



Introduction to Machine Learning

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

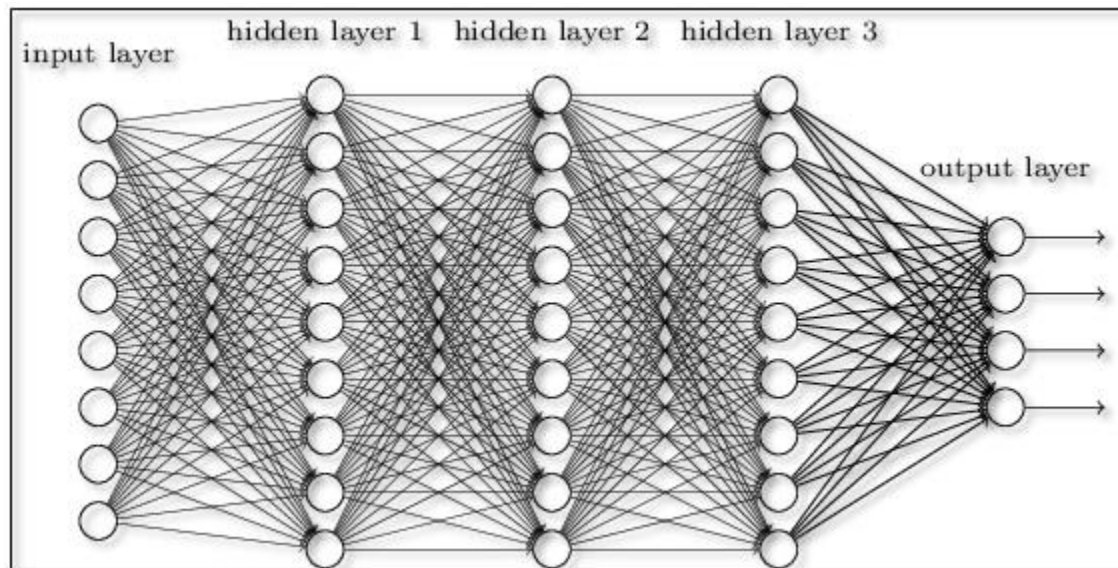
- A linear model for regression or classification

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

- Decision based on a linear combination of **fixed** nonlinear basis functions
- f is an identity function for regression
- 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

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

Examples of basis functions

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

$$\phi_j(x) = x^j$$

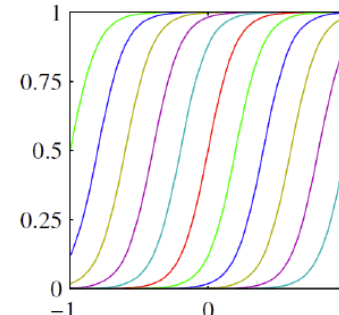
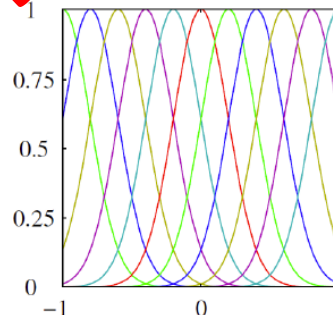
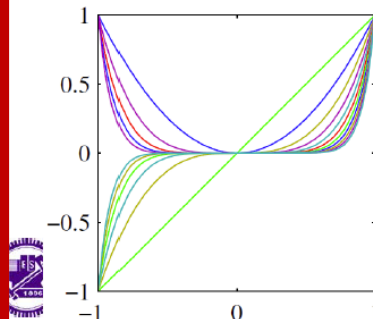
- Gaussian basis function: governed by μ_j and s

➤ μ_j governs the location while s governs the scale

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

- Sigmoidal basis function: governed by μ_j and s

$$\phi_j(x) = \sigma \left(\frac{x - \mu_j}{s} \right) \text{ where } \sigma(a) = \frac{1}{1 + \exp(-a)}$$



Activations

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

- Construct M linear combinations of the inputs x_1, \dots, x_D

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

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

$$z_j = h(a_j)$$

- $\{z_j = h(a_j)\}_{j=1}^M$ 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

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

- where a_k is the **output activation** for $k = 1, 2, \dots, K$
- $\{w_{kj}^{(2)}\}_{j=1}^M$ 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 $\xrightarrow{a_j}$ $\xrightarrow{a_k}$ y_k

- where \mathbf{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**

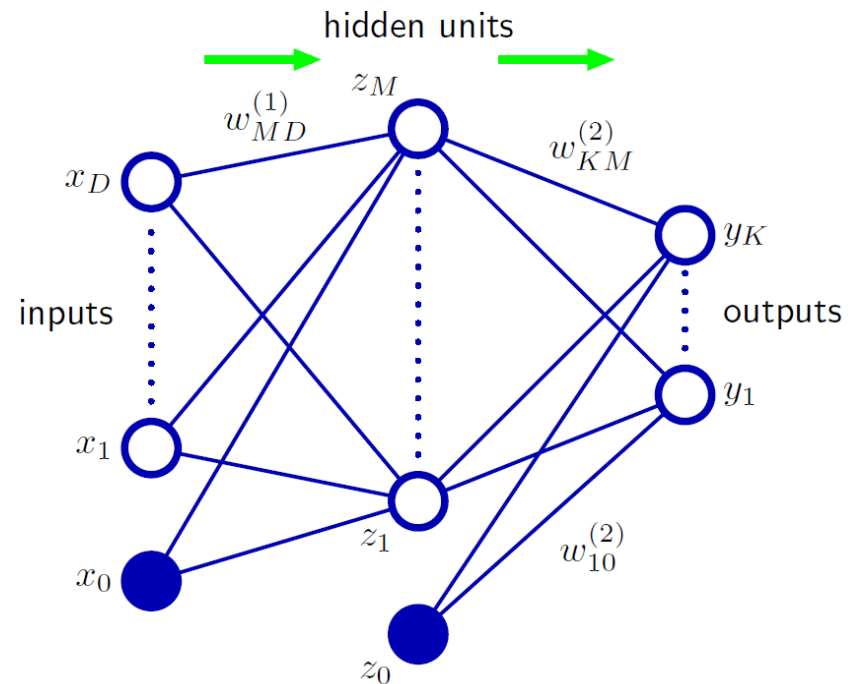
$$y_k(\mathbf{x}, \mathbf{w}) = \sigma \left(\sum_{j=0}^M w_{kj}^{(2)} h \left(\sum_{i=0}^D w_{ji}^{(1)} x_i \right) \right)$$

