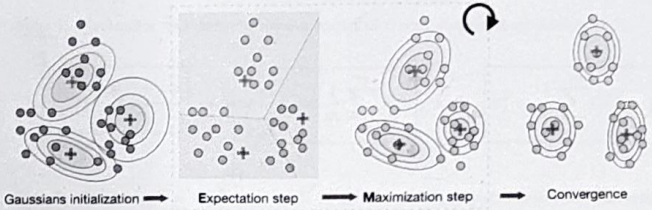
VIP Cheatsheet: Unsupervised Learning

Afshine Amidi and Shervine Amidi

September 9, 2018



Introduction to Unsupervised Learning

❒ **Motivation** – The goal of unsupervised learning is to find hidden patterns in unlabeled data $\{x^{(1)},...,x^{(m)}\}$.

❒ **Jensen's inequality** – Let f be a convex function and X a random variable. We have the following inequality:

$$\boxed{E[f(X)] \geqslant f(E[X])}$$

Expectation-Maximization

❒ **Latent variables** – Latent variables are hidden/unobserved variables that make estimation problems difficult, and are often denoted z. Here are the most common settings where there are latent variables:

Setting	Latent variable z	$x\|z$	Comments
Mixture of k Gaussians	Multinomial(ϕ)	$\mathcal{N}(\mu_j,\Sigma_j)$	$\mu_j \in \mathbb{R}^n, \phi \in \mathbb{R}^k$
Factor analysis	$\mathcal{N}(0,I)$	$\mathcal{N}(\mu+\Lambda z,\psi)$	$\mu_j \in \mathbb{R}^n$

❒ **Algorithm** – The Expectation-Maximization (EM) algorithm gives an efficient method at estimating the parameter θ through maximum likelihood estimation by repeatedly constructing a lower-bound on the likelihood (E-step) and optimizing that lower bound (M-step) as follows:

- E-step: Evaluate the posterior probability $Q_i(z^{(i)})$ that each data point $x^{(i)}$ came from a particular cluster $z^{(i)}$ as follows:

$$\boxed{Q_i(z^{(i)}) = P(z^{(i)}|x^{(i)};\theta)}$$

- M-step: Use the posterior probabilities $Q_i(z^{(i)})$ as cluster specific weights on data points $x^{(i)}$ to separately re-estimate each cluster model as follows:

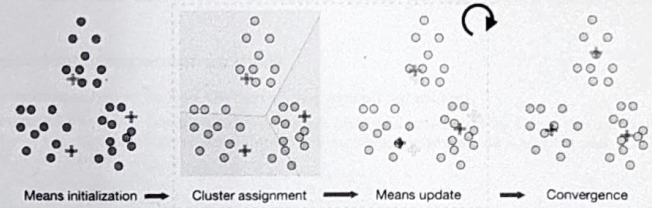
$$\boxed{\theta_i = \underset{\theta}{\text{argmax}} \sum_i \int_{z^{(i)}} Q_i(z^{(i)}) \log\left(\frac{P(x^{(i)},z^{(i)};\theta)}{Q_i(z^{(i)})}\right) dz^{(i)}}$$

k-means clustering

We note $c^{(i)}$ the cluster of data point i and μ_j the center of cluster j.

❒ **Algorithm** – After randomly initializing the cluster centroids $\mu_1,\mu_2,...,\mu_k \in \mathbb{R}^n$, the k-means algorithm repeats the following step until convergence:

$$\boxed{c^{(i)} = \arg\min_j ||x^{(i)} - \mu_j||^2} \quad \text{and} \quad \boxed{\mu_j = \frac{\sum_{i=1}^m 1_{\{c^{(i)}=j\}} x^{(i)}}{\sum_{i=1}^m 1_{\{c^{(i)}=j\}}}}$$



❒ **Distortion function** – In order to see if the algorithm converges, we look at the distortion function defined as follows:

$$\boxed{J(c,\mu) = \sum_{i=1}^m ||x^{(i)} - \mu_{c^{(i)}}||^2}$$

Hierarchical clustering

❒ **Algorithm** – It is a clustering algorithm with an agglomerative hierarchical approach that build nested clusters in a successive manner.

❒ **Types** – There are different sorts of hierarchical clustering algorithms that aims at optimizing different objective functions, which is summed up in the table below:

Ward linkage	Average linkage	Complete linkage
Minimize within cluster distance	Minimize average distance between cluster pairs	Minimize maximum distance of between cluster pairs

Clustering assessment metrics

In an unsupervised learning setting, it is often hard to assess the performance of a model since we don't have the ground truth labels as was the case in the supervised learning setting.

