## 1. Regularizations

## L1 Regularization (Lasso Regression)

$$\sum_{i=1}^{n} \left( y_i - \sum_{j=1}^{p} x_{ij} \beta_j \right)^2 + \lambda \sum_{j=1}^{p} |\beta_j|$$

• L1 regularization tends to produce sparse weight vectors, meaning it encourages some of the weights to be exactly zero. This can be useful for *feature selection*, as it effectively removes irrelevant features.

## L2 Regularization (Ridge Regression)

$$\sum_{i=1}^{n} \left( y_i - \sum_{j=1}^{p} x_{ij} \beta_j \right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2$$

• L2 regularization tends to produce weight vectors with smaller values overall. It penalizes large individual weights but does not typically force them to become exactly zero. *It helps to prevent overfitting by controlling the magnitude of the weights.* 

<u>Note</u>: the regularization methods can also be applied on logistic regression models. L1 versus L2 – See Ace the Data Science Interview Page 130 Solution #7.20.

# 2. Logistic Regressions – sigmoid & softmax functions

In the two-class logistic regression, the predicted probabilities are as follows, using **the sigmoid function**:

$$P(Y_i = 1) = \frac{1}{1 + e^{-\beta \cdot X_i}}$$

In the multiclass logistic regression, with K classes, the predicted probabilities are as follows, using **the softmax function**:

$$P(Y_i = k) = \frac{e^{\beta_k \cdot X_i}}{\sum_{0 \le c \le K} e^{\beta_c \cdot X_i}}$$

## 3. Variance-Bias Trade-off

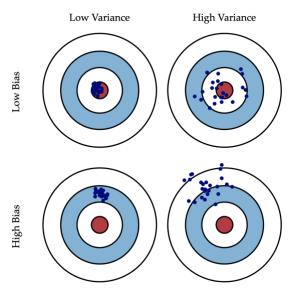
### **Conceptual Definition**

Bias: Error introduced by simplifying a model; high bias can lead to underfitting.

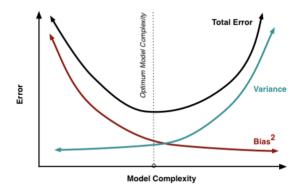
Variance: Error introduced by model sensitivity to training data; *high variance can lead to overfitting*.

The trade-off aims for an optimal balance, minimizing both bias and variance to achieve a model that generalizes well to new, unseen data.

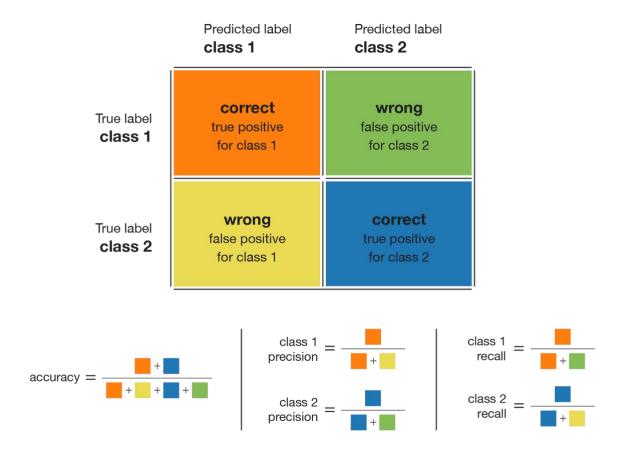
## **Graphical Illustration**



At its root, dealing with bias and variance is really about dealing with over- and under-fitting. *Bias is reduced and variance is increased in relation to model complexity*. As more and more parameters are added to a model, the complexity of the model rises and variance becomes our primary concern while bias steadily falls. For example, as more polynomial terms are added to a linear regression, the greater the resulting model's complexity will be.



## 4. Confusion Matrix



- The **precision** of a class define *how trustable* is the result when the model answer that a point belongs to that class. **Precision**: True Positive/**Predicted Positive**
- The **recall** of a class expresses *how well* the model is able to detect that class/what proportion of samples are correctly classified. Low recall value means our model is not doing well for this class. **Recall**: True Positive/**Real** Positive
- The **accuracy** of the model is basically the total number of correct predictions divided by total number of predictions.
- The **F1** score of a class is given by the harmonic mean of precision and recall (2×precision×recall / (precision + recall)), it combines precision and recall of a class in one metric.
- More generally, recall is simply the complement of the type II error rate, i.e. one minus the type II error rate. Precision is related to the type I error rate, but in a slightly more complicated way, as it also depends upon the prior distribution of seeing a relevant vs an irrelevant item. (Wikipedia)

<u>Note</u>: when there is a serious downside to predicting false negative, such as to detect a cancer or a transaction fraud, use *Recall* as the metric (VISA Sr DS interview as of 22/7).

# 5. F1 Score vs. Accuracy

### Accuracy:

**Pro**: Easy to interpret. If we say that a model is 90% accurate, we know that it correctly classified 90% of observations.

**Con**: *Does not take into account how the data is distributed.* For example, suppose 90% of all players do not get drafted into the NBA. If we have a model that simply predicts every player to not get drafted, the model would correctly predict the outcome for 90% of the players. This value seems high, but the model is actually unable to correctly predict any player who gets drafted.

#### F1-score:

**Pro:** Takes into account how the data is distributed. For example, if the data is highly imbalanced (e.g. 90% of all players do not get drafted and 10% do get drafted) then F1-score will provide a better assessment of model performance.

**Con**: Harder to interpret. The F1-score is a blend of the precision and recall of the model, which makes it a bit harder to interpret.

#### As a rule of thumb:

- We often use accuracy when *the classes are balanced* and there is no major downside to predicting false negatives.
- We often use F1 score when the classes are imbalanced and there is a serious downside to predicting false negatives (? This item might not be true as recall is more important).
- When working on problems with heavily imbalanced datasets AND you care more about detecting positives than detecting negatives (outlier detection / anomaly detection) then you would prefer the F1-score more.

## 6. ROC & AUC

The ROC curve is a graphical representation of the model's performance across different classification thresholds. Each value of the threshold T generates a point (false positive, true

positive) and, then, the ROC curve is the curve described by the ensemble of points generated when the threshold T varies from 1 to 0.

- x-axis False Positive Rate = 1 Precision
- y-axis True Positive Rate = Recall

AUC is the area under the ROC curve. It quantifies the overall performance of the model across various thresholds. AUC values range from 0 to 1, where 0.5 represents a random classifier, and 1 indicates a perfect classifier.

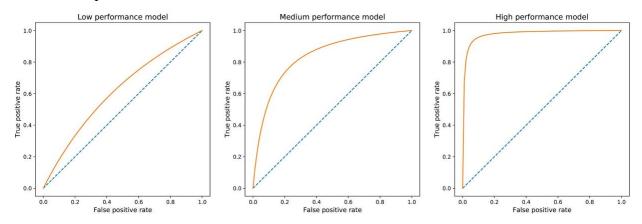


Illustration of possible ROC curves depending on the effectiveness of the model. On the left, the model has to sacrifice a lot of precision to get a high recall. On the right, the model is highly effective: it can reach a high recall while keeping a high precision.

<u>Note</u>: AUC=0.5 means the model does a random guess. AUC=0.3 (very likely) means your label might be wrong, it could be actual AUC=0.7 (VISA Sr DS interview as of 22/7).

# 7. Type I and Type II Errors

## Type I error (False Positive)

Rejecting the null hypothesis when it should not be rejected.

It is denoted by the Greek letter  $\alpha$  and is also called the  $\alpha$  level. The smaller value of  $\alpha$ , the smaller rate of type I error.

## Type II error (False Negative)

Not rejecting the null hypothesis when it should be rejected.

The rate of the type II error is denoted by the Greek letter  $\beta$  and related to *the power* of a test, which equals  $1 - \beta$ . The larger value of  $\beta$ , the smaller rate of type II error.

