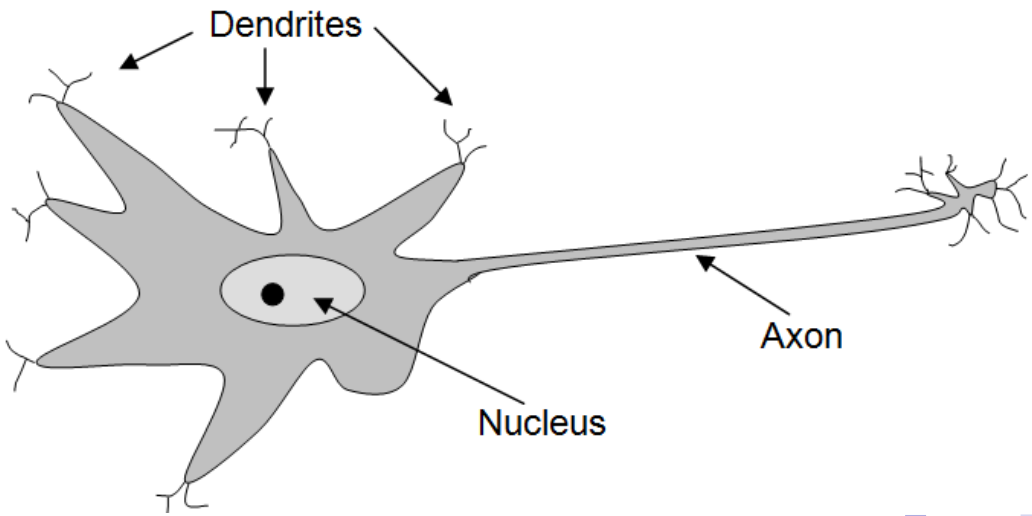
PQHS 471
Lecture 11: Neural Network, Deep Learning

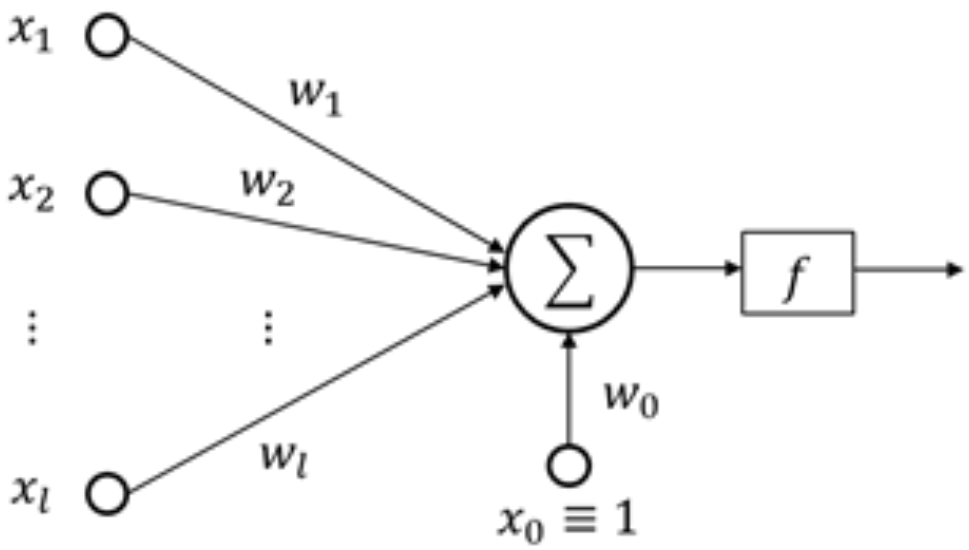
Introduction to artificial neural network (ANN or NN)

- A machine learning algorithm for classification, clustering, function approximation, etc.
- Motivated by how biological neural network learn and process information.
  - Cerebral cortex contains 10^{11} neurons that are deeply connected into a massive network.
  - Each neuron is connected to $10^3 - 10^4$ other neurons.
  - A neuron can receive information from other neurons, process the information, and then pass it to other neurons.



Simple perceptron model

- A perceptron model is the simplest, single-nueron model for supervised learning.
- Training data contains: inputs x_i, $i = 1, \ldots, l$. Each x_i is a n-vector; and output d, a n-vector. The output can be continuous (regression) or binary (classification).
- An activation function f is specified by user for binary outcome.



Learn the perceptron model

The learning algorithm is based on gradient search to minimize the squared loss: $\sum_{j=1}^{n}(d_j - y_j)^2$, where $y_j = f(w_0 + \sum_{i=1}^{l} w_i x_{ij})$.

1. Initialize w's to random numbers. Then at iteration r:
2. Compute $y_j^r = f(w_0^r + \sum_{i=1}^{l} w_i^r x_{ij})$.
3. Update weights by:
   - $w_0^{(r+1)} = w_0^r + \gamma_1^r \sum_{j=1}^{n}(d_j - y_j^r) f'(z_j^r)$.
   - $w_i^{(r+1)} = w_i^r + \gamma_2^r \sum_{j=1}^{n}(d_j - y_j^r) f'(z_j^r) x_{ij}$,

   Here $z_j^r = w_0^r + \sum_{i=1}^{l} w_i^r x_{ij}$. γ_1^r and γ_2^r are the learning rate (step size).

Compare with regression model:

- For continuous outcome, when f is identity function, the perceptron model is similar to a linear regression.
- For binary outcome, when f is logit/expit function, the perceptron model is similar to a logistic regression.

Artificial neural network

ANN is a glorified perceptron model with multiple neurons and (optionally) multiple layers (has at least one hidden layer of neurons).

