Day 6: Neural Networks

Summer STEM: Machine Learning

Nikola Janjušević, Akshaj Kumar Veldanda, Jacky Yuan, Tejaishwarya Gagadam

Department of Electrical and Computer Engineering
NYU Tandon School of Engineering
Brooklyn, New York

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Outline

Regression or Classification?

- **Problem 1:** Categorizing credit card applications into those who have good credit, bad credit and those who fall in the gray area.

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  - Target Variable: Predicting the amount of energy needed in the future

Machine Learning Problem Pipeline

1. Gather data
2. Visualize the data
3. Formulate ML problem
   - Regression vs Classification
   - Choose an appropriate cost function
4. Design the model and train to find the optimal parameters of the model
   - Prepare a design matrix
   - Perform feature engineering
   - Validate your choice of hyper-parameters using a cross-validation set
5. Evaluate the model on a test set
   - If the performance is not satisfactory, go back to step 4

Data

- Always save your data file as an .csv file
  - It is easy to edit in both excel and text file
  - Easy to load the data using Pandas
- Visualize the data
  - To get an rough estimate of how your machine learning model should be
  - Do you have sufficient training and testing data
- Always plot the data before pre-processing

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Supervised Learning

Type	Linear Regression	Logistic Regression
Use	Modeling Continuous Data	Classification
Features	Any Numerical Data, $\mathbf{x} = [x_1, x_2, ..., x_M]^T$	
Targets	Any Numerical Data, $\mathbf{y}$	Class Labels, $\mathbf{y}$
Model	$\hat{\mathbf{y}} = \mathbf{Wx} + \mathbf{b}$	$\hat{\mathbf{y}} = \sigma(\mathbf{Wx} + \mathbf{b})$
Loss Function	Error between $\mathbf{y}$ and $\hat{\mathbf{y}}$	Cross-Entropy

Optimization

- Use loss/error/cost function to find best model-parameters

Problem	Loss Function	Formula
Regression	Squared/L2 Loss	$\sum_i (\mathbf{y}_i - \hat{\mathbf{y}}_i)^2$
Binary Classification	Binary Cross-Entropy	$-\sum_i (y_i \ln(\hat{y}_i) + (1 - y_i)\ln(1 - \hat{y}_i))$
Multi-Class Classification	Cross-Entropy	$-\sum_i \sum_k (y_{ik} \ln(\hat{y}_{ik}))$

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- Non-linear opt. can use arbitrary Loss function

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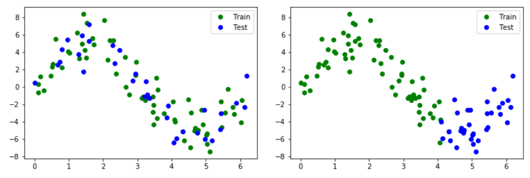
  - Classification Accuracy: $\frac{1}{N}\sum_i(\mathbf{y}_i == \hat{\mathbf{y}}_i)$

Train, Validation, and Test Sets

- Always split your data into train and test sets to see how well it does against new data
- Train set: set of data to be used for training
  - e.g. model.fit(x_train,y_train)
- Test set: After training is done, evaluate how well it does against unseen data using test set
- Validation set: If tuning hyper-paramters, perform one more split to get a validation set. Use validation set to tune parameters

Train and Test Sets (Dealing with Time Series)

- Train and test split is usually done by taking samples at random from the entire data set
- But when using time series to predict future, it is better to select test set to be a continuous chunk at the end of the time series
- Because we want to see how well the model does in predicting the future



Regularization

- Prevent over-fitting by adding a term to loss function
- $\mathit{Loss\ Function} = \mathit{Target\ loss\ function} + \lambda\, \mathit{Regularization}$
- λ hyper-parameter determine how much to emphasize on regularizing
- Large weights usually lead to over-fitting
- Weight-based regularization is most commonly used
  - L2 (Ridge) Regularization: $\sum_{j=1}^{D} |w_j|^2$
  - L1 (Lasso) Regularization: $\sum_{j=1}^{D} |w_j|$
- First over-estimate the model order you need, then use regularization to prevent over-fitting

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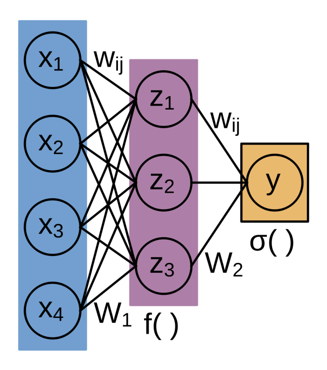

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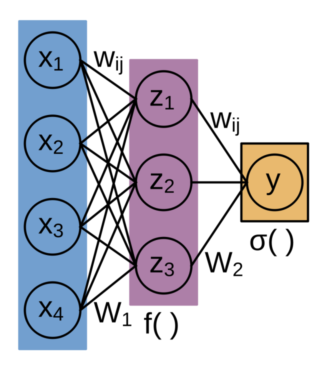