Network Diagram

Nodes: Input, hidden, and output variables

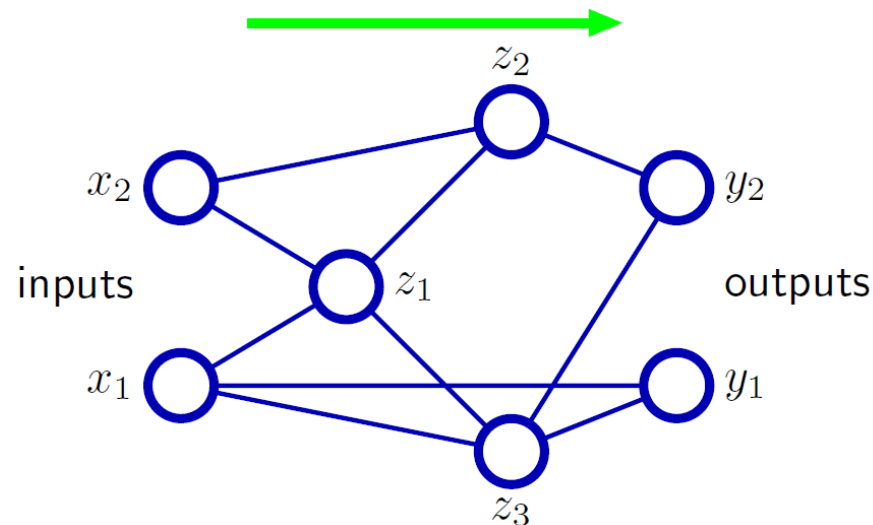
Links: Weights and biases

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

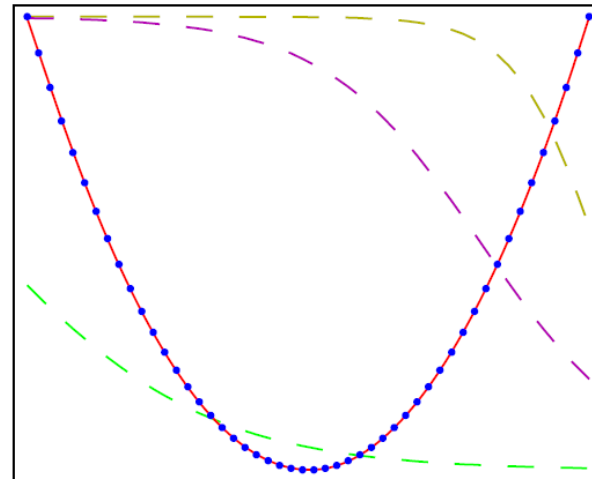


Neural networks as universal approximators

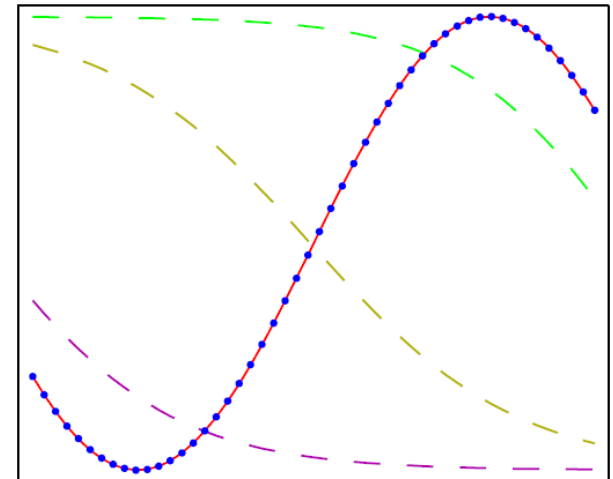
Points:
training data

Dashed curves:
Outputs of
three hidden
units

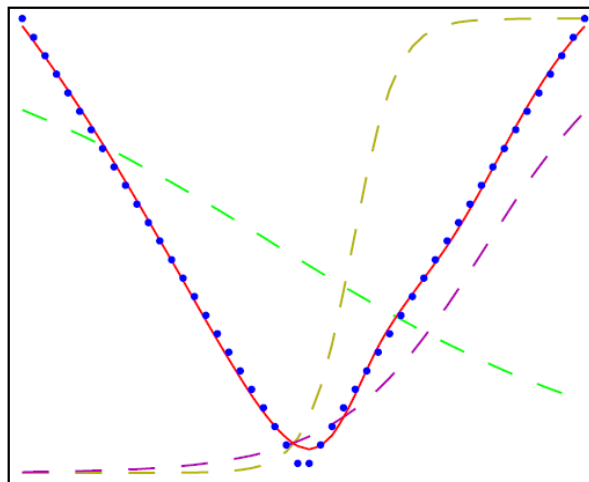
Curve:
Prediction by
the NN



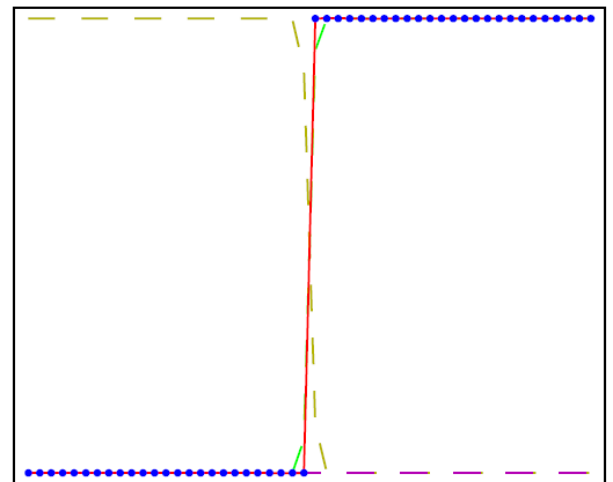
$$f(x) = x^2$$



$$f(x) = \sin(x)$$



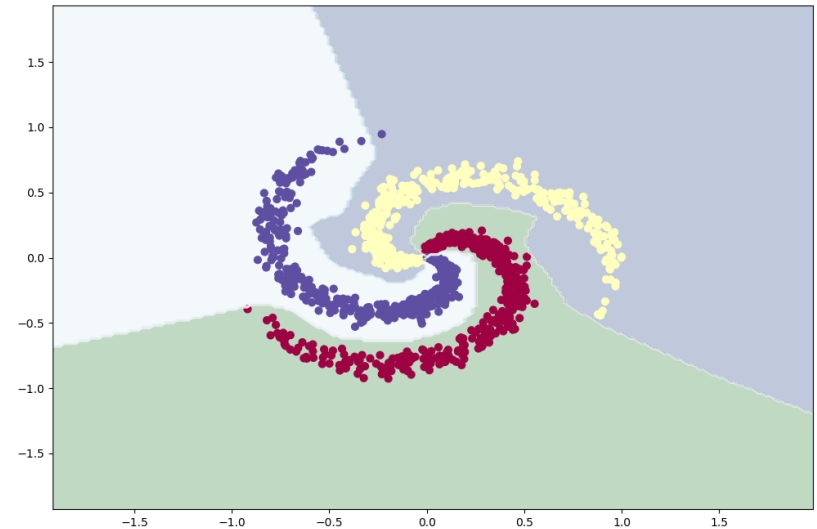
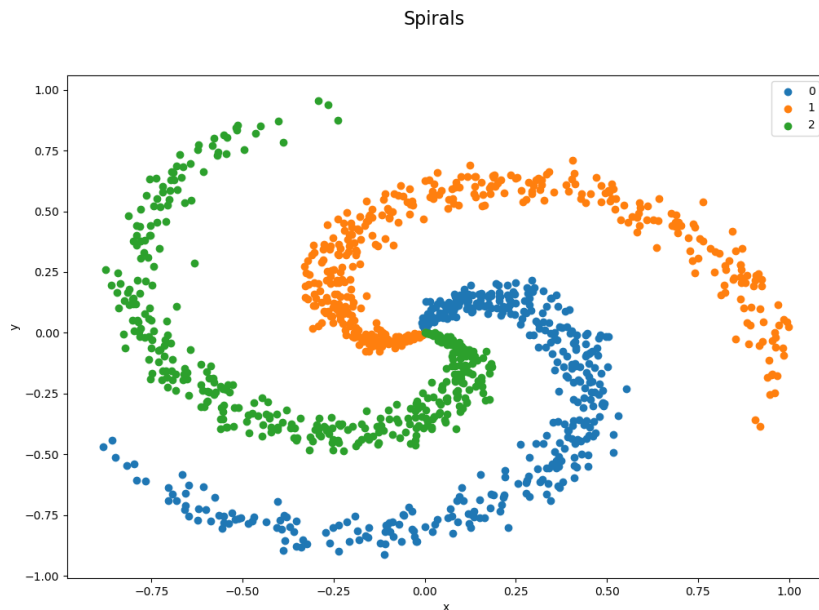
$$f(x) = |x|$$



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 $n = 1, 2, \dots, N$, 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

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

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

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

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



ML solution for 1D regression

- 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 \mathbf{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

ML solution for 1D regression

- Optimization by using gradient descent, stochastic gradient descent, or 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}_{ML} , the value of β can be found by minimizing the negative log likelihood