❒ **Silhouette coefficient** – By noting a and b the mean distance between a sample and all other points in the same class, and between a sample and all other points in the next nearest cluster, the silhouette coefficient s for a single sample is defined as follows:

$$\boxed{s = \frac{b-a}{\max(a,b)}}$$

❒ **Calinski-Harabaz index** – By noting k the number of clusters, B_k and W_k the between and within-clustering dispersion matrices respectively defined as

$$B_k = \sum_{j=1}^{k} n_{c(i)}(\mu_{c(i)} - \mu)(\mu_{c(i)} - \mu)^T, \qquad W_k = \sum_{i=1}^{m}(x^{(i)} - \mu_{c(i)})(x^{(i)} - \mu_{c(i)})^T$$

the Calinski-Harabaz index $s(k)$ indicates how well a clustering model defines its clusters, such that the higher the score, the more dense and well separated the clusters are. It is defined as follows:

$$\boxed{s(k) = \frac{\text{Tr}(B_k)}{\text{Tr}(W_k)} \times \frac{N-k}{k-1}}$$

Principal component analysis

It is a dimension reduction technique that finds the variance maximizing directions onto which to project the data.

❒ **Eigenvalue, eigenvector** – Given a matrix $A \in \mathbb{R}^{n\times n}$, λ is said to be an eigenvalue of A if there exists a vector $z \in \mathbb{R}^n \backslash \{0\}$, called eigenvector, such that we have:

$$\boxed{Az = \lambda z}$$

❒ **Spectral theorem** – Let $A \in \mathbb{R}^{n\times n}$. If A is symmetric, then A is diagonalizable by a real orthogonal matrix $U \in \mathbb{R}^{n\times n}$. By noting $\Lambda = \text{diag}(\lambda_1,...,\lambda_n)$, we have:

$$\boxed{\exists \Lambda \text{ diagonal}, \quad A = U\Lambda U^T}$$

Remark: the eigenvector associated with the largest eigenvalue is called principal eigenvector of matrix A.

❒ **Algorithm** – The Principal Component Analysis (PCA) procedure is a dimension reduction technique that projects the data on k dimensions by maximizing the variance of the data as follows:

- Step 1: Normalize the data to have a mean of 0 and standard deviation of 1.

$$\boxed{x_j^{(i)} \leftarrow \frac{x_j^{(i)} - \mu_j}{\sigma_j}} \quad \text{where} \quad \boxed{\mu_j = \frac{1}{m}\sum_{i=1}^{m} x_j^{(i)}} \quad \text{and} \quad \boxed{\sigma_j^2 = \frac{1}{m}\sum_{i=1}^{m}(x_j^{(i)} - \mu_j)^2}$$

- Step 2: Compute $\Sigma = \frac{1}{m}\sum_{i=1}^{m} x^{(i)}x^{(i)T} \in \mathbb{R}^{n\times n}$, which is symmetric with real eigenvalues.
- Step 3: Compute $u_1,...,u_k \in \mathbb{R}^n$ the k orthogonal principal eigenvectors of Σ, i.e. the orthogonal eigenvectors of the k largest eigenvalues.
- Step 4: Project the data on $\text{span}_{\mathbb{R}}(u_1,...,u_k)$. This procedure maximizes the variance among all k-dimensional spaces.

Independent component analysis

It is a technique meant to find the underlying generating sources.

❒ **Assumptions** – We assume that our data x has been generated by the n-dimensional source vector $s = (s_1,...,s_n)$, where s_i are independent random variables, via a mixing and non-singular matrix A as follows:

$$\boxed{x = As}$$

The goal is to find the unmixing matrix $W = A^{-1}$ by an update rule.

❒ **Bell and Sejnowski ICA algorithm** – This algorithm finds the unmixing matrix W by following the steps below:

- Write the probability of $x = As = W^{-1}s$ as:

$$p(x) = \prod_{i=1}^{n} p_s(w_i^T x) \cdot |W|$$

- Write the log likelihood given our training data $\{x^{(i)}, i \in [\![1,m]\!]\}$ and by noting g the sigmoid function as:

$$l(W) = \sum_{i=1}^{m}\left(\sum_{j=1}^{n}\log\left(g'(w_j^T x^{(i)})\right) + \log|W|\right)$$

Therefore, the stochastic gradient ascent learning rule is such that for each training example $x^{(i)}$, we update W as follows:

$$\boxed{W \longleftarrow W + \alpha \left(\begin{pmatrix} 1 - 2g(w_1^T x^{(i)}) \\ 1 - 2g(w_2^T x^{(i)}) \\ \vdots \\ 1 - 2g(w_n^T x^{(i)}) \end{pmatrix} x^{(i)^T} + (W^T)^{-1} \right)}$$

VIP Cheatsheet: Machine Learning Tips

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Metrics

Given a set of data points $\{x^{(1)},...,x^{(m)}\}$, where each $x^{(i)}$ has n features, associated to a set of outcomes $\{y^{(1)},...,y^{(m)}\}$, we want to assess a given classifier that learns how to predict y from x.

Classification

In a context of a binary classification, here are the main metrics that are important to track to assess the performance of the model.

