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Introduction to Neural Networks

GU 4241/GR 5241

Statistical Machine Learning

Xiaofei Shi

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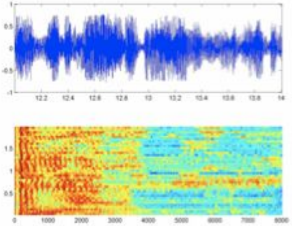
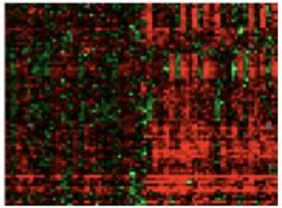


Gene Expression

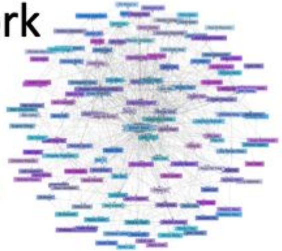


Product
Recommendation

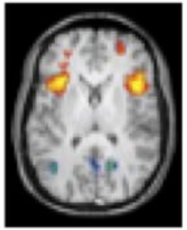
amazon
NETFLIX
ebay

Relational Data/
Social Network

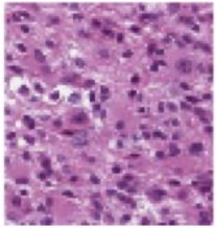
facebook
twitter



fMRI



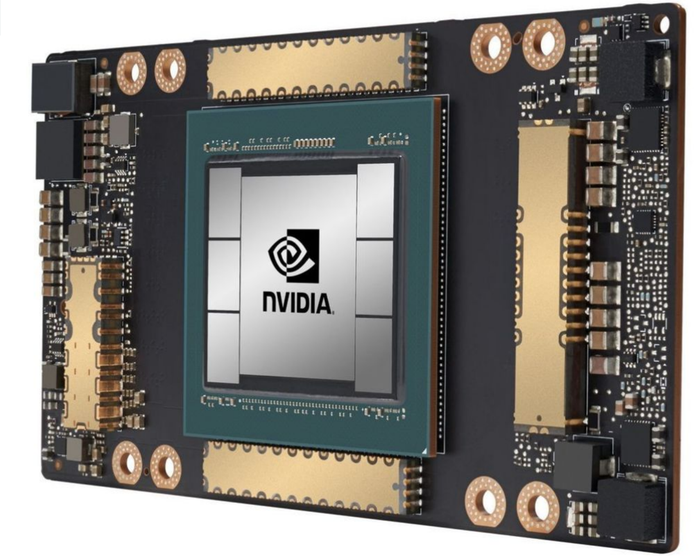
Tumor region



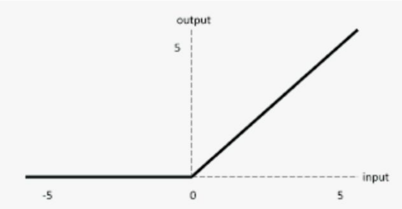
Overview

- A neural network is a supervised learning method. It can be applied to both regression and classification problems.
- The main idea is to extract linear combinations of the inputs as derived features, and then model the target as a nonlinear function of these features.
- The nonlinear transformation contributes to the model flexibility.
- Today, we will focus on the most widely used ``vanilla'' neural net, also called the single hidden layer feedforward neural networks.

Why deep architecture works



- Enough computational power
- Large training dataset:
  MNIST, CI-FAR, IMAGENET
- Architectures adapted to
  current computational methods



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Overview

- Derived features Z_m are obtained by applying the *activation function* σ to linear combinations of the inputs:

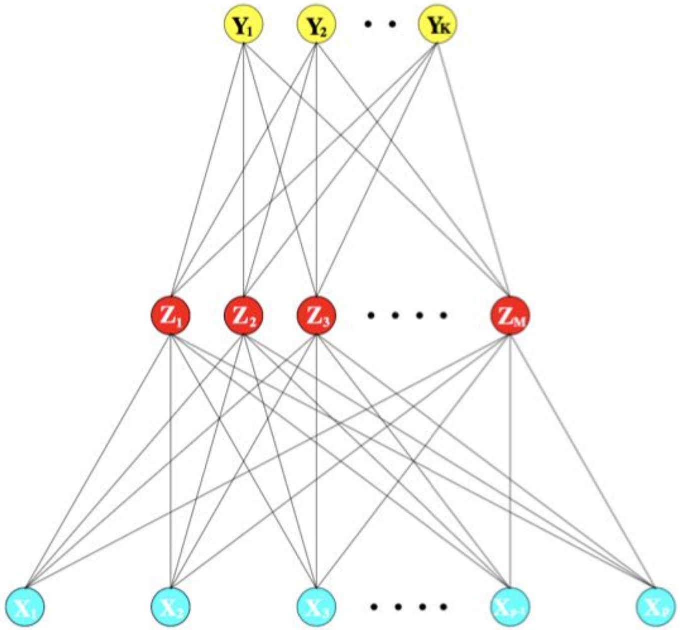
$$Z_m = \sigma(\alpha_{0m} + \alpha_m^T X), m = 1, \ldots, M.$$

- The target Y_k (or T_k in the figure) is modeled as a function of linear combinations of the Z_m:

$$T_k = \beta_{0k} + \beta_k^T Z, \quad k = 1, \ldots, K.$$

- The output function $g_k(T)$ allows a final transformation of the vector of outputs T:

$$f_k(X) = g_k(T), \quad k = 1, \ldots, K.$$



Schematic of a single hidden layer, feed-forward neural network

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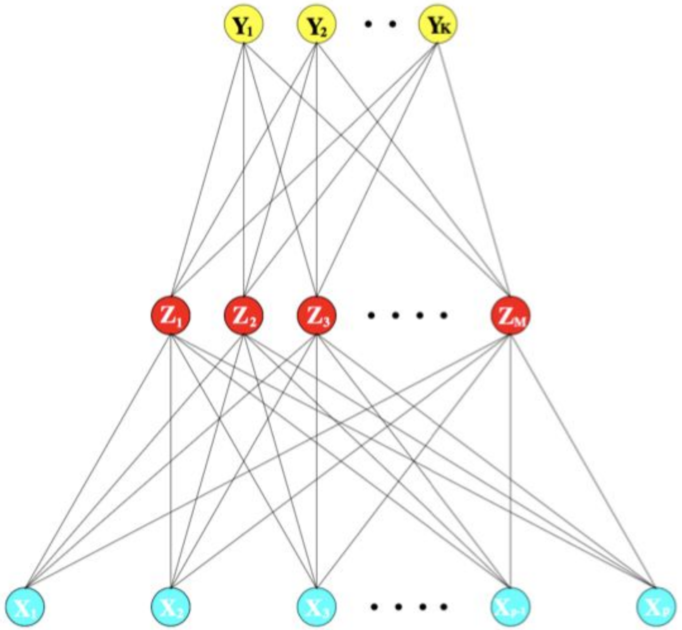
Artificial neurons

- Each artificial neuron has inputs and produces a single output which can be sent to multiple other neurons. The inputs can be the feature values of a sample of external data, such as images or documents, or they can be the outputs of other neurons.
- The outputs of the final output neurons of the neural net accomplish the task.



Schematic of a single hidden layer, feed-forward neural network

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Artificial neurons

- Neuron pre-activation (or input activation):

$$a(\mathbf{x}) = b + \sum_i w_i x_i = b + \mathbf{w}^\top \mathbf{x}$$

- Neuron output activation:

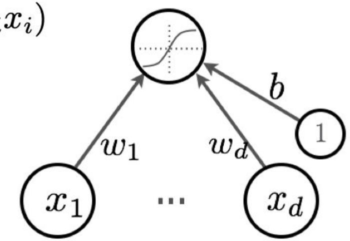
$$h(\mathbf{x}) = g(a(\mathbf{x})) = g(b + \sum_i w_i x_i)$$

where

$\mathbf{w}$ are the weights (parameters)

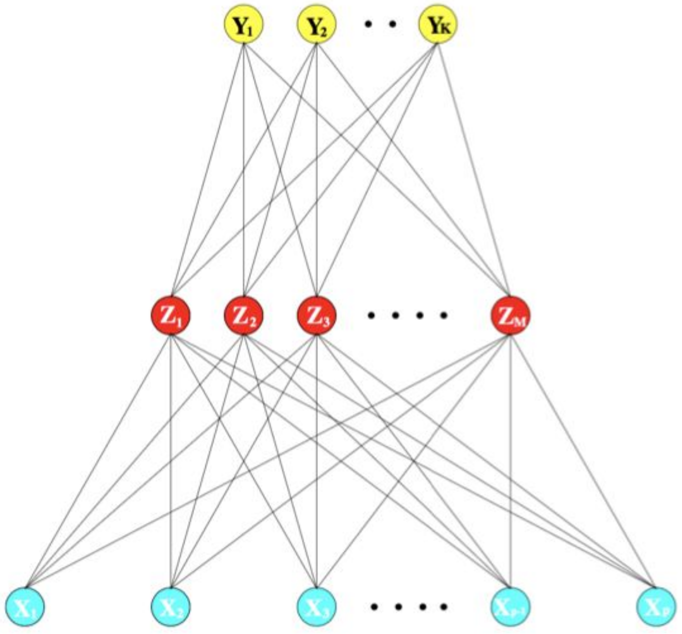
b is the bias term

$g(\cdot)$ is called the activation function



Activation functions

- An activation function of a node defines the output of that node given an input or set of inputs.
- Usually nonlinear.



