Mahalanobis Distance

Brendan McCane

March 2, 2009

1 Mahalanobis Distance for Continuous Variables

Let's say we have two independent and identically distributed random variables X and Y - two-dimensional space. Without loss of generality, let's assume that both X and Y have a variance equal to 1. It doesn't matter how they are distributed but let's assume we are interested in the Euclidean distance between two points, $p_1 = (x_1, y_1)$ and $p_2 = (x_2, y_2)$ in this space. As we all know the Euclidean distance is:

$$d^2(p_1, p_2) = (x_1 - x_2)^2 + (y_1 - y_2)^2. \tag{1}$$

We can reformulate this distance function as an inner-product in vector space:

$$d^2(p_1, p_2) = (p_1 - p_2)^T (p_1 - p_2), \tag{2}$$

where ^{T} represents matrix transpose.

OK, so far no problems. What if we can't actually directly observe X and Y, but can only observe scaled versions, s_1X and s_2Y, where $s_1, s_2 \neq 0$, but are otherwise arbitrary. Let's indicate a scaled observation point as p'_i. Can we still calculate $d^2(p_1, p_2)$?

$$\begin{aligned} d^2(p_1, p_2) &= (x_1 - x_2)^2 + (y_1 - y_2)^2 \\ &= (\frac{x'_1}{s_1} - \frac{x'_2}{s_1})^2 + (\frac{y'_1}{s_2} - \frac{y'_2}{s_2})^2 \\ &= \frac{(x'_1 - x'_2)^2}{s_1^2} + \frac{(y'_1 - y'_2)^2}{s_2^2}. \end{aligned}$$

So as long as we know the scale factor, we can calculate d^2. Well, it's pretty easy to calculate the scale factor and there are many ways to do it. For reasons that should become clear below, let's use the variance of each of the variables as a measure of spread. It is a basic fact from statistics that $Var(sX) = sVar(X)$, and since, by definition, $Var(X) = 1$, we have $Var(X') = s$ and we can calculate the scale factor for each variable and subsequently the distance in the undistorted space.

Now, let's try to be a bit trickier. What if we can't directly observe X and Y, but can only observe linear combinations:

$$\begin{aligned} X' &= a_{11}X + a_{12}Y \\ Y' &= a_{21}X + a_{22}Y. \end{aligned} \tag{3}$$

Can we still calculate $d^2(p_1, p_2)$? First, let's write equation 3 in a more convenient form:

$$p' = Ap, \tag{4}$$

where $A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$. We could have done a similar thing in the previous paragraph, but I think it's more intuitive the way it is. So, our Euclidean distance formula becomes:

$$\begin{aligned} d^2(p_1, p_2) &= (A^{-1}(p_1' - p_2'))^T (A^{-1}(p_1' - p_2')) \\ &= (p_1' - p_2')^T {A^{-1}}^T A^{-1} (p_1' - p_2') \end{aligned}$$

If we do a bit of manipulation and actually calculate the matrix ${A^{-1}}^T A^{-1}$, then we get:

$${A^{-1}}^T A^{-1} = \frac{1}{(a_{12}a_{21} - a_{11}a_{22})^2} \begin{bmatrix} a_{21}^2 + a_{22}^2 & -a_{11}a_{21} - a_{12}a_{22} \\ -a_{11}a_{21} - a_{12}a_{22} & a_{11}^2 + a_{12}^2 \end{bmatrix} \tag{5}$$

Now let's take a bit of a side-track and calculate the covariance matrix for X' and Y'. First the variance of X' and Y':

$$\begin{aligned} Var(X') =& E[(X' - \bar{X}')^2] \\ =& E[(a_{11}X + a_{12}Y - a_{11}\bar{X} - a_{12}\bar{Y})^2] \\ =& E[a_{11}^2 X^2 - 2a_{11}^2 \bar{X}^2 + a_{11}^2 \bar{X}^2 + 2a_{11}a_{12}\bar{X}\bar{Y} - 2a_{11}a_{12}\bar{X}\bar{Y} \\ & + a_{12}^2 Y^2 - 2a_{11}a_{12}\bar{X}\bar{Y} + 2a_{11}a_{12}\bar{X}\bar{Y} - 2a_{12}^2\bar{Y}^2 + a_{12}^2\bar{Y}^2] \\ =& a_{11}^2(X^2 - \bar{X}^2) + a_{12}^2(Y^2 - \bar{X}^2) \\ =& a_{11}^2 Var(X) + a_{12}^2 Var(Y) \\ =& a_{11}^2 + a_{12}^2, \end{aligned}$$

where $E[]$ represents expectation. We get similar results for the variance of Y', and can follow a similar treatment to get the covariance of X' and Y':

$$Cov(X', Y') = a_{11}a_{21} + a_{12}a_{22}. \tag{6}$$

Which leaves us with the covariance matrix:

$$\Sigma(X', Y') = \begin{bmatrix} a_{11}^2 + a_{12}^2 & a_{11}a_{21} + a_{12}a_{22} \\ a_{11}a_{21} + a_{12}a_{22} & a_{21}^2 + a_{22}^2. \end{bmatrix} \tag{7}$$

Now if we take the inverse of Σ, then we get:

$$\Sigma(X', Y')^{-1} = \frac{1}{(a_{12}a_{21} - a_{11}a_{22})^2} \begin{bmatrix} a_{21}^2 + a_{22}^2 & -a_{11}a_{21} - a_{12}a_{22} \\ -a_{11}a_{21} - a_{12}a_{22} & a_{11}^2 + a_{12}^2 \end{bmatrix}. \tag{8}$$

Which looks surprisingly like equation 5.

Thus we are led to the remarkable result that to measure the Euclidean distance in an underlying uncorrelated space, we need to use the Mahalanobis distance:

$$d^2(p_1, p_2) = (p_1' - p_2')^T \Sigma^{-1} (p_1' - p_2') \tag{9}$$