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



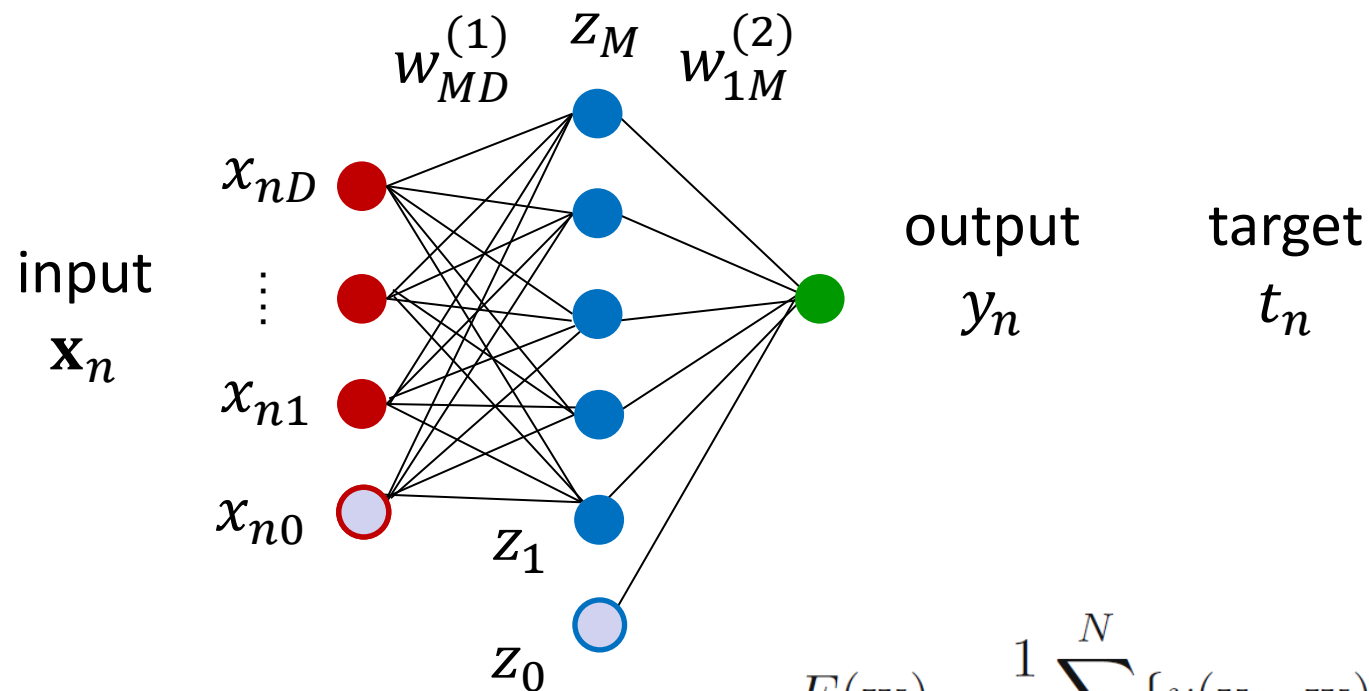
ML solution for 1D regression

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

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

ML solution for 1D regression

- Two-layer neural networks for one-dimensional regression



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

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

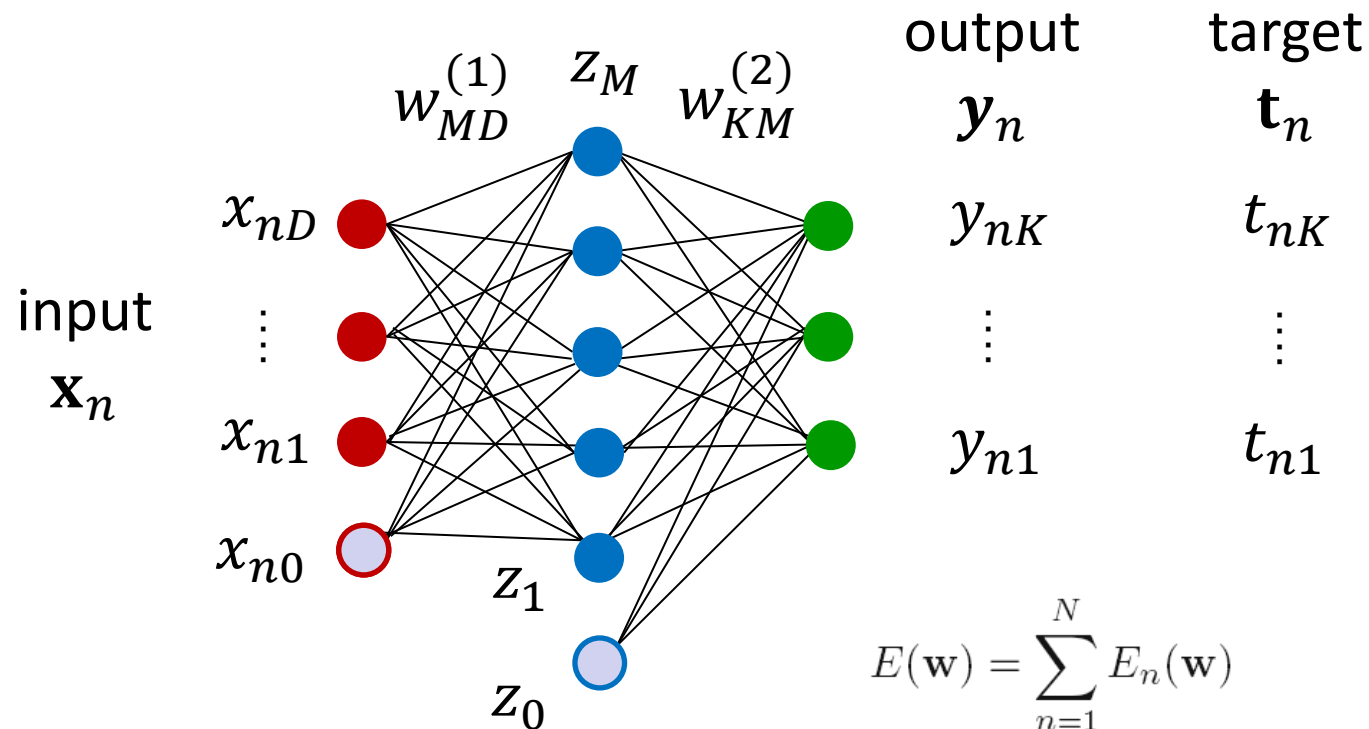
$$p(\mathbf{t}|\mathbf{x}, \mathbf{w}) = \mathcal{N}(\mathbf{t}|\mathbf{y}(\mathbf{x}, \mathbf{w}), \beta^{-1}\mathbf{I})$$

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



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

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

Neural networks for binary classification

- Neural networks can be used for classification
- Given a set of training data $\{\mathbf{x}_n\}$ where $n = 1, 2, \dots, N$, together with a corresponding set of target labels $\{t_n\}$, where $t_n = 1$ denotes class C_1 and $t_n = 0$ denotes class C_2
- Construct (two-layer) neural networks having a single output whose activation function is a logistic sigmoid

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

- where $0 \leq y(\mathbf{x}, \mathbf{w}) \leq 1$
- $y(\mathbf{x}, \mathbf{w})$ is the conditional probability $p(C_1|\mathbf{x})$
- The conditional probability $p(C_2|\mathbf{x})$ 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