Schematic of a single hidden layer, feed-forward neural network

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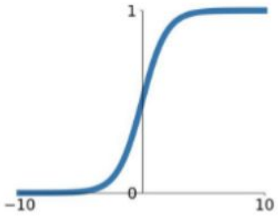
Activation functions

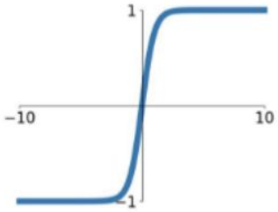
Sigmoid

$\sigma(x) = \frac{1}{1+e^{-x}}$



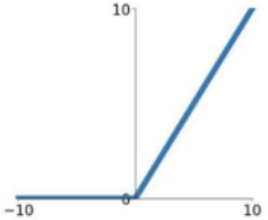
tanh

$\tanh(x)$



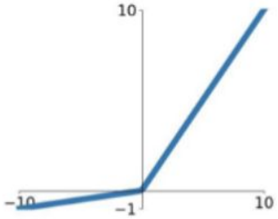
ReLU

$\max(0, x)$



Leaky ReLU

$\max(0.1x, x)$

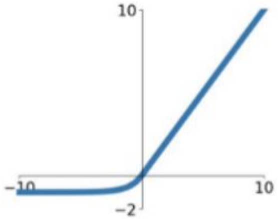


Maxout

$\max(w_1^T x + b_1, w_2^T x + b_2)$

ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



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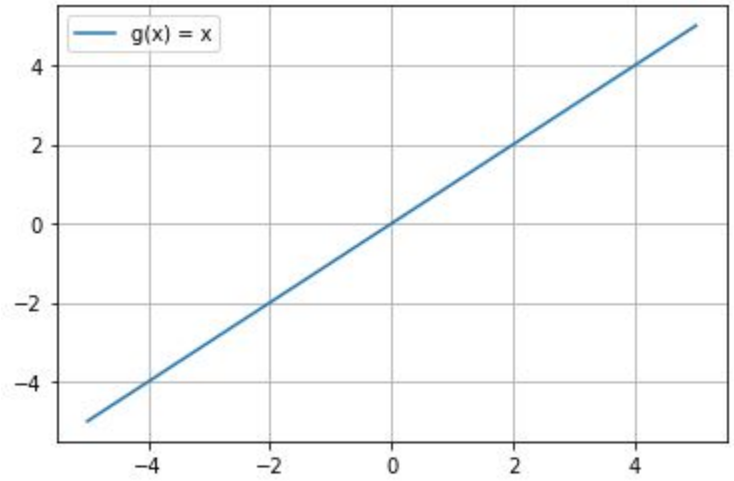
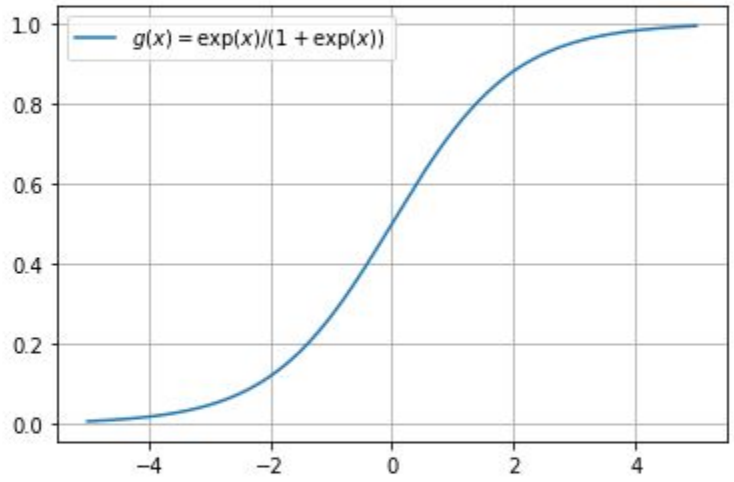
Activation function: linear

- No nonlinear transformation
- No input squashing



Activation function: sigmoid

- Always positive.
- Squashing the neuron's output between 0 and 1.
- Strictly increasing.



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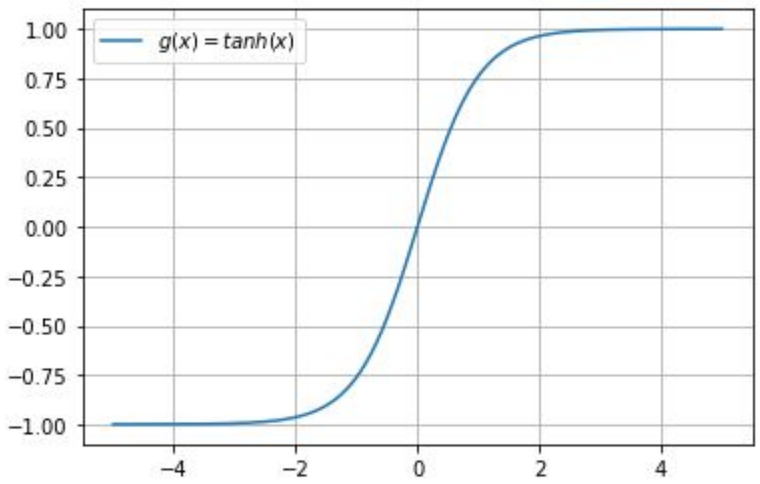
Activation function: tanh

- Can be positive and negative.
- Squashing the neuron's output between -1 and 1.
- Strictly increasing.



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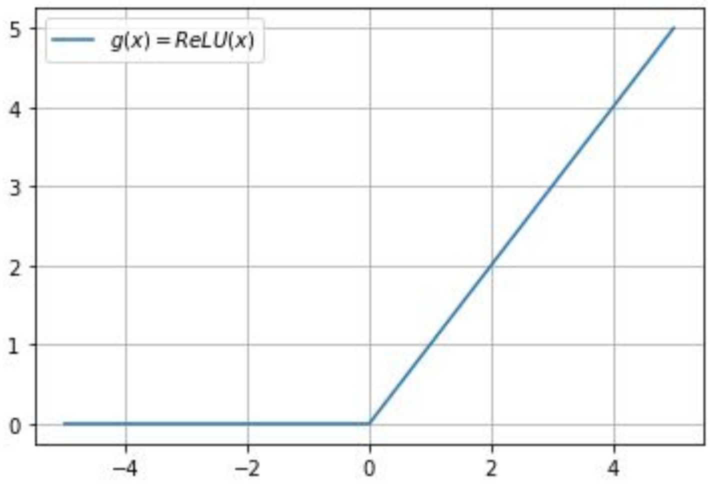
Activation function: sigmoid

- Always positive.
- Pushing the neuron's output above 0.
- Strictly increasing.