## 8. Linear Regression Assumptions

- (a) **Linearity**: The relationship between the independent variables (predictors) and the dependent variable (response) is linear.
- (b) **Independence**: The observations in the dataset are independent of each other. In other words, there should be no correlation or relationship between the residuals (errors) of different observations.
- (c) **Normality of Residuals**: The residuals (the differences between the observed and predicted values) should be normally distributed. This assumption ensures that the statistical tests and confidence intervals derived from the model are valid.
- (d) **Homoscedasticity**: Also known as constant variance, this assumption states that the variance of the errors is constant across all levels of the independent variables. In simpler terms, the spread of the residuals should be consistent along the range of predicted values.
- (e) **No or little multicollinearity**: There should be no perfect linear relationship among the predictor variables (multicollinearity). Perfect multicollinearity occurs when one predictor variable can be perfectly predicted from another predictor variable. It can lead to unstable parameter estimates and inflated standard errors.

# 9. Linear Regression Outliers

## How to identify outliers?

Standard residuals

#### How to deal with outliers?

- A measurement error or data entry error, correct the error if possible. If you can't fix it, remove that observation because you know it's incorrect.
- Not a part of the population you are studying (i.e., unusual properties or conditions), you can legitimately remove the outlier.
- A natural part of the population you are studying, you should not remove it.
  - What you should do in that case is two separate analyses, one with the outlier in the analysis and one with the outlier removed from the analysis. Then report both analyses and let the reader make the decision as to which one should be used.

### How to make outliers less influence to the linear regression?

Robust regression uses a method called *iteratively reweighted least squares to assign a weight to each data point*. This method is less sensitive to large changes in small parts of

the data. As a result, robust linear regression is less sensitive to outliers than standard linear regression.

# 10. Linear Regression Multicollinearity

## How to detect multicollinearity?

1. The Variance Inflation Factor (VIF) quantifies how much the variance is inflated. The VIF for the  $j^{th}$  predictor is:

$$VIF_j = \frac{1}{1 - R_i^2}$$

where  $R_j^2$  is the  $R^2$ -value obtained by regressing the  $j^{th}$  predictor on the remaining predictors (considering the  $x_j$  as the dependent variable and all others are independent variables). VIF is 1 means that there is no correlation among the  $j^{th}$  predictor and the remaining predictor variables, and hence the variance of  $b_j$  is not inflated at all. The general rule of thumb is that VIFs exceeding 4 warrant further investigation, while VIFs exceeding 10 are signs of serious multicollinearity requiring correction.

2. Calculate the correlation coefficient matrix for all the independent variables.

### How to deal with multicollinearity?

One solution to dealing with multicollinearity is to remove some of the violating predictors from the model.

# 11. Linear Regression on Time Series

- a) Violation of Independence Assumption: Time series data typically exhibit autocorrelation, meaning that observations are dependent on previous observations. This violates the independence assumption of linear regression, where observations are assumed to be independent of each other.
- b) Trend and Seasonality: Time series data often contain trends and seasonal patterns, which linear regression may not adequately capture. Linear regression assumes a linear relationship between the predictor variables and the response variable, which may not be appropriate for time series data with nonlinear trends or seasonal effects.
- c) Stationarity: Linear regression assumes that the relationship between variables remains constant over time. *However, many time series exhibit non-stationarity, where the mean, variance, or other statistical properties change over time.* Ignoring non-stationarity can lead to biased parameter estimates and incorrect inferences.

# 12. Linear Regression High Cardinality

## What is the high cardinality?

A *categorical* feature is said to possess *high cardinality* when there are too many of these unique values. One-hot Encoding becomes a big problem in such a case since we have a separate column for each unique value in the categorical variable. This leads to two problems (1) storage space consumption; (2) *the curse of dimensionality* (当维数增大时,空间数据会变得更稀疏,这将导致 bias 和 variance 的增加,最后影响模型的预测效果。解决办法:增加 sample size 或者使用 dimensionality reduction).

## How to deal the feature with a high cardinality?

A simple aggregation method. Leave instances belonging to a value with high frequency as they are and replace the other instances with a new category which we will call other.

Say our column color has 100 values and our threshold is 90% (that is 90). We have 5 different categories of colors: Red (50), Blue(40), Yellow (5), Green (3) and Orange (2). The numbers within the bracket indicate how many instances of that category are present in the column.

We see that Red (50) + Blue (40) reaches our threshold of 90. In that case, we retain only 2 categories (Red, Blue) and mark all other instances of other colors as the "Other". Thus we have reduced cardinality from 5 to 3 (Red, Blue, Other).

### What is the curse of dimensionality and how to cure the "curse"?

- Increase in dimensionality without increasing the number of samples will increase the
  sparsity in the training instances, which makes it difficult for any learning method to produce
  reliable results.
- Increase in dimensionality also increase the "sparsity" of the data distribution and it makes the distance between samples are more identical.
- Add more training samples.
- Reduce the dimension of the data for instance using PCA.

## Embedding vs. one-hot encoding

The one-hot encoding technique has two main drawbacks:

- 1. For high-cardinality variables those with many unique categories the dimensionality of the transformed vector becomes large (see previous high cardinality).
- 2. The mapping is completely uninformed: "similar" categories are not placed closer to each other in embedding space.

What is embedding? More details to be added...

An embedding is a mapping of a discrete — categorical — variable to a vector of continuous numbers.

https://towardsdatascience.com/neural-network-embeddings-explained-4d028e6f0526

## **Boosting Algorithms**

What's the differences between AdaBoost and Gradient Boosting?

See Ace the Data Science Interview page 100.

# **Bagging/Boosting Variance and Bias**

- Bagging algorithm (random forest) decreases ensemble variance by averaging, but has little effect on the ensemble bias, and solves the overfitting issues in a model.
- Boosting (AdaBoost/GBM) decreases the bias, not variance. It is because these mislabeled samples are with more weights, then the model would have less ensemble bias.
- Bagging algorithm (random forest) uses the bootstrapping sampling a dataset w/
  replacement. Boosting algorithm (AdaBoost/GBM/Xgboost) uses the full sample set for each
  iteration. Thus, they perform like sampling w/o replacement. While for Xgboost, the ratio of
  sampling of each tree can be modified with the following hyperparameter: subsample
  [default=1]

### **XGBoost**

Q: How does XGBoost do the parallel computation?

A: XGBoost doesn't run \*multiple trees\* in parallel, you need predictions after each tree to update gradients. Rather it does the parallelization \*WITHIN\* a single tree my using openMP to create branches independently. To observe this, build a giant dataset and run with n\_rounds=1. You will see all your cores firing on one tree. This is why it's so fast-well engineered.

Q: How does XGBoost treat the missing values?

A: (Answered by Tianqi Chen) Internally, XGBoost will automatically learn what is the best direction to go when a value is missing. Equivalently, this can be viewed as automatically "learn" what is the best imputation value for missing values based on reduction on training loss.

Q: How does XGBoost calculate the important score? What are the options?

A: Get feature importance of each feature. For tree model Importance type can be defined as:

- 'weight': the number of times a feature is used to split the data across all trees.
- 'gain': the average gain across all splits the feature is used in.
- 'cover': the average coverage across all splits the feature is used in.
- 'total gain': the total gain across all splits the feature is used in.
- 'total\_cover': the total coverage across all splits the feature is used in.