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

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

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

ML solution for binary classification

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

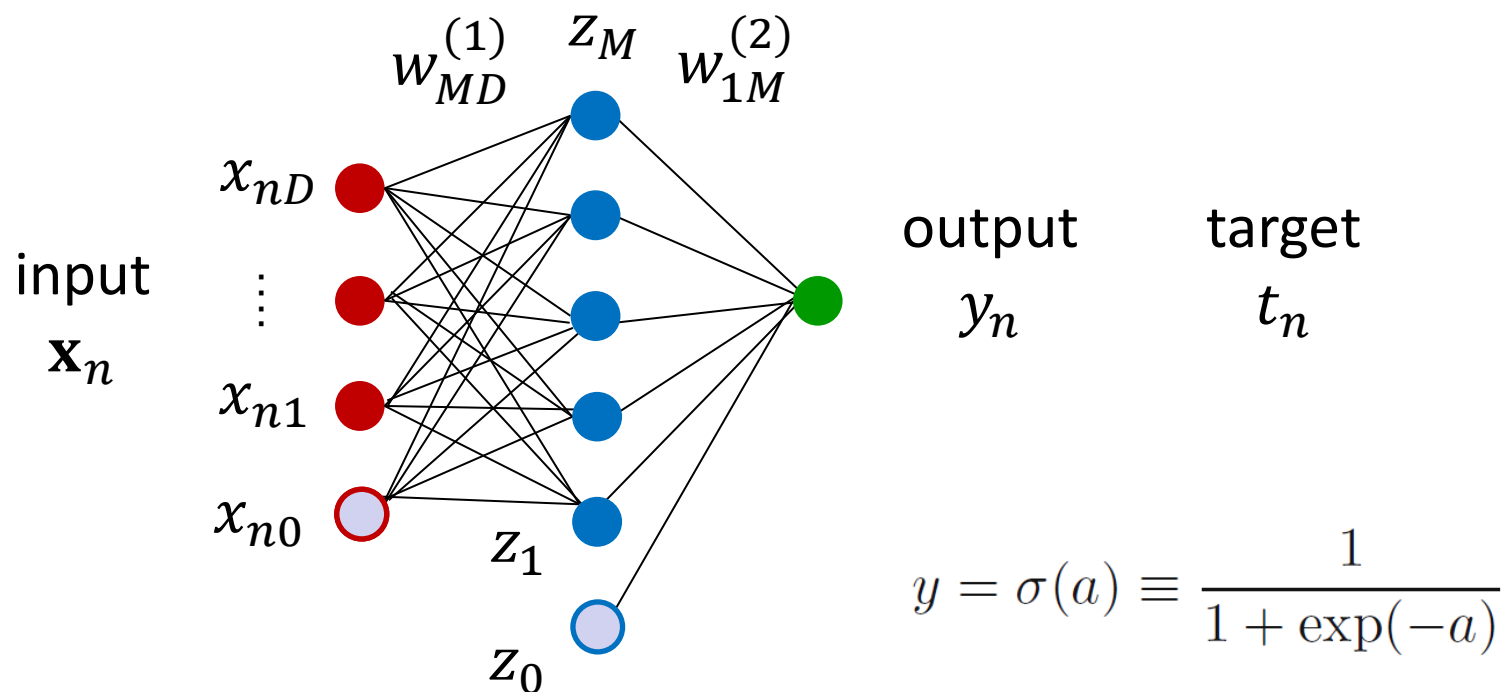
$$E(\mathbf{w}) = - \sum_{n=1}^N \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$

➤ where y_n denotes $y(\mathbf{x}_n, \mathbf{w})$

- Optimize \mathbf{w} by using gradient descent or its variant
- After getting \mathbf{w}_{ML} , binary classification is carried out by

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

ML solution for binary classification



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

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 $n = 1, 2, \dots, N$, 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

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

➤ where $0 \leq y_k \leq 1$ and $\sum_k y_k = 1$

ML solution for multi-class classification

- The negative log likelihood or the cross-entropy error is

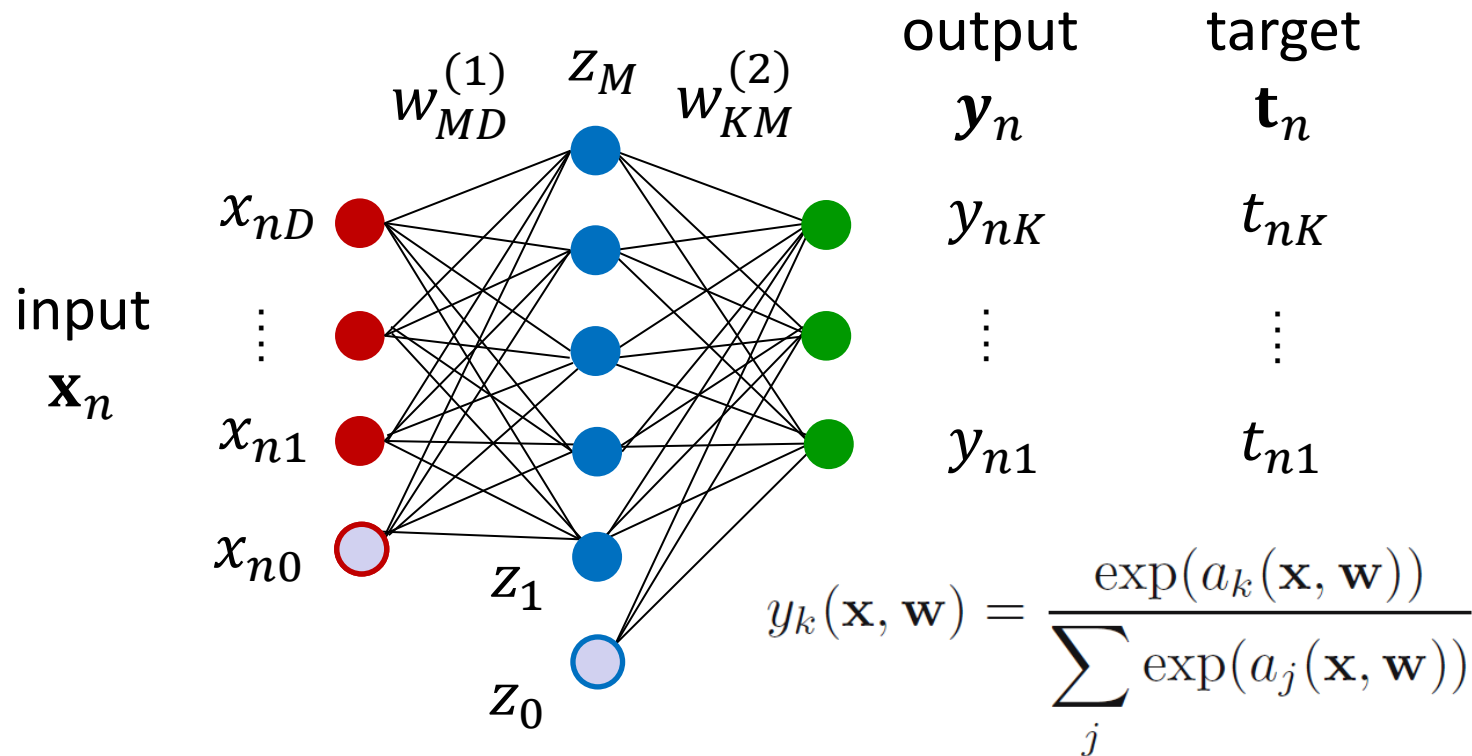
$$E(\mathbf{w}) = - \sum_{n=1}^N \sum_{k=1}^K t_{kn} \ln y_k(\mathbf{x}_n, \mathbf{w})$$

- Optimize \mathbf{w} by using gradient descent or its variant
- After getting \mathbf{w}_{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 \mathbf{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
- $\eta > 0$ is the **learning rate**
- This is a batch method, as evaluation of ∇E involves the entire data set
- 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