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Fitting neural networks: regression tasks

Recall our model is:

$$
\begin{aligned}
Z_m &= \sigma(\alpha_{0m} + \alpha_m^T X), \quad m = 1, \ldots, M. \\
T_k &= \beta_{0k} + \beta_k^T Z, \quad k = 1, \ldots, K. \\
f_k(X) &= g_k(T), \quad k = 1, \ldots, K.
\end{aligned}
$$

The unknow parameters of the model are often called *weights*. We denote the complete set of weights by θ, which consists of

$$
\begin{aligned}
\{\alpha_{0m}, \alpha_m;\ m = 1, 2, \ldots, M\} &\quad M(p+1) \text{ weights}, \\
\{\beta_{0k}, \beta_k;\ k = 1, 2, \ldots, K\} &\quad K(M+1) \text{ weights}.
\end{aligned}
$$

For regression, we use the squared error loss

$$
R(\theta) = \sum_{k=1}^{K} \sum_{i=1}^{n} (y_{ik} - f_k(x_i))^2.
$$

Fitting neural networks: classification tasks

Recall our model is:

$$\begin{aligned} Z_m &= \sigma(\alpha_{0m} + \alpha_m^T X), \quad m = 1, \ldots, M. \\ T_k &= \beta_{0k} + \beta_k^T Z, \quad k = 1, \ldots, K. \\ f_k(X) &= g_k(T), \quad k = 1, \ldots, K. \end{aligned}$$

The unknow parameters of the model are often called *weights*. We denote the complete set of weights by θ, which consists of

$$\begin{aligned} \{\alpha_{0m}, \alpha_m;\ m = 1, 2, \ldots, M\} & \qquad M(p+1) \text{ weights}, \\ \{\beta_{0k}, \beta_k;\ k = 1, 2, \ldots, K\} & \qquad K(M+1) \text{ weights}. \end{aligned}$$

For classification we use either squared error or corss-entropy

$$R(\theta) = -\sum_{i=1}^{n} \sum_{k=1}^{K} y_{ik} \log f_k(x_i),$$

and the correponding classifier is $G(x) = \text{argmax}_k f_k(x)$.

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Connection to gradient descent

Assume we use squared error loss. Let $z_{mi} = \sigma(\alpha_{0m} + \alpha_m^T x_i)$ and let $z_i = (z_{1i}, z_{2i}, \ldots, z_{Mi})$. Then we have

$$R(\theta) \equiv \sum_{i=1}^{n} R_i = \sum_{i=1}^{n} \sum_{k=1}^{K} (y_{ik} - f_k(x_i))^2,$$

where

$$f_k(x_i) = g_k(\beta_{0k} + \beta_k^T z_i) = g_k\left(\beta_{0k} + \sum_{m=1}^{M} \beta_{km}\sigma(\alpha_{0m} + \alpha_m^T x_i)\right).$$

The derivatives are

$$\begin{aligned}
\frac{\partial R_i}{\partial \beta_{km}} &= -2(y_{ik} - f_k(x_i))g_k'(\beta_k^T z_i)z_{mi}, \\
\frac{\partial R_i}{\partial \alpha_{ml}} &= -\sum_{k=1}^{K} 2(y_{ik} - f_k(x_i))g_k'(\beta_k^T z_i)\beta_{km}\sigma'(\alpha_m^T x_i)x_{il},
\end{aligned}$$

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Connection to gradient descent

Assume we use squared error loss. Let $z_{mi} = \sigma(\alpha_{0m} + \alpha_m^T x_i)$ and let $z_i = (z_{1i}, z_{2i}, \ldots, z_{Mi})$. Then we have

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The derivatives are

$$\begin{aligned}
\frac{\partial R_i}{\partial \beta_{km}} &= -2(y_{ik} - f_k(x_i)) g_k'(\beta_k^T z_i) z_{mi}, \\
\frac{\partial R_i}{\partial \alpha_{ml}} &= -\sum_{k=1}^{K} 2(y_{ik} - f_k(x_i)) g_k'(\beta_k^T z_i) \beta_{km} \sigma'(\alpha_m^T x_i) x_{il},
\end{aligned}$$

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Updating rule

Assume we use squared error loss. Let $z_{mi} = \sigma(\alpha_{0m} + \alpha_m^T x_i)$ and let $z_i = (z_{1i}, z_{2i}, \ldots, z_{Mi})$. Then we have

$$R(\theta) \equiv \sum_{i=1}^{n} R_i = \sum_{i=1}^{n} \sum_{k=1}^{K} (y_{ik} - f_k(x_i))^2,$$

where

$$f_k(x_i) = g_k(\beta_{0k} + \beta_k^T z_i) = g_k\left(\beta_{0k} + \sum_{m=1}^{M} \beta_{km}\sigma(\alpha_{0m} + \alpha_m^T x_i)\right).$$

A gradient update at the $(r+1)$st iteration has the form

$$\beta_{km}^{(r+1)} = \beta_{km}^{(r)} - \gamma_r \sum_{i=1}^{N} \frac{\partial R_i}{\partial \beta_{km}^{(r)}},$$

$$\alpha_{ml}^{(r+1)} = \alpha_{ml}^{(r)} - \gamma_r \sum_{i=1}^{N} \frac{\partial R_i}{\partial \alpha_{ml}^{(r)}}.$$

Updating rule

If we write the gradients as

$$
\begin{aligned}
\frac{\partial R_i}{\partial \beta_{km}} &= -2(y_{ik} - f_k(x_i))g_k'(\beta_k^T z_i)z_{mi}, \\
\frac{\partial R_i}{\partial \alpha_{ml}} &= -\sum_{k=1}^{K} 2(y_{ik} - f_k(x_i))g_k'(\beta_k^T z_i)\beta_{km}\sigma'(\alpha_m^T x_i)x_{il}.
\end{aligned}
$$

Back propagation

If we write the gradients as

$$\frac{\partial R_i}{\partial \beta_{km}} = -2(y_{ik} - f_k(x_i))g_k'(\beta_k^T z_i)z_{mi},$$

$$\frac{\partial R_i}{\partial \alpha_{ml}} = -\sum_{k=1}^{K} 2(y_{ik} - f_k(x_i))g_k'(\beta_k^T z_i)\beta_{km}\sigma'(\alpha_m^T x_i)x_{il}.$$

$$\frac{\partial R_i}{\partial \beta_{km}} = \delta_{ki} z_{mi},$$

$$\frac{\partial R_i}{\partial \alpha_{ml}} = s_{mi} x_{il}.$$

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Back propagation

If we write the gradients as

$$\frac{\partial R_i}{\partial \beta_{km}} = \delta_{ki} z_{mi},$$
$$\frac{\partial R_i}{\partial \alpha_{ml}} = s_{mi} x_{il}.$$

In some sense, δ_{ki} and s_{mi} are "errors" at the output and hidden layer units. The errors satisfy

$$s_{mi} = \sigma'(\alpha_m^T x_i) \sum_{k=1}^{K} \beta_{km} \delta_{ki}.$$

They are called the *back-propagation equations*. The updates can be implemented with a two-pass algorithm:

- *forward pass*: fix weights, compute the predicted values $\hat{f}_k(x_i)$.
- *backward pass*: errors δ_{ki} are computed, and back-propagated to give the errors s_{mi}. Then use both sets of errors to compute the gradients.

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Starting values

- If the weights are near zero, then the operative part of the sigmoid is roughly zero.
- Usually starting values for weights are chosen to be random values near zero.
- Hence the model starts out nearly linear, and becomes nonlinear as the weights increases.

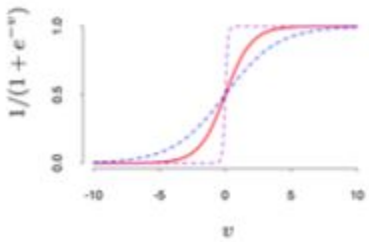


FIGURE 11.3. *Plot of the sigmoid function* $\sigma(v) = 1/(1+\exp(-v))$ *(red curve), commonly used in the hidden layer of a neural network. Included are* $\sigma(sv)$ *for* $s = \frac{1}{2}$ *(blue curve) and* $s = 10$ *(purple curve). The scale parameter* s *controls the activation rate, and we can see that large* s *amounts to a hard activation at* $v = 0$*. Note that* $\sigma(s(v - v_0))$ *shifts the activation threshold from 0 to* v_0*.*

Multiple minima

The error function $R(\theta)$ is nonconvex, possessing many local minima.

The solution we obtained from back-propagation is a local minimum.

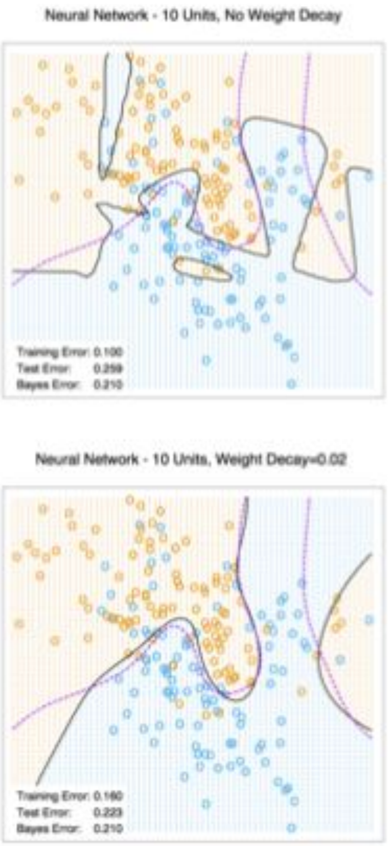
Usually, we try a number of random starting configuration, and choose the solution giving lowest error, or use the average predictions over the collection of networks as the final prediction.

