Deep Neural Networks for Scalable Prediction

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Agenda

- Neural Networks (NN's) basics and inspirations
- Problem domains
- Architectures: various and popular
- Training and testing basics
- A simple application example:
  - Marketing campaign response application
- As time allows:
  - “Try it at Home” using a downloadable Jupyter Notebook

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NN's, ML, and Prediction

- NN's are a class of machine learning (ML) methods
- Like many other ML methods, a common objective is maximizing predictive accuracy
- ML methods are in general not for theory or hypothesis testing (Not yet, at least)

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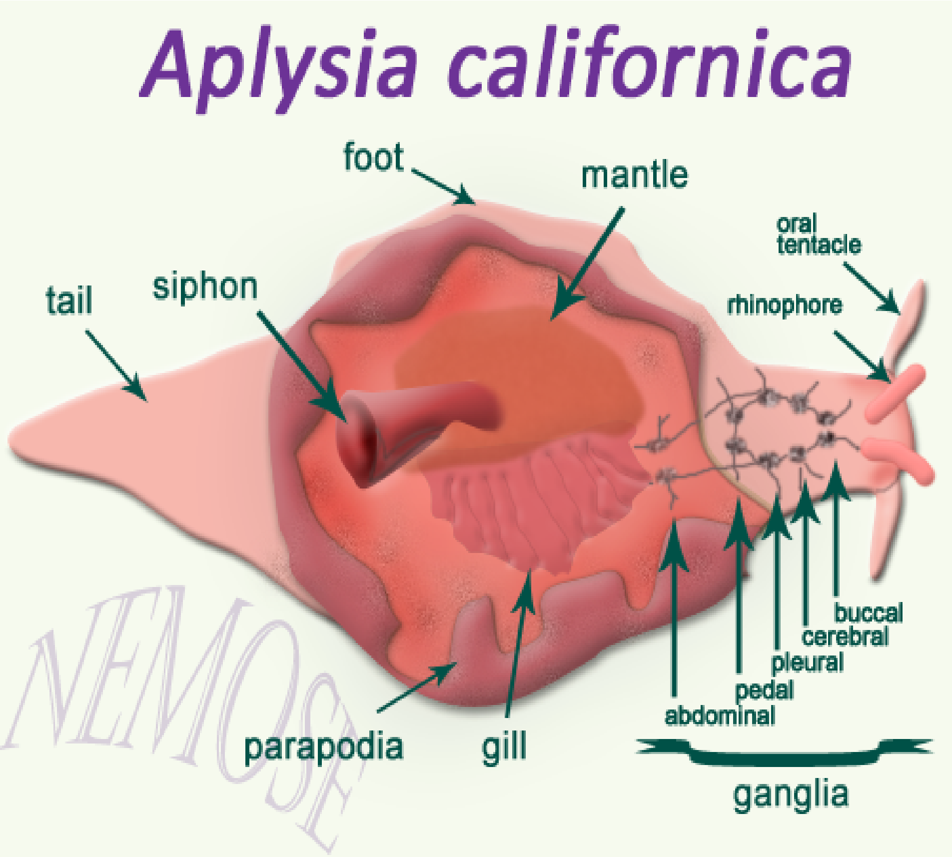
NN Progress in Problem Domains

- NLP
- Image recognition
- Autonomous vehicles
- Drug repurposing and discovery
- Security

