MACHINE LEARNING CHEATSHEET

Summary of Machine Learning Algorithms descriptions, advantages and use cases. Inspired by the very good book and articles of *MachineLearningMastery,* with added math, and *ML Pros & Cons* of *HackingNote.* Design inspired by *The Probability Cheatsheet* of W. Chen. Written by Rémi Canard.

GNERAL

Definition

We want to learn a target function ***f*** that maps input variables ***X*** to output variable ***Y***, with an error ***e***:

$$Y = f(X) + e$$

Linear, Nonlinear

Different algorithms make different assumptions about the shape and structure of f, thus the need of testing several methods. Any algorithm can be either:

- **Parametric (or Linear):** simplify the mapping to a known linear combination form and learning its coefficients.
- **Non parametric (or Nonlinear):** free to learn any functional form from the training data, while maintaining some ability to generalize.

Linear algorithms are usually simpler, faster and requires less data, while Nonlinear can be are more flexible, more powerful and more performant.

Supervised, Unsupervised

Supervised learning methods learn to predict Y from X given that the data is labeled.

Unsupervised learning methods learn to find the inherent structure of the unlabeled data.

Bias-Variance trade-off

In supervised learning, the prediction error ***e*** is composed of the **bias**, the **variance** and the **irreducible** part.

Bias refers to **simplifying assumptions** made to learn the target function easily.

Variance refers to sensitivity of the model to changes in the training data.

The **goal of parameterization** is to achieve a **low bias** (underlying pattern not too simplified) and **low variance** (not sensitive to specificities of the training data) **tradeoff**.

Underfitting, Overfitting

In statistics, ***fit*** refers to how well the target function is approximated.

Underfitting refers to poor inductive learning from training data and poor generalization.

Overfitting refers to learning the training data detail and noise which leads to poor generalization. It can be **limited** by using resampling and defining a validation dataset.

Optimization

Almost every machine learning method has an optimization algorithm at its core.

Gradient Descent

Gradient Descent is used to **find the coefficients** of f that **minimizes a cost function** (for example MSE, SSR).

Procedure:

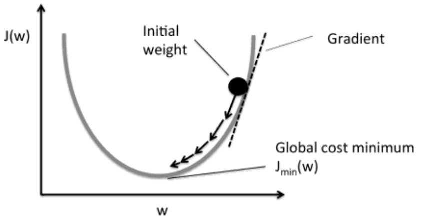
→ Initialization $\theta = 0$ (coefficients to 0 or random)

→ Calculate cost $J(\theta) = evaluate(f\ (coefficients\ J))$

→ Gradient of cost $\frac{\partial}{\partial\theta_j}J(\theta)$ we know the uphill direction

→ Update coeff $\theta j = \theta j - \alpha\ \frac{7}{789}J(\theta)$ we go downhill

The cost updating process is repeated until convergence (minimum found).



Batch Gradient Descend does summing/averaging of the cost over all the observations.

Stochastic Gradient Descent apply the procedure of parameter updating for each observation.

Tips:

- Change **learning rate** α ("size of jump" at each iteration)

- Plot *Cost vs Time* to assess learning rate performance

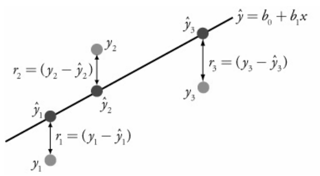
- Rescaling the input variables

- Reduce passes through training set with SGD

- Average over 10 or more updated to observe the learning trend while using SGD

Ordinary Least Squares (OLS)

OLS is used to find the estimator $\hat{\beta}$ that **minimizes the sum of squared residuals:** $\sum_{iCD}^{n}(y_i - \beta_@ - \sum_{9CD}^{p}\beta_9 x_{i9})^F = y - X\,\beta$


