Improved Convergence Speed of Fully Symmetric Learning Rules for Principal Component Analysis

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Fully symmetric learning rules for principal component analysis can be derived from a novel objective function suggested in our previous work. We observed that these learning rules suffer from slow convergence for covariance matrices where some principal eigenvalues are close to each other. Here we describe a modified objective function with an additional term which mitigates this convergence problem. We show that the learning rule derived from the modified objective function inherits all fixed points from the original learning rule (but may introduce additional ones). Also the stability of the inherited fixed points remains unchanged. Only the steepness of the objective function is increased in some directions. Simulations confirm that the convergence speed can be noticeably improved, depending on the weight factor of the additional term.
1. Introduction

In our previous work (Möller, 2020), we derived several fully symmetric learning rules for principal component analysis (PCA), starting from a novel objective function (in this paper referred to as “original” objective function). We analyzed the fixed points of these learning rules and (indirectly via the objective function) their stability. We could show that the learning rules have stable, desired fixed points in the eigenvectors of the covariance matrix, but exhibit additional undesired fixed points; however, the latter are unstable. Preliminary simulations confirmed that the learning rules converge towards the desired fixed points, but also revealed a disadvantage: If some principal eigenvalues of the covariance matrix are close to each other, the learning rules operate close the undesired fixed points which noticeably slows down convergence.

In this continuation of our work, we introduce an additional term into our objective function which mitigates the convergence problem. We derive a learning rule from this modified objective function. We determine the fixed points of the learning rule and show that the modified learning rule shares the fixed points of the original one, but may introduce additional fixed points. Using the same indirect method as in our previous work, we study the stability at the shared fixed points and show that it is unchanged compared to the original objective function. Simulations confirm both the theoretical results and the improved convergence speed of the novel learning rule.

We recapitulate the notation in section 2 and our Lagrange-multiplier approach in section 3. The original objective function and the corresponding (“short”) learning rule are recapitulated in section 4 together with insights on the fixed-point structure which motivate the modifications introduced here. Section 5.1 introduces the modified objective function from which we derive a (“short”) learning rule in section 5.2. The fixed points of this modified learning rule are analyzed in section 5.3. The stability of the fixed points is analyzed indirectly from the modified objective function in section 5.4. Simulations are presented in section 6. The report ends with a discussion (section 7) and conclusions (section 8).

2. Notation

We use the same notation as in our previous work (Möller, 2020). Table 1 shows the names of widely used matrices. Column vector \( i \) of a matrix \( X \) is written as \( x_i \). Fixed-

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1In a fully symmetric learning rule, all units see the same input and perform exactly the same computations. Earlier symmetric learning rules required a distinct weight factor in each unit to ensure convergence to the principal eigenvectors and not just to the principal subspace.

2Our analysis focuses on the simplest (“short”) learning rule from our previous work, since our simulations show that the more complex (“long”) learning rules differ only marginally in their behavior, probably since terms coincide in the vicinity of the Stiefel manifold of the eigenvector estimates; see appendix A.
Table 1: Notation: matrices

| Symbol | Description |
|--------|-------------|
| C      | n × n covariance matrix |
| V      | n × n matrix of eigenvectors v_i (columns) of C |
| Λ      | n × n diagonal matrix of eigenvalues λ_i (distinct, descending) of C |
| W      | n × m matrix of principal eigenvector estimates w_i (columns) of C |
| A      | n × m projection of W onto the eigenvectors V |
| Q      | n × n orthogonal matrix: Q^T Q = QQ^T = I_n |
| B      | m × m matrix used to form the Lagrange multipliers |
| I_n    | n × n unit matrix |
| 0_{n,m} | n × m null matrix |

Table 2: Notation: operators

| Symbol | Description |
|--------|-------------|
| δ_{ij} | Kronecker’s delta |
| dg{X}  | diagonal matrix with diagonal elements from X |
| diag^n_i {x_i} | diagonal matrix with n diagonal elements x_i |
| blkdiag_{k=1}^k {X_l} | block-diagonal matrix with k blocks X_l |
| ||X||_F^2 = tr{X^T X} | squared Frobenius norm of X |

References to equations and lemmata from our previous work (Möller, 2020) are printed in bold font.

3. Lagrange-Multiplier Approach

We use the Lagrange-multiplier approach from our previous work (Möller, 2020). For a given objective function J, we write the extended objective function J^* as

\[ J^*(B, W) = J(W) + C(B, W) \]  (1)

where C is the constraint term which includes the matrix B (elements β_{jk}) which forms the Lagrange multipliers. We use the same symmetric construction for the Lagrange multipliers as in equation (39), here with Ω_j = 1 (i.e. operating on a Stiefel manifold):

\[ C(B, W) = \frac{1}{2} \sum_{j=1}^{m} \sum_{k=1}^{m} \frac{1}{2}(β_{jk} + β_{kj}) (w_j^T w_k - δ_{jk}) . \]  (2)
4. Original Objective Function

The original “novel” objective function from equation (23) is

\[ J(W) = \frac{1}{4} \sum_{j=1}^{m} (w_j^T C w_j)^2. \]  

(3)

We are interested in the local maxima of this function. From (3) we derived a fully symmetric learning rule “N2S”, either from our “short” form derivation (450) or from the canonical metric on the Stiefel manifold (486):

\[ \tau \dot{W} = CWD - WDW^T CW \]  

(4)

where \( \tau \) is a time constant and

\[ D = \frac{m}{j=1} \text{diag}\{w_j^T C w_j\}. \]  

(5)

The fixed-point structure of this equation is relatively complex. If all diagonal elements of \( D \) are pairwise different, we obtain the special solution (270)

\[ \bar{W} = VP \left( \begin{array}{c} I_m \\ 0 \end{array} \right) \]  

(6)

where \( P \) is an arbitrary \( n \times n \) permutation matrix. If some diagonal elements of \( D \) may coincide, we obtain the general solution for the fixed points

\[ \bar{W} = VP \left( \begin{array}{c} U^*^T P^* \\ 0 \end{array} \right). \]  

(7)

Here \( U^* \) is an orthogonal block-diagonal matrix (where the size of each block depends on the number of identical diagonal elements in \( D \)), and \( P^* \) another permutation matrix (which is chosen such that identical diagonal elements in \( D \) are contiguous in a rearranged matrix \( D^* \), see (249)).

To motivate our modified objective function below, we look at the term \( \bar{W}^T CW \). From equations (282) and (284) we know that, in the fixed points, we have

\[ \bar{W}^T CW = P^*^T \text{blkdiag}\left\{ U^*_l \hat{\Lambda}_l^* U^*_{l'}^T \right\} P^* \]  

(8)

under the constraint (295)

\[ \text{dg}\{U^*_l \hat{\Lambda}_l^* U^*_{l'}^T\} = d_{l'}^* I_l. \]  

(9)

Each diagonal matrix \( \hat{\Lambda}_l^* \) is a block of the upper-left \( m \times m \) part of a permuted version of the eigenvalue matrix \( \Lambda \).
It is not clear which matrices $U_i^*$ fulfill constraint (9). However, we can say that if the constraint is fulfilled and $U_i^*$ is not of size $1 \times 1$, the matrix $U_i^* \Lambda_i^* U_i^{*T}$ cannot be diagonal (Lemma 5). Therefore the block-diagonal matrix in (8) has non-zero off-diagonal elements. A permutation transformation of a matrix as in (8) permutes the positions of the diagonal elements (see (516)), which entails that off-diagonal elements remain at off-diagonal positions. Therefore $\tilde{W}^T C \tilde{W}$ from (8) has non-zero off-diagonal elements if we are at an undesired fixed point.

In contrast, if we look at the desired fixed points from (6), we see that $\tilde{W}^T C \tilde{W}$ is diagonal:

$$\tilde{W}^T C \tilde{W} = (I_m \ 0) \ P^T V^T C V P (I_m \ 0)$$

$$= (I_m \ 0) \ P^T \Lambda P (I_m \ 0)$$

$$= (I_m \ 0) \ \Lambda^* (I_m \ 0)$$

$$= \Lambda^*.$$

Therefore we introduce a term into the objective function where off-diagonal elements in $\tilde{W}^T C \tilde{W}$ are pushed towards zero.

5. Modified Objective Function

In the following, we suggest a modified objective function by introducing an additional term, derive a learning rule, analyze its fixed points, and study the stability of the fixed points indirectly through the behavior of the objective function.

5.1. Modified Objective Function

We suggest the following modified objective function:

$$J(W) = \frac{1}{4} \left[ (1 + \alpha) \sum_{j=1}^{m} (w_j^T C w_j)^2 - \alpha \sum_{j=1}^{m} \sum_{k=1}^{m} (w_j^T C w_k)^2 \right].$$

Again, we are interested in the local maxima of this function. The first term of (14) coincides with the original objective function (3). A second term with negative sign is added which penalizes non-zero off-diagonal elements in $W^T C W$ as motivated in section 4. A weight factor $\alpha$ is introduced which expresses the influence of the second term. The

$^3$Note that $\Lambda^*$ in this derivation may differ from the one in (8) and (9).

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factors of the two terms are chosen such that terms \((w_j^T C w_k)^2\) with \(j = k\) are weighted with 1, and terms with \(j \neq k\) are weighted with \(-\alpha\). By writing the equation in this way we can avoid the use of Kronecker’s delta. Due to the negative sign and the squared expressions, the terms with \(j \neq k\) are maximized if they are zero.

### 5.2. Derivation of Modified Learning Rule

To derive a learning rule from the modified objective function (14), we first determine its derivative with respect to a single weight vector \(w_l\):

\[
\frac{\partial J}{\partial w_l} = \frac{1}{2} \left[ (1 + \alpha) \sum_{j=1}^{m} (w_j^T C w_j) \frac{\partial w_j^T C w_j}{\partial w_l} - \alpha \sum_{j=1}^{m} \sum_{k=1}^{m} (w_j^T C w_k) \frac{\partial w_j^T C w_k}{\partial w_l} \right]
\]  

\[
= (1 + \alpha) \sum_{j=1}^{m} (w_j^T C w_j) C w_j \delta_{jl} - \frac{1}{2} \alpha \sum_{j=1}^{m} \sum_{k=1}^{m} (w_j^T C w_k) (C w_k \delta_{jl} + C w_j \delta_{kl})
\]

\[
= (1 + \alpha) \left( w_l^T C w_l \right) C w_l - \frac{1}{2} \alpha \left[ \sum_{k=1}^{m} (w_k^T C w_k) C w_k + \sum_{j=1}^{m} (w_j^T C w_l) C w_j \right]
\]

\[
= (1 + \alpha) \left( w_l^T C w_l \right) C w_l - \frac{1}{2} \alpha \left[ \sum_{j=1}^{m} (w_j^T C w_j) C w_j + \sum_{j=1}^{m} (w_j^T C w_l) C w_j \right]
\]

\[
= (1 + \alpha) \left( w_l^T C w_l \right) C w_l - \alpha \sum_{j=1}^{m} (w_j^T C w_l) C w_j
\]

\[
= (1 + \alpha) \left( w_l^T C w_l \right) C w_l - \alpha \sum_{j=1}^{m} C w_j w_j^T C w_l
\]

\[
= (1 + \alpha) \left( w_l^T C w_l \right) C w_l - \alpha C \sum_{j=1}^{m} w_j w_j^T C w_l
\]

\[
= (1 + \alpha) \left( w_l^T C w_l \right) C w_l - \alpha C W W^T C w_l.
\]

Now we combine the expression above into a derivative with respect to the entire matrix \(W\) (with \(m\) columns \(w_l, l = 1, \ldots, m\)):

\[
M := \frac{\partial J}{\partial W} = (1 + \alpha) C W \text{diag}\{w_j^T C w_j\} - \alpha C W W^T C W
\]

\[
= (1 + \alpha) C W D - \alpha C W W^T C W.
\]

In our previous work (Möller, 2020) we found that there are two variants to eliminate the Lagrange multipliers, the first leading to “uninteresting” principal subspace rules,
the second to “interesting” PCA rules. We use the second variant and our “short” form derivation and obtain the following “modified” learning rule which we henceforth refer to as “M2S”:

\[
\tau \dot{W} = M - W M^T W
\]

\[
\tau \dot{W} = (1 + \alpha) C W D - \alpha C W W^T C W
\]

\[
\tau \dot{W} = W \left[ (1 + \alpha) D W^T C - \alpha W^T C W W^T C \right] W
\]

\[
\tau \dot{W} = (1 + \alpha) C W D - \alpha C W (W^T C W)
\]

\[
\tau \dot{W} = (1 + \alpha) W D (W^T C W) + \alpha W (W^T C W) (W^T C W).
\]

We can arrange equation (27) in two ways. In the first arrangement, we sort the terms according to the common factors \((1 + \alpha)\) and \(-\alpha\):

\[
\tau \dot{W} = (1 + \alpha) (C W D - W D W^T C W) - \alpha (C W - W W^T C W) (W^T C W).
\]

This arrangement leads to an interesting insight on the fixed-point structure of “M2S” which is elaborated in section 5.3.

The second arrangement is obtained from (27) by combining the first with the second and the third with the forth term, and factoring out common terms:

\[
\tau \dot{W} = C W \left[ (1 + \alpha) D - \alpha W^T C W \right] - W \left[ (1 + \alpha) D - \alpha W^T C W \right] W^T C W
\]

\[
\tau \dot{W} = C W D'_{\alpha} - W D'_{\alpha} W^T C W.
\]

We see that we obtain the same form as in “N2S” (4), but with a matrix

\[
D'_{\alpha} = (1 + \alpha) D - \alpha W^T C W
\]

instead of \(D\). Note that \(D'_{\alpha}\) is not generally diagonal (but \(D'_{\alpha}\) would be diagonal if the rule actually converges to the principal eigenvectors).

5.3. Fixed Points of Modified Learning Rule

We can gain an interesting insight on the fixed-point structure of “M2S” from an analysis of the first arrangement of terms in (28). We see that the first term coincides with the original learning rule “N2S” from (4). The second term contains the right-hand side of Oja’s subspace rule (110)

\[
\tau \dot{W} = C W - W W^T C W
\]
as the first factor (Oja, 1989). We know from (113) that the fixed points of (32) are
\[
\bar{W} = VP \begin{pmatrix} R \\ 0 \end{pmatrix}
\] (33)
where \( R \) is an arbitrary orthogonal matrix, thus the subspace factor in the second term of (28) will disappear as soon as the eigenvector estimates span the same subspace as an arbitrary selection of \( m \) eigenvectors of \( C \). The general fixed-point solution of “N2S” (7) always fulfills (33) with \( R = U^*P^* \) (U* and P* are orthogonal, as is their product), thus the second term of (28) disappears in the fixed points of “N2S”. This leads to the insight that all fixed points of “N2S” are also present in “M2S”. The additional term in the modified objective function apparently only shapes the landscape outside the fixed points. Note, however, that learning rule “M2S” may have additional fixed points compared to “N2S”.

Aside from this observation, the interpretation of the second term is difficult. The entire second term may also disappear for other values of \( W \), depending on the interplay between first and second factor. Moreover, the negative sign of the second term implies that this term will probably not push \( W \) towards the subspace described above.

For the fixed-point analysis of “M2S”, we proceed as in our previous work (Möller, 2020). We express \( \bar{W} \) through the projections \( \bar{A} \) onto the eigenvectors by \( W = VA \), apply \( V^T CV = \Lambda \), insert the ansatz (84)
\[
\bar{A} = Q \begin{pmatrix} I_m \\ 0 \end{pmatrix}
\] (34)
where \( Q \) is an orthogonal matrix and therefore \( \bar{A} \) is semi-orthogonal (located on a Stiefel manifold defined by \( \bar{A}^T\bar{A} = I_m \)), and define
\[
M := Q^T AQ = \begin{pmatrix} S & T^T \\ T & U \end{pmatrix}.
\] (35)
In appendix C we describe two attempts — starting from either (28) or (30) — at deriving constraints on \( S \) and \( T \) which lead to the same result, namely
\[
SD\bar{D} = \bar{D}S
\] (36)
\[
T [(1 + \alpha)\bar{D} - \alpha S] = 0.
\] (37)
While the constraint on \( S \) (36) coincides with the one for “N2S”, the constraint on \( T \) (37) differs from the one for “N2S” (where it is \( TD = 0 \) with the only solution \( T = 0 \)). The constraint (37) also has the solution \( T = 0 \), but can have additional, non-zero solutions if the factor \( \bar{D}_\alpha = (1 + \alpha)\bar{D} - \alpha S \) is singular. A simulation shows that \( \text{det}\{\bar{D}_\alpha\} \) can actually be zero, see figure 3 in appendix B. We will focus on the case \( T = 0 \) which coincides with “N2S”. For this case, the derivation completely coincides with the one of “N2S” (from equation (248) onward) and leads to the special solution (6) and the general solution (7).
5.4. Stability Analysis

The stability analysis uses the same indirect approach as in our previous work (Möller, 2020, Sec. 8). We can use the following expressions from (330), (335), and (338):

$$\tilde{W}^T C \tilde{W} = U^T_m \Lambda^* U_m =: H$$  
(38)

$$W^T C W = F^T H F + B^T \Lambda^* B$$  
(39)

$$F^T H F \approx H + A^T H + HA + A^T H A$$

$$- \frac{1}{2} (A^T A + B^T B) H - \frac{1}{2} H (A^T A + B^T B).$$  
(40)

We compute the change in the objective function under a small step from fixed point $\tilde{W}$ (on the Stiefel manifold) to point $W$ obtained by an approximated back-projection onto the Stiefel manifold. The step is parametrized by a skew-symmetric $m \times m$ matrix $A$ and an $(n - m) \times m$ matrix $B$. For the modified objective function from equation (14) we get

$$\Delta J = J(W) - J(\tilde{W})$$  
(41)

$$= (1 + \alpha) \frac{1}{4} \left[ \sum_{j=1}^{m} (w_j^T C w_j)^2 - \sum_{j=1}^{m} (\tilde{w}_j^T C \tilde{w}_j)^2 \right]_{\Delta J_1}$$

$$+ \alpha \frac{1}{4} \left[ \sum_{j=1}^{m} \sum_{k=1}^{m} (\tilde{w}_j^T C \tilde{w}_k)^2 - \sum_{j=1}^{m} \sum_{k=1}^{m} (w_j^T C w_k)^2 \right]_{\Delta J_2}$$  
(43)

where the negative sign was incorporated into $\Delta J_2$. We see that $\Delta J_1$ describes the change of the original objective function (3) for which we derived (413)

$$\Delta J_1 \approx$$

$$\frac{1}{2} \sum_{j=1}^{m} H_{jj} \left\{ (A^T H A)_{jj} - [(A^T A + B^T B) H]_{jj} + (B^T \Lambda^* B)_{jj} \right\} + \sum_{j=1}^{m} [(A^T H)_{jj}]^2.$$  
(44)

For $\Delta J_2$ we obtain

$$\Delta J_2 = \frac{1}{4} \sum_{j=1}^{m} \sum_{k=1}^{m} [(\tilde{w}_j^T C \tilde{w}_k)^2 - (w_j^T C w_k)^2]$$

$$= \frac{1}{4} \sum_{j=1}^{m} \sum_{k=1}^{m} [e_j^T \tilde{W}^T C \tilde{W} e_k]^2 - (e_j^T W^T C W e_k)^2]$$  
(45)

$$= \frac{1}{4} \sum_{j=1}^{m} \sum_{k=1}^{m} [(e_j^T H e_k)^2 - (e_j^T \{F^T H F + B^T \Lambda^* B\} e_k)^2]$$  
(46)

$$= \frac{1}{4} \left[ \|H\|_F^2 - \|F^T H F + B^T \Lambda^* B\|_F^2 \right]$$  
(47)
\[
\frac{1}{4} \left[ \| U_m^* \Lambda U_m \|_F^2 - \text{tr}\{ (F^T H F + B^T \Lambda * B)^2 \} \right] \tag{48}
\]
\[
\frac{1}{4} \left[ \| \Lambda * \|_F^2 - \text{tr}\{ (F^T H F + B^T \Lambda * B)^2 \} \right] \tag{49}
\]
\[
\approx \frac{1}{4} \left[ \| \Lambda * \|_F^2 - \text{tr}\{ (F^T H F)^2 + 2(F^T H F)(B^T \Lambda * B) \} \right] \tag{50}
\]
\[
\frac{1}{4} \left[ \| \Lambda * \|_F^2 - \text{tr}\{ (F^T H F)^2 \} - 2 \text{tr}\{ (F^T H F)(B^T \Lambda * B) \} \right] \tag{51}
\]

where we omitted terms above second order in the approximation. Note that for symmetric \( X \) we have \( \| X \|_F^2 = \text{tr}\{ X^T X \} = \text{tr}\{ X^2 \} \).

We further process the second term of (51), using the invariance of the trace to cyclic permutation, exploiting skew-symmetry \( A^T = -A \) and symmetry \( H^T = H \), and omitting terms above second order in \( A \) and \( B \):

\[
\text{tr}\{ (F^T H F)^2 \}
\]
\[
\approx \text{tr}\left\{ \left[ H + A^T H + HA + A^T HA - \frac{1}{2}(A^T A + B^T B)H - \frac{1}{2} H(A^T A + B^T B) \right]^2 \right\} \tag{52}
\]
\[
\approx \text{tr}\left\{ H^2 + HA^T H + H^2 A + HA^T HA - \frac{1}{2} H(A^T A + B^T B)H - \frac{1}{2} H^2(A^T A + B^T B) + A^T H^2 + A^T HA^T H + A^T HHA + HAH + HAA^T H + HAHA + A^T HAH - \frac{1}{2} (A^T A + B^T B)H^2 - \frac{1}{2} H(A^T A + B^T B)H \right\} \tag{53}
\]
\[
= \text{tr}\left\{ H^2 + H^2 A^T + H^2 A + HA^T HA - \frac{1}{2} H^2(A^T A + B^T B) - \frac{1}{2} H^2(A^T A + B^T B) + H^2 A^T + HA^T HA^T + H^2 AA^T + H^2 A + H^2 AA^T + HAHA + HA^T HA - \frac{1}{2} H^2(A^T A + B^T B) - \frac{1}{2} H^2(A^T A + B^T B) \right\} \tag{54}
\]
\[ \Delta J_2 \approx \frac{1}{2} \left[ \text{tr}\{\hat{\Lambda}^* B^T B\} - \text{tr}\{\Lambda^* B^T \hat{\Lambda}^* B\} \right] \]

For the special case with pairwise different elements in \( \tilde{D} \) we have \( U_m = I_m \) and thus \( H = \hat{\Lambda}^* \). We apply (576) and obtain

\[ \Delta J_2 \approx \frac{1}{2} \left[ \text{tr}\{\hat{\Lambda}^* B^T B\} - \text{tr}\{\Lambda^* B^T \hat{\Lambda}^* B\} \right] \]

For the special case we also have with (376)

\[ \Delta J_1 \approx \frac{1}{2} \sum_{j=1}^{m} \left[ \hat{\lambda}_j^s (A^T \hat{\Lambda}^* A)_{jj} - \hat{\lambda}_j^{s^2} (A^T A)_{jj} \right] \]

\[ + \frac{1}{2} \sum_{j=1}^{m} \left[ \hat{\lambda}_j^s (B^T \hat{\Lambda}^* B)_{jj} - \hat{\lambda}_j^{s^2} (B^T B)_{jj} \right] \]

thus by combining the two expressions we obtain

\[ \Delta J \approx \frac{1}{2} (1 + \alpha) \sum_{j=1}^{m} \left[ \hat{\lambda}_j^s (A^T \hat{\Lambda}^* A)_{jj} - \hat{\lambda}_j^{s^2} (A^T A)_{jj} \right] \]
\[
\frac{1}{2}(1 + \alpha) \sum_{j=1}^{m} \left[ \hat{\lambda}_j^*(B^T \hat{\Lambda}^* B)_{jj} - \hat{\lambda}_j^{*2}(B^T B)_{jj} \right] \\
- \frac{1}{2} \alpha \sum_{j=1}^{m} \left[ \hat{\lambda}_j^*(A^T \hat{\Lambda}^* A)_{jj} - \hat{\lambda}_j^{*2}(A^T A)_{jj} \right] \\
- \frac{1}{2} \sum_{j=1}^{m} \left[ \hat{\lambda}_j^*(B^T \hat{\Lambda}^* B)_{jj} - \hat{\lambda}_j^{*2}(B^T B)_{jj} \right].
\]

(67)

\[
\frac{1}{2}(1 + \alpha) \sum_{j=1}^{m} \left[ \hat{\lambda}_j^*(B^T \hat{\Lambda}^* B)_{jj} - \hat{\lambda}_j^{*2}(B^T B)_{jj} \right] \\
- \frac{1}{2} \sum_{j=1}^{m} \left[ \hat{\lambda}_j^*(B^T \hat{\Lambda}^* B)_{jj} - \hat{\lambda}_j^{*2}(B^T B)_{jj} \right].
\]

(68)

As in the original objective function (3), we can demonstrate the existence of a maximum \((\Delta J < 0)\) if the first \(m\) eigenvectors are associated with the \(m\) largest eigenvalues (section 8.4.1); these are the “desired” fixed points. Otherwise we obtain a saddle point or a minimum \((\Delta J > 0)\) in some directions.

For the general case where diagonal elements in \(\hat{\Lambda}^*\) may coincide and where we have \(H = U^T \hat{\Lambda}^* U_m\), we could show that \(\Delta J > 0\) for \(B = 0\) and a specific choice of \(A\) (section 8.4.2). Since \(\Delta J_2\) only depends on \(B\) and disappears for \(B = 0\), we can demonstrate that the “undesired” fixed points are either saddle points or minima.

We conclude that the additional term introduced in the modified objective function (14) leaves the stability of the fixed points unchanged. We also see that the factor \((1 + \alpha)\) leads to a steeper shape of the objective function in the vicinity of the fixed points, at least in some directions (determined by step parameter \(A\)).

### 6. Simulations

As in our previous work, we restrict our simulations to averaged learning rules operating on the covariance matrix \(C = E\{xx^T\}\) (in contrast, online learning rules operate on individual data vectors \(x\)).

### 6.1. Methods

We explore the behavior of the following learning rules:

“TwJ2S” from (449), which is the same as rule (15a) from [Xu (1993)](https://dx.doi.org/10.1162/neco.1993.5.3.437), with \(\Theta = \text{diag} \{ j/m \}\),

“N2S” from (4), which is the same as “M2S” with \(\alpha = 0\), and

“M2S” from (30) for \(\alpha \in \{ 1.0, 2.0, 5.0, 10.0, 20.0 \}\).
We determine eigenvector estimates $W$ with $n = 10$ and $m = 4$. We start from a random initial $W$ located on the Stiefel manifold ($W^T W = I_m$) which is the same for all learning rules and all figures.

We generate a $n \times n$ covariance matrix $C$ from a random orthogonal $V$ and a diagonal eigenvalue matrix $\Lambda$ through $C = V\Lambda V^T$. The matrix $\Lambda$ is generated from one of the following eigenvalue sets, either

"nearby eigenvalues" $\{0.91, 0.9, 0.8, \ldots, 0.1\}$ or

"evenly spaced eigenvalues" $\{1.0, 0.9, 0.8, \ldots, 0.1\}$

through $\Lambda = \text{diag}^n_i \lambda_i$.

The simulation uses an Euler step $W_{t+1} = W_t + \dot{W}_t$ where $\dot{W}_t$ contains the parameter $\gamma = 1/\tau$. Three different subsequent back-projection modes are tested:

"exact back-projection to Stiefel manifold"

$$W_{t+1} = W_{t+1}' (W_{t+1}'^T W_{t+1}')^{-\frac{1}{2}},$$

(69)

"approximated back-projection to Stiefel manifold" from (630)

$$W_{t+1} = W_{t+1}' - \frac{1}{2} W_t \dot{W}_t^T \dot{W}_t,$$

(70)

"no back-projection"

$$W_{t+1} = W_{t+1}'.$$

(71)

To evaluate the deviation of $W$ from semi-orthogonality ("orthonormality" for short) and the deviation of $W$ from the true principal eigenvectors (in arbitrary order), we define three error measures $e_1$, $e_2$, and $e'_2$ on square matrices of size $m$:

$$e_1(X) = \frac{1}{m^2} \sum_{i=1}^m \sum_{j=1}^m |X_{ij} - \delta_{ij}|$$

(72)

$$e_2(X) = \frac{1}{m} \sum_{j=1}^m \max_{i=1}^m \{|(x_j)_i| - 1\}$$

(73)

$$e'_2(X) = \frac{1}{2} \left( e_2(X) + e_2(X^T) \right)$$

(74)

Error measure $e_1$ is zero if $X$ coincides with the identity matrix of the same size. Error measure $e_2$ is zero if the maximal absolute element in each column of $X$ is 1. Error measure $e'_2$ considers $e_2$ in both columns and rows. We define the orthonormality error $e_o$ and the error of the projection to the eigenvectors $e_p$ as

$$e_o(W) = e_1(W^T W)$$

(75)
\[ e_p(W, \hat{V}) = e'_2(\hat{V}^T W) \]  

(76)

where \( \hat{V} \) (size \( n \times m \)) contains the \( m \) principal eigenvectors in its columns. Error measure \( e_o \) is zero for a semi-orthogonal \( W \). Error measure \( e_p \) is zero if each eigenvector estimate \( w_j \) corresponds to a true eigenvector \( \pm v_i \) (arbitrary sign) in a one-to-one mapping. To motivate the error measure \( e_p \), we show two examples of final values of \( \hat{V}^T W \) which lead to \( e_p \approx 0 \). The first is from learning rule “TwJ2S” where the ordering of the estimated eigenvectors with respect to the eigenvalues is determined by the fixed matrix \( \Theta \):

\[
\hat{V}^T W = \begin{pmatrix}
0.00 & 0.00 & 0.00 & -1.00 \\
-0.00 & -0.00 & 1.00 & 0.00 \\
0.00 & -1.00 & -0.00 & -0.00 \\
1.00 & 0.00 & 0.00 & 0.00
\end{pmatrix} .
\]  

(77)

The corresponding eigenvalue estimates \( w_j^T C w_j \) are, in the same order: 0.70, 0.80, 0.90, 1.00. The second example is from learning rule “N2S” where the approached ordering is arbitrary:

\[
\hat{V}^T W = \begin{pmatrix}
-0.00 & -1.00 & 0.00 & 0.00 \\
0.00 & 0.00 & -0.00 & 1.00 \\
1.00 & -0.00 & 0.00 & -0.00 \\
-0.00 & 0.00 & 1.00 & 0.00
\end{pmatrix} .
\]  

(78)

The eigenvalue estimates are, in the same order: 0.80, 1.00, 0.70, 0.90.

6.2. Results

Figure 1 shows the simulation results for the evenly spaced eigenvector set for the three back-projection methods (note the reduced number of simulation steps). Looking at the projection error \( e_p \) (right diagrams), we see fast convergence for all learning rules, particularly for the exact back-projection where the learning rate \( \gamma \) can be higher than in the other two back-projection methods. “N2S” converges more slowly than “TwJ2S”, but is in the same convergence range. “M2S” converges faster with increasing \( \alpha \) and even surpasses “TwJ2S” (but see section 7), but the gain decreases for the highest values of \( \alpha \). The orthonormality error \( e_o \) (left diagrams) stays small for exact back-projection, reduces very fast for approximated back-projection, and reduces somewhat slower for no back-projection. In the latter two cases, increasing \( \alpha \) accelerates the convergence of the orthonormality error. The improved convergence of the orthonormality error from no back-projection to approximated back-projection is not reflected in faster reduction of the projection error, though.

Figure 2 shows the simulation results for nearby eigenvalues \( \lambda_1 \approx \lambda_2 \). Looking at the projection error (right diagrams), both “N2S” and “TwJ2S” show slower convergence than for evenly spaced eigenvalues (note the larger number of simulation steps), but we see
that “N2S” converges considerably slower than “TwJ2S” which confirms the observation reported before (Möller, 2020). However, with increasing $\alpha$ in “M2S”, the time course of the projection error approaches that of “TwJ2S”. Looking at the orthonormality error (left diagrams), we see small values for exact back-projection, fast convergence for approximated back-projection, and much slower convergence with no back-projection. In the latter case, there is a tendency for faster convergence with increasing $\alpha$ in “M2S”, approaching “TwJ2S” for $\alpha = 20$. Again, the projection error does not differ between no back-projection and approximated back-projection, even though the latter shows a noticeably faster reduction of the orthonormality error.

All learning rules seem to approach a lower limit in both $e_o$ and $e_p$ which can probably be explained by numerical effects.

7. Discussion

The simulations show a marked improvement of the convergence speed of the modified learning rule “M2S” for increasing $\alpha$, particularly if some principal eigenvalues are close to each other. Nearby principal eigenvalues slow down both the “N2S” and the “M2S” rule, but the latter is affected more strongly for which we can provide the explanation that the “symmetry-breaking” effect of $D$ is reduced if the eigenvalue estimates on its diagonal are close to each other (Möller, 2020). Introducing the additional terms in the modified objective function mitigates this effect. However, we originally expected that the additional terms will also modify or suppress the “undesired” fixed points, but our analysis shows that all fixed points of “N2S” are also present in “M2S”. We assume that the contributions by the different terms of the additional sum cancel out in the fixed points which therefore remain unchanged. Only the steepness of the landscape outside of the fixed points is increased. Additional fixed points may be present in “M2S”, but this was not analyzed here (particularly the different constraint on $T$ may lead to additional fixed points).

