Companion to Machine Learning

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Contents

Sources

Throughout this compendium, each piece of information will be formatted as such.

Name / Description of fact Source

Information about fact.

The location which currently contains "Source" could potentially be filled with a variety of sources. Here is how to find the source based off the shortened form.

- **Hands-On Machine Learning** refers to Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow, 2nd Edition by Aurélien Géron

0 Notation

0.1 Data

$\boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ ... \\ x_M \end{pmatrix}$: data point corresponding to a column vector of M features

$\overline{\boldsymbol{x}} = \begin{pmatrix} 1 \\ x_1 \\ x_2 \\ ... \\ x_M \end{pmatrix}$: concatenation of 1 with the vector$\boldsymbol{x}$

$\boldsymbol{X} = \begin{pmatrix} x_{1,1} & ... & x_{1,N} \\ ... & ... & ... \\ x_{M,1} & ... & x_{M,N} \end{pmatrix}$: dataset consisting of N data points and M features

$\overline{\boldsymbol{X}} = \begin{pmatrix} 1 & ... & 1 \\ x_{1,1} & ... & x_{1,N} \\ ... & ... & ... \\ x_{M,1} & ... & x_{M,N} \end{pmatrix}$: concatenation of a vector of 1's with the matrix $\boldsymbol{X}$

$y =$: output target (regression) or label (classification)

$\boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ ... \\ y_N \end{pmatrix}$: vector of outputs for a dataset of N points

$\boldsymbol{x}_* =$: test input / unknown input

$\boldsymbol{y}_* =$: predicted output

$N =$: Number of data points in the dataset

$M =$: Number of a features in a data point

$\boldsymbol{w} = \begin{pmatrix} w_1 \\ w_2 \\ ... \\ w_M \end{pmatrix}$

$\boldsymbol{w}^T = (w_1, w_2, ..., w_M)$ or $(w_0, w_1, w_2, ..., w_M)$ w_0 multiplies the first entry of $\overline{\boldsymbol{x}}$ (bias)

Note: bold symbols represents a vector

1 Introduction

1.1 What is Machine Learning

Machine Learning is the field of study that gives computers the ability to learn from data without being explicitly programmed. This is good for problems that require a lot of fine-tuning or for which using a traditional approach yields no good solution. Machine Learning's data dependency allows it to adapt to new data and gain insight for complex problems and large amounts of data.

1.2 Applications of Machine Learning

Machine Learning can be used for a range of tasks and can be seen used in:

- Analyzing images of products on a production line to automatically classify them (Convolutional Neural Net)
- Forecasting company revenue based on performance metrics (Regression or Neural Net)
- Automatically classifying news articles (NLP using Recurrent Neural Networks)
- Summarizing long documents automatically (Natural Language Processing)
- Building intelligent bot for a game (Reinforcement Learning)

1.3 Types of Machine Learning

1.3.1 Supervised Learning

In supervised learning, the training set you feed to the algorithm includes the desired solutions, called labels. (e.g determining if an email is spam would be trained a dataset of example emails labelled as spam or not spam.)

Some commonly used supervised learning algorithms are:

- k-Nearest Neighbors
- Linear Regression
- Logistic Regression
- Support Vector Machines (SVMs)
- Decision Trees and Random Forests
- Neural Networks

1.3.2 Unsupervised Learning

In unsupervised learning, the training data is unlabeled and the system tries to learn without guidance. The system will try and automatically draw inferences and conclusions about the

data and group it as such. (e.g. having a lot of data about blog visitors. Using a clustering algorithm we can group and detect similar visitors).

Some important unsupervised learning algorithms are:

- Clustering
  - K-Means
  - DBSCAN
  - Hierarchical Cluster Analysis
- Anomaly detection and novelty detection
  - One-class SVM
  - Isolation Forest
- Visualization and dimensionality reduction
  - Principal Component Analysis (PCA)
  - Kernel PCA
  - Locally Linear Embedding (LLE)
  - t-Distributed Stochastic Neighbor Embedding (t-SNE)
- Association rule learning
  - Apriori
  - Eclat

1.3.3 Semisupervised Learning

Labelling can be very time-consuming and costly, often there will be plenty of unlabelled and a few labelled instances. Algorithms that deal with data that is partially labeled is called semi-supervised learning. A good example of this is Google Photos. Google clusters and groups your photos based on facial recognition (unsupervised) and then you can label one photo and it will be able to label every picture like that (supervised). Most semi-supervised learning algorithms are combinations of unsupervised and supervised algorithms.

1.3.4 Reinforcement Learning

Reinforcement Learning is a learning algorithm based on a reward system. The learning system, called an agent, can observe the environment, select and perform actions, and get rewards in return (or penalties in the form of negative rewards). It will then learn by itself what the best strategy, called a policy, to get the most reward over time. A policy defines what action the agent should choose when it is in a given situation.

2 Data Analysis

2.1 Limitations of Data

2.1.1 Nonrepresentative Training Data

One thing to look out for when using training data is whether the data is representative of the new cases you want to generalize to. For example if you are training linear regression life satisfaction vs GDP of countries, if some countries are missing from the dataset then the dataset is not fully representative of the problem.

2.1.2 Poor Quality Data

If your data is full of errors, outliers and noise, it will make it harder for the system to detect the underlying patterns, so your system is less likely to perform well. In order to mitigate this we need to clean the training data.

- If some instances are outliers, it may help to discard them or try to fix the errors manually
- If some instances are missing features, you may decide to ignore that attribute, ignore the instance, fill in the missing values, or train one model with the feature and one without

2.1.3 Irrelevant Features

A critical part of the success of a Machine Learning project is coming up with a good set of features to train on. This process is called *feature engineering*.

- *Feature selection*: Selecting the most useful features to train on among the existing features
- *Feature extraction*: Combining existing features to produce a more useful one (dimensionality reduction algorithms can help)
- *Ad hoc Features*: Creating new features by gathering new data.

2.2 Feature Engineering

2.2.1 Feature Construction

Features can be modified for various reasons, including to increase predictor performance and to reduce time or memory requirements. Below are common techniques for constructing features.

2.2.1.1 Transformation

Common feature transformations include:

- **Centering** each feature to be around the origin.
- **Scaling** each feature to be of the same scale. For example, scaling can be done to make sure each feature has the same variance or the same maximum absolute value.
- **Logarithmically** transforming each feature to reduce the skewness of feature distributions.

Note that feature transformation runs the risk of discarding useful information. For example, scaling to make each feature have the same variance should not be done if the differing variances of the features are actually relevant to the problem.

2.2.1.2 Feature Extraction

Feature expansion involves combining multiple features into new features when first order interactions are not good enough. For example, given features x_1 and x_2, $x_1 \cdot x_2$ is a new feature (i.e. meta-feature) formed by an expansion of x_1 and x_2.

2.2.1.3 "Ad hoc" Features

Constructing ad hoc features involves applying domain knowledge to introduce custom features.

2.2.2 Feature Selection

Irrelevant features are features that are uncorrelated with a prediction task. Redundant features are features that are highly correlated with one another, so using multiple redundant features does not help with predictions much more than using a single such feature.

Different learning algorithms have differing levels of robustness to irrelevant or redundant features. For example, decision trees are robust to redundant features, since such features have low information gain, while KNN is not, since the set of redundant features will behave as one heavily weighted feature. When possible, these feature should not be selected in the first place. Below are common ways to avoid selecting such features.

2.2.2.1 Wrapper Methods

Wrapper methods involve building a model for feature subsets, and then selecting the best performing model. A "forward search" approach starts with no features and then adds the feature that best improves the model until a certain number of features are selected. A "backward" search approach starts with all features and removes the feature that improves the model the least until a certain number of features have been removed.

Computing all possible feature subsets would guarantee finding the optimal one. However, a problem with M features has 2^M possible feature subsets, so finding all possible subsets is infeasible for large values of M. The forward and backward search approaches approximate this but with a time complexity of $O(M^2)$.

2.2.2.2 Filter Methods

Filter methods, also known as variable ranking, involve assigning each feature a score measuring how informative it is in predictions. This score is determined by some "scoring function" S. Features are then ranked by score, and a number of top features are selected.

2.2.2.3 Embedded Methods

Embedded methods involve modifying the cost function to constrain the choice of model. A common example of this is regularization, which can be used to penalize complex models and encourage a sparse feature set.

2.3 Overfitting

Overfitting is when the model performs well on the training data, but does not generalize well. Complex models can detect subtle patterns in the data, but if the training set is noise, or if it is too small, then the model will likely detect patterns in the noise itself. These patterns will not generalize to new instances. Overfitting often happens when the training data has many features, which allows for an approximation of the target function with many degrees of freedom. We can use regularization to constrain a model to make it simpler to reduce the risk of overfitting.

2.4 Underfitting

Underfitting is the opposite of overfitting: it occurs when the model is too simple to learn the underlying structure of the data. Methods of fixing the problem include:

- Select a more powerful model, with more parameters.
- Feed better features to the learning algorithm
- Reduce the constraints on the model (e.g., reduce the regularization hyperparameter)

2.5 Bias Variance Decomposition

Many machine learning algorithms are based on building a formal model based on the training data (e.g. a decision tree). Models have parameters, which are characteristics that can help in classification (e.g. a node in a decision tree). Models may also have hyper-parameters, which in turn control other parameters in a model (e.g. max height of decision tree).

Generalization errors result from a combination of noise, variance, and bias. Bias concerns how well the type of model fits the data. Models with high bias pay little attention to training data and suffer from underfitting, while models with low bias may pay too much attention to training data and become overfitted. Bias and variance tend to be at odds with one another (high bias typically leads to low variance, and vice versa).

3 Evaluation of Learning

3.1 Performance Formulation

Let y_* be an output generated by a function f approximating some target function. Let y be the corresponding output of the target function. A loss function $l(y, y_*)$ can be used to measure the accuracy of the approximation function f. Some common loss functions include:

- Squared Loss: $l(y, y_*) = (y - y_*)^2$
- Absolute Loss: $l(y, y_*) = |y - y_*|$
- Zero/One Loss: $l(y, y_*) = 1_{y \neq y_*}$

We assume that the data coming from our target function comes from some probability distribution D, and that our training data is a random sample of (x, y) pairs from D. A Bayes Optimal Classifier is a classifier that for any input x, returns the y most likely to be generated by D.

Based on the available training data, the goal of supervised learning is to find a mapping f from x to y such that generalization error $\sum_{(x,y)} D(x, y) l(y, f(x))$ is minimized. However, since D is unknown, we instead estimate the error from the average error in our training or test data, which is $\frac{1}{N} \sum_{n=1}^{N} l(y_n, f(x_n))$.

3.2 Testing and Validation

Models are initially built based on a training dataset. Test sets (also known as holdout sets) are then used to estimate the generalization error. Validation sets are also used to measure the model's performance, but unlike test sets, validation sets can make changes to the model's parameters.

3.2.1 Cross Validation

Cross validation is a technique for measuring how well a model generalizes. The idea behind it is to break up a training data set into K equally sized partitions, and use $K - 1$ of the partitions as training data and the remaining partition for testing. This should be repeated K times, so that all points of data are at some point used for testing. Higher values of K lower the amount of variance of in the error estimation. To avoid training and testing data having a different probability distribution, the data should be shuffled before being split.

3.2.2 Bootstrapping

Bootstrapping is an alternative to cross validation where instead of dividing a training data set into partitions, a random sample of points (with possible duplicates) is used as training data. The remaining points are then used as testing data, with the goal being similar to that of cross validation.

3.3 Performance Evaluation of Classifiers

Consider the following terminology for classification problems:

- True positive (TP) - Examples of class 1 predicted as class 1
- False positive (FP) - Examples of class 0 predicted as class 1 (Type 1 Error)
- True negative (TN) - Examples of class 0 predicted as class 0
- False negative (FN) - Examples of class 1 predicted as class 0 (Type 2 Error)

3.3.1 Accuracy and Error

The following formulas can be used to measure accuracy and error:

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$$

$$ErrorRate = \frac{FP + FN}{TP + TN + FP + FN}$$

3.3.2 Precision and Recall

Precision and recall can be measured as follows:

$$P = \frac{TP}{TP + FP}$$

$$R = \frac{TP}{TP + FN}$$

Precision measures the ratio of positive predictions that were correct, while recall measures the ratio of total positive instances that were predicted. Similarly to how variance and bias are often at odds with one another, so are precision and recall.

3.3.3 F-Measure

An F-measure (also known as a F1 score) measures a model's accuracy by taking into account both precision and recall as follows:

$$F = \frac{2PR}{P + R}$$

To adjust the relative importance of precision vs recall, a weighted F-measure can be used, which is defined as follows:

$$F = \frac{(1 + \beta^2)PR}{\beta^2 P + R}$$

In a standard F-measure, $\beta = 1$, $\beta < 1$ means that precision is valued over recall, while $\beta > 1$ means recall is valued over precision.

3.3.4 Sensitivity and Specificity

Sensitivity is the same measure as recall. Specificity is a measure of how well a classifier avoids false positives, and is measured as:

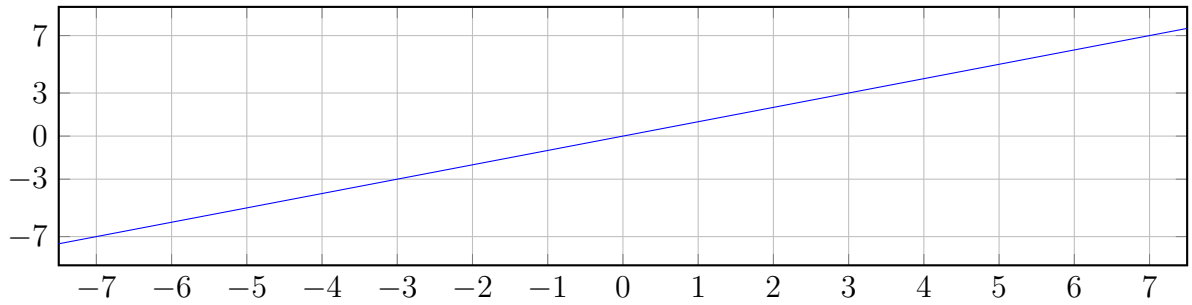
$$Specificity = \frac{TN}{TN + FP}$$

4 Activation Functions

4.1 Linear/Identity

The *linear function* is an activation function where the output is proportional to the input and the *identity function* is a subset of the linear function where $a = 1$.

$$h(x) = ax$$

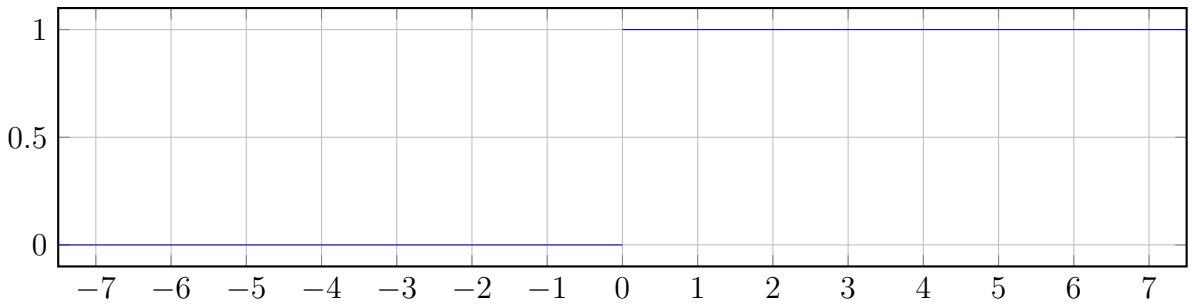


The linear function gives a range of activations so it is not a binary activation. The derivative is constant so the gradient has no relationship with $\boldsymbol{X}$ and therefore backpropagation and gradient descent would not work with this activation function.

4.2 Threshold

The *threshold function* denoted $heaviside(\cdot)$ outputs a number 0 or 1 based on its input z. It is defined as a piecewise function

$$heaviside(z) = \begin{cases} 0 & \text{if } z < 0 \\ 1 & \text{if } z \geq 0 \end{cases}$$

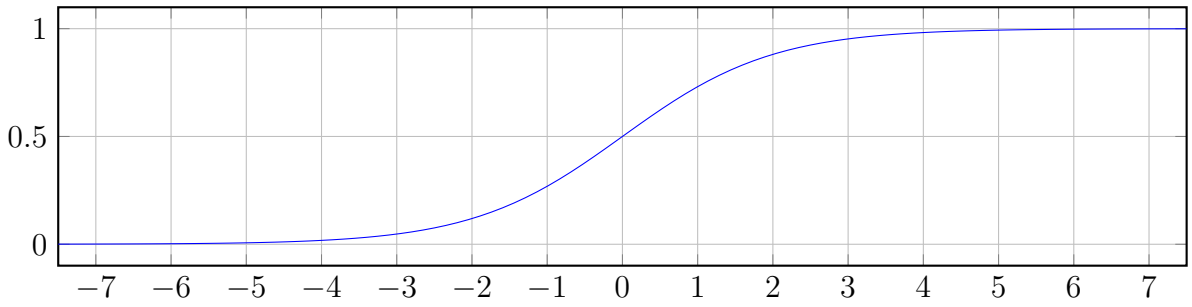


The key property of the threshold function is that it will predict 1 when z, which will generally be our prediction $\boldsymbol{w}^T\boldsymbol{x}$, is greater than 0 else it will predict 0.

4.3 Sigmoid Function

The *sigmoid function* denoted $\sigma(\cdot)$ outputs a number between 0 and 1. It is defined as

$$\sigma(t) = \frac{1}{1 + exp(-t)}$$

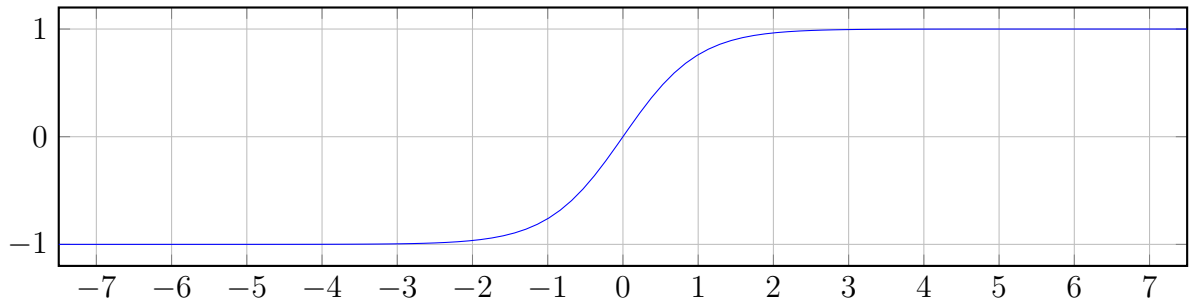


The key property of the sigmoid function is that $\sigma(t) < 0.5$ when $t < 0$, and $\sigma(t) \geq 0.5$ when $t \geq 0$, so a sigmoid function is useful for classification since it can predict 1 when $\boldsymbol{w}^T\boldsymbol{x}$ is positive and 0 if it is negative.

4.4 Tanh

The *tanh function* denoted $tanh(\cdot)$ outputs a number between -1 and 1. It is zero-centered function making it easier to model inputs that have strongly negative, neutral, and strongly positive values, otherwise it is similar to the sigmoid function.

$$h(a) = tanh(a) = \frac{e^a - e^{-a}}{e^a + e^{-a}}$$



The gradient is stronger for tanh than sigmoid, however, tanh also has the vanishing gradient problem.

