Extended CIL Summary
FS 2013

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July 16, 2013

This summary is based on the course slides of the Computational Intelligence Lab slides[1] from spring semester 2013.

[1] http://cil.inf.ethz.ch

Part I.
Dimensionality Reduction

Select the *most interesting* dimensions.

1. Intrinsic Dimensionality

Pairwise Distances

Assume components of data $x = (x_1, \ldots, x_D)^T \in \mathbb{R}^D$ are i.i.d. Gaussian distributed:

$$x_d \sim \mathcal{N}(0,1) \implies x_d - y_d \sim \mathcal{N}(0,2).$$

Using χ^2-distribution:

$$\frac{1}{2}(x_d - y_d)^2 \sim \chi^2(1),$$

and extending to D dimensions:

$$\frac{1}{2}\sum_{d=1}^{D}(x_d - y_d)^2 \sim \chi^2(D) = \Gamma\left(\frac{D}{2}, 2\right)$$

$$\text{Recall: } \forall z, k, \theta > 0,\ \Gamma(z;k,\theta) = \frac{\theta^k}{\Gamma(k)} y^{k-1} e^{-\theta z}$$

Hence, the dimension-normalised squared distance is:

$$\frac{1}{D}\sum_{d=1}^{D}(x_d - y_d)^2 \sim \Gamma\left(\frac{D}{2}, \frac{4}{D}\right)$$

is Gamma distributed with mean 2 and variance $\frac{8}{D}$.
$\Gamma\left(\frac{D}{2}, \frac{4}{D}\right)$ tends towards normality with shrinking width for large D. Therefore, most points have *constant* pairwise distances in this limit.

2. Principal Component Analysis

Objectives of PCA:

1. Minimise error $\|x_n - \tilde{x}_n\|$ of point x_n and its approximation $\tilde{x}_n$.
2. Reveal "interesting" information: maximise *variance*.

Both objectives are show to be formally equivalent.
Consider a set of observations $\{x_n\},\ n = 1, \ldots, N$ and $x_n \in \mathbb{R}^D$.

Goal Project data onto $K < D$ dimensional space while maximising variance of the projected data.

For K = 1 Define direction of projection as u_1. Set $\|u_1\|_2 = 1$ (only the direction of the projection is important.

2.1. Statistics of Projected Data

Original Data

Mean is given by the sample mean $\bar{x}$.

Covariance of the Data:

$$\Sigma = \frac{1}{N}\sum_{n=1}^{N}(x_n - \bar{x})(x_n - \bar{x})^T$$

Projected Data

Mean is given by: $u_1^T\bar{x}$.

Variance is given by:

$$\begin{aligned}\frac{1}{N}\sum_{n=1}^{N}\left\{u_1^T x_n - u_1^T\bar{x}\right\}^2 &= \frac{1}{N}\sum_{n=1}^{N}\left\{u_1^T(x_n - \bar{x})\right\}^2 \\ &= \frac{1}{N}\sum_{n=1}^{N}u_1^T(x_n - \bar{x})(x_n - \bar{x})^T u_1 \\ &= u_1^T\Sigma u_1.\end{aligned}$$

2.2. Maximisation Problem

These statistics now can be fed into a maximisation problem:

$$\max_{u_1}\ u_1^T\Sigma u_1$$

such that $\|u_1\|_2 = 1$.
Writing the Lagrangian results in in:

$$\mathcal{L} := u_1^T\Sigma u_1 + \lambda_1(1 - u_1^T u_1).$$

Setting $\frac{\delta}{\delta u_1}\mathcal{L} \stackrel{!}{=} 0$ results in:

$$\Sigma u_1 = \lambda_1 u_1$$

We observe that u_1 is an *eigenvector* of Σ and λ_1 it's associated *eigenvalue*. Furthermore λ_1 is also the variance of the projected data:

$$\lambda_1 = u_1^T\Sigma u_1$$

2.2.1. Second principal direction

The second principal direction can be obtained by maximising the variance $u_2^T \Sigma u_2$, subject to $\|u_2\|_2 = 1$ and $u_2^T u_1 = 0$:

$$\mathcal{L} = u_2^T \Sigma u_2 + \lambda_2 \left(1 - u_2^T u_2\right) + \nu \left(u_2^T u_1\right).$$

The maximum i found by setting $\frac{\delta \mathcal{L}}{\delta u_2} \stackrel{!}{=} 0$:

$$2\Sigma u_2 - 2\lambda_2 u_2 + \nu u_1 = 0.$$

Because of the orthogonality between u_2 and u_1 we observe that u_2 contains no component of u_1 and hence $\nu = 0$. We get:

$$\Sigma u_2 = \lambda_2 u_2.$$

We observe that u_2 is an eigenvector of Σ with the second largest eigenvalue of λ_2.

2.3. Solution: Eigenvalue Decomposition

Hence we see that the eigenvalue decomposition of the covariance matrix

$$\Sigma = U \Lambda U^T$$

contains all relevant information.
For a projection space of size $K \leq D$ we choose the K eigenvectors $\{u_1, \ldots, u_k\}$ with the largest associated eigenvalues $\{\lambda_1, \ldots, \lambda_2\}$.

2.4. Error Formulation

We define an *orthonormal* basis $\{u_d\}$, $d = 1, \ldots, D$ of $\mathbb{R}^D$. The scalar projection of x_n onto u_d (magnitude) is given by:

$$z_{n,d} = x_n^T u_d.$$

The associated projection onto u_d amounts to $z_{n,d} u_d$. Therefore, each data point can be represented in the basis by:

$$x_n = \sum_{d=1}^{D} z_{n,d} u_d = \sum_{d=1}^{D} \left(x_n^T u_d\right) u_d.$$

Restricted representation using $K < D$ basis vectors can be written as:

$$\tilde{x}_n = \sum_{d=1}^{K} a_{n,d} u_d + \sum_{d=K+1}^{D} b_d u_d,$$

where b_d does not depend on the data point x_n.

The approximation error can be represented by:

$$J(\{a_{n,d}\},\{b_d\}) = \frac{1}{N}\sum_{n=1}^{N}\|x_n - \tilde{x}_n\|_2^2$$

$$\text{Minimisation of } J \text{ w.r.t.} a_{n,d} = x_n^T$$

$$\text{Minimisation of } J \text{ w.r.t.} b_d = \bar{x}^T u_d$$

The displacement can be obtained by resubsittuing $a_{n,d}$ and b_d:

$$x_n - \tilde{x}_n = \sum_{d=K+1}^{D}\left\{(x_n - \bar{x})^T u_d\right\} u_d.$$

We observe that the displacement vector is orthogonal to the principal space! Resubstituting the displacement into the error criterion leads to:

$$J = \frac{1}{N}\sum_{n=1}^{N}\sum_{d=K+1}^{D}\left(x_n^T u_d - \bar{x}^T u_d\right)^2 = \sum_{d=K+1}^{D} u_d^T \Sigma u_d$$

2.5. Matrix viewpoint

The data can be represented as matrix:

$$X = [x_1, \ldots, x_n, \ldots, x_N]$$

The corresponding zero-centered data is:

$$\bar{X} = X - M,$$

where $M = \underbrace{[\bar{x}, \ldots, \bar{x}]}_{N \text{ times}}$.
Compute the projection of $\bar{X}$ on $U_k = [u_1, \ldots, u_K]$ with:

$$\underbrace{\bar{Z}_K}_{K\times N} = \underbrace{U_K^T}_{K\times D} \cdot \underbrace{\bar{X}}_{D\times N}.$$

To approximate $\bar{X}$, we return to the original basis:

$$\tilde{\bar{X}} = U_K \cdot \bar{Z}_K.$$

For $K = D$ we obtain a perfect reconstruction.

2.6. Computation

First compute the *empirical mean*:

$$\bar{x} = \frac{1}{N}\sum_{n=1}^{N} x_n$$

Then *center the data* by subtracting the mean from each sample:

$$\bar{X} = X - M,$$

where $M = \underbrace{[\bar{x}, \ldots, \bar{x}]}_{N \text{ times}}$. Now compute the *Covariance matrix*:

$$\Sigma = \frac{1}{N}\sum_{n=1}^{N}(x_n - \bar{x})(x_n - \bar{x})^T = \frac{1}{N}\underbrace{\bar{X}\bar{X}^T}_{\text{Scatter Matrix } \mathbf{S}}.$$

Σ is *symmetric.*
Now the *Eigenvalue decomposition* can be computed:

$$\Sigma = U\Lambda U^T,$$

where $\Lambda = diag[\lambda_1, \ldots, \lambda_D]$, such that $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_D$ with orthonormal eigenvectors.

Transformation the data can be transformed on to the new basis of K dimensions:

$$\tilde{\bar{Z}} = U_K^T \bar{X},$$

$\bar{Z} \in \mathbb{R}^{K \times N}$: We obtain a dimension reduction of the data.

Reconstruction Go back to the original basis by computing

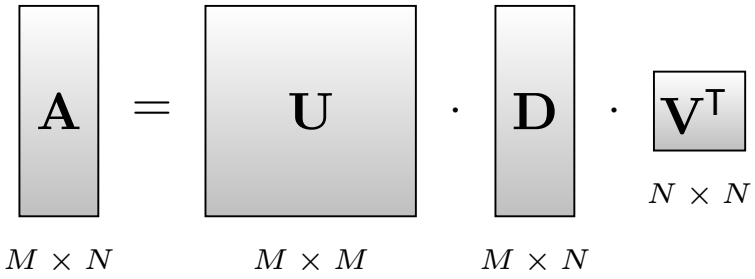
$$\tilde{\bar{X}} = U_K \bar{Z}$$
$$\tilde{X} = \tilde{\bar{X}} + M$$

3. Singular Value Decomposition

3.1. Introduction

The *Singular Value Decomposition* (SVD) is a widely used technique to decompose a matrix into several component matrices exposing many of the useful and interesting properties of the original matrix like rank, null-space, orthogonal basis of column and row space.
Every rectangular, real or complex matrix S has an SVD decomposition into a set of three matrix factors.

Let A be any real M by N matrix, $A \in \mathbb{R}^{M \times N}$, then A can be decomposed as $A = UDV^T$:



- U is an $M \times M$ orthogonal matrix, $U^T U = I$
- D is an $M \times N$ diagonal matrix
- V^T is an $N \times N$ orthogonal matrix, $V^T V = I$

3.2. Singular values

The elements of D are only non-zero on the diagonal and are called the *singular values*. By convention, the order of the singular vectors is determined by the *high-to-low* sorting of singular values, with the highest singular value in the upper left index of the D matrix. The first r columns of U are called *left singular vectors*, they form an orthogonal basis for the space spanned by the columns of the original matrix A.
Similarly the first r rows of V^T are the *right singular vectors*, they form an orthonormal basis for the row space of A.
SVD provides an explicit representation of the range and null-space of a matrix A.

- The right side singular vectors corresponding to vanishing singular values of A, span the null space of A:

$$d_i = 0 \quad \Longrightarrow \quad Av_i = 0 \quad \Longrightarrow \quad v_i \in Null(A).$$

- The left singular vectors corresponding to the non-zero singular values of A span the range of A.

As a consequence, the rank of A equals the number of non-zero singular values (= the number of non-zero elements in D).

$$Rank(A) = \#d_i > 0.$$

3.3. Closest Rank-k Matrix

Let the SVD of $A \in \mathbb{R}^{M \times N}$ be given by $A = UDV^T$. If $k < r = Rank(A)$ and

$$A_k = \sum_{i=1}^{k} d_i u_i v_i^T.$$

Then

$$\min_{Rank(B)=k} \|A - B\|_2 = \|A - A_k\|_2.$$

This means that A_k is the closest $Rank(k)$ approximation to A in the Eculidean matrix norm sense hence:

$$\|A - A_k\|_2 = d_{k+1}.$$

3.4. Properties

The columns of U are the eigenvectors of AA^T. This claim can be verified using the SVD decomposition:

$$AA^T = UDV^T VDU^T = UD^2U^T.$$

Similarly the rows of V^T (or columns of V) are the eigenvectors of A^TA as:

$$A^TA = VDU^T UDV^T = VD^2V^T.$$

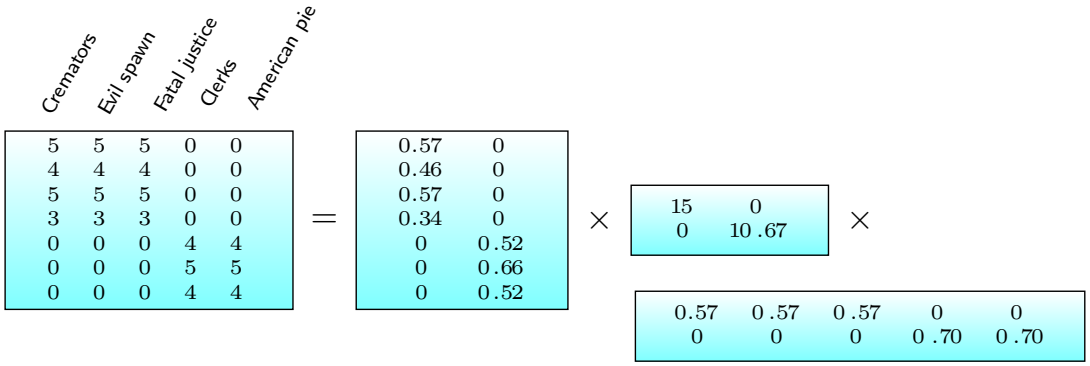
3.5. Movie Example

Let A be a list of users with their respective movie preferences. Then the SVD decomposition

$$A = UDV^T,$$

can be interpreted in the following way:

- **U**: Users-to-concept affinity matrix.
- **D**: Expression level of the different concepts in the data.
- **V**: Movies-to-concept similarity matrix.


Cremators
Evil spawn
Fatal justice
Clerks
American pie
5 5 5 0 0
4 4 4 0 0
5 5 5 0 0
3 3 3 0 0
0 0 0 4 4
0 0 0 5 5
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15 0
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0.57 0.57 0.57 0 0
0 0 0 0.70 0.70

Part II.
Clustering

4. Introduction

A set of datapoints in a d-dimensional Euclidean space is given.

Aim The aim is to find a *meaningful partition* of the data; i.e. label each data point with a unique value $\{1, \ldots, k\}$.

Objective The partition should group together similar data points, while the different groups/clusters should be as dissimilar as possible from each other.

This way we can uncover similarities between data points and give rise to data compression schemes.

4.1. Problem

Consider N data points in a D-dimensional space. Each data vector is denoted by x_n, $n = 1, \ldots, N$. Our goal is to partition the data set into K clusters: Find vectors $u_1, \ldots, u_K$ that represent the centroid of each cluster.
A datapoint x_n belongs to cluster k if the Euclidean distance between x_n and u_k is smaller than the distance to any any other centroid.
Mathematically, the clustering problem defines a mixed discrete continuous optimisation problem.

4.1.1. The Cost Function of Vector Quantisation

Objective Minimise the cost function

$$J(U, Z) = \|X - UZ\|_F^2 = \sum_{n=1}^{N} \sum_{k=1}^{K} z_{k,n} \|x_n - u_k\|_2^2$$

where

$$\begin{aligned} X &= [x_1, \ldots, x_N] \in \mathbb{R}^{D \times N} \\ U &= [u_1, \ldots, u_K] \in \mathbb{R}^{D \times K}, && \text{centroids} \\ Z &\in \{0, 1\}^{K \times N}, && \text{assignments} \end{aligned}$$

with $\sum_k z_{k,n} = 1 \forall n$ i.e., one element per columns set to 1.

Assignment notation:

Assignment Notation : Vector $\hat{z} \in \{1, \ldots, K\}^N$ indicating for each data point to which cluster index it is assigned:

$$\hat{z} = \begin{pmatrix} 2 \\ 3 \\ 4 \\ 2 \\ 2 \\ 1 \end{pmatrix}$$

Matrix Notation : The matrix $Z \in \{0, 1\}^{K \times N}$ with only one non-zero entry per column, assigns data points to clusters:

$$Z = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$

5. K-Means

5.1. Overview

The algorithm alternates between two steps:

- *Assigning data points* to clusters Let $k^*(x_n)$ denote the cluster index with the minimal distance between a cluster centroid and the data point x_n:

$$k^*(x_n) = \arg\min_k \left\{ \|x_n - u_1\|_2^2, \ldots, \|x_n - u_k\|_2^2, \ldots, \|x_n - u_K\|_2^2 \right\}$$

- *Updating the cluster centroids* based on all the data points assigned to it. Compute the mean/centroid of a cluster that can be written as:

$$u_k = \frac{\sum_{n=1}^N z_{k,n} x_n}{\sum_{n=1}^N z_{k,n}} \quad \forall k, \quad k \in \{1, \ldots, K\}$$

5.2. Algorithm

1. Initiate with a random choice of $u_1^{(0)}, \ldots, u_K^{(0)}$ (or let $u_1^{(0)}, \ldots, u_K^{(0)}$ equal data points from the set). Set $t = 1$.

2. **Cluster assignment.** Solve $\forall n$:

$$k^*(x_n) = \arg\min_k \left\{ \left\| x_n - u_1^{(t)} \right\|_2^2, \ldots, \left\| x_n - u_K^{(t)} \right\|_2^2 \right\}.$$

   Then, $z_{k*(x_n),n}^{(t)} = 1$ and $z_{j,n}^{(t)} = 0 \; \forall j \neq k, \quad j = 1, \ldots, K$.

3. **Centroid update**

$$u_k^{(t)} = \frac{\sum_{n=1}^{N} z_{k,n}^{(t)} x_n}{\sum_{i=1}^{N} z_{k,n}^{(t)}} \; \forall k, \; k \in \{1, \ldots, K\}$$

4. Increment t. Repeat step 2 until $\left\| u_k^{(t)} - u_k^{(t-1)} \right\|_2^2 < \varepsilon \; \forall K \; (0 < \varepsilon << 1)$ or until $t = t_{\text{finish}}$.

Aspects:

- The computational cost of each iteration is $\mathcal{O}(KN)$.
- Convergence is guaranteed
- Optimises a *non-convex* objective. Hence only a local minimum can be guaranteed.
- Can be used to compress data: store only the centroids and the assignments of data point to clusters.

Problems:

- Non-convex objective, local minima and sensitive to initialisations.
- Not appropriate for non-Euclidean data $\mapsto$ need to use other distances.
- The optimal number of clusters K is unknown: One has to find a balance between total compression ($K = 1$) and no loss of information ($K = N$).

5.3. Stability

5.3.1. High-Level Stability test

The following is a high-level stability test for a given set of data points and a given number of clusters:

1. Generate perturbed versions of the set for example by adding noise or drawing sub-samples.
2. Apply the clustering algorithm on all versions.
3. Compute pair-wise distances between all clusterings (using some distance measure).
4. Compute the *instability* as the mean distance between all clusterings.

Repeat this for different numbers of clusters and choose the one that minimises the instability.

5.3.2. Distance between Clusterings

For two clusterings C and C' that are defined on the same data points we compute the distance between clusterings d in the following procedure:

1. Compute the distances between the two clusterings by counting points on which the two clusterings agree or disagree.
2. Repeat over all permutations of the cluster labels (since the same cluster might be sometimes labeled 1 and sometimes 2 etc...).
3. Choose the permutation with minimal distance and the corresponding distances is d.

In other words,

$$d = \min_{\pi} \left\| Z - \pi(Z') \right\|_0$$

where $\pi(Z')$ is one of the possible row permutations of Z' and $\|Z\|_0$ denotes the cardinality of Z. If two clusterings are defined on different data sets but many points overlap, we use only these for comparison, otherwise, a mapping from one domain to the other is required.

5.3.3. Calculation of Stability

The rate of inconsistent data items r is computed as follows"

1. Cluster data sets X, X' to infer assignments Z, Z'.
2. Train a classifier φ on (X, Z) to transfer the clustering results Z on X to X'.
3. Apply φ on X' and compare the optimally permuted output with Z':

$$r := \frac{1}{N} \min_{\pi \in \mathbb{S}_K} \left\{ \sum_{i=1}^{N} \mathbb{I}_{\{\pi(\varphi(x_i')) \neq \hat{z}_i'\}} \right\}.$$

   The indicator function $\mathbb{I}_{\{p\}}$ is 1 if predicate p is true, and 0 otherwise.

   Minimisation of $\pi \in \mathbb{S}_K$ compensates for the permutation of the cluster numbers.

The higher the number of clusters, the more difficult it is to have a small rate r of inconsistent cluster assignments. Given K clusters of equal size, a random assignment yields

$$r_{rand} = \frac{K-1}{K}.$$

To be able to compare hypotheses with different K, relate r to r_{rand}. The *stability* is this defined as:

$$stab := 1 - \frac{r}{r_{rand}}.$$

- $stab = 1$: No inconsistent assignments
- $stab = 0$: Not better than a random assignment

6. Clustering as Matrix Factorisation

SVD is a class matrix factorisation technique according to which every matrix matrix can be decomposed into $X = UDV^T$. With $U \in \mathbb{R}^{D\times D}$, $D \in \mathbb{R}^{D\times N}$ and $V \in \mathbb{R}^{N\times N}$. By setting UD in the decomposition as U and renaming V^T to Z, we can write

$$X = UZ.$$

Approximating X using the K largest singular values we get a factorisation involving matrices of the same dimensionality as K-Means.

7. Mixture Models

7.1. Soft Clustering

The term Soft clustering is ambiguous since it can refer to the algorithm or to the model:

Algorithmic Soft K-Means: Instead of assigning a point to exactly one cluster. Consider assigning a probability that a data point belongs to a certain cluster.

Model relaxation

Part III.
Appendix

A. Matrix Definitions and Theorems

A.1. Norms

A *norm* is a function $\|\circ\| : V \mapsto \mathbb{R}$ quantifying the size of a vector. It must satisfy

- *Positive scalability:*

$$\|a \cdot x\| = |a| \cdot \|x\|.$$

- *Triangle inequality*

$$\|x + y\| \leq \|x\| + \|y\| \quad \forall x, y \in V.$$

- *Separability*:

$$\|x\| = 0 \implies x = 0.$$

A.1.1. Vector norms

p-norms The most commonly used matrix norms are p-norms.

$$\|x\|_p := \left(\sum_{i-1}^{n} |x_i|^p \right)^{1/p}$$

for $p \in [1, \infty]$, where $|x_i|$ denotes the absolute value of coordinate x_i.

A special case of the p norm is the *Eclidean norm*:

$$\|x\|_2 := \sqrt{\sum_{i=1}^{n} x_i^2}.$$

0-**norm** technically not really a norm is defined by:

$$\|x\|_0 := \text{number of nonzero coordinates in } x.$$

A.1.2. Matrix norms

p-norm for matrices:

$$\|X\|_p := \max_{x \neq 0} \frac{\|Ax\|_p}{\|x\|_p}.$$

A special case is the Euclidean or *spectral norm*:

$$\|X\|_2 = \sigma_{\max}(X),$$

the largest singular value of X.

Frobenius norm is defined as:

$$\|X\|_F := \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n} x_{ij}^2} = \sum_{i=1}^{\min(m,n)} \sigma_i^2,$$

where σ_i are the singular values of X.

A.2. Orthogonality

Orthogonal vectors Two vectors in an inner product are orthogonal if their inner product is zero.

Orthonormal vectors Orthogonal vectors that have unit length 1

Orthogonal matrix An orthogonal matrix is a square matrix with real entries whose columns and rows are orthogonal unit vectors (i.e. orthonormal vectors). For orthogonal matrices it also holds that

$$A^T A = I \quad \Longrightarrow \quad A^T = A^{-1} \text{ since,}$$

$$(A^T A)_{i,j} = a_i^T a_j = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

B. Occam's Razor

> Entities must not be multiplied beyond necessity.

It states that among competing hypotheses, the hypothesis with the fewest assumptions should be selected. It is often understood as 'the simplest explanation is usually the correct one', although this is potentially misleading. The application of the principle often shifts the burden of proof in a discussion.[a] The razor states that one should proceed to simpler theories until simplicity can be traded for greater explanatory power. The simplest available theory need not be most accurate. Philosophers also point out that the exact meaning of simplest may be nuanced.[2]

[2] http://en.wikipedia.org/wiki/Occam's_razor

C. Probability

We denote Ω the sample space and by A an event, which is a subset of Ω.

Probability distribution A function p that assigns a real number $p(A)$ to each event A is a *probability distribution* if it satisfies the following three axioms:

- $p(A) \geq 0$ for every A.
- $p(\Omega) = 1$.
- If A_1, A_2, ... are disjoint then

$$p\left(\bigcup_{i=1}^{\infty}\right) = \sum_{i=1}^{\infty} p(A_i)$$

Random Variable A random variable is a mapping:

$$\begin{aligned} X \ : \ \Omega \ &\to \ \mathcal{K} \\ \omega \ &\mapsto \ X(\omega) \end{aligned}$$

that assigns an element $X(\omega) \in \mathcal{K}$ to each outcome ω.

Notation and types of random variables (sample spaces):

Notation :

X	Random variable
x	a value taken by the r.v. X.

Discrete random variables :

- Finite: e.g. $X \in \mathcal{B} \equiv \{0, 1\}$ or $X \in \mathcal{S}_n$ (set of permutations)
- Contably Infinite: e.g $X \in \mathbb{N}, \mathbb{Z}$ etc...

Continous random variables : e.g $X \in \mathbb{R}, [a, b]$ etc...

C.1. Distributions

C.1.1. Categorical distribution

Example The sample space of throwing two dice is $\Omega = [1, \ldots, 6] \times [1, \ldots, 6]$. We consider the two random variables $X_1 + X_2$ given by summing up the numbers x_1, x_2 of the two dice. The random variable can thus take values in $[2, \ldots, 12]$. This leads to the following probabilites:

Random variable	2	3	4	5	6	7	8	9	10	11	12
Probability	$\frac{1}{36}$	$\frac{2}{36}$	$\frac{3}{36}$	$\frac{4}{36}$	$\frac{5}{36}$	$\frac{6}{36}$	$\frac{5}{36}$	$\frac{4}{36}$	$\frac{3}{36}$	$\frac{2}{36}$	$\frac{1}{36}$

The random variable $X_1 + X_2$ is an example of the *categorical distribution*: A discrete distribution over K events. Each event has the probability π_k of occurring.

Definition The categorical distribution is a discrete probability distribution whose sample space is the set of $1-\text{of}-K$ encoded random vectors x of dimensions K having the property:

$$\sum_{k=1}^{K} z_k = 1, \quad z_k \in \{0, 1\}.$$

The probability mass function is defined as

$$p(z|\pi) = \prod_{k=1}^{K} \pi_k^{z_k},$$

where π_k represents the probability of seeing element k ($\pi_k \geq 0$, $\sum_{k=1}^{K} \pi_k = 1$).

C.1.2. Gaussian Distribution

The probability density function of the Gaussian distribution is given by:

$$p(x|\mu, \sigma) = \mathcal{N}(x|\mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}$$
$$\mu = \text{ mean of distribution}$$
$$\sigma^2 = \text{ variance of distribution.}$$

Probability for $X \in [a, b]$ is given by an integral:

$$P(a < X < b) = \int_a^b p(x)dx = \frac{1}{\sqrt{2\pi}\sigma} \int_a^b exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\} dx.$$

C.1.3. Multivariate Gaussian Distribution

Generalises the univaraite Gaussian distribution to higher dimensions. The distribution samples the space $\mathcal{X} \subseteq \mathbb{R}^D$. A random vector $X = (X_1, \ldots, X_D)^T$ has a multivariate normal distribution if every linear combination of its components (i.e., $Y = a_1X_1 + \ldots + a_DX_D$) has a univariate normal distribution.

Definition :

$$p(x|\mu\Sigma) = \mathcal{N}(x|\mu, \Sigma) := \frac{1}{(\sqrt{2\pi})^D|\Sigma|^{1/2}} exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)$$

C.1.4. Multidimensional Moment Statistics

Expectation Vector of component expectations:

$$\mathbb{E}[X] = \begin{pmatrix} \mathbb{E}[X_1] \\ \vdots \\ \mathbb{E}[X_D] \end{pmatrix}$$

Variance Generalised covariance:

$$\begin{aligned} Cov[X, Y] : &= \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x, y)(x - \mu_X)(y - \mu_Y) dx dy \\ &= \mathbb{E}_{X,Y}[(x - \mu_X)(y - \mu_Y)] \end{aligned}$$

Covariance Matrix For random variables $X_1, \ldots, X_D$ we record covariances in the covariance matrix Σ:

$$\Sigma_{i,j} := Cov[X_i, Y_i] \quad i, j \in \{1, \ldots, D\}.$$

Σ generalises the notion of variance to sets of random variables for multiple dimensions.