VIP Cheatsheet: Supervised Learning

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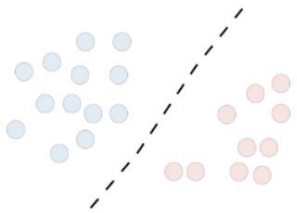
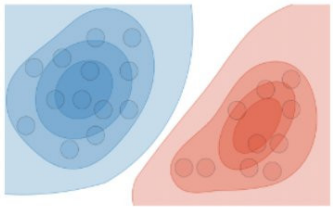
Introduction to Supervised Learning

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

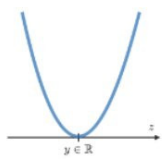
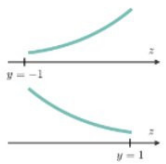
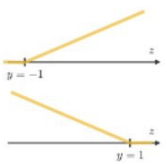
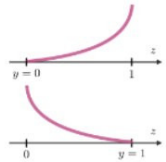
❒ **Type of model** – The different models are summed up in the table below:

	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:

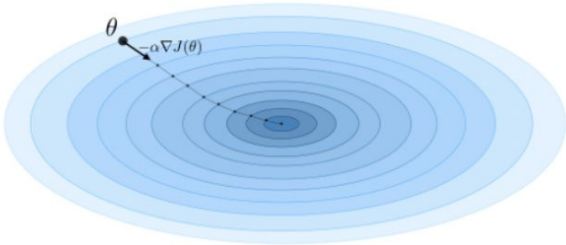
Least squared	Logistic	Hinge	Cross-entropy
$\frac{1}{2}(y-z)^2$	$\log(1+\exp(-yz))$	$\max(0,1-yz)$	$-\left[y\log(z)+(1-y)\log(1-z)\right]$
			
Linear regression	Logistic regression	SVM	Neural Network

❒ **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:

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

❒ **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:

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

VIP Cheatsheet: Unsupervised Learning

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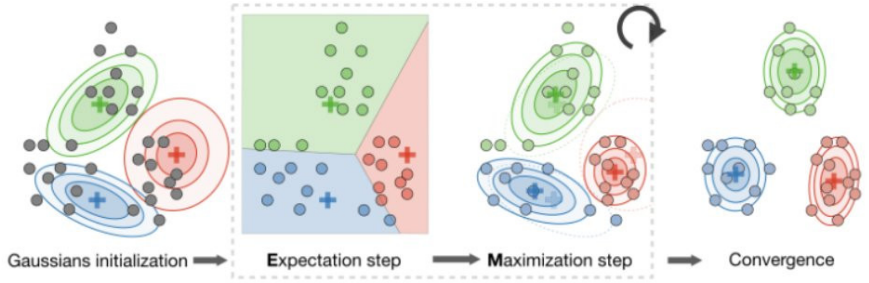


Introduction to Unsupervised Learning

❒ **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:

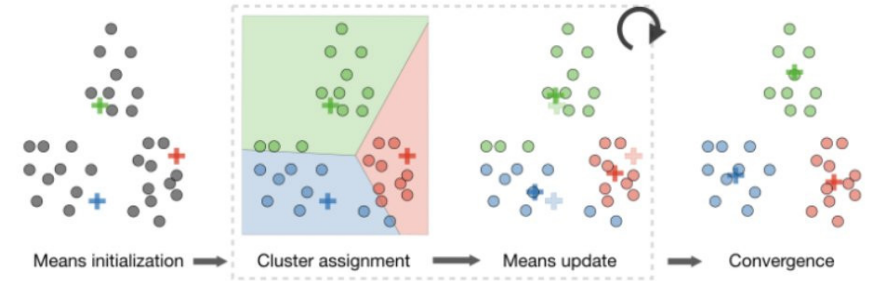
$$\boxed{\theta_i = \underset{\theta}{\text{argmax}} \sum_i \int_{z^{(i)}} Q_i(z^{(i)}) \log\left(\frac{P(x^{(i)},z^{(i)};\theta)}{Q_i(z^{(i)})}\right) dz^{(i)}}$$