Alypsia



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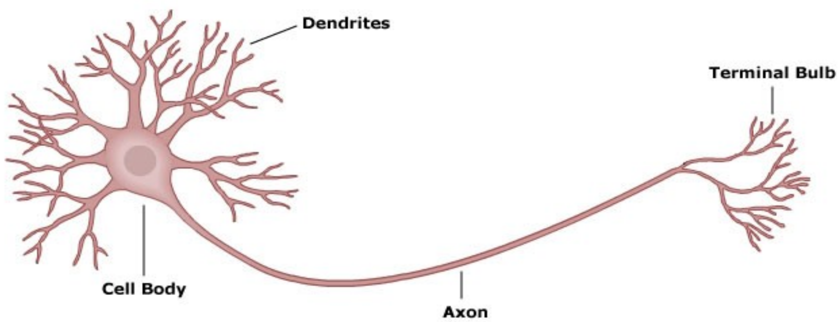
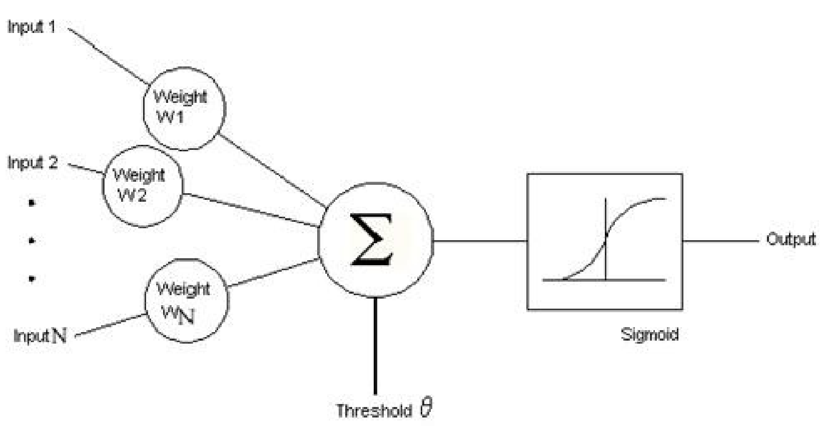
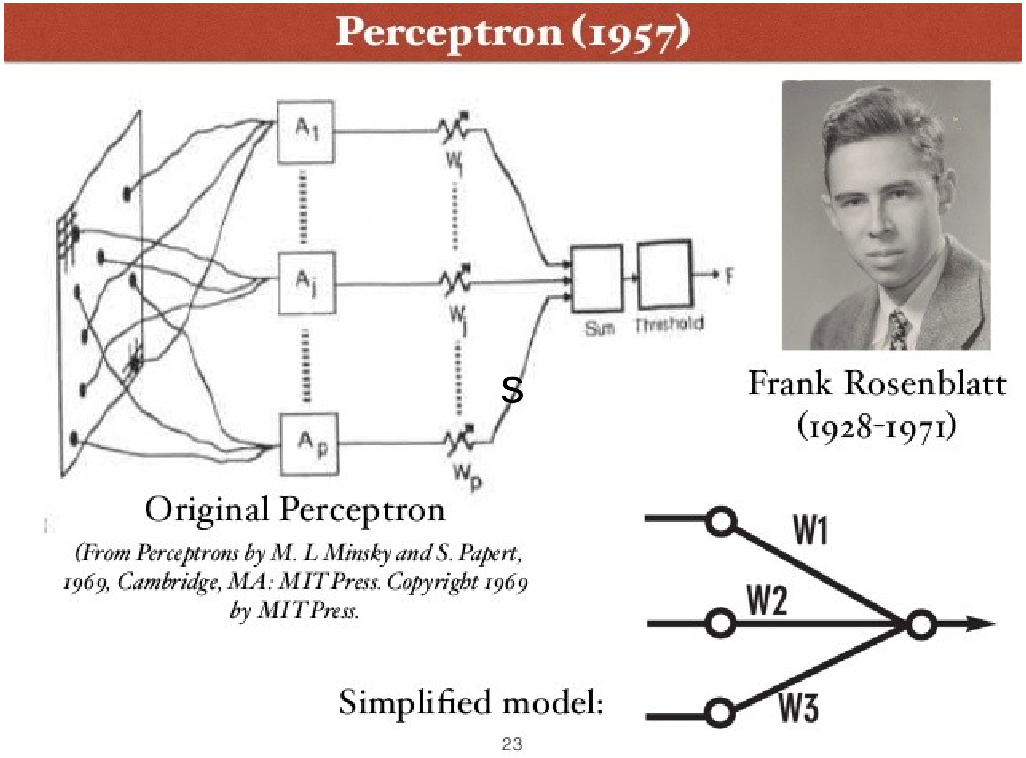
Getting from There to Here: Some Key Developments

- Carew, Castellucci & Kandel (1971): learning at the level of the single neuron
- McCulloch & Pitts (1943): artificial neuron
- Hubel & Wiesel (1959): organization of central nervous system in cats, primates
- Rosenblatt (1957), Minsky & Papert (1969, 1987): “perceptron”
- Rumelhart & McClelland (1986, 1987): parallel distributed processing

Perceptron







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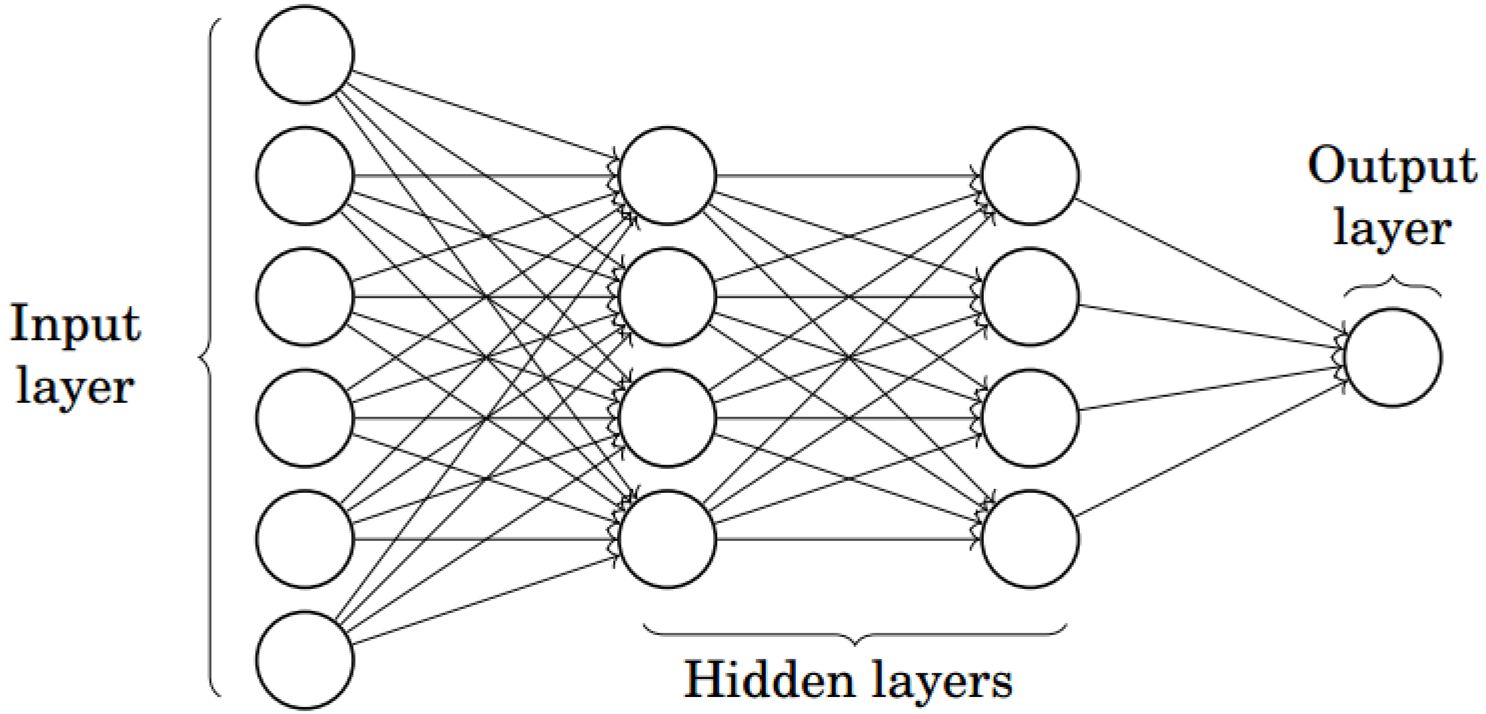
Multilayer Perceptron