Multiple minima

- Often neural networks have too many weights and will overfit the data at the global minimum of R.
- A regularization method is *weight decay*. We add a penalty to the error function $R(\theta) + \lambda J(\theta)$, where

$$J(\theta) = \sum_{k,m} \beta_{km}^2 + \sum_{m,l} \alpha_{ml}^2.$$

- $\lambda \geq 0$ is a tuning parameter, can be chosen by cross-validation.



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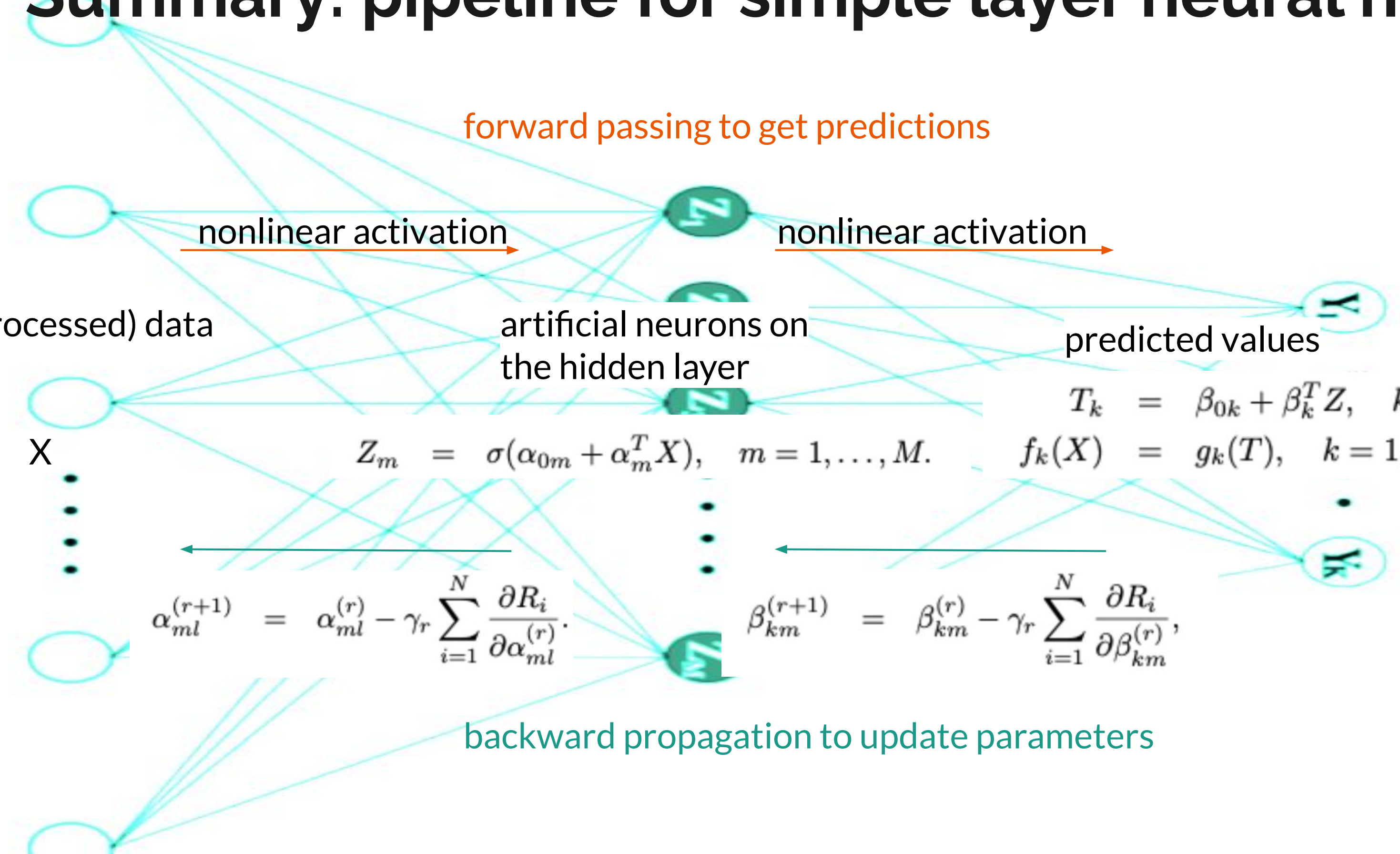
Summary: pipeline for simple layer neural net



forward passing to get predictions

nonlinear activation

nonlinear activation

(preprocessed) data

artificial neurons on the hidden layer

predicted values

X

$$Z_m = \sigma(\alpha_{0m} + \alpha_m^T X), \quad m = 1, \ldots, M.$$

$$T_k = \beta_{0k} + \beta_k^T Z, \quad k = 1, \ldots, K.$$

$$f_k(X) = g_k(T), \quad k = 1, \ldots, K.$$

$$\alpha_{ml}^{(r+1)} = \alpha_{ml}^{(r)} - \gamma_r \sum_{i=1}^{N} \frac{\partial R_i}{\partial \alpha_{ml}^{(r)}}.$$

$$\beta_{km}^{(r+1)} = \beta_{km}^{(r)} - \gamma_r \sum_{i=1}^{N} \frac{\partial R_i}{\partial \beta_{km}^{(r)}},$$

backward propagation to update parameters

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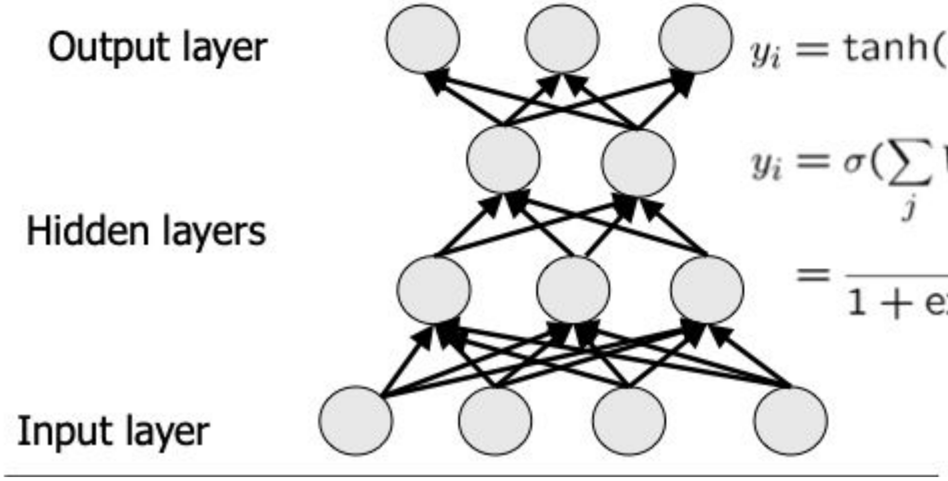
Deep neural network

Definition: Deep architectures are composed of *multiple levels* of non-linear operations, such as neural nets with many hidden layers.



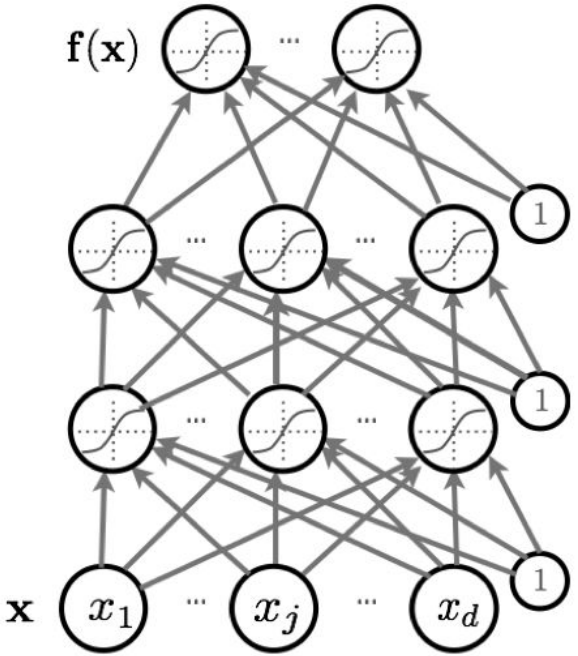
$$y_i = \tanh\left(\sum_j W_{ij} x_j + W_{i0}\right)$$

$$y_i = \sigma\left(\sum_j W_{ij} x_j + W_{i0}\right)$$

$$= \frac{1}{1 + \exp\left[-\left(\sum_j W_{ij} x_j + W_{i0}\right)\right]}$$

Deep neural network: architecture

- How neural networks predict f(x) given an input x:
  - Feed forward
  - Types of activations
  - Capacity of neural networks
- How to train neural networks:
  - Loss function
  - Backward propagation with gradient descent
- More recent techniques:
  - Architecture
  - Dropout
  - SGD
  - Batch normalization