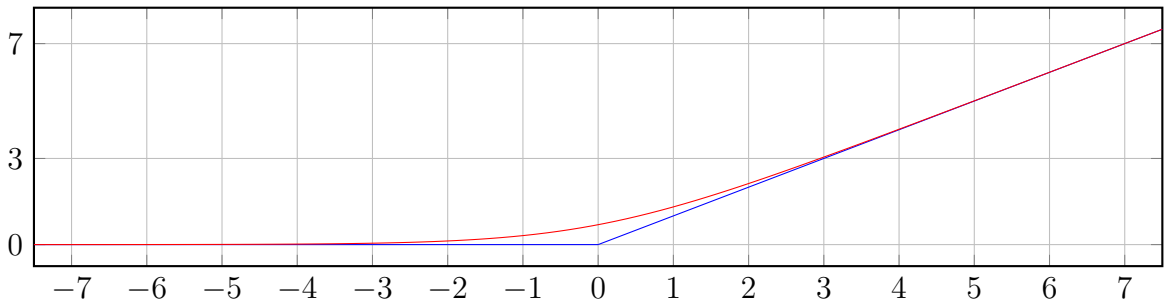
4.5 Rectified Linear Units

The *reLU function* plotted in blue is defined as

$$h(a) = max(0, a)$$

and the soft version ("Softplus") plotted in red is defined as

$$h(a) = log(1 + e^a)$$



The benefit of using the reLU activation function is that the gradient is 0 or 1 so it helps mitigate the vanishing problem for deep neural networks. The softplus function does not prevent gradient vanishing.

4.5.1 Maxout Units

Generalization of rectified linear units where we can have several linear parts and having them be whatever we want rather than having a 0 part. They can be thought of as the aggregation of a hidden layer of identity units with a max unit.

$$max\{\sum_i w_i^{(1)x_i, \sum_i w_i^{(2)}} x_i, \sum_i w_i^{(3)} x_i, ...\}$$

5 Convex Optimization

In machine learning we can often turn problems into convex functions and simplify the problem into finding the global minima of the function, which in essence is minimizing the training error. One of the key theorem's of a convex function is that the local minimum of a convex function is also a global minimum. Therefore we can apply many methods to find parameters that satisfy the global minima.

5.1 Normal Solution

To find the value of our parameter (generally $\boldsymbol{w}$) that minimizes the cost function, there is a closed-form solution. We can express this closed form solution for any convex loss function as follows.

$$\frac{\partial J(\boldsymbol{w})}{\partial \boldsymbol{w}} = 0$$

The limitations of using the Normal Solution is that we usually have to compute the inverse of $\boldsymbol{X}^T\boldsymbol{X}$ which is a $(M+1) \times (M+1)$ matrix (where M is the number of features). The computational complexity of inverting such a matrix is typically about $O(M^{2.4})$ to $O(M^3)$, depending on the implementation. Some of the other approaches below are better suited for cases where there are a large number of features or too many training instances to fit in memory.

5.2 Gradient Descent

Gradient Descent is a generic optimization algorithm capable of finding optimal solution to a wide range of problems. The general ida is to tweak parameters iteratively in order to minimize a cost function. The main concept utilized in gradient descent is to measure the local gradient of the error with regard to the parameter vector and move in the direction of the descending gradient. Once the gradient is zero, you have reached the minimum.

You start with filling your parameter $\boldsymbol{w}$ with random values (random initialization. Then you improve it gradually, taking small steps at a time, each step attempting to decrease the cost function, until the algorithm converges to a minimum. One important parameter of Gradient Descent is the size of the steps, determined by the *learning rate* hyperparameter. If the learning rate is too small, then the algorithm will have to go through many iterations to converge, if the learning rate is too high, you might jump across the minimum possibly, higher than you were before and potentially make the algorithm diverge. One gradient descent technique is having a learning rate that changes as you approach the minimum to prevent overshoot, also called the learning schedule.

A limitation of Gradient Descent is when the cost function we are dealing with is not a convex function. In this case holes, ridges, irregular terrain will make the convergence to the minimum difficult.

5.2.1 Batch Gradient Descent

To implement Gradient Descent, you need to compute the gradient of the cost function with regard to each model parameter w_j - how much the cost function will change if you change w_j a little bit. This is equivalent to the partial derivative of the cost function with regard to the parameter w_j. For the entire parameter vector $\boldsymbol{w}$ we can denoted the gradient vector as $\nabla_{\boldsymbol{w}} J(\boldsymbol{w})$.

Once we have the gradient vector, which points uphill, we descend in the opposite direction (subtract $\nabla_{\boldsymbol{w}} J(\boldsymbol{w})$ from $\boldsymbol{w}$). This is where we use our learning rate α to determine the size of the downhill step.

$$\boldsymbol{w}^{(nextstep)} = \boldsymbol{w} - \alpha \nabla_{\boldsymbol{w}} J(\boldsymbol{w})$$

The limitation of Batch Gradient Descent is the fact that it uses the whole training set to compute the gradients at every step, which makes it very slow when the training set is large.

5.2.2 Stochastic Gradient Descent

Stochastic Gradient Descent picks a random instance in the training set at every step and computes the gradients based on only that single instance. This makes the algorithm much faster and also makes it possible to train on huge training sets. However, due to its stochastic nature, this algorithm will bounce up and down, decreasing only on average. Over time it will end up very close to the minimum, but once it gets there it will continue to bounce around, never settling down. Therefore, once the algorithm stops, the final parameter values are good, but not optimal.

This can actually help when the cost function is very irregular (not convex) as it can help the algorithm jump out of a local minima. One solution to the problem of being unable to settle at the minimum is gradually reducing the learning rate. The steps start out large (helps make quick progress and escape local minima), then get smaller and smaller, allowing the algorithm to settle at the global minima. The function that determines the learning rate is called the *learning schedule*.

5.2.3 Mini-batch Gradient Descent

Mini-batch GD is a combination of Batch GD and Stochastic GD. At each step, instead of computing the gradients based on the full training set or based on just one instance, Mini-batch GD computes the gradient on small random sets of instances called *mini-batches*. The main advantage of this over Stochastic GD is that you get a performance boost from hardware optimization of matrix operations. Mini-batch will perform better to get closer to the minimum than Stochastic GD but it may be harder for it to escape local minima.

5.3 Gradient Descent Optimization

When training neural networks there can be issues involving slow convergence, dimensionality and magnitude. So other methods were introduced to be able to quickly train neural networks with accuracy for large amounts of data.

5.3.1 Adaptive Gradients

Adagrad is an algorithm for gradient-based optimization that adapts to the learning rate to the parameters, performing smaller updates for parameters associated with frequently occurring features and larger updates for parameters associated with infrequent features. It is well suited for dealing with sparse features.

$$r_t \leftarrow r_{t-1} + (\frac{\partial E_n}{\partial w_{ji}})^2$$

$$w_{ji} \leftarrow w_{ji} - \frac{\alpha}{\sqrt{r_t}} \frac{\partial E_n}{\partial w_{ji}}$$

The problem is that the learning rate $\frac{\alpha}{\sqrt{r_t}}$ decays too quickly.

5.3.2 RMS Prop

To combat the problem with AdaGrad we can instead divide by the root mean square of partial derivatives.

$$r_t \leftarrow \beta r_{t-1} + (1-\beta)(\frac{\partial E_n}{\partial w_{ji}})^2 \quad \text{where } 0 \leq \beta \leq 1$$

$$w_{ji} \leftarrow w_{ji} - \frac{\alpha}{\sqrt{r_t}} \frac{\partial E_n}{\partial w_{ji}}$$

The problem now is that the gradient lacks momentum.

5.3.3 Adaptive Moment Estimate

Now to induce momentum, Adam replaces the gradient by the moving average.

$$r_t \leftarrow \beta r_{t-1} + (1-\beta)(\frac{\partial E_n}{\partial w_{ji}})^2 \quad \text{where } 0 \leq \beta \leq 1$$

$$s_t \leftarrow \gamma s_{t-1} + (1-\gamma)(\frac{\partial E_n}{\partial w_{ji}}) \quad \text{where } 0 \leq \gamma \leq 1$$

$$w_{ji} \leftarrow w_{ji} - \frac{\alpha}{\sqrt{r_t}} s_t$$

6 Instance-Based Learning

6.1 Parametric vs Non-Parametric Methods

Datasets can be represented as a set of points in a high-dimensional space; a data point with n features $x_1, x_2, ..., x_n$ can be represented with the feature vector $(x_1, x_2, ..., x_n)$ in n-dimensional space. Parametric methods of supervised learning attempt to model the data using these features, while non-parametric (also known as instance-based) methods do not.

6.1.1 Approximation

Parametric methods use parameters to create global approximations. Non-parametric methods instead create approximations based on local data.

6.1.2 Efficiency

Parametric methods do most of their computation beforehand, and the summarize their results in a set of parameters. Non-parametric methods tend to have a shorter training time but a longer query answering time.

6.2 K-Nearest Neighbors

K-nearest neighbors (KNN) is a common non-parametric method. The idea is to predict the value of a new point based on the values of the K most similar (i.e. closest) points.

6.2.1 Implementation

A common implementation of KNN involves looping through all N points in a training set and computing their distance to some point x. Then the K nearest points are selected. This process can be sped up by storing the data points in a data structure that helps facilitate distance-based search (e.g. a k-d tree).

6.2.2 Distance Function

"Nearby" means of minimal distance, which is commonly defined by Euclidean distance. Other distance functions $d(x, x')$ can be used, though must meet the following conditions:

- $d(x, x') = d(x', x)$ (i.e. symmetric)
- $d(x, x) = 0$ (i.e. definite)
- $d(a, c) \leq d(a, b) + d(b, c)$ (i.e. triangle inequality holds)

6.2.3 Decision Boundaries

Decision boundaries define the borders of a single classification of input. These boundaries are formed of sections of straight lines that are equidistant to two points of different classes. A highly jagged line is an indicator of overfitting, while a simple line is an indicator of underfitting.

6.2.4 Selection of K

The selection of the value of K is a bias-variance tradeoff. Low values of K have high variance but low bias, while high values of K have low variance but high bias. High-values of K result in smoother decision boundaries, which can be a sign of underfitting, and vice versa.

K can be selected experimentally by evaluating the performance for different values of K through cross-validation or against a testing set. In theory, as the number of training examples approaches infinity, the error rate of a 1NN classifier is at worst twice that of the Bayes Optimal Classifier.

6.2.5 Pre-Processing

Some common forms of pre-processing for KNN include:

- Removing undesirable inputs. Common removal methods are:
  - Editing methods, which involve eliminating noisy points of data.

  - Condensation methods, which involve selecting a subset of data that produces the same or very similar classifications.
- Use custom weights for each feature (not all features may be equally relevant for the situation)

6.2.6 Distance-Weighted Nearest Neighbor

A common problem with KNN is that it can be sensitive to small changes in the training data. One way to mitigate with drawback is to compute a weight for each neighbor based on its distance (e.g. through a Gaussian distribution), and this weight determines how much of an influence that point's value has. This differs from standard KNN which weighs the values of the K nearest neighbors equally and ignores all other values.

6.2.7 High Dimensionality

In uniformly distributed high-dimensional spaces, distances between points tend to be roughly equal, since there are so many features that changing a few features results in only a small change in distance. However, KNN can still be applied in practice for high-dimensional spaces, since data in high-dimensional spaces tends to be concentrated around certain hubs rather than uniformly distributed.

7 Statistical Learning

Data is often incomplete, indirect, or noisy. Statistical learning lets us consider forms of uncertainty to help us build better models. If we have access to the underlying probability distribution of the data, then we can form an optimal regression or classifier. In practice we typically do not know the underlying probability distributions, so we have to estimate them from the available training data. It is generally best to choose a family of parametric distributions (e.g. Gaussian or Binomial) and then determine which parameters describe the available training data the best. This is known as a density estimate and we assume that each point of training data is independently selected from the same distribution.

7.1 Bayesian Learning

Bayes' theorem describes the probability of an event H given evidence e.

$$P(H|e) = \frac{P(e|H)P(H)}{P(e)} \tag{1}$$

$$= kP(e|H)P(H) \tag{2}$$

where:

- $P(H|e)$: Posterior probability
- $P(e|P)$: Likelihood

- $P(H)$: Prior probability
- $P(e)/k$: Normalizing constant

Bayesian Learning consists of determining the posterior probability using Bayes' theorem.

Suppose we want to make a prediction about an unknown quantity $\boldsymbol{X}$ we can consider the hypothesis space which represents all possible models h_i to predict the scenario.

$$P(\boldsymbol{X}|\boldsymbol{e}) = \sum_i P(\boldsymbol{X}|e, h_i)P(h_i|e) \tag{3}$$

$$= \sum_i P(\boldsymbol{X}|h_i)P(h_i|e) \tag{4}$$

This prediction yields the weighted combination of all the hypothesis' in the hypothesis space based on it's likelihood from the evidence. The prior $P(h_i|e)$ is yields the weight for each hypothesis and $P(\boldsymbol{X}|h_i)$ yields the likelihood of the hypothesis for the unknown quantity $\boldsymbol{X}$.

Bayesian probability is:

- Optimal: give a prior probability, no prediction is correct more often than the Bayesian prediction.
- Overfitting-free: all hypothesis are weighted and considered, eliminating overfitting.

One of the constraints of bayesian learning is that it can be intractable when the hypothesis space grows very large, often as a result of approximating a continuous hypothesis space with many discrete hypothesis. This requires us to approximate Bayesian Learning.

7.2 Approximate Bayesian Learning

7.2.1 Maximum a Posteriori

Maximum a Posteriori (MAP) makes predictions based on only the most probable hypothesis $h_{MAP} = argmax_{h_i} P(h_i|e)$. This differs from Bayesian learning, which makes predictions for all hypothesis weighted by their probability. MAP and Bayesian learning predictions tend to converge as the amount of data increases, and overfitting can be mitigated by giving complex hypothesis a low prior probability. However, finding h_{MAP} may be difficult or intractable.

7.2.2 Maximum Likelihood

Maximum Likelihood (ML) simplifies MAP by assuming uniform prior probabilities and then makes a prediction based on the most probable hypothesis h_{ML}. ML tends to be less accurate than MAP and Bayesian predictions, it is also subject to overfitting due to the prior probabilities being uniform. Finding h_{ML} is easier than finding h_{MAP} since finding h_{ML} for $P(e|h)$ is equivalent to calculating it for $argmax_h \sum_n logP(e_n|h)$.

7.3 Bayesian Linear Regression

Instead of taking the hypothesis $\boldsymbol{w}$ that maximizes the posterior, we can compute the posterior and work with that directly as follows:

$$\begin{aligned} P(\boldsymbol{w}|\boldsymbol{y},\boldsymbol{X}) &= \frac{P(\boldsymbol{y}|\boldsymbol{w},\boldsymbol{X})P(\boldsymbol{w}|\boldsymbol{X})}{P(\boldsymbol{y}|\boldsymbol{x})} \\ &= ke^{-\frac{1}{2}(\boldsymbol{w}-\overline{\boldsymbol{w}})^T\boldsymbol{A}(\boldsymbol{w}-\overline{\boldsymbol{w}})} \\ &= N(\overline{\boldsymbol{w}},\boldsymbol{A^{-1}}) \end{aligned}$$

where

$$\begin{aligned} \overline{w} &= \sigma^{-2}\boldsymbol{A^{-1}}\overline{\boldsymbol{X}}\boldsymbol{y} \\ A &= \sigma^{-2}\overline{\boldsymbol{X}}\overline{\boldsymbol{X}}^T + \boldsymbol{\Sigma^{-1}} \end{aligned}$$

7.3.1 Prediction

Let us consider an input $\boldsymbol{x_*}$ for which we want a corresponding prediction y_*.

$$\begin{aligned} P(y_*|\overline{\boldsymbol{x_*}},\overline{\boldsymbol{X}},\boldsymbol{y}) &= \int_{\boldsymbol{w}} P(y_*|\overline{\boldsymbol{x_*}},\boldsymbol{w})P(\boldsymbol{w}|\overline{\boldsymbol{X}},\boldsymbol{y})d\boldsymbol{w} \\ &= k\int_{\boldsymbol{w}} e^{-\frac{(y_*-\overline{\boldsymbol{x}}^T\boldsymbol{w})^2}{2\sigma^2}} ke^{-\frac{1}{2}(\boldsymbol{w}-\overline{\boldsymbol{w}})^T\boldsymbol{A}(\boldsymbol{w}-\overline{\boldsymbol{w}})}d\boldsymbol{w} \\ &= N(\overline{\boldsymbol{x_*}}^T\boldsymbol{A}^{-1}\overline{\boldsymbol{X}}\boldsymbol{y},\overline{\boldsymbol{x_*}}^T\boldsymbol{A}^{-1}\overline{\boldsymbol{x_*}}) \end{aligned}$$

This gives us a gaussian distribution of the solution. Generally for the prediction we take the mean of the distribution.

7.4 Noisy Linear Regression

Linear Regression data is often noisy and isn't distributed in a perfectly straight line.

$$\boldsymbol{y} = f(\overline{\boldsymbol{X}}) + \varepsilon$$

Now assuming our noise ε is a Gaussian distribution (good in practice and mathematically) then we get the likelihood distribution:

$$\begin{aligned} P(\boldsymbol{y}|\overline{\boldsymbol{X}},\boldsymbol{w},\sigma) &= N(\boldsymbol{y}|\boldsymbol{w}^T\overline{\boldsymbol{X}},\sigma^2) \\ &= \prod_{n=1}^{N}\frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{(y_n-\boldsymbol{w}^T\overline{\boldsymbol{x}}_n)^2}{2\sigma^2}} \end{aligned}$$

7.4.1 Maximum Likelihood Solution

We can apply maximum likelihood to this and find the best $\boldsymbol{w}^*$ by maximizing the likelihood of the data.

$$\begin{aligned}\boldsymbol{w}^* &= argmax_{\boldsymbol{w}} P(\boldsymbol{y}|\overline{\boldsymbol{X}}, \boldsymbol{w}, \sigma) \\ &= argmax_{\boldsymbol{w}} \prod_n e^{-\frac{(y_n - \boldsymbol{w}^T \overline{\boldsymbol{x}}_n)^2}{2\sigma^2}} \\ &= argmax_{\boldsymbol{w}} \sum_n -\frac{(y_n - \boldsymbol{w}^T \overline{\boldsymbol{x}}_n)^2}{2\sigma^2} \\ &= argmin_{\boldsymbol{w}} \sum_n (y_n - \boldsymbol{w}^T \overline{\boldsymbol{x}}_n)^2\end{aligned}$$

This leads us to least square problem derived in the Linear Regression section using the Mean Squared Error.

7.4.2 Maximum A Posteriori Solution

Alternatively we can apply MAP to our noisy linear regression problem and find $\boldsymbol{w}^*$ with the highest posterior probability (most probable hypothesis).