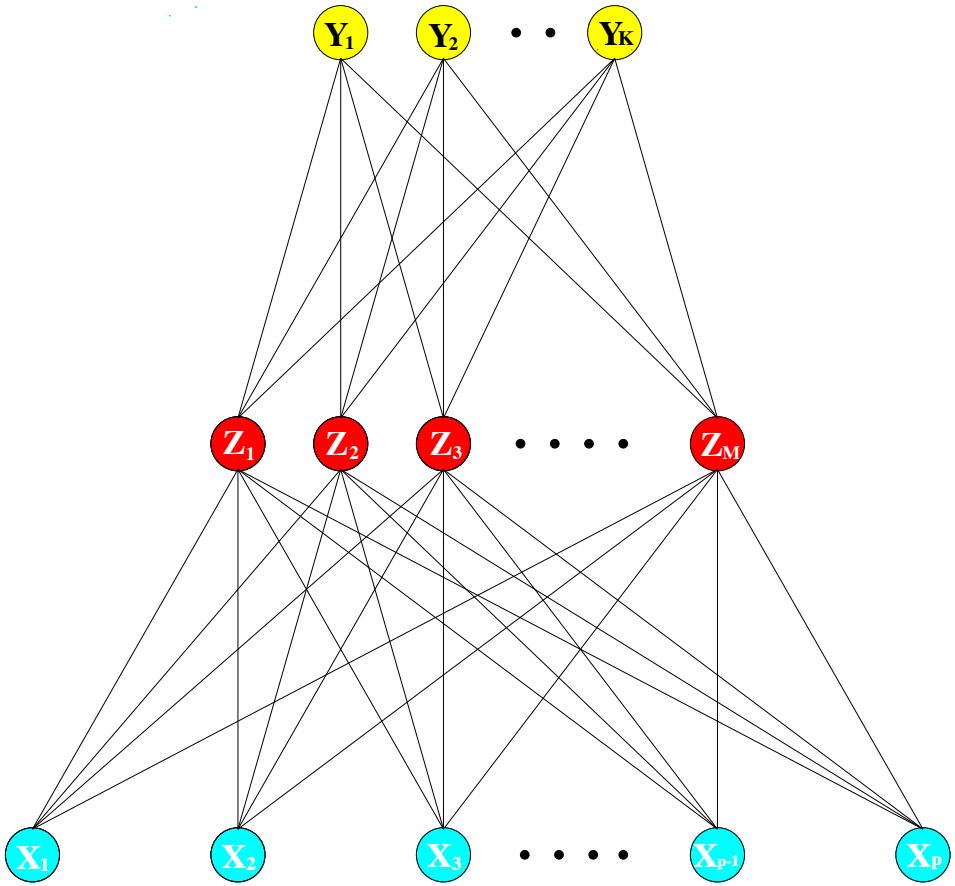


Figure is from "elements of statistical learning" chapter 11, figure 11.2

- The neural network has input (X), output (Y), and hidden variable Z.
- It works for continuous or categorial outcomes.
- In an ANN, a mathematical neuron works the same as a perceptron. It receives a number of inputs, computes the weighted sum and then generate outputs through activation functions.
- The mathematical model for an ANN for K-class classification (Y is categorial with K classes):

$$z_m = \sigma(\alpha_{0m} + \alpha_m^T X),\ m = 1, \ldots, M.$$
$$T_k = \beta_{0k} + \beta_k^T Z,\ k = 1, \ldots, K.$$
$$f_k(X) = g_k(\mathbf{T}),\ k = 1, \ldots, K.$$

  Here, σ is "activation function".
- In K-class classification, usually use softmax function for g:

$$g_k(\mathbf{T}) = \frac{e^{T_k}}{\sum_l e^{T_l}}$$

- $K = 1$ for continuous outcome.

A little bit on the activation function

- Determines the output of a neuron.
- Nonlinear activation functions can turn the linear model to a non-linear one, which can better capture the nonlinearity in the data.
- Some activation functions (such as the sigmoid functions) can help normalize the output of each neuron to a range between 1 and 0 or between -1 and 1.
- Needs to be computationally easy.

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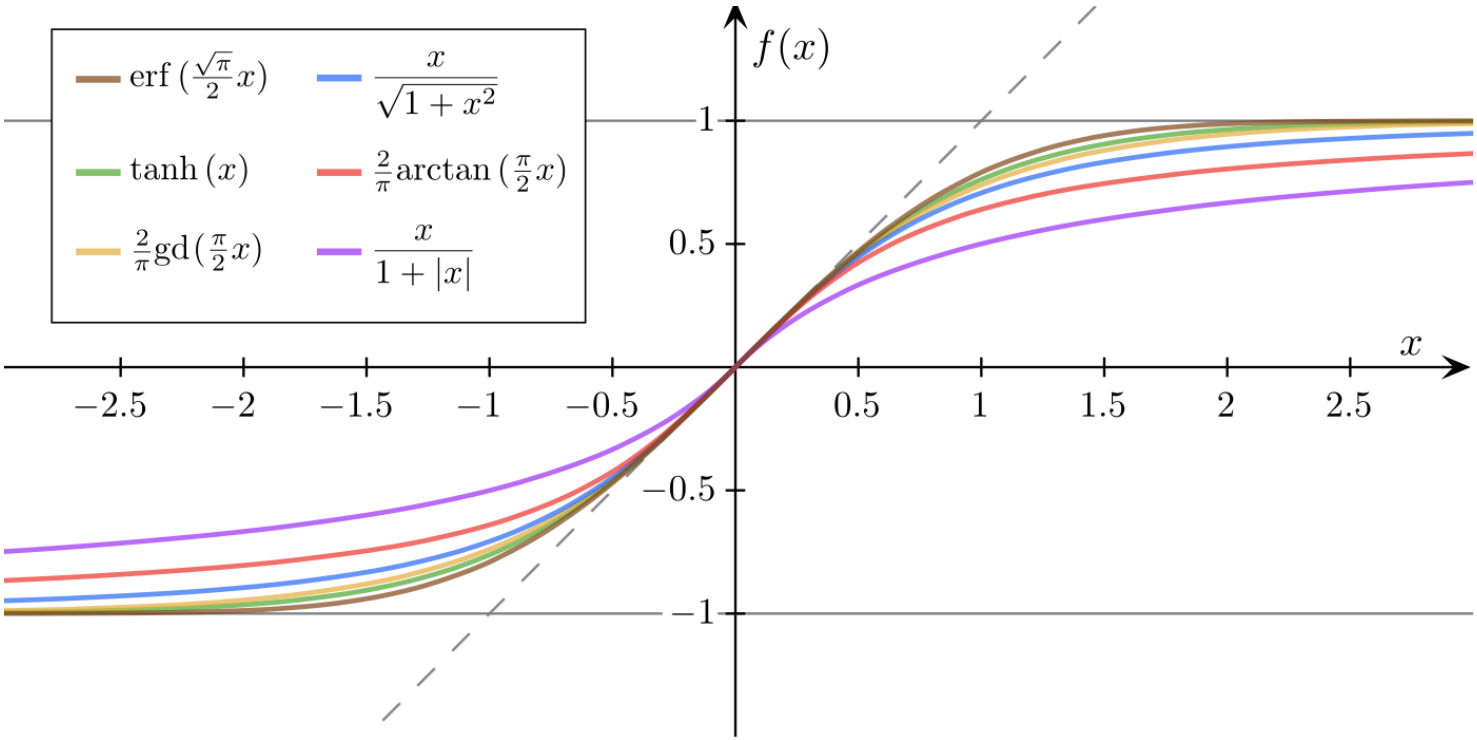
Often used activation functions:

- Linear activation functions: linear function or step function.
- Nonlinear activation functions:
  - Sigmoid functions: S-shaped. Examples: logistic, tanh.
  - ReLU (Rectified Linear Unit): similar to a linear spline.

