On determination of *T* matrix in TLS modelling

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1. Introduction

Uncertainty in an atomic position is characterised, in a harmonic approximation, by a quadratic function of the vector of atomic displacement. In mathematics, such a scalar function of a vector is called quadratic form. In a chosen coordinate system, each vector is presented by a vector-column $\mathbf{u}$ of its coordinates and a quadratic form is characterised by a quadratic symmetric matrix U. When moving from one coordinate system to another, a matrix of a quadratic form changes following the rule

$$U_{new} = Q^t U Q \qquad (1.1)$$

where Q is the matrix of transition to the new basis and Q^t stands for transposed matrix Q. To obtain Q, one expresses the vectors of the new basis in the initial basis and takes corresponding coefficients as columns of Q.

By definition, matrices of quadratic forms describing atomic uncertainties are positively definite, or, in singular cases, positive semidefinite. We remind that a quadratic matrix U is positive definite if for any vector $\mathbf{u}$ the scalar product $(\mathbf{u},U\mathbf{u})>0$; in the text below we shall note this as $U>0$. For a positive semidefinite (alias non-negatively definite) matrix U such that $(\mathbf{u},U\mathbf{u}) \geq 0$ for any $\mathbf{u}$ we shall use notation $U \geq 0$.

TLS modelling is an efficient way to treat uncertainties in atomic positions in X-ray crystallography considering an atomic group displacing as a rigid body (to simplify the presentation, in what follows we consider a model composed from a single rigid group). In such a model an uncertainty of each atom m=1, …n is described by a quadratic form whose matrix $U_{TLS,m}$ is a sum of three components (Schomaker & Trueblood, 1968)

$$U_{TLS,m} = T + A_m L A_m^t + (A_m S + S^t A_m^t) \qquad (1.2)$$

Here T stands for the common component due to a translation (vibration) of the group as a rigid body, and two other terms,

$$U_{LS,m} = A_m L A_m^t + (A_m S + S^t A_m^t) \qquad (1.3)$$

different for different atoms, describe uncertainties due to rigid body libration. Of course, the total uncertainty of atom m may have a contribution from other sources

$$U_m = U_{TLS,m} + U_{add,m} \qquad (1.4)$$

that we do not discuss here. By the definition, U_m, $U_{TLS,m}$, T, $U_{LS,m}$, $U_{add,m}$ are positive semidefinite.

A knowledge of matrices T, L and S allows calculating $U_{TLS,m}$ for each atom of the group. The inverse problem of finding T, L and S arises when one analyses the collective vibration of molecular fragments given the set of individual U_m. This problem is commonly solved by least-squares fit

$$\sum_{m=1}^{n} \sum_{j,k=1,3} \left(U_{TLS,m}^{(jk)}(T,L,S) - U_m^{(jk)} \right)^2 \to \min_{t,l,s} \qquad (1.5)$$

where variables are independent elements $t^{(j,k)}$, $l^{(j,k)}$, $s^{(j,k)}$ of T, L and S (20 elements per each rigid group; Schomaker & Trueblood, 1968). As a rule, refinement starts from zero values that means that initially all atomic uncertainties supposed to be individual with no common terms. When the model is composed from several rigid groups, (1.5) includes also a sum over the groups.

In fact this approach is not good since by minimising (1.5) we are looking for $U_{TLS,m}$ that are 'in average equal to U_m' (sometimes 'smaller', sometimes 'larger') and the difference U_m-$U_{TLS,m}$ (commonly referenced as a local or residual B-factor) is not guaranteed to be positive definite as it must be.

Below we propose an algorithm to directly estimate the matrix T starting from a set of U_m and without involving a least-squares fit (1.5). This algorithm is accompanied by comments making it more understandable for a reader not very familiar with linear algebra. In what follows, capital italic (M) stand for matrices of quadratic forms and small italic greeks (μ) stand for their eigenvalues. Small bold ($\mathbf{u}$) stand for vector-columns composed from three vector coordinates in the chosen basis.

2. Determination of a common component for isotropic and anisotropic cases

2.1. Problem and definitions

Let U_m, m=1, …n, be symmetric 3×3 matrices representing positive definite forms $\mathbf{U}_m$ in some previously chosen *orthonormal* basis common for all of them. We want to present all U_m as

$$U_m = U_{res,m} + T_{max} \qquad (2.1)$$

where T_{max} is a positive definite matrix such that all residual $U_{res,m}$ are positive semidefinite and that for any positive semidefinite matrix subtracting it from the set of residual $U_{res,m}$ breaks this condition of non-negativity at least for one of them. In what follows we shall call such a matrix T_{max} 'maximal'.

2.2. Isotropic models

In the case of an isotropic model, all U_m are proportional to the unit matrix,

$$U_m = \begin{pmatrix} u_m & 0 & 0 \\ 0 & u_m & 0 \\ 0 & 0 & u_m \end{pmatrix} = u_m \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = u_m I \quad , u_m>0 \, , m=1, \ldots n. \qquad (2.2)$$

Matrix T is also diagonal, and L and S are zero.

For isotropic models the solution T_{max} is unique and presented by the matrix $T_{max}= t_{max}I$ with the element

$$t_{\max} = \min_{m=1,\ldots,n} \{u_m\} \tag{2.3}$$

everywhere at its diagonal. Obviously, if we are back from the purely algebraic problem formulated in 2.1 to the original crystallographic one, (2.2-2.3) is equivalent to a search for the minimal value of the isotropic *B* factor for the group of atoms.

2.3. Anisotropic models

When working with anisotropic atomic displacement, that is the case of TLS modelling, the matrices U_m are no more diagonal and the solution is no more unique (in fact, one may show that it is not unique even in the case of matrices in two-dimensional space) and imposing different extra conditions leads to different solution.