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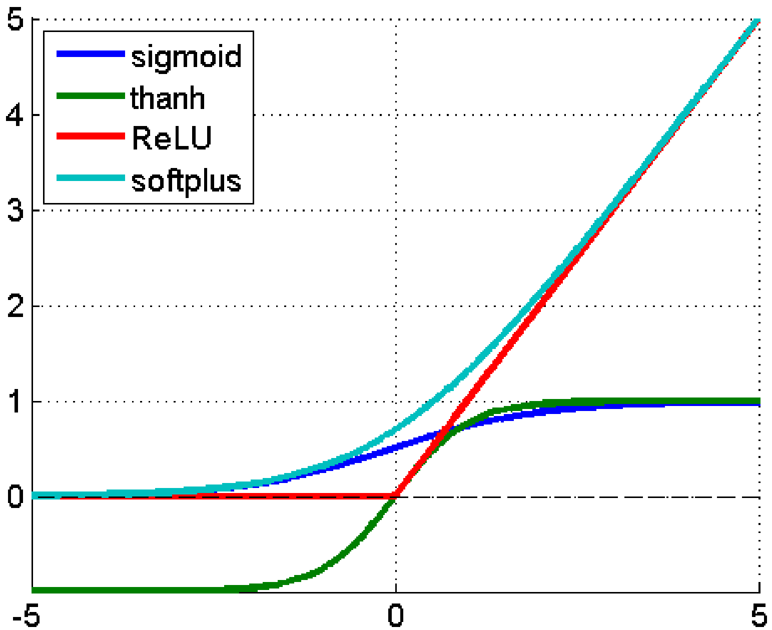
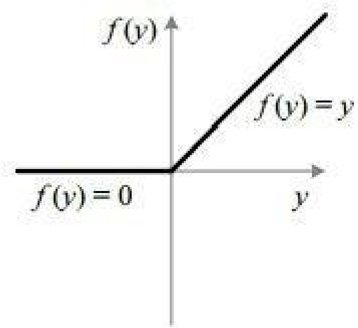
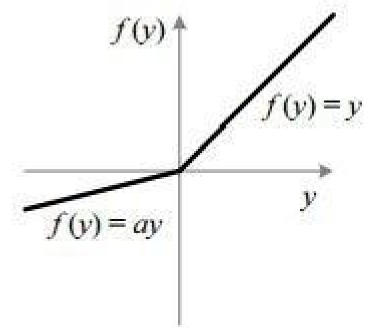
Common Activation Functions

