### **Neural networks for classification**

- 3-class classification
- 2-layer neural networks with 64 hidden units



https://www.annytab.com/neural-network-classification-in-python/



# **Network training**

• Given a set of training data  $\{\mathbf{x}_n\}$  where n=1,2,...,N, together with a corresponding set of target vectors  $\{\mathbf{t}_n\}$ , we can learn the neural networks by minimizing

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \|\mathbf{y}(\mathbf{x}_n, \mathbf{w}) - \mathbf{t}_n\|^2$$

 Let's consider how to train the networks by giving a probabilistic interpretation to the network output



# **Neural networks for 1D regression**

- We aim to minimize the error between  $y(\mathbf{x}_n,\mathbf{w})$  and  $t_n$
- We assume that the target is a scalar-valued function, which is normally distributed around the prediction

$$p(t|\mathbf{x}, \mathbf{w}) = \mathcal{N}\left(t|y(\mathbf{x}, \mathbf{w}), \beta^{-1}\right)$$

- ightharpoonup where  $y(\mathbf{x}, \mathbf{w})$  is the prediction by neural networks and  $\beta^{-1}$  is the variance
- Suppose data are i.i.d. The likelihood is

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \prod_{n=1}^{N} p(t_n|\mathbf{x}_n, \mathbf{w}, \beta)$$

ightharpoonup where  $\mathbf{X}=\{\mathbf{x}_1,\ldots,\mathbf{x}_N\}$  and  $\mathbf{t}=\{t_1,\ldots,t_N\}$ 



Taking the negative logarithm, we get negative log likelihood

$$\frac{\beta}{2} \sum_{n=1}^{N} \{y(\mathbf{x}_n, \mathbf{w}) - t_n\}^2 - \frac{N}{2} \ln \beta + \frac{N}{2} \ln(2\pi)$$

 The maximum likelihood solution for w is equivalent to minimizing the sum-of-squares error

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \{y(\mathbf{x}_n, \mathbf{w}) - t_n\}^2$$

- Does setting the gradient of  $E(\mathbf{w})$  to zero work?
  - No closed-form solution

- Optimization by using gradient descent, stochastic gradient descent,
   Newton-Raphson iterative optimization scheme
- The nonlinearity of  $y(\mathbf{x}_n, \mathbf{w})$  makes  $E(\mathbf{w})$  to be nonconvex
- In practice, local minima of the negative log likelihood may be found
- After having found  $\mathbf{w}_{\mathrm{ML}}$ , the value of  $\beta$  can be found by minimizing the negative log likelihood

$$\frac{1}{\beta_{\mathrm{ML}}} = \frac{1}{N} \sum_{n=1}^{N} \{y(\mathbf{x}_n, \mathbf{w}_{\mathrm{ML}}) - t_n\}^2$$

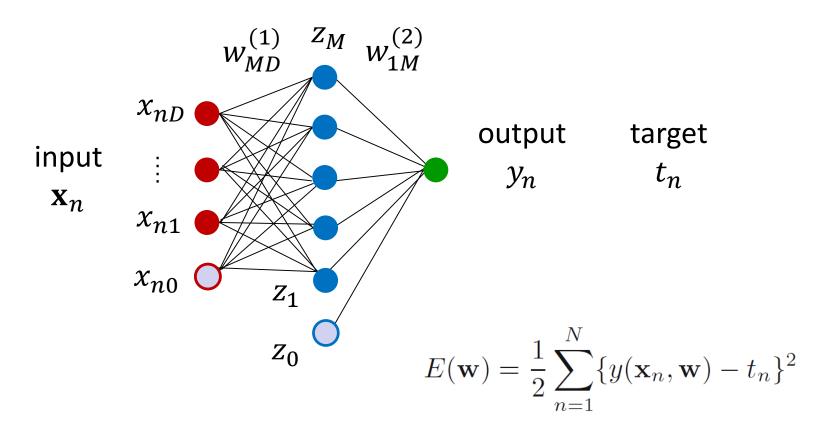


• After getting  $\mathbf{w}_{\mathrm{ML}}$  and  $\beta_{\mathrm{ML}}$ , we can predict the distribution of the target value t for an input testing data point  $\mathbf{x}$  via

$$p(t|\mathbf{x}, \mathbf{w}) = \mathcal{N}\left(t|y(\mathbf{x}, \mathbf{w}), \beta^{-1}\right)$$