Gaussian Prior:

$$P(\boldsymbol{w}) = N(0, \boldsymbol{\Sigma})$$

Posterior:

$$\begin{aligned}P(\boldsymbol{w}|\boldsymbol{X}, \boldsymbol{y}) &\propto P(\boldsymbol{w}) P(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{w}) \\ &= k e^{-\frac{\boldsymbol{w}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{w}}{2}} e^{-\frac{\sum_n (y_n - \boldsymbol{w}^T \boldsymbol{x}_n)^2}{2\sigma^2}}\end{aligned}$$

We can now simplify this to an optimization problem of finding

$$\begin{aligned}\boldsymbol{w}^* &= argmax_{\boldsymbol{w}} P(\boldsymbol{w}|\overline{\boldsymbol{X}}, \boldsymbol{y}) \\ &= argmax_{\boldsymbol{w}} -\sum_n (y_n - \boldsymbol{w}^T \overline{\boldsymbol{x}}_n)^2 - \boldsymbol{w}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{w} \\ &= argmin_{\boldsymbol{w}} \sum_n (y_n - \boldsymbol{w}^T \overline{\boldsymbol{x}}_n)^2 + \boldsymbol{w}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{w}\end{aligned}$$

Let $\boldsymbol{\Sigma}^{-1} = \lambda \boldsymbol{I}$ then

$$\boldsymbol{w}^* = argmin_{\boldsymbol{w}} \sum_n (y_n - \boldsymbol{w}^T \overline{\boldsymbol{x}}_n)^2 + \lambda \|\boldsymbol{w}\|^2$$

This is the ridge regularized least square problem that reduces overfitting.

7.5 Mixture of Gaussians

Now we consider the probabilistic generative model for classification. We can compute the posterior $P(C|\boldsymbol{x})$ according to Bayes' theorem to estimate the probability of the class for a given data point. Here we are using Bayes theorem for inference rather than for Bayesian learning (estimating parameters of a model).

$$\begin{aligned} P(C|\boldsymbol{x}) &= \frac{P(\boldsymbol{x}|C)P(C)}{\sum_C P(\boldsymbol{x}|C)P(C)} \\ &= kP(\boldsymbol{x}|C)P(C) \end{aligned}$$

where:

- $P(C)$: Prior probability of class C
- $P(\boldsymbol{x}|C)$: class conditional distribution of $\boldsymbol{x}$

with the following assumptions:

- In classification the number of classes is finite, so a natural prior $P(C)$ is the multinomial $P(C = c_k) = \pi_k$
- when $\boldsymbol{x} \in \mathbb{R}$ then it is often ok to assume that $P(\boldsymbol{x}|C)$ is Gaussian.
- Assume the same covariance matrix $\boldsymbol{\Sigma}$ is used for each class.

From our assumptions we get

$$P(\boldsymbol{x}|c_k) \propto e^{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_k)^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_k)}$$

7.5.1 Binary Classification

Subbing our assumptions into Bayes theorem for binary classification and simplifying, we get the following posterior distribution for classes c_k, c_j.

$$P(c_k|\boldsymbol{x}) = \frac{1}{1 + e^{(-\boldsymbol{w}^T\boldsymbol{x}+w_0)}}$$

where:

$$\begin{aligned} \boldsymbol{w} &= \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_k - \boldsymbol{\mu}_j) \\ w_0 &= \boldsymbol{\mu}_k^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_k + \frac{1}{2}\boldsymbol{\mu}_j^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_j + log\frac{\pi_k}{\pi_j} \end{aligned}$$

We can observe that this equation is the logistic sigmoid and we can draw the class boundary/linear separator at $\sigma(\boldsymbol{w}^T\boldsymbol{x} + w_0) = 0.5$ which is equivalent to $\boldsymbol{w}_k^T\overline{\boldsymbol{x}} = 0$.

7.5.2 Multinomial Classification

Now similarly for a multi-class problem where all K classes are a gaussian distribution we get.

$$P(c_k|\boldsymbol{x}) = \frac{e^{\boldsymbol{w}_k^T \boldsymbol{x}}}{\sum_j e^{\boldsymbol{w}_j^T \boldsymbol{x}}}$$

where

$$\boldsymbol{w}_k^T = (-\frac{1}{2}\boldsymbol{\mu}_k^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_k + log(\pi_k), \boldsymbol{\mu}_k^T \boldsymbol{\Sigma}^{-1})$$

This process can be extrapolated for classes that aren't all distributed with a gaussian distribution (e.g exponential, poisson, bernoulli etc ...). We can see that this is a specific case of the softmax distribution which is a generalization of the sigmoid and is discussed in further detail in the next section.

7.5.3 Parameter Estimation

Let $\pi = P(y = C_1)$ and $1 - \pi = P(y = C_2)$ where $P(\boldsymbol{x}|C_1) = N(\boldsymbol{x}|\boldsymbol{\mu}_1, \boldsymbol{\Sigma})$ and $P(\boldsymbol{x}|C_2) = N(\boldsymbol{x}|\boldsymbol{\mu}_2, \boldsymbol{\Sigma})$. In order to actually use bayesian inference to get the classification probability of our input data, we need to learn the parameters π, $\boldsymbol{\mu}_1$, $\boldsymbol{\mu}_2$ and $\boldsymbol{\Sigma}$. We can estimate the parameters by maximum likelihood, maximum a posteriori or bayesian learning. This example will demonstrate using maximum likelihood to learn these parameters.

We can express the Likelihood of our training set as $L(\boldsymbol{X}, \boldsymbol{y}) = P(\boldsymbol{X}, \boldsymbol{y}|\pi, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\Sigma})$. We want to maximize the likelihood in order to use Bayes inference.

$$L(\boldsymbol{X}, \boldsymbol{y}) = \prod_n [\pi|\boldsymbol{\mu}_1, \boldsymbol{\Sigma}]^{y_n} [(1-\pi)|N(\boldsymbol{x}_n|\boldsymbol{\mu}_2, \boldsymbol{\Sigma})]^{1-y_n}$$

Taking the log we can turn this into an optimization problem of finding

$$argmax_{\pi, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\Sigma}} \sum_n y_n [log(\pi) - \frac{1}{2}(\boldsymbol{x}_n - \boldsymbol{\mu}_1)^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x}_n - \boldsymbol{\mu}_1)] + (1 - y_n)[log(1-\pi) - \frac{1}{2}(\boldsymbol{x}_n - \boldsymbol{\mu}_2)^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x}_n - \boldsymbol{\mu}_2)]$$

7.5.3.1 Estimate π (probability of class)

$$0 = \frac{\partial log(L(\boldsymbol{X}, \boldsymbol{y}))}{\partial \pi}$$
$$\pi = \frac{\sum_n y_n}{N}$$

7.5.3.2 Estimate $\boldsymbol{\mu}$ (mean of classes)

$$0 = \frac{\partial log(L(\boldsymbol{X}, \boldsymbol{y}))}{\partial \boldsymbol{\mu}_1}$$
$$\boldsymbol{\mu}_1 = \frac{\sum_n y_n \boldsymbol{x}_n}{N_1}$$

and

$$0 = \frac{\partial log(L(\boldsymbol{X}, \boldsymbol{y}))}{\partial \boldsymbol{\mu}_2}$$
$$\boldsymbol{\mu}_2 = \frac{\sum_n (1 - y_n) \boldsymbol{x}_n}{N_2}$$

7.5.3.3 Estimate $\boldsymbol{\Sigma}$ (covariance matrix)

$$0 = \frac{\partial log(L(\boldsymbol{X}, \boldsymbol{y}))}{\partial \boldsymbol{\Sigma}}$$
$$\boldsymbol{\Sigma} = \frac{N_1}{N} \boldsymbol{S}_1 + \frac{N_2}{N} \boldsymbol{S}_2$$

where S_k are the empirical covariance matrices of the class k

$$\boldsymbol{S}_1 = \frac{1}{N_1} \sum_{n \in C_1} (\boldsymbol{x}_n - \boldsymbol{\mu}_1)(\boldsymbol{x}_n - \boldsymbol{\mu}_1)^T$$
$$\boldsymbol{S}_2 = \frac{1}{N_1} \sum_{n \in C_2} (\boldsymbol{x}_n - \boldsymbol{\mu}_2)(\boldsymbol{x}_n - \boldsymbol{\mu}_2)^T$$

8 Linear Models

8.1 Linear Regression

8.1.1 Formulation

Linear Regression is a supervised machine learning algorithm where the predicted output is continuous and has a constant slope. Our main objective is to generate a line that minimizes the distance from the line to all of data points. This is essentially minimizing the error and maximizing our prediction accuracy.

8.1.2 Simple Regression

A simple two variable linear regression uses the slope-intercept form, where m and b are the variables our algorithm will try to "learn". $\boldsymbol{x}$ represents our input data and y represents the prediction.

$$y = m\boldsymbol{x} + b$$

8.1.3 Multivariable Regression

Often times there are more than one feature in the data and we need a more complex multi-variable linear equation as our hypothesis. We can represent our hypothesis with the follow multi-variable linear equation, where $\boldsymbol{w}$ are the weights and $\boldsymbol{x}$ is the input data.

$$\begin{aligned} h_{\boldsymbol{w}}(\boldsymbol{x}) &= w_0 x_0 + w_1 x_1 w_2 x_2 + ... + w_n x_n \\ &= \boldsymbol{w}^T \boldsymbol{x} \end{aligned}$$

8.1.4 Cost Function

To predict based on a dataset we first need to learn the weights that minimize the mean squared error (euclidean loss) of our hypothesis. We can define the following to be our cost function to minimize with N being the number of data points and n being the n^{th} training example. This can be proven with statistical linear regression.

$$J(\boldsymbol{w}) = \frac{1}{2N} \sum_{n=1}^{N} (h_{\boldsymbol{w}}(\overline{\boldsymbol{x}}_n) - y_n)^2$$

8.1.5 Gradient Descent Solution

Now to solve for $\boldsymbol{w}$ we can use Gradient Descent and iteratively update $\boldsymbol{w}$ until it converges. We get the slope of the cost function to be:

$$\frac{\partial J \boldsymbol{w}}{\partial \boldsymbol{w}_j} = \frac{1}{N} \sum_{n=1}^{N} (\boldsymbol{w}^T \overline{\boldsymbol{x}}_n - y_n) x_{j,n}$$

now applying a step α we can iteratively change $\boldsymbol{w}$ until it reaches the global minima.

$$\boldsymbol{w}_j := \boldsymbol{w}_j - \alpha \frac{1}{N} \sum_{n=1}^{N} (h_{\boldsymbol{w}}(\overline{\boldsymbol{x}}_n) - y_n)$$

8.1.6 Normal Equation Solution

The closed form solution to the linear system in $\boldsymbol{w}$

$$\frac{\partial J \boldsymbol{w}}{\partial \boldsymbol{w}_j} = \frac{1}{N} \sum_{n=1}^{N} (\boldsymbol{w}^T \overline{\boldsymbol{x}}_n - y_n) x_{j,n}$$

writing this as a linear system in w we get $A\boldsymbol{w} = b$ where

$$A = \sum_{n=1}^{N}(\boldsymbol{x}_n \boldsymbol{x}_n^T) \text{ and } b = \sum_{n=1}^{N}(\boldsymbol{x}_n y_n)$$

so we can solve for $\boldsymbol{w} = \boldsymbol{A}^{-1}\boldsymbol{b}$ and get the following vectorized solution.

$$\boldsymbol{w} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

8.2 Logistic Regression

8.2.1 Formulation

Logistic regression is an algorithm used for classification. It is used to estimate the probability that an instance belongs to a particular class. If the estimated probability is greater than 50%, then the model predicts the instance belongs to that class, and otherwise it predicts it does not. Logistic Regression is form of discriminative learning as it attempts to model $P(c_k|\boldsymbol{x})$ directly, this is unlike the generative model where $P(c_k)$ and $P(\boldsymbol{x}|c_k)$ are found by max likelihood and $P(c_k|\boldsymbol{x})$ by Bayesian Inference.

8.2.2 Prediction

Logistic Regression computers the weighted sum of the input features (plus a bias term) and outputs the logistic (Sigmoid Function) of the result. The hypothesis for class k is given by

$$\pi_k = h_{\boldsymbol{w}}(\boldsymbol{x}) = \sigma(\boldsymbol{w}^T\overline{\boldsymbol{x}})$$

Once the Logistic Regression model has estimated the probability that an instance $\boldsymbol{x}$ belongs to the positive class, it can make its prediction y easily.

$$y = \begin{cases} 0 & \pi_k < 0.5 \\ 1 & \pi_k \geq 0.5 \end{cases}$$

8.2.3 Cost Function

The objective of training the model is such that the model estimates high probabilities for positive instances ($y = 1$) and low probabilities for negative instances ($y = 0$). This concept is captured through the cost function shown below.

$$J(\boldsymbol{w}) = \begin{cases} -log(\pi_k) & y = 1 \\ -log(1 - \pi_k) & y = 0 \end{cases}$$

This makes intuitive sense because $-log(t)$ grows very large when t approaches 0, so the cost will be large if the model estimates a probability close to 0 for a positive instance. The cost will also be very large if the model estimates a probability close to 1 for a negative instance.

On the other hand $-log(t)$ is close to 0 when t is close to 1, so the cost will be close to 0 if the estimated probability is close to 0 for a negative instance or close to 1 for a positive instance.

We can express the cost as a single expression called the *log loss*.

$$J(\boldsymbol{w}) = -\frac{1}{N}\sum_{n=1}^{N}[y_n log(h_{\boldsymbol{w}}(\overline{\boldsymbol{x}}_n)) + ((1-y_n) log(1-h_{\boldsymbol{w}}(\overline{\boldsymbol{x}}_n))]$$

8.2.4 Solution

Unfortunately, there is no known closed-form solution to compute the value of $\boldsymbol{w}$ that minimizes the cost function. The cost function however, is convex, so Gradient Descent or any other convex optimization algorithm is guaranteed to find the global minimum. The gradient can be expressed as:

$$\frac{\partial J\boldsymbol{w}}{\partial \boldsymbol{w}_j} = \frac{1}{N}\sum_{n=1}^{N}(\sigma(\boldsymbol{w}^T\overline{\boldsymbol{x}}) - y_n)x_{j,n})$$

Some faster more sophisticated methods are

- Conjugate Gradient
- BFGS
- L-BFGS

8.2.5 Softmax Regression

The Logistic Regression model can be generalized to support multiple classes. When given an instance $\boldsymbol{x}$, the Softmax Regression model computes a score $f_k(\boldsymbol{x})$ for each class k, then estimates the probability of each class by applying the *softmax function* to the scores.

$$f_k(\boldsymbol{x}) = \boldsymbol{w}_k^T\overline{\boldsymbol{x}}$$

Once the score of every class for the instance $\boldsymbol{x}$ is computed, you can estimate the probability π_k that the instance belongs to class k. The function computes the exponential of each score, the normalizes them.

$$\pi_k = P(y_n = k|\boldsymbol{x}_n, \boldsymbol{w}) = \frac{e^{f_k(\boldsymbol{x})}}{\sum_{j=1}^{K} e^{f_j(\boldsymbol{x})}}$$

The Softmax Regression classifier predicts the class with the highest estimated probability.

The cost function associated with the Softmax Regression Classifier is the Cross Entropy cost function; it penalizes the model when it estimates a low probability for a target class. Cross entropy is used to measure how well a set of estimates class probabilities matches the target class. The cost function is represented as such

$$J(\boldsymbol{w}) = -\frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K}(y_n == k) log(\pi_k^{(n)})$$

where $y_n == k$ is the target probability the n^{th} instance belongs to class k and $\pi_k^{(n)}$ is the estimated probability that instance $\boldsymbol{x}_n$ belongs to class k.

The gradient vector is

$$\nabla_{\boldsymbol{w}_k} J(\boldsymbol{w}) = \frac{1}{N} \sum_{n=1}^{N} (\pi_k^{(n)} - (y_n == k)) \boldsymbol{x}_n$$

that can be paired with an optimization algorithm to solve.

8.3 Generalized Linear Models

Often times our data won't be linear and it could be of a higher degree polynomial or a completely different distribution altogether. We can turn this non-linear problem into a linear regression problem by mapping the data to a different vector space using a basis function.

To demonstrate, let us consider Linear Regression on a nonlinear M x 1 (feature) dataset. Let ϕ denote the polynomial basis function where $\phi_j(\boldsymbol{x}) = x^j$. Then we can express our hypothesis as:

$$h_{\boldsymbol{w}}(\boldsymbol{x}) = w_0\phi(x) + w_1\phi_1(x) + w_2\phi_2(x) + ... + w_m\phi_m(x)$$

A dataset with 3 features with a polynomial basis would have a hypothesis as such

$$h_{\boldsymbol{w}}(\boldsymbol{x}) = w_0 + w_1x_1 + w_2x_2 + w_3x_1^2 + w_4x_2^2 + w_5x_1^2x_2 + w_6x_1x_2^2 + w_7x_1^2x_2^2 + w_8x_1^3 + w_9x_2^3$$

This can then be extrapolated to logisitic regression and m-features. Some commonly used basis functions are:

- Polynomial: $\phi_j(\boldsymbol{x}) = x^j$
- Gaussian: $\phi_j(\boldsymbol{x}) = e^{(\frac{x-\mu_j}{2s^2})}$
- Sigmoid: $\phi_j(\boldsymbol{x}) = \sigma(\frac{x-\mu_j}{s})$
- Fourier Basis, Wavelets, etc ...

8.4 Regularization

Small outliers can drastically change our values of $\boldsymbol{w}$ so rely on regularization to reduce over-fitting. Polynomial models can be easily regularized by reducing the number of polynomial degrees. For a linear model, regularization is typically achieved by constraining the weights of the model. The regularization term should only be added to the cost function during training. Once the model is trained, the non-regularized cost should be used to measure the model's performance. The bias term w_0 is not regularized.

8.4.1 Ridge Regression

Ridge Regression (Tikhonov Regularization) is a regularized version of Linear regression with a regularization term of $\frac{\lambda}{2}\|\boldsymbol{w}\|_2^2$ (l_2-norm) added to the cost function. This forces the learning algorithm to fit the data but also keep the model weights as small as possible. The hyperparameter λ controls how much you want to regularize the model.

$$J(\boldsymbol{w}) = ERROR(\boldsymbol{w}) + \frac{\lambda}{2}\|\boldsymbol{w}\|_2^2$$

8.4.2 Lasso Regression

Least Absolute Shrinkage and Selection Operator Regression is another regularized version of Linear Regression, it adds a regularization term to the cost function but uses the l_1 norm of the weight vector instead of half the square of the l_2 norm.

$$J(\boldsymbol{w}) = ERROR(\boldsymbol{w}) + \lambda \sum_{i=1}^{n} |\boldsymbol{w}_i|$$

An important characteristic of Lasso Regression is that it tends to eliminate the weights of the least important features (i.e, set them to zero). Lasso Regression automatically performs feature selection and outputs a *sparse model*.

8.4.3 Elastic Net

Elastic Net is a middle ground between Ridge Regression and Lasso Regression. The regularization term is a simple mix of both Ridge and Lasso's regularization terms and you can control the mix ratio r. When $r = 0$, Elastic Net is equivalent to Ridge Regression, and when $r = 1$, it is equivalent to Lasso Regression.

$$J(\boldsymbol{w}) = ERROR(\boldsymbol{w}) + \frac{(1-r)\lambda}{2}\|\boldsymbol{w}\|_2^2 + r\lambda \sum_{i=1}^{n} |\boldsymbol{w}_i|$$

8.4.4 Early Stopping

Early Stopping is a different way to regularize iterative learning algorithms such as Gradient Descent. This method aims to stop training as soon as the validation error reaches a minimum. For all convex optimization problems there will be a global minima, once that global minima is reached the curve will start going up. This proposes to stop as soong as we reach the minimum.

9 Kernel Methods

9.1 Kernel Trick

9.1.1 Formulation

When we consider generalized linear models we have to come up with some basis functions, our hypothesis space is limited because we have fixed basis functions. To have a non-limited

hypothesis space we need to be able to consider an infinite number of basis functions. Using kernel trick we can change the complexity of the problem to depend on the number of data rather than the number of basis functions.

Examples:

- Gaussian Processes
- Support Vector Machine

9.1.2 Dual Problem

Given a constrained optimization problem, known as the *primal problem*, it is possible to express a different but closely related problem, called its *dual problem*. The dual problem is generally achieved by constraint based optimization (e.g taking the lagrangian and representing the problem as an optimization in other simpler variables). The solution to the dual problem typically gives a lower bound to the solution of the primal problem, but under some conditions it can have the same solution as the primal problem. The complexity of the primal solution depends on the number of basis functions while the complexity of the dual problem depends on the number of data points.

9.1.3 Kernel Function

Let $\phi(\boldsymbol{x})$ be a set of basis functions that map inputs x to a feature space. In many cases this feature space only appears in the dot product $\phi(\boldsymbol{x})^T\phi(\boldsymbol{x}')$ of input pairs $\boldsymbol{x}, \boldsymbol{x}'$, therefore we can define the kernel function

$$k(\boldsymbol{x}, \boldsymbol{x}') = \phi(\boldsymbol{x})^T\phi(\boldsymbol{x}')$$

to be the dot product of any pair $\boldsymbol{x}, \boldsymbol{x}'$ in feature space. Now we only need to know $k(\boldsymbol{x}, \boldsymbol{x}')$, not $\phi(\boldsymbol{x})$. If we know $k(\boldsymbol{x}, \boldsymbol{x}')$ then we know the output to any input $\boldsymbol{x}, \boldsymbol{x}'$ without having to compute $\phi(\boldsymbol{x})$. Intuitively a kernel is a measure of the similarity of the input.

9.1.4 Constructing Kernels

Two main methods:

- Find mapping $\boldsymbol{\phi}$ to feature space and let $\boldsymbol{K = \phi^T\phi}$
- Directly specify K

A valid kernel must be a positive semi-definite. This means that k must factor into the product of a transposed matrix by itself (e.g., $\boldsymbol{K = \phi^T\phi}$) or, all eigenvalues must be greater than or equal to 0.

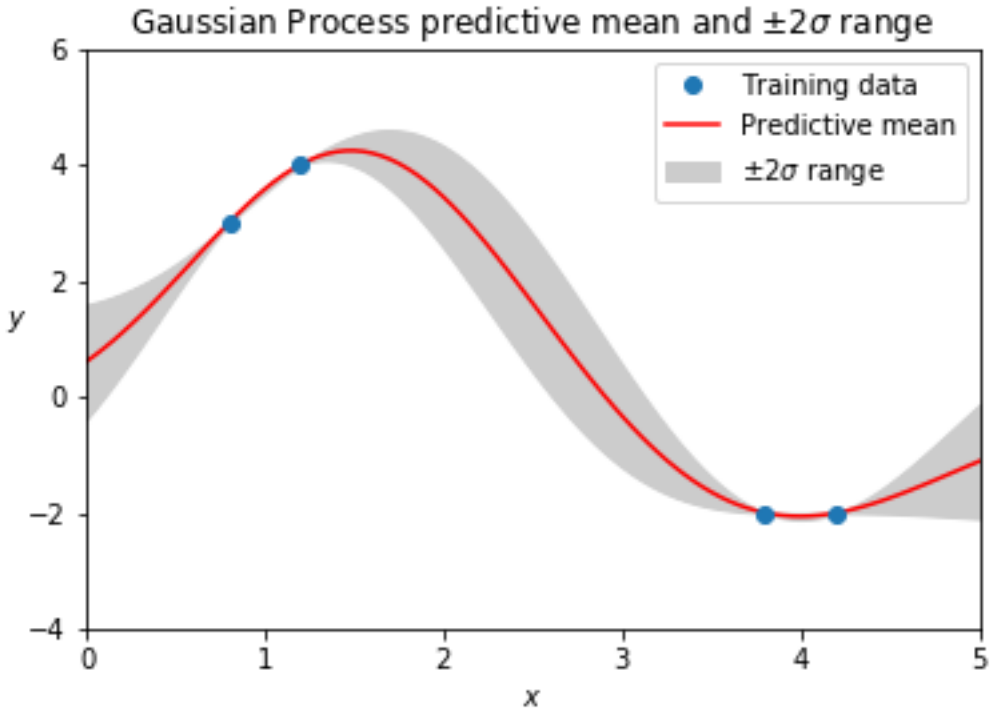
9.1.5 Common Kernels

- Linear/Identity: $k(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{x}^T\boldsymbol{x}'$
- Polynomial: $k(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x}^T\boldsymbol{x}' + 1)^d$

- Gaussian RBF: $k(\boldsymbol{x}, \boldsymbol{x}') = exp(-\gamma \|\boldsymbol{x} - \boldsymbol{x}'\|^2)$
- Sigmoid Kernel: $k(\boldsymbol{x}, \boldsymbol{x}') = tanh(\alpha \boldsymbol{x}^T \boldsymbol{x}' + c)$

9.2 Gaussian Processes

The idea behind Gaussian processes is that given a dataset it is able to capture any function that happens to be going through those points. It is does not assume any parametric form for the underlying data. The gaussian process essentially learns a distribution over what is the outcome of that function at any point. Between two points in the dataset it does not know what the function should look like, so it models the uncertainty of the prediction with a distribution between the data points, the bounds being + and - some multiple of standard deviation.



9.2.1 Function Space

In Bayesian Linear Regression we saw that it was a parametric form of learning the weight $\boldsymbol{w}$. Now instead we can consider the function space view were we can instead directly learn the function $f(\boldsymbol{x}) = \boldsymbol{w}^T \phi(\boldsymbol{x})$. We can express this function space view as:

- Prior: $P(f(\boldsymbol{x}_*)) = \int_{\boldsymbol{w}} P(f|\boldsymbol{w}, \boldsymbol{x}_*) P(\boldsymbol{w})) d\boldsymbol{w}$
- Posterior: $P(f(\boldsymbol{x}_*)|\boldsymbol{X}, \boldsymbol{y}) = \int_{\boldsymbol{w}} P(f|\boldsymbol{w}, \boldsymbol{x}_*) P(\boldsymbol{w}|\boldsymbol{X}, \boldsymbol{y}) d\boldsymbol{w}$

According to every function view, there is a Gaussian at $f(\boldsymbol{x}_*)$ for every $\boldsymbol{x}_*$. Those Gaussians are correlated through $\boldsymbol{w}$.

9.2.2 Representation

We can represent a Gaussian Process, a distribution over functions as:

$$f(\boldsymbol{x}) \sim GP(m(\boldsymbol{x}), k(\boldsymbol{x}, \boldsymbol{x}'))\forall \boldsymbol{x}, \boldsymbol{x}'$$

where $m(\boldsymbol{x}) = E(f(\boldsymbol{x}))$ is the mean and $k(\boldsymbol{x}, \boldsymbol{x}') = E((f(\boldsymbol{x} - m(\boldsymbol{x})))(f(\boldsymbol{x}') - m(\boldsymbol{x}')))$ is the kernel covariance matrix.

9.2.3 Gaussian Process Regression

The gaussian process regression is the kernel version of Bayesian Linear Regression where we learn based on the function space view, computing the posterior over f rather than over w. This allows for the complexity to be cubic in the number of training points rather than the number of features. We can perform regression using the following formulae.

Prior: $P(f(\cdot)) = N(m(\cdot), k(\cdot, \cdot))$

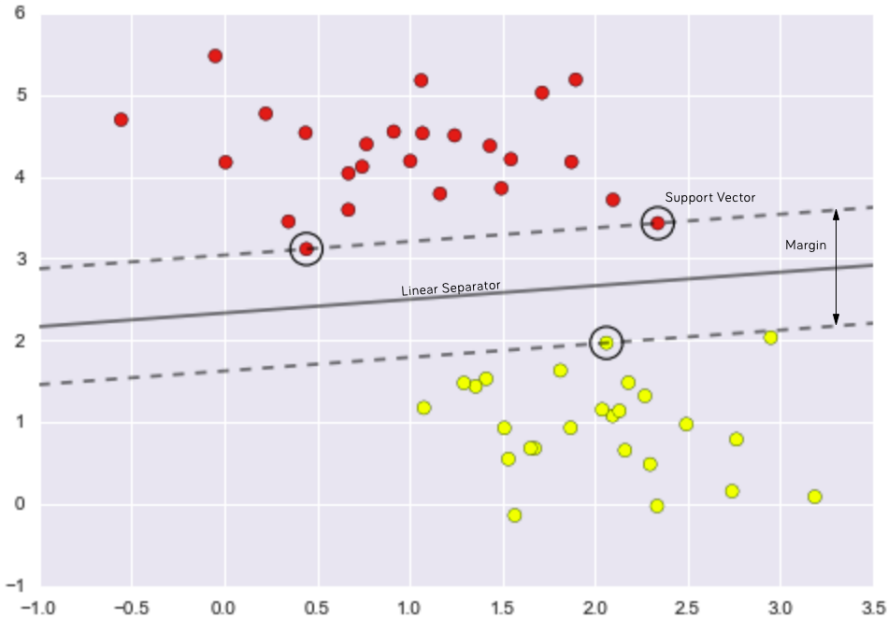
Likelihood: $P(\boldsymbol{y}|\boldsymbol{X}, f) = N(f(\cdot), \sigma^2\boldsymbol{I})$

Posterior: $P(f(\cdot)|\boldsymbol{X}, \boldsymbol{y}) = N(\overline{f}(\cdot), k'(\cdot, \cdot))$ where
$\overline{f}(\cdot) = k(\cdot, \boldsymbol{X})(\boldsymbol{K} + \sigma^2\boldsymbol{I})^{-1}\boldsymbol{y}$ and
$k'(\cdot, \cdot) = k(\cdot, \cdot) - k(\cdot, \boldsymbol{X})(\boldsymbol{K} + \sigma^2\boldsymbol{I})^{-1}k(\boldsymbol{X}, \cdot)$

Prediction: $P(\boldsymbol{y}_*|\boldsymbol{x}_*, \boldsymbol{X}, \boldsymbol{y}) = N(\overline{f}(\boldsymbol{x}_*), k'(\boldsymbol{x}_*, \boldsymbol{x}_*))$

9.3 Support Vector Machines

Support Vector Machines is a kernel based method that can be used for classification and regression. It performs extremely well for small amounts of data and can even beat out Neural Networks.



9.3.1 Max-Margin Classifier

Max-Margin classifier is generally only used for binary classification where the data is linearly separable. The intuition behind the max-margin classifier is that we want to find a linear separator for the data that maximizes the distance to the closest data points. We formulate this method as we need to consider noise, a larger margin will allow room for noise, otherwise if it is too narrow then there is room for possible misclassification.

We can turn the problem into an optimization problem of finding the max margin as follows.

Linear Separator: $\boldsymbol{w}^T\phi(\boldsymbol{x}) = 0$.

Distance to Linear Separator:

$$\frac{y\boldsymbol{w}^T\phi(x)}{\|\boldsymbol{w}\|}, y \in \{-1, 1\}$$

Maximum Margin:

$$max_{\boldsymbol{w}} \frac{1}{\|\boldsymbol{w}\|}\{min_n y_n \boldsymbol{w}^T\phi(\boldsymbol{x}_n)\}$$

We can transform this expression by fixing the minimal distance to 1 and minimizing our scale $\|\boldsymbol{w}\|$ to be:

$$min_w \frac{1}{2}\|\boldsymbol{w}\|^2 \text{ s.t. } y_n\boldsymbol{w}^T\phi(\boldsymbol{x}_n) \geq 1 \ \forall n$$

This now becomes a convex quadratic optimization problem with linear constraints, which is a form of that is quite easy. The points where $y_n\boldsymbol{w}^T\phi(\boldsymbol{x}_n) = 1$ define the active constraints, called the support vectors.

9.3.1.1 Dual Representation

To compute this problem we want to reformulate such that $\phi(\boldsymbol{x})$ only appears in a kernel. From the kernel trick we see we can achieve this by finding the dual of the optimization. This will result in a sparse kernel since only the points on the margin matter.

We want to transform the constrained optimization problem

$$min_w \frac{1}{2}\|\boldsymbol{w}\|^2 \text{ s.t. } y_n\boldsymbol{w}^T\phi(\boldsymbol{x}_n) \geq 1 \ \forall n$$

into an unconstrained optimization problem. We can use the lagrangian to obtain the following.

$$max_{a\geq 0} \ min_{\boldsymbol{w}} L(\boldsymbol{w}, \boldsymbol{a})$$

where

$$L(\boldsymbol{w}, \boldsymbol{a}) = \frac{1}{2}\|\boldsymbol{w}\|^2 - \sum_n a_n[y_n\boldsymbol{w}^T\phi(\boldsymbol{x}_n) - 1]$$

where the second term is the penalty for violating the n^th constraint.

We can then solve the inner minimization $min_{\boldsymbol{w}} L(\boldsymbol{w}, \boldsymbol{a})$ to obtain:

$$L(\boldsymbol{a}) = \sum_n a_n - \frac{1}{2} \sum_n \sum_n a_n a_n, y_n y_n, k(\boldsymbol{x}_n, \boldsymbol{x}_n)$$

We are then left with the optimization problem in $\boldsymbol{a}$ only known as the dual problem.

$$max_{\boldsymbol{a}} L(\boldsymbol{a}) \text{ s.t. } a_n \geq 0$$

This is sparse optimization since many of the a_n's are 0 when the data point is already ≥ 1, so the penalty is 0 for theses since they already satisfy the constraint.

9.3.1.2 Classification

Primal Problem:

$$y_* = sgn(\boldsymbol{w}^T \phi(\boldsymbol{x}_*))$$

Dual Problem:

$$y_* = sgn(\sum_n a_n y_n \phi(\boldsymbol{x}_n)^T \phi(\boldsymbol{x}_*))$$
$$y_* = sgn(\sum_n a_n y_n k(\boldsymbol{x}_n, \boldsymbol{x}_*))$$

Intuitively what is happening here is we are taking the sum of the degree of similarity between each query point and every point in the training set that is a support vector.

9.3.2 Soft Margin Classifier

Often times the data is not linearly separable and we have overlapping class distributions. We want a method such that we can relax the constraints yet keep the maximum margin as maximizing the margin is equivalent to minimizing an upper bound on the worst case loss. To achieve this we introduce Soft Margins which formulates that we can relax the constraints by introducing a slack variable $\xi \geq 0$. We can now impose the following constraint.

$$y_n \boldsymbol{w}^T \phi(\boldsymbol{x}_n) \geq 1 - \xi_n \ \forall n$$

This introduces a new optimization problem

$$min_{\boldsymbol{w}, \boldsymbol{\xi}} \ C \sum_{n=1}^{N} \xi_n + \frac{1}{2} \|\boldsymbol{w}\|^2 \quad \text{s.t. } y_n \boldsymbol{w}^T \phi(\boldsymbol{x}_n) \geq 1 - \xi_n, \ \xi_n \geq 0 \ \forall n$$

$C > 0$ controls the tradeoff between the slack variable penalty and the margin.

Some intuition behind this is further explored.

- Since $\sum_n \xi_n$ is an upper bound on the number of misclassifications, C can also be thought as a regularized coefficient that controls the tradeoff between error minimization and model complexity
- We can see that if we let $C \to \infty$ then we recover the original hard margin problem.
- Soft margins can only handle minor misclassifications and are still sensitive to outliers.

9.3.3 Multiclass SVM

There are many approaches to train multi class SVM's the best one being the continuous ranking approach. The idea behind this, is that instead of computing the sign of a linear separator, we compare the values of linear functions for each class k. The SVM returns a continuous value to rank all classes.

9.3.3.1 Constraint

Now for each class $k \neq y$ we define a linear constraint that guarantees a margin of at least 1 between classes.

$$\boldsymbol{w}_y^T \phi(\boldsymbol{x}) - \boldsymbol{w}_k^T \phi(\boldsymbol{x}) \geq 1 \ \forall k \neq y$$

9.3.3.2 Classification

With the constraint we can achieve the optimization problem used for classification. For multiclass dataset that is linearly separable we get:

$$min_{\boldsymbol{w}} \frac{1}{2} \sum_k \|\boldsymbol{w}_k\|^2 \quad \text{s.t. } \boldsymbol{w}_{y_n}^T \phi(\boldsymbol{x_n}) - \boldsymbol{w}_k^T \phi(\boldsymbol{x}_n) \geq 1 \ \forall n, k \neq y_n$$

For overlapping classes we can add the slack variable ξ

$$min_{\boldsymbol{w},\boldsymbol{\xi}} \ C \sum_n \xi_n + \frac{1}{2} \sum_k \|\boldsymbol{w}_k\|^2 \quad \text{s.t. } \boldsymbol{w}_{y_n}^T \phi(\boldsymbol{x_n}) - \boldsymbol{w}_k^T \phi(\boldsymbol{x}_n) \geq 1 - \xi_n \ \forall n, k \neq y_n$$

10 Artificial Neural Networks Primer

10.1 Origins

The concept of a Artificial Neural Network (ANN) stems from the anatomy of the brain. They are modelled directly after biological neurons, a neural cell, found in the brain. Biological neurons produce short electrical impulses called *action potentials* which travel along the neurons and make synapses release chemical signals called *neurotransmitters*. When a neuron receives a sufficient amount of these neurotransmitters within a few milliseconds, it fires its own electrical impulses. These, individual neurons behave in a simple way but they are organized in a vast network of billions, with each neuron typically connect to thousands of other neurons. Highly complex computations can be performed by a network of fairly simple neurons.

10.2 ANN Unit

Now the idea behind Artificial Neural Networks is to mimic the brain by making Artificial Neurons. The Perceptron is one of the simplest ANN architectures and is based on a slightly different artificial neuron called a *threshold logic unit* (TLU), or sometimes a *linear threshold unit* (LTU). The TLU computes a weighted sum of its inputs ($a = w_1x_1 + w_2x_2 + ... + w_nx_n = \boldsymbol{w}^T\boldsymbol{x}$), then applies an activation function to that sum and outputs the result: $h_{\boldsymbol{w}}(a)$. When picking an activation function, it should be nonlinear, otherwise the network is just a linear function. The activation function should be chosen such that it mimics firing in neurons: the unit should be "active" (output near 1) when fed with the "right" inputs and the unit should be "inactive" (output near 0) when fed with the wrong inputs.

10.3 Perceptron

A perceptron is a type of single layer feed-forward network. It is simply composed of a single layer of threshold logic units, with each TLU connected to all the inputs. When all the neurons in a layer are connected to every neuron in the previous later, the layer is called a *fully connected layer*, or a *dense layer*. The inputs of the perceptron are fed to special pass through neurons called input neurons: they output whatever input they are fed. All the input neurons form the *input layer*. Moreover, an extra bias feature is generally added ($x_0 = 1$): it is typically represented using a special type of neuron called a *bias neuron*, which outputs 1 all the time.

10.3.1 Threshold Perceptron Learning

10.3.1.1 Threshold Perceptron Algorithm

For threshold perceptron algorithm, learning is done separately for each unit j since units do not share weights. The learning algorithm is as follows, for each unit j, for each $(\boldsymbol{x}, \boldsymbol{y})$ pair do until the output is correct for all training instances:

- Case 1: Correct output produced then $\forall i W_{ji} \leftarrow W_{ji}$
- Case 2: Output produced 0 instead of 1 then $\forall i W_{ji} + x_i$
- Case 3: Output produced is 1 instead of 0 then $\forall i W_{ji} - x_i$

Now we will demonstrate the intuition behind this. If we consider using a threshold activation function then the perceptron computes:

- 1 when $\boldsymbol{w}^T\overline{\boldsymbol{x}} = \sum_i x_i w_i + w_0 > 0$
- 0 when $\boldsymbol{w}^T\overline{\boldsymbol{x}} = \sum_i x_i w_i + w_0 < 0$

Now leveraging the fact that $\overline{\boldsymbol{x}}^T\overline{\boldsymbol{x}} \geq 0$ and $\overline{\boldsymbol{x}}^T\overline{\boldsymbol{x}} \leq 0$ then we can we can come up with the following statements.

- If the output should be 1 instead of 0 then $\boldsymbol{w} \leftarrow \boldsymbol{w} + \overline{\boldsymbol{x}}$ since $(\boldsymbol{w} + \overline{\boldsymbol{x}})^T\overline{\boldsymbol{x}} \geq \boldsymbol{w}^T\overline{\boldsymbol{x}}$
- If the output should be 0 instead of 1 then $\boldsymbol{w} \leftarrow \boldsymbol{w} - \overline{\boldsymbol{x}}$ since $(\boldsymbol{w} - \overline{\boldsymbol{x}})^T\overline{\boldsymbol{x}} \leq \boldsymbol{w}^T\overline{\boldsymbol{x}}$

10.3.1.2 Sequential Gradient Descent Algorithm

Alternatively we can use gradient descent to minimize misclassification error to train the perceptron.

Let $y \in \{-1, 1\} \forall y$ and let $M = \{(\boldsymbol{x}_n, y_n)_{\forall n}\}$ be the set of misclassified examples (i.e., $y_n \boldsymbol{w}^T \overline{\boldsymbol{x}}_n < 0$).

We need to find a $\boldsymbol{w}$ that minimizes the misclassification error

$$E(\boldsymbol{w}) = -\sum_{(\boldsymbol{x}_n, y_n) \in M} y_n \boldsymbol{w}^T \overline{\boldsymbol{x}}_n$$

and the gradient is:

$$\nabla \boldsymbol{E} = -\sum_{(\boldsymbol{x}_n, y_n) \in M} y_n \overline{\boldsymbol{x}}_n$$

Now applying this to the gradient descent algorithm we have:

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + \alpha y \overline{\boldsymbol{x}}$$

We adjust $\boldsymbol{w}$ one sample at a time. Here α is the learning rate and we see that if we let $\alpha = 1$ then we recover the threshold perceptron algorithm.

10.3.1.3 Limitations

The decision boundary of each output neuron is linear, so Perceptrons are incapable of learning complex However, if the training instances are linearly separable then this algorithm will converge to a solution.

10.3.2 Sigmoid Perceptron Learning

Similar to Threshold perceptron learning, Sigmoid Perceptron Learning hinges on the same concepts. We can set our objective to minimizing the minimum squared error or maximum likelihood which will yield the same algorithm as for logistic regression.

$$E(\boldsymbol{w}) = \frac{1}{2} \sum_n E_n(\boldsymbol{w})^2 = \frac{1}{2} \sum_n (y_n - \sigma(\boldsymbol{w}^T \overline{\boldsymbol{x}}_n))^2$$

We can compute the gradient to be

$$\nabla \boldsymbol{E} = -\sum_n E_n(\boldsymbol{w}) \sigma(\boldsymbol{w}^T \overline{\boldsymbol{x}}_n)(1 - \sigma(\boldsymbol{w}^T \overline{\boldsymbol{x}}_n)) x_i$$

Now using sequential gradient descent we repeat the following for each $(\boldsymbol{x}_n, y_n)$ until some stopping criterion is satisfied.

$$\epsilon_n \leftarrow y_n - \sigma(\boldsymbol{w}^T \overline{\boldsymbol{x}}_n)$$
$$\boldsymbol{w} \leftarrow \boldsymbol{w} + \alpha \epsilon_n \sigma(\boldsymbol{w}^T \overline{\boldsymbol{x}}_n)(1 - \sigma(\boldsymbol{w}^T \overline{\boldsymbol{x}}_n)) \overline{\boldsymbol{x}}_n$$

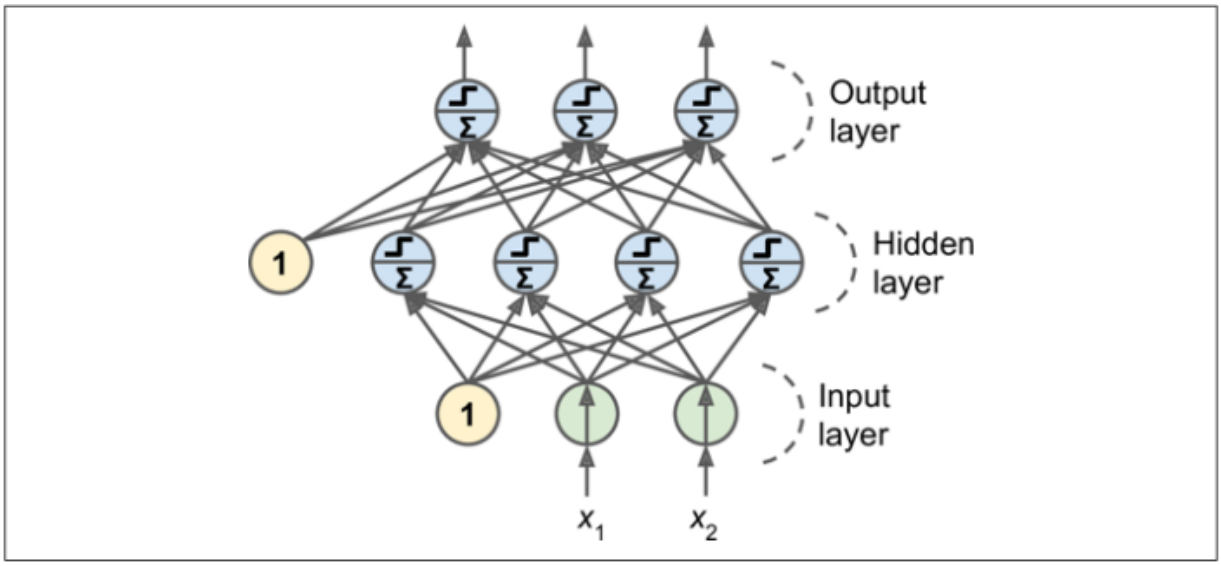
It possesses the same limitations as threshold perceptron learning.

10.4 Multi-Layer Neural Nets

We previously saw the limitations of the perceptron as it was only able to learn on linearly separable data. Unfortunately a lot of data is not linear and this led to the birth of Multi-layer Neural Networks: which are able to learn non-linear basis functions.

10.4.1 n-Layer Perceptron

The follow diagram depicts a 2 layer perceptron. Multilayer perceptron are composed of one (passthrough) *input layer*, one or more layers of ANN's units called *hidden layers*, and one final layer of ANN units called the *output layer*. The layers close to the input layer are usually called the *lower layers*, and the ones close to the outputs are usually called the *upper layers*. Every layer except the output layer includes a bias neuron and is fully connected to the next layer.



Let us denote the hidden units with $\boldsymbol{z}$, the output units with $\boldsymbol{y}$ and the weights between the layers with $\boldsymbol{w}^(layer_num)$.

Hidden Units: $z_j = h_1(\boldsymbol{w}_j^{(1)}\overline{\boldsymbol{x}})$

Output Units: $y_k = h_2(\boldsymbol{w}_k^{(2)}\overline{\boldsymbol{z}})$

Overall: $y_k = h_2(\sum_j w_{kj}^{(2)} h_1(\sum_i w_{ji}^{(1)} x_i))$

10.4.1.1 Non-linear Regression

We can use a multi-layer neural network to equivalently represent regression with the following expression.

$$y_k = \sum_j w_{kj}^{(2)} \sigma(\sum_i w_{ji} x_i)$$

We can interpret the sigmoid as a non linear basis function and the outer summation to be the linear combination.

10.4.1.2 Non-linear Classification

We can use a multi-layer neural network to equivalently represent binary classification with the following expression.

$$P(c_k|\boldsymbol{x}) = \sigma(\sum_j w_{kj}^{(2)} \sigma(\sum_i w_{ji} x_i))$$

We can interpret the sigmoid as a non-linear basis function and the outer summation to be the linear combination. The outer sigmoid is the normalization to return the probability.

What is happening in both regression and classification is we are allowing the basis functions to adapt and vary and we are no longer restricted to fixed basis functions.

10.4.2 Backpropagation

One of the most common forms of weight training for multi-layer neural nets is error minimization using backpropagation. This allows us to compare the errors at the output and backpropagate the error back through the error through the network to train the weights.

We can then use gradient descent to to adjust the weights. Generally based on the size of the model and the data it is more favorable to use faster gradient descent algorithms and we can consider gradient descent optimizations for training.

10.4.2.1 Algorithm

Forward Phase: Propagate units forward to compute the output of each unit. We want to obtain the output z_j for each unit j.

$$z_j = h(a_j) \quad \text{where} \quad a_j = \sum_i w_{ji} z_i$$

Backward Phase: compute delta δ_j at each unit j. We can use chain rule to recursively compute the gradient and follow the following process.

For each weight w_{ji}

$$\frac{\partial E_n}{\partial w_{ji}} = \frac{\partial E_n}{\partial a_j} \frac{\partial a_j}{\partial w_{ji}} = \delta_j z_i$$

Let $\delta_j = \frac{\partial E_n}{\partial a_j}$ then

$$\delta_j = \begin{cases} h'(a_j)(z_j - y_j) & \text{base case: } j \text{ is an output unit} \\ h'(a_j) \sum_k w_k \delta_k & \text{recursion: } j \text{ is a hidden unit} \end{cases}$$

Since $a_j = \sum_i w_{ji} z_i$ then $\frac{\partial a_j}{\partial w_{ji}} = z_i$.

11 Deep Learning

A Deep Neural Network is a neural network with many hidden layers. The main advantage of a DNN is its high expressivity, it is able to learn very complex underlying functions. As we increase the number of layers, the number of ANN units needed may decrease (with the number of layers). The power and basis of deep learning is that instead of having to have domain knowledge about what features to apply machine learning to, deep neural networks are able to learn hierarchical feature representations. For example for facial classification the first hidden layer detects certain strokes, the next is able to detect facial features such as eyes and noses and so on until it is able to reconstruct and detect the face.

11.1 Vanishing/Exploding Gradients Problem

One of the problems of backpropagation in deep neural networks consisting of sigmoid and hyperbolic units is that they often suffer from *vanishing gradients*. The problem here is that the computed gradients get smaller and smaller as the algorithm progresses down to the lower layers. As a result, the gradient descent update leaves the lower layers' connection weights virtually unchanged, and training never converges to a good solution. This is because when moving in the forward phase the variance keeps increasing after each layer until the activation saturates at the top layer when using the sigmoid or tanh activation function. When the function saturates at 0 or 1, with a derivative extremely close to 0, then when backpropagation kicks in it has virtually no gradient to propagate back through the network. The little gradient that exists keeps getting diluted as backpropagation progresses down through the top layers, so there is really nothing left for the lower layers.

Some popular solutions for this problem are:

- Pre-training
- Recfitified Linear Units and Maxout Units
- Residual Networks/Skip Connections
- Batch Normalization

11.1.1 Batch Normalization

Although using the reLU activation function can reduce the danger of vanishing/exploding gradient problem, it doesn't guarantee that it won't come back. Batch Normalization addresses this problem. The technique consists of adding an operation in the model just before or after the activation function of each hidden layer. This operation simply zero-centers and normalizes each input, then scales and shifts the result using two new parameter vectors per layer: one for scaling, the other for shifting. The operations lets the model learnt the optimal scale and mean of each of the layer's inputs. In many cases if you add a BN layer as the very first layer of your neural network, you do not need to standardize your training set; the BN will do it for you.

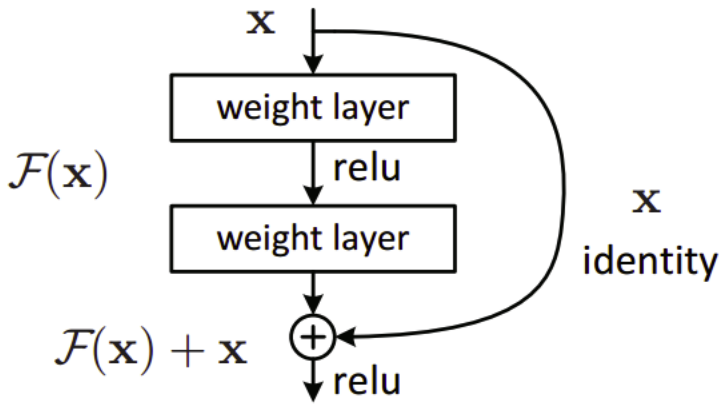
In order to zero-center and normalize the inputs, the algorithm needs to estimate each input's mean and standard deviation. It does so by evaluating the mean and standard deviation fo the input over the current mini-batch.

When testing the trained network we need to make predictions for individual instances rather than for batches of instances: in this case, we have no way to compute each input's mean and standard deviation. One solution is to wait till the end of training and run the whole training set through the neural network and compute the mean and standard deviation of each input of the BN layer. However, most implementations of Batch Normalization estimate these final statistics during training by using a moving average of the layer's input means and standard deviations.

Batch Normalization does, however, add some complexity to the model. Moreover there is a runtime penalty: the neural network makes slow predictions due to the extra computations required at each layer. Fortunately, it's often possible to fuse the BN layer with the previous layer, after training, thereby avoiding the runtime penalty. This is done by updating the previous layer's weights and biases so that it directly produces outputs of the appropriate scale and offset.

11.1.2 Residual Networks

Even with reLU, very deep networks suffer from vanishing gradients. Residual Networks leverages an architecture with sip connections, which are essentially connections from early layers to later layers bypassing certain layers. In Residual Networks the input $\boldsymbol{x}$ of the skip connection is added to the output of the layers it skipped thus the overall output is $f(\boldsymbol{x})+\boldsymbol{x}$. The intuition behind this type of skip connection sit that they have an uninterrupted gradient flow from the first layer to the last layer. If the output of some combination of layers results in a gradient of almost then by using skip connections we pass the original input x to the output, allowing us to use that gradient rather than the diminished one.



11.2 Overfitting

Since deep neural networks are so highly expressive this increases the risk of overfitting. Often times the number of parameters is larger than the amount of data. We can use some

of the follow techniques to help mitigate overfitting.

- Regularization
- Dropout
- Data augmentation

11.2.1 Dropout

The idea behind dropout is to randomly "drop" some units from the network when training, this effectively is the same as saying to reduce their values to 0. Now we train the model with missing nodes (that could represent features) making the network robust if it is able to still perform well and making it impervious to overfitting since it can perform well with some features removes. In each training iteration, a different subnetwork is trained. At test time, these subnetworks are merged by averaging their weights.

At training during each iteration of gradient descent:

- Each input unit is dropped with probability p_1
- Each hidden unit is dropped with probability p_2.

For prediction, since we scaled down the inputs by probability p_1 and the hidden units by p_2, so we need to multiply by their complementary probability to increase their magnitude accordingly.

- Multiply each input unit by $1 - p_1$
- Multiply each hidden unit by $1 - p_2$

11.2.1.1 Algorithm

Let $\odot$ denote elementwise multiplication. For each training example $(\boldsymbol{x}_n, y_n)$ do

Sample $\boldsymbol{z}_n^{(1)}$ from Bernoulli$(1 - p_i)^{k_i}$ for $1 \leq l \leq L$
Neural Network with dropout applied:
$f_n(\boldsymbol{x}_n, \boldsymbol{z}_n; \boldsymbol{W}) = h_i(\boldsymbol{W}^{(L)}[...h_2(\boldsymbol{W}^{(2)}[h_1(\boldsymbol{W}^{(1)}[\overline{\boldsymbol{x}}_n \odot \boldsymbol{z}_n^{(1)}]) \odot \boldsymbol{z_n}^{(2)}])... \odot \boldsymbol{z}_n^{(L)}])$
Loss: $Err(y_n, f_n(\boldsymbol{x}_n, \boldsymbol{z}_n; \boldsymbol{W}))$
Update: $w_{kj} \leftarrow w_{kj} - \alpha \dfrac{\partial Err}{\partial w_{kj}}$

Until convergence.

Prediction:

$$f(\boldsymbol{x}_n; \boldsymbol{W}) = h_i(\boldsymbol{W}^{(L)}[...h_2(\boldsymbol{W}^{(2)}[h_1(\boldsymbol{W}^{(1)}[\overline{\boldsymbol{x}}_n(1 - p_1)])(1 - p_2)])...(1 - p_L)])$$

11.2.2 Data Augmentation

Data augmentation artificially increases the size of the training set by generating many realistic variants of each training instance. This reduces overfitting, making this a possible regularization technique. The generated instances should be as realistic as possible,: ideally, given an image from the augmented training set, a human should not be able to tell whether it was augmented or not.

Some data augmentation methods are things like, slightly shifting, rotating or resizing every picture in the training set by various amounts and add the resulting pictures to the training set. This forces the model to be more tolerant to variations in the position, orientation, and size of the objects in the pictures. You can also play around with lighting and flip the pictures horizontally. By combining these transformations, you can greatly increase the size of your training set.

12 Convolutional Neural Networks

Convolutional networks are a specialized king of neural network for processing data that has a known grid-like topology. Examples include time-series data, which can be thought of as a 1-D grid taking samples at regular time intervals, and image data, which can be thought of as a 2-D grid of pixels.

12.1 Convolution

In its most general form, convolution is a mathematical operation on two functions of real-valued argument. In essence it uses a weighted function $w(\tau)$, where τ is the age of the measurement. It applies this weight average operation at every moment to obtain a new function y providing a smoothed estimate of the original function x.

$$y(t) = \int_t x(\tau)w(t-\tau)d\tau$$

This is the convolution and it is typically denoted with an asterisk.

$$y(t) = (x * w)(t)$$

In convolutional network terminology, the first argument (x) to the convolution is referred to as the *input*, and the second argument (w) as the *kernel*. The output is sometimes referred to as the *feature map*.