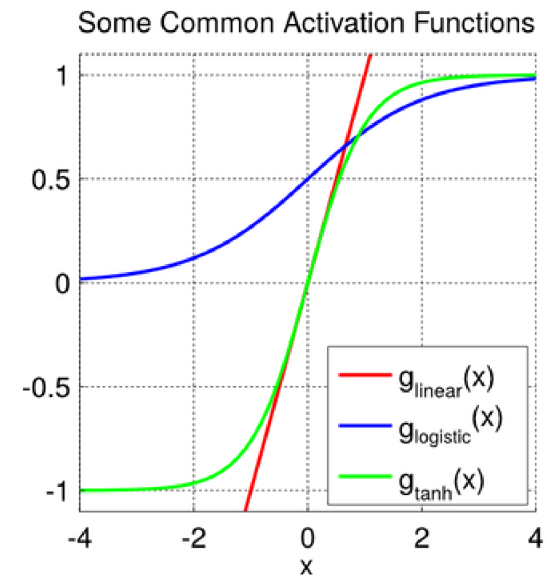


ReLU



Leaky ReLU





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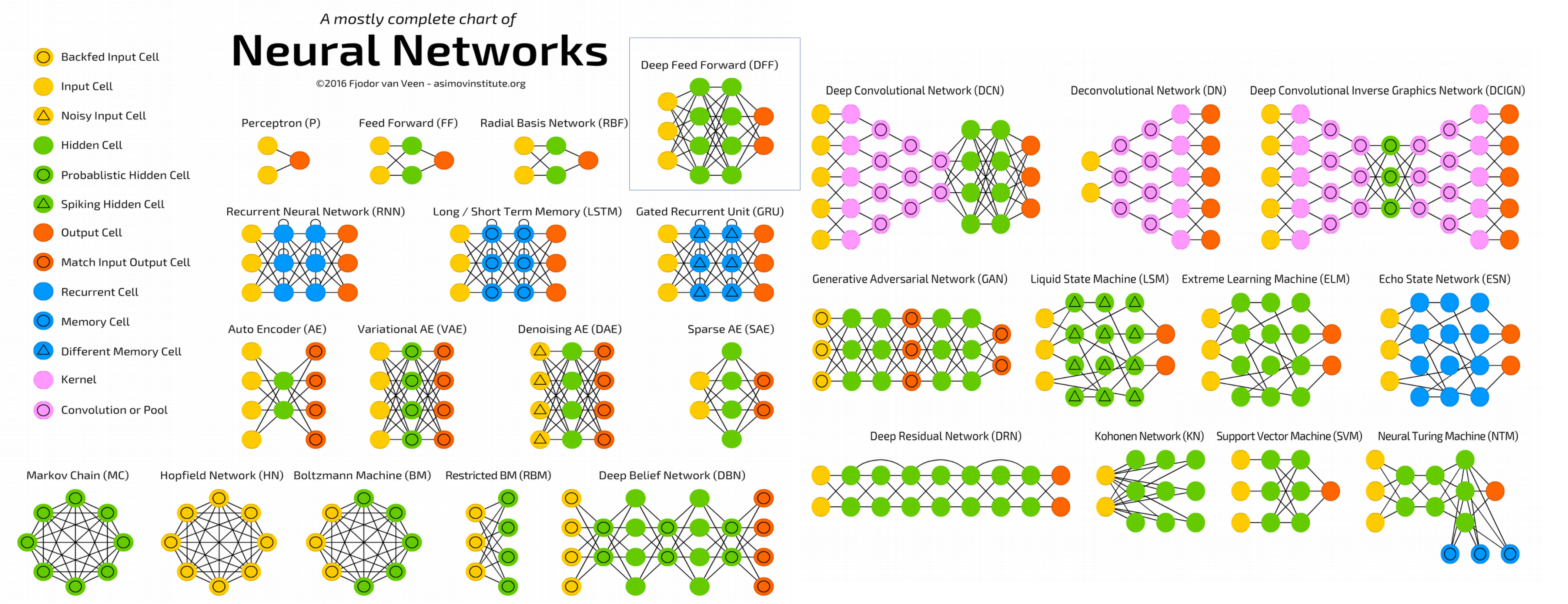
A Diversity of Network Architectures

van Veen, 2016



http://www.asimovinstitute.org/neural-network-zoo/

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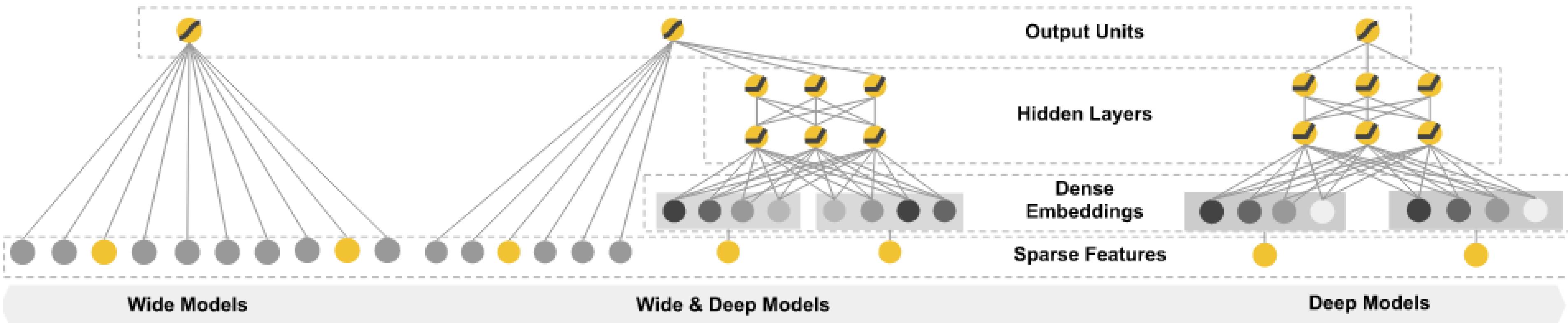
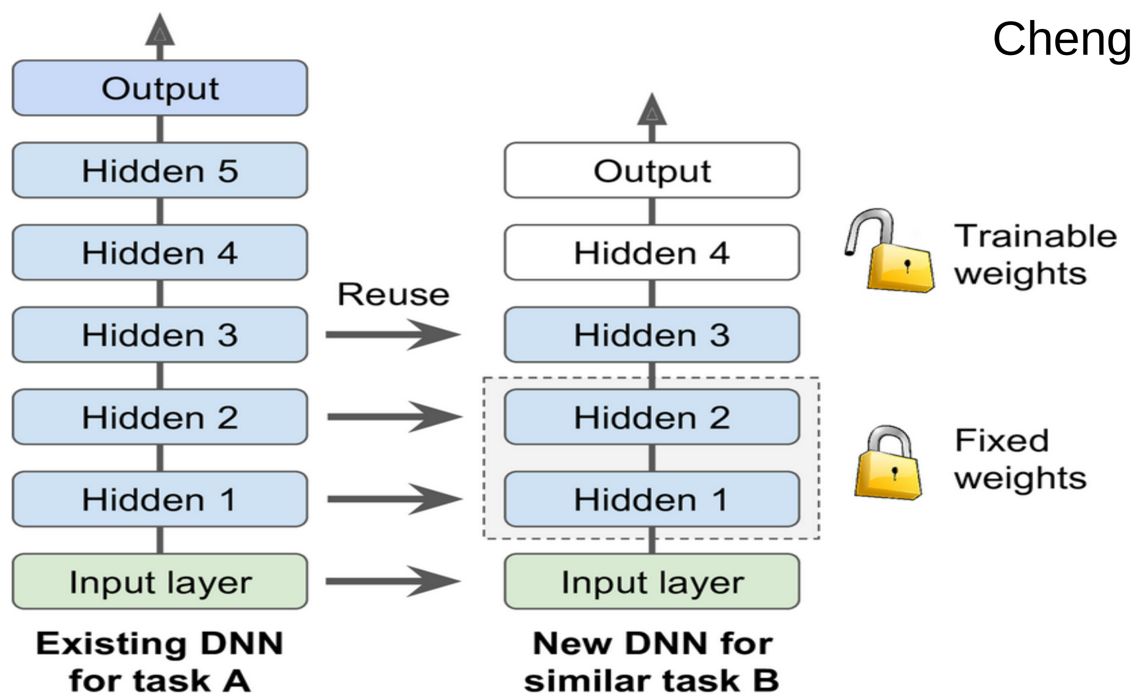
Some Variations and Extensions