$\hat{y} = b_0 + b_1 x$
$\hat{y}_3$
y_2
$r_2 = (y_2 - \hat{y}_2)$
$r_3 = (y_3 - \hat{y}_3)$
y_3
$\hat{y}_2$
$\hat{y}_1$
$r_1 = (y_1 - \hat{y}_1)$
y_1

Using linear algebra such that we have $\hat{\beta} = (X^T X)^{-D} X^T y$

Maximum Likelihood Estimation (MLE)

MLE is used to find the estimators that **minimizes the likelihood function:**

$f(\theta|x) = f_8(x)$ density function of the data distribution

Linear Algorithms

All linear Algorithms assume a linear relationship between the input variables X and the output variable Y.

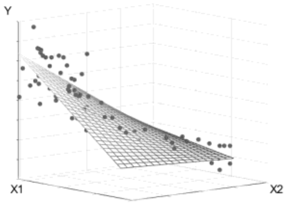
Linear Regression

Representation:

A LR model representation is a linear equation:

$$y = \beta_@ + \beta_D x_D + \cdots + \beta_i x_i$$

$\beta_@$ is usually called intercept or **bias** coefficient. The dimension of the hyperplane of the regression is its **complexity**.



Learning:

Learning a LR means estimating the coefficients from the training data. Common methods include **Gradient Descent** or **Ordinary Least Squares**.

Variations:

There are extensions of LR training called **regularization** methods, that aim to **reduce the complexity** of the model:

- **Lasso Regression**: where OLS is modified to minimize the sum of the coefficients (*L1 regularization*)

$$\sum_{\text{iCD}}^{n}(y_\text{i} - \beta_@ - \sum_{\text{9CD}}^{p}\beta_9 x_{\text{i9}})^\text{F} + \lambda\sum_{\text{9CD}}^{p}|\beta_9| = RSS + \lambda\sum_{\text{9CD}}^{p}|\beta_9|$$

- **Ridge Regression**: where OLS is modified to minimize the squared sum of the coefficients (*L2 regularization*)

$$\sum_{\text{iCD}}^{n}(y_\text{i} - \beta_@ - \sum_{\text{9CD}}^{p}\beta_9 x_{\text{i9}})^\text{F} + \lambda\sum_{\text{9CD}}^{p}\beta_9^\text{F} = RSS + \lambda\sum_{\text{9CD}}^{p}\beta_9^\text{F}$$

where $\lambda \geq 0$ is a tuning parameter to be determined.

Data preparation:

- Transform data for linear relationship (ex: log transform for exponential relationship)

- Remove noise such as outliers

- Rescale inputs using standardization or normalization

Advantages:

+ Good regression baseline considering simplicity

+ Lasso/Ridge can be used to avoid overfitting

+ Lasso/Ridge permit feature selection in case of collinearity

Use case examples:

- Product sales prediction according to prices or promotions

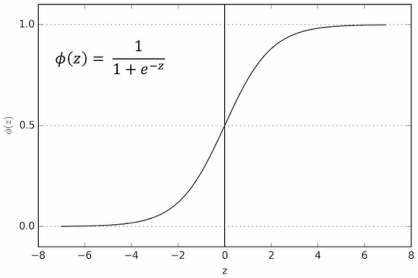
- Call-center waiting-time prediction according to the number of complaints and the number of working agents

Logistic Regression

It is the go-to for **binary classification.**

Representation:

Logistic regression a linear method but predictions are transformed using the **logistic function** (or sigmoid):



ϕ is *S*-shaped and map real-valued number in (0,1).