Two-layer neural networks for one-dimensional regression





# Neural networks for multi-dimensional regression

- Neural networks can be used for K-dimensional regression
- Construct neural networks with K outputs
- Make the following assumption

$$p(\mathbf{t}|\mathbf{x}, \mathbf{w}) = \mathcal{N}(\mathbf{t}|\mathbf{y}(\mathbf{x}, \mathbf{w}), \beta^{-1}\mathbf{I})$$

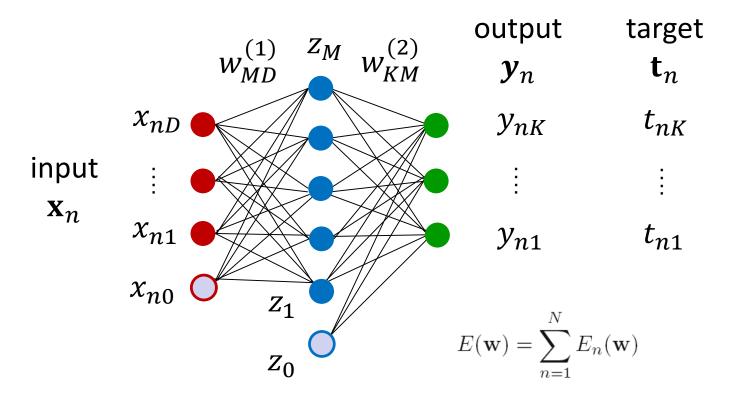
- We can use maximum likelihood solution, which is equivalent to minimizing the sum-of-squares errors, to get  $\mathbf{w}_{\mathrm{ML}}$
- Similarly given  $\mathbf{w}_{\mathrm{ML}}$ , the optimal  $eta_{\mathrm{ML}}$  is obtained

$$\frac{1}{\beta_{\text{ML}}} = \frac{1}{NK} \sum_{n=1}^{N} \|\mathbf{y}(\mathbf{x}_n, \mathbf{w}_{\text{ML}}) - \mathbf{t}_n\|^2$$



### Neural networks for multi-dimensional regression

Two-layer neural networks for K-dimensional regression





$$E_n(\mathbf{w}) = \frac{1}{2} \|\mathbf{y}_n - \mathbf{t}_n\|^2 = \frac{1}{2} \sum_{k=1}^K (y_{nk} - t_{nk})^2$$

# Neural networks for binary classification

- Neural networks can be used for classification
- Given a set of training data  $\{\mathbf{x}_n\}$  where n=1,2,...,N, together with a corresponding set of target labels  $\{t_n\}$ , where  $t_n=1$  denotes class  $\mathcal{C}_1$  and  $t_n=0$  denotes class  $\mathcal{C}_2$
- Construct (two-layer) neural networks having a single output whose activation function is a logistic sigmoid

$$y = \sigma(a) \equiv \frac{1}{1 + \exp(-a)}$$

- $\triangleright$  where  $0 \leqslant y(\mathbf{x}, \mathbf{w}) \leqslant 1$
- $\rightarrow y(\mathbf{x}, \mathbf{w})$  is the conditional probability  $p(\mathcal{C}_1|\mathbf{x})$
- ightharpoonup The conditional probability  $p(\mathcal{C}_2|\mathbf{x})$  is given by  $1-y(\mathbf{x},\mathbf{w})$