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Deep neural network: architecture

- Consider a network with L hidden layers.
  - layer pre-activation for k>0

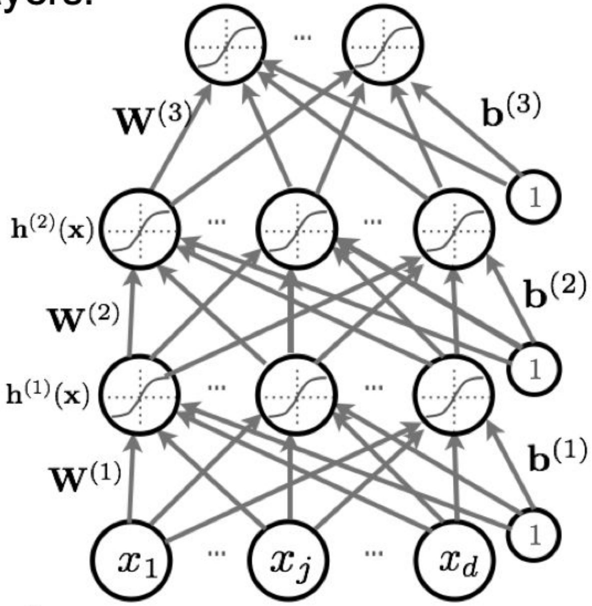
$$\mathbf{a}^{(k)}(\mathbf{x}) = \mathbf{b}^{(k)} + \mathbf{W}^{(k)}\mathbf{h}^{(k-1)}(\mathbf{x})$$

  - hidden layer activation from 1 to L:

$$\mathbf{h}^{(k)}(\mathbf{x}) = \mathbf{g}(\mathbf{a}^{(k)}(\mathbf{x}))$$

  - output layer activation (k=L+1):

$$\mathbf{h}^{(L+1)}(\mathbf{x}) = \mathbf{o}(\mathbf{a}^{(L+1)}(\mathbf{x})) = \mathbf{f}(\mathbf{x})$$



$$(\mathbf{h}^{(0)}(\mathbf{x}) = \mathbf{x})$$

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Neural network structure

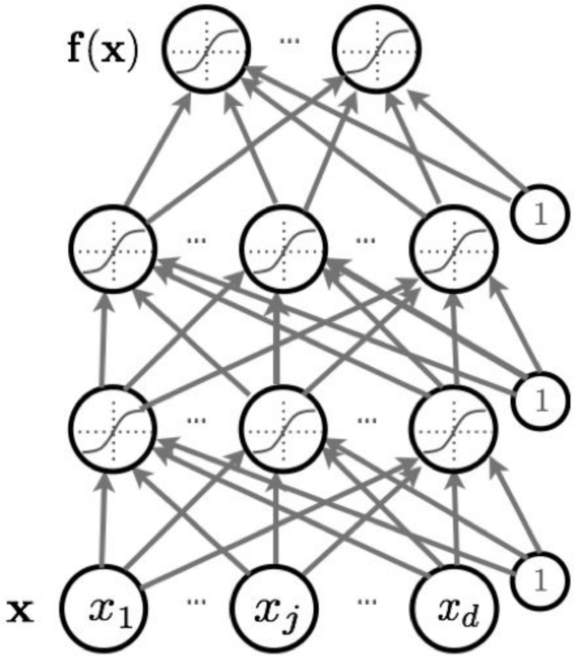
- Fully connected layer
- Deep architecture

  - LeNet5

  - AlexNet

  - ResNet

  - ......
- Semi-supervised learning



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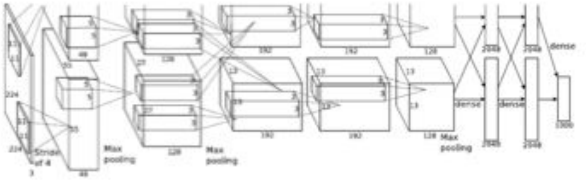
Deep neural network: important breakthrough

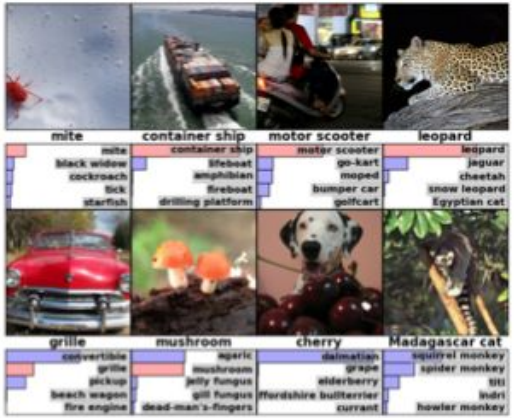
- Deep Convolutional Nets for Vision (Supervised)

  Krizhevsky, A., Sutskever, I. and Hinton, G. E., ImageNet Classification with Deep Convolutional Neural Networks, NIPS, 2012.



IMAGENET

1.2 million training images
1000 classes



- Deep Nets for Speech (Supervised)

  Hinton et. al. Deep Neural Networks for Acoustic Modeling in Speech Recognition: The Shared Views of Four Research Groups, IEEE Signal Processing Magazine. 2012.

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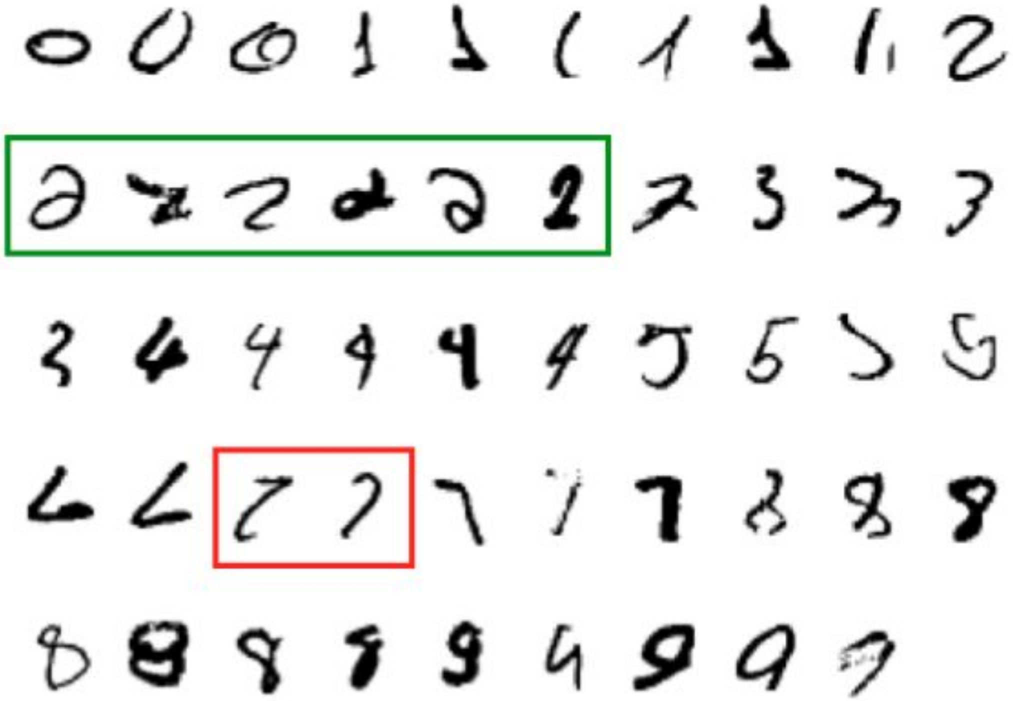
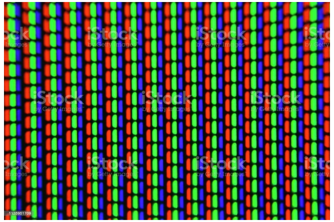
MNIST