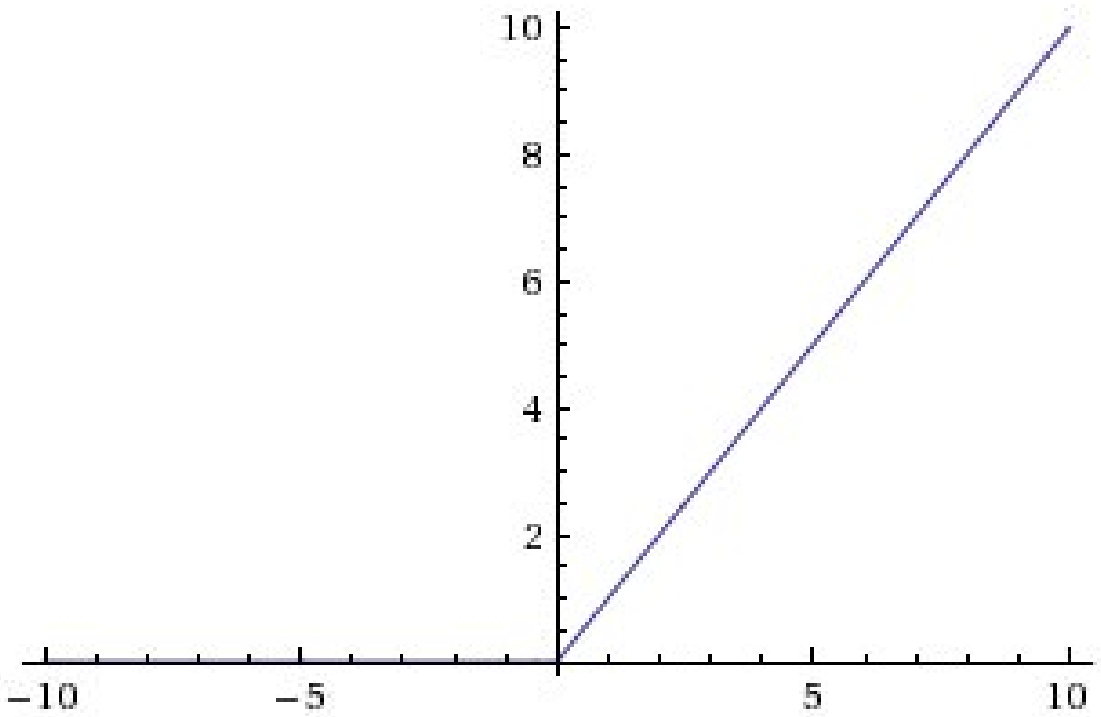
Activation functions

Sigmoid functions



Activation functions

ReLU



ANN model fitting

Numbers of parameters in an ANN are:

- α_{0m}, α_m: $M \times (P+1)$
- β_{0m}, β_k: $K \times (M+1)$

Objective function of an ANN:

- For continuous outcome, residual sum of squares:

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

- For categorical outcome, cross-entropy (or NLL, negative log likelihood):

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

Model fitting is done by "**back propagation algorithm**".

Back propagation algorithm

Essentially a gradient descent algorithm.

- Initialization: pick random weights (model parameters).
- Forward: given weights, compute predicted values.
- Backward: update the weights, using first derivatives as direction. The first derivatives can be obtained using chain rule.

Detailed derivations are skipped. Please refer to ESL chpt 11.

Back propagation algorithm

Note:

- Be careful of overfitting: the model is too flexible and has too many parameters.
- Regularization technique (e.g., L1 penalty) can be used to stabilize the model fitting.
- Number of neurons and the number of layers are set by user.
- Compared with the perceptron model, ANN can capture highly non-linear relationships. With adequate numbers of neurons and hidden layers, arbitrary decision boundary can be formed.

Neural network in R

The neuralnet package in R provides functions to train a neural network.

```
library(neuralnet)
data(infert, package="datasets")

## fit NN
fit <- neuralnet(case~parity+induced+spontaneous, infert)
predicted <- fit$net.result[[1]]>0.5
table(infert$case, predicted)
predicted
FALSE TRUE
0   143   22
1    37   46

## compare with SVM
library(e1071)
fit.svm <- svm(case~parity+induced+spontaneous, infert)
predicted <- predict(fit.svm)>0.5
table(infert$case, predicted)
predicted
FALSE TRUE
0   149   16
1    43   40
```

Deep learning

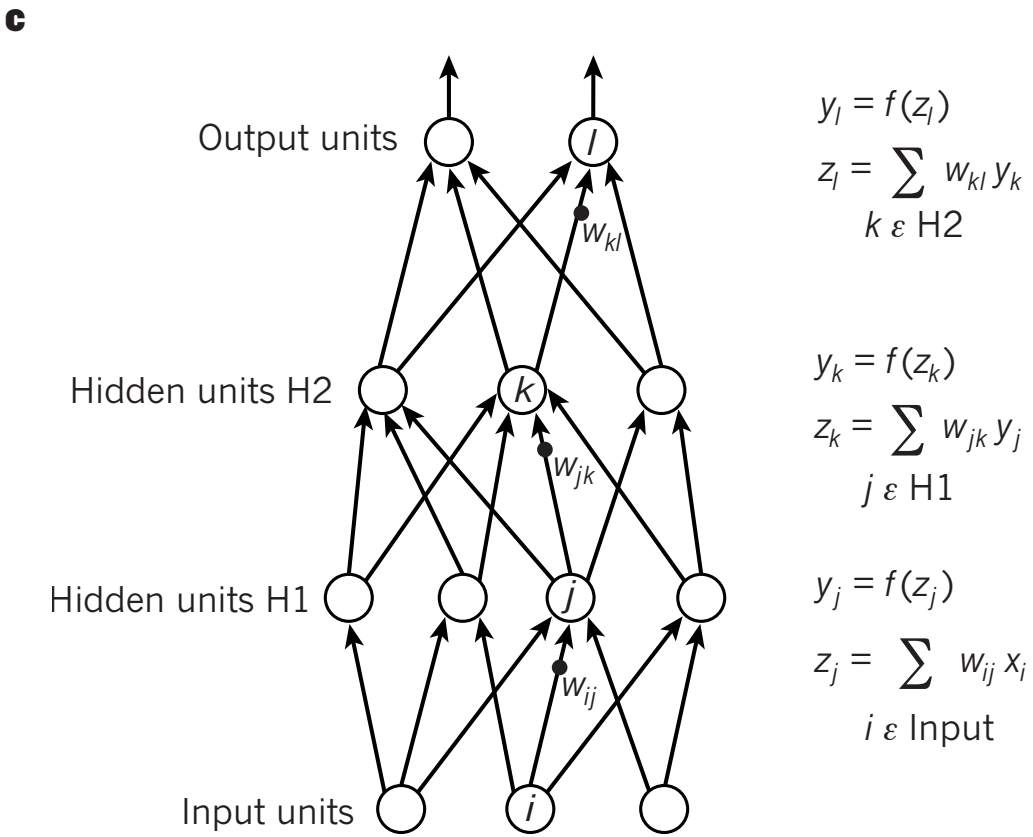
Deep learning

- Appeared quite a while ago (1980's), but gained tremendous attention fairly recently, mostly due to the increased computational power and availability of large-scale training data.
- Becomes a social buzz word, and widely applied to many fields.

Google AlphaGo beats the world champion 4-1 in a set of five GO games.

Deep Architecture

There are different types, but the most common is the feed-forward multilayer neural network.



Why go deep, since one can approximate any function as close as possible with shallow architecture?

- Deep machines are more efficient for representing certain classes of functions.
- So deep architecture trades breadth for depth (more layers, but less neurons in each layer).
- Demo: Tensorflow Playground: http://playground.tensorflow.org/

Advantages:

- Traditional machine learning algorithm requires feature extraction from data: Data $\rightarrow$ Feature $\rightarrow$ Model. Finding the correct features is critical in the success of a ML model.
- In complex pattern recognition/prediction problem (such as audio/image recognition, natural language processing), the input signals are highly non-linear and feature extraction is difficult.
- Deep learning can better capture the non-linearity in the data, thus potentially automate the feature selection step.