# ML solution for binary classification

 Regression: the target is a real-valued function, which is normally distributed around the prediction

$$p(t|\mathbf{x}, \mathbf{w}) = \mathcal{N}\left(t|y(\mathbf{x}, \mathbf{w}), \beta^{-1}\right)$$

 Classification: the conditional distribution of a target given its input is a Bernoulli distribution of the form

$$p(t|\mathbf{x}, \mathbf{w}) = y(\mathbf{x}, \mathbf{w})^t \left\{ 1 - y(\mathbf{x}, \mathbf{w}) \right\}^{1-t}$$



# ML solution for binary classification

 When using ML optimization, we minimize the negative log likelihood, here called cross-entropy error

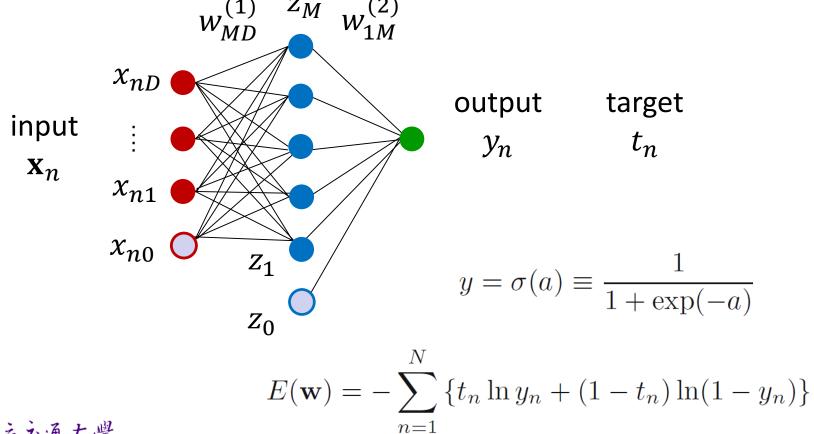
$$E(\mathbf{w}) = -\sum_{n=1}^{N} \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$

- $\triangleright$  where  $y_n$  denotes  $y(\mathbf{x}_n, \mathbf{w})$
- Optimize w by using gradient descent or its variant
- After getting  $\mathbf{w}_{\mathrm{ML}}$ , binary classification is carried out by

$$p(t|\mathbf{x}, \mathbf{w}) = y(\mathbf{x}, \mathbf{w})^t \left\{ 1 - y(\mathbf{x}, \mathbf{w}) \right\}^{1-t}$$



# ML solution for binary classification





#### Neural networks for multi-class classification

- Neural networks can be extended to K-class classification
- Given a set of training data  $\{\mathbf{x}_n\}$  where n=1,2,...,N, together with a corresponding set of target vectors  $\{\mathbf{t}_n\}$ , where  $\mathbf{t}_n$  is encoded by using 1-of- K coding scheme
- Construct (two-layer) neural networks having K outputs and use softmax as the activation function

$$y_k(\mathbf{x}, \mathbf{w}) = \frac{\exp(a_k(\mathbf{x}, \mathbf{w}))}{\sum_j \exp(a_j(\mathbf{x}, \mathbf{w}))}$$

 $\blacktriangleright$  where  $0 \leqslant y_k \leqslant 1$  and  $\sum_k y_k = 1$ 



#### ML solution for multi-class classification

The negative log likelihood or the cross-entropy error is

$$E(\mathbf{w}) = -\sum_{n=1}^{N} \sum_{k=1}^{K} t_{kn} \ln y_k(\mathbf{x}_n, \mathbf{w})$$

