Interpreting multivariate normal via eigen-decomposition of covariance matrix

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See here for a PDF version of this vignette.

Prerequisites

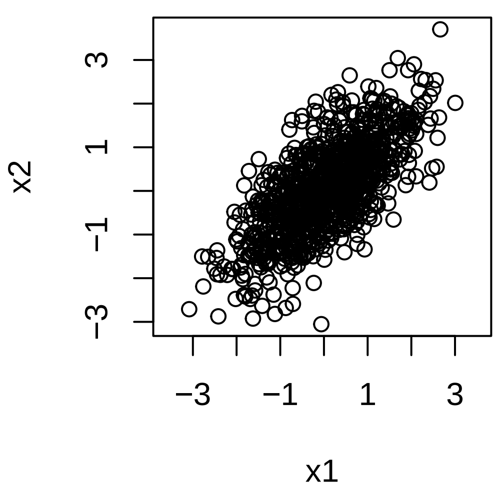
You should be familiar with the multivariate normal distribution, and with the eigen-decomposition for symmetric positive semi-definite (PSD) matrices.

Introduction

Getting an intuition for what the p-dimensional multivariate normal distribution $N_p(\mu, \Sigma)$ "looks like" can be difficult. For $p = 1$ or 2, things are not too bad; we can directly visualize a univariate normal distribution by plotting its density, and visualize a bivariate normal distribution by plotting a contour plot of the density, or by simulating samples from the distribution and visualizing them using a 2-d scatterplot. For example, the following code does this for $N(0, \Sigma)$, where

$$\Sigma = \begin{pmatrix} 1.0 & 0.7 \\ 0.7 & 1.0 \end{pmatrix}:$$

```r
library(mvtnorm)
Sigma <- cbind(c(1,0.7),c(0.7,1))
X <- rmvnorm(1000,c(0,0),Sigma)
plot(X[,1],X[,2],xlab = "x1",ylab = "x2",asp = 1)
```



But in $p = 100$ dimensions, or even just $p = 4$ dimensions, things become much harder because direct visualization is impractical. So how can we get intuition about the multivariate normal distribution, $N_p(\mu, \Sigma)$ when p is large?

Note first that the mean μ is just a vector of p numbers, and generally causes few problem in interpretation: you can just think of each number as specifying the mean in each of the p coordinates one at a time.

In contrast, the covariance matrix Σ is a $p \times p$ matrix that captures potentially more complex patterns, and creates more challenges for intuition. One possible approach is to plot a heatmap of this matrix, and this can certainly be helpful in certain situations. However, this vignette describes a more algebraic approach based on the eigen-decomposition of Σ.

Some linear algebra

Recall that any valid $p \times p$ covariance matrix Σ must be symmetric and positive semi-definite (PSD). Furthermore, recall that any such PSD matrix must have eigen-decomposition:

$$\Sigma = V \Lambda V',$$

where

- Λ is a $K \times K$ diagonal matrix with the non-zero eigenvalues of Σ, $\lambda_1, \ldots, \lambda_K$, on the diagonal ($K \leq p$ is the rank of Σ).
- V is a $p \times K$ orthonormal matrix ($V^T V = I_K$), whose columns $v_1, \ldots, v_K$ are the normalized eigenvectors of Σ corresponding to the non-zero eigenvalues.

Recall also that if $Z \sim N_p(0, I_p)$, A is any $n \times p$ matrix, and $X = \mu + AZ$, then $X \sim N(\mu, AA^T)$.

Now apply this last result with $A = V\Lambda^{1/2}$ where $\Lambda^{1/2}$ is the diagonal matrix with $\lambda_1^{1/2}, \ldots, \lambda_K^{1/2}$ on the diagonal. For $X = \mu + AZ$, we get

$$X \sim N_p(\mu, V\Lambda^{1/2}\Lambda^{1/2}V^T).$$

That is,

$$X \sim N_p(\mu, \Sigma).$$

We can write the matrix multiple $V\Lambda^{1/2}Z$ as a sum to make the structure more obvious:

$$\mu + \sum_{k=1}^{K} \lambda_k^{1/2} z_k v_k \sim N_p(\mu, \Sigma).$$

Here, μ and $v_1, \ldots, v_K$ are all column vectors of length p, whereas the λ_k and z_k are all scalars.

Interpration as a random linear combination of eigenvectors

From this algebra, if $X \sim N_p(\mu, \Sigma)$, then we can think of X as being generated by taking the mean μ, and adding a *random linear combination* of the eigenvectors of Σ. Specifically,

$$X = \mu + \sum_{k=1}^{K} b_k v_k,$$

where the weights

$$b_k = \lambda_k^{1/2} z_k \sim N(0, \lambda_k).$$

are independent of one another.

Note that if λ_k is "small" then $b_k \approx 0$, so the eigenvectors with small eigenvalues contribute little to X, and we can focus on the eigenvectors with large eigenvalues. Indeed, this approach provides the simplest insights when most of the λ_k are negligible and only one or two eigenvectors contribute meaningfully to the sum.

Example: rank-1 covariance

To make a simple example, set $\mu = 0$ and assume Σ is a rank-1 matrix. That is, Σ has only one eigenvector:

$$\Sigma = \lambda v v^T$$

for some vector v of length p.

In this case, the algebra above gives the representation $X = bv$ where $b \sim N(0, \lambda)$. That is X is simply a multiple of v, where the multiplier is randomly distributed from a univariate normal. Thus, in this case the randomness in X boils down to the randomness in a single random univarate normal, which is easy to visualize.

To give an example, suppose that v is the vector of all ones, $v = (1, \ldots, 1)$, and $\lambda = 1$. That is, Σ is a matrix of all ones. Then $X = (b, \ldots, b)$, a vector filled with b, where $b \sim N(0, 1)$.

To give another example, if $v = (-1, -1, -1, 1, 1)$ and $\lambda = 2$, then $X = (-b, -b, -b, b, b)$, where $b \sim N(0, 2)$.