The representation is an equation with binary output:

$$y = \frac{e^{\beta_\text{R}\text{S}\beta_\text{T}x_\text{T}\text{S}\cdots\text{S}\beta_\text{i}x_\text{i}}}{1 + e^{\beta_\text{R}\text{S}\beta_\text{T}x_\text{T}\text{S}\cdots\text{S}\beta_\text{i}x_\text{i}}}$$

Which actually models the probability of default class:

$$p(X) = \frac{e^{\beta_\text{R}\text{S}\beta_\text{T}x_\text{T}\text{S}\cdots\text{S}\beta_\text{i}x_\text{i}}}{1 + e^{\beta_\text{R}\text{S}\beta_\text{T}x_\text{T}\text{S}\cdots\text{S}\beta_\text{i}x_\text{i}}} = p(Y = 1|X)$$

Learning:

Learning the Logistic regression coefficients is done using **maximum-likelihood estimation**, to predict values close to 1 for default class and close to 0 for the other class.

Data preparation:

- Probability transformation to binary for classification

- Remove noise such as outliers

Advantages:

+ Good classification baseline considering simplicity

+ Possibility to change cutoff for precision/recall tradeoff

+ Robust to noise/overfitting with L1/L2 regularization

+ Probability output can be used for ranking

Use case examples:

- Customer scoring with probability of purchase

- Classification of loan defaults according to profile

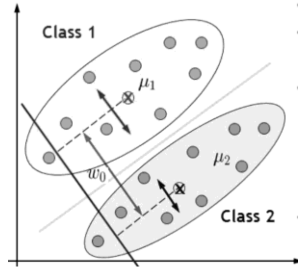
Linear Discriminant Analysis

For **multiclass classification**, LDA is the preferred linear technique.

Representation:

LDA representation consists of **statistical properties** calculated for **each class**: **means** and the **covariance matrix**:

$$\mu_k = \frac{\text{D}}{n_k}\sum_{\text{iCD}}^{n} x_\text{i} \quad \text{and} \quad \sigma^\text{F} = \frac{\text{D}}{n-K}\sum_{\text{iCD}}^{n}(x_\text{i} - \mu_k)^\text{F}$$



LDA assumes **Gaussian** data and attributes of **same σ^2**.

Predictions are made using **Bayes Theorem:**

$$P(Y = k|X = x) = \frac{P(k)\times P(x|k)}{\sum_{l\text{CD}}^{K} P(l)\times P(x|l)}$$

to obtain a discriminate function (latent variable) for each class k, estimating $P(x|k)$ with a Gaussian distribution:

$$D_k(x) = x \times \frac{\mu_k}{\sigma^\text{F}} - \frac{\mu_k{}^\text{F}}{2\sigma^\text{F}} + \ln(P(k))$$

The class with largest **discriminant value** is the **output class.**

Variations:

- **Quadratic DA**: Each class uses its own variance estimate

- **Regularized DA**: Regularization into the variance estimate

Data preparation:

- Review and modify univariate distributions to be Gaussian

- Standardize data to $\mu = 0, \sigma = 1$ to have same variance

- Remove noise such as outliers

Advantages:

+ Can be used for dimensionality reduction by keeping the latent variables as new variables

Use case example:

- Prediction of customer churn

Nonlinear Algorithms

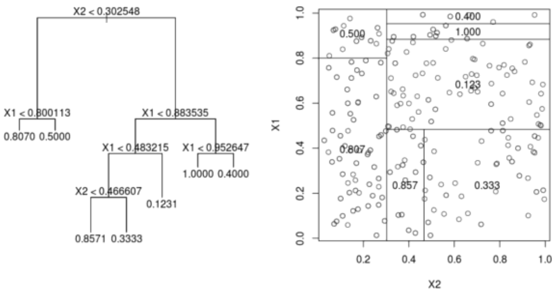
All Nonlinear Algorithms are non-parametric and more flexible. They are not sensible to outliers and do not require any shape of distribution.

Classification and Regression Trees

Also referred as CART or Decision Trees, this algorithm is the foundation of Random Forest and Boosted Trees.

Representation:

The model representation is a **binary tree**, where each **node** is an **input variable** *x* with a split point and each **leaf** contain an **output variable** *y* for prediction.



The model actually **split the input space** into (hyper) rectangles, and predictions are made according to the **area** observations *fall* into.