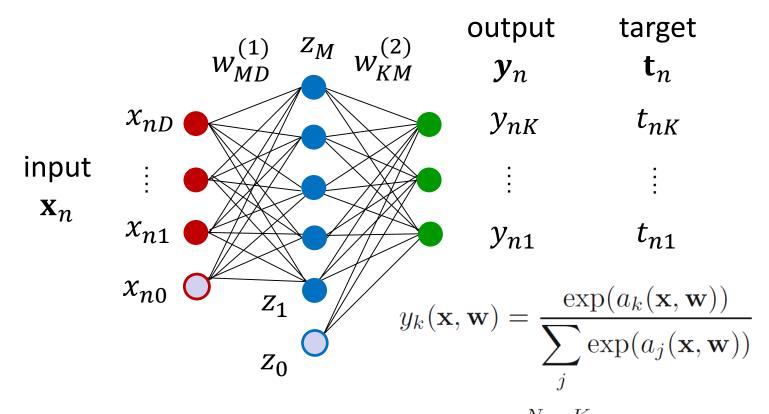
- Optimize w by using gradient descent or its variant
- After getting  $\mathbf{w}_{\mathrm{ML}}$ , multi-class classification is carried out by using the softmax function

$$y_k(\mathbf{x}, \mathbf{w}) = \frac{\exp(a_k(\mathbf{x}, \mathbf{w}))}{\sum_j \exp(a_j(\mathbf{x}, \mathbf{w}))}$$



#### ML solution for multi-class classification

Two-layer neural networks for K-class classification





$$E(\mathbf{w}) = -\sum_{n=1}^{N} \sum_{k=1}^{K} t_{kn} \ln y_k(\mathbf{x}_n, \mathbf{w})$$

#### **Gradient descent**

• The simplest approach is to update  ${f w}$  by a displacement in the negative gradient direction

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E(\mathbf{w}^{(\tau)})$$

- ➤ This is a steepest descent algorithm
- $\triangleright \eta > 0$  is the learning rate
- $\blacktriangleright$  This is a batch method, as evaluation of  $\nabla E$  involves the entire data set
- ightharpoonup A range of starting points  $\{\mathbf{w}^{(0)}\}$  may be needed, in order to find a satisfactory minimum



### Stochastic gradient descent

- Stochastic gradient descent (or called sequential gradient descent) has proved useful in practice when training neural networks on a large data set
- The error function needs to comprise a sum of terms, one for each data point, i.e.,

$$E(\mathbf{w}) = \sum_{n=1}^{N} E_n(\mathbf{w})$$

Sum-of-squares error for regression

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \{y(\mathbf{x}_n, \mathbf{w}) - t_n\}^2$$

Cross-entropy error for classification



国立立通大学 
$$E(\mathbf{w}) = -\sum_{n=1}^{N} \left\{ t_n \ln y_n + (1-t_n) \ln(1-y_n) \right\}$$
National Chiao Tung University

### Stochastic gradient descent

 Stochastic gradient descent makes an update to the weight vector based on one data point at a time

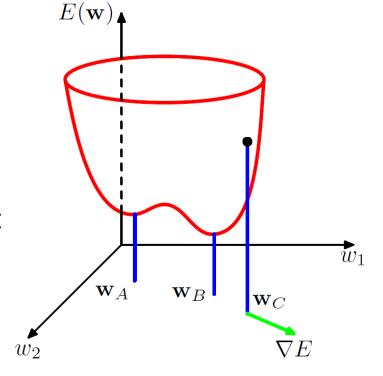
$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E_n(\mathbf{w}^{(\tau)})$$



### Geometric view of gradient descent

• The error function  $E(\mathbf{w})$  is a surface sitting over the weight space

- W<sub>A</sub> is a local minimum
- $oldsymbol{\mathbf{w}}_B$  is a global minimum
- At any point  $\mathbf{w}_C$ , the local gradient of the error surface is given by the vector  $\nabla E$





 The computational cost of gradient descent mainly lies in the evaluation of gradient at each iteration