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



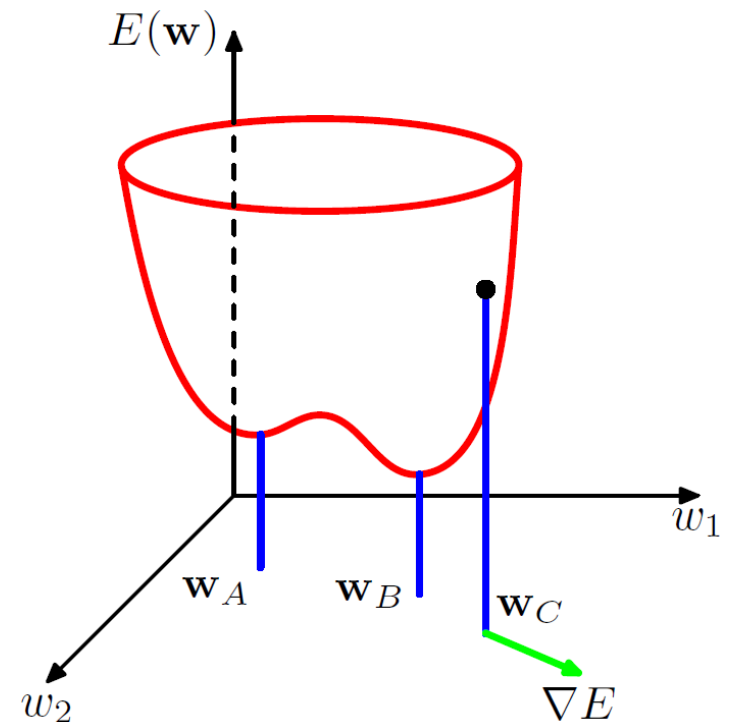
Stochastic gradient descent

- 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
- \mathbf{w}_A is a local minimum
- \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 ∇E

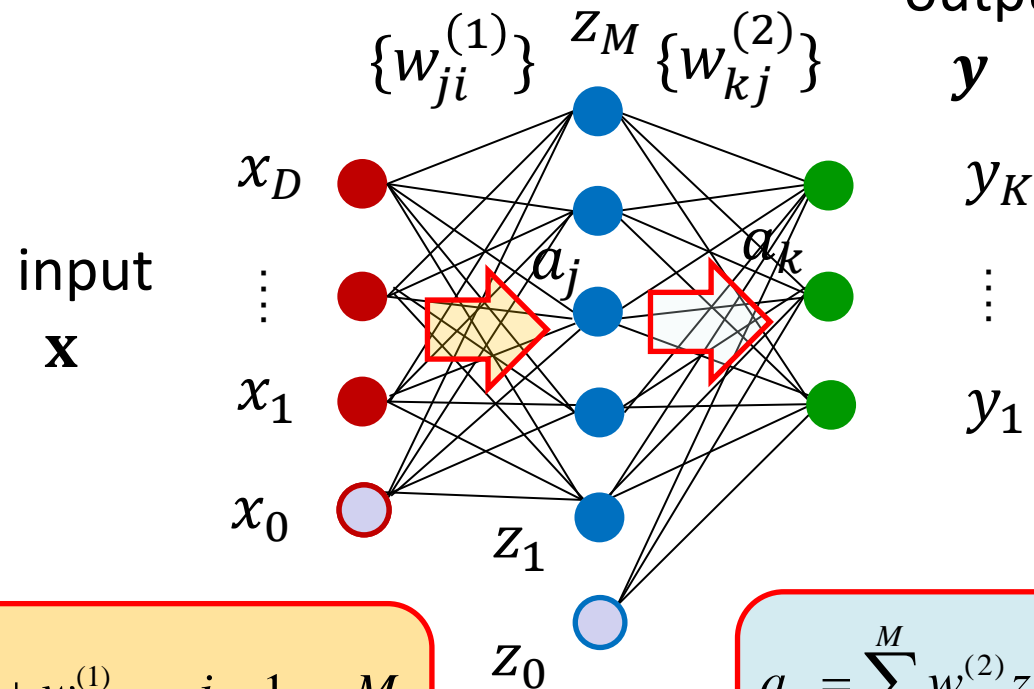


Error backpropagation

- The computational cost of gradient descent mainly lies in the evaluation of gradient at each iteration
 - $\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E_n(\mathbf{w}^{(\tau)})$
 - 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 output



$$a_j = \sum_{i=1}^D w_{ji}^{(1)} x_i + w_{j0}^{(1)}, \quad j = 1, \dots, M$$

$$z_j = h(a_j)$$

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

$$y_k = a_k$$

Error backpropagation

- Variables/Activations dependency:

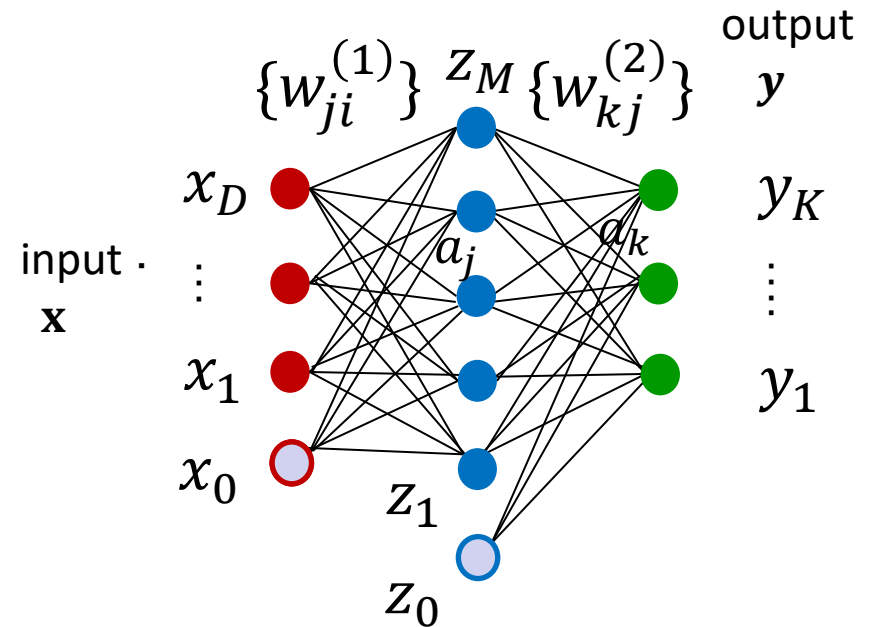
$$\{x_i\} \rightarrow \{w_{ji}^{(1)}\} \rightarrow \{a_j\} \rightarrow \{z_j\} \rightarrow \{w_{kj}^{(2)}\} \rightarrow \{a_k\} \rightarrow \{y_k\} \rightarrow E$$

- Our goal in gradient computation:

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

- In backpropagation, we also need to compute

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



Error backpropagation

- Stochastic gradient descent

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

- Multi-dimensional regression

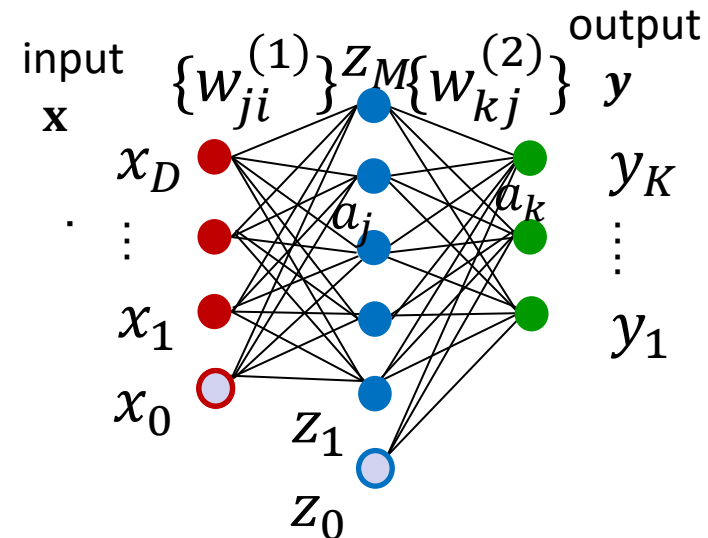
$$a_j = \sum_{i=1}^D w_{ji}^{(1)} x_i + w_{j0}^{(1)}, \quad j = 1, \dots, M$$

$$z_j = h(a_j)$$

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

$$y_k = a_k$$

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



Hidden layer

$$\delta_j \equiv \frac{\partial E}{\partial a_j} = \sum_k \frac{\partial E}{\partial a_k} \frac{\partial a_k}{\partial a_j}$$

