

Decomposition of Covariance [3]

Qi Zhao

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1. Introduction

Given a normal distribution [5] with mean zero and a full covariance matrix [1], it can be known that the iso-contours take an ellipsoidal form with the major and minor axes at arbitrary orientations. Now consider viewing the distribution in a new coordinate frame where the axes are aligned with the axes of the normal (Figure 1): in this new frame of reference, the covariance matrix Σ_{diag} will be diagonal. Denote the data vector in the new coordinate system by $x = [x_1, x_2]^T$ where the frames of reference are related by x

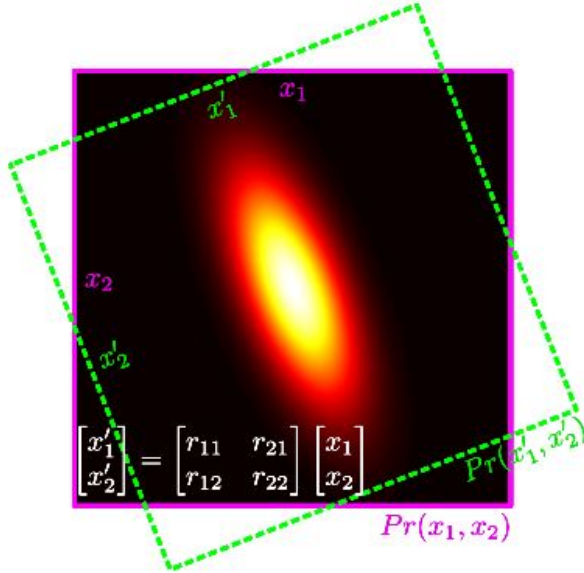


Figure 1. Decomposition of full co-variance. For every bivariate normal distribution in variables x_1 and x_2 with full covariance matrix, there exists a coordinate system with variables x_1' and x_2' where the covariance is diagonal: the ellipsoidal iso-contours align with the coordinate axes x_1' and x_2' in this canonical coordinate frame. The two frames of reference are related by the rotation matrix \mathbf{R} which maps (x_1', x_2') to (x_1, x_2) . From this it follows (see text) that any covariance matrix Σ can be broken down into the product $R^T \Sigma'_{diag} R$ of a rotation matrix \mathbf{R} and a diagonal covariance matrix Σ'_{diag} .

$$Pr(x) = \frac{1}{2\pi^{\frac{D}{2}} \sqrt{|\Sigma'_{diag}|}} \exp[-0.5 x'^T \Sigma'^{-1}_{diag} x'] \quad (1)$$

If we convert back to the original axes by substituting in $x = R x'$ to get in Equation 2.

$$\begin{aligned} Pr(x) &= \frac{1}{2\pi^{\frac{D}{2}} \sqrt{|\Sigma'_{diag}|}} \exp[-0.5 (R x')^T \Sigma'^{-1}_{diag} R x'] \\ &= \frac{1}{2\pi^{\frac{D}{2}} \sqrt{|R^T \Sigma'_{diag} R|}} \exp[-0.5 (x')^T (R^T \Sigma'^{-1}_{diag} R) x'] \end{aligned} \quad (2)$$

where we have used $|R^T \Sigma R| = |R^T| \cdot |\Sigma| \cdot |R| = 1 \cdot |\Sigma| \cdot 1 = |\Sigma|$. Equation 3 is a multivariate normal with covariance.

$$\Sigma_{full} = R^T \Sigma'_{diag} R \quad (3)$$

2. Conclusions

It can be concluded that full covariance matrices are expressible as a product of this form involving a rotation matrix [2] \mathbf{R} and a diagonal covariance matrix Σ , which is possible to retrieve these elements from an arbitrary valid covariance matrix Σ_{full} by decomposing it in this way using the singular value decomposition.

The matrix \mathbf{R} contains the principal directions of the ellipsoid in its columns. The values on the diagonal of Σ_{diag} encode the variance (and hence the width of the distribution) along each of these axes. Hence the results of the eigen-decomposition can be used to answer questions about which directions in space are most and least certain.

References

- [1] C. A. Guevara, E. Cherchi, and M. Moreno. Estimating random coefficient logit models with full covariance matrix. *Transportation Research Record: Journal of the Transportation Research Board*, 137(2132):87–95, 2009. 1
- [2] A. Horn. Doubly stochastic matrices and the diagonal of a rotation matrix. *American Journal of Mathematics*, 76(3):620–630, 1954. 1

- [3] D. Koutsoyiannis. Optimal decomposition of covariance matrices for multivariate stochastic models in hydrology. *Water Resources Research*, 35(4):1219C1229, 1999. [1](#)
- [4] B. Rannala and Z. Yang. Probability distribution of molecular evolutionary trees: a new method of phylogenetic inference. *Journal of Molecular Evolution*, 43(3):304–311, 1996. [1](#)
- [5] C. M. Stein. Estimation of the mean of a multivariate normal distribution. *Annals of Statistics*, 9(6):1135–1151, 1981. [1](#)