Cheng et al., 2016

Géron, 2017



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NN Training: Basic Elements

- Four basic elements:
  - Data
  - Model
  - Optimization Method
    - Some kind of gradient descent
  - Loss functions
    - Cross entropy: $H(y,p) = -\sum_i y_i \log(p_i)$
    - Mean squared error
- Evaluation
  - Predictive accuracy performance metrics using training and test data

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“Features” (input data)

- NN models do math operations using continuous data
- Input data, or “features,” that are categorical are transformed
- Methods include:
  - Dummy, or “one hot,” encoding
  - “Hashing” : “bucketing” a large number of categories
  - “Embedding” : many categories respresented in a low dim space

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Back Propagation and Gradient Descent

- NN training involves:
  - Calculating the gradient of the loss function with respect to parameters ("weights")
  - Adjusting the weights to decrease the loss function
- "Backprop" is used to calculate the gradient
  - Most loss functions are nonconvex due to NN nonlinearity
- "Gradient descent"
  - Decrease loss in small, "learning rate" steps
  - *Stochastic* GD: use random samples of training data
- Parameter estimates during training can be examined
  - e.g. whether weights are "stuck" at some value like zero

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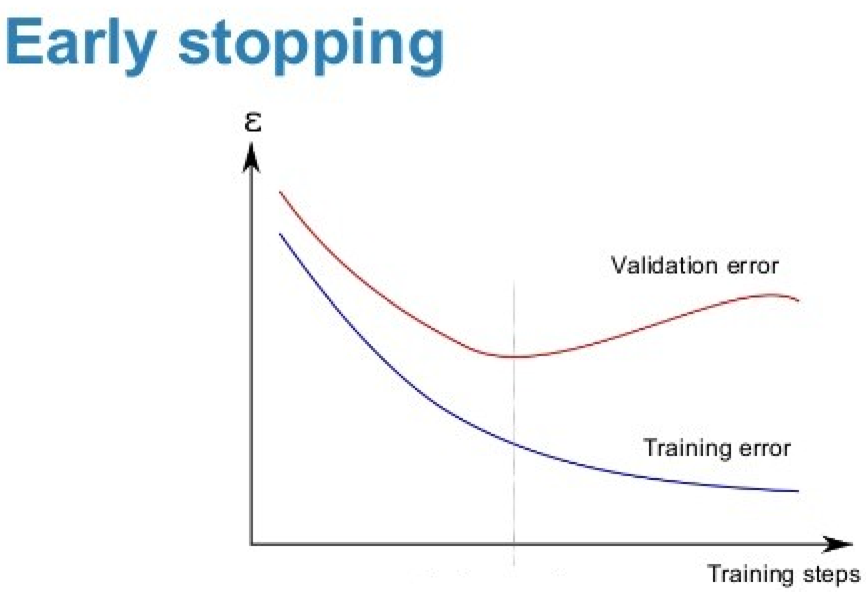
Regularization

- Goal: reduce generalization error without decreasing training error
  - accept some bias in trade-off to variance reduction
- Methods:
  - Parameter penalties
  - Data augmentation
  - Noise “injection”
  - Multitask learning
  - Parameter sharing
  - Bagging / ensembles
  - Dropout
  - Early stopping



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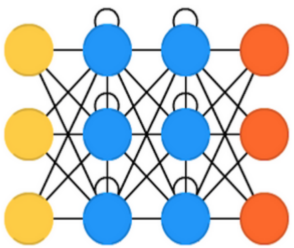
Performance Assessment

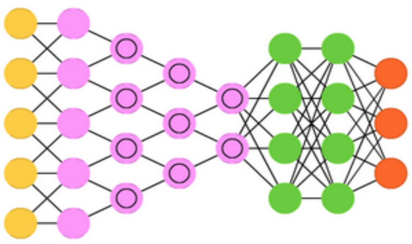
- On both training and test data sets
- For classifiers, the “usual” methods
    - Classification error or accuracy rate
    - Loss
    - LL
    - AUC
    - F1, precision, recall
  - For continuous outcomes, MSE