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

Output layer

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

Error function

Error backpropagation

- Variables/Activations dependency:

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

$$a_j = \sum_{i=1}^D w_{ji}^{(1)} x_i + w_{j0}^{(1)}, \quad j = 1, \dots, M$$

$$z_j = h(a_j)$$

Hidden layer

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

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

$$y_k = a_k$$

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

$$\delta_k = y_k - t_k$$



Error backpropagation

- Variables/Activations dependency:

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

$$a_j = \sum_{i=1}^D w_{ji}^{(1)} x_i + w_{j0}^{(1)}, \quad j = 1, \dots, M$$

$$z_j = h(a_j)$$

Hidden layer

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

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

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

$$y_k = a_k$$

Output layer

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

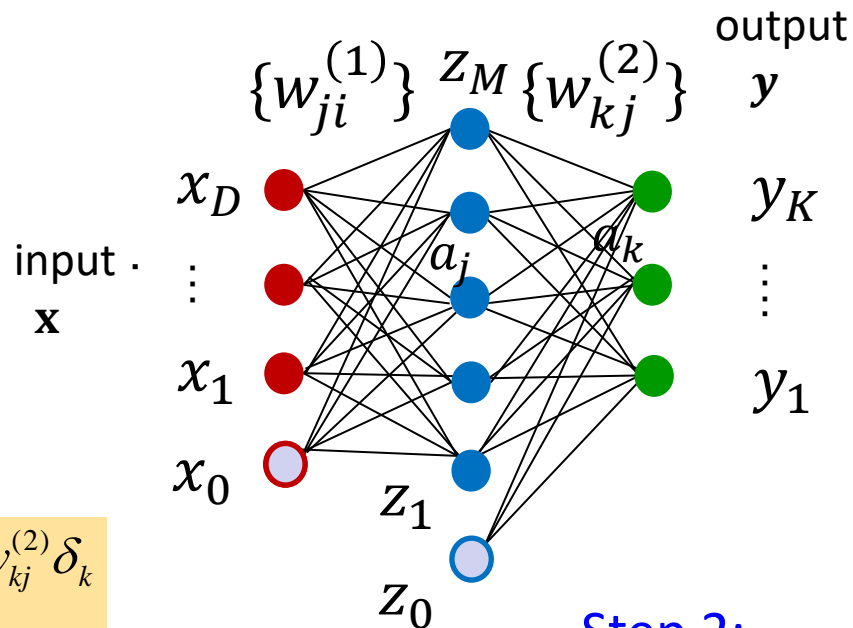
$$E(\mathbf{w}) = \frac{1}{2} \sum_{k=1}^K (y_k - t_k)^2$$

Error function

$$\delta_k = y_k - t_k$$



A review of error backpropagation



Step 3:

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

Step 1:

$$\delta_k = y_k - t_k$$

Step 2:

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

Step 4:

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

Error backpropagation for other tasks

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

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

$$y_k = a_k \quad \text{regression}$$

$$y = \frac{1}{1 + e^{-a}} \quad \text{binary classification}$$

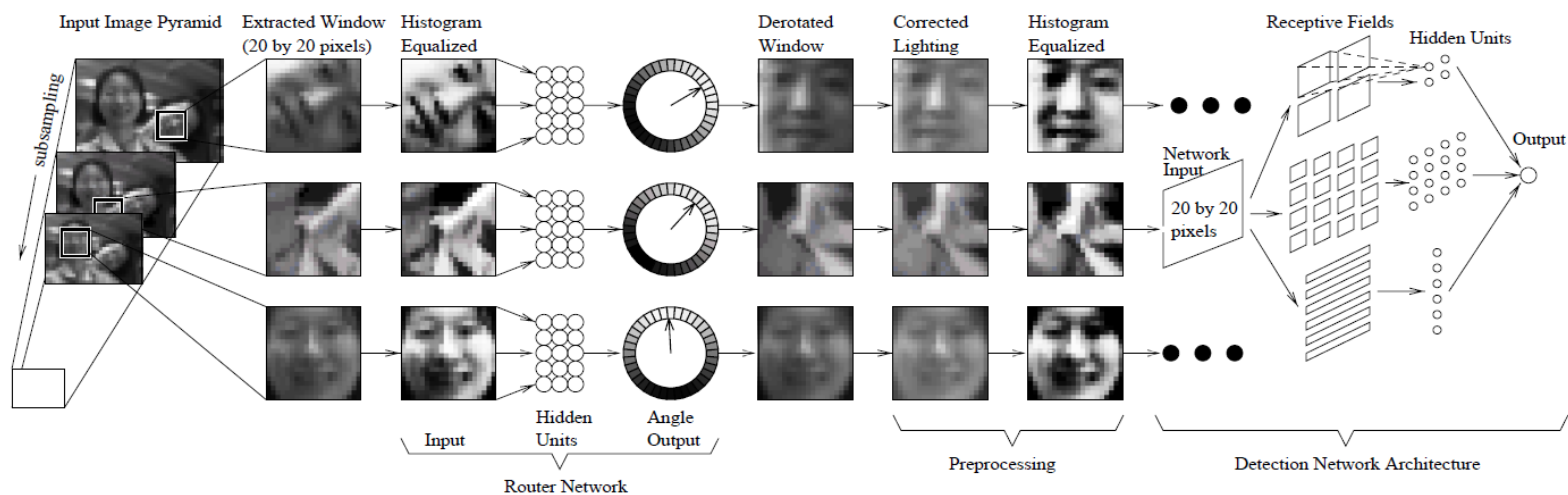
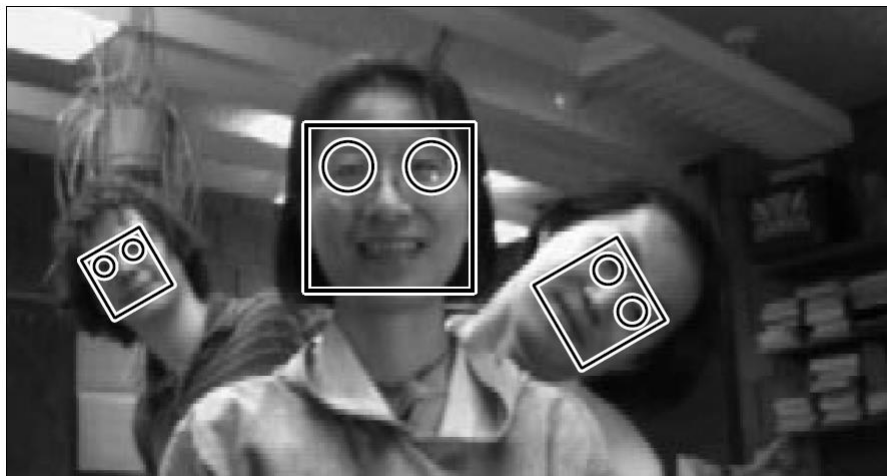
$$y_k = \frac{e^{a_k}}{\sum_j e^{a_j}} \quad \text{multi-class classification}$$