In our algorithm we replace a simultaneous search of the maximal matrix T_{max} for all matrices by a consecutive search for two matrices at a time. To do so, we find first the maximal matrix $T_{1\text{-}2}$, say, for U_1 and U_2. We apply then the same procedure for $T_{1\text{-}2}$ and U_3 getting $T_{1\text{-}3}$, etc., finishing with $T_{max}=T_{1\text{-}n}$. Determination of the maximal matrix T_{max} for two matrices is done using the algorithm described below.

3. Determination of a maximal matrix for two positive definite matrices – general case

3.1. General comments

Fig. 1 schematizes the search algorithm for the maximal matrix T_{max} for two positive definite quadratic 3×3 matrices. More formally, let $M>0$ and $N>0$ be two positive definite matrices presenting in some Cartesian coordinate system two quadratic forms $\mathbf{M}$ and $\mathbf{N}$. We search for a matrix $T_{max}>0$ such that $M\text{-}T_{max}\geq 0$, $N\text{-}T_{max}\geq 0$, and for any other matrix $\widetilde{T}\geq 0$ at least one of two conditions $M\text{-}T_{max}\text{-}\widetilde{T}\geq 0$, $N\text{-}T_{max}\text{-}\widetilde{T}\geq 0$ is broken. The text below illustrates and comments the scheme. Numbers in parentheses at the beginning of paragraph corresponds to the numbers in yellow rectangulars at the scheme.

Let $\tau_1 \geq \tau_2 \geq \tau_3 > 0$ stand for the eigenvalues of T_{max}. As we mentioned above, an extra condition should be imposed to define which of possible maximal T_{max} we are looking for. Let's choose T_{max} such that its minimal eigenvalue is as large as possible, $\tau_3 \to \max$, and then from all possible matrices with this τ_3 to choose the one for which its second eigenvalue is also maximal, $\tau_2 \to \max$.

It is easy to show (see Appendix B, P1) that each $T_{max}>0$ may be presented as a sum

$$T_{max} = T_3 + T_{res} \tag{3.1}$$

where $T_3>0$ has equal positive eigenvalues (and is diagonal in any orthonormal basis, Appendix B, P2) and $T_{res}\geq 0$ has at least one eigenvalue equal to 0. In its turn, T_{res} also can be presented as a sum

$$T_{res} = T_2 + T_1 \tag{3.2}$$

where $T_2\geq 0$ has two equal positive and one zero eigenvalues, and $T_1\geq 0$ has one positive and two zero eigenvalues (in a singular situation any of T_2 and T_1 may be absent). By this reason, we search for T_{max} presenting it as

$$T_{max} = T_3 + T_2 + T_1 \tag{3.3}$$

with the properties indicated above.

3.2. Initialisation and search for the maximal matrix T_3 with three equal eigenvalues

(1) In what follows let $\mu_1 \geq \mu_2 \geq \mu_3 > 0$ and $\nu_1 \geq \nu_2 \geq \nu_3 > 0$ be eigenvalues of M and N, respectively, and $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$ and $\mathbf{g}_1$, $\mathbf{g}_2$, $\mathbf{g}_3$ be the corresponding normalised eigenvectors. Let's suppose also that the minimal eigenvalues of M are larger than those of N, that means $\mu_3 > \nu_3$; or if $\mu_3 = \nu_3$ then $\mu_2 > \nu_2$; finally if $\mu_3 = \nu_3$ and $\mu_2 = \nu_2$ then $\mu_1 > \nu_1$. Otherwise we simply exchange the name of the matrices.

(2) If $\mu_3 \geq \nu_1$ then the situation is singular, we directly get the final answer $T_{max} = N$ (see Appendix B, P3) and interrupt the procedure.

(3) In a non singular situation, $\mu_3 < \nu_1$,

$$T_3 = \begin{pmatrix} \nu_3 & 0 & 0 \\ 0 & \nu_3 & 0 \\ 0 & 0 & \nu_3 \end{pmatrix} \tag{3.4}$$

(see Appendix B, P4). Residual matrices are

$$\widetilde{M} = M - T_3 \,, \quad \widetilde{N} = N - T_3 \tag{3.5}$$

respectively. Note that their eigenvectors are the same as for M and N and that for the eigenvector $\mathbf{g}_3$ corresponding to ν_3 we have a condition

$$\widetilde{N}\mathbf{g}_3 = (N - T_3)\mathbf{g}_3 = \nu_3\mathbf{g}_3 - \nu_3\mathbf{g}_3 = 0 \tag{3.6}$$

Eigenvalues of the new matrices $\widetilde{M}$ and $\widetilde{N}$ are

$$\widetilde{\mu}_1 = \mu_1 - \nu_3 \geq \widetilde{\mu}_2 = \mu_2 - \nu_3 \geq \widetilde{\mu}_3 = \mu_3 - \nu_3 \geq 0 \text{ and } \widetilde{\nu}_1 = \nu_1 - \nu_3 \geq \widetilde{\nu}_2 = \nu_2 - \nu_3 \geq \widetilde{\nu}_3 = 0, \tag{3.7}$$

It follows from (3.6) that $T_{res}\mathbf{g}_3 = 0$ (Appendix B, P5) meaning that $\mathbf{g}_3$ defines a one-dimensional subspace in which no more common displacement described by M and N may be found.

3.3. Additional maximal degenerate matrix

The matrix T_{res} that should be added to T_3 has at least one of its eigenvalues equal to zero and is no more positive but only non-negative definite. We want to exclude from further analysis the direction $\mathbf{g}_3$, following the notes of step (3).

In this Section we consider only a general situation when $\widetilde{\mu}_1 \geq \widetilde{\mu}_2 \geq \widetilde{\mu}_3 > 0$ and $\widetilde{\nu}_1 \geq \widetilde{\nu}_2 > \widetilde{\nu}_3 = 0$. All other situations, considered as singular, are studied separately in Section 4.

(4) We change the basis in which the matrices are given. The vectors of the new basis are eigenvectors of N (and those of $\widetilde{N}$), $\mathbf{g}_1$, $\mathbf{g}_2$, $\mathbf{g}_3$. This basis is orthogonal,

by the properties of eigenvectors, and normal, by the initial choice. The residual matrices of the quadratic forms in the new basis are given by

$$M_G = G^t \widetilde{M} G \,,\; N_G = G^t \widetilde{N} G \tag{3.8}$$

In the new basis, N_G is diagonal,

$$N_G = \begin{pmatrix} \widetilde{\nu}_1 & 0 & 0 \\ 0 & \widetilde{\nu}_2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{3.9}$$

The latter presentation means that in this basis any matrix $T \geq 0$, such that $N_G - T \geq 0$, has zero in the right column and the bottom line (see Appendix B, P6-P7). In particular, this is true for T_{res}.

3.4. Additional single degenerate maximal matrix T_2

The fact that $T_{res} \geq 0$ has $\mathbf{g}_3$ as its eigenvector corresponding to $\widetilde{\tau}_3 = 0$ means that in the basis of its own eigenvectors $\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3 = \mathbf{g}_3$ this matrix is presented as a diagonal one

$$T_{res} = \begin{pmatrix} \widetilde{\tau}_1 & 0 & 0 \\ 0 & \widetilde{\tau}_2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{3.10}$$

with $\widetilde{\tau}_1 \geq \widetilde{\tau}_2 \geq 0$. An analysis similar to the previous one leads to the conclusion that in this basis

$$T_2 = \begin{pmatrix} \widetilde{\tau}_2 & 0 & 0 \\ 0 & \widetilde{\tau}_2 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \; T_1 = \begin{pmatrix} \widetilde{\tau}_1 - \widetilde{\tau}_2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{3.11}$$

One may note that T_2 has exactly the same form in any orthonormal basis with the third vector equal to $\mathbf{g}_3$, in particular, in the basis of vector $\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3$ (demonstration similar to P2 in Appendix B). Therefore we need to search for the matrix in the form

$$T_2 = \begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{3.12}$$

where $a \geq 0$ is as large as possible such that $M_G - T_2 \geq 0$ and $N_G - T_2 \geq 0$.

(5a) Condition $N_G - T_2 \geq 0$ gives, similarly to the previous analysis, $t \leq \widetilde{\nu}_2$. Condition $M_G - T_2 \geq 0$ in a non-singular case may be expressed using the function $\alpha(M_G)$ defined in Appendix A. Summarising,

$$a = \min\{\alpha(\widetilde{M}_G), \widetilde{\nu}_2\} \tag{3.13}$$

After matrix T_2 is defined, new residual matrices are calculated as

$$\widetilde{M}_G = M_G - T_2 \,,\; \widetilde{N}_G = N_G - T_2 \tag{3.14}$$

3.5. Additional double degenerate maximal matrix T_1

(6a) In (3.13) we consider as a general situation the case when $a = \alpha(\widetilde{M}_G)$. This means that each of two matrices $\widetilde{M}_G$ and $\widetilde{N}_G$ has at least one zero eigenvalue and the corresponding eigenvectors $\widetilde{\mathbf{e}}_3$ ($\widetilde{M}_G\widetilde{\mathbf{e}}_3=0$) and $\mathbf{g}_3$ ($\widetilde{N}_G\mathbf{g}_3=0$) are non collinear (if they were collinear, then $\widetilde{\mathbf{e}}_3=\lambda\mathbf{g}_3$, $\widetilde{M}_G\mathbf{g}_3=0$ that would mean $(M_G-T_2)\mathbf{g}_3 = M_G\mathbf{g}_3 - T_2\mathbf{g}_3 = M_G\mathbf{g}_3 =0$ contradicting the condition $\widetilde{\mu}_3>0$). The maximal matrix T_1 has both $\widetilde{\mathbf{e}}_3$, $\mathbf{g}_3$ and any their linear combination as its eigenvectors corresponding to zero eigenvalue (see Appendix B, P8).

We change once more the basis. Similarly to step (4), Section 3.3, the vectors of the new basis are defined as

$$\mathbf{p}_3=\mathbf{g}_3,\ \mathbf{p}_2=[\ \widetilde{\mathbf{e}}_3-(\widetilde{\mathbf{e}}_3,\mathbf{p}_3)\mathbf{p}_3\ ]\cdot\|\widetilde{\mathbf{e}}_3-(\widetilde{\mathbf{e}}_3,\mathbf{q}_3)\mathbf{q}_3\|^{-1},\ \mathbf{p}_1=\mathbf{p}_2\wedge\mathbf{p}_3 \qquad (3.15)$$

Here $\mathbf{u}\wedge\mathbf{v}$ stands a vector product of $\mathbf{u}$ and $\mathbf{v}$ and $\|\mathbf{u}\|$ stands for the module of the vector $\mathbf{u}$, which in the orthonormal basis can be calculated by the Pythagor theorem. This new basis is orthonormal. The property that $T_1\mathbf{p}_3=T_1\mathbf{p}_2=T_2\mathbf{p}_3=0$ proves that indeed $\{\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3\}$ is the basis of eigenvectors of T_{res} considered above in (3.11).

(7a) We build the matrix P of transition to the new basis. This matrix is composed in columns from the coordinates of the vectors $\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3$ in the previous basis $\{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3\}$

$$M_P = P^t\widetilde{M}_G P\ ,\ N_P = P^t\widetilde{N}_G P \qquad (3.16)$$

In the new basis, T_1 is searched in form

$$T_1=\begin{pmatrix} b & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0\end{pmatrix} \qquad (3.17)$$

(8) The value of *b* for the maximal T_1 to be subtracted from M_P and N_P can be calculated using the function β defined in Appendix A:

$$b = \min\{\beta(M_P), \beta(N_P)\} \qquad (3.18)$$

4. Maximal matrix for two positive semidefinite matrices: singular cases

The analysis in Section 3 does not consider singular situations. These cases are studied below completing the algorithm

(5b-7b) After step (3) $\widetilde{N}$ is a double degenerate matrix, $\widetilde{\nu}_2=\widetilde{\nu}_3=0$. Then T_2 is a zero matrix and T_1 may be searched for as (3.17-3.18) directly in the basis $\{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3\}$ of the eigenvectors of N.

(5c-6b-7b) After step (3) $\widetilde{\nu}_2>0$ and $\widetilde{M}$ is a degenerate matrix, $\widetilde{\mu}_3=0$, with the same eigenvector $\mathbf{g}_3$ ($\mathbf{e}_3=\mathbf{g}_3$). Both M_G and N_G have 0 in the right column and the bottom line, and the problem is reduced to a two-dimensional. Condition $\widetilde{\mu}_3=0$ means that

$\mu_3=\nu_3$ and then by the initial choice, $\tilde{\mu}_2 \geq \tilde{\nu}_2>0$. Then in (3.12-3.13) the value of a for T_2 becomes

$$a = \tilde{\nu}_2 \tag{4.1}$$

and we can search for T_1 as (3.17-3.18) directly in the basis $\{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3\}$.

(5d-7a) After step (3) $\tilde{\nu}_2>0$ and $\tilde{M}$ is a degenerate matrix, $\tilde{\mu}_3=0$, with the eigenvector $\mathbf{e}_3 \neq \mathbf{g}_3$. This condition may be formally expressed, for example, by $(\mathbf{g}_3, \tilde{M}\mathbf{g}_3)>0$. Condition $\tilde{\mu}_3=0$ means that $\mu_3=\nu_3$ and then by the initial choice, $\tilde{\mu}_2 \geq \tilde{\nu}_2>0$. The situation is absolutely similar to the case (6a) except that here the zero-value eigenvector is computed for the initial matrix M (the same eigenvectors as for $\tilde{M}$) and not for the updated one, $\tilde{M}_G$, as in (6a). Therefore, we change the basis to

$$\mathbf{p}_3 = \mathbf{g}_3 \,,\ \mathbf{p}_2 = [\mathbf{e}_3 - (\mathbf{e}_3, \mathbf{p}_3)\mathbf{p}_3] \cdot \|\mathbf{e}_3 - (\mathbf{e}_3, \mathbf{p}_3)\mathbf{p}_3\|^{-1} \,,\ \mathbf{p}_1 = \mathbf{p}_2 \wedge \mathbf{p}_3 \tag{4.2}$$

define T_2 as zero matrix and search for T_1 as (3.17-3.18) directly in the new basis.

(6b) If in (3.12-3.13) the value of $a = \tilde{\nu}_2$, then T_1 may be searched for as (3.17-3.18) directly in the basis $\{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3\}$ of the eigenvectors of N. Also immediately

$$\beta(N_P) = \tilde{\nu}_1 - \tilde{\nu}_2 \,. \tag{4.3}$$

5. Algorithm termination and concluding remarks

(9) Finally, collecting T_1, T_2 and T_3 together in the initial coordinate system gives

$$T_{max} = T_3 + G(T_2 + PT_1P^t)G^t \tag{5.1}$$

where in some cases either G or P may be unitary matrices and either T_2 or T_1 be zero matrices.

This algorithm was realised in the frame of the program complex *PHENIX* (Adams *et al*., 2002; *www.phenix-online.org*) and extensively tested.