A Few Notable Special Types

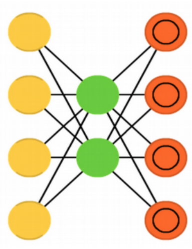
- Recurrent NN
  - text processing, e.g. NER, POS



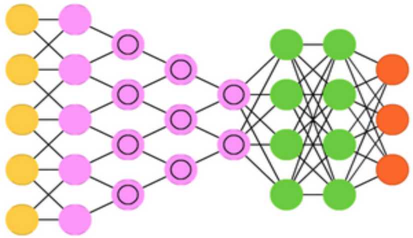
- Convolutional NN
  - image, audio recognition, text processing



- Autoencoder
  - *un*supervised learner
  - data compression

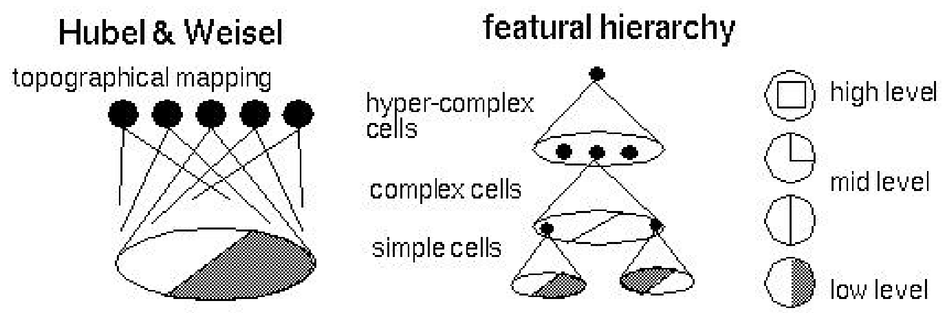


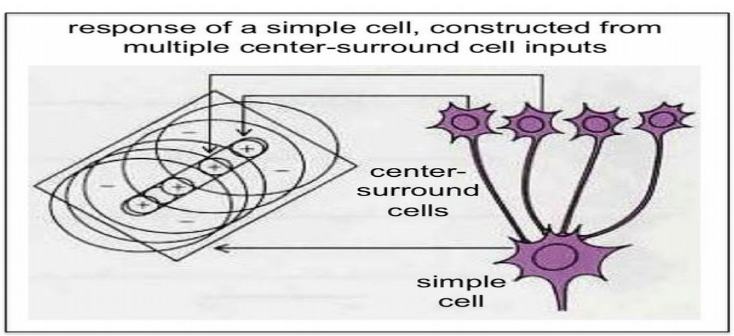
Convolutional NNs

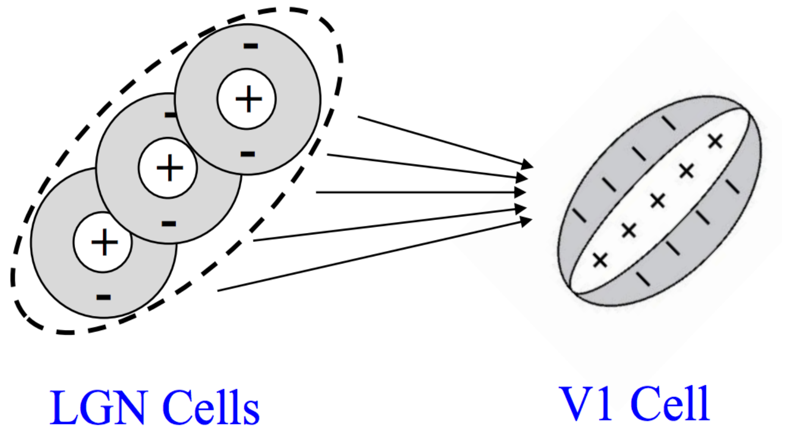


- Grid-like data in one or more dimensions
- Somewhat functionally similar to visual system elements
  - Inspired by Nobel work on mammalian visual processing
- Convolution : applying a kernel to input to produce a “feature map”
- Convolutional layers include both convolution and pooling
- CNN attributes: sparse connections, parameter sharing, equivariance.

Visual Input Processing







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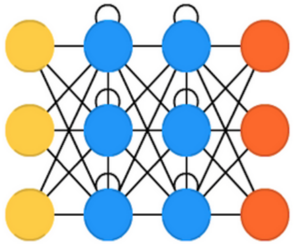
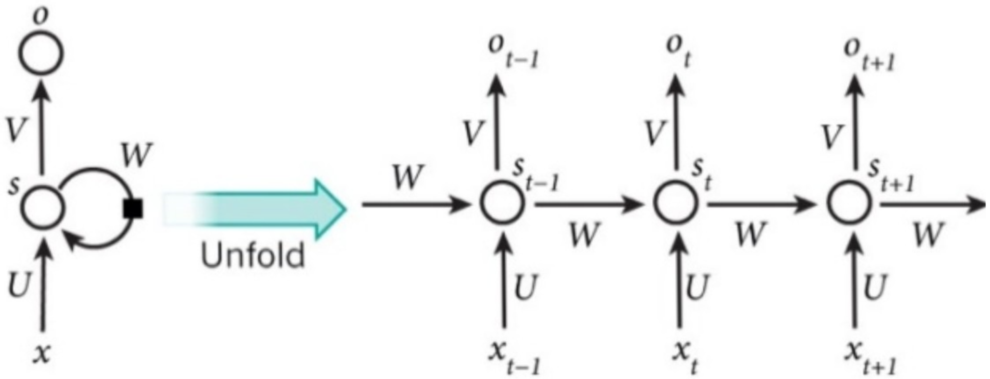
Recurrent NN's

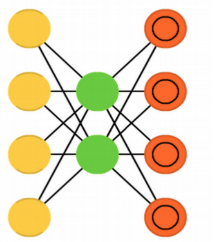


- Sequential data, e.g. for part of speech labeling of text data
- Sequences can vary in lengths
- Sequential dependencies “unfolded” to model state-to-state transitions



- Scalability and generalization facilitated by parameter sharing.