Learning:

Learning of a **CART** is done by a greedy approach called **recursive binary splitting** of the input space:

At each step, the best **predictor** X_9 and the best **cutpoint** s are selected such that $\{X|X_9 < s\}$ and $\{X|X_9 \geq s\}$ **minimizes the cost**.

- For **regression** the cost is the **Sum of Squared Error:**

$$\sum_{iCD}^{n}(y_i - \hat{y})^{F}$$

- For **classification** the cost function is the **Gini index:**

$$G = \sum_{iCD}^{n} p_k(1 - p_k)$$

The Gini index is **an indication of how *pure* are the leaves**, if all observations are the same type G=0 (perfect purity), while a 50-50 split for binary would be G=0.5 (worst purity).

The most common **Stopping Criterion** for splitting is a minimum of **training observations per node**.

The simplest form of pruning is **Reduced Error Pruning:**

Starting at the leaves, each node is replaced with its most popular class. If the prediction accuracy is not affected, then the change is kept

Advantages:

+ Easy to interpret and no overfitting with pruning

+ Works for both regression and classification problems

+ Can take any type of variables without modifications, and do not require any data preparation

Use case examples:

- Fraudulent transaction classification

- Predict human resource allocation in companies

Naive Bayes Classifier

Naive Bayes is a **classification** algorithm interested in selecting the **best hypothesis *h* given data *d*** assuming there is no interaction between features.

Representation:

The representation is the based on Bayes Theorem:

$$P(h|d) = \frac{P(d|h) \times P(h)}{P(d)}$$

with naïve hypothesis $P(d|h) = P(x_D|h) \times \ldots \times P(x_i|h)$

The prediction is the **Maximum A posteriori Hypothesis**:

$$MAP(h) = \max(P(h|d)) = \max(P(d|h) \times P(h))$$

The denominator is not kept as it is only for normalization.

Learning:

Training is **fast** because only **probabilities** need to be calculated:

$$P(h) = \frac{instances_w}{all\ instances} \text{ and } P(x|h) = \frac{count(x \text{ A} \{\})}{instances_w}$$

Variations:

Gaussian Naive Bayes can extend to numerical attributes by assuming a Gaussian distribution.

Instead of $P(x|h)$ are calculated with $P(h)$ during **learning**:

$$\mu(x) = \frac{D}{n}\sum_{iCD}^{n} x_i \text{ and } \sigma = \sqrt{\frac{D}{n}\sum_{iCD}^{n}(x_i - \mu(x))^{F}}$$

and **MAP** for **prediction** is calculated using Gaussian PDF

$$f(x|\mu(x),\sigma) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{(x-\mu)^{Ç}}{F\sigma^{Ç}}}$$

Data preparation:

- Change numerical inputs to categorical (binning) or near-Gaussian inputs (remove outliers, log & boxcox transform)

- Other distributions can be used instead of Gaussian

- Log-transform of the probabilities can avoid overflow

- Probabilities can be updated as data becomes available

Advantages:

+ Fast because of the calculations

+ If the naive assumptions work can converge quicker than other models. Can be used on smaller training data.

+ Good for few categories variables

Use case examples:

- Article classification using binary word presence

- Email spam detection using a similar technique

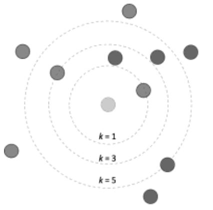
K-Nearest Neighbors

If you are like your neighbors, you are one of them.

Representation:

KNN uses the **entire training set**, **no training** is required.

Predictions are made by searching the ***k* similar instances**, according to a **distance**, and **summarizing the output**.



For **regression** the output can be the **mean**, while for **classification** the output can be the **most common class**.

