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# The Fréchet Distance between Multivariate Normal Distributions

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The Fréchet distance between two multivariate normal distributions having means $\mu_X$, $\mu_Y$ and covariance matrices $\Sigma_X$, $\Sigma_Y$ is shown to be given by $d^2 = |\mu_X - \mu_Y|^2 + \mathrm{tr}(\Sigma_X + \Sigma_Y - 2(\Sigma_X \Sigma_Y)^{1/2})$. The quantity $d_0$ given by $d_0^2 = \mathrm{tr}(\Sigma_X + \Sigma_Y - 2(\Sigma_X \Sigma_Y)^{1/2})$ is a natural metric on the space of real covariance matrices of given order.

## 1. INTRODUCTION

In [1], M. Fréchet introduced a metric on the space of probability distributions on $R$ having first and second moments. The Fréchet distance $d(F, G)$ between two distributions $F$ and $G$ is defined by

$$d^2(F, G) = \min_{X,Y} E\,|X - Y|^2 \tag{1}$$

where the minimization is taken over all random variables $X$ and $Y$ having distributions $F$ and $G$, respectively. The bivariate distribution $H$ which minimizes the right-hand side of (1) is well-known [1, 2] to be the singular distribution with distribution function

$$H(x, y) = \min[F(x), G(y)], \tag{2}$$

where $F$ and $G$ are the distribution functions of $F$ and $G$, respectively. In the particular case when $F$ and $G$ belong to a family of distributions which is closed with respect to changes of location and scale, the Fréchet distance takes the simple form

$$d^2(F, G) = (\mu_X - \mu_Y)^2 + (\sigma_X - \sigma_Y)^2 \tag{3}$$

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where $\mu_X$, $\mu_Y$ and $\sigma_X$, $\sigma_Y$ are the respective means and standard deviations of $F$ and $G$.

Definition [1] generalises in an obvious way to define a metric on the space of probability distributions on $R^n$ having second moments. The solution (2) does not apply in the case when $X$ and $Y$ are vectors and the evaluation of the Fréchet distance is extremely difficult in general. Again, however, the distance $d(F, G)$ is easy to determine when $F$ and $G$ belong to a family of $n$-dimensional distributions which is closed with respect to linear transformations of the random vector. We shall prove that in this case, the Fréchet distance is given by

$$d^2(F, G) = |\mu_X - \mu_Y|^2 + \operatorname{tr}[\Sigma_X + \Sigma_Y - 2(\Sigma_X \Sigma_Y)^{1/2}] \tag{4}$$

where $\mu_X$, $\mu_Y$ and $\Sigma_X$, $\Sigma_Y$ are the respective means and covariance matrices of $F$ and $G$, and the positive square root is taken. The above formula holds in particular when $F$ and $G$ are normal distributions on $R^n$. Additionally it will be seen that

$$d_0^2(\Sigma_X, \Sigma_Y) = \operatorname{tr}[\Sigma_X + \Sigma_Y - 2(\Sigma_X \Sigma_Y)^{1/2}] \tag{5}$$

defines a metric on the space of all covariance matrices of order $n$.

## 2. Main Result

Since the results (4) and (5) generalise easily to the complex case, it will be convenient to take $X$ and $Y$ as complex-valued random vectors in $C^n$ having, initially, zero means. We prove the following theorem.

THEOREM. *Let $X$, $Y$ be random vectors taking values in $C^n$ and having zero means and covariance matrices $\Sigma_X$, $\Sigma_Y$ respectively. Then*

$$\operatorname{tr}[\Sigma_X + \Sigma_Y - 2(\Sigma_X \Sigma_Y)^{1/2}] \leqslant E\,|X - Y|^2 \leqslant \operatorname{tr}[\Sigma_X + \Sigma_Y + 2(\Sigma_X \Sigma_Y)^{1/2}] \tag{6}$$

*where the square roots are the positive roots.*

*The bounds in* (6) *are attained when $X - Y$ has covariance matrix*

$$\Sigma_{X-Y} = \Sigma_X + \Sigma_Y \pm [(\Sigma_X \Sigma_Y)^{1/2} + (\Sigma_Y \Sigma_X)^{1/2}], \tag{7}$$

*and, for non-singular $\Sigma_X$, this occurs when $X$ and $Y$ are related by*

$$Y = \pm \Sigma_X^{-1} (\Sigma_X \Sigma_Y)^{1/2} X. \tag{8}$$

*Proof.* Let $W$ be the random vector taking values in $C^{2n}$ defined by $W = [{}^X_Y]$, and denote the covariance matrix of $W$ by

$$\Sigma_W = \begin{bmatrix} \Sigma_X & V \\ V^* & \Sigma_Y \end{bmatrix}$$

where * denotes conjugate transpose. Clearly,

$$E\,|X - Y|^2 = \operatorname{tr}[\Sigma_X + \Sigma_Y - V - V^*]$$

so that we require extreme values of $\operatorname{tr}(V + V^*)$ subject to the condition that $\Sigma_W$ is a covariance matrix. We note that $\operatorname{tr}(V + V^*)$ is a linear functional defined on a convex region of the $\Sigma_W$ space and hence we can apply the method of Lagrange multipliers. Let $Q$ denote the Hermitian form $w^* \Sigma_W w$ so that

$$Q = x^*\Sigma_X x + x^*Vy + y^*V^*x + y^*\Sigma_Y y.$$

Since $Q$ is non-negative definite, it must be capable of being written

$$Q = \sum_{i=1}^{m} |a_i^* x + b_i^* y|^2,$$

where $a_i, b_i \in C^n$ for $i = 1,..., m$ and $m \leqslant 2n$.