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:

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



❒ **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:

VIP Cheatsheet: Deep Learning

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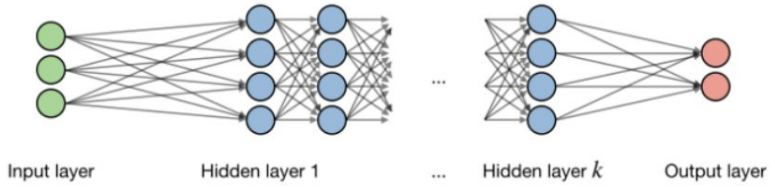
Neural Networks

Neural networks are a class of models that are built with layers. Commonly used types of neural networks include convolutional and recurrent neural networks.

❒ **Architecture** – The vocabulary around neural networks architectures is described in the figure below:

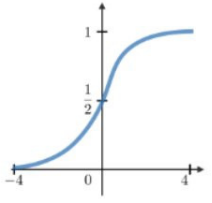
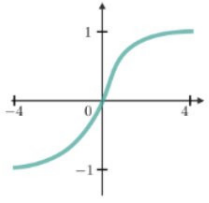
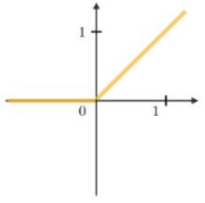
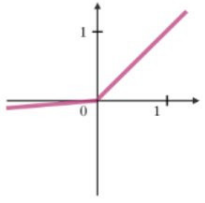


By noting i the i^{th} layer of the network and j the j^{th} hidden unit of the layer, we have:

$$\boxed{z_j^{[i]} = {w_j^{[i]}}^T x + b_j^{[i]}}$$

where we note w, b, z the weight, bias and output respectively.

❒ **Activation function** – Activation functions are used at the end of a hidden unit to introduce non-linear complexities to the model. Here are the most common ones:

Sigmoid	Tanh	ReLU	Leaky ReLU
$g(z) = \frac{1}{1+e^{-z}}$	$g(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$	$g(z) = \max(0,z)$	$g(z) = \max(\epsilon z, z)$ with $\epsilon \ll 1$
			

❒ **Cross-entropy loss** – In the context of neural networks, the cross-entropy loss $L(z,y)$ is commonly used and is defined as follows:

$$\boxed{L(z,y) = -\Big[y\log(z) + (1-y)\log(1-z)\Big]}$$

❒ **Learning rate** – The learning rate, often noted η, indicates at which pace the weights get updated. This can be fixed or adaptively changed. The current most popular method is called Adam, which is a method that adapts the learning rate.

❒ **Backpropagation** – Backpropagation is a method to update the weights in the neural network by taking into account the actual output and the desired output. The derivative with respect to weight w is computed using chain rule and is of the following form:

$$\boxed{\frac{\partial L(z,y)}{\partial w} = \frac{\partial L(z,y)}{\partial a} \times \frac{\partial a}{\partial z} \times \frac{\partial z}{\partial w}}$$

As a result, the weight is updated as follows:

$$\boxed{w \longleftarrow w - \eta \frac{\partial L(z,y)}{\partial w}}$$

❒ **Updating weights** – In a neural network, weights are updated as follows:

- Step 1: Take a batch of training data.
- Step 2: Perform forward propagation to obtain the corresponding loss.
- Step 3: Backpropagate the loss to get the gradients.
- Step 4: Use the gradients to update the weights of the network.

❒ **Dropout** – Dropout is a technique meant at preventing overfitting the training data by dropping out units in a neural network. In practice, neurons are either dropped with probability p or kept with probability $1-p$.