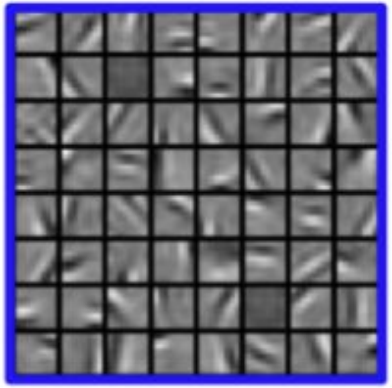


Convolutional neural network

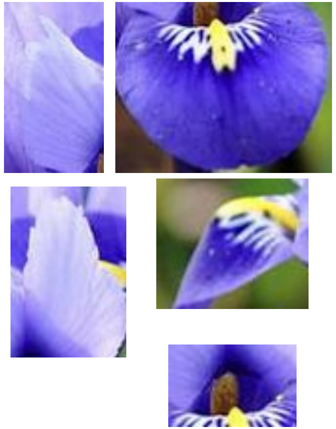
pixels



features



object parts/
combination of features



objects

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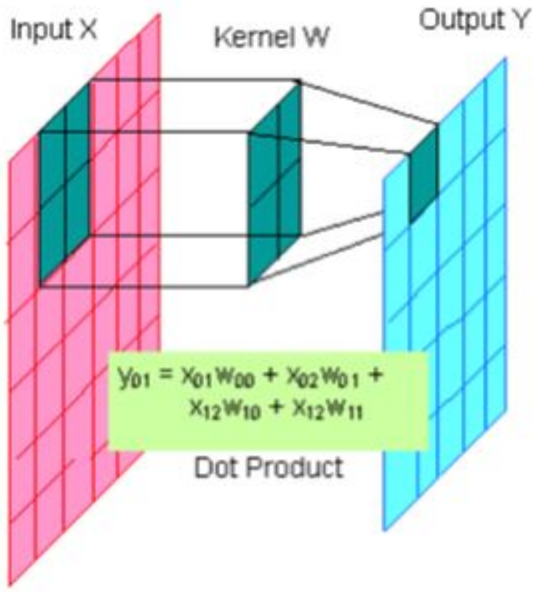
Convolutional neural network

- Instead of focusing on individual, CNN provides a automatic algorithm to study groups of nearby pixels.
- Very successful in
  - computer vision (CV)
  - natural language processing (NLP)



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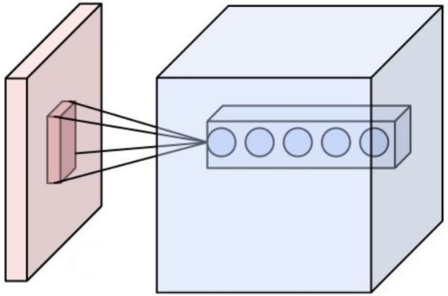
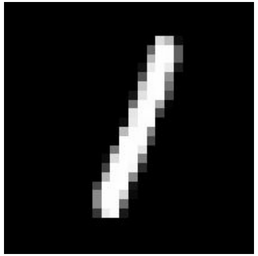
Convolutional neural network





- Hyperparameters in convolutional layer:

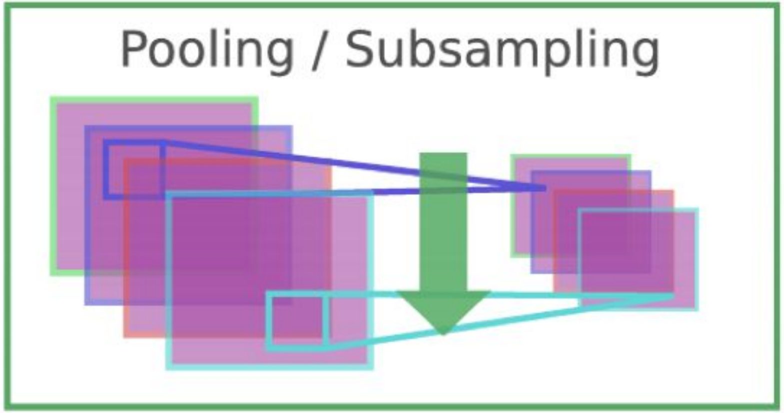
  (pytorch, MNIST data)
- The input sample size is (1,28,28)

```
torch.nn.Conv2d(
in_channels   = 1,  # we only have grayscale figure
out_channels = 16, # number of filters
kernel_size   = 5,   # filter size
stride            = 1,   # filter movement
padding         = 2   # when stride = 1,
                           padding = (kernel_size -1)/2
)
```

- Output size is (16,28,28)

Convolutional neural network

- Pooling/subsampling hidden units in same neighborhood
  - Introduces invariance to local translations
  - Reduces the number of hidden units in hidden layer
- Hyperparameters in pooling layers
  torch.nn.MaxPool2d(2)



Jarret et al. 2009

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Convolutional neural network

(1,28,28)

convolutional layer

(16, 28, 28)

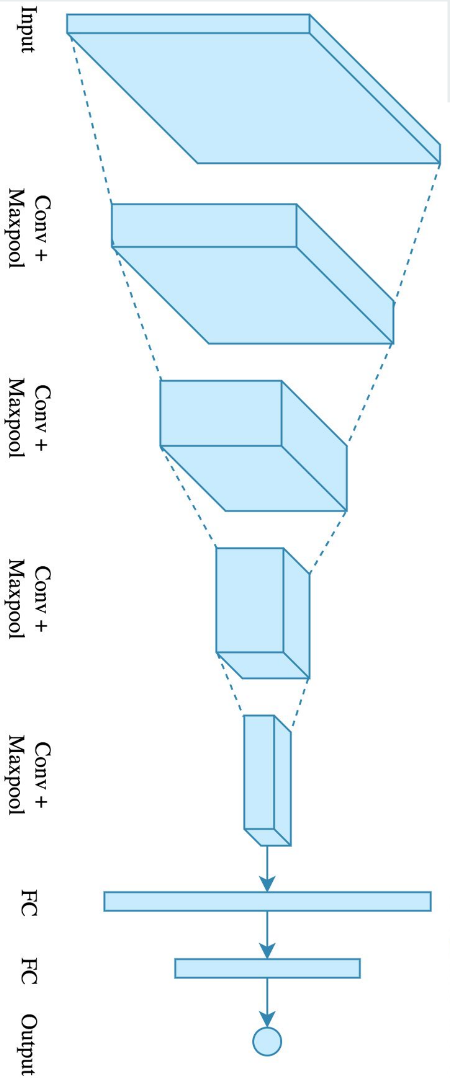
nonlinear activation

layer (usually ReLU)

(16, 28, 28)

max pooling

(16, 14, 14)



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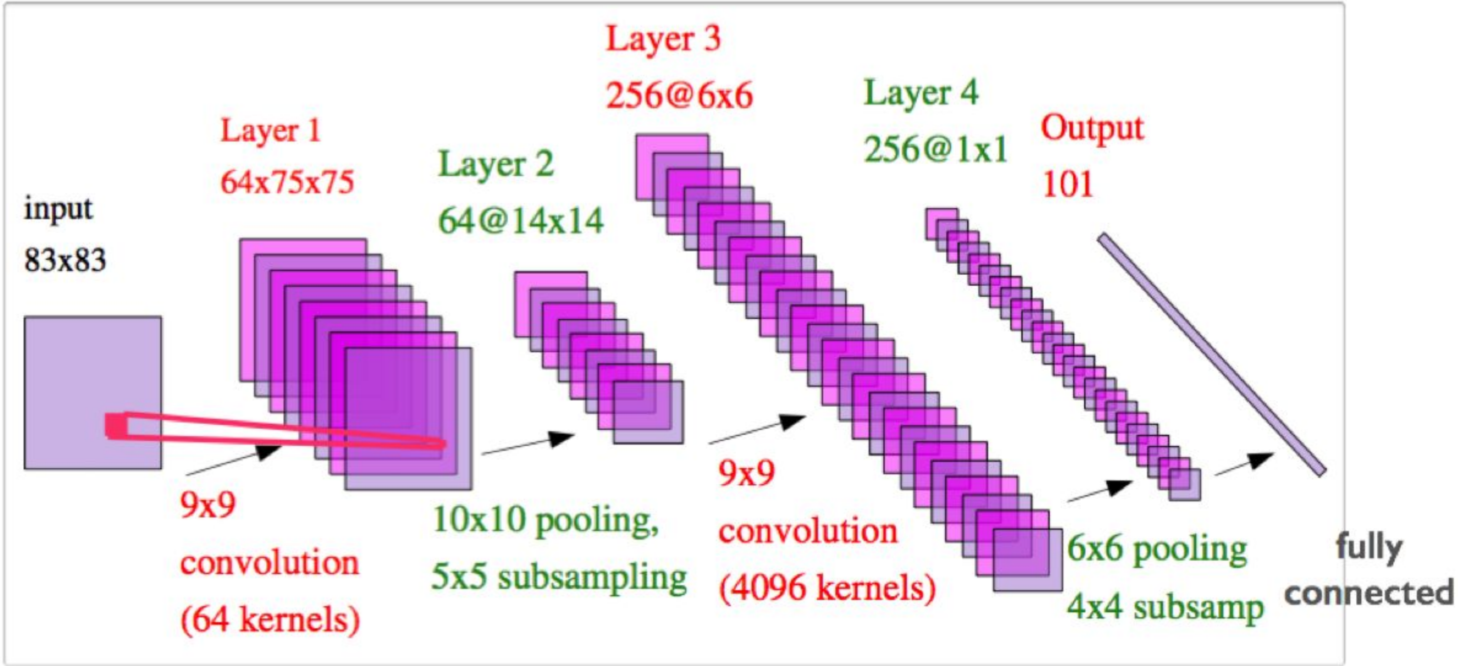
Convolutional neural network