It follows that $\Sigma_X$, $\Sigma_Y$ and $V$ must have simultaneous representations of the form

$$\Sigma_X = \sum_{i=1}^{m} a_i a_i^*, \qquad \Sigma_Y = \sum_{i=1}^{m} b_i b_i^*, \qquad V = \sum_{i=1}^{m} a_i b_i^*. \tag{9}$$

We seek to minimize $\operatorname{tr} \sum_{i=1}^m (a_i b_i^* + b_i a_i^*)$ subject to the matrices $\sum_{i=1}^m a_i a_i^*$ and $\sum_{i=1}^m b_i b_i^*$ having given values $\Sigma_X$ and $\Sigma_Y$, respectively. Introducing Hermitian matrices $\Lambda$ and $M$ of Lagrange multipliers we seek unconstrained extreme values of the real quantity

$$S = \operatorname{tr} \sum_{i=1}^{m} (a_i b_i^* + b_i a_i^*) + \operatorname{tr}\left(\sum_{i=1}^{m} a_i a_i^*\right) \Lambda + \operatorname{tr}\left(\sum_{i=1}^{m} b_i b_i^*\right) M.$$

It is easily seen that extreme values satisfy the conditions

$$\begin{matrix} b_i = \Lambda a_i \\ a_i = M b_i \end{matrix} \qquad (i = 1,..., m).$$

Thus, $\Lambda$ is a Hermitian matrix which by virtue of conditions (9) must satisfy the equations

$$\Lambda \Sigma_X \Lambda = \Sigma_Y \tag{10}$$

and

$$V=\Sigma_X A, \tag{11}$$

which together imply $V^2=\Sigma_X\Sigma_Y$.

For non-singular $\Sigma_X$ we may put

$$A=\Sigma_X^{-1/2}R\Sigma_X^{-1/2} \tag{12}$$

so that $R$ is Hermitian and, because of (10), $R^2$ simplifies to the non-negative definite $\Sigma_X^{1/2}\Sigma_Y\Sigma_X^{1/2}$. If the latter has eigenvalues $\lambda_i$ and eigenvectors $s_i$ with $s_i^*s_j=\delta_{ij}$, then all its Hermitian square roots are of the form $\sum_{i=1}^m \varepsilon_i\lambda_i^{1/2}s_is_i^*$ where, for each $i$, $\varepsilon_i^2=1$. From (11) and (12), $V=\Sigma_X^{1/2}R\Sigma_X^{-1/2}$ has the same eigenvalues as $R$, so the maximum and minimum of tr $V$, viz., $\pm\sum_{i=1}^m \lambda_i^{1/2}$, are attained when

$$V=\pm\,\Sigma_X^{1/2}(\Sigma_X^{1/2}\Sigma_Y\Sigma_X^{1/2})^{1/2}\,\Sigma_X^{-1/2}.$$

The latter product is a way of expressing $(\Sigma_X\Sigma_Y)^{1/2}$, the positive square root of $\Sigma_X\Sigma_Y$, when $\Sigma_X$ is non-singular. (More generally $\Sigma_X\Sigma_Y$ has the same non-negative eigenvalues $\lambda_i$ as $\Sigma_X^{1/2}\Sigma_Y\Sigma_X^{1/2}$ above, and its positive square root is $\sum_{i=1}^m \lambda_i^{1/2}u_it_i^*$ where $t_i$, $u_i$ are left and right eigenvectors of $\Sigma_X\Sigma_Y$ with $t_i^*u_j=\delta_{ij}$.) Thus, $\mathrm{tr}(V+V^*)$ is maximised or minimised by taking

$$V=\pm(\Sigma_X\Sigma_Y)^{1/2} \tag{13}$$

That the covariance matrix of $X-Y$ is given by (7) and that relation (8) between $X$ and $Y$ yields the upper and lower bounds is now routine. Moreover, by continuity considerations (13) carries over to the case where $\Sigma_X$ is singular; consequently (6) and (7) hold generally and the theorem is proved.

For singular $\Sigma_X$, (8) obviously no longer applies; but if the null space of $\Sigma_X$ is contained in that of $\Sigma_Y$, it holds with $\Sigma_X^{-1}$ replaced by the pseudo-inverse of $\Sigma_X$.