Convolutional Neural Networks

❒ **Convolutional layer requirement** – By noting W the input volume size, F the size of the convolutional layer neurons, P the amount of zero padding, then the number of neurons N that fit in a given volume is such that:

$$\boxed{N = \frac{W - F + 2P}{S} + 1}$$

❒ **Batch normalization** – It is a step of hyperparameter γ, β that normalizes the batch $\{x_i\}$. By noting μ_B, σ_B^2 the mean and variance of that we want to correct to the batch, it is done as follows:

$$\boxed{x_i \longleftarrow \gamma \frac{x_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}} + \beta}$$

It is usually done after a fully connected/convolutional layer and before a non-linearity layer and aims at allowing higher learning rates and reducing the strong dependence on initialization.

VIP Cheatsheet: Machine Learning Tips

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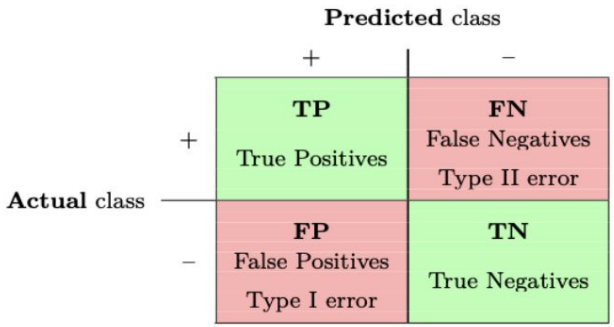
Metrics

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:



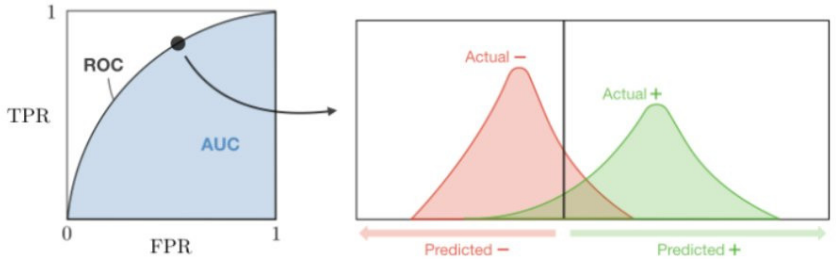
❒ **Main metrics** – The following metrics are commonly used to assess the performance of classification models:

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
$\frac{\text{SS}_{\text{res}} + 2(n+1)\widehat{\sigma^2}}{m}$	$2\left[(n+2) - \log(L)\right]$	$\log(m)(n+2) - 2\log(L)$	$1 - \frac{(1-R^2)(m-1)}{m-n-1}$

VIP Refresher: Probabilities and Statistics

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Introduction to Probability and Combinatorics

❒ **Sample space** – The set of all possible outcomes of an experiment is known as the sample space of the experiment and is denoted by S.

❒ **Event** – Any subset E of the sample space is known as an event. That is, an event is a set consisting of possible outcomes of the experiment. If the outcome of the experiment is contained in E, then we say that E has occurred.

❒ **Axioms of probability** – For each event E, we denote $P(E)$ as the probability of event E occuring. By noting $E_1,...,E_n$ mutually exclusive events, we have the 3 following axioms:

(1) $\boxed{0 \leqslant P(E) \leqslant 1}$ (2) $\boxed{P(S) = 1}$ (3) $\boxed{P\left(\bigcup_{i=1}^{n} E_i\right) = \sum_{i=1}^{n} P(E_i)}$

❒ **Permutation** – A permutation is an arrangement of r objects from a pool of n objects, in a given order. The number of such arrangements is given by $P(n,r)$, defined as:

$$\boxed{P(n,r) = \frac{n!}{(n-r)!}}$$

❒ **Combination** – A combination is an arrangement of r objects from a pool of n objects, where the order does not matter. The number of such arrangements is given by $C(n,r)$, defined as:

$$\boxed{C(n,r) = \frac{P(n,r)}{r!} = \frac{n!}{r!(n-r)!}}$$

Remark: we note that for $0 \leqslant r \leqslant n$, we have $P(n,r) \geqslant C(n,r)$.