Often times we will be working with discretized data and we can define the discrete convolution as:

$$y(t) = (x * w)(t) = \sum_{\tau=-\infty}^{\infty} x(\tau)w(t-\tau)$$

In machine learning applications, the input is usually a multidimensional array of data, and the kernel is usually a multidimensional array of parameters that are adapted by the learning

algorithm. For this we often require to use convolutions over more than one axis at a time. In this case we would want to use a two-dimensional kernel K and express the convolution as:

$$y(i,j) = (I * K)(i,j) = \sum_m \sum_n I(m,n)K(i-m, j-n)$$

and by commutativity:

$$y(i,j) = (I * K)(i,j) = \sum_m \sum_n I(i-m, j-n)K(m,n)$$

Many neural network libraries will also implement a related function called the *cross-correlation*, which is that same as convolution but without flipping the kernel:

$$y(i,j) = (I * K)(i,j) = \sum_m \sum_n I(i+m, j+n)K(m,n)$$

12.1.1 Convolutions for Feature Extraction

In neural networks a convolution denotes the linear combination of a subset of units based on a specific pattern of weights.

$$a_j = \sum_i w_{ji} z_i$$

Convolutions are often combined with an activation function to produce a feature

$$z_j = h(a_j) = h(\sum_i w_{ji} z_i)$$

12.2 Architecture

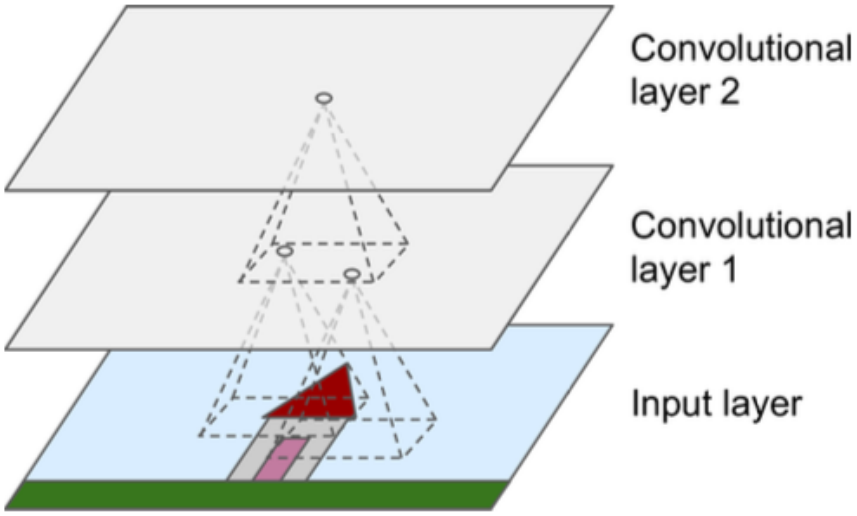
The architecture of a CNN refers to any network that includes an alternation of convolution and pooling layers, where some of the convolution weights are shared.

12.2.1 Filters

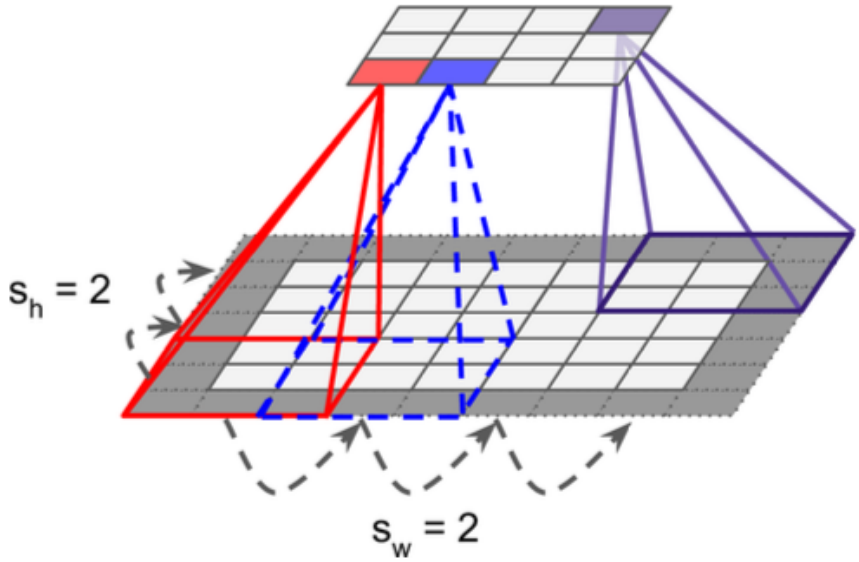
A neuron's weights can be represented as a small image the size of the receptive field or window called filters. When applying a filter over a receptive field the neurons using those weights will ignore everything in their receptive field except for what that filter dictates. E.g a vertical filter will cause all neurons to ignore everything except for the central vertical line (since all inputs will get multiplied by 0, except for the ones located on the central vertical line). A layer full of neurons using the same filter outputs a feature map, which highlights the areas in an image that activate the filter the most. You do not have to define the filters manually, during training the convolutional layer wil automatically learn the most useful filters for its task.

12.2.2 Convolutional Layers

The most important building block of a CNN is the *convolutional layer*, neurons in the first convolutional layer are not connected to every single pixel in the input image, but only to pixels in their receptive field. In turn each neuron in the second convolutional layer is connected only to neurons located within the small window in the first layer. This architecture allows the network to concentrate on small low-level features in the first hidden layer, then assemble them into larger higher-level features in the next hidden layer, and so on. For each window we apply the same filter / set of weights.



It is also possible to connect a large input layer to a smaller layer by spacing out the receptive fields, which reduces the complexity and dimensionality. The shift from one receptive field to the next is called the stride.



12.2.3 Pooling Layers

The goal of pooling layers is to *subsample* the input image in order to reduce the computational load, the memory usage, and the number of parameters (reducing risk of overfitting). Just like in convolutional layers, each neuron in a pooling layer is connected to the outputs of a limited number of neurons in the previous layer, located within a small rectangular receptive field. For each receptive field we must define its size, stride and padding type similar to the Convolutional Layer. The difference is that a pooling neuron has no weights; all it does is aggregate the inputs using an aggregation function such as max or mean. For example in a max pooling layer only the max value in each receptive field makes it to the next layer.

The pooling layers also introduce some level of *invariance* to small translations. For example when if you have a max pooling layer and you shift some pixels around in the receptive field the output for that receptive field will still be the same.

12.2.4 Parameters

- **Number of Filters**: integer indicating the number of filters applied to each window/receptive field.
- **Kernel Size**: tuple(width, height) indicating the size of the window/receptive field.
- **Stride**: tuple(horizontal, vertical) indicating the horizontal and vertical shift between each window/receptive field.
- **Padding**: "valid" or "same". Valid indicates no input padding. Same indicates that the input is padded with a border of zeros to ensure that the output has the same size as the input.

12.3 Benefits/Advantages

12.3.1 Sparse Interactions

Since there are fewer connections between layers due to the organization of the receptive fields then it is easier to train and less computationally expensive.

12.3.2 Parameter Sharing

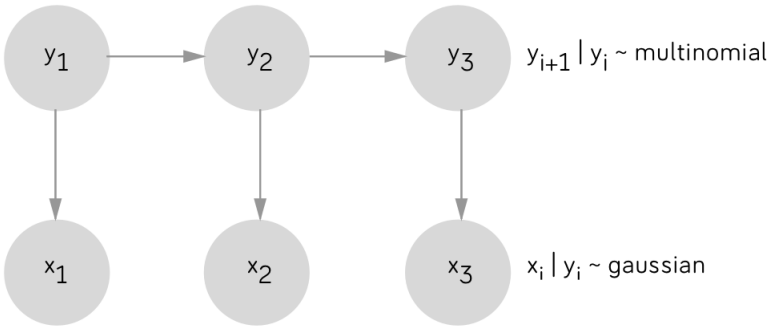
For each receptive field the same filter is applied so there are fewer weights that have to be computed also making it less computationally expensive and less complex.

12.3.3 Locally Equivariant Representation

With pooling layers we are able to make the network robust and invariant to translations as well as handle inputs of varying length.

13 Hidden Markov Models

Hidden Markov models provide a way to make predictions for a sequence of data where the prediction for one data point is dependent or correlated with the prediction for the next data point. This is different than other models that treat each data point independently. For example in speech recognition words can be recognized/interpreted based on the sound of the syllables before it. Hidden Markov models are a generalization of Mixture of Gaussians.



13.1 Assumptions

13.1.1 Stationary Process

Transition and emission distributions are identical at each step

$$P(x_t|y_t) = P(x_{t+1}|y_{t+1}) \; \forall t$$
$$P(y_t|y_{t-1}) = P(y_{t+1}|y_t) \; \forall t$$

13.1.2 Markovian Process

Next state is independent of previous states given the current statements

$$P(y_{t+1}|y_t, y_{t-1}, ..., y_1) = P(y_{t+1}|y_t) \; \forall t$$

13.1.3 Distributions

Initial Distribution

$$P(y_i) \sim multinomial$$

Transition Distribution

$$P(y_{i+1}|y_i) \sim multinomial$$

Emission Distribution

$$P(x_t|y_t) \sim gaussian(continuous)$$
$$\sim multinomial(discrete)$$

Joint Distribution

$$P(y_{1..t}, x_{1..t}) = P(y_1)\prod_{i=1}^{t-1} P(y_{i+1}|y_i)\prod_{i=1}^{t} P(x_i|y_i)$$

13.2 Inference in Temporal Models

There are many applications of Hidden Markov Models for example mobile robot localisation. In scenarios like we generally want to compute 4 common tasks:

- **Monitoring:** $P(y_t|x_{1..t})$
- **Prediction:** $P(y_{t+k}|x_{1..t})$
- **Hindsight:** $P(y_k|x_{1..t})$ where $k < t$
- **Most Likely Explanation:** $argmax_{y_1,\ldots,y_t} P(y_{1..t}|x_{1..t})$

13.2.1 Monitoring

$P(y_t|x_{1..t})$: distribution of current state given observations. We can employ recursive computation to decompose the query to be in terms of the probability of the previous hidden state.

$$P(y_t|x_{1..t}) \propto P(x_t)P(y_t)\sum_{y_{t-1}} P(y_t|y_{t-1})P(y_{t-1}|x_{1..t-1})$$

Now with this derivation we can compute $P(y_t|x_{1..t})$ by forward computation.

$P(y_1|x_1) \propto P(x_1|y_1)P(y_1)$
For $i = 2$ to t do

$$P(y_i|x_{1..i}) \propto P(x_i|y_i)\sum_{y_{i-1}} P(y_i|y_{i-1})P(y_{i-1}|x_{1..i-1})$$

End

Linear complexity in t

13.2.2 Prediction

$P(y_{t+k}|x_{1..t})$: distribution over future state up to k given observations. Using recursive computation we obtain

$$P(y_{t+k}|x_{1..t} = \sum_{y_{t+k-1}} P(y_{t+k}|y_{t+k-1})P(y_{t+k-1}|x_{1..t})$$

where we predict based on the previous state.

Now computing $P(y_{t+k}|x_{1..t})$ by forward computation, we first have to use monitoring until we need to do prediction.

For $j = 1$ to k do

$$P(y_{t+j}|x_{1..t}) = \sum_{y_{t+j-1}} P(y_{t+j}|y_{t+j-1})P(y_{t+j-1}|x_{1..t})$$

End

Linear complexity in $t + k$.

13.2.3 Hindsight

$P(y_k|x_{1..t})$ for $k < t$: distribution over a paste state give observations. Some examples of this are delayed activity/speech recognition.

Computation:

$$P(y_k|x_{1..t}) = P(y_k|x_{1..k})P(x_{k+1..t}|y_k)$$

We see this is composed of two parts the first being the forward monitoring and the latter being the backward part where we take the future observations and propagate them back. The latter can be expressed as:

$$P(x_{k+1..t}|y_k) = \sum_{y_{k+1}} P(y_{k+1}|y_k)P(x_{k+1}|y_{k+1})P(x_{k+2..t}|y_{k+1})$$

The algorithm for computation is the forward-backward algorithm expressed as follows.

1. Compute $P(y_k|x_{1..k})$ by forward computation (monitoring)

2. Compute $P(x_{k+1..t}|y_k)$ by backward computation

$$P(x_t|y_{t-1}) = \sum_t P(y_t|y_{t-1})P(x_t|y_t)$$

For $j = t - 1$ downto k do

$$P(x_{j..t}|y_{j-1}) = \sum_{y_j} P(y_j|y_{j-1})P(x_j|y_j)P(x_{j+1..t}|y_j)$$

End

3. $P(y_k|x_{k+1..t}) \propto P(y_k|x_{1..k})P(x_{k+1..t}|y_k)$

Linear complexity in t.

13.2.4 Most Likely Explanation

$argmax_{y_{1..t}} P(y_{1..t}|x_{1..t})$: most likely state sequence given observations.

Computation:

$$max_{y_{1..t}} P(y_{1..t}|x_{1..t}) = max_{y_t} P(x_t|y_t) max_{y_{1..t-1}} P(y_{1..t}|x_{1..t-1})$$

By Recursive Computation we get:

$$max_{y_{1..i-1}} P(y_{1..i}|x_{1..i-1}) \propto max_{y_{i-1}} P(y_i|y_{i-1}) P(x_{i-1}|y_{i-1}) max_{y_{1..i-2}} P(y_{1..i-1}|x_{1..i-2})$$

Now we can use this to compute $max_{y_{1..t}} P(y_{1..t}|x_{1..t})$ by dynamic programming.

13.2.4.1 Viterbi Algorithm

$max_{y_1} P(y_{1..2}|x_1) \propto max_{y_1} P(y_2|y_1) P(x_1|y_1) P(y_1)$
For $i = 2$ to $t-1$ do
    $max_{y_{1..i}} P(y_{1..i+1}|x_{1..i}) \propto max_{y_i} P(y_{i+1}|y_i) P(x_i|y_i) max_{y_{1..i-1}} P(y_{1..i}|x_{1..i-1})$
End
$max_{y_{1..t}} P(y_{1..t}|x_{1..t}) \propto max_{y_t} P(x_t|y_t) max_{y_{1..t-1}} P(y_{1..t}|x_{1..t-1})$

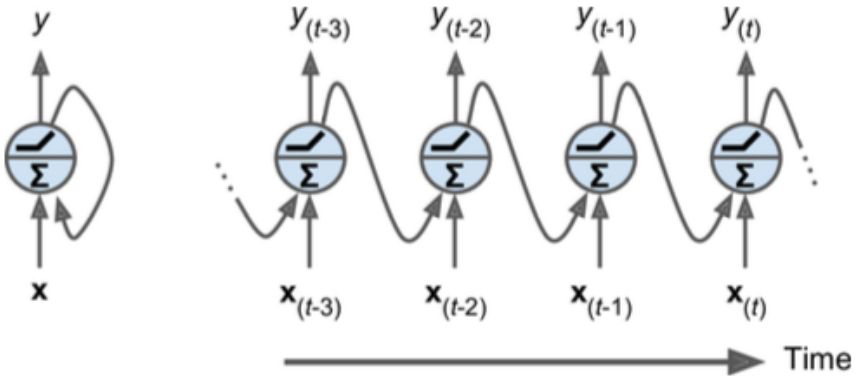
Linear complexity in t.

14 Recurrent Neural Networks

When posed with the problem of handling variable length data (e.g., sequences, time-series, spatial data) this poses a problem of a variable number of parameters. Using Recurrent Neural Networks we can handle sequences of variable length data, we can generalize this to handle trees and graphs using Recursive Neural Networks.

14.1 Recurrent Neurons

In Recurrent Neural Networks, the outputs can be fed back to the network as inputs, creating a recurrent structure that can be unrolled to handle varying length data. The simplest possible RNN, composed of one neuron receiving inputs, producing an output, and sending that output back to itself. At each time step t, this recurrent neuron receives the inputs $\boldsymbol{x}_t$ as well as its own output from the previous time step $\boldsymbol{y}_{t-1}$. Since there is no previous output at the first time step, it is generally set to 0.



To create a layer of recurrent neurons. At each time step t, every neuron receives both the input vector $\boldsymbol{x}_t$ and the output vector from the previous step $\boldsymbol{y}_{t-1}$. Each recurrent neuron has two sets of weights: one for the inputs $\boldsymbol{x}_t$ and the other for the outputs of the previous time step $\boldsymbol{y}_{t-1}$. call these weight vectors $\boldsymbol{w}_x$ and $\boldsymbol{w}_y$. If we consider the whole recurrent layer we can place all weight vectors in two weight matrices, $\boldsymbol{W}_x$ and $\boldsymbol{W}_y$.

The output of a recurrent layer for a single instance can be represented with the following equation where b is the bias vector and $\phi(\cdot)$ is the activation function.

$$\boldsymbol{y}_t = \phi(\boldsymbol{W}_x^T \boldsymbol{x}_t + \boldsymbol{W}_y^T \boldsymbol{y}_{t-1} + \boldsymbol{b})$$

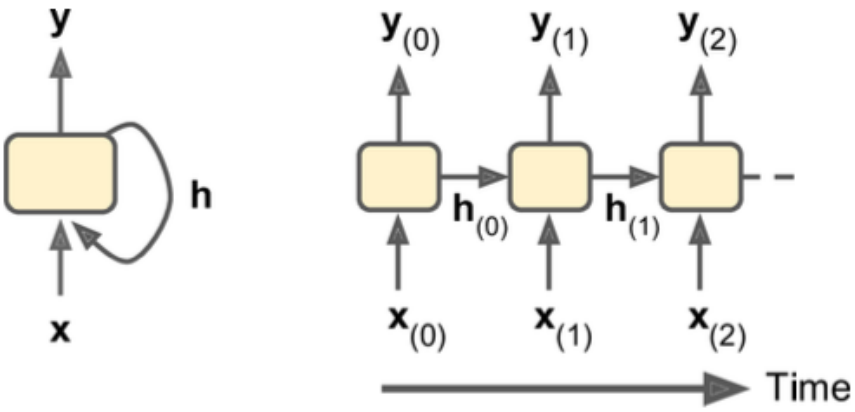
Similarly we can compute a recurrent layer's output using mini-batch by placing all the inputs at time step t in an input matrix $\boldsymbol{X}_t$.

$$\boldsymbol{Y}_t = \phi(\begin{bmatrix}\boldsymbol{X}_t & \boldsymbol{Y}_{t-1}\end{bmatrix} \boldsymbol{W} + \boldsymbol{b}) \text{ with } \boldsymbol{W} = \begin{bmatrix}\boldsymbol{W}_x \\ \boldsymbol{W}_y\end{bmatrix}$$

14.1.1 Memory Cells

The output of a recurrent neuron at time step t is a function of all the inputs from the previous steps, so it has some form of *memory*. A part of neural network that preservers some state across time steps is called a memory cell. A single recurrent neuron, or a layer of neurons is a very basic cell, capable of learning only short patterns.

In general a cell's tate at time step t, denoted $\boldsymbol{h}_t$, is a function of some inputs at that time step and its state at the previous time step: $\boldsymbol{h}_t = f(\boldsymbol{h}_{t-1}, \boldsymbol{x}_t)$. Its output at time step t, denoted $\boldsymbol{y}_t$, is also a function of the previous state and the current inputs. In the case of basic cells the output is equal to the state, but in more complex cells this is not always the case.



14.2 Bi-directional RNN

The recurrent networks we have considered up to now have a "causal" structure, meaning that the state at time t captures only information from the past, and the present input. In many applications, however, we what to output a prediction of $\boldsymbol{y}_t$ that may depend on the *whole input sequence*. For example, in speech recognition, the correct interpretations of the current sound as a phoneme may depend on the new fex phonemes because of co-articulation and may even depend on the next few words because of the linguistic dependencies between nearby words. This is also true of handwriting recognition and many other sequence-to-sequence learning tasks.

Bidirectional recurrent neural networks were invented to address that need. Bidirectional RNNs combine an rNN that moves forward through time, beginning from the start of the sequence with another RNN that moves backwards through time, beginning from the end of the sequence.