Autoencoders



- Network that reproduces its inputs
- An *unsupervised* learning method
- Two basic components
  - An *encoder* that reduces the dimensionality of inputs
  - A *decoder* that attempts to reproduce inputs from the outputs of the encoder
- Analogous to PCA

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A Growing Host of Libraries and Platforms

- **TensorFlow** http://www.tensorflow.com
- **Theano** http://deeplearning.net/software/theano
- **Keras** https://keras.io/
- **PyTorch** http://pytorch.org
- **Blocks** http://blocks.readthedocs.io/en/latest
- **MxNet** http://mxnet.io
- **Lasagne** http://lasagne.readthedocs.org
- **H_2O** https://www.h2o.ai/

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NN's at Scale

- “Scalability” can be accomplished in scope and in time
- GPU processing
- Using a cluster
- Parameter tying and sharing
- More machine “grunt”
- Care in coding and serializing

A Simple TensorFlow Example

- Tensorflow - machine learning numerical computation library
- Released by Google for public use
- Programmable with Python (also Java, C++, Go; other APIs in development, e.g. for Ruby, Haskell)
- Programming paradigm:
  - define model in graph form
  - execute using optimized C++ code
- Can take advantage of multiple CPUs and GPUs
- Scalable from small platforms to big ones
- Models deployable to diverse environments
- Somewhat of a “learning curve”
- www.tensorflow.org

An Example Application: Predicting Customer Segment Membership

- Customer data from a retailer, the “ZETA” company
- Sample from an enhanced CRM DB
- N=50,000
- Three “Buyer Engagement” segments
  - Low, Med, Hi = 21%, 44%, 35%
- 22 predictor variables from 3rd party suppliers
  - 5 continuous, 17 categorical
  - various degrees of missingness in categoricals
  - mostly inferred or aggregate measures

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A Baseline “Shallow” MNL model

- Using TensorFlow
- 200,000 “training” iterations
- 80%/20% random training/test split

Training Data

```
accuracy:0.581
```

Test Data

```
accuracy: 0.581
```

DNN's for Predicting Engagement

- Two or three hidden layers
- 10 or 15 nodes per hidden layer
- Fully connected MLP
- Categorical feature embedding
- “Leaky ReLU” activation function
- Adaptive gradient optimizer
- “drop-out” probability of 0.10
- 200,000 training iterations
- Classification accuracy calculated for training and test samples

Classification Accuracy: Proportion Correct

Nodes per Hidden Layer	Data	Two Hidden Layers	Three Hidden Layers
10	Training	0.766	0.790
	Test	0.765	0.785
15	Training	0.789	0.789
	Test	0.784	0.785

Resources

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Try It At Home!

- In an Jupyter Notebook,

  A simple DNN Binary Classifier Predicting Response to a Marketing Campaign
- Python,Tensorflow, scikit-learn, Other bits and pieces
- Bank marketing data available in the UCI Machine Learning Repository
- You'll find the Jupyter Notebook:

  CSP 2018 DNN Binary Classifier Example vx.ipynb

  where 'x' is an integer version number.

  at:

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- Supplementary Material -

Jupyter Notebook Example:

High Notes
and
Code Snippets

The Notebook:
“A Toe In The Tensorflow DNN Water”

- Python 3 + packages that include Tensorflow and Scikit Learn
- Trains and assesses the predictive accuracy of a two hidden layer binary classifier NN
- Bank marketing data from the UCI machine learning Repository
- Also, a binary logistic regression model for comparison purposes
- Assembled using Continuum.io Anaconda

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The Data

UCI Machine Learning Repository: Bank Marketing Data Set https://archive.ics.uci.edu/ml/datasets/Bank+Marketing#

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UCI

Machine Learning Repository

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Bank Marketing Data Set

Download: Data Folder, Data Set Description

Abstract: The data is related with direct marketing campaigns (phone calls) of a Portuguese banking institution. The classification goal is to predict if the client will subscribe a term deposit (variable y).

Data Set Characteristics:	Multivariate	**Number of Instances:**	45211	**Area:**	Business
Attribute Characteristics:	Real	**Number of Attributes:**	17	**Date Donated**	2012-02-14
Associated Tasks:	Classification	**Missing Values?**	N/A	**Number of Web Hits:**	321450

Source:

[Moro et al., 2014] S. Moro, P. Cortez and P. Rita. A Data-Driven Approach to Predict the Success of Bank Telemarketing. Decision Support Systems, Elsevier, 62:22-31, June 2014

Packages and “Features”

Required packages are loaded into the Notebook's Python environment. Then, after reading the UCI ML Repository, variables are selected to use as inputs, “features.

```
import pandas as pd
import numpy as np
import tensorflow as tf
from sklearn.model_selection import train_test_split
from sklearn.metrics import roc_auc_score
from sklearn import preprocessing

# The following allows output from multiple statements to come out in a single output cell.
from IPython.core.interactiveshell import InteractiveShell
InteractiveShell.ast_node_interactivity = "all"
```