## **Light GBM**

Light GBM (LGB) is a gradient boosting framework that uses a tree based learning algorithm that offer the following advantages over prior implementations of GBM's:

- Faster training speed and higher efficiency: Light GBM uses a \*histogram based algorithm\*
   (i.e. it buckets continuous feature values into discrete bins which fasten the training procedure).
- Lower memory usage: Replaces continuous values to discrete bins which result in \*lower memory usage\*.
- Better accuracy than other boosting algorithm: It produces much more complex trees by following \*a leaf-wise split approach (BFS)\* rather than \*a level-wise approach (DFS)\* which is the main factor in achieving higher accuracy. However, it can sometimes lead to overfitting which can be avoided by setting the max\_depth & num\_leaves parameter.
- Compatibility with Large Datasets: It is capable of performing equally good with large datasets with a significant reduction in training time as compared to XGBOOST.
- Parallel learning is supported.

## Parameters in Random Forest (Link)

a. **n\_estimators**: Number of trees. The default number of estimators is 100 in scikit-learn.

- b. **max\_features**: Random forest takes random subsets of features and tries to find the best split. max\_features helps to find the number of features to take into account in order to make the best split. It can take four values "auto", "sqrt", "log2" and None. In case of auto: considers max\_features = sqrt(n\_features). In case of sqrt: considers max\_features = sqrt(n\_features), it is same as auto. In case of log2: considers max\_features = log2(n\_features). In case of None: considers max\_features = n\_features.
- c. max\_depth: It governs the maximum height up to which the trees inside the forest can grow. It is one of the most important hyperparameters when it comes to increasing the accuracy of the model, as we increase the depth of the tree the model accuracy increases upto a certain limit but then it will start to decrease gradually because of overfitting in the model. It is important to set its value appropriately to avoid overfitting. The default value is set to None, None specifies that the nodes inside the tree will continue to grow until all leaves become pure or all leaves contain less than min\_samples\_split (another hyperparameter).
- d. **min\_samples\_split**: It specifies the minimum amount of samples an internal node must hold in order to split into further nodes. If we have a very low value of min\_samples\_splits then, in this case, our tree will continue to grow and start overfitting. By increasing the value of min\_samples\_splits we can decrease the total number of splits thus limiting the number of parameters in the model and thus can aid in reducing the overfitting in the model. However, the value should not be kept very large that a number of parameters drop extremely causing the model to underfit. We generally keep min\_samples\_split value between 2 and 6. However, the default value is set to 2.
- e. **min\_samples\_leaf**: The minimum number of samples at the leaf node
- f. **max\_leaf\_nodes**: It sets a limit on the splitting of the node and thus helps to reduce the depth of the tree, and effectively helps in reducing overfitting.

## Parameters in XGBoost (Link)

#### Tree complexity parameters

- a. **n\_estimators**: Specifies the number of boosting rounds or trees to build. A higher number can lead to better performance, but it also increases the risk of overfitting.
- b. **max\_depth**: maximum depth of a tree. Deeper trees can capture more complex patterns in the data, but may also lead to overfitting.

c. **min\_child\_weight**: minimum sum of instance weight (hessian) needed in a child. This can be used to control the complexity of the decision tree by preventing the creation of too small leaves. Higher values make the algorithm more conservative.

## Sampling parameters

- d. **subsample**: percentage of rows used for each tree construction. Lowering this value can prevent overfitting by training on a smaller subset of the data.
- e. **colsample\_bytree**: percentage of columns used for each tree construction. Lowering this value can prevent overfitting by training on a subset of the features.

## Learning task specific parameters

- f. **learning\_rate** (or eta): Controls the contribution of each tree to the final prediction. Lower values make the model more robust, but a smaller learning rate typically requires more boosting rounds.
- g. **gamma**: minimum loss reduction required to make a further partition on a leaf node of the tree. Higher values increase the regularization.
- h. **lambda**: L2 regularization term on weights. Higher values increase the regularization.
- i. alpha: L1 regularization term on weights. Higher values increase the regularization.

# Parameter tuning in LGB (steps apply to XGB as well)

- (1) Firstly, tree-specific parameters which controls each individual tree in the model, such as:
- a. *max\_depth*: the max depth of a tree, it's used to control overfitting as higher depth will allow model to learn relations very specific to a particular sample.
- b. *max\_bin*: the maximum numbers of bins that feature values are bucketed in. A smaller number will reduce overfitting.
- c. *num\_leaves*: number of leaves to use in the full tree. Having a large number of leaves will improve accuracy, but will also lead to overfitting.
- d. min\_data\_in\_leaf: (alias min\_child\_samples) the minimum number of samples to group into a leaf. Larger number will reduce overfitting (but may lead to under-fitting).
- e. min\_split\_gain: (alias gamma) minimum loss reduction required to make a further partition on a leaf node of the tree.
- (2) Secondly, boosting parameters.
- a. *num\_iterations*: the number of sequential trees to be modeled. Though GBM is fairly robust at higher number of trees but it can still overfit at a point.
- b. learning\_rate: the importance ratio applied to residual for the next tree prediction. For example, if the current prediction for a particular example is 0.2, the actual prediction with

adding next tree is 0.8, then learning rate 0.1 would adjust the actual prediction from 0.8 to 0.2+0.1\*(0.8-0.2)=0.26.

- (3) Thirdly, miscellaneous parameters. These chosen two are mainly for improving model accuracy.
- a. objective: the loss function the model is trying to minimizing, e.g., mae, mse, etc. We use mae because the target model performance is the absolute error metrics (MAE and MAE90) that more directly relates to PnL than squared error.
- b. boosting (or booster in XGBOOST): the boosting method the model is using, e.g., gbdt, rf, dart, goss. We use the 'dart' (dropout meets multiple additive regression trees) method for higher accuracy according to the parameters-tuning guidance.

## **Cross Validation (Model Selection)**

### Version 1.

Cross-validation usually helps to avoid the need of a validation set.

The basic idea with training/validation/test data sets is as follows:

- 1. Training: You try out different types of models with different choices of hyperparameters on the training data (e.g. linear model with different selection of features, neural net with different choices of layers, random forest with different values of mtry).
- 2. Validation: You compare the performance of the models in Step 1 based on the validation set and select the winner. This helps to avoid wrong decisions taken by overfitting the training data set.
- 3. Test: You try out the winner model on the test data just to get a feeling how good it performs in reality. This unravels overfitting introduced in Step 2. Here, you would not take any further decision. It is just plain information.

Now, in the case where you replace the validation step by cross-validation, the attack on the data is done almost identically, but you only have a training and a test data set. There is no need for a validation data set.

- 1. Training: See above.
- 2. Validation: You do cross-validation on the training data to choose the best model of Step 1 with respect to cross-validation performance (here, the original training data is repeatedly split into a temporary training and validation set). The models calculated in cross-validation

are only used for choosing the best model of Step 1, which are all computed on the full training set.

3. Test: See above.

## Version 2. (From Andrew Ng and similar to Version 1. (a))

Suppose we want to select different models with different d values. The data set is separated into 2 sets - train/test data sets.

$$d=1, h_{\theta}(x)=\theta_0+\theta_1 x$$
, train the model and get  $\theta^{(1)}$  such that  $J_{test}(\theta^{(1)})$  is minimized.

$$d=2, h_{\theta}(x)=\theta_0+\theta_1x+\theta_2x^2$$
, then where  $\theta^{(2)}\to J_{test}(\theta^{(2)})$ 

. . .

$$d = 10, h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \dots + \theta_{10} x^{10}$$
, then where  $\theta^{(10)} \to J_{test}(\theta^{(10)})$ 

Suppose d=5 is the optimal solution. Then how wells does the model generalizes? Report test set error  $J_{test}(\theta^{(5)})$ .

**Problem**:  $J_{test}(\theta^{(5)})$  is likely to be an optimistic estimate of *generalization error*. i.e. our extra parameter (d=degree of polynomial) is fit to test set.