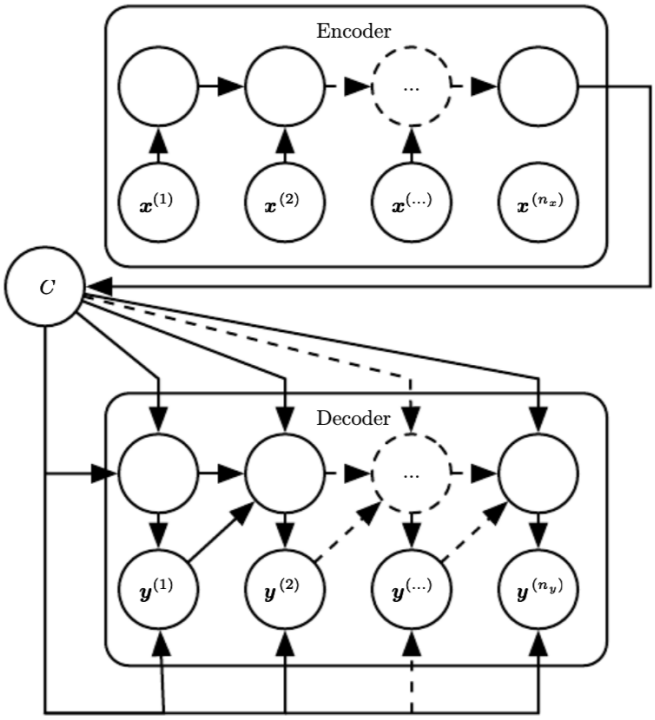
14.3 Encoder-Decoder Model

Often times when dealing with sequences of data the output sequence is not necessarily the same length as the input sequence. Additionally, sometimes the output is not always a one to one mapping with the input. A good example of this is language translation where translation from english to another language does not guarantee the sentence will be the same length or that the first word in an english sentence matches the first word in the output language. Here we discuss how an RNN can be trained to map an input sequence to an output sequence that is not necessarily of the same length.

We often call the input to the RNN the context. We want to produce a representation of this context, C. The context C might be a vector or sequence of vectors that summarize the input sequence $\boldsymbol{X}$.

The simplest RNN architecture for mapping a variable-length sequence to another variable-length sequence is the encoder-decoder or sequence-to-sequence architecture. The idea is illustrated with the following items. Let $\boldsymbol{x}^{(i)}$ be the i^{th} input and $\boldsymbol{y}^{(i)}$ by the i^{th} output.

- An encoder or reader or input RNN processes the input sequence. The encoder emits the context C, as a simple function of its final hidden state.
- A decoder or writer or output RNN is conditioned on that fixed-length vector to generate the output sequence $\boldsymbol{Y} = (\boldsymbol{y}^{(1)}, ..., \boldsymbol{y}^{(n_y)})$.



The innovation in this kind of architecture is that the lengths of the input (n_x) and the outputs (n_y) vary from each. Previous architectures constrained $n_x = n_y$. In a sequence-to-sequence architecture, the two RNNs are trained jointly to maximize the average of log $P(\boldsymbol{y}^{(1)}, ..., \boldsymbol{y}_{(n_y)} | \boldsymbol{x}^{(1)}, ...\boldsymbol{x}_{(n_x)})$ over all the pairs of $\boldsymbol{x}$ and $\boldsymbol{y}$ sequences in the training set. The last state $\boldsymbol{h}_{n_x}$ of the encoder RNN is typically used as a representation C of the input sequence that is provided as input to the decoder RNN.

One clear limitation of this architecture is when the context C output by the encoder RNN has a dimension that is too small to properly summarize a long sequence. To adapt to this they proposed to make C a variable-length sequence rather than a fixed-size vector. Additionally, attention mechanisms were introduced to associate elements of the sequence C to elements of the output sequence.

14.4 Long-Term Dependencies

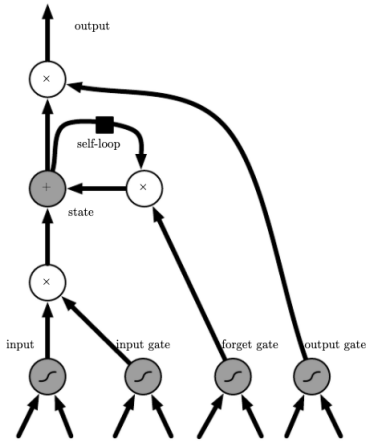
The mathematical challenge of learning long-term dependencies in recurrent networks is that gradients propagated over many staged tend to either vanish or explode (gradient vanishing problem). Even if we assume that the parameters are such that the recurrent network is stable. the difficulty with long-term dependencies arises from the exponentially smaller

weights give to long-term interactions compared to short-term ones. We will discuss some approaches to overcoming the problem.

The following methods discuss gated RNNs which are based on the idea of creating paths through time that have derivatives that neither vanish nor explode. Gated RNNs generalize this to connection weights that may change at each time step. Another mechanism that is introduced in gated RNNs is if a sequence is made of subsequences and we need to accumulate evidence inside each sub-sequence, we need a mechanism to forget the old state by setting it to zero. Instead of manually deciding when to clear the state, we want the neural network to learn to decide when to do it. This is what gated RNNs do.

14.4.1 Long Short-Term Memory

The clever idea of introducing self-loops to produce paths where the gradient can flow for long durations is a core contribution of the initial LSTM model. A crucial addition has been to make the weight on this self-loop conditioned on the context, rather than fixed. By making the weight of this self-loop gated (controlled by another hidden unit), the time scale of integration can be changed dynamically. This means that even for an LSTM with fixed parameters, the time scale of integration can change based on the input sequence, because the time constants are output by the model itself.



Instead of a unit that simply applies an element-wise nonlinearity to the affine transformation of inputs and recurrent units, LSTM recurrent networks have "LSTM" cells that have an internal recurrence, in addition to the outer recurrence of the RNN. Each cell has the same inputs and outputs as an ordinary recurrent network, but also has more parameters and a system of gating units that controls the flow of information. The most important component is the cell state unit, which has a linear self-loop. Here the self-loop weight is controlled by a forget gate unit. The learning equations for the LSTM cell are as follows:

- Input gate: $i_t = \sigma(W^{(ii)}\overline{x}_t + W^{(hi)}h_{t-1})$
- Forget gate: $f_t = \sigma(W^{(if)}\overline{x}_t + W^{(hf)}h_{t-1})$
- Output gate: $o_t = \sigma(W^{(io)}\overline{x}_t + W^{(ho)}h_{t-1})$

- Process input: $\overline{c}_t = tanh(W^{(i\overline{c})} + W^{(h\overline{c})}h_{t-1})$
- Cell update: $c_t = f_t * c_{t-1} + i_t + \overline{c}_t$
- Output: $y_t = h_t = o_t * tanh(c_t)$

14.4.2 Gated Recurrent Units

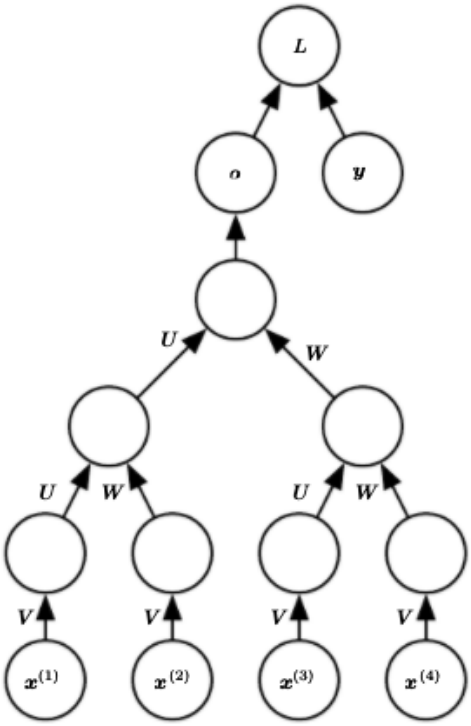
Not all pieces of the LSTM architecture are actually necessary. The main difference with the LSTM and the GRU is that a single gating unity simultaneously controls the forgetting factor and the decision to update the state unit. The update equations are the following:

- Reset gate: $r_t = \sigma(W^{(ir)}\overline{x}_t + W^{(hr)}h_{t-1})$
- Update gate: $z_t = \sigma(W^{(iz)}\overline{x}_t + W^{(hz)}h_{t-1})$
- Process input: $\overline{h}_t = tanh(W^{(i\overline{h})}\overline{x}_t + r_t * (W^{(h\overline{h})}h_{t-1}))$
- Hidden state update: $h_t = (1 - z_t) * h_{t-1} + z_t * \overline{h}_t$
- Output: $y_t = h_t$

The reset and update gates can individually "ignore" parts of the state vector. The update gates act like conditional leaky integrators that can linearly gate any dimension, thus choosing to copy it or completely ignore it by replacing it with the new target state value. The reset gates control which parts of the state get used to compute the next target state, introducing an additional nonlinear effect in the relationship between past state and future state.

14.5 Recursive Neural Networks

Recursive Neural Networks represent a generalization of recurrent neural networks, with a different kind of computational graph, which is structured as a deep tree, rather than chain-like structure of RNNs. Recursive networks have been successfully applied to processing data structures as inputs to neural nets, in natural language processing, as well as in computer vision.



One advantage of recursive nets over recurrent nets is that for a sequence of the same length τ, the depth can be drastically reduced from τ to $O(log\tau)$, which might help deal with long term dependencies. The key question is how to best structure the tree. One option is to have a tree structure that does not depend on the data. In some application domains, external methods can suggest the appropriate tree structure. Ideally one would like the learner itself to discover and infer the tree structure that is appropriate for any give input.

14.6 Attention

Attention is a mechanism for alignment in models where the output and input are of variable-length. This lets us align inputs with their corresponding outputs in applications such as machine translation, image captioning and more. Attention in machine translation is where we align each output word with relevant input words by computing a softmax of the inputs as follows.

Context vector c_i: weighted sum of input encodings h_j

$$c_i = \sum_j a_{ij} h_j$$

a_{ij} is an alignment weight between input encoding h_j and output encoding s_i.

$$a_{ij} = \frac{exp(alignment(s_i, h_j))}{\sum_{ji} exp(alignment(s_i, h_{j'}))}$$

Alignment example: $alignment(s_i, h_j) = s_i^T h_j$

14.7 Training

To train a RNN, the trick is to unroll it through time and then use regular back propagation. This strategy is called backpropagation through time. The algorithm will also consider weight sharing will also play a part where we combine gradients of shared weights into a single gradient.

There is first a forward pass through the unrolled network. Then the output sequence is evaluated using a cost function. The gradients of that cost function are then propagated backward through the unrolled network. Finally the model parameters are updated using the gradients computed during backpropagation through time.

14.7.1 Challenges

Some challenges that training brings up, is the gradient vanishing and explosion problem. Another issue is the Long Range memory problem, although a RNN can handle sequences of events but there is no guarantee it will remember information from the first input. This is specifically important applications like machine translation where every input is equally important so you need the long term memory. Lastly, prediction drift is another challenge when training RNN's. Prediction drift is the idea that predictions far into the future will have error from the previous predictions propagated through to it and therefore be less accurate.

15 Transformer Networks

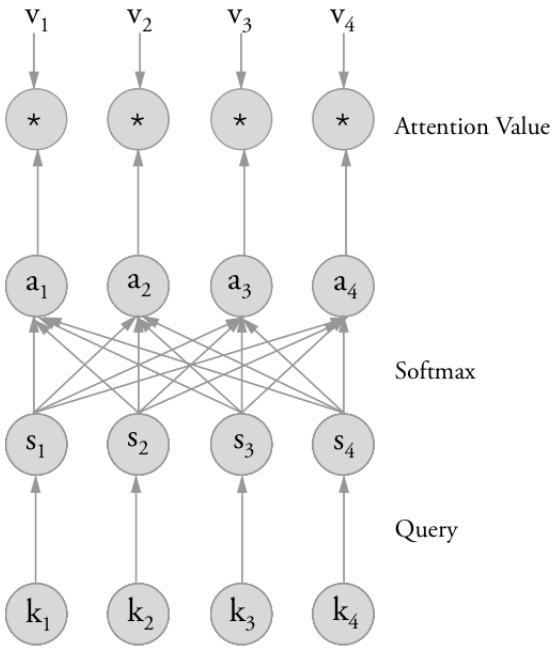
There exist many challenges with RNNs and so Transformer Networks were creating to overcome these challenges. RNNs possessed challenges like having long range dependencies, gradient vanishin and explosion, large number of training steps, and recurrence prevents parallel computation. Transformer network are able to mitigate or resolve all of these challenges.

15.1 Attention Mechanism

We can think about attention as some form of approximation of a SELECT that you would do on a database. If you want to retrieve a value based on a query to find some key. We can think about attention being a neural process that mimics the retrieval of a value $\boldsymbol{v}_i$ for a query q based on a key k_i, in a more fuzzy probabilistic way.

$$attention(q, \boldsymbol{k}, \boldsymbol{v}) = \sum_i similarity(q, k_i) \times v_i$$

We can outline the neural architecture for the attention mechanism as follows.



s_i is the similarity and is commonly computed as the following:

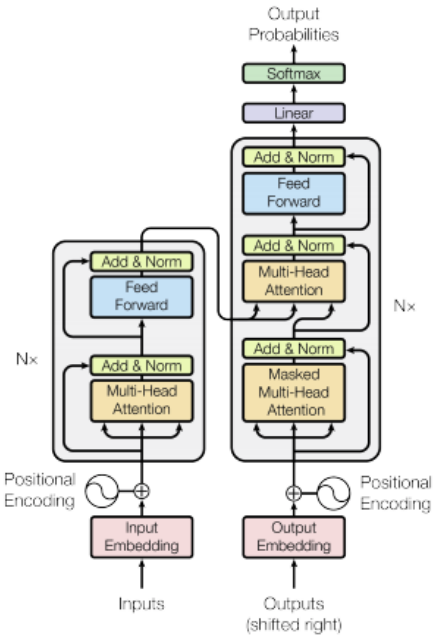
$$s_i = f(q, k_i) \begin{cases} q^T k_i & \text{dot product} \\ \frac{q^T k_i}{\sqrt{d}} & \text{scaled dot product, } d \text{ is dimensionality} \\ q^T \boldsymbol{W} k_i & \text{general dot product} \\ w_q^T q + w_k^T k_i & \text{additive similarity} \end{cases}$$

a_i is the output of the softmax and can be computed as:

$$a_i = \frac{exp(s_i)}{\sum_j exp(s_j)}$$

Finally the $*$ is the attention value computed as $\sum_i a_i v_i$.

15.2 Architecture



15.2.1 Encoder

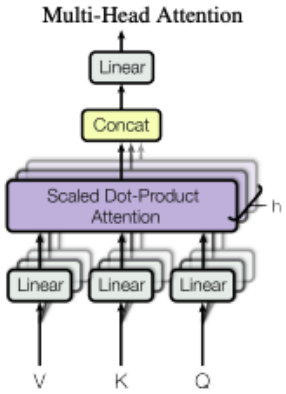
The path of the data starts from feeding an entire sequence into the encoder. It first goes through positional encoding, which captures the order of the sequence of the input. It then passes to the multi-head attention which is computing the attention between every position and every other position. This treats every input as a query and finds some keys that correspond to the other inputs and take a convex combination of the corresponding values and then take a dot product of that to produce a better embedding. In essence it finds similar inputs and merges them together to form better inputs. Now if we repeat this N times, then in the first iteration we look at pairs and then the next iteration pairs of pairs and so on, so we can find similarities between groups of inputs to create optimal embeddings for sequences. The add and norm layer following the multi-head attention is essentially adding a residual connection that takes the original to what comes out of the multi-head attention and then it normalizes (0 mean and 1 variance) this. The output of this is a sequence of embeddings that captures each input but also the relation to other inputs in the sequence.

15.2.2 Decoder

The decoder is required to produce an output so it is complemented at the top with a softmax and linear layer. The first masked multi-head attention on the decoder side that is used for simply combining output words with previous output words. This is a masked multi-head attention because you want to ensure that you are only generating future words based on the previous words so we "mask" the future words. The other multi-head attention block combines output words with input words and then finally a feed forward neural network again.

15.2.3 Multi-head Attention

Multi-head attention: compute multiple attentions per query with different weights.



$$multihead(Q, K, V) = W^o concat(head_1, head_2, ..., head_h)$$
$$head_i = attention(W_i^Q Q, W_i^K K, W_i^V V)$$
$$attention(Q, K, V) = softmax(\frac{Q^T K}{\sqrt{d_k}})V$$

15.2.4 Masked Multi-head Attention

Masked multi-head attention is where some values are masked. When decoding, an output value should only depend on previous outputs (not future outputs). Hence we mask future outputs.

$$attention(Q, K, V) = softmax(\frac{Q^T K}{\sqrt{d_k}})V$$
$$maskedAttention(Q, K, V) = softmax(\frac{Q^T K + M}{\sqrt{d_k}})V$$

where M is a mask matrix of 0's and $-\infty$'s

15.2.5 Layer Normalization

The normalization layer exists above every multi-head attention. Essentially what it does is reduce the number of steps required by gradient descent to optimize the network. This normalizes the values in each layer to have 0 mean and 1 variance.

For each hidden unit h_i we compute

$$h_1 \leftarrow \frac{g}{\sigma}(h_i - \mu)$$

where g is a variable and

$$\mu = \frac{1}{H}\sum_{i=1}^{H} h_i$$

$$\sigma = \sqrt{frac1H \sum_{i=1}^{H} (h_i - \mu)^2}$$

This reduces covariate shift (gradient dependencies between each layer) and therefore fewer training iterations are needed.

15.2.6 Positional Embedding

The attention mechanism does not care about the position of the input, they could be all shuffled, if it wasn't for the positional embedding we could get the same output. The ordering carries meaning in many cases and so we use this positional encoding to keep track of this ordering.

$$PE_{position,2i} = sin(position/10000^{2i/d})$$
$$PE_{position,2i+1} = cos(position/10000^{2i/d})$$

16 Autoencoder

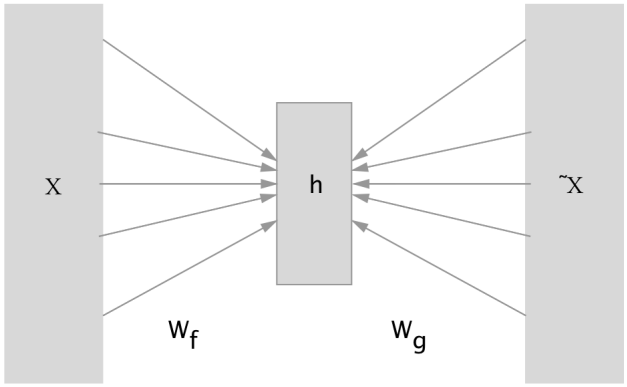
An autoencoder is a special type of feed forward neural network used for:

- Compression
- Denoising
- Sparse Representation
- Data Generation

An autoencoder is a neural network that is trained to attempt to copy its input to its output. Internally, it has a hidden layer $\boldsymbol{h}$ that describes a code used to represent the input. The network consists of tow parts: an encoder function $\boldsymbol{h} = f(\boldsymbol{x})$ and a decoder that produces a reconstruction $\boldsymbol{r} = g(\boldsymbol{h})$.

16.1 Linear Autoencoder

Let f and g be linear and their respective weight matrices be $\boldsymbol{W}_f$ and $\boldsymbol{W}_g$. We then represent the network as below where $\boldsymbol{h} = \boldsymbol{W}_f \boldsymbol{x}$ and $\tilde{X} = \boldsymbol{W}_g \boldsymbol{h}$.



