Notes on Gaussian Processes

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# Introductory Notes

## Gaussian Models

The PDF of an MVN in dimensions is defined by the following:

(1)

where is the mean vector , and is the covariance matrix.

is known as the *precision matrix* or *concentration matrix*. The normalization constant ensures that the pdf integrates to 1.

A *full* *covariance matrix* has parameters since is symmetric. A *diagonal* *covariance* *matrix* has parameters, and has 0s in the off-diagonal terms. A spherical (or isotropic) covariance, , has one free parameter.

The expression inside the exponent is the Mahalanobis distance between a data vector and the mean vector .

Let us look more closely into the Mahalanobis distance by performing *eigendecomposition* of **.**

So we can write , where is an orthonormal matrix of eigenvectors satisfying , and is a diagonal matrix of eigenvalues. Thus we can write:

where is the th column of , containing the th eigenvector. Hence, we can rewrite the Mahalanobis distance as follows:

where .

Thus the contours of equal probability density of a Gaussian lie along ellipses. The eigenvectors determine the orientation of the ellipse, and the eigenvalues determine how elongated it is. In general the Mahalanobis distance corresponds to Euclidean distance in a transformed coordinate system , shifted by and rotated by .

**Theorem**: (MLE for a Gaussian)

If we have N iid samples , then the MLE for the parameters is given by

(1)

(2)

Proof:

We use the following notation and identities

– trace of a matrix

(3)

Here . We use the notation .

(4)

In order to prove (4) we use the following tensor notation:

(superscript corresponds to row vector, subscript - to column vector)

, (superscript-subscript combination on the same index implies summation)

Thus we write

## Gaussian Processes (GP)

A Gaussian Process is a Gaussian distribution over functions:

## Noiseless Gaussian Process Regression

We observe a training set where

Given the test set of size , we want to predict the function outputs .

where is matrix, is matrix, and is

Here

Computing predictions is just a question of deriving the conditional distribution from the joint distribution.

# Appendix

## Covariance and Correlation

Covariance between two r.v.’s and measures the degree to which X and Y are related linearly. Covariance is defined as:

A group of symbols with numbers

Description automatically generated with medium confidence

Figure: several sets of points, with the correlation coefficient of and for each set. Note that the correlation reflects the noisiness and the direction of a linear relationship (top row) but not the slope of the relationship (middle), nor the shape indicating non-linear relationship (bottom). Source: <http://en.wikipedia.org/wiki/File:Correlation_examples.png>

If x is a d-dimensional vector, its covariance matrix is defined as the following symmetric positive definite matrix

The Pearson correlation coefficient between and is defined as:

The correlation matrix has the form

**Statement**:

Proof: We have to prove that (A.1)

Cauchy-Schwarz in : (A.2)

Clearly for discrete r.v.’s and (A.1) follows from (A.2).

For continuous r.v.’s and we use the Cauchy-Schwarz in

(A.3) where the integration is performed over some domain of .

A substitution of the distribution function of with and the distribution function of with in (A.3) yields (A1) for the case of continuous r.v.’s.

# References

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[6] [Machine Learning Tutorial at Imperial College London: Gaussian Processes, Richard Turner, U of Cambridge, Nov 23th, 2016](https://youtu.be/92-98SYOdlY?si=K6cMS8998JFbpMi9)

[7] [Machine Learning: Probabilistic Perspective, Kevin P. Murphy, 2012](https://github.com/dimitarpg13/probabilistic_machine_learning/blob/main/books/MachineLearningProbabilisticPerspective.pdf)