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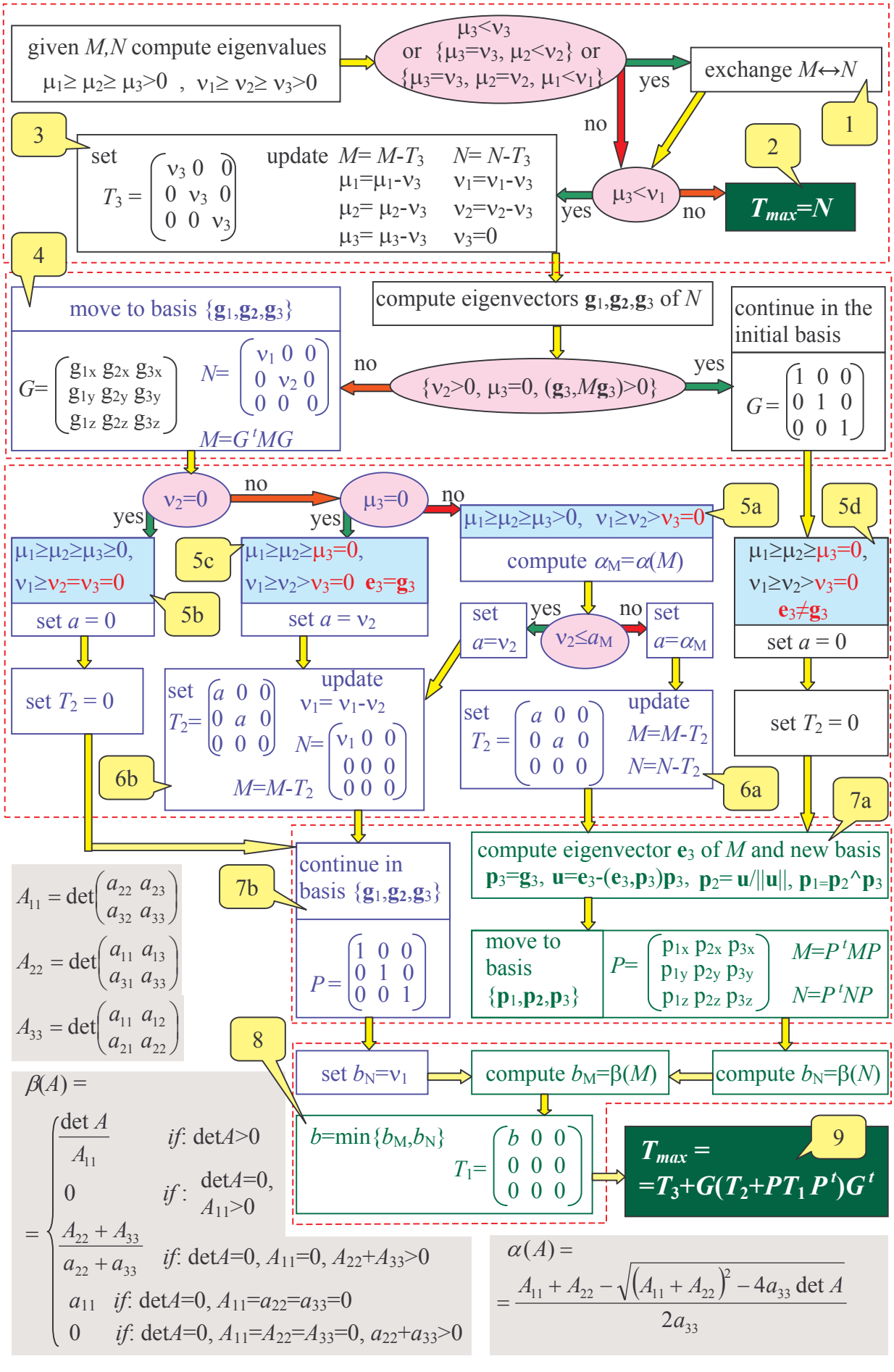
Fig. 1. Scheme of the determination of the maximal matrix T_{max} for two positive definite 3×3 matrices M and N. Different colours (black, blue, green) of rectangulars correspond to different bases. Ping ellipses indicate the conditions, and light blue highlights the condition with which corresponding rectangular can be reached. Grey rectangular show the formula to calculate the functions α and β. Red broken contours indicate the principals steps of the procedure: initialisation, search for T_3, change of the basis, search for T_2, second change of the basis, search for T_1 and final computing of T_{max}. Numbers in yellow rectangulars correspond to the numbers of the steps in the text.


given M,N compute eigenvalues
μ1≥ μ2≥ μ3>0 , ν1≥ ν2≥ ν3>0
μ3<ν3 or {μ3=ν3, μ2<ν2} or {μ3=ν3, μ2=ν2, μ1<ν1}
yes
exchange M↔N
1
no
2
μ3<ν1
yes
no
Tmax=N
3
set T3 = ν3 0 0 / 0 ν3 0 / 0 0 ν3
update M= M-T3 N= N-T3
μ1=μ1-ν3 ν1=ν1-ν3
μ2= μ2-ν3 ν2=ν2-ν3
μ3= μ3-ν3 ν3=0
4
move to basis {g1,g2,g3}
G= g1x g2x g3x / g1y g2y g3y / g1z g2z g3z
N= ν1 0 0 / 0 ν2 0 / 0 0 0
M=G^tMG
compute eigenvectors g1,g2,g3 of N
{ν2>0, μ3=0, (g3,Mg3)>0}
no
yes
continue in the initial basis
G= 1 0 0 / 0 1 0 / 0 0 1
ν2=0
no
μ3=0
no
yes
yes
μ1≥μ2≥μ3>0, ν1≥ν2>ν3=0
5a
compute αM=α(M)
5d
μ1≥μ2≥μ3≥0, ν1≥ν2=ν3=0
5b
set a = 0
5c
μ1≥μ2≥μ3=0, ν1≥ν2>ν3=0 e3=g3
set a = ν2
set a=ν2
ν2≤aM
yes
no
set a=αM
μ1≥μ2≥μ3=0, ν1≥ν2>ν3=0 e3≠g3
set a = 0
set T2 = 0
set T2 = a 0 0 / 0 a 0 / 0 0 0
update ν1= ν1-ν2
N= ν1 0 0 / 0 0 0 / 0 0 0
M=M-T2
6b
set T2 = a 0 0 / 0 a 0 / 0 0 0
update M=M-T2 N=N-T2
6a
set T2 = 0
7a
compute eigenvector e3 of M and new basis
p3=g3, u=e3-(e3,p3)p3, p2= u/||u||, p1=p2^p3
7b
continue in basis {g1,g2,g3}
P= 1 0 0 / 0 1 0 / 0 0 1
move to basis {p1,p2,p3}
P= p1x p2x p3x / p1y p2y p3y / p1z p2z p3z
M=P^tMP
N=P^tNP
8
set bN=ν1
compute bM=β(M)
compute bN=β(N)
b=min{bM,bN}
T1= b 0 0 / 0 0 0 / 0 0 0
9
Tmax = =T3+G(T2+PT1P^t)G^t
A11 = det a22 a23 / a32 a33
A22 = det a11 a13 / a31 a33
A33 = det a11 a12 / a21 a22
β(A) = det A / A11 if: detA>0
0 if: detA=0, A11>0
(A22 + A33) / (a22 + a33) if: detA=0, A11=0, A22+A33>0
a11 if: detA=0, A11=a22=a33=0
0 if: detA=0, A11=A22=A33=0, a22+a33>0
α(A) = (A11 + A22 − √((A11 + A22)^2 − 4a33 det A)) / 2a33

Appendix A. Definition of $\alpha(A)$ and $\beta(A)$

For a given matrix $A \geq 0$ of dimension 3×3 with the elements a_{jk} we define two functions $\alpha(A)$ and $\beta(A)$ of its elements.

We define $\alpha(A)$ as a value such that $A\text{-}T(\alpha) \geq 0$ for $0 \leq \alpha \leq \alpha(A)$, where $T(\alpha) = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & 0 \end{pmatrix}$,

and for $\alpha > \alpha(A)$ this condition breaks. Let A_{jj} be determinants of its principal minors:

$$A_{11} = \det \begin{pmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{pmatrix},\ A_{22} = \det \begin{pmatrix} a_{11} & a_{13} \\ a_{31} & a_{33} \end{pmatrix},\ A_{33} = \det \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}. \tag{A.1}$$

Then for $A > 0$ this maximal value of α is given by

$$\alpha(A) = \frac{A_{11} + A_{22} - \sqrt{(A_{11} + A_{22})^2 - 4a_{33}\det A}}{2a_{33}} > 0 \tag{A.2}$$

(for a proof see Appendix B, P9).

We define $\beta(A)$ as a value such that $A\text{-}T(\beta) \geq 0$ for $0 \leq \beta \leq \beta(A)$, where $T(\beta) = \begin{pmatrix} \beta & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$,

and for $\beta > \beta(A)$ this condition breaks. This value is given by

a) $\beta(A) = \dfrac{\det A}{A_{11}} > 0$, if $\det A > 0$ (A.3)

b) $\beta(A) = 0$, if $\det A = 0$ and $A_{11} > 0$ (A.4)

c) $\beta(A) = \dfrac{A_{22} + A_{33}}{a_{22} + a_{33}} > 0$, if $\det A = 0$ and $A_{11} = 0$ and $A_{22} + A_{33} > 0$ (A.5)

d) $\beta(A) = a_{11} \geq 0$, if $\det A = 0$ and $A_{11} = a_{22} = a_{33} = 0$ (A.6)

e) $\beta(A) = 0$, if $\det A = 0$ and $A_{11} = A_{22} = A_{33} = 0$ and $a_{22} + a_{33} > 0$ (A.7)

(for a proof see Appendix B, P10).

Appendix B. Proofs of some propositions

P1. Presentation of T as $T = T_3 + T_2 + T_1$ (Section 3.1)

In the (orthonormal) basis of its own eigenvectors the matrix T is diagonal,

$$T = \begin{pmatrix} \tau_1 & 0 & 0 \\ 0 & \tau_2 & 0 \\ 0 & 0 & \tau_3 \end{pmatrix} \tag{B.1}$$

and can be decomposed into a sum

$$T = \begin{pmatrix} \tau_3 & 0 & 0 \\ 0 & \tau_3 & 0 \\ 0 & 0 & \tau_3 \end{pmatrix} + \begin{pmatrix} \tau_2 - \tau_3 & 0 & 0 \\ 0 & \tau_2 - \tau_3 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} \tau_1 - \tau_2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{B.2}$$

of one positive definite and two positive semidefined matrices, with 1 and 2 zero eigenvalues, respectively.

P2. Diagonal presentation of T_3 (Section 3.1)

In the *orthonormal* basis of its own eigenvectors the matrix T_3 is

$$T_3 = \begin{pmatrix} \tau_3 & 0 & 0 \\ 0 & \tau_3 & 0 \\ 0 & 0 & \tau_3 \end{pmatrix} = \tau_3 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \tau_3 I \qquad \text{(B.3)}$$

In any other *orthonormal* basis obtained with the transition matrix Q (a rotation or rotoinversion matrix) the matrix of T_3 is

$$T_{3,Q} = Q^t T_3 Q = Q^{-1} T_3 Q = Q^{-1} \tau_3 I Q = \tau_3 Q^{-1} Q = \tau_3 I \qquad \text{(B.4)}$$

P3. $T_{max} = N$ if $\mu_3 \geq \nu_1$ (Section 3.2)

Let $\mu_1 \geq \mu_2 \geq \mu_3 \geq \nu_1 \geq \nu_2 \geq \nu_3 > 0$. With the notation used, for any vector $\mathbf{u}$

$$(\mathbf{u},M\mathbf{u}) \geq \mu_3(\mathbf{u},\mathbf{u}) \,,\; \nu_1(\mathbf{u},\mathbf{u}) \geq (\mathbf{u},M\mathbf{u}) \geq \nu_3(\mathbf{u},\mathbf{u}) \,. \qquad \text{(B.5)}$$

Therefore,

$$(\mathbf{u},(M\text{-}N)\mathbf{u}) \geq (\mathbf{u},M\mathbf{u}) - (\mathbf{u},N\mathbf{u}) \geq (\mu_3\text{-}\nu_1)(\mathbf{u},\mathbf{u}) \geq 0. \qquad \text{(B.6)}$$

In other words, $M\text{-}N \geq 0$. It is clear that nothing more can be subtracted from the second matrix, that proves the proposition.

P4. $T_3 = \nu_3 I$ (Section 3.2).