Conditional Probability

❒ **Bayes' rule** – For events A and B such that $P(B) > 0$, we have:

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

Remark: we have $P(A \cap B) = P(A)P(B|A) = P(A|B)P(B)$.

❒ **Partition** – Let $\{A_i, i \in [\![1,n]\!]\}$ be such that for all i, $A_i \neq \varnothing$. We say that $\{A_i\}$ is a partition if we have:

$$\boxed{\forall i \neq j, A_i \cap A_j = \emptyset \quad \text{and} \quad \bigcup_{i=1}^{n} A_i = S}$$

Remark: for any event B in the sample space, we have $P(B) = \sum_{i=1}^{n} P(B|A_i)P(A_i)$.

❒ **Extended form of Bayes' rule** – Let $\{A_i, i \in [\![1,n]\!]\}$ be a partition of the sample space. We have:

$$\boxed{P(A_k|B) = \frac{P(B|A_k)P(A_k)}{\sum_{i=1}^{n} P(B|A_i)P(A_i)}}$$

❒ **Independence** – Two events A and B are independent if and only if we have:

$$\boxed{P(A \cap B) = P(A)P(B)}$$

Random Variables

❒ **Random variable** – A random variable, often noted X, is a function that maps every element in a sample space to a real line.

❒ **Cumulative distribution function (CDF)** – The cumulative distribution function F, which is monotonically non-decreasing and is such that $\lim_{x \to -\infty} F(x) = 0$ and $\lim_{x \to +\infty} F(x) = 1$, is defined as:

$$\boxed{F(x) = P(X \leqslant x)}$$

Remark: we have $P(a < X \leqslant B) = F(b) - F(a)$.

❒ **Probability density function (PDF)** – The probability density function f is the probability that X takes on values between two adjacent realizations of the random variable.

❒ **Relationships involving the PDF and CDF** – Here are the important properties to know in the discrete (D) and the continuous (C) cases.

Case	CDF F	PDF f	Properties of PDF
(D)	$F(x) = \sum_{x_i \leqslant x} P(X = x_i)$	$f(x_j) = P(X = x_j)$	$0 \leqslant f(x_j) \leqslant 1$ and $\sum_j f(x_j) = 1$
(C)	$F(x) = \int_{-\infty}^{x} f(y)dy$	$f(x) = \frac{dF}{dx}$	$f(x) \geqslant 0$ and $\int_{-\infty}^{+\infty} f(x)dx = 1$

❒ **Variance** – The variance of a random variable, often noted $\text{Var}(X)$ or σ^2, is a measure of the spread of its distribution function. It is determined as follows:

$$\boxed{\text{Var}(X) = E[(X - E[X])^2] = E[X^2] - E[X]^2}$$

❒ **Standard deviation** – The standard deviation of a random variable, often noted σ, is a measure of the spread of its distribution function which is compatible with the units of the actual random variable. It is determined as follows:

$$\boxed{\sigma = \sqrt{\text{Var}(X)}}$$

VIP Refresher: Linear Algebra and Calculus

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General notations

❒ **Vector** – We note $x \in \mathbb{R}^n$ a vector with n entries, where $x_i \in \mathbb{R}$ is the i^{th} entry:

$$x = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \in \mathbb{R}^n$$

❒ **Matrix** – We note $A \in \mathbb{R}^{m \times n}$ a matrix with m rows and n columns, where $A_{i,j} \in \mathbb{R}$ is the entry located in the i^{th} row and j^{th} column:

$$A = \begin{pmatrix} A_{1,1} & \cdots & A_{1,n} \\ \vdots & & \vdots \\ A_{m,1} & \cdots & A_{m,n} \end{pmatrix} \in \mathbb{R}^{m \times n}$$

Remark: the vector x defined above can be viewed as a $n \times 1$ matrix and is more particularly called a column-vector.