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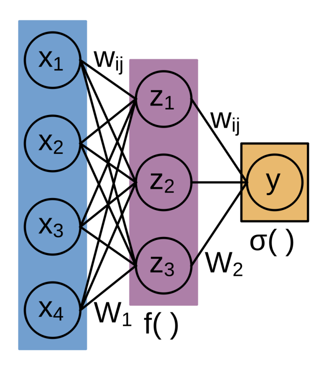

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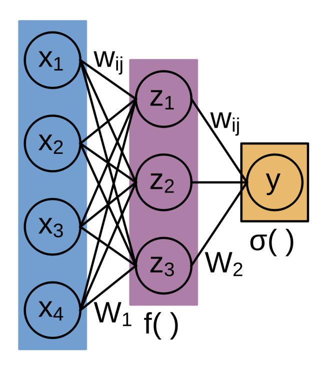

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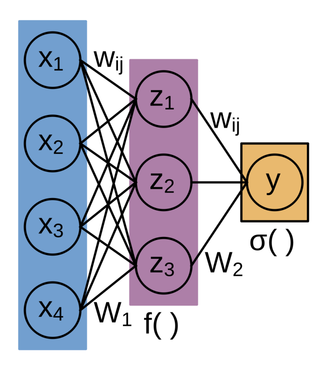
- But why stop here?...



Mathematical Model: Multi-Layer Perceptron

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$$\hat{\mathbf{y}} = f_{out}(W_{out}\mathbf{z}_L + b_{out})$$

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- Model:

$$\hat{\mathbf{y}} = f_{out}(W_{out}\mathbf{z}_L + b_{out})$$

  - Where, $z_l = f_l(W_l\mathbf{z}_{l-1} + b_l)$ for $1 \leq l \leq L$, $z_0 := \mathbf{x}$, and L is the number of hidden layers

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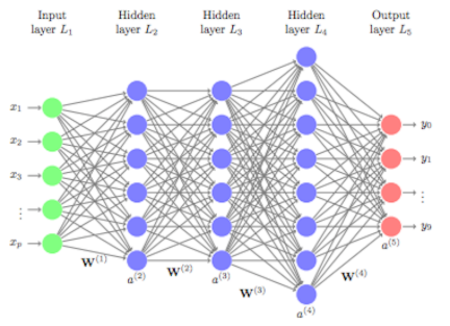

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  - easy to compute, performs well in practice

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- This can be overwhelming...

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  - for all hidden layers

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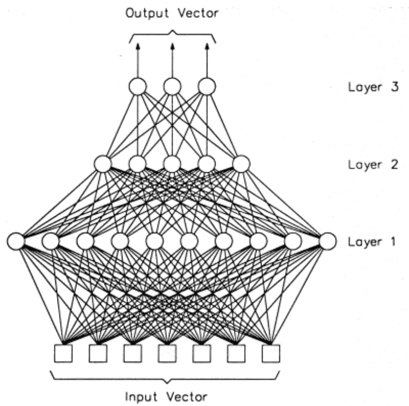

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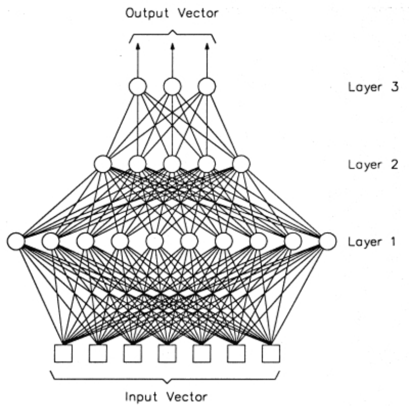

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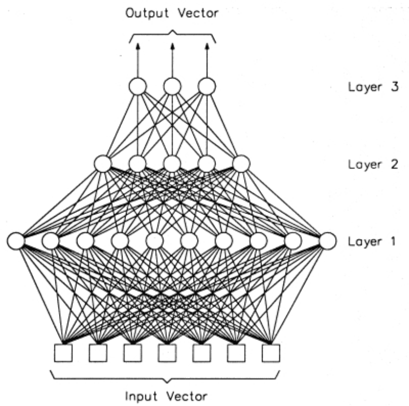
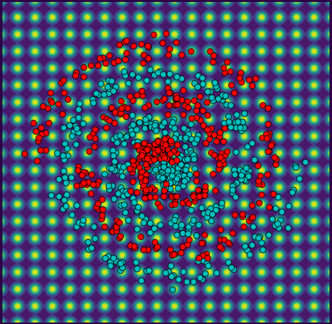
  - Expand, combine & reduce



Toy Example: Spiral Classification

Human Engineered
Feature Transformations:



NN Engineered
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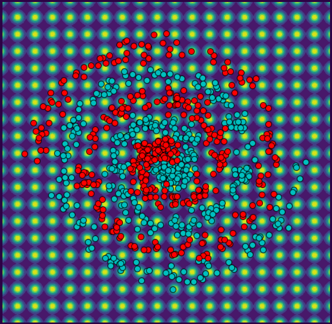

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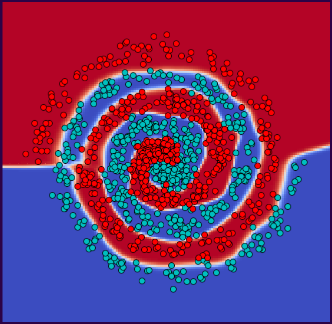


Advantages and Disadvantages

Advantages	Disadvantages
■ Further removed need for domain knowledge ■ Infinitely expressive	■ Less control over behavior of model ■ Computationally expensive (kind of...)

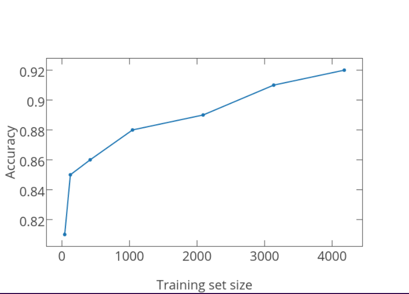
Biological Justification

- Example: Steps for Processing Vision
  1. Eyes gather light
  2. Light intensities converted to shapes
  3. Shapes recognized as objects
  4. Objects associated with ideas
  5. Idea recognized as Akshaj

Outline

Large Scale Machine Learning

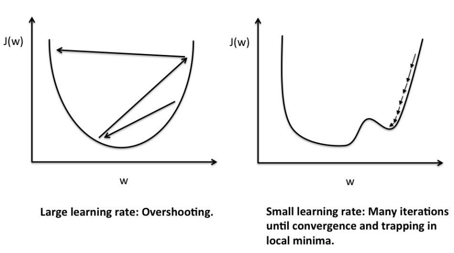
- Learning with large data sets
- Algorithms today perform so much better than five years ago due to shear amount of data availability
- "It's not who has the best algorithm that wins. It's who has the most data"
  - So we want to learn from large data sets

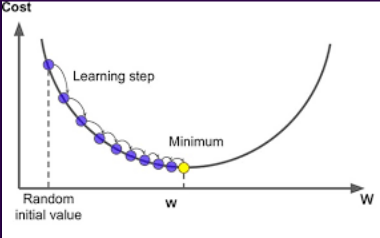


Learning with Large Data Sets

- Challenges:
  - Computationally very expensive to compute gradients
  - And each gradient computation performs only one step of update
- In large scale machine learning, we want to come up with computationally reasonable ways to deal with large data sets
  - Batch Gradient Descent
  - Stochastic Gradient Descent
  - Mini-batch Gradient Descent

Digression: Revisiting Learning Rate





Correct learning rate

Batch Gradient Descent

- **Batch Gradient Descent** takes all the examples in the training data to compute one step of gradient descent update
- Algorithm: Consider linear regression (N = 100,000,000)
  - $\hat{y} = \sum_{i=0}^{N} w_i x_i$
  - $Cost, J = \frac{1}{N} \sum_{i=0}^{N} (y_i - \hat{y}_i)^2$
  - Gradient Descent Update $w_{new} = w_{old} - \alpha \frac{dJ}{dw}$

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Stochastic Gradient Descent

- **SGD** takes only one example in the training example to perform one step of gradient descent
  - The algorithm modifies the parameters a little bit to fit just the first example (x_1, y_1)
  - Then again modify the parameters to fit the second training example (x_2, y_2) and so on...
- Algorithm (Let N be the total number of training examples):

  Repeat{

  for $i = 1, 2 ... N${

  $Cost, J = (y_i - \hat{y}_i)^2$

  Gradient Descent Update $w_{new} = w_{old} - \alpha \frac{dJ}{dw}$

  }

  }

Batch Gradient Descent

- **Batch Gradient Descent** uses 'b' training examples to perform one update step
  - 'b' is called batch size
  - Number of iterations = $\frac{N}{b}$
- Algorithm:

$Repeat\{$

$j = 0$

for i in range(iterations){

$Cost, J = \frac{1}{b}\sum_{j=1}^{i+b}(y_j - \hat{y}_j)^2$

Gradient Descent Update $w_{new} = w_{old} - \alpha\frac{dJ}{dw}$

$j = j + b$

}

}

Outline

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1 Review of Week 1

2 Neural Network Model

3 Training with Neural Networks

4 Introduction to Keras

5 Neural Network Lab

6 (Optional) Lab: Cat vs. Non-Cat

Thank You!

- Next Class: Convolutional Neural Networks