From Yann LeCun's slides

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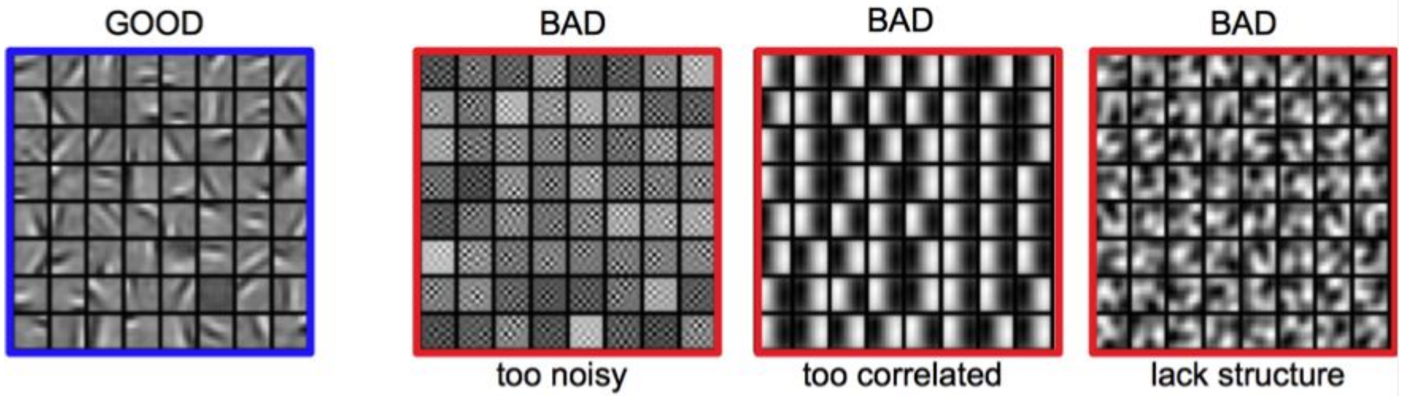
Convolutional neural network

- Visualize parameters:
  learned features should exhibit structure and should be uncorrelated and are uncorrelated

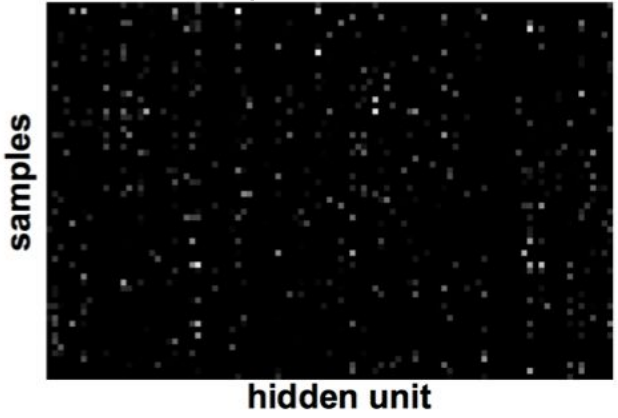


[From Marc'Aurelio Ranzato, CVPR 2014 tutorial]

Convolutional neural network

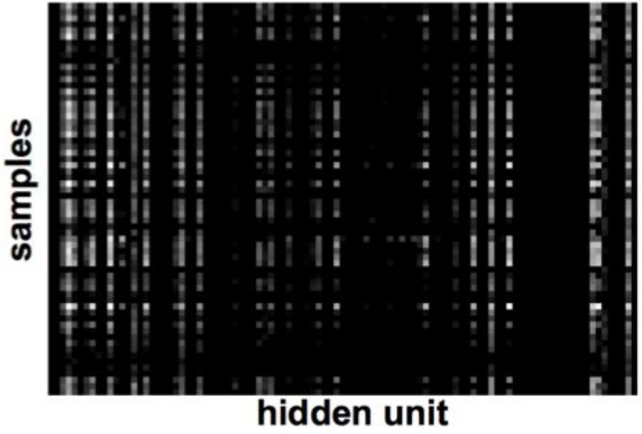
- Visualize features (feature maps need to be uncorrelated)

Good training:
hidden units are sparse
across samples.



[From Marc'Aurelio Ranzato, CVPR 2014 tutorial]

Bad training:
hidden units are highly
correlated.



[From Marc'Aurelio Ranzato, CVPR 2014 tutorial]

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Why training is hard

- Underfitting: use better optimization:

  - use better optimization tools (e.g. batch-normalization, 2nd-order methods).

  - use GPUs, distributed computing.
- Overfitting: use better regularization:

  - unsupervised pre-training

  - stochastic drop-out training
- For many large-scale practical problems, have to scale up:

  - ReLu nonlinearity

  - initialization (e.g. Kaiming He's initialization)

  - stochastic gradient descent

  - momentum, batch-normalization, and drop-out

Preprocessing

- One-hot representation: class 0 or class 1 → (1,0) or (0,1)
- Normalizing the inputs will speed up training (Lecun et al. 1998)

  - could normalization be useful at the level of the hidden layers?
- Batch normalization is an attempt to do that

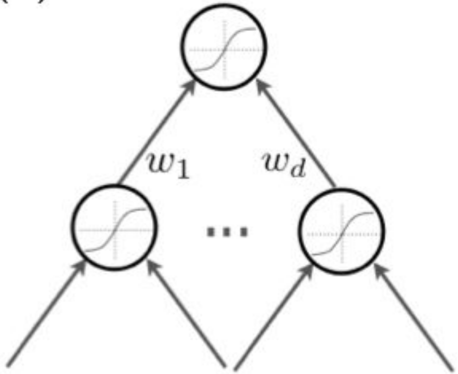
  - each unit's pre-activation is normalized (mean subtraction, stddev division)

  - during training, mean and stddev is computed for each minibatch

  - backpropagation takes into account the normalization

  - at test time, the global mean / stddev is used

$$\mathbf{a}^{(k)}(\mathbf{x}) = \mathbf{b}^{(k)} + \mathbf{W}^{(k)}\mathbf{h}^{(k-1)}(\mathbf{x})$$



Initialization of parameters

- Initialize biases to 0
- For weights
  - Can not initialize weights to 0 with tanh activation
    - ➢ All gradients would be zero (saddle point)
  - Can not initialize all weights to the same value
    - ➢ All hidden units in a layer will always behave the same
    - ➢ Need to break symmetry
  - Sample $\mathbf{W}_{i,j}^{(k)}$ from $U\left[-b, b\right]$, where

$$b = \frac{\sqrt{6}}{\sqrt{H_k + H_{k-1}}}$$

Sample around 0 and break symmetry

Size of $\mathbf{h}^{(k)}(\mathbf{x})$

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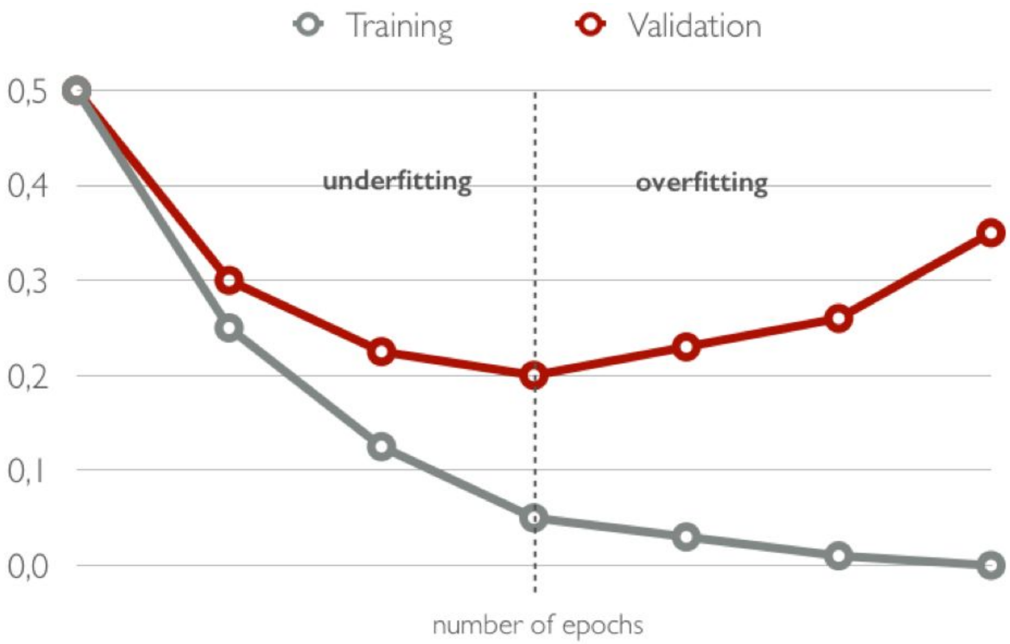
Deep neural network: overfitting

- Overfitting often occurs in applications of neural networks.
- Ways to overcome:
  - Early stopping:
    Stop training process early.
  - Dropout:
    Use random binary masks.