Example: DL in image recognition

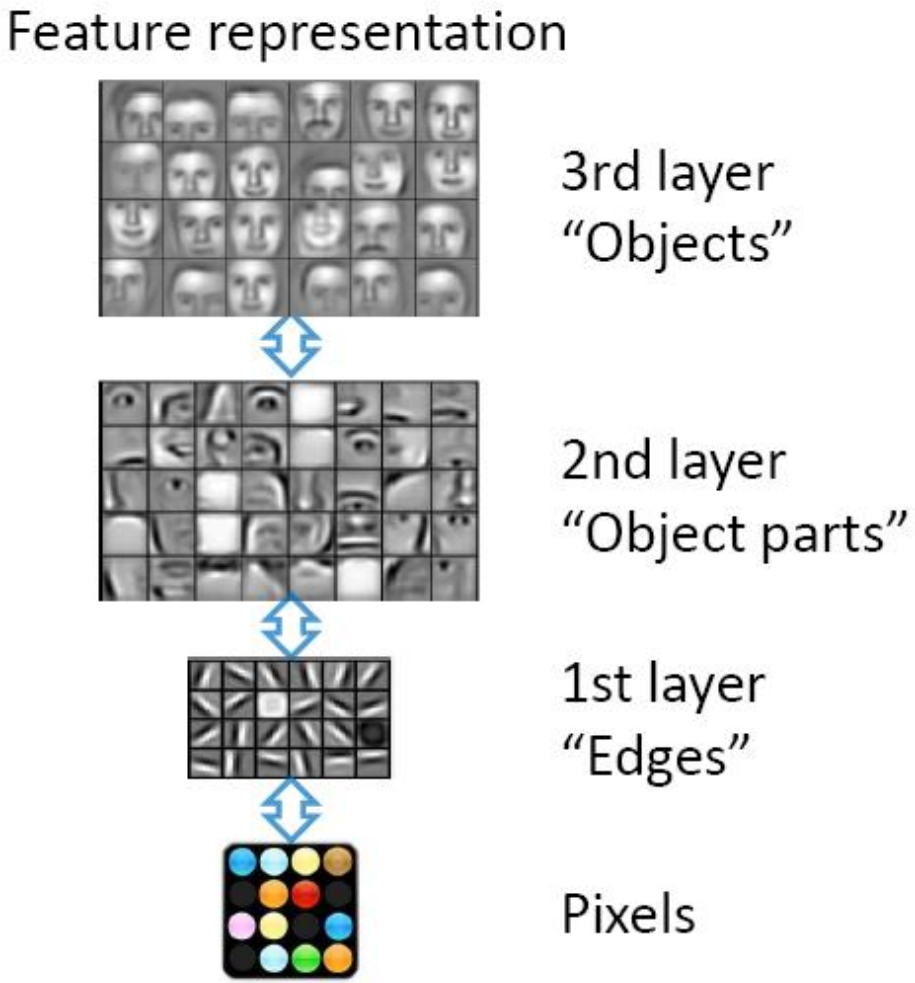
In image recognition problem, the inputs are color intensity values for all pixels in a picture. Tradition method that directly link pixels to outcome doesn't work well, because the higher order interactions (patterns) are not captured efficiently.

In deep learning (such as convolutional neural network):

- Layer 1: presence/absence of edge at particular location and orientation.
- Layer 2: motifs formed by particular arrangements of edges; allows small variations in edge locations.
- Layer 3: assemble motifs into larger combinations of familiar objects.
- Layer 4 and beyond: higher order combinations.

Key: the layers are not designed, but learned from data using a general-purpose learner.

Example: DL in image recognition (cont.)



Train a deep neural network

Back propagation does not work well if randomly initialized.

It was shown that deep networks trained with back propagation (without unsupervised pre-training) perform worse than shallow networks.

	train.	valid.	test
DBN, unsupervised pre-training	0%	1.2%	1.2%
Deep net, auto-associator pre-training	0%	1.4%	1.4%
Deep net, supervised pre-training	0%	1.7%	2.0%
Deep net, no pre-training	.004%	2.1%	2.4%
Shallow net, no pre-training	.004%	1.8%	1.9%

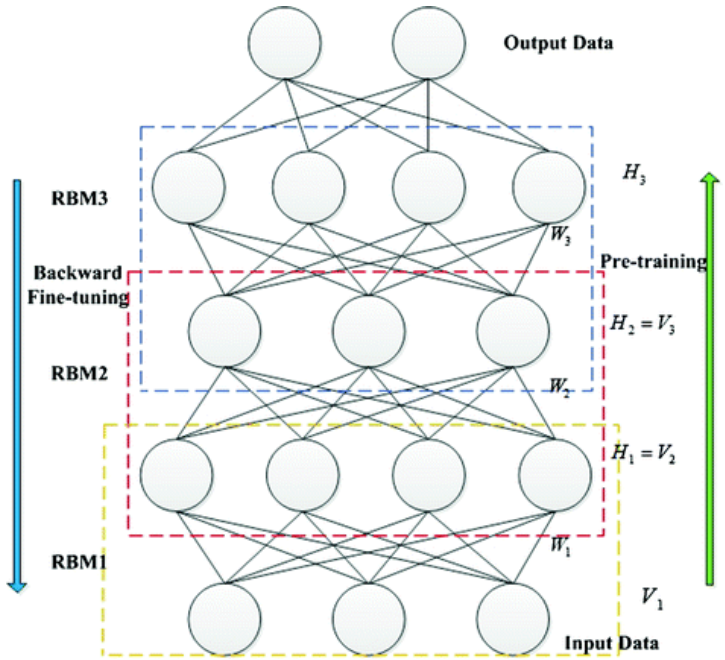
(Bengio et al., NIPS 2007)

Problems with Back Propagation: gradient is progressively getting more dilute below top few layers.

Deep Network Training

Hinton *et al.*, (2006) **A fast learning algorithm for deep belief nets** proposes greedy layer-wise training for trainning a deep belief network (DBN).

DBN is a type of deep neural network, which can be viewed as a stack of simple, unsupervised networks such as restricted Boltzmann machines (RBMs, similar to factor analysis).