Various distances can be used, for example:

- **Euclidean** Distance, good for **similar** type of variables

$$d(a,b) = \sqrt{\sum_{\text{iCD}}^{n} (a_{\text{i}} - b_{\text{i}})^{\text{F}}}$$

- **Manhattan** Distance, good for **different** type of variables

$$d(a,b) = \sum_{\text{iCD}}^{n} |a_{\text{i}} - b_{\text{i}}|$$

The **best value of *k*** must be found by **testing**, and the algorithm is **sensible** to the ***Curse of dimensionality***.

Data preparation:

- Rescale inputs using standardization or normalization

- Address missing data for distance calculations

- Dimensionality reduction or feature selection for *COD*

Advantages:

+ Effective if the training data is large

+ No learning phase

+ Robust to noisy data, no need to filter outliers

Use case examples:

- Recommending products based on similar customers

- Anomaly detection in customer behavior

Support Vector Machines

SVM is a go-to for high performance with little tuning

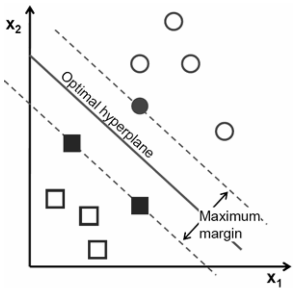
Representation:

In SVM, a **hyperplane** is selected to **separate the points** in the input variable space by their class, with the **largest margin**.

The closest datapoints (defining the margin) are called the **support vectors**.

But real **data cannot be perfectly separated**, that is why a ***C*** defines the amount of **violation** of the margin allowed.

The lower C, the more sensitive SVM is to training data.



The **prediction** function is the signed **distance** of the new input *x* to the separating hyperplane *w*:

$f(x) = < w, x > + \rho = w^T x + \rho$ with ρ the bias Which gives for **linear kernel**, with x_{i} the support vectors:

$$f(x) = \sum_{\text{iCD}}^{n} a_{\text{i}} \times (x \times x_{\text{i}})) + \rho$$

Learning:

The hyperplane learning is done by transforming the problem using linear algebra, and minimizing:

$$\left[\frac{1}{n}\sum_{\text{iCD}}^{n} \max\left(0, 1 - y_{\text{i}}\ (\vec{w}.\vec{x_{\text{Ü}}} - b\ )\right)\right] + \lambda||\vec{w}||^{\text{F}}$$

Variations:

SVM is implemented using various kernels, which define the measure between new data and support vectors:

- **Linear** (dot-product): $K(x, x_{\text{i}}) = \sum(x \times x_{\text{i}})$

- **Polynomial**: $K(x, x_{\text{i}}) = 1 + \sum(x \times x_{\text{i}})^{d}$

- **Radial**: $K(x, x_{\text{i}}) = e^{-\text{â}\ \sum(x - x_{\text{i}})^{\text{ç}})}$

Data preparation:

- SVM assumes numeric inputs, may require dummy transformation of categorical features

Advantages:

+ Allow nonlinear separation with nonlinear Kernels

+ Works good in high dimensional space

+ Robust to multicollinearity and overfitting

Use case examples:

- Face detection from images

- Target Audience Classification from tweets

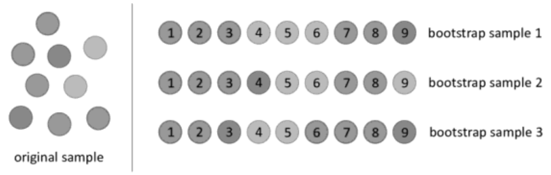
Ensemble Algorithms

Ensemble methods use multiple, simpler algorithms combined to obtain better performance.

Bagging and Random Forest

Random Forest is part of a bigger type of ensemble methods called **Bootstrap Aggregation** or **Bagging**. Bagging can **reduce the variance** of high-variance models.