❒ **Identity matrix** – The identity matrix $I \in \mathbb{R}^{n \times n}$ is a square matrix with ones in its diagonal and zero everywhere else:

$$I = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 1 \end{pmatrix}$$

Remark: for all matrices $A \in \mathbb{R}^{n \times n}$, we have $A \times I = I \times A = A$.

❒ **Diagonal matrix** – A diagonal matrix $D \in \mathbb{R}^{n \times n}$ is a square matrix with nonzero values in its diagonal and zero everywhere else:

$$D = \begin{pmatrix} d_1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & d_n \end{pmatrix}$$

Remark: we also note D as $diag(d_1,...,d_n)$.

Matrix operations

❒ **Vector-vector multiplication** – There are two types of vector-vector products:

- inner product: for $x,y \in \mathbb{R}^n$, we have:

$$\boxed{x^T y = \sum_{i=1}^{n} x_i y_i \in \mathbb{R}}$$

- outer product: for $x \in \mathbb{R}^m, y \in \mathbb{R}^n$, we have:

$$\boxed{xy^T = \begin{pmatrix} x_1 y_1 & \cdots & x_1 y_n \\ \vdots & & \vdots \\ x_m y_1 & \cdots & x_m y_n \end{pmatrix} \in \mathbb{R}^{m \times n}}$$

❒ **Matrix-vector multiplication** – The product of matrix $A \in \mathbb{R}^{m \times n}$ and vector $x \in \mathbb{R}^n$ is a vector of size $\mathbb{R}^m$, such that:

$$\boxed{Ax = \begin{pmatrix} a_{r,1}^T x \\ \vdots \\ a_{r,m}^T x \end{pmatrix} = \sum_{i=1}^{n} a_{c,i} x_i \in \mathbb{R}^m}$$

where $a_{r,i}^T$ are the vector rows and $a_{c,j}$ are the vector columns of A, and x_i are the entries of x.

❒ **Matrix-matrix multiplication** – The product of matrices $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{n \times p}$ is a matrix of size $\mathbb{R}^{n \times p}$, such that:

$$\boxed{AB = \begin{pmatrix} a_{r,1}^T b_{c,1} & \cdots & a_{r,1}^T b_{c,p} \\ \vdots & & \vdots \\ a_{r,m}^T b_{c,1} & \cdots & a_{r,m}^T b_{c,p} \end{pmatrix} = \sum_{i=1}^{n} a_{c,i} b_{r,i}^T \in \mathbb{R}^{n \times p}}$$

where $a_{r,i}^T, b_{r,i}^T$ are the vector rows and $a_{c,j}, b_{c,j}$ are the vector columns of A and B respectively.

❒ **Transpose** – The transpose of a matrix $A \in \mathbb{R}^{m \times n}$, noted A^T, is such that its entries are flipped:

$$\boxed{\forall i,j, \qquad A_{i,j}^T = A_{j,i}}$$

Remark: for matrices A,B, we have $(AB)^T = B^T A^T$.

❒ **Inverse** – The inverse of an invertible square matrix A is noted A^{-1} and is the only matrix such that:

$$\boxed{AA^{-1} = A^{-1}A = I}$$

Remark: not all square matrices are invertible. Also, for matrices A,B, we have $(AB)^{-1} = B^{-1}A^{-1}$

❒ **Trace** – The trace of a square matrix A, noted $\text{tr}(A)$, is the sum of its diagonal entries:

$$\boxed{\text{tr}(A) = \sum_{i=1}^{n} A_{i,i}}$$

Remark: for matrices A,B, we have $tr(A^T) = tr(A)$ and $tr(AB) = tr(BA)$

❒ **Determinant** – The determinant of a square matrix $A \in \mathbb{R}^{n \times n}$, noted $|A|$ or $\det(A)$ is expressed recursively in terms of $A_{\backslash i,\backslash j}$, which is the matrix A without its i^{th} row and j^{th} column, as follows: