null_discriminability

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Setup

Given the following two-class problem:

$$X_i \stackrel{d}{\sim} \mathcal{N}\left(\mu_i^{(x)}, \Sigma_i^{(x)}\right)$$

with $\mu_i^{(x)} \in \mathbb{R}^p$, $\Sigma_i^{(x)} \in \mathbb{R}^{p \times p}$, then the goal is the distribution of $||Y|| = ||X_1 - X_2||$, where:

$$Y = X_1 - X_2 \stackrel{d}{\sim} \mathcal{N} \Big(\mu^{(y)} = \mu_1^{(x)} - \mu_2^{(x)}, \Sigma^{(y)} = \Sigma_1^{(x)} + \Sigma_2^{(x)} \Big)$$

To simplify the math, assume that $\Sigma_{i,j}^{(x)} = \sigma_i^{(x)}$ when i=j, and 0 otherwise. That is, observations between dimensions are assumed to be independent. Let $Y = (Y_i)_{i=1}^p$, so Y_i is a random variable for each dimension, where $\Sigma_{i,j}^{(y)} = \sigma_i^{(y)}$ when i=j and zero otherwise. Then:

$$||Y||^2 = \sum_{i=1}^p Y_i$$

and:

$$||Y|| = \sqrt{\sum_{i=1}^{p} Y_i}$$

Theoretical Approach

Approach 1

Note that for $A = Z_1 + \mu$ where $A \stackrel{d}{\sim} \mathcal{N}(\mu, 1)$ and Z_1 is the standard gaussian, we can find the MGF:

$$M_{A}(t) = \mathbb{E}\left[e^{tA^{2}}\right] = \mathbb{E}\left[e^{t(Z+\mu)^{2}}\right]$$

$$= \int_{-\infty}^{\infty} e^{t(z+\mu)^{2}} \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}z^{2}} dz$$

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$$\begin{split} &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\left(\frac{1}{2} - t\right)z^2 + 2\mu tz + \mu^2 t\right) \, \mathrm{d}z \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\left(\frac{1}{2} - t\right)\left(z - \frac{2\mu t}{1 - 2t}\right)^2 + \mu^2 t + \frac{2\mu^2 t^2}{1 - 2t}\right) \, \mathrm{d}z \\ &= \frac{\sqrt{1 - 2t}}{\sqrt{2\pi}\sqrt{1 - 2t}} \exp\left(\mu^2 t + \frac{2\mu^2 t^2}{1 - 2t}\right) \int_{-\infty}^{\infty} \exp\left(-\left(\frac{1}{2} - t\right)\left(z - \frac{2\mu t}{1 - 2t}\right)^2\right) \, \mathrm{d}z \\ &= \frac{\sqrt{1 - 2t}}{\sqrt{2\pi}\sqrt{1 - 2t}} \exp\left(\mu^2 t + \frac{2\mu^2 t^2}{1 - 2t}\right) \int_{-\infty}^{\infty} \exp\left(-\frac{\left(z - \frac{2\mu t}{1 - 2t}\right)^2}{2(1 - 2t)^{-1}}\right) \, \mathrm{d}z \\ &= \frac{1}{\sqrt{1 - 2t}} \exp\left(\mu^2 t + \frac{2\mu^2 t^2}{1 - 2t}\right) \frac{\sqrt{1 - 2t}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2}\left(z - \frac{2\mu t}{1 - 2t}\right)^2 (1 - 2t)\right) \, \mathrm{d}z \\ &= \frac{1}{\sqrt{1 - 2t}} \exp\left(\mu^2 t + \frac{2\mu^2 t^2}{1 - 2t}\right) & \text{pdf of Gaussian} \\ &= \frac{1}{\sqrt{1 - 2t}} \exp\left(\frac{\mu^2 t}{1 - 2t}\right) \end{split}$$

which is the MGF of the non-central chi-squared distribution with non-centrality parameter μ^2 . Then:

$$\left(\frac{Y_i}{\sigma_{y,i}}\right)^2 \stackrel{d}{\sim} \chi_1^2 \left(\lambda_i^{(y)}\right), \ \lambda_i^{(y)} = \left(\frac{\mu_i^{(y)}}{\sigma_i^{(y)}}\right)^2$$

is non-central chi-squared with 1 degree of freedom and non-centrality parameter $\lambda_i^{(y)} = \left(\frac{\mu_i^{(y)}}{\sigma_i^{(y)}}\right)^2$. Then we can write:

$$||Y||^2 = \sum_{i=1}^p \sigma_i^2 \left(\frac{Y_i}{\sigma_i^{(y)}}\right)^2$$

which is a linear combination of non-central chi-squareds, which is the definition of the generalized chi-squared distribution.