Divide the data set into 3 sets:

Training Set/Cross Validation Set (CV)/Test Set and the ratio is like 60%/20%/20%

Model Selection using Cross Validation

$$d = 1$$
  $h_{\theta}(x) = \theta_0 + \theta_1 x$ , then  $\min_{\alpha} J(\theta) \to \theta^{(1)} \to J_{CV}(\theta^{(1)})$ 

$$d = 2 h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2, \text{ then } \min_{\theta} J(\theta) \to \theta^{(2)} \to J_{CV} \left(\theta^{(2)}\right)$$

. . .

$$d=10\;h_{\theta}(x)=\theta_0+\theta_1x+\theta_2x^2+\cdots+\theta_{10}x^{10}, \text{ then } \min_{\theta}J(\theta)\rightarrow\theta^{(10)}\rightarrow J_{CV}\big(\theta^{(10)}\big)$$

Suppose  $J_{CV}(\theta^{(4)})$  has the smallest CV error and pick d=4.

Estimate the generalization error for test set  $J_{test}(\theta^{(4)})$ .

# **Optimizations**

Gradient Descent (also called batch gradient descent)

$$\begin{split} J_{train}(\theta) &= \frac{1}{2m} \sum_{i=1}^m \left( h_\theta \big( x^{(i)} \big) - y^{(i)} \right)^2 \\ \text{Repeat } \{ \\ \text{for every } j = 0, \dots, n \\ \theta_j &\coloneqq \theta_j - \alpha \frac{1}{m} \sum_{i=1}^m \left( h_\theta \big( x^{(i)} \big) - y^{(i)} \right) x_j^{(i)} \end{split}$$

Notes: where n is the number of features and m is number of samples. Suppose update K iterations, the total computation is O(Kmn). When m is large, computing is very expensive to update one iteration.

### Stochastic Gradient Descent

$$J_{train}(\theta) = \frac{1}{2m} \sum_{i=1}^m \left( h_{\theta} \left( \boldsymbol{x}^{(i)} \right) - \boldsymbol{y}^{(i)} \right)^2$$

- 1. Randomly shuffle dataset
- 2. Repeat {

For i=1,...,m { // GD on each observation, so the convergence path is the zigzag shape for every j=0,...,n  $\theta_j \coloneqq \theta_j - \alpha \big(h_\theta\big(x^{(i)}\big) - y^{(i)}\big) x_j^{(i)}$  }

Suppose update K iterations, the total computation is O(Kn). Each iteration only takes 1 observation, so the convergence path is a zigzag shape.

#### Mini-Batch Gradient Descent

```
\begin{split} J_{train}(\theta) &= \frac{1}{2m} \sum_{i=1}^{m} \left( h_{\theta} \left( x^{(i)} \right) - y^{(i)} \right)^{2} \\ \text{Say } b &= 10 \text{ (batch size) and } m = 1000 \\ \text{Repeat } \{ \\ \text{For } i &= 1,11,21,...,991 \ \{ \\ \theta_{j} &\coloneqq \theta_{j} - \alpha \frac{1}{10} \sum_{k=i}^{i+9} \left( h_{\theta} \left( x^{(k)} \right) - y^{(k)} \right) x_{j}^{(k)} \\ &\text{ (for every } j = 0,...,n) \\ &\text{ } \} \end{split}
```

Note: It's between batch GD and stochastic GD and the vectorization can be parallelized. Suppose update K iterations, the total computation is O(Kbn).

## RMSprop (Root Mean Square Propagation)

On iteration *t*:

Compute dW, db on current mini-batch

$$S_{dW} = \beta_2 S_{dW} + (1 - \beta_2) dW^2$$

$$S_{db} = \beta_2 S_{db} + (1 - \beta_2) db^2$$

$$w \coloneqq w - \alpha \frac{dW}{\sqrt{S_{dW}} + \epsilon}$$

$$b \coloneqq b - \alpha \frac{db}{\sqrt{S_{db}} + \epsilon}$$

Notes:

The algorithm damps out the oscillations in the gradient descent, so a larger learning rate can be applied to speed up the learning algorithm.

### Adam (ADAptive Moment estimation)

$$V_{dW} = 0, S_{dW} = 0, V_{db} = 0, S_{db} = 0$$

On iteration *t*:

Compute

$$\begin{split} V_{dW} &= \beta_1 V_{dW} + (1-\beta_1) dW, V_{db} = \beta_1 V_{db} + (1-\beta_1) db \text{ // the "momentum" } \beta_1 \\ S_{dW} &= \beta_2 S_{dW} + (1-\beta_2) dW^2, S_{db} = \beta_2 S_{db} + (1-\beta_2) db^2 \text{ // the "RMSProp" } \beta_2 \\ V_{dW}^{corrected} &= V_{dW} / (1-\beta_1^t), V_{db}^{corrected} = V_{db} / (1-\beta_1^t) \text{ // } t \text{ is the iteration number} \\ S_{dW}^{corrected} &= S_{dW} / (1-\beta_2^t), S_{db}^{corrected} = S_{db} / (1-\beta_2^t) \\ w &\coloneqq w - \alpha \frac{V_{dW}^{corrected}}{\sqrt{S_{dW}^{corrected}} + \epsilon} \\ b &\coloneqq b - \alpha \frac{V_{db}^{corrected}}{\sqrt{S_{db}^{corrected}} + \epsilon} \end{split}$$

Configuration parameters:

 $\alpha$ : needs to be tuned

 $\beta_1$ : 0.9 // the first moment

 $\beta_2$ : 0.999 // the second moment

*ϵ*: 10E-8

Note:

- Adam combines the best properties of the AdaGrad (1<sup>st</sup> moment) & RMSProp (2<sup>nd</sup> moment) algorithms to provide an optimization algorithm that can handle sparse gradients on noisy problems.
- Adam is relatively easy to configure where default parameters do well on most cases.

## **Feature Selection in Machine Learning**

#### **Embedded Methods**

They are used to optimize the objective function or performance if a learning algorithm or model. The intrinsic model building metric is used during learning.

**Regularization**: Regularization adds a penalty term to different parameters of the machine learning model for avoiding overfitting in the model. This penalty term is added to the coefficients; **hence it shrinks some coefficients to zero. Those features with zero coefficients can be removed from the dataset.** The types of regularization techniques are L1 Regularization (Lasso Regularization) or Elastic Nets (L1 and L2 regularization).

## Filter Methods (on the basis of statistics measures)

The filter methods pick up the intrinsic properties of the features (i.e. the relevance of the features) measured via univariate statistics.

**Chi-squared test** is used for categorical features in a dataset. We calculate the Chi-square between *a categorical feature* and *a categorial target* and select the desired number of features with the best Chi-square scores. Note that the Fisher's exact test is for a small-sized samples. **Correlation (Pearson's correlation)** is a measure of the linear relationship of *2 or more continuous variables*. If two variables are correlated, we can predict one from the other. Therefore, the model only really needs one of them.

# Model explainability/interpretation

- Feature importance Which features impact most model predictions
- Partial dependence plots How is ONE feature impacting predictions
- SHAP values How are ALL features impacting ONE prediction

## Partial Dependent Plot

The partial dependent plot (PDP) shows the global effect that a single input feature has on the model prediction. The input feature of interest is set to a constant value for \*all examples\* in the training data. The model then scores this adjusted data and average over the training data to calculate a single point on the PDP. This process is repeated to calculate the PDP over the input feature range in the training data.

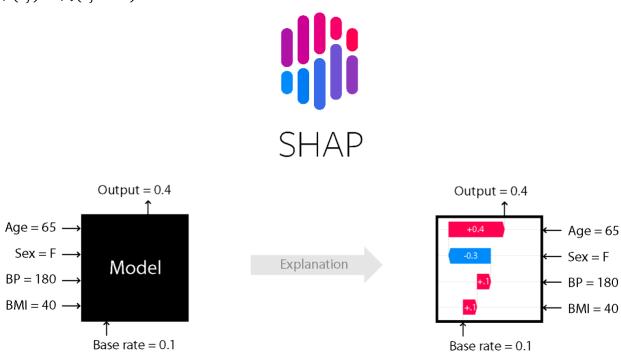
The original dataset is {obs1:[2,4,6], obs2:[1,3,5], obs3:[4,2,1]}. Consider the PDP on x2, the possible new dataset is {obs1:[2,2,6], obs2:[1,2,5], obs3:[4,2,1]} and then compute y\_hat1, y\_hat2, and y\_hat3, then average y\_hat's. Repeat the process for a different x2 value say x2=3 and so on.