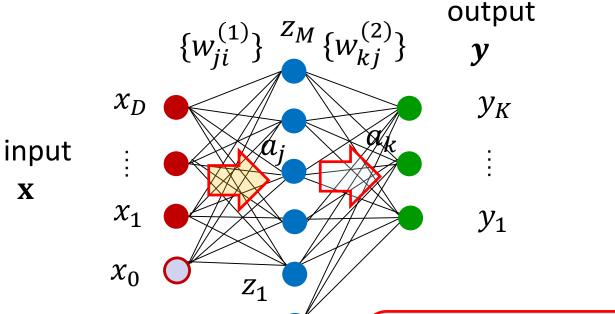
$$\triangleright \mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E_n(\mathbf{w}^{(\tau)})$$

- > The dimension of gradient is the number of learnable parameters
- In feed-forward neural networks, the gradient of an error function  $E(\mathbf{w})$  can be efficiently evaluated via an algorithm called error backpropagation



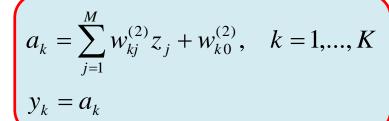
#### Feed-forward neural networks

Two-layer feed-forward neural networks for regression



$$a_{j} = \sum_{i=1}^{D} w_{ji}^{(1)} x_{i} + w_{j0}^{(1)}, \quad j = 1,..., M$$

$$z_{j} = h(a_{j})$$





Variables/Activations dependency:

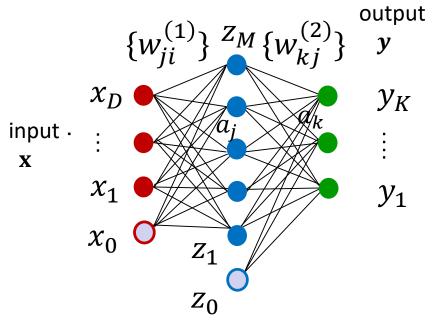
$$\{x_i\} \to \{w_{ji}^{(1)}\} \to \{a_j\} \to \{z_j\} \to \{w_{kj}^{(2)}\} \to \{a_k\} \to \{y_k\} \to E$$

Our goal in gradient computation:

$$\frac{\partial E}{\partial w_{kj}^{(2)}}$$
 and  $\frac{\partial E}{\partial w_{ji}^{(1)}}$ 

 In backpropagation, we also need to compute

$$\delta_k = \frac{\partial E}{\partial a_k}$$
 and  $\delta_j = \frac{\partial E}{\partial a_j}$ 





Stochastic gradient descent

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E_n(\mathbf{w}^{(\tau)})$$

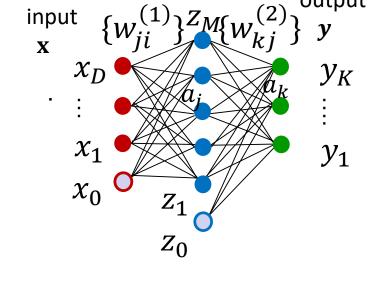
Multi-dimensional regression

$$a_{j} = \sum_{i=1}^{D} w_{ji}^{(1)} x_{i} + w_{j0}^{(1)}, \quad j = 1,..., M$$

$$z_{j} = h(a_{j})$$

$$a_k = \sum_{j=1}^{M} w_{kj}^{(2)} z_j + w_{k0}^{(2)}, \quad k = 1, ..., K$$
$$y_k = a_k$$

$$E(\mathbf{w}) = \frac{1}{2} \sum_{k=1}^{K} (y_k - t_k)^2$$



Hidden layer 
$$\delta_{j} \equiv \frac{\partial E}{\partial a_{j}} = \sum_{k} \frac{\partial E}{\partial a_{k}} \frac{\partial a_{k}}{\partial a_{j}}$$

$$= h'(a_{j}) \sum_{k} w_{kj}^{(2)} \delta_{k}$$

$$\delta_k \equiv \frac{\partial E}{\partial a_k} = y_k - t_k$$

**Error function** 



Variables/Activations dependency:

$$\{x_i\} \to \{w_{ji}^{(1)}\} \to \{a_j\} \to \{z_j\} \to \{w_{kj}^{(2)}\} \to \{a_k\} \to \{y_k\} \to E$$

$$a_{j} = \sum_{i=1}^{D} w_{ji}^{(1)} x_{i} + w_{j0}^{(1)}, \quad j = 1,..., M$$

$$z_{j} = h(a_{j})$$

$$\delta_j = h'(a_j) \sum_k w_{kj}^{(2)} \delta_k$$

Hidden layer

$$a_k = \sum_{j=1}^{M} w_{kj}^{(2)} z_j + w_{k0}^{(2)}, \quad k = 1, ..., K$$

$$y_k = a_k$$

Output layer 
$$\frac{\partial E}{\partial w_{kj}^{(2)}} = \frac{\partial E}{\partial a_k} \frac{\partial a_k}{\partial w_{kj}^{(2)}} = \delta_k z_j$$

$$E(\mathbf{w}) = \frac{1}{2} \sum_{k=1}^{K} (y_k - t_k)^2$$

Error function 
$$\delta_k = y_k - t_k$$





Variables/Activations dependency:

$$\{x_i\} \to \{w_{ji}^{(1)}\} \to \{a_j\} \to \{z_j\} \to \{w_{kj}^{(2)}\} \to \{a_k\} \to \{y_k\} \to E$$

$$a_{j} = \sum_{i=1}^{D} w_{ji}^{(1)} x_{i} + w_{j0}^{(1)}, \quad j = 1, ..., M$$

$$z_{j} = h(a_{j})$$

$$\delta_{j} = h'(a_{j}) \sum_{k} w_{kj}^{(2)} \delta_{k}$$

$$\partial F = \partial F = \partial a_{k}$$

Hidden layer 
$$\frac{\partial E}{\partial w_{ji}^{(1)}} = \frac{\partial E}{\partial a_j} \frac{\partial a_j}{\partial w_{ji}^{(1)}} = \delta_j x_i$$

$$a_k = \sum_{j=1}^{M} w_{kj}^{(2)} z_j + w_{k0}^{(2)}, \quad k = 1, ..., K$$

Output layer 
$$\frac{\partial E}{\partial w_{kj}^{(2)}} = \frac{\partial E}{\partial a_k} \frac{\partial a_k}{\partial w_{kj}^{(2)}} = \delta_k z_j$$

$$E(\mathbf{w}) = \frac{1}{2} \sum_{k=1}^{K} (y_k - t_k)^2$$

Error function 
$$\delta_k = y_k - t_k$$

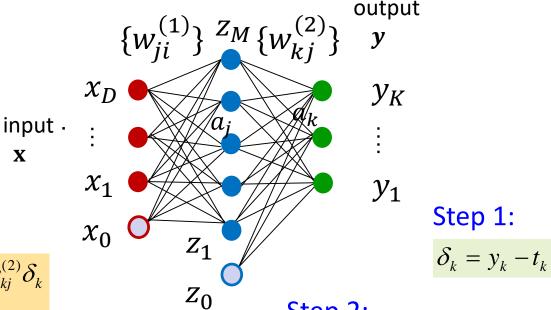
$$\delta_k = y_k - t_k$$





 $y_k = a_k$ 

# A review of error backpropagation



#### Step 3:

$$\delta_j = h'(a_j) \sum_k w_{kj}^{(2)} \delta_k$$

#### Step 4:

$$\frac{\partial E}{\partial w_{ji}^{(1)}} = \frac{\partial E}{\partial a_j} \frac{\partial a_j}{\partial w_{ji}^{(1)}} = \delta_j x_i$$

### Step 2:

$$\frac{\partial E}{\partial w_{kj}^{(2)}} = \frac{\partial E}{\partial a_k} \frac{\partial a_k}{\partial w_{kj}^{(2)}} = \delta_k z_j$$



