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ERRATA

In the paper "The Theory and Practice of Distance Geometry', T. F. Havel, I. D. Kuntz and B. Crippen, *Bulletin of Mathematical Biology,* 1983, **45**, 665-720, the following corrections should be made:

Line 4 of p. 672 the expression should read:

$$\tfrac{1}{2}(\mathbf{x}_i \cdot \mathbf{x}_i + \mathbf{x}_j \cdot \mathbf{x}_j + d^2(\mathbf{x}_i, \mathbf{x}_j))$$

equation (2.11) on p. 686 should read:

$$l_{k'm'} - u_{ik'} - u_{jm'} < l_{k'n} - u_{m'n} - u_{ik'} - u_{jm'}.$$

The caption to Figure 6 on p. 693 should read:

How to decide if the triangle inequality is limiting.

Upper triangle limits, left; lower triangle limits, right.

Statement 10 and the preceding comment in Procedure for Algorithm 2.3 on p. 694 should read:

comment: in this case all four points are colinear.

10. **if** DLB(p_1, p_2) $\leqslant$ | DUB(p_0, p_1) $-$ DUB(p_0, p_2) | $\leqslant$ DUB(p_1, p_2) **then**

Equation (3.5) pp. 703–704 should read:

$$\begin{aligned}
\langle \mathbf{A}, \mathbf{B} \rangle &= Tr(\mathbf{A}^T \ \mathbf{B}) = Tr(\mathbf{A} \ \mathbf{B}) \text{ by symmetry} \\
&= Tr(\mathbf{U}^T \Gamma \mathbf{U} \mathbf{V}^T \Omega \mathbf{V}) \\
&= Tr\left[\left\{\sum_k \left(\sum_l u_{li}\gamma_l u_{lk}\right)\left(\sum_m v_{mk}\omega_k v_{mj}\right)\right\}\right] \\
&= Tr\left[\left\{\sum_{l,m} \gamma_l \omega_m u_{li} v_{mj} \sum_k u_{lk} v_{mk}\right\}\right] \\
&= \sum_{l,m} \gamma_l \omega_m (\mathbf{u}_l \cdot \mathbf{v}_m)^2 \\
&\leqslant \sum_n \gamma_n \omega_{\pi(n)}
\end{aligned}$$

for some permutation π of the indices $\{1, \ldots, N\}$, where $\mathbf{u}_l$ and $\mathbf{v}_m$ are the eigenvectors of **A** and **B**, respectively.

The second line of equation (3.10) on p. 705 should read:

$$= \frac{1}{2N^2} \sum_{j=2}^{N} \sum_{k=2}^{N} d_{1j}^2 + d_{1k}^2 - d_{jk}^2.$$

The line following equation (3.14) on p. 711 should read:

which has eigenvalues 0 and $12 d_{01}^{-4}$ on the half-planes $x_0 > x_1$ and $x_0 < x_1$.

On p. 711, the expression in the second line of the second paragraph should read:

$$d_{01}^{-6}[6(x_0 - x_1)^2 + 2(y_0 - y_1)^2].$$