### SHAP interpretability

Shapley Additive Explainability (SHAP) is another popular interpretability method to explain individual predictions (local/global). Shapley values are obtained by incorporating concepts from Cooperative Game Theory and local explanations (i.e. given a set of features, Cooperate Game Theory defines how to fairly distribute the attribution amongst all the features that are working in coordination).

The value of the i-th feature of j-th instance is its contribution to the prediction  $f(x_i)$ , weighted and summed over all possible feature value combinations. An abstract intuition to understand this measure can be shown in simple linear model

 $y = \beta_0 + \beta_1 x^1 + \dots + \beta_m x^m$ , the Shaply value of the i-th feature on the j-th sample is simply  $\phi(x_i^i) = \beta_i (x_i^i - \bar{x}^i)$ 



For example, for a particular feature X with a feature\_value=0.39, mean\_feature\_value=-0.04 and shap\_value=0.34. It means the feature\_value=0.39 has a positive contribution shap\_value=0.34 to the prediction.

# **Comparison of Two Means**

The hypothesis is

$$H_0: \mu_1 = \mu_2$$
  
 $H_a: \mu_1 \neq \mu_2$ 

Tests of Significance for *Two Unknown Means and Known Standard Deviations* Given samples from two normal populations of size  $n_1$  and  $n_2$  with unknown means  $\mu_1$  and  $\mu_2$  and known standard deviations  $\sigma_1$  and  $\sigma_2$ , the test statistic comparing the means is known as *the two-sample z statistic* 

$$z = \frac{(\bar{x}_1 - \bar{x}_2) - (\bar{\mu}_1 - \bar{\mu}_2)}{\sqrt{\sigma_1^2/n_1 + \sigma_2^2/n_2}}$$

Which has the standard normal distribution N(0,1).

Tests of Significance for *Two Unknown Means and Unknown Standard Deviations* In general, the population standard deviations are not known, and are estimated by the calculated values  $s_1$  and  $s_2$ . In this case, the test statistic is defined by *the two-sample t statistic* 

$$t = \frac{(\bar{x}_1 - \bar{x}_2) - (\bar{\mu}_1 - \bar{\mu}_2)}{\sqrt{s_1^2/n_1 + s_2^2/n_2}}$$

Although the two-sample statistic does not exactly follow the t distribution (since two standard deviations are estimated in the statistic), conservative p-values may be obtained using the t(k) distribution where k represents the smaller of  $n_1 - 1$  and  $n_2 - 1$ .

## P-value

#### What is the p-value?

- A p-value is a statistical measurement used to validate a hypothesis against observed data.
- The lower the p-value, the greater the statistical significance of the observed difference.
- A p-value of 0.05 or lower is generally considered statistically significant.
- A p-value measures the probability of obtaining the observed results, assuming that the null hypothesis is true.
- P-value can serve as an alternative to or in addition to preselected confidence levels for hypothesis testing.

A/B Testing

What's the A/B testing?

A/B testing is to compare 2 or more versions.

What's the null hypothesis and the alternative hypothesis?

The null hypothesis is that the change in the design made for the test group **would results in no change in the conversion rate.** The alternative hypothesis is the opposing that the change in the design for the test group **would results in an improvement (or reduction) in the conversion** 

rate.

•  $p \le 0.05$  (*Note that the equal sign means 'significant'*)

o Reject H0 -> Change in the conversion rate -> Significant test result

• *p* > 0.05

o Fail to reject H0 -> No change in the conversion rate -> Not significant test result

How to determine the minimum sample size?

You will need the baseline conversion rate and the minimum detectable effect (MDE)/minimum effect of interest (MEI), which is the minimum difference between the control and test group that you or your team will determine to be worth the investment of making the design change in the first place. The equation for minimum sample size in each group (assumes equal sized groups) is

$$n = \frac{2(\bar{p}(1-\bar{p}))(Z_{\beta} - Z_{\alpha/2})^{2}}{(p_{B} - p_{A})^{2}}$$

 $Z_{\beta}$ : z-score represents the desired Power (typically 0.84 for 80% power – see below for explanation of the Power)

 $Z_{\alpha/2}$ : z-score represents the desired level of statistical significance (typically 1.96)

 $\bar{p}$ : pooled probability or the average of  $p_A$  and  $p_B$ 

 $p_A$ : success rate of control group

 $p_B$ : success rate of test group

#### What is the Power?

Power is also known as  $1 - \beta$ , it can be explained as the strength of your test to detect an actual difference in your variant. Conversely,  $\beta$  is the probability that your test does not reject the null hypothesis when it should actually be rejecting the null hypothesis. *The higher the Power, the lower the probability of a Type II error.* Experiments are usually set at a power level of 80%, or  $\beta = 20\%$ . Another way of putting it is: if there is a difference in the test, you're willing to make Type II error 20% of the time.

### How to deal with small sample sizes?

We can lower the required sample size by:

- Reducing the confidence threshold / increasing the significance threshold accepting higher risk of false positives
- Increasing the minimum effect of interest (MEI/MDE)
- By accepting the test will have lower power against a particular MEI

## Can you run an A/B test with unequal sample sizes? (<u>Hyperlink</u>)

TL;DR: Yes, but you wouldn't want to.

You can run an experiment with an unequal allocation (e.g. 10–90) as long as you don't modify the allocation while the experiment is running. However it will be less efficient than a 50–50 allocation – either your test will have less power, or you will need to run it longer to achieve a comparable result.

例如原计划两周的 AB testing,一周后发现 p-value<0.05 了, 这时候能不能结束? 怎么从统计上解释不能提前结束?

答案:一般做 ab test 都是根据想要达到的 statistical power,一般是 0.8,来计算一个 sample size,然后用 sample size 来预计需要做 testing 的时间。在你的 case 里面算出来的 时间是两周,如果你只做了一周,预设的 sample size 没达到,那么 power 就会偏低,导致 type 2 error 太高,实验结果不可信。*p-value 小于 0.05 只能保证 type 1 error 比较小,但* 

*sample size 没达到会导致 type 2 error 太高。*我们做 ab test 要两种 error 都低实验结果才可信。

An example: Ads Click Through Rate (CLR) (Hyperlink)

$$\begin{split} \bar{X}_1 \sim & N(p_1, p_1(1-p_1)/n_1) \\ \bar{X}_2 \sim & N(p_2, p_2(1-p_2)/n_2) \\ \bar{X}_1 - \bar{X}_2 \sim & N\left(p_1 - p_2, \frac{p_1(1-p_1)}{n_1} + \frac{p_2(1-p_2)}{n_2}\right) \end{split}$$

Hypothesis:

$$H_0: \bar{X}_1 - \bar{X}_2 = 0, H_a: \bar{X}_1 - \bar{X}_2 \neq 0$$

t-test statistic:

$$t = \frac{\bar{X}_1 - \bar{X}_2 - 0}{SE} = \frac{\bar{X}_1 - \bar{X}_2 - 0}{\sqrt{\frac{p_1(1 - p_1)}{n_1} + \frac{p_2(1 - p_2)}{n_2}}}$$

Since standard deviation of the sample  $S_1 = \sqrt{p_1(1-p_1)/n_1}$  is different from  $S_2 = \sqrt{p_2(1-p_2)/n_2}$ , we use the unpooled standard error t-test (usually one SE should twice more than another SE, but in this case they're not that different). For unpooled t-test, the degree of freedom we choose min $(n_1 - 1, n_2 - 1)$ .