# Error backpropagation for other tasks

• Step 1:  $\delta_k \equiv \frac{\partial E}{\partial a_k} = \frac{\partial E}{\partial y_k} \frac{\partial y_k}{\partial a_k}$ 

$$E(\mathbf{w}) = \begin{cases} \frac{1}{2} \sum_{k=1}^{K} (y_k - t_k)^2 & \text{regression} \\ -\{t \ln y(\mathbf{x}, \mathbf{w}) + (1 - t) \ln(1 - y(\mathbf{x}, \mathbf{w}))\} & \text{binary classification} \\ -\sum_{k=1}^{K} t_k \ln y_k(\mathbf{x}, \mathbf{w}) & \text{multi-calss classification} \end{cases}$$

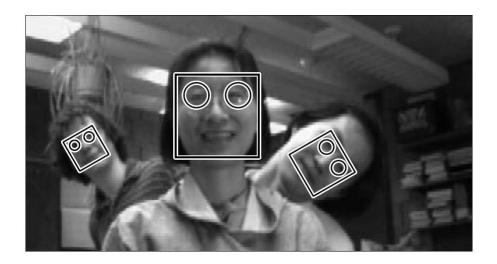
$$y_k = a_k$$
 regression  $y = \frac{1}{1 + e^{-a}}$  binary classification  $y_k = \frac{e^{a_k}}{\sum_j e^{a_j}}$  multi-class classification