$\mu_1 \geq \mu_2 \geq \mu_3 > 0,\; \nu_1 \geq \nu_2 \geq \nu_3 > 0, \mu_3 \geq \nu_3$. With the notation used, for any vector $\mathbf{u}$

$$(\mathbf{u},(M\text{-}\nu_3 I)\mathbf{u}) = (\mathbf{u},M\mathbf{u}) - \nu_3(\mathbf{u},\mathbf{u}) \geq (\mu_3\text{-}\nu_3)(\mathbf{u},\mathbf{u}) \geq 0 \,, \qquad \text{(B.7)}$$

$$(\mathbf{u},(N\text{-}\nu_3 I)\mathbf{u}) = (\mathbf{u},N\mathbf{u}) - \nu_3(\mathbf{u},\mathbf{u}) \geq (\nu_3\text{-}\nu_3)(\mathbf{u},\mathbf{u}) = 0 \,. \qquad \text{(B.8)}$$

At the same time, for any $\nu > \nu_3$ the matrix $N\text{-}\nu I$ is not positive semidefinite. For example, if $\mathbf{g}_3$ is eigenvector of N corresponding to ν_3 then

$$(\mathbf{g}_3,(N\text{-}\nu I)\mathbf{g}_3) = (\mathbf{g}_3,N\mathbf{g}_3\text{-}\nu\mathbf{g}_3) = (\nu_3\text{-}\nu)(\mathbf{g}_3,\mathbf{g}_3) < 0. \qquad \text{(B.9)}$$

P5. $T_{res}\mathbf{g}_3=0$ (Section 3.2).

If $N\geq 0$, $T\geq 0$, $N\text{-}T\geq 0$, and $N\mathbf{u} = 0$, then

$$0 \leq (\mathbf{u},(N\text{-}T)\mathbf{u}) = (\mathbf{u},\text{-}T\mathbf{u}) = \text{-}(\mathbf{u},T\mathbf{u}) \leq 0 \qquad \text{(B.10)}$$

that is possible only if $(\mathbf{u},T\mathbf{u})=0$. Since T is positive semidefinite with eigenvalues $\tau_1\geq\tau_2\geq\tau_3\geq 0$, presenting $\mathbf{u}$ by its coordinates u_1, u_2, u_3 in the basis of eigenvectors of T we obtain that $(\mathbf{u},T\mathbf{u}) = \tau_1 u_1^2 + \tau_2 u_2^2 + \tau_3 u_3^2 = 0$ that proves $T\mathbf{u}=0$.

P6. $a_{j3} = a_{3j} = 0$, $j=1,2,3$ if $A\geq 0$ with $a_{33} = 0$ (Section 3.3).

General theory tells that for a matrix $A\geq 0$ the determinants of the principal minors of A are non negative. For a matrix of dimension 3×3 with the elements $a_{jk} = a_{kj}$ this means that

$$A_{11}=\det\begin{pmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{pmatrix}\geq 0,\; A_{22}=\det\begin{pmatrix} a_{11} & a_{13} \\ a_{31} & a_{33} \end{pmatrix}\geq 0,\; A_{33}=\det\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}\geq 0, \qquad \text{(B.11)}$$

$$a_{11}\geq 0,\; a_{22}\geq 0,\; a_{33}\geq 0$$

If $a_{33}=0$ then $A_{11}\geq 0$ and $A_{22}\geq 0$ give immediately $a_{13}=a_{31}=a_{23}=a_{32}=0$. Similar results may be obtained for $a_{11}=0$ or $a_{22}=0$.

P7. $T\geq 0$ has 0 in the right column and bottom line if $N\geq 0$ has (Section 3.3).
Let n_{jk} and t_{jk} be the elements of $N\geq 0$ and $T\geq 0$, respectively. If $n_{33}=0$ the condition $N\text{-}T\geq 0$ leads to $n_{33}\text{-}t_{33}\geq 0$ (see P6) that with $t_{33}\geq 0$ gives $t_{33}=0$. Then by (P6)

$$t_{13}=t_{31}=t_{23}=t_{32}=0\ . \tag{B.12}$$

P8. $\tilde{\mathbf{e}}_3$ and $\mathbf{g}_3$ are two non collinear eigenvectors of T_1 (Section 3.5).
Let $M\geq 0$, $N\geq 0$, $T\geq 0$, $M\text{-}T\geq 0$, $N\text{-}T\geq 0$ and $M\mathbf{u}=0$, $N\mathbf{v}=0$. Then

$$\begin{aligned} 0 \leq (\mathbf{u},(M\text{-}T)\mathbf{u}) &= (\mathbf{u},M\mathbf{u}) - (\mathbf{u},T\mathbf{u}) = -(\mathbf{u},T\mathbf{u}) \leq 0 \\ 0 \leq (\mathbf{v},(N\text{-}T)\mathbf{v}) &= (\mathbf{v},N\mathbf{v}) - (\mathbf{v},T\mathbf{v}) = -(\mathbf{v},T\mathbf{v}) \leq 0 \end{aligned} \tag{B.13}$$

that is possible only if $(\mathbf{u},T\mathbf{u}) = (\mathbf{v},T\mathbf{v}) = 0$ and then $T\mathbf{u} = T\mathbf{v} = \mathbf{0}$ (as in P5). That means also that for any linear combination of $\mathbf{u}$ and $\mathbf{v}$ we have $T(\alpha\mathbf{u}+\beta\mathbf{v}) = \mathbf{0}$.