❒ **Confusion matrix** – The confusion matrix is used to have a more complete picture when assessing the performance of a model. It is defined as follows:

		Predicted class +	**Predicted** class −
Actual class	+	**TP** True Positives	**FN** False Negatives Type II error
	−	**FP** False Positives Type I error	**TN** True Negatives

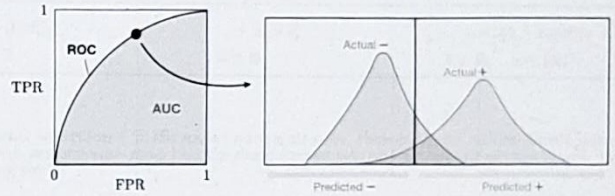
❒ **Main metrics** – The following metrics are commonly used to assess the performance of classification models:

Metric	Formula	Interpretation
Accuracy	$\frac{\text{TP}+\text{TN}}{\text{TP}+\text{TN}+\text{FP}+\text{FN}}$	Overall performance of model
Precision	$\frac{\text{TP}}{\text{TP}+\text{FP}}$	How accurate the positive predictions are
Recall Sensitivity	$\frac{\text{TP}}{\text{TP}+\text{FN}}$	Coverage of actual positive sample
Specificity	$\frac{\text{TN}}{\text{TN}+\text{FP}}$	Coverage of actual negative sample
F1 score	$\frac{2\text{TP}}{2\text{TP}+\text{FP}+\text{FN}}$	Hybrid metric useful for unbalanced classes

❒ **ROC** – The receiver operating curve, also noted ROC, is the plot of TPR versus FPR by varying the threshold. These metrics are are summed up in the table below:

Metric	Formula	Equivalent
True Positive Rate TPR	$\frac{\text{TP}}{\text{TP}+\text{FN}}$	Recall, sensitivity
False Positive Rate FPR	$\frac{\text{FP}}{\text{TN}+\text{FP}}$	1-specificity

❒ **AUC** – The area under the receiving operating curve, also noted AUC or AUROC, is the area below the ROC as shown in the following figure:



Regression

❒ **Basic metrics** – Given a regression model f, the following metrics are commonly used to assess the performance of the model:

Total sum of squares	Explained sum of squares	Residual sum of squares
$\text{SS}_{\text{tot}}=\sum_{i=1}^{m}(y_i-\overline{y})^2$	$\text{SS}_{\text{reg}}=\sum_{i=1}^{m}(f(x_i)-\overline{y})^2$	$\text{SS}_{\text{res}}=\sum_{i=1}^{m}(y_i-f(x_i))^2$

❒ **Coefficient of determination** – The coefficient of determination, often noted R^2 or r^2, provides a measure of how well the observed outcomes are replicated by the model and is defined as follows:

$$R^2=1-\frac{\text{SS}_{\text{res}}}{\text{SS}_{\text{tot}}}$$

❒ **Main metrics** – The following metrics are commonly used to assess the performance of regression models, by taking into account the number of variables n that they take into consideration:

Mallow's Cp	AIC	BIC	Adjusted R^2
$\frac{\text{SS}_{\text{res}}+2(n+1)\widehat{\sigma^2}}{m}$	$2\big[(n+2)-\log(L)\big]$	$\log(m)(n+2)-2\log(L)$	$1-\frac{(1-R^2)(m-1)}{m-n-1}$

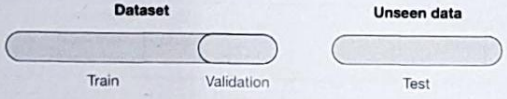
where L is the likelihood and $\widehat{\sigma}^2$ is an estimate of the variance associated with each response.

Model selection

❒ **Vocabulary** – When selecting a model, we distinguish 3 different parts of the data that we have as follows:

Training set	Validation set	Testing set
- Model is trained - Usually 80% of the dataset	- Model is assessed - Usually 20% of the dataset - Also called hold-out or development set	- Model gives predictions - Unseen data

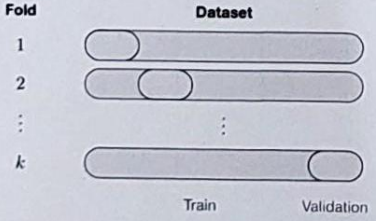
Once the model has been chosen, it is trained on the entire dataset and tested on the unseen test set. These are represented in the figure below:



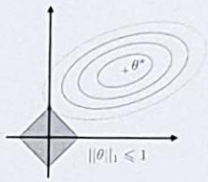
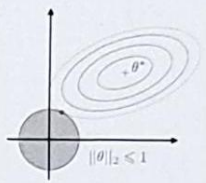
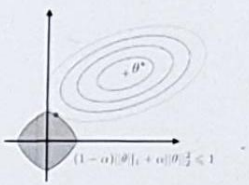
❒ **Cross-validation** – Cross-validation, also noted CV, is a method that is used to select a model that does not rely too much on the initial training set. The different types are summed up in the table below:

k-fold	Leave-p-out
- Training on $k-1$ folds and assessment on the remaining one - Generally $k = 5$ or 10	- Training on $n-p$ observations and assessment on the p remaining ones - Case $p = 1$ is called leave-one-out

The most commonly used method is called k-fold cross-validation and splits the training data into k folds to validate the model on one fold while training the model on the $k-1$ other folds, all of this k times. The error is then averaged over the k folds and is named cross-validation error.