It uses the **Bootstrap statistical procedure**: estimate a quantity from a sample by creating many random subsamples with replacement, and computing the mean of each subsample.


original sample
1 2 3 4 5 6 7 8 9 bootstrap sample 1
1 2 3 4 5 6 7 8 9 bootstrap sample 2
1 2 3 4 5 6 7 8 9 bootstrap sample 3

Representation:

For **bagged decision trees**, the steps would be:

- Create many subsamples of the training dataset

- Train a CART model on each sample

- Given a new dataset, calculate the average prediction

However, combining models works best if submodels are **weakly correlated** at best.

Random Forest is a tweaked version of bagged decision trees to **reduce tree correlation**.

Learning:

During learning, each **sub-tree** can only access a random **sample of features** when **selecting the split points**. The size of the feature sample at each split is a parameter *m*.

A good default is $\sqrt{p}$for classification and $\frac{p}{\text{ä}}$for regression.

The **OOB** estimate is the performance of **each model on its Out-Of-Bag** (not selected) samples. It is a reliable estimate of test error.

Bagged method can provide **feature importance**, by calculating and averaging the **error function drop for individual variables** (depending of samples where a variable is selected or not).

Advantages:

In addition to the advantages of the CART algorithm

+ Robust to overfitting and missing variables

+ Can be parallelized for distributed computing

+ Performance as good as SVM but easier to interpret

Use case examples:

- Predictive Maintenance (PdM) models

- Optimizing line decision for credit cards

Boosting and AdaBoost

AdaBoost was the first successful boosting algorithm developed for binary classification.

Representation:

A boost classifier is of the form

$$F_T(x) = \sum_{t\text{CD}}^{T} f_t(x)$$

where each f_t is a **week learner correcting the errors** of the previous one.

Adaboost is commonly used with decision trees with one level (***decision stumps***).

Predictions are made using the weighted average of the weak classifiers.

Learning:

Each training set instance is initially weighted $w(x_{\text{i}}) = \frac{\text{D}}{n}$

One *decision stump* is prepared using the weighted samples, and a **misclassification rate** is calculated:

$$\epsilon = \frac{\sum_{\text{iCD}}^{n}(w_{\text{i}} \times p_{error\ \text{i}})}{\sum_{\text{iCD}}^{n} w}$$

Which is the weighted sum of the misclassification rates, where w is the training instance *i* weight and $p_{error\ \text{i}}$ its prediction error (1 or 0).

A **stage value** is computed from the misclassification rate:

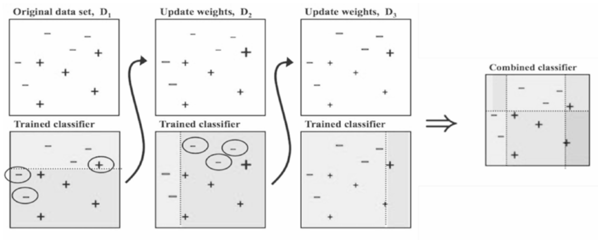
$$stage = \ln\left(\frac{1-\epsilon}{\epsilon}\right)$$

This stage value is used to **update the instances weights**:

$$w = w \times e^{sta\text{èe}\times\text{g}}$$

The **incorrectly** predicted instance are given **more** weight.

Weak models are added sequentially using the training weights, until no improvement can be made or the number of rounds has been attained.



Data preparation:

- Outliers should be removed for AdaBoost

Advantages:

+ High performance with no tuning (only number of rounds)

Interesting Resources

Machine Learning Mastery website

> *https://machinelearningmastery.com/*

Scikit-learn website*, for python implementation*

> *http://scikit-learn.org/*

W.Chen probability cheat sheet

> *https://github.com/wzchen/probability_cheatsheet*

HackingNote*, for interesting, condensed insights*

> *https://www.hackingnote.com/*

Seattle Data Guy blog*, for business-oriented articles*

> *https://www.theseattledataguy.com/*

Explained visually*, making hard ideas intuitive*

> *http://setosa.io/ev/*

This Machine Learning Cheat sheet

> *aimlbobbilithinks/digitaltransformation (github.com)*