P9. Demonstration of the formula for $\alpha(A)$ (Appendix A).
Let $a_{jk}=a_{kj}$, $j,k=1,2,3$, be the elements of the matrix $A>0$. We define the matrix A_α

$$A_\alpha = A - \alpha\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = A - \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{B.14}$$

For $\alpha=0$ by definition $A_\alpha>0$. When $\alpha>>1$, two of diagonal elements of A_α are negative that is impossible for positive definite matrix. The question is to find minimal positive value of α such that the condition $A_\alpha>0$ breaks. This is equivalent to the condition when one of eigenvalues of A_α becomes equal to zero. A product of eigenvalues is equal to the determinant of A_α, *i.e.*

$$\det A_\alpha = \alpha^2 a_{33} - \alpha\left[A_{11} + A_{22}\right] + \det A = P_2(\alpha) \tag{B.15}$$

where A_{kk} are corresponding principal minors of A. By the properties of positive definite matrix, $a_{33}>0$, $A_{11}+A_{22}>0$, $\det A>0$. The quadratic equation $P_2(\alpha) = 0$ has two real roots

$$\frac{A_{11}+A_{22}\pm\sqrt{\left(A_{11}+A_{22}\right)^2-4a_{33}\det A}}{2a_{33}}>0 \tag{B.16}$$

and that taken with sign '-' is $\alpha(A)$. The presence of solutions, *i.e.* the fact that

$$\left(A_{11}+A_{22}\right)^2-4a_{33}\det A\geq 0 \tag{B.17}$$

may be justified, for example, by the same argument that for large α the matrix A_α is not positive definite (the condition $\det A_\alpha>0$ simply means that both eigenvalues are negative). Therefore, due to continuity of the problem there should be values of α when each of the eigenvalues becomes negative (in a singular situation, both at the same time).

It may be noted that, as it has been shown in the text, if $A\geq 0$ with one zero and two positive eigenvalues then $\alpha(A)$ is equal to the minimal positive eigenvalue; finally for $A\geq 0$ with two zero eignevalues $\alpha(A)=0$.

P10. Demonstration of the formula for $\beta(A)$ (Appendix A).

Let $a_{jk}=a_{kj}$, j,k=1,2,3, be the elements of the matrix $A\geq 0$. We define the matrix A_β

$$A_\beta = A - \beta\begin{pmatrix}1&0&0\\0&0&0\\0&0&0\end{pmatrix} = A - \begin{pmatrix}\beta&0&0\\0&0&0\\0&0&0\end{pmatrix} \tag{B.18}$$

For β=0 by definition $A_\beta\geq 0$. When $\beta>>1$, one of diagonal elements of A_β is negative that is impossible for positive semidefinite matrix. The question is to find minimal non-negative value of β such that the condition $A_\beta\geq 0$ breaks.

When $\det A>0$, this corresponds to the (positive) root of

$$\det A_\beta = -\beta A_{11} + \det A = P_1(\beta) = 0 \tag{B.19}$$

giving (A.3).

When $\det A=0$ (one zero eigenvalue exists already) a search for β with $\det A_\beta=0$ cannot be applied any more and we shall use the characteristic equation for the eigenvalues of A_β

$$\begin{aligned} &P_3(\lambda,\beta)= \\ &= -\lambda^3 +\lambda^2(a_{11}+a_{22}+a_{33}-\beta) -\lambda[A_{11}+A_{22}+A_{33}-\beta(a_{22}+a_{33})] +(\det A-\beta A_{11}) = \\ &\quad = -\lambda^3 +\lambda^2(a_{11}+a_{22}+a_{33}-\beta) -\lambda[A_{11}+A_{22}+A_{33}-\beta(a_{22}+a_{33})] -\beta A_{11} = 0 \end{aligned} \tag{B.20}$$

If $A_{11}>0$, for any $\beta>0$ we have $P_3(0,\beta)<0$ that necessary means an existence of a negative root of the characteristic equation, thus $\beta(A)=0$ as (A.4).

When $\det A=0$ and $A_{11}=0$, the characteristic polynomial becomes

$$\begin{aligned} &P_3(\lambda,\beta)= -\lambda^3 +\lambda^2(a_{11}+a_{22}+a_{33}-\beta) -\lambda[A_{22}+A_{33}-\beta(a_{22}+a_{33})] = \\ &\quad = -\lambda\ \{\lambda^2 -\lambda(a_{11}+a_{22}+a_{33}-\beta) +[A_{22}+A_{33}-\beta(a_{22}+a_{33})]\ \} = -\lambda\ Q_2(\lambda,\beta) \end{aligned} \tag{B.21}$$

Here

$$Q_2(0,\beta)= A_{22}+A_{33}-\beta(a_{22}+a_{33}),\ Q_2'(0,\beta) = -a_{11}-a_{22}-a_{33}+\beta \tag{B.22}$$

$$Q_2(0,0)= A_{22}+A_{33}\geq 0\ ,\ Q_2'(0,0) = -a_{11}-a_{22}-a_{33} < 0 \tag{B.23}$$

($Q_2'(0,0)=0$ only for zero matrix), that confirms non-negativity of A eigenvalues. If $Q_2(\lambda,\beta)=0$ has two positive roots for β=0 (corresponding condition $A_{22}+A_{33}>0$), then the smallest of them becomes equal to 0 for

$$\beta(A) = \frac{A_{22}+A_{33}}{a_{22}+a_{33}} \tag{B.24}$$

(here $a_{22}+a_{33}>0$, otherwise $a_{22}=a_{33}=0$ would give $a_{k2}=a_{2k}=a_{k3}=a_{3k}=0$ by (P6), and $A_{22}=A_{33}=0$). If A has a single positive root and two zeros (the corresponding condition $\det A=A_{11}=A_{22}=A_{33}=0$), then

$$P_3(\lambda,\beta)= -\lambda\ Q_2(\lambda,\beta)= -\lambda\ \{\lambda^2 -\lambda(a_{11}+a_{22}+a_{33}-\beta) -\beta(a_{22}+a_{33})]\ \} \tag{B.25}$$

If $a_{22}+a_{33}>0$ then $Q_2(0,\beta)<0$ for any $\beta>0$ indicating a negative root that proves (A.6). Finally, $\det A=A_{11}=0$ and $a_{22}=a_{33}=0$ gives (A.7) (as noted above, condition $A_{22}=A_{33}=0$ follows from $a_{22}=a_{33}=0$).