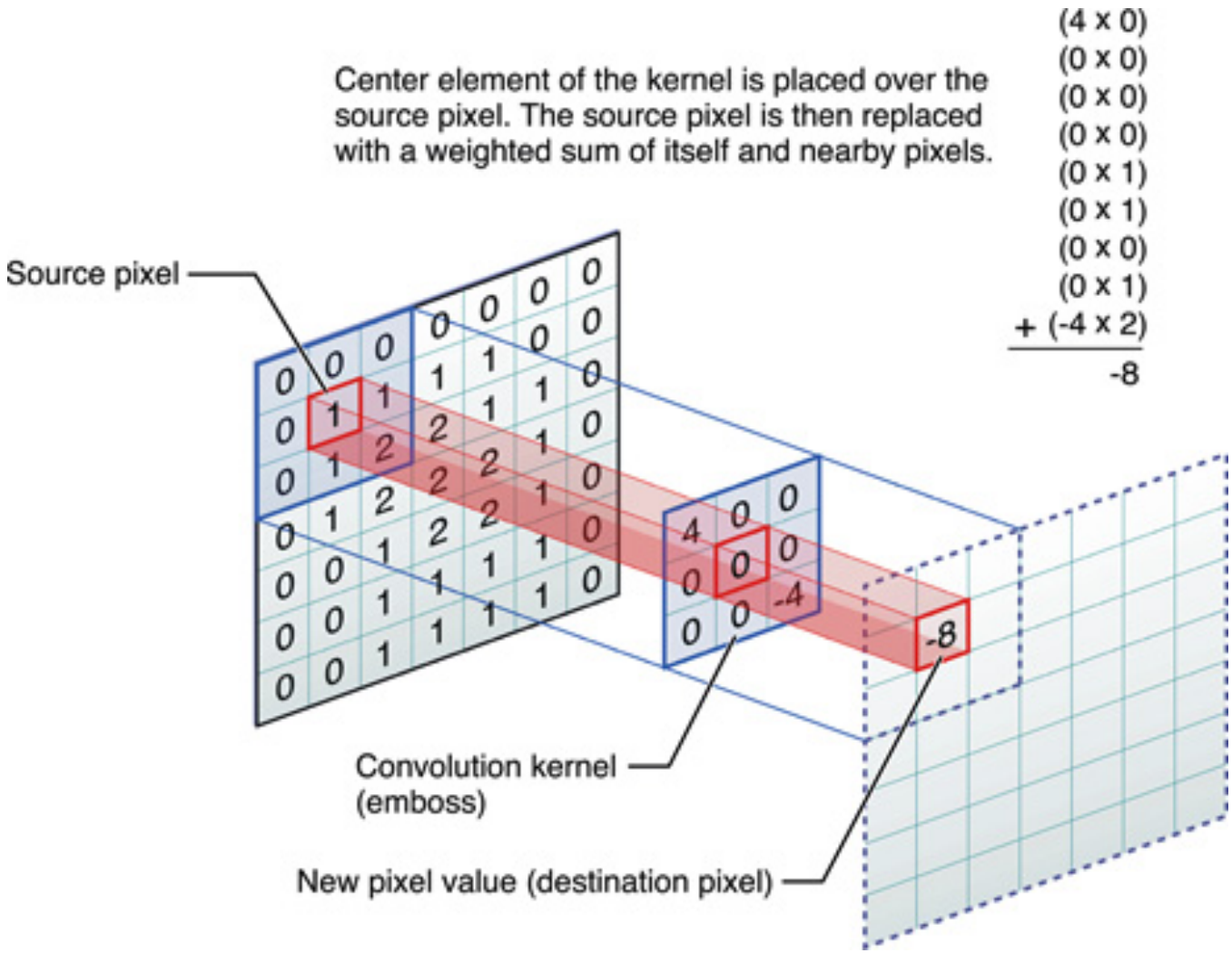
DBN Greedy Training

Let v be the input data (visible layer).

- First construct an RBM with input layer v and hidden layer h^1. The trained RBM provides $p(h^1|v)$.
- Obtain a set of realization of hidden layer h^1 (denoted by $\tilde{h}^1$) based on the trained RBM. One can either sample from $p(h^1|v)$, or compute $E[p(h^1|v)]$.
- With $\tilde{h}^1$ and hidden layer h^2, train another RBM, and so on.
- Once all parameters are estimated, perform supervised top-down training (backprop) to refine the parameters.

Convolutional neural network (CNNs / ConvNet)

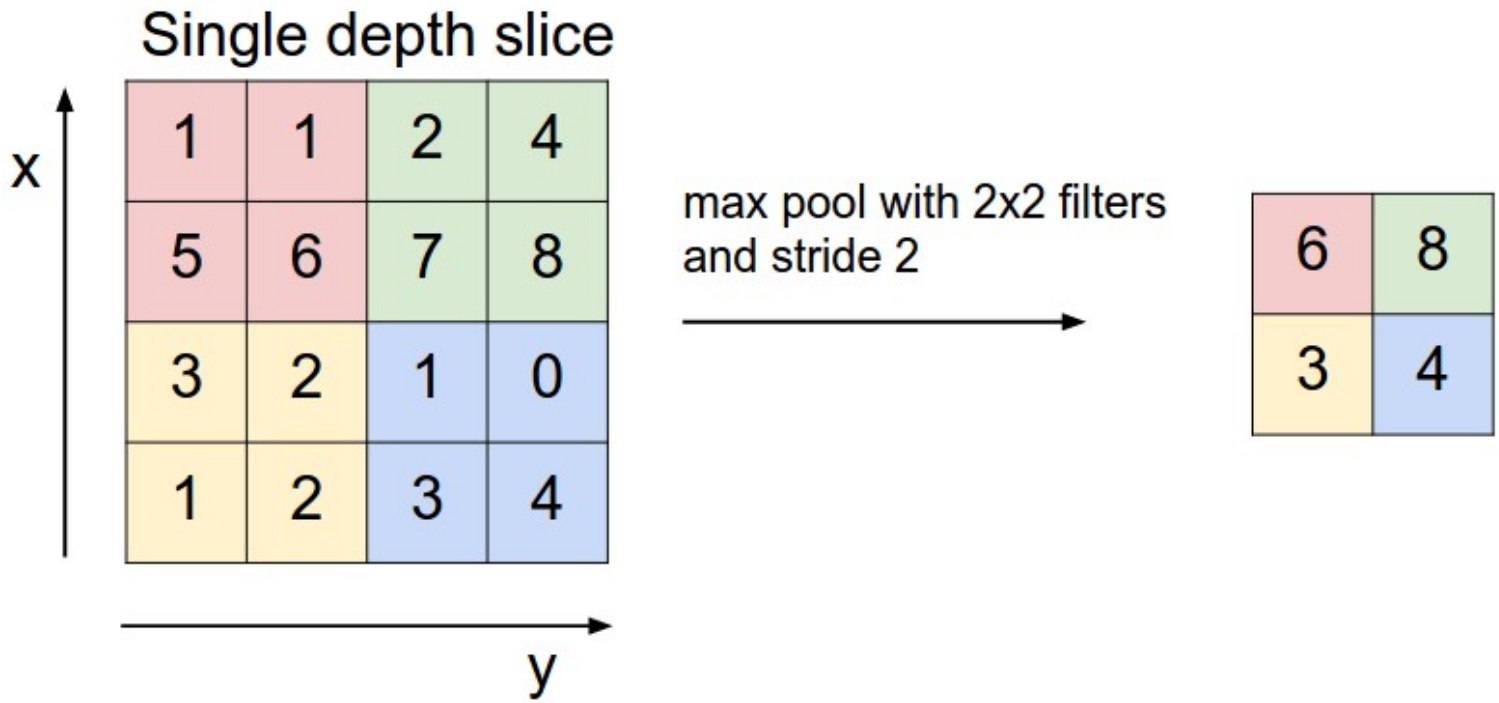
- ConvNet is a type of feed forward neural network.
- Widely applied to data where nearby values are correlated, for example, images (pixel values are spatially correlated), sound (frequencies are temporally correlated), etc.
- The network are stacked by convolutional and pooling layers for feature extraction.
- The final layer of the network is a fully connected layer to connect the extracted features to the output.


Center element of the kernel is placed over the source pixel. The source pixel is then replaced with a weighted sum of itself and nearby pixels.
(4 x 0)
(0 x 0)
(0 x 0)
(0 x 0)
(0 x 1)
(0 x 1)
(0 x 0)
(0 x 1)
+ (-4 x 2)
-8
Source pixel
Convolution kernel (emboss)
New pixel value (destination pixel)