- Steps 2 ~ 4 remain unchanged



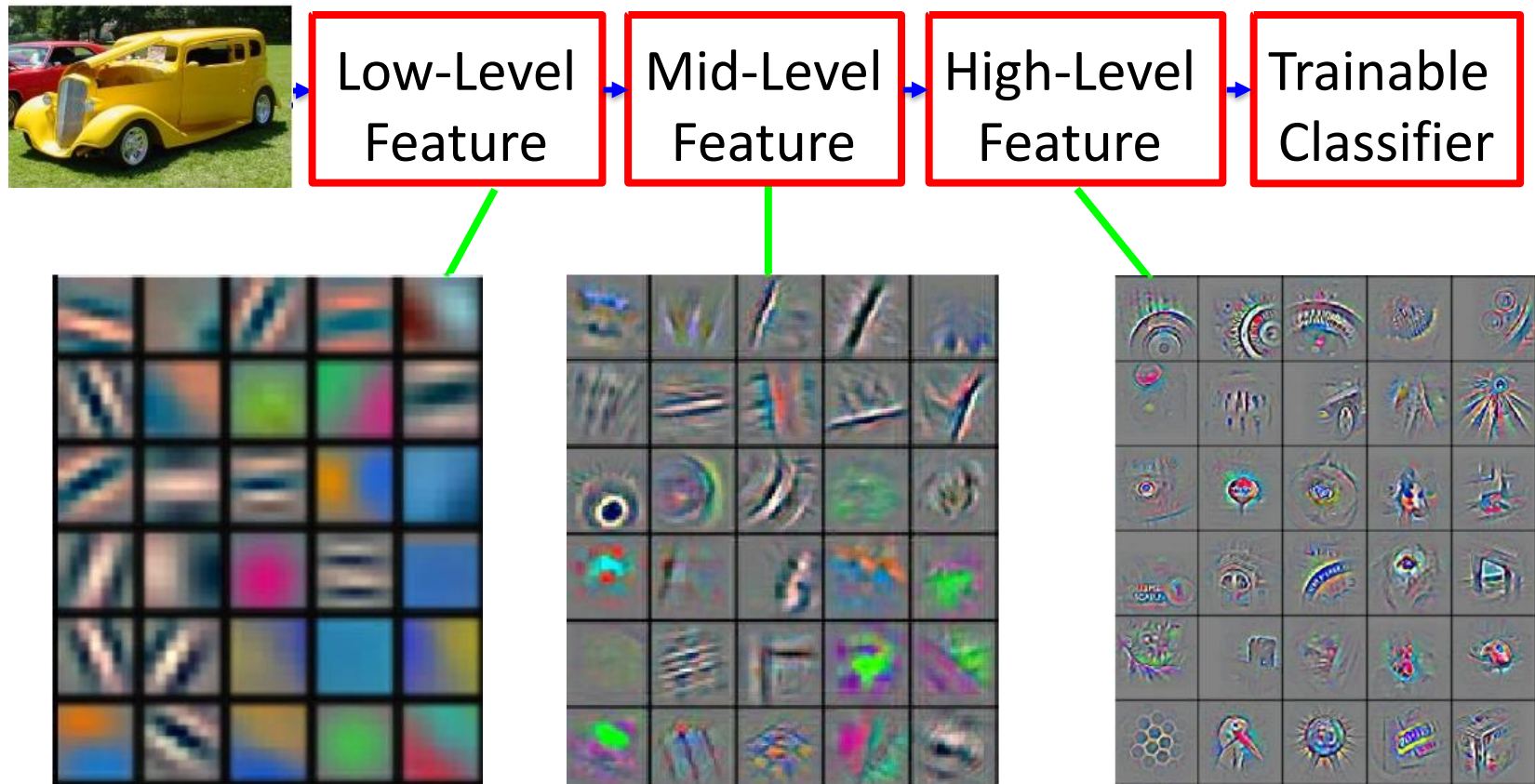
Neural networks' applications

- Face detection

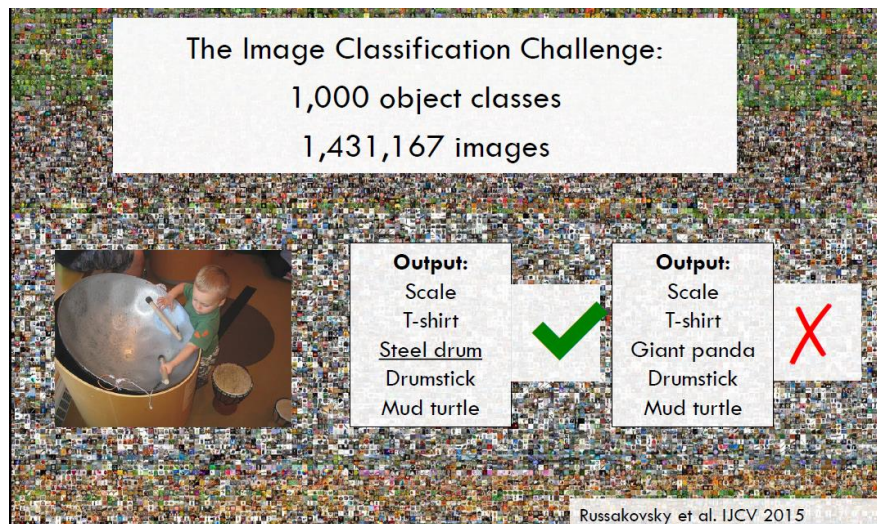


Rowley et al.

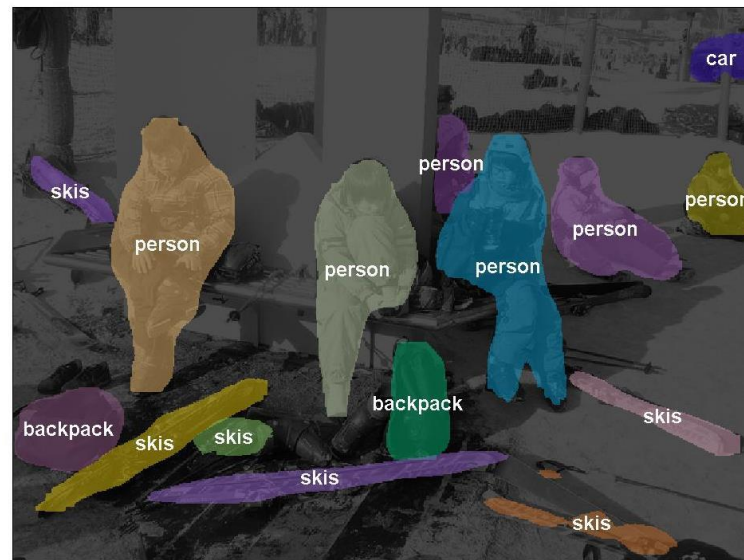
Convolutional neural networks



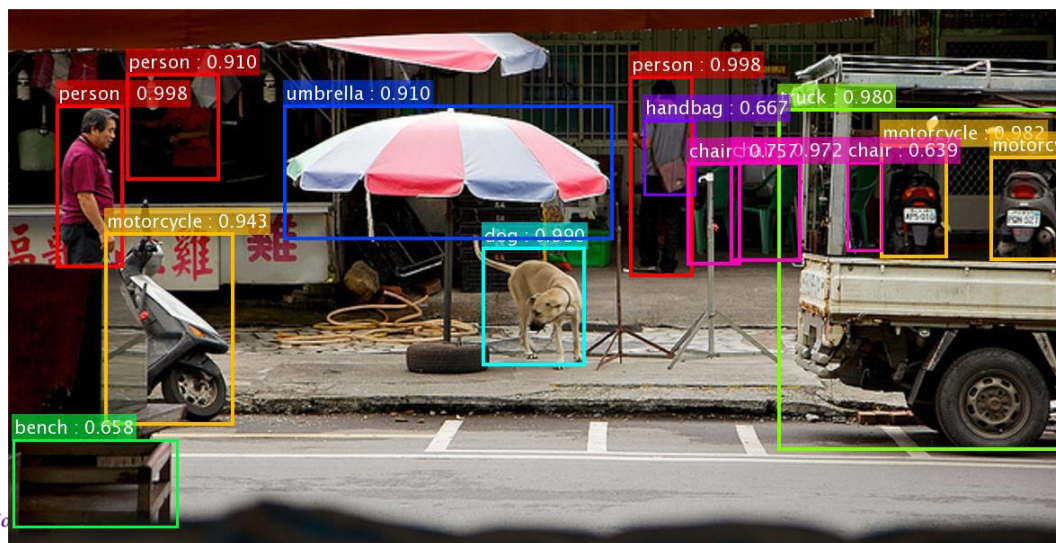
Convolutional neural networks' applications