❒ **Regularization** – The regularization procedure aims at avoiding the model to overfit the data and thus deals with high variance issues. The following table sums up the different types of commonly used regularization techniques:

LASSO	Ridge	Elastic Net
- Shrinks coefficients to 0 - Good for variable selection	Makes coefficients smaller	Tradeoff between variable selection and small coefficients
		
$... + \lambda\|\|\theta\|\|_1$ $\lambda \in \mathbb{R}$	$... + \lambda\|\|\theta\|\|_2^2$ $\lambda \in \mathbb{R}$	$... + \lambda\left[(1-\alpha)\|\|\theta\|\|_1 + \alpha\|\|\theta\|\|_2^2\right]$ $\lambda \in \mathbb{R}$, $\alpha \in [0,1]$

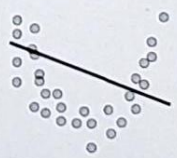
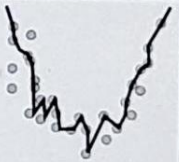
❒ **Model selection** – Train model on training set, then evaluate on the development set, then pick best performance model on the development set, and retrain all of that model on the whole training set.

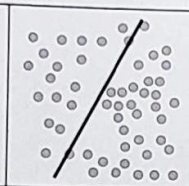
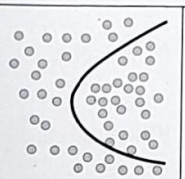
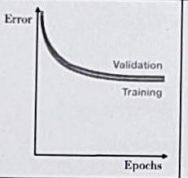
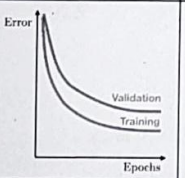
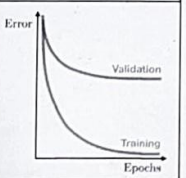
Diagnostics

❒ **Bias** – The bias of a model is the difference between the expected prediction and the correct model that we try to predict for given data points.

❒ **Variance** – The variance of a model is the variability of the model prediction for given data points.

❒ **Bias/variance tradeoff** – The simpler the model, the higher the bias, and the more complex the model, the higher the variance.

	Underfitting	Just right	Overfitting
Symptoms	- High training error - Training error close to test error - High bias	- Training error slightly lower than test error	- Low training error - Training error much lower than test error - High variance
Regression			

Classification			
Deep learning			
Remedies	- Complexify model - Add more features - Train longer		- Regularize - Get more data

❒ **Error analysis** – Error analysis is analyzing the root cause of the difference in performance between the current and the perfect models.

❒ **Ablative analysis** – Ablative analysis is analyzing the root cause of the difference in performance between the current and the baseline models.

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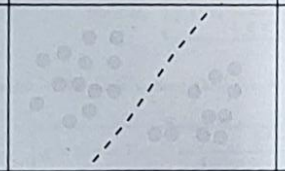
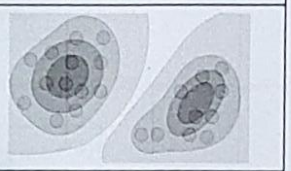
Introduction to Supervised Learning

Given a set of data points $\{x^{(1)},...,x^{(m)}\}$ associated to a set of outcomes $\{y^{(1)},...,y^{(m)}\}$, we want to build a classifier that learns how to predict y from x.

❒ **Type of prediction** – The different types of predictive models are summed up in the table below:

	Regression	Classifier
Outcome	Continuous	Class
Examples	Linear regression	Logistic regression, SVM, Naive Bayes

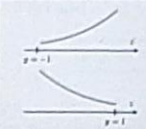
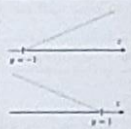
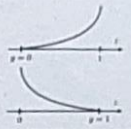
❒ **Type of model** – The different models are summed up in the table below:

	Discriminative model	Generative model
Goal	Directly estimate $P(y\|x)$	Estimate $P(x\|y)$ to deduce $P(y\|x)$
What's learned	Decision boundary	Probability distributions of the data
Illustration		
Examples	Regressions, SVMs	GDA, Naive Bayes

Notations and general concepts

❒ **Hypothesis** – The hypothesis is noted h_θ and is the model that we choose. For a given input data $x^{(i)}$, the model prediction output is $h_\theta(x^{(i)})$.

❒ **Loss function** – A loss function is a function $L:(z,y)\in\mathbb{R}\times Y\longmapsto L(z,y)\in\mathbb{R}$ that takes as inputs the predicted value z corresponding to the real data value y and outputs how different they are. The common loss functions are summed up in the table below:

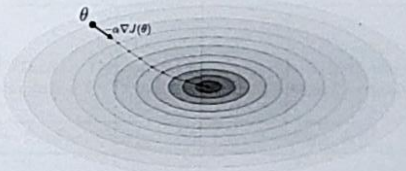
Least squared	Logistic	Hinge	Cross-entropy
$\frac{1}{2}(y-z)^2$	$\log(1+\exp(-yz))$	$\max(0,1-yz)$	$-\left[y\log(z)+(1-y)\log(1-z)\right]$
			
Linear regression	Logistic regression	SVM	Neural Network

❒ **Cost function** – The cost function J is commonly used to assess the performance of a model, and is defined with the loss function L as follows:

$$\boxed{J(\theta)=\sum_{i=1}^{m}L(h_\theta(x^{(i)}),y^{(i)})}$$

❒ **Gradient descent** – By noting $\alpha\in\mathbb{R}$ the learning rate, the update rule for gradient descent is expressed with the learning rate and the cost function J as follows:

$$\boxed{\theta\longleftarrow\theta-\alpha\nabla J(\theta)}$$



Remark: Stochastic gradient descent (SGD) is updating the parameter based on each training example, and batch gradient descent is on a batch of training examples.

❒ **Likelihood** – The likelihood of a model $L(\theta)$ given parameters θ is used to find the optimal parameters θ through maximizing the likelihood. In practice, we use the log-likelihood $\ell(\theta)=\log(L(\theta))$ which is easier to optimize. We have:

$$\boxed{\theta^{\text{opt}}=\underset{\theta}{\arg\max}\ L(\theta)}$$

❒ **Newton's algorithm** – The Newton's algorithm is a numerical method that finds θ such that $\ell'(\theta)=0$. Its update rule is as follows:

$$\boxed{\theta\leftarrow\theta-\frac{\ell'(\theta)}{\ell''(\theta)}}$$

Remark: the multidimensional generalization, also known as the Newton-Raphson method, has the following update rule:

$$\theta\leftarrow\theta-\left(\nabla^2_\theta\ell(\theta)\right)^{-1}\nabla_\theta\ell(\theta)$$

Linear regression

We assume here that $y|x;\theta \sim \mathcal{N}(\mu,\sigma^2)$

❒ **Normal equations** – By noting X the matrix design, the value of θ that minimizes the cost function is a closed-form solution such that:

$$\boxed{\theta = (X^TX)^{-1}X^Ty}$$

❒ **LMS algorithm** – By noting α the learning rate, the update rule of the Least Mean Squares (LMS) algorithm for a training set of m data points, which is also known as the Widrow-Hoff learning rule, is as follows:

$$\boxed{\forall j, \quad \theta_j \leftarrow \theta_j + \alpha \sum_{i=1}^{m} \left[y^{(i)} - h_\theta(x^{(i)})\right] x_j^{(i)}}$$

Remark: the update rule is a particular case of the gradient ascent.

❒ **LWR** – Locally Weighted Regression, also known as LWR, is a variant of linear regression that weights each training example in its cost function by $w^{(i)}(x)$, which is defined with parameter $\tau \in \mathbb{R}$ as:

$$\boxed{w^{(i)}(x) = \exp\left(-\frac{(x^{(i)}-x)^2}{2\tau^2}\right)}$$

Classification and logistic regression

❒ **Sigmoid function** – The sigmoid function g, also known as the logistic function, is defined as follows:

$$\forall z \in \mathbb{R}, \quad \boxed{g(z) = \frac{1}{1+e^{-z}} \in]0,1[}$$

❒ **Logistic regression** – We assume here that $y|x;\theta \sim \text{Bernoulli}(\phi)$. We have the following form:

$$\boxed{\phi = p(y=1|x;\theta) = \frac{1}{1+\exp(-\theta^Tx)} = g(\theta^Tx)}$$

Remark: there is no closed form solution for the case of logistic regressions.

❒ **Softmax regression** – A softmax regression, also called a multiclass logistic regression, is used to generalize logistic regression when there are more than 2 outcome classes. By convention, we set $\theta_K = 0$, which makes the Bernoulli parameter ϕ_i of each class i equal to:

$$\boxed{\phi_i = \frac{\exp(\theta_i^Tx)}{\sum_{j=1}^{K}\exp(\theta_j^Tx)}}$$

Generalized Linear Models

❒ **Exponential family** – A class of distributions is said to be in the exponential family if it can be written in terms of a natural parameter, also called the canonical parameter or link function, η, a sufficient statistic $T(y)$ and a log-partition function $a(\eta)$ as follows:

$$\boxed{p(y;\eta) = b(y)\exp(\eta T(y) - a(\eta))}$$

Remark: we will often have $T(y) = y$. Also, $\exp(-a(\eta))$ can be seen as a normalization parameter that will make sure that the probabilities sum to one.

Here are the most common exponential distributions summed up in the following table:

Distribution	η	$T(y)$	$a(\eta)$	$b(y)$
Bernoulli	$\log\left(\frac{\phi}{1-\phi}\right)$	y	$\log(1+\exp(\eta))$	1
Gaussian	μ	y	$\frac{\eta^2}{2}$	$\frac{1}{\sqrt{2\pi}}\exp\left(-\frac{y^2}{2}\right)$
Poisson	$\log(\lambda)$	y	e^η	$\frac{1}{y!}$
Geometric	$\log(1-\phi)$	y	$\log\left(\frac{e^\eta}{1-e^\eta}\right)$	1

❒ **Assumptions of GLMs** – Generalized Linear Models (GLM) aim at predicting a random variable y as a function fo $x \in \mathbb{R}^{n+1}$ and rely on the following 3 assumptions:

(1) $\boxed{y|x;\theta \sim \text{ExpFamily}(\eta)}$ (2) $\boxed{h_\theta(x) = E[y|x;\theta]}$ (3) $\boxed{\eta = \theta^Tx}$

Remark: ordinary least squares and logistic regression are special cases of generalized linear models.

Support Vector Machines

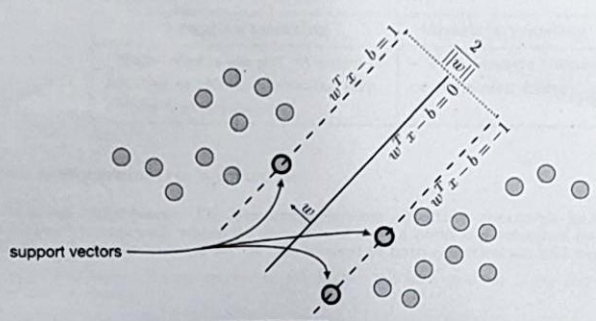
The goal of support vector machines is to find the line that maximizes the minimum distance to the line.

❒ **Optimal margin classifier** – The optimal margin classifier h is such that:

$$\boxed{h(x) = \text{sign}(w^Tx - b)}$$

where $(w,b) \in \mathbb{R}^n \times \mathbb{R}$ is the solution of the following optimization problem:

$$\boxed{\min \frac{1}{2}||w||^2} \quad \text{such that} \quad \boxed{y^{(i)}(w^Tx^{(i)} - b) \geqslant 1}$$



Remark: the line is defined as $\boxed{w^T x - b = 0}$.

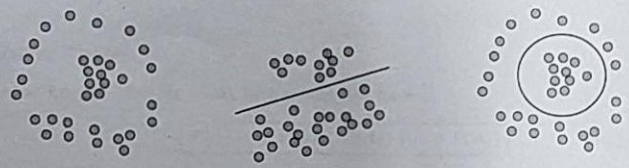
❒ **Hinge loss** – The hinge loss is used in the setting of SVMs and is defined as follows:

$$\boxed{L(z,y) = [1-yz]_+ = \max(0,1-yz)}$$

❒ **Kernel** – Given a feature mapping ϕ, we define the kernel K to be defined as:

$$\boxed{K(x,z) = \phi(x)^T \phi(z)}$$

In practice, the kernel K defined by $K(x,z) = \exp\left(-\frac{||x-z||^2}{2\sigma^2}\right)$ is called the Gaussian kernel and is commonly used.



Non-linear separability ⟶ Use of a kernel mapping ϕ ⟶ Decision boundary in the original space

Remark: we say that we use the "kernel trick" to compute the cost function using the kernel because we actually don't need to know the explicit mapping ϕ, which is often very complicated. Instead, only the values $K(x,z)$ are needed.

❒ **Lagrangian** – We define the Lagrangian $\mathcal{L}(w,b)$ as follows:

$$\boxed{\mathcal{L}(w,b) = f(w) + \sum_{i=1}^{l} \beta_i h_i(w)}$$

Remark: the coefficients β_i are called the Lagrange multipliers.

Generative Learning

A generative model first tries to learn how the data is generated by estimating $P(x|y)$, which we can then use to estimate $P(y|x)$ by using Bayes' rule.

Gaussian Discriminant Analysis

❒ **Setting** – The Gaussian Discriminant Analysis assumes that y and $x|y=0$ and $x|y=1$ are such that:

$$\boxed{y \sim \text{Bernoulli}(\phi)}$$

$$\boxed{x|y=0 \sim \mathcal{N}(\mu_0,\Sigma)} \quad \text{and} \quad \boxed{x|y=1 \sim \mathcal{N}(\mu_1,\Sigma)}$$

❒ **Estimation** – The following table sums up the estimates that we find when maximizing the likelihood:

$\widehat{\phi}$	$\widehat{\mu_j}$ $(j=0,1)$	$\widehat{\Sigma}$
$\frac{1}{m}\sum_{i=1}^{m} 1_{\{y^{(i)}=1\}}$	$\frac{\sum_{i=1}^{m} 1_{\{y^{(i)}=j\}} x^{(i)}}{\sum_{i=1}^{m} 1_{\{y^{(i)}=j\}}}$	$\frac{1}{m}\sum_{i=1}^{m}(x^{(i)}-\mu_{y^{(i)}})(x^{(i)}-\mu_{y^{(i)}})^T$

Naive Bayes

❒ **Assumption** – The Naive Bayes model supposes that the features of each data point are all independent:

$$\boxed{P(x|y) = P(x_1,x_2,...|y) = P(x_1|y)P(x_2|y)... = \prod_{i=1}^{n} P(x_i|y)}$$

❒ **Solutions** – Maximizing the log-likelihood gives the following solutions, with $k \in \{0,1\}$, $l \in [\![1,L]\!]$

$$\boxed{P(y=k) = \frac{1}{m} \times \#\{j|y^{(j)}=k\}} \quad \text{and} \quad \boxed{P(x_i=l|y=k) = \frac{\#\{j|y^{(j)}=k \text{ and } x_i^{(j)}=l\}}{\#\{j|y^{(j)}=k\}}}$$

Remark: Naive Bayes is widely used for text classification and spam detection.

Tree-based and ensemble methods

These methods can be used for both regression and classification problems.

❒ **CART** – Classification and Regression Trees (CART), commonly known as decision trees, can be represented as binary trees. They have the advantage to be very interpretable.

❒ **Random forest** – It is a tree-based technique that uses a high number of decision trees built out of randomly selected sets of features. Contrary to the simple decision tree, it is highly uninterpretable but its generally good performance makes it a popular algorithm.

Remark: random forests are a type of ensemble methods.

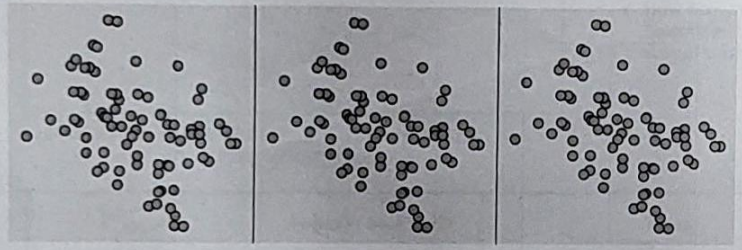
❒ **Boosting** – The idea of boosting methods is to combine several weak learners to form a stronger one. The main ones are summed up in the table below:

Adaptive boosting	Gradient boosting
- High weights are put on errors to improve at the next boosting step - Known as Adaboost	- Weak learners trained on remaining errors

Other non-parametric approaches

❒ **k-nearest neighbors** – The k-nearest neighbors algorithm, commonly known as k-NN, is a non-parametric approach where the response of a data point is determined by the nature of its k neighbors from the training set. It can be used in both classification and regression settings.

Remark: The higher the parameter k, the higher the bias, and the lower the parameter k, the higher the variance.

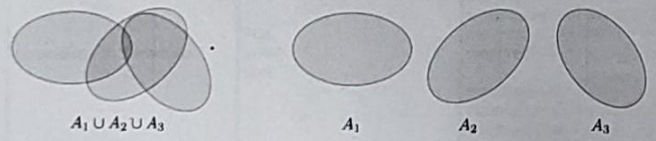


$k = 1$ $k = 3$ $k = 11$

Learning Theory

❒ **Union bound** – Let $A_1, ..., A_k$ be k events. We have:

$$\boxed{P(A_1 \cup ... \cup A_k) \leqslant P(A_1) + ... + P(A_k)}$$



$A_1 \cup A_2 \cup A_3$ A_1 A_2 A_3

❒ **Hoeffding inequality** – Let $Z_1, .., Z_m$ be m iid variables drawn from a Bernoulli distribution of parameter ϕ. Let $\widehat{\phi}$ be their sample mean and $\gamma > 0$ fixed. We have:

$$\boxed{P(|\phi - \widehat{\phi}| > \gamma) \leqslant 2\exp(-2\gamma^2 m)}$$

Remark: this inequality is also known as the Chernoff bound.