#### **Causal Inference**

How to discover causal inference?

Randomized Controlled Tests (or A/B test)

An example and steps

Goal: Does sending promotion emails increase customer's purchase conversion? The RCT consists of 5 steps

- 1. Select participants (randomly)
- 2. Split them into 2 groups (randomly)
- 3. Participants in the treatment group get emails & participants in the control group gets no emails
- 4. Monitor purchase conversion over time
- 5. Make decision & draw conclusion: sending emails "causes" purchase conversion increase

## Challenges & Concepts

1. Confounders

Some factors, rather than the control variables, impact the outcome as well. The randomization is important in selection and split the groups.

2. Selection bias

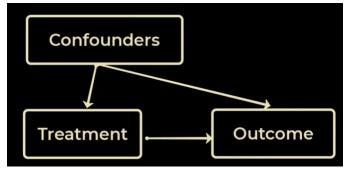
The selected group isn't a good representative for the whole population.

3. Counterfactuals

A sample in the control group also outputs an outcome with the treatment, but the outcome is imputed using machine learning. Control 组中没有接受 Treatment 的也产生一个 outcome,但是这个 outcome 是人为的。

### Causal inference assumptions

- 1. Causal Markov Condition (Markov assumption)
- Causal graph
- Directed Acyclic Graph (DAG)



- SUTVA (Stable Unit Treatment Value Assumption)Control and Treatment groups do not influence each other
- IgonorabilityNo unknown confounders.

#### How to measure the causal inference?

Average Treatment Effect (ATE) and conditional ATE.

#### Central limit theorem

In probability theory, the central limit theorem (CLT) establishes that, in many situations, when independent random variables are summed up, their properly normalized sum tends toward a normal distribution even if the original variables themselves are not normally distributed.

If  $X_1, X_2, \ldots, X_n, \ldots$  are random samples drawn from a population with overall mean  $\mu$  and finite variance  $\sigma^2$ , and if  $\bar{X}_n$  is the sample mean of first n samples, then the limiting form of the distribution,  $Z = \lim_{n \to \infty} \left( \frac{\bar{X}_n - \mu}{\frac{\sigma}{\sqrt{n}}} \right)$ , is a standard normal distribution.

### Law of large numbers

In probability theory, the law of large numbers (LLN) is a theorem that describes the result of performing the same experiment a large number of times. According to the law, the average of the results obtained from a large number of trials should be close to the expected value and tends to become closer to the expected value as more trials are performed.

It is also important to note that the LLN only applies to the average. Therefore, while

$$\lim_{n \to \infty} \sum_{i=1}^{n} \frac{X_i}{n} = \bar{X}$$

Bayes' Theorem

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

where A and B are events and  $P(B) \neq 0$ .

# What are gradient vanishing/exploding in deep neural networks

#### Vanishing

As the backpropagation algorithm advances downwards (or backward) from the output layer towards the input layer, the gradients often get smaller and smaller and approach zero which eventually leaves the weights of the initial or lower layers nearly unchanged. As a result, the gradient descent never converges to the optimum. This is known as the vanishing gradients problem.

## **Exploding**

On the contrary, in some cases, the gradients keep on getting larger and larger as the backpropagation algorithm progresses. This, in turn, causes very large weight updates and causes the gradient descent to diverge. This is known as the exploding gradients problem.

## Why it happens?

Certain activation functions, like the logistic function (sigmoid), have a very huge difference between the variance of their inputs and the outputs. In simpler words, they shrink and transform a larger input space into a smaller output space that lies between the range of [0,1]. Observing the above graph [...missing...] of the sigmoid function, we can see that for larger inputs (negative or positive), its output saturates at 0 or 1 [...but...] with *a derivative* very close to zero. Thus, when the backpropagation algorithm chips in, it virtually has no gradients to propagate backward in the network, and whatever little residual gradients exist keeps on diluting as the algorithm progresses down through the top layers. So, this leaves nothing for the lower layers.

### What are the solutions?

#### 1. Weight initializations

Randomly initialize the connection weights for each layer in the network as described in the following equation which is popularly known as Xavier initialization (after the author's first name) or Glorot initialization (after his last name).

Weights follows a normal distribution with mean 0 and variance  $\sigma^2 = 1/n_{avg}$  where  $n_{avg} = (n_{input} + n_{output})/2$  and  $n_{input}$  and  $n_{output}$  are numbers of layer input and number of neuron for that layer.

2. Using Non-saturating Activation Functions (this one is for the vanishing of gradients) such as ReLU (Rectified Linear Unit)

$$R(z) = \max(0, z)$$

#### 3. Gradient Clipping

Another popular technique to mitigate the exploding gradients problem is to clip the gradients during backpropagation so that they never exceed some threshold. This is called Gradient Clipping. *This optimizer will clip every component of the gradient vector to a value between -1.0 and 1.0.* Meaning, all the partial derivatives of the loss w.r.t each trainable parameter will be clipped between -1.0 and 1.0

# Popular activation functions and their pro's & con's

- sigmoid
- Non-zero derivatives concentrate around origin; while small derivatives away from origin and it causes *the gradient vanishing*.
- tanh (hyperbolic tangent)
- It is very similar to sigmoid function but it is symmetric to the origin.
- The derivatives of the tanh are larger than the derivatives of the sigmoid, so to minimize the cost function is faster.
- ReLU
- More computationally efficient than sigmoid/tanh
- Accelerates the convergence of gradient descend.
- The zero derivatives on the negative x-axis makes some neurons not updated at all (dead neurons).
- Leaky ReLU
- Add small positive derivative value to the negative x-axis to avoid the dead neurons happening.

## **Batch Normalization**

https://deepai.org/machine-learning-glossary-and-terms/batch-normalization

$$\mu = \frac{1}{m} \sum z^{(i)}, \, \sigma^2 = \frac{1}{m} \sum \left( z^{(i)} - \mu \right)^2, \, z_{norm}^{(i)} = \frac{z^{(i)} - \mu}{\sqrt{\sigma^2 + \epsilon}} \, \text{and} \, \, \tilde{z}^{(i)} = \gamma z_{norm}^{(i)} + \beta$$

where  $\gamma$  and  $\beta$  are learnable parameters and  $z^{(i)}$  means  $z^{[l](i)}$  for lth layer. We are mapping from  $z_{norm}^{(i)}$  to  $\tilde{z}^{(i)}$  because we don't want to the hidden units always have zero mean and one variance.

Special case is when  $\gamma = \sqrt{\sigma^2 + \epsilon}$  and  $\beta = \mu$ , then  $\tilde{z}^{(i)} = z^{(i)}$ .

$$x \xrightarrow{w^{[1]},b^{[1]}} \overline{z^{[1]}} \xrightarrow{\beta^{[1]},\gamma^{[1]}BN} \tilde{z}^{[1]} \to a^{[1]} = g^{[1]} (\tilde{z}^{[1]}) \xrightarrow{w^{[2]},b^{[2]}} z^{[2]} \xrightarrow{\beta^{[2]},\gamma^{[2]}} \tilde{z}^{[2]} \to \cdots$$

Parameters are  $w^{[1]}, b^{[1]}, \beta^{[1]}, \gamma^{[1]}, \dots, w^{[l]}, b^{[l]}, \beta^{[l]}, \gamma^{[l]}$  and  $b^{[t]}$  are actually all zeros.