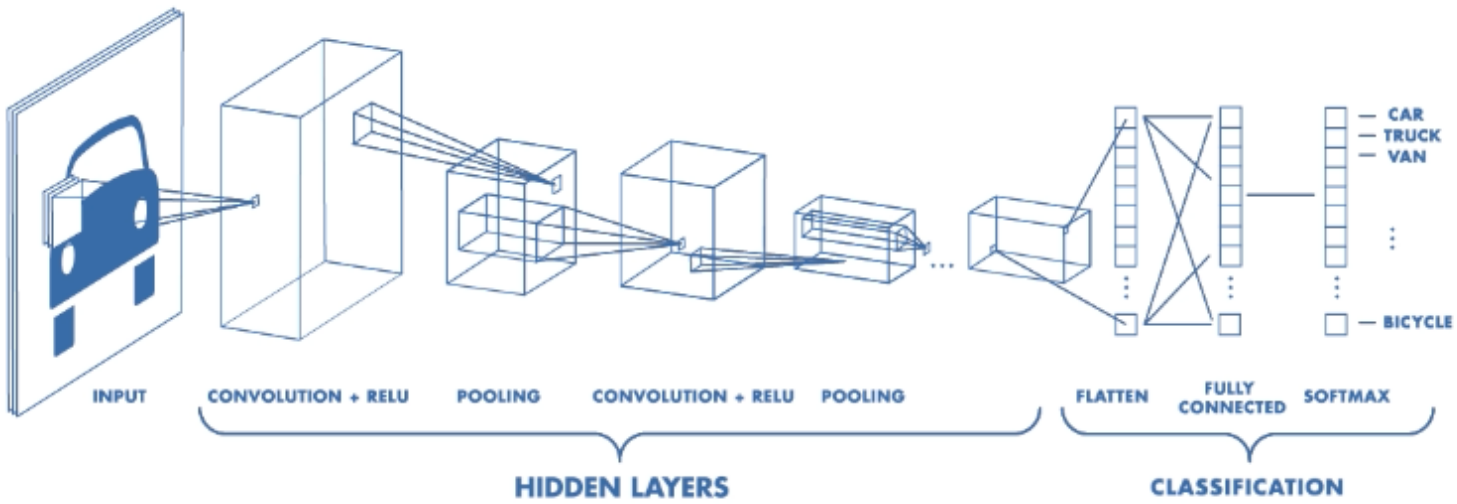
Pooling layers

- After the convolution, scan the data and apply a pooling function (usually max).
- Reduce the size of the representation, reduce the amount of parameters and computation, and alleviate overfitting.
- For example, a pooling layer with filters of size 2x2 downsamples the input by 2 along both width and height, retaining only 25% of the data.
- In backpropagation, one only routes the gradient to the input that had the highest value in the forward pass. So it's important to keep track of the index of the max activation during the forward pass of a pooling layer.

Pooling layers



ConvNet diagram



https://www.mathworks.com/videos/introduction-to-deep-learning-what-are-convolutional-neural-networks--1489512765771.html

- The model learning is based on back propagation.
- Pre-training is helpful.
- Large number of parameters (often millions). Require large training set.

Transfer learning

Problems in training a large ConvNet:

- Training data is not large enough.
- Model training requires significant computing resources.

Transfer learning

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Transfer learning:

- "Transfer" of knowledge: knowledge gained while learning to recognize cars could apply when trying to recognize trucks.
- Similar to the Bayesian statistics ideas of using prior from historical data.
- Pre-trained networks from large training set (e.g., ImageNet, which contains 1.2 million images with 1000 categories) can be borrowed in different ways.
  - Only retrain the last (fully-connected) layer. Previous layers are used as fixed feature extractor.
  - Train some layers while freeze others.
  - As the initial values and retrain the whole network.

Transfer learning (cont.)

- There are a number of pre-trained networks (VGGnet, AlexNet, GoogLeNet, ResNet) available for transfer learning.
- One needs to download the pre-trained network (can be big, due to large number of paremters).
- Most deep learning packages provide easy interface for transfer learning.

Our experiences show that transfer learning can significantly improve the performance, even though the image to be classified are very different from the training ones.

Deep learning software package

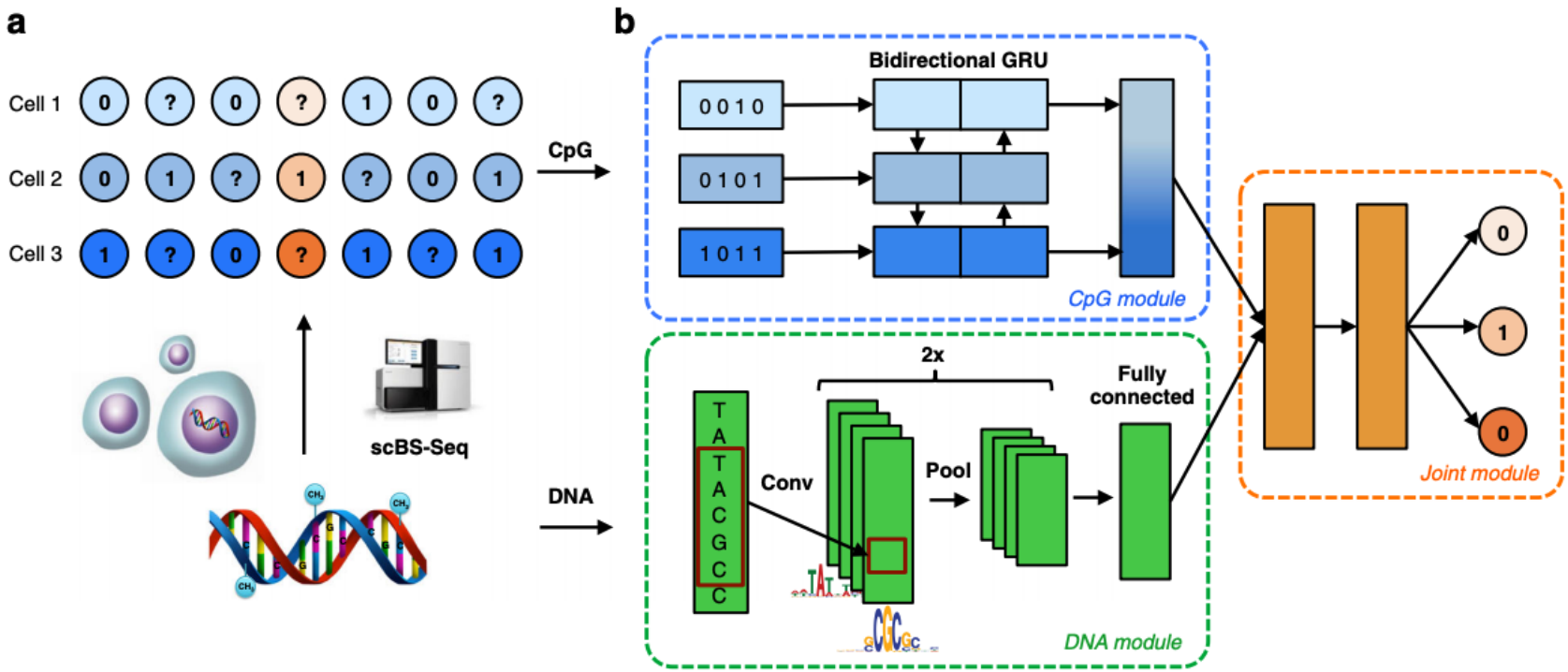
Most of the popular deep learning software packages are written in Python, for example,

- Tensorflow by Google: https://www.tensorflow.org.
- PyTorch by Facebook: https://pytorch.org.
- Theano: http://deeplearning.net/software/theano.
- Keras: https://keras.io.

