The problem is now to find a symmetric matrix L of Lagrange multipliers such that U is orthogonal. If both sides of (9) are multiplied by their transposed matrices, the unknown orthogonal matrix U can be eliminated:

$$\mathsf{U}(\widetilde{\mathsf{S}+\mathsf{L}})\mathsf{U}(\mathsf{S}+\mathsf{L})=(\widetilde{\mathsf{S}+\mathsf{L}})\tilde{\mathsf{U}}\mathsf{U}(\mathsf{S}+\mathsf{L})$$
$$=(\mathsf{S}+\mathsf{L})\,(\mathsf{S}+\mathsf{L})=\tilde{\mathsf{R}}\mathsf{R}\,. \quad (10)$$

Since $\tilde{\mathsf{R}}\mathsf{R}$ is a symmetric positive definite matrix the positive eigenvalues μ_k and the corresponding eigenvectors $\mathbf{a}_k$ can be found by well established procedures. Since $\mathsf{S}+\mathsf{L}$ is symmetric and positive definite also, it is evident from (10) that it must have the same normalized eigenvectors $\mathbf{a}_k$ and the positive eigenvalues $\sqrt{\mu_k}$.

It can be easily verified that the Lagrange multipliers are then

$$l_{ij}=\sum_k \sqrt{\mu_k} \qquad a_{ki}a_{kj}-s_{ij} \quad (11)$$

where a_{ki} denotes the ith component of $\mathbf{a}_k$. The effect of the orthogonal matrix U on these eigenvectors $\mathbf{a}_k$ is determined from (9) and defines unit vectors $\mathbf{b}_k$ as

$$\mathbf{b}_k=\mathsf{U}\,.\,\mathbf{a}_k=\frac{1}{\sqrt{\mu_k}}\,\mathsf{U}(\mathsf{S}+\mathsf{L})\mathbf{a}_k=\frac{1}{\sqrt{\mu_k}}\,\mathsf{R}\mathbf{a}_k\,. \quad (12)$$

The orthogonal matrix U is finally constructed as

$$u_{ij}=\sum_k b_{ki}a_{kj} \quad (13)$$

and the problem to find the constraint minimum of the function E is solved.

Sometimes it may happen that all of the vectors $\mathbf{x}_n$ or $\mathbf{y}_n$ lie in a plane. Then one of the eigenvalues of $\tilde{\mathsf{R}}\mathsf{R}$, *e.g.* μ_3, will be zero. In this case a complete set of vectors $\mathbf{a}_k, \mathbf{b}_k$ is constructed by setting

$$\mathbf{a}_3=\mathbf{a}_1\times\mathbf{a}_2 \qquad \mathbf{b}_3=\mathbf{b}_1\times\mathbf{b}_2\,. \quad (14)$$

Note that the procedure described in this article can be easily extended to vector spaces of higher dimensions.

It is possible also to replace the constraints of equation (2) by the more general constraints

$$\tilde{\mathsf{U}}\mathsf{U}=\mathsf{M}\,, \quad (15)$$

where M is a symmetric and positive definite matrix. If B is any specific solution of (15), it is easy to prove that all possible other solutions U of that equation can be written as

$$\mathsf{U}=\mathsf{V}\,.\,\mathsf{B} \quad (16)$$

with an orthogonal matrix V. If the initial vector set $\mathbf{x}_n$ is transformed into $\mathbf{x}'_n=\mathsf{B}\mathbf{x}_n$ then this problem is reduced to minimizing $E'=\frac{1}{2}\sum_n w_n(\mathsf{V}\mathbf{x}'_n-\mathbf{y}_n)^2$ with the constraint $\tilde{\mathsf{V}}\mathsf{V}=1$.

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A comment on the close-packing of hyperspheres.

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The packing of hyperspheres in more than three dimensions is discussed.

Lifchitz (1976) has drawn attention to a type of lattice packing for hyperspheres in which there is one hypersphere per unit cell (at the origin) and where the unit cell has a metric matrix in which the diagonal elements are 1 and all other elements are $\frac{1}{2}$. This matrix can be factorized into an upper triangular matrix and its transpose to obtain the orthonormal coordinates as required.

This packing is, however, except for dimensions 1, 2 and 3, by no means the closest packing of hyperspheres. The general solution remains unknown but the packing fraction for four-dimensional close-packing is $\pi^2/16=0{\cdot}61685$ and corresponds to a hypercubic cell centred at $(\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2})$ with 24 contacts per sphere. This is denser than the type of packing described by Lifchitz, which for four dimensions gives the value $\pi^2/(8\times5^{1/2})=0{\cdot}55173$ for the packing fraction and 20 contacts per sphere. Leech (1964) has given a table of what, up to that date, were believed to be the closest packings in up to 12 dimensions. The packing fraction for 12 dimensions exceeded by a factor of more than 8 that for the Lifchitz type of packing, and there are 756 contacts per hypersphere as compared with 156.

The French words 'assemblage compact' might thus be better translated as 'close-ish packing' rather than as 'close-packing'.

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