BN works within a mini-batch

• For the  $t^{th}$  mini-batch

$$X^{\{t\}} \xrightarrow{w^{[1]},b^{[1]}} z^{[1]} \xrightarrow{\beta^{[1]},\gamma^{[1]}} \tilde{z}^{[1]} \xrightarrow{} \tilde{z}^{[1]} \rightarrow a^{[1]} = g^{[1]} \big(\tilde{z}^{[1]}\big) \xrightarrow{w^{[2]},b^{[2]}} z^{[2]} \xrightarrow{\beta^{[2]},\gamma^{[2]}} \tilde{z}^{[2]} \rightarrow \cdots$$

- Compute forward prop on  $X^{\{t\}}$
- In each hidden layer, use BN to replace  $z^{[1]}$  with  $\tilde{z}^{[l]}$
- Use back prop to compute gradient  $dw^{[l]}$ ,  $db^{[l]}$ ,  $d\beta^{[l]}$ ,  $d\gamma^{[l]}$
- Update the parameters  $w^{[l]} := w^{[l]} + a dw^{[l]}, \dots$

## Why BN works?

- Normalized the inputs for the hidden layers (similar idea as to normalize the inputs for the model)
- Covariate shift. Consider a mapping  $x \to y$ , when x changes, the mapping needs to be retrained. The batch normalization reduces the covariate shift for each hidden layer even small changes in the input won't affect the layer output too much.
- Batch norm as regularization. For each mini-batch, the mapping  $z^{[l]} \to \tilde{z}^{[l]}$  within that mini batch add some noise. Similar to dropout, this has a *slight* regularization effect.

#### BN at test time

At the training time, for each mini-batch  $\{t\}$ , to keep records for l layer,  $\mu^{\{1\}[l]}$ ,  $\mu^{\{2\}[l]}$ ,  $\mu^{\{3\}[l]}$ , ... and compute  $\mu$  (exponentially weighted average) likewise for  $\sigma^2$  at l layer,  $\sigma^{2\{1\}[l]}$ ,  $\sigma^{2\{3\}[l]}$ , ... and compute  $\sigma^2$ . Then

$$z_{norm}^{(i)} = \frac{\left(z^{(i)} - \mu\right)}{\sqrt{\sigma^2 + \epsilon}}$$
$$\tilde{z}^{(i)} = \gamma z_{norm}^{(i)} + \beta$$

## **Imbalanced Dataset**

https://github.com/scikit-learn-contrib/imbalanced-learn

All these approaches aim at rebalancing (partially or fully) the dataset:

- Undersampling consists in sampling from the majority class in order to keep only a part of these points
  - Random undersampling: Randomly remove samples from the majority class, with or
    without replacement. This is one of the earliest techniques used to alleviate imbalance in
    the dataset, however, it may increase the variance of the classifier and is very likely to
    discard useful or important samples.

- Cluster: Cluster centroids is a method that replaces cluster of samples by the cluster centroid of a K-means algorithm, where the number of clusters is set by the level of undersampling.
- O <u>Disadvantages</u>: (1) It can discard useful information about the data itself which could be necessary for building rule-based classifiers such as Random Forests. (2) The sample chosen by random undersampling may be a biased sample. And it will not be an accurate representation of the population in that case. Therefore, it can cause the classifier to perform poorly on real unseen data.
- Oversampling consists in replicating some points from the minority class in order to increase its cardinality
  - o Random Oversampling: Random Oversampling involves supplementing the training data with multiple copies of some of the minority classes. Oversampling can be done more than once (2x, 3x, 5x, 10x, etc.) This is one of the earliest proposed methods, that is also proven to be robust. Instead of duplicating every sample in the minority class, *some of them may be randomly chosen with replacement*.
  - Generating synthetic data consists in creating new synthetic points from the minority class (see SMOTE method for example) to increase its cardinality.
  - O <u>Disadvantages</u>: (1) It increases the likelihood of overfitting since it replicates the minority class events. (2) While generating synthetic examples, SMOTE does not take into consideration neighboring examples can be from other classes. This can increase the overlapping of classes and can introduce additional noise. (3) SMOTE is not very practical for high dimensional data.
- It's possible to combine oversampling and undersampling techniques into a hybrid strategy. Common examples include SMOTE and Tomek links or SMOTE and Edited Nearest Neighbors (ENN).

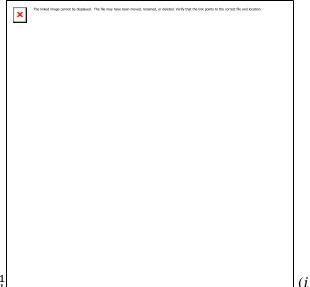
#### **SMOTE**

SMOTE (synthetic minority oversampling technique) is one of the most commonly used oversampling methods to solve the imbalance problem. It aims to balance class distribution by randomly increasing minority class examples by replicating them. SMOTE synthesizes new minority instances between existing minority instances. It generates the **virtual training records by linear interpolation** for the minority class.

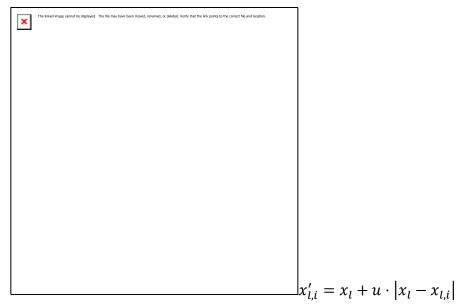
- Step 1: Setting the minority class set A, for each  $x \in A$ , the k-nearest neighbors of x are obtained by calculating the Euclidean distance between x and every other sample in set A.
- **Step 2:** The sampling rate N is set according to the imbalanced proportion. For each  $x_l \in A$ , N examples (i.e  $x_{l,1}, x_{l,2}, ..., x_{l,n}$ ) are *randomly selected* from its k-nearest neighbors, and



they construct the set  $A_l^1$ . For example if n = 3 and k = 5, 3 of the 5-nearest neighbors of  $x_l$  are randomly selected and n can be either less or greater than k.



• Step 3: For each example  $x_{l,i} \in A_l^1$  (*i* 1,2,..., *N*), the following formula is used to generate a new example



in which u follows a uniform distribution between 0 and 1.

## K-mean

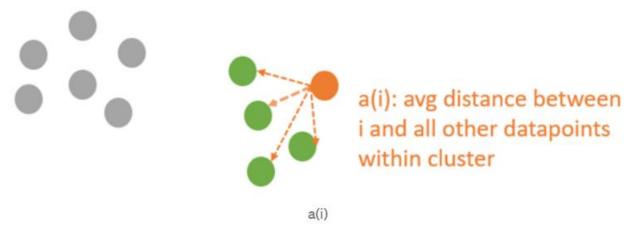
Details of implementation of the algorithm is saved in KMeans.py

**NOTE**: The Silhouette Method is used in combination with the Elbow Method for a more confident decision.

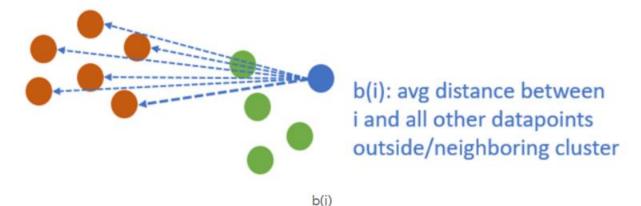
Silhouette coefficient for a particular data point i

$$S(i) = \frac{b(i) - a(i)}{\max(a(i), b(i))}$$

a(i) is the average distance between i and all the other data points in the cluster which i belongs to.



b(i) is the average distance from i to all clusters which i does not belong to.



For a value of K, to calculate the average Silhouette coefficient  $AverageSilhouette = mean\{S(i)\}$ 

Points to remember while calculating the Silhouette coefficient:

- The value of the silhouette coefficient is between [-1, 1].
- A score of 1 denotes the best meaning that the data point *i* is very compact within the cluster to which it belongs and far away from the other clusters.
- The worst value is -1. Values near 0 denote overlapping clusters.