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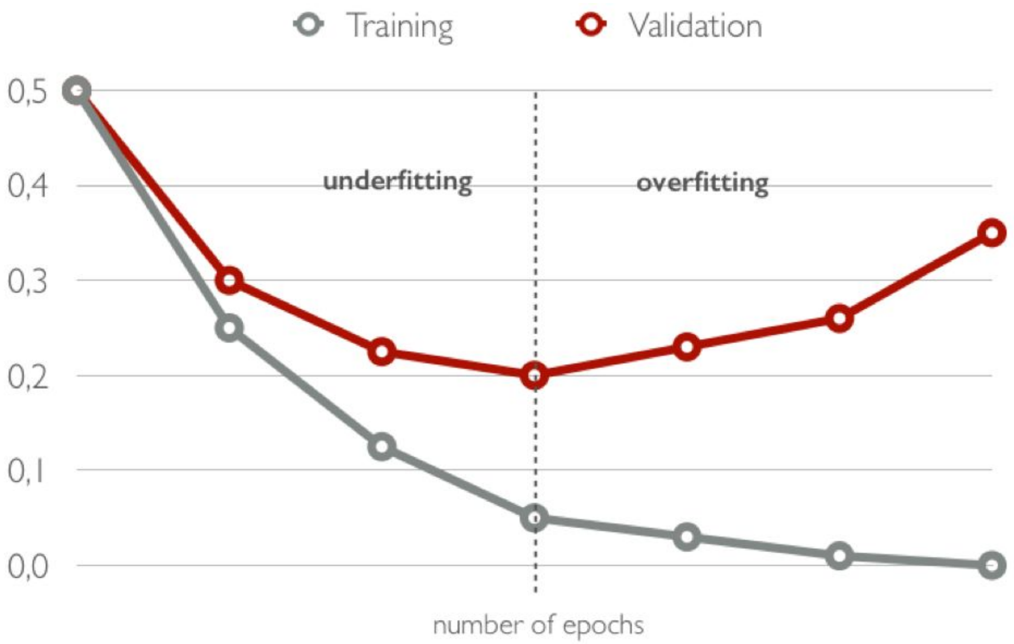
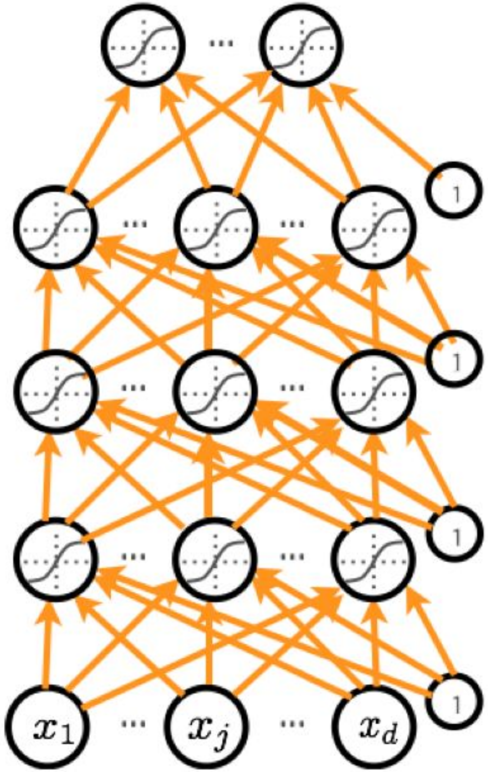
Early stopping



Dropouts

- Cripple neural network by removing hidden units stochastically
  - each hidden unit is set to 0 with probability 0.5
  - hidden units cannot co-adapt to other units
  - hidden units must be more generally useful
- Could use a different dropout probability, but 0.5 usually works well



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Model selection

- Training Protocol:
  - Train your model on the Training Set $\mathcal{D}^{\text{train}}$
  - For model selection, use Validation Set $\mathcal{D}^{\text{valid}}$
    - Hyper-parameter search: hidden layer size, learning rate, number of iterations/epochs, etc.
  - Estimate generalization performance using the Test Set $\mathcal{D}^{\text{test}}$
- Remember: Generalization is the behavior of the model on **unseen examples**.

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Optimization

- SGD with momentum, batch-normalization, and dropout usually works very well
- Pick learning rate by running on a subset of the data

  - Start with large learning rate & divide by 2 until loss does not diverge

  - Decay learning rate by a factor of ~100 or more by the end of training

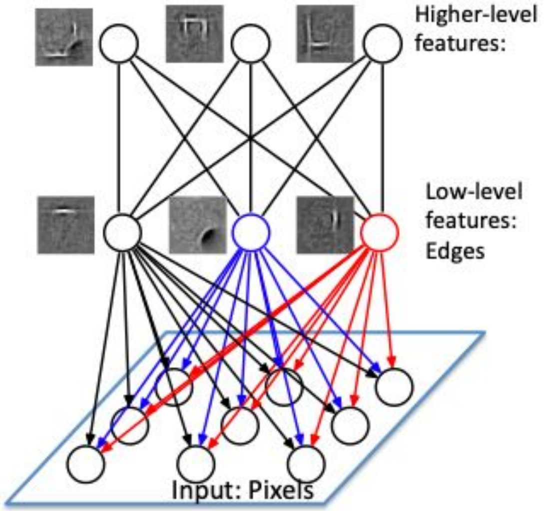
  - Use ReLU nonlinearity

  - Initialize parameters so that each feature across layers has similar variance. Avoid units in saturation.
- Use adapted learning rate

Deep neural network: important breakthrough

- Deep Belief Networks, 2006 (Unsupervised)

  Hinton, G. E., Osindero, S. and Teh, Y., A fast learning algorithm for deep belief nets, Neural Computation, 2006.



Theoretical Breakthrough:

- Adding additional layers improves variational lower-bound.

Efficient Learning and Inference with multiple layers:

- Efficient greedy layer-by-layer learning learning algorithm.
- Inferring the states of the hidden variables in the top most layer is easy.

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Deep neural network: important breakthrough

- Conditional generative model P(zebra images| horse images)

- Style Transfer

Input Image

Monet

Van Gogh

Zhou el al., Cycle GAN 2017

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Summary: pipeline for deep neural net

forward passing to get predictions

(preprocessed) data $\xrightarrow{\text{nonlinear activation}}$ hidden layers $\xrightarrow{\text{nonlinear activation}}$ hidden layers $\xrightarrow{\text{nonlinear activation}}$ hidden layers $\xrightarrow{\text{nonlinear activation}}$ ...... $\xrightarrow{\text{nonlinear activation}}$ hidden layers $\xrightarrow{\text{nonlinear activation}}$ predicted values

(preprocessed) data $\longleftarrow$ hidden layers $\longleftarrow$ hidden layers $\longleftarrow$ hidden layers $\longleftarrow$ ...... $\longleftarrow$ hidden layers $\longleftarrow$ predicted values

backward propagation to update parameters

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Summary:

- Usually the loss function is non-convex
- To have better performance, we can

  - Try different loss function

  - Try different penalty on learnt parameters

  - Try different initializations

  - Try different learning rate (1e-2, 1e-3)/ adapted learning rate

  - Try dropout

  - Try early stopping

  - Try different optimizer (SGD+momentum, Adam, RMSprop)

  - Try different activation function + batch normalization

  - Try different/deeper architecture

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References

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- https://towardsdatascience.com/neural-network-architectures-156e5bad51ba
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