Objective: find weights $\boldsymbol{W}_f$ and $\boldsymbol{W}_g$ that minimize the reconstruction error

$$min_{\boldsymbol{w}} \frac{1}{2} \sum_n \|\boldsymbol{W}_g \boldsymbol{W}_f \boldsymbol{x}_n - \boldsymbol{x}_n\|_2^2$$

We can use back propagation to train the neural network. When using Euclidean Norm (i.e squared loos), the solution is the same as principal component analysis (PCA).

16.1.1 Principal Component Analysis

PCA is typically used to project higher dimensional data and map it on to a lower dimensional hyper plane such that it preserves as much as possible variations in the data. In principle this means we could reconstruct the original data as closely as possible.

16.2 Non-linear Autoencoder

Let f and g be non-linear functions then we can represent the objective as:

$$min_{\boldsymbol{w}} \frac{1}{2} \sum_n \|g(f(\boldsymbol{x}_n; \boldsymbol{W}_f); \boldsymbol{W}_g) - \boldsymbol{x}_n\|_2^2$$

The hidden nodes in a non-linear autoencoder represent a non-linear manifold. What we are doing by computing some hidden representation here would be to take our data and project it on to a lower dimensional space that is not linear anymore because I allow myself to have non-linear mappings.

16.3 Deep Autoencoders

In deep autoencoders we have multiple layers (f) before we reach the hidden layers and we have multiple layers (g) to reconstruct as well. In theory, one hidden layer in f and g is sufficient to represent any possible compression, however, multiple layers in f and g is often better.

16.4 Regularizing Autoencoders

16.4.1 Sparse Representations

When there are more hidden nodes than inputs, we need to use regularization to constrain the autoencoder. We can do this by forcing the hidden nodes to be sparse:

$$min_{\boldsymbol{w}} \frac{1}{2} \sum_n \|g(f(\boldsymbol{x}_n; \boldsymbol{W}_f); \boldsymbol{W}_g) - \boldsymbol{x}_n\|_2^2 + c\, nnz(f(\boldsymbol{x}_n; \boldsymbol{W}_f))$$

where $nnz(f(\boldsymbol{x}_n; \boldsymbol{W}_f))$is the number of non-zero entries in the vector produced by f.

Approximate objective: L1 regularization becomes:

$$min_{\boldsymbol{w}} \frac{1}{2} \sum_n \|g(f(\boldsymbol{x}_n; \boldsymbol{W}_f); \boldsymbol{W}_g) - \boldsymbol{x}_n\|_2^2 + c\|f(\boldsymbol{x}_n; \boldsymbol{W}_f)\|_1$$

16.4.2 Denoising Autoencoders

Let us consider the noisy version $\tilde{\boldsymbol{x}}$ of the input $\boldsymbol{x}$. Then we can denoise the data with the following objective.

$$min_{\boldsymbol{w}} \frac{1}{2} \sum_n \|g(f(\tilde{\boldsymbol{x}}_n; \boldsymbol{W}_f); \boldsymbol{W}_g) - \boldsymbol{x}_n\|_2^2 + c\|f(\tilde{\boldsymbol{x}}_n; \boldsymbol{W}_f)\|_1$$

16.5 Probabilistic Autoencoder

Probabilistic or stochastic encoders have interesting properties that allow us to generate data. We can express an probabilistic autoencoder as follows. Let f and g represent conditional distributions $f : P(\boldsymbol{h}|\boldsymbol{x}; \boldsymbol{W}_f)$ and $g : P(\boldsymbol{x}|\boldsymbol{h}; \boldsymbol{W}_g)$. The encoder is essentially a conditional distribution over the intermediate representation and the decoder is a conditional with respect to the input we are trying to produce. We can use sigmoid, softmax at the hidden and output layers to output classifications based on distributions of data.

16.5.1 Generative Model

Based on probabilistic autoencoders we use this architecture to generate new data. If we want to generate new data points that are similar to the data point we had in the data set then the beauty of having a distribution is that we can sample from distribution over the intermediate representation $\boldsymbol{h}$. Then for every point h we sampled we can produce some output. The formal steps are as follows

- Sample $\boldsymbol{h}$ from some distribution $P(\boldsymbol{h})$.
- Sample $\boldsymbol{x}$ from decoder $P(\boldsymbol{x}|\boldsymbol{h}; \boldsymbol{W}_g)$

The one underlying problem with this is that we need some distribution that we can sample from. This distribution is conditioned on $\boldsymbol{X}$ so the new data generated we are producing is still going to be relativisitically similar to the input data.

17 Generative Networks

Generative Networks are is a learning task that involves automativally discovering and learning the regularities of patterns in input data in such a way that the model can be used to generate or output new data that could have been drawn from the original dataset.

17.1 Variational Autoencoder

Variational autoencoders were created to combat the problem of generative modelling using probabilistic autoencoders. The idea behind a variational autoencoder is to train an encoder $P(\boldsymbol{h}|\boldsymbol{x};\boldsymbol{W}_f)$ to approach a simple and fixed distribution e.g. $N(\boldsymbol{h};0,\boldsymbol{I})$. This way we can set the prior distribution $P(\boldsymbol{h})$ to $N(\boldsymbol{h};0,\boldsymbol{I})$.

We construct the objective

$$max_{\boldsymbol{w}} \sum_n logP(\boldsymbol{x}_n;\boldsymbol{W}_f,\boldsymbol{W}_g) - c\, KL(P(\boldsymbol{h}|\boldsymbol{x}_n;\boldsymbol{W}_f)||N(\boldsymbol{h};0,\boldsymbol{I}))$$

where the first part essentially tries to maximize the probability of reconstructing $\boldsymbol{x}$ and the second part is some sort of regularization term. The second part tries to make sure that our encoder has a distribution over $\boldsymbol{h}$ conditioned on $\boldsymbol{x}$ that is as close as possible to the fixed distribution $N(\boldsymbol{h};0,\boldsymbol{I})$.

17.1.1 Evaluation

How do we compute $P(\boldsymbol{x}_n;\boldsymbol{W}_f,\boldsymbol{W}_g)$?

$$\mathrm{P}\left(\boldsymbol{x}_n;\boldsymbol{W}_f,\boldsymbol{W}_g\right) = \int_{\boldsymbol{h}} \mathrm{P}\left(\boldsymbol{x}_n \mid \boldsymbol{h};\boldsymbol{W}_g\right) \mathrm{P}\left(\boldsymbol{h} \mid \boldsymbol{x}_n;\boldsymbol{W}_f\right) d\boldsymbol{h}$$

since $\mathrm{P}\left(\boldsymbol{h} \mid \boldsymbol{x_n};\boldsymbol{W}_f\right)$ should approach $N(\boldsymbol{h};0,\boldsymbol{I})$ then force $\mathrm{P}\left(\boldsymbol{h} \mid \boldsymbol{x_n};\boldsymbol{W}_f\right)$ to be Gaussian

$$\mathrm{P}\left(\boldsymbol{h} \mid \boldsymbol{x}_n;\boldsymbol{W}_f\right) = N\left(\boldsymbol{h};\mu_n\left(\boldsymbol{x}_n;\boldsymbol{W}_f\right),\sigma_n\left(\boldsymbol{x}_n;\boldsymbol{W}_f\right)\boldsymbol{I}\right)$$

where the mean μ_n and variance σ_n are obtained by a neural net in $\boldsymbol{x}_n$ parameterized by $\boldsymbol{W}_f$. Now we approximate the integral over $\boldsymbol{h}$

$$\begin{aligned}&\mathrm{P}\left(\boldsymbol{x}_n;\boldsymbol{W}_f,\boldsymbol{W_g}\right)\\ &= \textstyle\int_{\boldsymbol{h}} \mathrm{P}\left(\boldsymbol{x}_n \mid \boldsymbol{h};\boldsymbol{W}_g\right) N\left(\boldsymbol{h};\mu_n\left(\boldsymbol{x}_n;\boldsymbol{W}_f\right),\sigma_n\left(\boldsymbol{x}_n;\boldsymbol{W}_f\right)\boldsymbol{I}\right) d\boldsymbol{h}\end{aligned}$$

by a single sample

$$\mathrm{P}\left(\boldsymbol{x}_n;\boldsymbol{W}_f,\boldsymbol{W_g}\right) \approx \mathrm{P}\left(\boldsymbol{x}_n \mid \boldsymbol{h}_n;\boldsymbol{W}_g\right)$$

where $\boldsymbol{h}_n \sim N\left(\boldsymbol{h};\mu_n\left(\boldsymbol{x}_n;\boldsymbol{W}_f\right),\sigma_n\left(\boldsymbol{x}_n;\boldsymbol{W}_f\right)\boldsymbol{I}\right)$

17.1.2 Training

When doing training we want to do gradient descent, however, since we are taking a single sample between the encoder and decoder we can't use gradient descent through the entire network. Instead the key hear is that we want to use reparameterization so that we first sample from a different distribution, perform some operations on the sample until it becomes effectively a sample from the distribution that I was initially interested in. By doing this, when gradient is performed instead of having to propagate over a sampling step it is now a combination of mathematical operators over which it is traversing.

17.2 Generative Adverserial Networks

GAN's are generative networks with an approach based on game theory they consist of two networks:

- Generator $g\left(\boldsymbol{z}; \boldsymbol{W}_g\right) \rightarrow \boldsymbol{x}$
- Discriminator $d\left(\boldsymbol{x}; \boldsymbol{W}_d\right) \rightarrow \mathrm{P}(\boldsymbol{x}$ is real)

The generator is responsible of generating new datapoints. The discriminator's job is to predict whether some data point is real or not, it is basically providing feedback to the generator whether the produced data point is real or not.

The objective:

$$\min_{W_g} \max_{\boldsymbol{W}_d} \sum_n \log \mathrm{P}\left(\boldsymbol{x}_n \text{ is real}; \boldsymbol{W}_d\right) + \log \mathrm{P}\left(g\left(\mathbf{z}_n; \boldsymbol{W}_g\right) \text{ is fake}; \boldsymbol{W}_d\right)$$

$$= \min_{\boldsymbol{w}_g} \max_{\boldsymbol{W}_d} \sum_n \log d\left(\boldsymbol{x}_{\boldsymbol{n}}; \boldsymbol{W}_d\right) + \log\left(1 - d\left(g\left(\mathbf{z}_n; \boldsymbol{W}_g\right); \boldsymbol{W}_d\right)\right)$$

In this objective the discriminator is going to maximize the probability with which it can recognize data points from our training set as being real and it is also going to try to maximize the probability that the data points that are generated by the generator are fake. If it can distinguish between real data points and fake data points then it is still able to pick out some differences and that is what it will try to achieve. The generator is trying to fool the discriminator so it will try to minimize these probabilities.

17.2.1 Training

Repeat until convergence

- For k steps do
  - Sample $\boldsymbol{z}_1, \ldots, \boldsymbol{z}_N$ from $P(\boldsymbol{z})$
  - Sample $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$ from training set
  - Update discriminator by ascending its stochastic gradient

$$\nabla_{\boldsymbol{W}_d}\left(\frac{1}{N} \sum_{n=1}^{N}\left[\log d\left(\boldsymbol{x}_{\boldsymbol{n}}; \boldsymbol{W}_d\right) + \log\left(1 - d\left(g\left(\mathbf{z}_n; \boldsymbol{W}_g\right); \boldsymbol{W}_d\right)\right)\right]\right)$$

- Sample $\boldsymbol{z}_1, \ldots, \boldsymbol{z}_N$ from $P(\boldsymbol{z})$
- Update generator by descending its stochastic gradient

$$\nabla_{\boldsymbol{W}_g} \left(\frac{1}{N} \sum_{n=1}^{N} \log \left(1 - d \left(g \left(\mathbf{z}_n; \boldsymbol{W}_g \right); \boldsymbol{W}_d \right) \right) \right)$$

In the end we are looking for a distribution that corresponds to the true data distribution and so in the limit we would like the generator to have a distribution over the space of data to be the same as the distribution as that of the training set. $P(\boldsymbol{x}|\boldsymbol{z}; \boldsymbol{W}_g)$ should be equal to our true data distribution and similarly the discriminator should have a 50 % confidence about its prediction of real or fake data; $P(\boldsymbol{x} \text{ is real}; \boldsymbol{W}_d) = 0.5$.

Problems with this in practice are that there may be a training imbalance where one network may dominate the other and also there is a risk of local convergence.

18 Ensemble Learning

Sometimes individual learning techniques yields a different hypothesis and none of them are perfect. The idea here with ensemble learning is to combine multiple imperfect hypothesis to form a better hypothesis. The intuition here is that individuals often make mistakes, but the "majority" is less likely to make mistakes. Individuals can also pool knowledge together to make better decisions.

18.1 Formulation

Ensemble learning is the method of selecting and combining and ensemble of hypotheses into a better hypothesis. This allows us to enlarge the hypothesis space: when we have a pereceptrons we have linear separators but with an ensemble of perceptrons we get a polytope.

18.2 Bagging

The idea behind bagging is that we have a pool of hypotheses h that are fed an input $\boldsymbol{x}$. We then set the output to be the majority output from the pool of hypotheses. To formulate this we make the assumption that each h_i makes error with probability p and that each hypothesis is independent. We can them compute the following probabilities.

- k hypotheses make an error: $\binom{n}{k} p^k (1-p)^{(n-k)}$
- Majority makes an error: $\sum_{k>n/2} \binom{n}{k} p^k (1-p)^{(n-k)}$
- With $n = 5, p = 0.1 \rightarrow err(majority) < 0.01$

18.2.1 Weighted Majority

In practice the above is rarely the case. Hypotheses are rarely independent and some hypotheses have less than others. One way to tackle this problem is taking a weighted majority instead. The intuition being we can decrease the weight of correlated hypotheses and increase the weight of the good hypotheses.

18.2.2 Independent Classifiders/Predictors

If we want to obtain independent classifiers/predictors for bagging we can try one of two things. Boostrap sample and random projection.

Boostrap sampling involves sampling (without replacement) a subset of the data. Each time we train a base learner to produce a hypothesis then the hypothesis produced will have less correlation with the other hypotheses because they are trained on a subset of the data.

Similarly a method that does this with the features is called random projection. The idea is that we have a set of features and normally we want to use all the features when making a prediction, however, instead we can subsample the features to obtain predictors with less correlation.

With bootsrap sampling and random projection we learn different classifiers/predictors based on each data subset and feature subset.

18.2.2.1 Algorithm

- For $k = 1$ to K
  - $\boldsymbol{D}_k \leftarrow$ sample data subset
  - $\boldsymbol{F}_k \leftarrow$ sample feature subset
  - $h_k \leftarrow$ train classifier/predictor based on $\boldsymbol{D}_k$ and $\boldsymbol{F}_k$
- Classification: $majority(h_1(\boldsymbol{x}), ..., h_k(\boldsymbol{x}))$
- Regression: $average(h_1(\boldsymbol{x}), ..., h_k(\boldsymbol{x}))$

18.3 Boosting

Boosting is a popular ensemble learning technique that computes a weighted majority and it obtains hypotheses by using a base learning technique that produces classifiers. The base learner can be a weak learner (bad learning technique) and by pooling a lot of the resulting hypotheses we can obtain a higher accuracy and effectively boost the weak learner. The idea here is to boost weak learners and compensate for their weakness to increase accuracies. The way to do this in practice is by reweighting the training set, the weak learner will take the original dataset produce a hypothesis and then we will perturb the dataset and the weak learner will produce a new hypothesis. We then repeat till we are satisfied. The intuition behind this is that if have some instances that are misclassified by one hypothesis then we

increase their weight: make them more important so that the next time around the algorithm a better chance to classify those instances correctly.

We can boost anything that is weak learner which is classified as something that produces hypotheses that are at least as good as random classifiers (50%). It also has the following advantages:

- No need to learn perfect hypothesis
- Can boost any weak learning algorithm
- Boosting is simple to program
- Good generalization

18.3.1 Weighted Training Set

The main principle behind boosting is learning with a weighted training set. We will use supervised learning to minimize the train error and apply a bias algorithm to learn correctly the instances with high weights.

The idea is that when an instance is misclassified by a hypothesis, we are going to increase its weight so that the next hypothesis is more likely to classify it correctly.

18.3.2 Boosting Framework

- Set all instance weights $\boldsymbol{w}_x$ to 1.
- Repeat until sufficient nnumber of hypotheses
  - $h_i \leftarrow$ learn(dataset, weights)
  - Increase $\boldsymbol{w}_x$ of misclassified instances $\boldsymbol{x}$

Ensemble hypothesis is the weighted majority of h_i's with weights $\boldsymbol{w}_i$ proportional to the accuracy of h_i.

18.3.3 Adaptive Boosting

Let w be the vector of N instance weights and z be the vector of M hypothesis weights. This algorithm is used in the context of classification.

- $w_j \leftarrow \frac{1}{N} \forall_j$
- For $m = 1$ to M do
  - $h_m \leftarrow$ learn(dataset, w)
  - err $\leftarrow 0$
  - For each (x_j, y_j) in dataset do
    - if $h_m(x_j) \neq y_j$ then err $\leftarrow err + w_j$

- For each (x_j, y_j) in dataset do
  - if $h_m(x_j) \neq y_j$ then $w_j \leftarrow err/(1-err)$
- $w \leftarrow normalize(w)$
- $z_m \leftarrow log[(1-err)/err]$

- Return $weighted - majority(h, z)$

18.3.4 Gradient Boosting

Gradient boosting is a method designed to do boosting for regression. The idea is we start with a predictor f that is a regression technique (hypothesis/function) that makes a prediction for some input. The predictor f_k incurs loss $L(f_k(\boldsymbol{x}, y))$ at stage k.

Given the loss function we want to compute the negative gradient of the loss function with respect to the current predictor f_k. The idea is then to fit the next predictor to this negative gradient. We train h_{k+1} to approximate the negative gradient:

$$h_{k+1}(\boldsymbol{x}) \approx -\frac{\partial L(f_k \boldsymbol{x}, y)}{\partial f_k(\boldsymbol{x})}$$

Now we can update the predictor by adding a multiple α_{k+1} of h_{k+1} to simulate gradient descent since we are adding a multiple of the gradient which we are approximating with h_{k+1}.

$$f_{k+1}\boldsymbol{x} \leftarrow f_k(\boldsymbol{x}) + \alpha_{k+1} h_{k+1}(\boldsymbol{x})$$

The base learner h_{k+1} can be any non-linear predictor and is often a small decision tree.

18.3.4.1 Algorithm

- Initialize predictor with a constant c :

$$f_0\left(\boldsymbol{x}_n\right) = \text{argmin}_c \sum_n L\left(c, y_n\right)$$

- For $k = 1$ to K do
  - Compute pseudo residuals: $r_n = -\frac{\partial L(f_{k-1}(x_n), y_n)}{\partial f_{k-1}(x_n)}$
  - Train a base learner h_k with residual dataset $\{(\boldsymbol{x}_n, r_n)_{\forall n}\}$
  - Optimize step length:

$$\eta_k = \text{argmin}_\eta \sum_n L\left(f_{k-1}\left(\boldsymbol{x}_n\right) + \eta h_k\left(\boldsymbol{x}_n\right), y_n\right)$$

  - Update predictor: $f_k(\boldsymbol{x}) \leftarrow f_{k-1}(\boldsymbol{x}) + \eta_k h_k(\boldsymbol{x})$

This algorithm is still prone to overfitting. We can reduce overfitting by incorporating a validation and stopping when the loss starts increasing.