#### Generative Model vs. Discriminative Model

A Generative Model learns the joint probability distribution P(X,Y). It predicts the conditional probability with the help of Bayes Theorem. A Discriminative Model learns the conditional probability distribution P(Y|X).

*Generative models* use probability estimates and likelihood to model data points and distinguish between different class labels in a dataset. These models *are capable of generating new data instances*. However, they also have a major drawback. The presence of outliers affects these models to a significant extent.

Discriminative models, also called *conditional models*, tend to learn *the boundary between classes/labels* in a dataset. Discriminative models are *not capable of generating new data instances*.

In Math, training classifiers involve estimating f:  $X \rightarrow Y$  or P(Y|X)

#### Generative classifiers

- Assume some functional form for P(Y), P(X|Y)
- Estimate parameters of P(X|Y) and P(Y) directly from training data
- Use Bayes rule to calculate P(Y|X) = P(Y)P(X|Y)/P(X) = P(X,Y)/P(X)

### Discriminative Classifiers

- Assume some functional form for P(Y|X)
- Estimate parameters of P(Y|X) directly from training data

#### Generative Classifiers

- Naïve Bayes (Bayesian networks)
- Hidden Markov Models (HMM)

#### Discriminative Classifiers

- Logistic regression
- Support Vector Machine
- Decision Tree
- Random Forest

#### Dense & Sparse Features

Dense features incorporate information from users/items pairs, historical statistics, predictions from upstream models [1] and etc. Typically *sparse features* include IDs of users/items, demographics, keywords and etc. Many recommendation models rely on both dense and sparse features in conjunction in order to achieve the best results. Dense features cannot completely replace sparse features and vice versa.

Dense and sparse features have different properties. For example, the relative ordering of dense feature values are meaningful but this is rarer for sparse features. In an online production system values for sparse features are often restricted within a predefined dictionary while ranges of dense features can be undetermined. Due to the inherent differences of dense and sparse features, they are processed in different ways.

### Machine Learning System Design

- Search Ranking
- Feed Based System
- Recommendation System
- Self-Driving Car: Image Segmentation
- Entity Linking System
- Ad Prediction System

#### **CNN**

The pooling operation involves sliding a two-dimensional filter over each channel of feature map and summarizing the features lying within the region covered by the filter. For a feature map having dimensions  $n_h \times n_w \times n_c$ , the dimensions of output obtained after a pooling layer is

$$(n_h - f + 1)/s \times (n_w - f + 1)/s \times n_c$$

- $n_h$  height of feature map
- $n_w$  width of feature map
- $n_c$  number of channels in the feature map
- f size of filter
- s stride length

A common CNN model architecture is to have a number of convolution and pooling layers stacked one after the other.

Why to use Pooling Layers?

- Pooling layers are used to reduce the dimensions of the feature maps. Thus, it reduces
  the number of parameters to learn and the amount of computation performed in the
  network.
- The pooling layer summarizes the features present in a region of the feature map
  generated by a convolution layer. So, further operations are performed on summarized
  features instead of precisely positioned features generated by the convolution layer. This
  makes the model more robust to variations in the position of the features in the input
  image.

Type of pooling layers:

- Max pooling
- Average pooling
- Global pooling global max pooling or global average pooling Global pooling reduces each channel in the feature map to a single value. Thus, an  $n_h \times n_w \times n_c$  feature map is reduced to  $1 \times 1 \times n_c$  feature map. This is equivalent to using a filter of dimensions  $n_h \times n_w$  i.e. the dimensions of the feature map. Further, it can be either global max pooling or global average pooling.

The motivation of padding

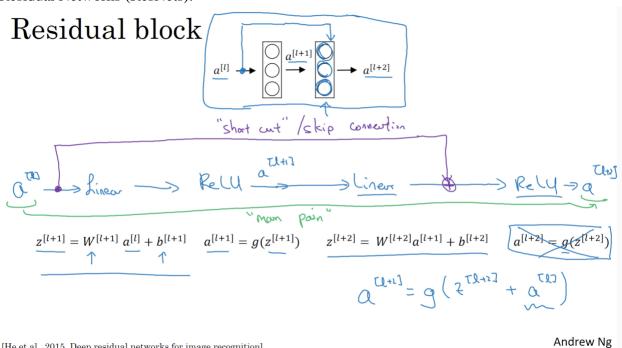
- For a gray scale  $(n \times n)$  image and  $(f \times f)$  filter/kernel, the dimensions of the image resulting from a convolution operation is  $(n f + 1) \times (n f + 1)$ . Thus, the image shrinks every time a convolution operation is performed. This places an upper limit to the number of times such an operation could be performed before the image reduces to nothing thereby precluding (阻止 v.) us from building deeper networks.
- Also, the pixels on the corners and the edges are used much less than those in the middle.

The same padding:

Same Padding: In this case, we add 'p' padding layers (p layers of zeros) such that the output image has the same dimensions as the input image.

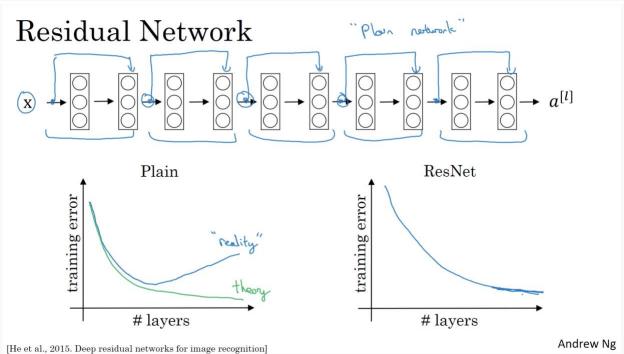
$$[(n+2p)\times(n+2p) \text{ image}] * [(f\times f) \text{ filter}] -> [(n\times n) \text{ image}]$$
 where \* represents a convolution operation which gives  $p = (f-1)/2$  (because  $n+2p-f+1=n$ ).

Residual Networks (ResNets):



[He et al., 2015. Deep residual networks for image recognition]





# Why ResNets work?

• **The identity function** is easy for residual block to learn. It won't hurt the overall performance as the depth increases. Deep networks hard to learn even the identity function.

A bag has 18 black balls and 9 white balls. On each turn you randomly select two balls and set them aside. If both balls are the same color you then add a black ball, otherwise you add a white ball. What is the probability that the last ball left in the bag is white? What if we instead start with 18 black balls and 36 white balls?

B(t) and W(t) are number of black balls and white balls at t

So we have B(0) = 18 and W(0) = 9 and also each time number of balls in the bag decreased by 1

So B(t+1) + W(t+1) = B(t) + W(t) - 1 and at the  $26^{th}$  step, B(26) + W(26) = 1

If we have BB, then B(t+1) = B(t) - 1 and W(t+1) = W(t)

If we have BW, then B(t+1) = B(t) - 1 and W(t+1) = W(t)

If we have WW, then B(t+1) = B(t) + 1 and W(t+1) = W(t) - 2

Notice that W is \*always\* odd because W(0) = 9 and it is decreased by 2 and B(26) + W(26) = 1. So the last one must be a white ball.

If there are 18 blacks balls and 36 white balls.

Because W(0) = 36, so W is \*always\* even and B(53) + W(53) = 1. So the last one must be a black ball.

You know that the probability it rains on any given day is 0.4. You are wondering if you should bring your umbrella with you today. You ask your friend if it's raining right now and he says yes. Knowing that your friend may be lying to you with probability 0.2, what is the true probability that it is raining now?

R standards for prob of raining and Y stands for friends says yes.

So the question is asking for P(R|Y) and we know P(R) = 0.4 and P(Y|NR) = 0.2.

$$P(R|Y) = \frac{P(Y|R)P(R)}{P(Y|R)P(R) + P(Y|NR)P(NR)} = \frac{0.8 \times 0.4}{0.8 \times 0.4 + 0.2 \times 0.6} = \frac{8}{11}$$