Approach 2

Let $Z_p \overset{d}{\sim} \mathcal{N}(0, I_p)$, the standard isotropic gaussian with p dimensions. Then by definition with $Y \overset{d}{\sim} \mathcal{N}(\mu^{(y)}, \Sigma^{(y)})$, since $\Sigma^{(y)} \succ 0$, Σ has the eigendecomposition $\Sigma = Q' \Lambda Q$ where Q is the orthonormal matrix of eigenvectors and Λ the square diagonal matrix of positive eigenvalues, where $\Lambda = W'W$ and $W = \Lambda^{\frac{1}{2}}$. Then $\Sigma = (WQ)'(WQ) = L'L$ is a cholesky decomposition of Σ . Then it is clear that $Y = LZ_p + \mu^{(y)}$, so:

$$||Y||^{2} = Y'Y = \left(LZ_{p} + \mu^{(y)}\right)' \left(LZ_{p} + \mu^{(y)}\right)$$
$$= \left(Z_{p} + L^{-1}\mu^{(y)}\right)' \Sigma \left(Z_{p} + L^{-1}\mu^{(y)}\right)$$
$$= \left(Z_{p} + L^{-1}\mu^{(y)}\right)' \Sigma \left(Z_{p} + L^{-1}\mu^{(y)}\right)$$

Then with $S = QZ_p$, S is also multivariate normal since it is a full-rank linear transformation of Z_p (recall Q is full-rank by definition of the eigendecomposition of $\Sigma \succ 0$). Note also that it is $S \stackrel{d}{\sim} \mathcal{N}(0, I_p)$ since $Q'Q = QQ' = I_p$ by definition of orthonormal. Then it is clear that:

$$Y'Y = (Z_p + L^{-1}\mu^{(y)})'Q'\Lambda Q(Z_p + L^{-1}\mu^{(y)})$$

$$= (QZ_p + QL^{-1}\mu^{(y)})'\Lambda (QZ_p + QL^{-1}\mu^{(y)})$$

$$= (S + QL^{-1}\mu^{(y)})'\Lambda (S + QL^{-1}\mu^{(y)})$$

$$= (S + u)'\Lambda (S + u)$$

$$= \sum_{i=1}^{p} (S_i + u_i)^2 \lambda_i$$

where $u = QL^{-1}\mu^{(y)}$. Then $u_i = Q\frac{\mu^{(y)}}{\sigma_i^{(y)}}$, since $L_{i,i} = \sigma_i^{(y)}$ as Σ is diagonal and 0 otherwise. Note than that by definition, $(S_i + u_i)^2$ is non-central chi-squared distributed, so again we see that $||Y||^2$ is a linear combination of independent chi-squareds.

Then by both of the above approaches, it is clear that ||Y|| is distributed as the generalized chi-distribution. In the case when the variances are the same, this is simply the Rice distribution.

I'm honestly shocked but apparently when Σ is not a simple scaling of the identity, this distribution does not have any real empirical methods associated with it (ie, nice pdf, cdf, etc).

Empirical Approach

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Algorithm 1: Empirical Discriminability
Data: \mu_i \in \mathbb{R}^p the means of our 2 classes.
          \Sigma_i \in \mathbb{R}^{p \times p} the covariances of our classes.
          n_i the number of elements in each class.
          n the number of realizations to empirically sample, per-class.
Result: D the theoretical discriminability using an empirical approximation.
for l = 1 : n \ do
     for i = 1 : p \text{ do}
          for j = 1 : p \text{ do}
            sample x_i from \mathcal{N}(\mu_i, \Sigma_i).
sample x_j from \mathcal{N}(\mu_j, \Sigma_j).
Let d_{l,i,j} = ||x_i - x_j||
         end
     end
end
for i = 1 : p do
     for j = 1 : p \ do
      Let P_{i,j} be the relative mass of d_{:,i,i} < d_{:,i,j}.
end
Let D = \sum_{i=1}^{p} \pi_i \pi_j P_{i,j}, where \pi_i = \frac{n_i}{n}.
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