COROLLARY. *Let $\mathscr{C}_n(\Sigma)$ be the set of all covariance (non-negative, Hermitian) matrices of order $n$. Then*

$$d_0(\Sigma_X,\Sigma_Y)=[\mathrm{tr}(\Sigma_X+\Sigma_Y-2(\Sigma_X\Sigma_Y)^{1/2})]^{1/2} \tag{14}$$

*defines a metric on $\mathscr{C}_n(\Sigma)$.*

In the particular case when the real covariance matrices $\Sigma_X$ and $\Sigma_Y$ have the same principal axes, the metric has the particularly simple form

$$d_0^2(\Sigma_X,\Sigma_Y)=\sum_{i=1}^n(\sigma_i-\rho_i)^2 \tag{15}$$

where $\sigma_i$, $\rho_i$ are the standard deviations of the (principal) components of $X$ and $Y$, respectively, along the $i$th principal axis.

## 3. Fréchet Distance between Multinormal Distributions

Since multinormal distributions are determined completely by their means and covariance matrices, it follows immediately that the Fréchet distance between normal distributions $F$ and $G$ on $R^n$ with means $\mu_X$, $\mu_Y$ and (real) covariance matrices $\Sigma_X$, $\Sigma_Y$ is given by

$$d^2(F, G) = |\mu_X - \mu_Y|^2 + \operatorname{tr}(\Sigma_X + \Sigma_Y - 2(\Sigma_X \Sigma_Y)^{1/2}). \tag{16}$$

Indeed, the above result holds for any two distributions from a family of real, elliptically contoured distributions having finite second-order moments and with density function of the form

$$p(x; \mu, A) = (\text{const}) \times f((x-\mu)^* A(x-\mu)), \tag{17}$$

where $f$ is a non-negative function on the positive real axis such that $0 < \int_0^\infty r^{n/2-1} f(r)\, dr < \infty$, and $A$ is a positive-definite, symmetric matrix. In particular, by taking

$$\begin{aligned} f(u) &= \text{const}, \qquad && 0 \leqslant u \leqslant c \\ &= 0 && \text{elsewhere,} \end{aligned} \tag{18}$$

we see that Eq. (16) also determines the Fréchet distance between uniform distributions on two ellipsoids centered at $\mu_X$, $\mu_Y$ and having covariance matrices $\Sigma_X$, $\Sigma_Y$. (This implies that the ellipsoids have the same shape and orientation as the principal ellipsoids of $\Sigma_X$, $\Sigma_Y$.) It is worth emphasizing that for non-singular $\Sigma_X$ the minimizing transformation (8) between $X$ and $Y$ is (a) linear and (b) Hermitian. This latter property has the interpretation that the transformation is a pure strain and does not involve a rotation. This non-rotational property holds in a certain sense even if $F$ and $G$ have arbitrary continuous density functions in $R^n$ provided that the minimum of $E|X-Y|^2$ is achieved by a differentiable transformation between $X$ and $Y$. By consideration of nearly uniform distributions over small ellipsoids, one may show the non-rotational property of the minimizing transformation to hold locally. This result can also be proved by a standard calculus of variations argument in which $E|X-Y|^2$ is minimized subject to the constraint that the Jacobian $\partial(y)/\partial(x)$ satisfies the equation

$$\frac{\partial(y)}{\partial(x)} = \frac{p_X(x)}{p_Y(y)} \tag{19}$$

where $p_X(x)$, $p_Y(y)$ are the given density functions of the vectors $X$ and $Y$, respectively.

## 4. Two Trace Inequalities for Real Covariance Matrices

The result

$$\min_{X,Y} E\,|X-Y|^2 = \operatorname{tr}[\Sigma_X + \Sigma_Y - 2(\Sigma_X\Sigma_Y)^{1/2}] \tag{20}$$

when $X$, $Y$ have zero means and covariance matrices $\Sigma_X$, $\Sigma_Y$ has two simple consequences, First,

$$\operatorname{tr}(\Sigma_X\Sigma_Y)^{1/2} \leqslant \operatorname{tr}\left(\frac{\Sigma_X+\Sigma_Y}{2}\right) \tag{21}$$

with equality iff $\Sigma_X = \Sigma_Y$. This well-known result is a generalisation of the fact that the geometric mean of two positive numbers is less than or equal to the arithmetic mean. Second, by replacing $Y$ in (20) by $tY$ where $t$ is any complex number we see that

$$\min_{X,Y} E\,|X-tY|^2 = (\operatorname{tr}\Sigma_Y)\,|t|^2 - 2\operatorname{tr}(\Sigma_X\Sigma_Y)^{1/2}\cdot|t| + \operatorname{tr}\Sigma_X \geqslant 0$$

which implies

$$\operatorname{tr}(\Sigma_X\Sigma_Y)^{1/2} \leqslant [\operatorname{tr}\Sigma_X\cdot\operatorname{tr}\Sigma_Y]^{1/2} \tag{22}$$

where equality holds iff $\Sigma_X = |t|^2\,\Sigma_Y$ for some complex scalar $t$. Inequality (22) is a generalisation of the Schwarz inequality. The quantity

$$\rho = \operatorname{tr}(\Sigma_X\Sigma_Y)^{1/2}\,[\operatorname{tr}\Sigma_X\cdot\operatorname{tr}\Sigma_Y]^{-1/2} \tag{23}$$

is the largest correlation coefficient possible between two random vectors $X$, $Y$ having prescribed covariance matrices $\Sigma_X$, $\Sigma_Y$.

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