The R development for deep learning lags behind, but gradually catches up: There are a few packages:

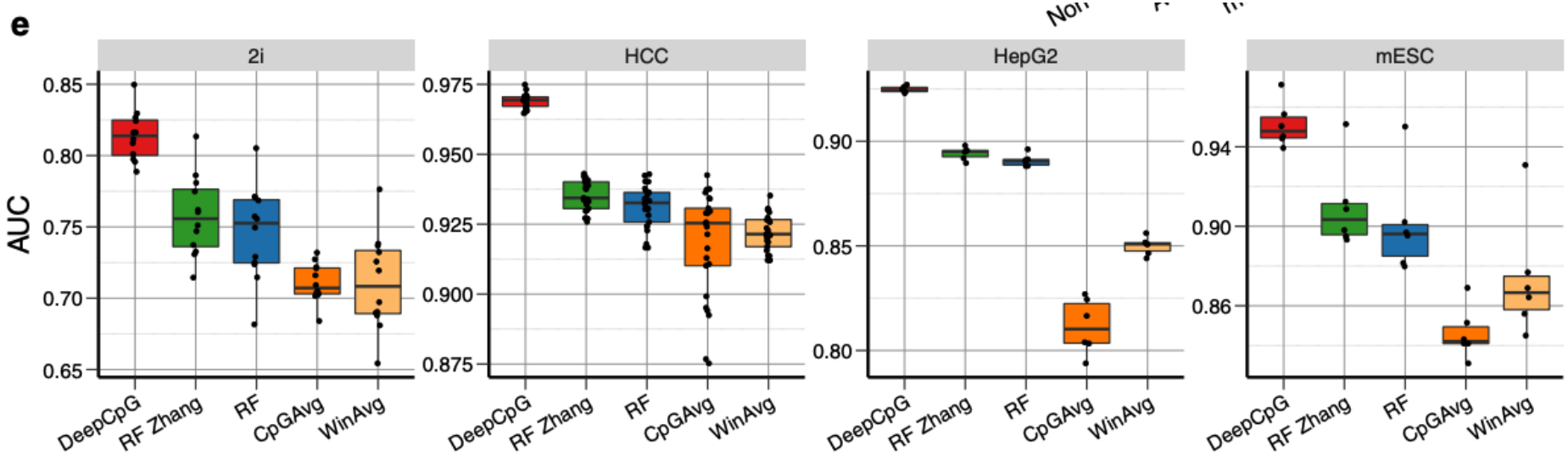
- MXNetR: https://mxnet.apache.org/versions/1.8.0/.
- Other available ones on CRAN include `RNN`, `LSTM`, `darch`, `deepnet`.

Deep learning examples



Angermueller, C., Lee, H.J., Reik, W. et al. DeepCpG: accurate prediction of single-cell DNA methylation states using deep learning. Genome Biol 18, 67 (2017).