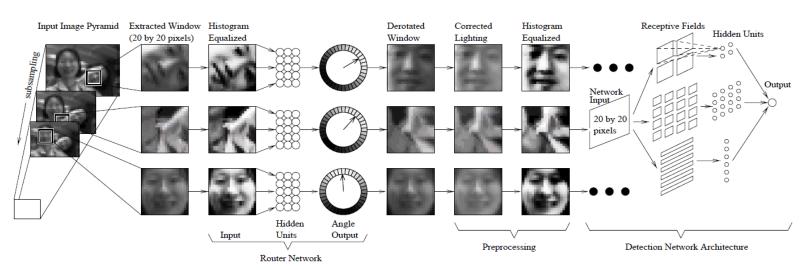
Steps 2 ~ 4 remain unchanged



# **Neural networks' applications**

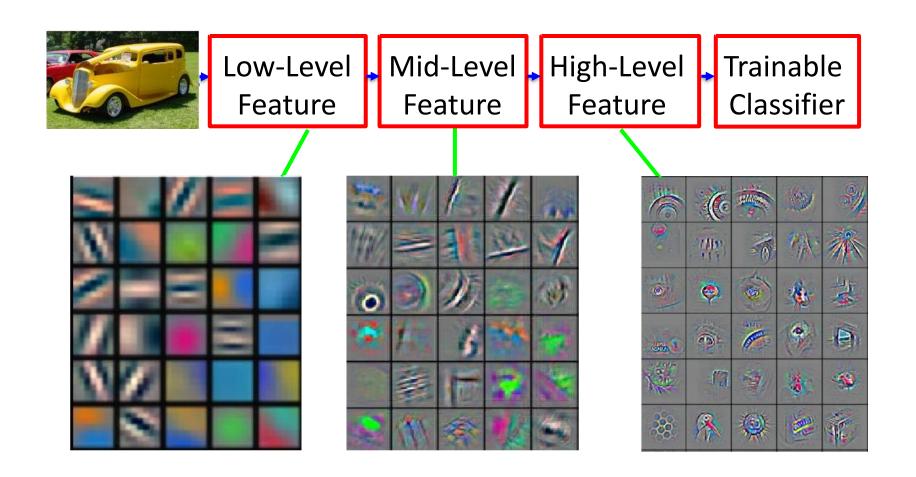
Face detection





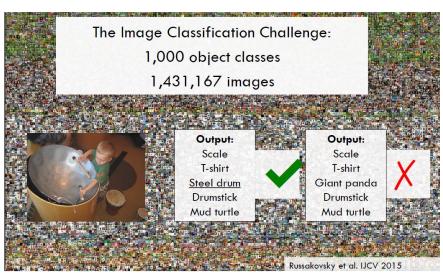


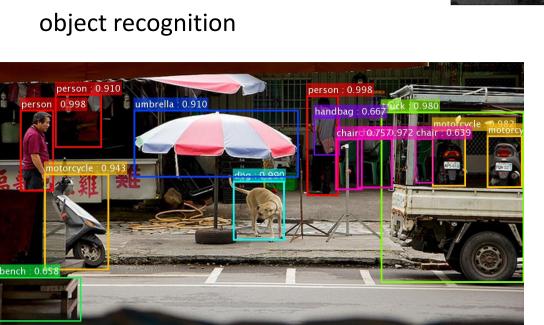
### **Convolutional** neural networks





### **Convolutional** neural networks' applications





skis person person person person backpack skis skis skis

object segmentation

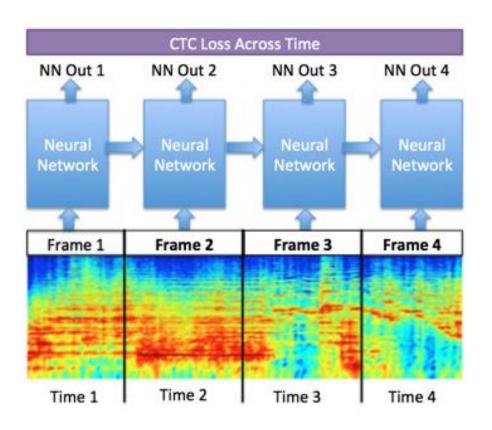
object detection





### **Recurrent** neural networks

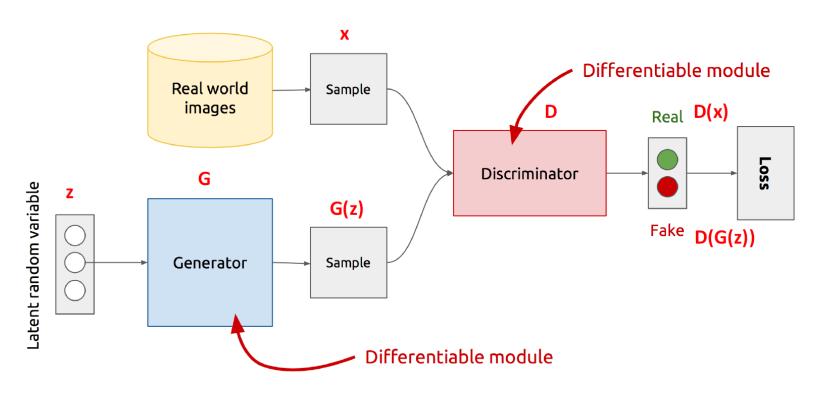
Speech recognition



https://gab41.lab41.org/speech-recognition-you-down-with-ctc-8d3b558943f0



### **Generative adversarial networks**



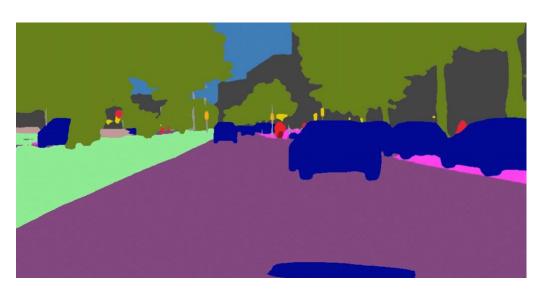
https://www.slideshare.net/xavigiro/deep-learning-for-computer-vision-generative-models-and-adversarial-training-upc-2016



# **Generative adversarial networks' applications**



Karras et al.



Wang et al.



### References

• Chapters 5.1, 5.2, and 5.3 in the PRML textbook



# **Thank You for Your Attention!**

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