❒ **Training error** – For a given classifier h, we define the training error $\widehat{\epsilon}(h)$, also known as the empirical risk or empirical error, to be as follows:

$$\boxed{\widehat{\epsilon}(h) = \frac{1}{m}\sum_{i=1}^{m} 1_{\{h(x^{(i)}) \neq y^{(i)}\}}}$$

❒ **Probably Approximately Correct (PAC)** – PAC is a framework under which numerous results on learning theory were proved, and has the following set of assumptions:

- the training and testing sets follow the same distribution
- the training examples are drawn independently

❒ **Shattering** – Given a set $S = \{x^{(1)}, ..., x^{(d)}\}$, and a set of classifiers $\mathcal{H}$, we say that $\mathcal{H}$ shatters S if for any set of labels $\{y^{(1)}, ..., y^{(d)}\}$, we have:

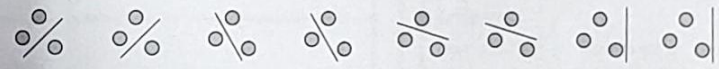
$$\boxed{\exists h \in \mathcal{H}, \quad \forall i \in [\![1, d]\!], \quad h(x^{(i)}) = y^{(i)}}$$

❒ **Upper bound theorem** – Let $\mathcal{H}$ be a finite hypothesis class such that $|\mathcal{H}| = k$ and let δ and the sample size m be fixed. Then, with probability of at least $1 - \delta$, we have:

$$\boxed{\epsilon(\widehat{h}) \leqslant \left(\min_{h \in \mathcal{H}} \epsilon(h)\right) + 2\sqrt{\frac{1}{2m}\log\left(\frac{2k}{\delta}\right)}}$$

❒ **VC dimension** – The Vapnik-Chervonenkis (VC) dimension of a given infinite hypothesis class $\mathcal{H}$, noted $\text{VC}(\mathcal{H})$ is the size of the largest set that is shattered by $\mathcal{H}$.

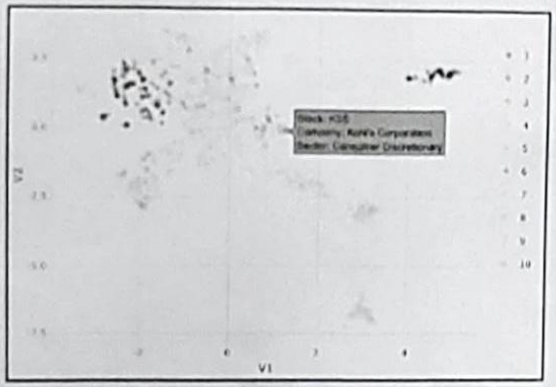
Remark: the VC dimension of $\mathcal{H} = \{$set of linear classifiers in 2 dimensions$\}$ is 3.



❒ **Theorem (Vapnik)** – Let $\mathcal{H}$ be given, with $\text{VC}(\mathcal{H}) = d$ and m the number of training examples. With probability at least $1 - \delta$, we have:

$$\boxed{\epsilon(\widehat{h}) \leqslant \left(\min_{h \in \mathcal{H}} \epsilon(h)\right) + O\left(\sqrt{\frac{d}{m}\log\left(\frac{m}{d}\right) + \frac{1}{m}\log\left(\frac{1}{\delta}\right)}\right)}$$

Segmentation & Clustering



Combining K-Means & UMAP to visualize clusters by Stock Price Movements

Summary:

- **Common Applications in Business**: Can be used for finding segments within Customers, Companies, etc.
- **Key Concept:** Transform data into a matrix enabling trends to be compared across units of measure (e.g. user-item matrix)
- **Gotchas:** Data must be normalized or standardized to enable comparison. This often requires calculation proportions of values by customer, company, etc to ensure the larger values do not dominate the trend mining operation.
- **How Many Components/Clusters?** Use a *Scree Plot* to determine the proportion of variance explained or total within sum of squares

Type	Popular Methods	Uses	Data Treatment
Clustering	K-Means Hierarchical Clustering	**Group Detection:** Methods use a measure of similarity (e.g. Euclidean distance) to detect groups within data set	Standardized or normalized
Dimensionality Reduction	PCA UMAP tSNE	**Reduce Width of Data:** Performing Machine Learning on wide data can drastically increase the time for algorithms to converge. Dimensionality reduction can be applied as a preprocessing step to reduce the width (number of columns) of the data but still maintain a high proportion of the overall structure. **Visualization:** Visualizing the first two components as X and Y often can enable cluster visualization. Combining with clustering techniques can provide a useful method of visualization.	Standardized or normalized

R Cheat Sheet

K-Means

```
set.seed(0)

kmeans_obj <- kmeans(X, centers = 4)
```

UMAP

```
library(umap)

umap_obj <- umap(X)
```

Python Cheat Sheet

K-Means

```
from sklearn.cluster import KMeans

kmeans = KMeans(
    n_clusters=4,
    random_state=0).fit(X)
```

UMAP

```
import umap

reducer = umap.UMAP()

embedding = reducer.fit_transform(X)
```

Resources

- Business Analysis With R Course (DS4B 101-R) - Modeling - Week 6
- Business Science Problem Framework
- Ultimate R Cheat Sheet | Ultimate Python Cheat Sheet

Data Science Courses for Business

Business Science University
university.business-science.io

version: 1.0