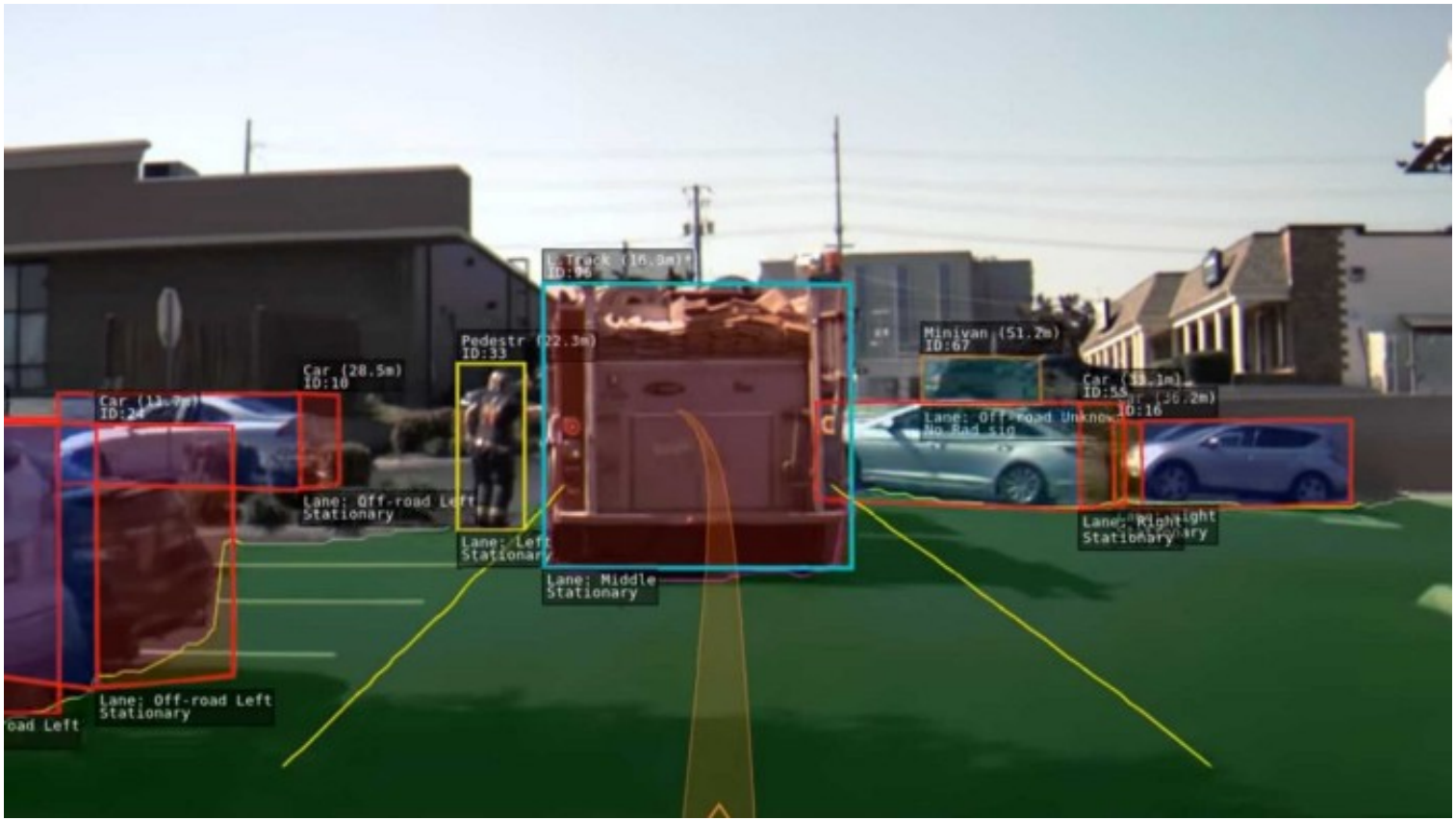
Deep learning examples



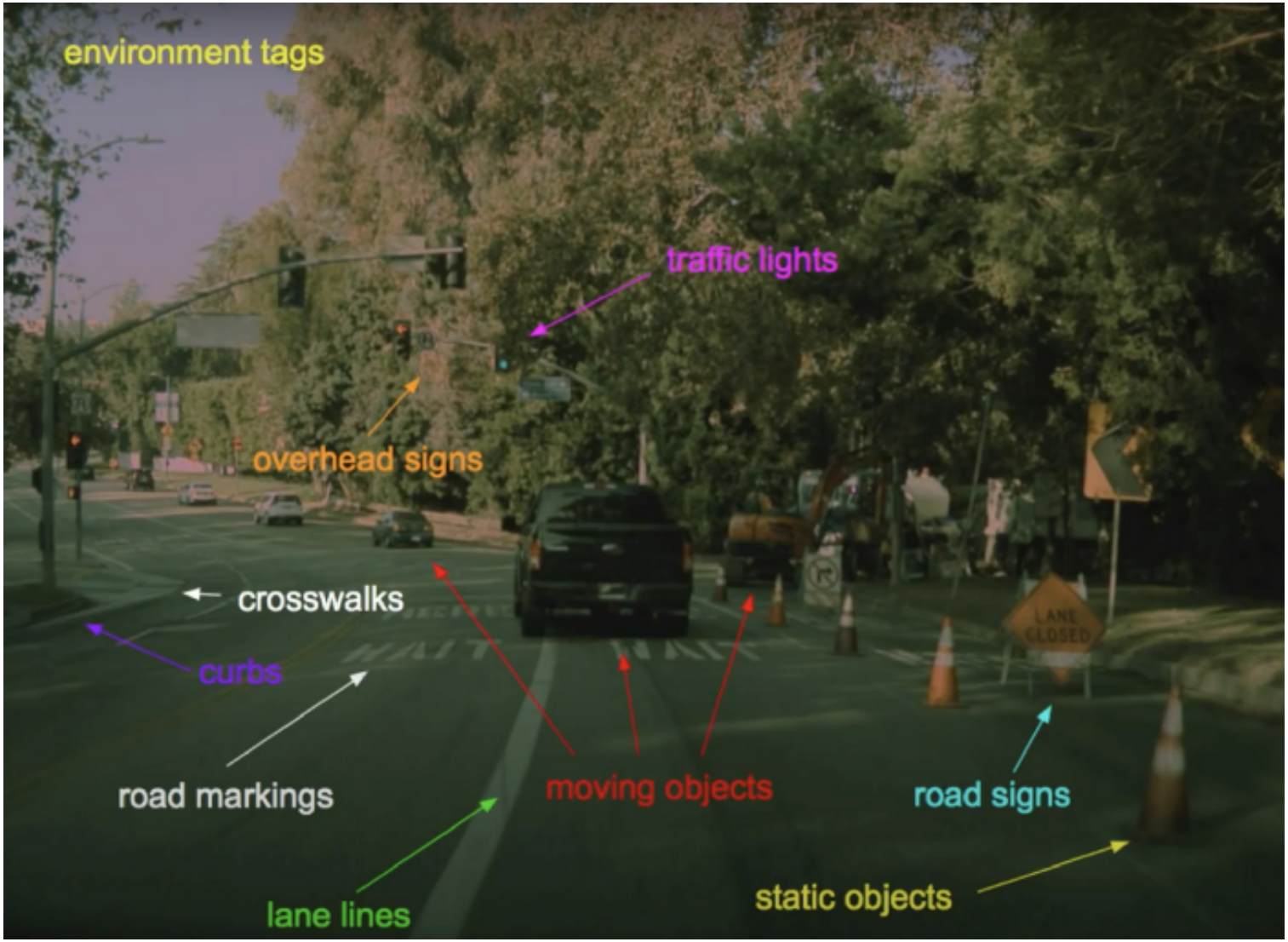
DNA module: CNN
CpG module: RNN
ReLU + sigmoid

Tesla: Autopilot by neural networks

Information from Andrej Karpathy, AI Lead at Tesla.



Goal: Fully self-driving, full autonomy(Level 5).



About 50 tasks must be done on-device, simultaneously.

HydraNets: Specialized Dynamic Architectures for Efficient Inference

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Abstract

There is growing interest in improving the design of deep network architectures to be both accurate and low cost. This paper explores semantic specialization as a mechanism for improving the computational efficiency (accuracy-per-unit-cost) of inference in the context of image classification. Specifically, we propose a network architecture template called HydraNet, which enables state-of-the-art architectures for image classification to be transformed into dynamic architectures which exploit execution for efficient inference. HydraNets are wide networks containing distinct components specialized to compute features for visually similar classes, but they retain efficiency by dynamically selecting only a small number of components to eval-

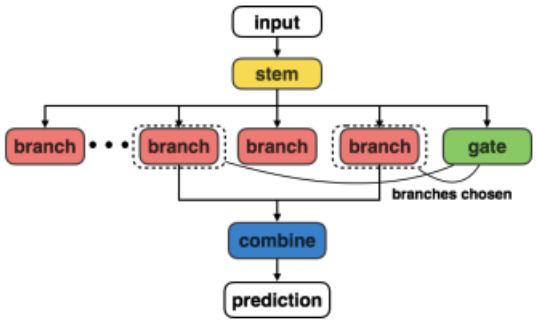
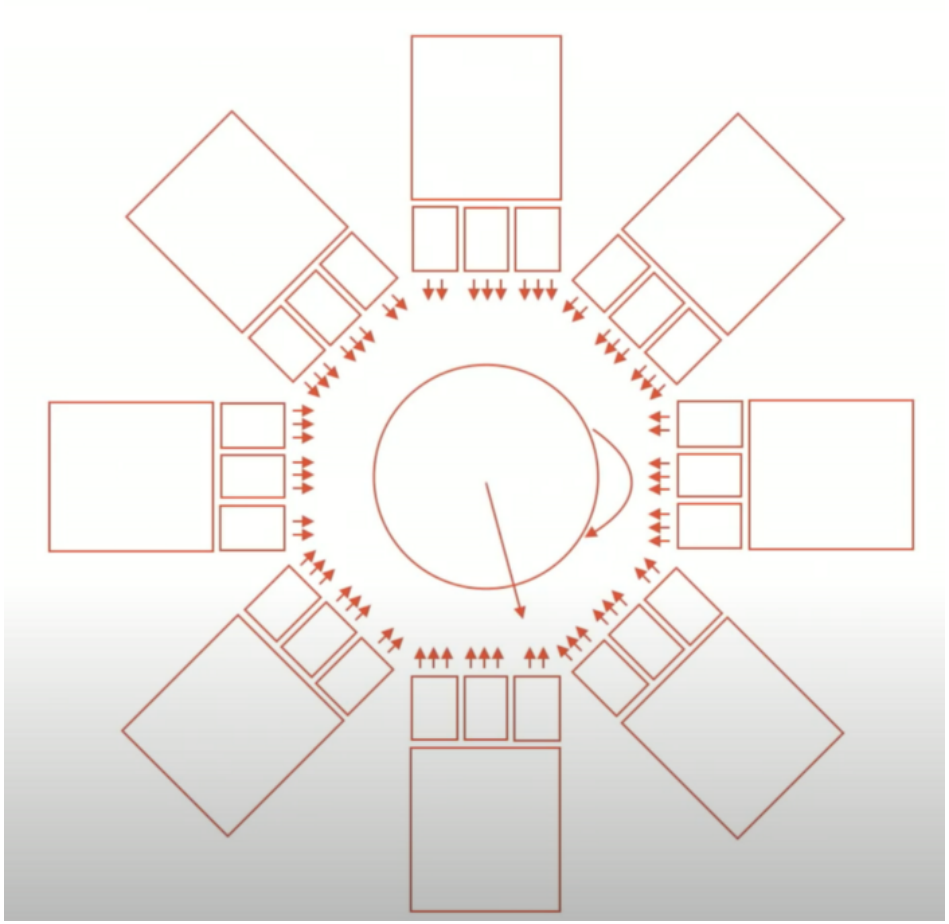


Figure 1: The HydraNet template architecture: contains multiple *branches* specialized for different inputs and a *gate* chooses which branches to run when performing inference on an input, and a *combiner* that aggregates branch outputs to make final predictions.

Backbone: HydraNets.

HydraNet architecture



One Tesla car: process 4,096 images on-device.

Summary

- Deep learning is a powerful technique in the machine learning field.
- So far the major areas of application include speech recognition, image classification, natural language processing.
- Demonstrate superior performance when there are many highly nonlinear patterns in the data.
- Application in biostatistics/bioinformatics field is relatively fewer so far, perhaps because
  - Training data size (subjects) is still too small.
  - Biological knowledge, in the form of existing networks, are already explicitly used, instead of being learned from data. They are hard to beat with a limited amount of data.
  - Lack of good inference procedure.

Textbook chapters

- ESL: chapter 11.