Avariables are selected from Pandas DataFrame “bankDat” of input data to be used as features. The data are then randomly split into training and test subsets.

```
varsToUse=['age','balance','housing','loan','campaign','previous','y']

campCusts=bankDat[varsToUse]
```

```
Xtrain, Xtest, yTrain, yTest = train_test_split(campCustX, convY,
                                                test_size=0.20, random_state=23)
```

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“Normalization”, Logistic Regression

The training data are normalized, and then the test data are rescaled using the normalization parameters of the test data.

```
Xtrain=Xtrain.astype(float)

scaler = preprocessing.StandardScaler().fit(Xtrain)

# XTrain's columns should be mean = 0, std = 1
Xtrain = scaler.transform(Xtrain)

# Xtest is rescaled based on Xtrain's means and std devs
Xtest = scaler.transform(Xtest.astype(float))
```

A logistic regression model is fit to the training data, and then applied to the test data.

```
from sklearn import linear_model
logReg=linear_model.LogisticRegression()
logMod1=logReg.fit(Xtrain,yTrain)
```

```
training data accuracy 0.882
training data auc 0.688
test data accuracy 0.881
test data auc 0.689
```

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NN: mini-batch generation

A function is used to randomly sample training data to be used in "mini-batches."

```
def get_batch(epoch, ncases, b_ndx, b_size):
    # epoch is the alg iteration, b_ndx is the batch no.
    # b_size is batch size

    ndxs= np.random.randint(ncases,size=b_size)
    X_bat=Xtrain[ndxs]
    y_bat=yTrain[ndxs]
    return X_bat, y_bat
```

NN: parameters

Various parameters are set. ;-)

Weights are initialized.

Tensors are defined to hold input and output data.

```
learn_rate = 0.1
b_size = 100                    # batch size
n_epochs = 100                  # no. of epochs
ncases=Xtrain.shape[0]          #no. of records
n_bats = int(np.ceil(ncases/b_size))  # no. of batches

# Inputs, nodes in hidden layers, classes in the output

n_hid_1 = 4 # 1st layer number of neurons
n_hid_2 = 4 # 2nd layer number of neurons
num_inp = 6 # selected campaign predictors
num_class = 2 # y values, 0 or 1


# tf placeholders for input data

X = tf.placeholder("float32", shape=(None, num_inp),name="X")
y = tf.placeholder("int32", shape=(None),name="y")

# Layer weights & biases

weights = {
    'h1': tf.Variable(tf.random_normal([num_inp, n_hid_1])),
    'h2': tf.Variable(tf.random_normal([n_hid_1, n_hid_2])),
    'out': tf.Variable(tf.random_normal([n_hid_2, num_class]))
     }
biases = {
    'b1': tf.Variable(tf.random_normal([n_hid_1])),
    'b2': tf.Variable(tf.random_normal([n_hid_2])),
    'out': tf.Variable(tf.random_normal([num_class]))
     }
```

NN: network, loss,optimizer, accuracy

Operations between layers and activation functions are specified.

```
def neural_net(x):
    # A two hidden fully connected layers each with 4 neurons, relu activation fcns
    layer_1 = tf.nn.relu(tf.matmul(X, weights['h1']))
    # Hidden fully connected layer with 4 neurons
    layer_2 = tf.nn.relu(tf.matmul(layer_1, weights['h2']))
    # Output fully connected layer with a neuron for each class
    out_layer = tf.matmul(layer_2, weights['out'])
    return out_layer
```

Loss function, optimizer, and accuracy metrics are specified.

```
logits = neural_net(X)

loss_op = tf.reduce_mean(tf.nn.sparse_softmax_cross_entropy_with_logits(
    logits=logits, labels=y))

optimizer = tf.train.AdamOptimizer(learning_rate=learn_rate)
train_op = optimizer.minimize(loss_op)

correct_pred=tf.nn.in_top_k(logits,y,1)
accuracy = tf.reduce_mean(tf.cast(correct_pred, tf.float32))
```

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Running in Tensorflow Session

A Tensorflow “session” is defined and executed. All variables initialized globally beforehand.

```
with tf.Session() as sess:
    init.run()
    print('epoch ',end='')
    for epoch in range(n_epochs):

        for b_ndx in range(n_bats):
            X_batch, y_batch=get_batch(epoch,ncases, b_ndx, b_size)
            sess.run(train_op, feed_dict={X: X_batch, y: y_batch})
        if epoch % 20 == 0:
            print(epoch, end=', ')

    print('done!\n')
    accTrain=accuracy.eval(feed_dict={X: Xtrain, y: yTrain})
    print('\ntraining data accuracy {:5.3f}'.format(accTrain))
    trainProbs=tf.nn.softmax(logits).eval(feed_dict={X: Xtrain, y: yTrain})
    print('training data auc {:5.3f}'.format(roc_auc_score(yTrain,trainProbs[:,1])))

    accTest=accuracy.eval(feed_dict={X: Xtest, y: yTest})
    print('test data accuracy {:5.3f}'.format(accTest))
    testProbs=tf.nn.softmax(logits).eval(feed_dict={X: Xtrain, y: yTrain})
    print('test data auc {:5.3f}'.format(roc_auc_score(yTrain,testProbs[:,1])))
```

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