object recognition



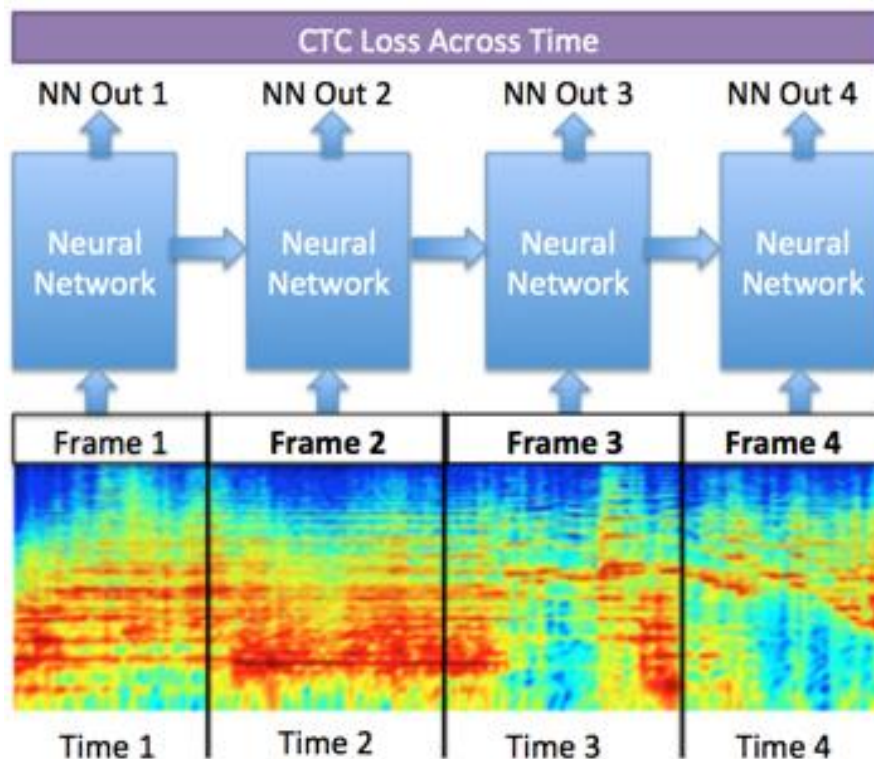
object segmentation



object detection

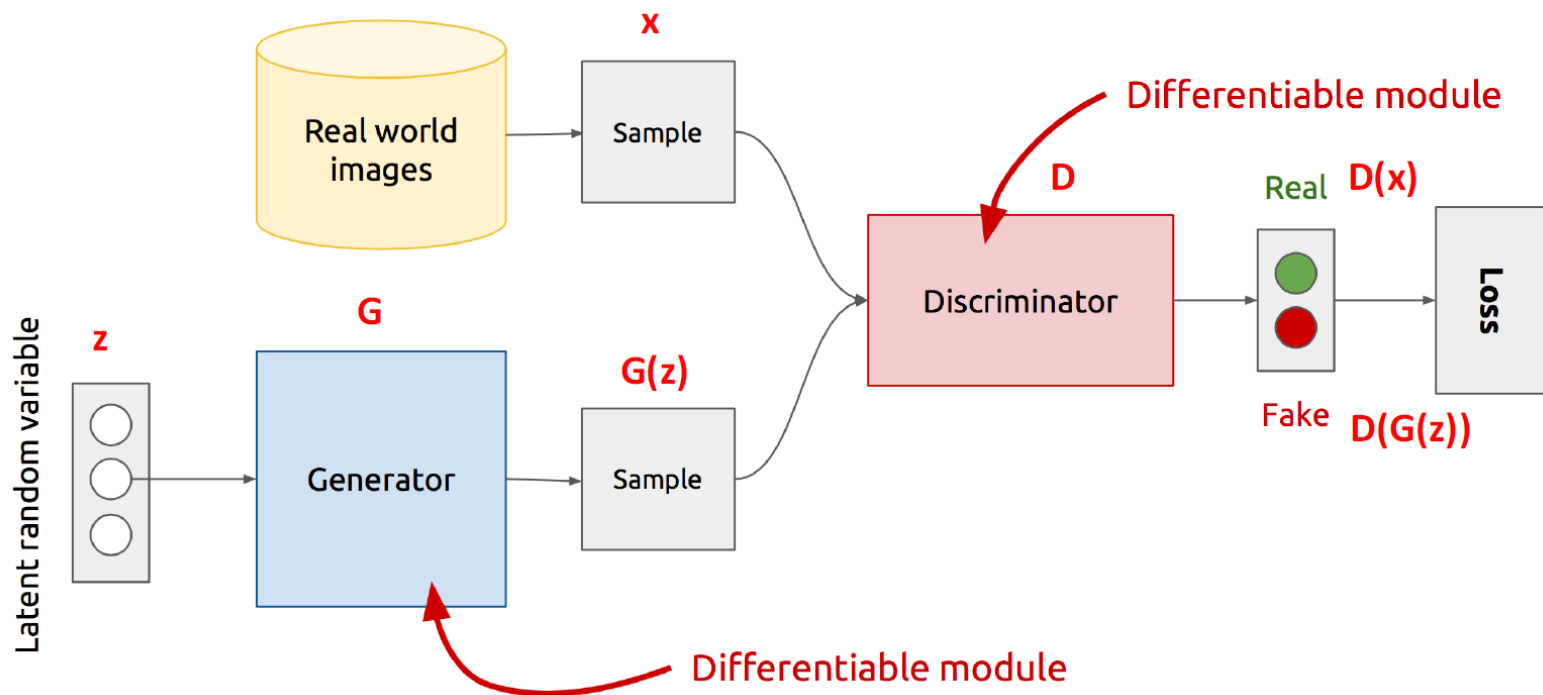
Recurrent neural networks

- Speech recognition



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

Generative adversarial networks

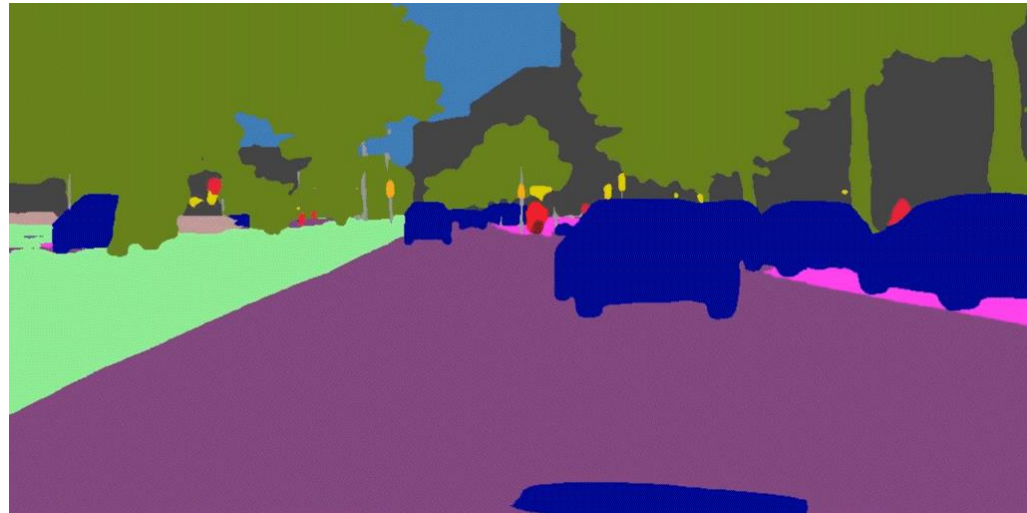


<https://www.slideshare.net/xavigiro/deep-learning-for-computer-vision-generative-models-and-adversarial-training-upc-2016>

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!

THANK YOU FOR YOUR ATTENTION!

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