It is always unfortunate if an additional parameter (in this case $\alpha$) has to be introduced. We currently cannot provide a universal guideline on how $\alpha$ has to be adjusted for different eigenvalue spectra and dimensions. We observed that higher values of $\alpha$ than the ones tested in the simulations sometimes lead to divergence. We could imagine that learning rules can be designed where $\alpha$ is suitably chosen depending on $W$. Note that also the suitable range for the learning rate $\gamma$ is not clear. With exact back-projection, it can be higher than with approximated back-projection (since the approximation is based on the assumption of small steps) or without back-projection, but suitable values may depend on the eigenvalue spectrum and the dimensions.

We compare “N2S” and “M2S” with the learning rule “TwJ2S” where we have a fixed diagonal weight-factor matrix $\Theta$ with distinct elements in the place of $D$ or $D'_\alpha$. The influence of the choice of the elements of $\Theta$ on the convergence speed has to be studied.
Figure 1: Orthonormality error $e_o$ (left) and error of projection to eigenvectors $e_p$ (right) for evenly spaced eigenvalues (logarithmic, 20,000 steps, subsampling 100).
Figure 2: Orthonormality error $e_o$ (left) and error of projection to eigenvectors $e_p$ (right) for nearby eigenvalues $\lambda_1 \approx \lambda_2$ (logarithmic, 50.000 steps, subsampling 100).

(a) Exact back-projection, $\gamma = 1$.  
(b) Approximated back-projection, $\gamma = 0.1$.  
(c) No back-projection, $\gamma = 0.1$.
An absolute statement like ‘rule “M2S” performs better than “TwJ2S” for a certain $\alpha$’ is therefore debatable. The time course of the projection error of “TwJ2S” should therefore only be taken as a coarse reference.

The stability analysis in section 5.4 revealed that the additional second term in the modified objective function (14) leads to a term depending only on the step parameter $B$, see equations (61) and (65). With inverted sign, this term alone would be sufficient to explain PCA behavior. One could therefore assume that the additional term in objective function alone (with inverted sign) could lead to a PCA rule. However, we have also shown that the corresponding terms in the learning rule “M2S” are characteristic for subspace behavior, thus the fixed-point structure is completely different without the original first term.

We did not explore the difference between the “short” learning rules studied here and the alternative of learning rules derived from the “embedded” metric on the Stiefel manifold.

8. Conclusion

We introduced an additional term into the objective function which improves the convergence speed of the corresponding learning rule, particularly in the case of nearby principal eigenvalues. The modified learning rule “M2S” is structurally similar to the original rule “N2S”, with a different matrix $D'_\alpha$ in place of $D$. Our analysis shows that the modified learning rule has all fixed points of the original rule but may introduce new fixed points (which was not studied further). Also the stability of the fixed points shared with the original rule is unaffected by the modification.

References

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Changes

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A. Terms of Learning Rules Close to the Stiefel Manifold

In our previous work, we derived different learning rules, either from a derivation in “short” or “long” form or from two different metrics on the Stiefel manifold, canonical and embedded (section 9). The “short” rules coincide with the “canonical” rules, so we have three groups: “short”, “long”, and “embedded”.

In this report we focus on “short” learning rules. In simulations (data not shown) comparing rules from the three groups for the “original” objective function (N2S, NL, NSE), the time course of the projection error $e_p$ was not markedly different, regardless of the back-projection method used. In the following we explore how the different terms can be approximated if the learning rule operates in the vicinity of the Stiefel manifold where $W^T W \approx I_m$. We start from learning rule NL which contains all types of terms known so far (476):

$$\tau \dot{W} = 5CWD - WW^T CWD - WDW^T CW - CWDW^T W - CWD^* - CWW^T WD$$

(79)

where

$$D = \text{diag}\{w_j^T Cw_j\} = \text{dg}\{W^T CW\} \quad (80)$$

$$D^* = \text{diag}\{w_j^T CW^T w_j\} = \text{dg}\{W^T CWW^T W\} \quad (81)$$

Close to the Stiefel manifold, we have $D^* \approx \text{dg}\{W^T CW\} = D$. We can approximate the different terms as

$$\tau \dot{W} = 5CWD - WW^T CWD - WDW^T CW - CWD - CWD^* - CWW^T WD$$

(82)

which leads to the rule called NSE (485):

$$\tau \dot{W} = 2CWD - WW^T CWD - WDW^T CW.$$

There is no obvious approximation which leads from here to N2S, so we assume that in the vicinity of the Stiefel manifold, there are essentially just the two forms N2S and NSE, which correspond to the gradient in the canonical or embedded metric (section 9.3), respectively. Even these two rules show very similar behavior.

It is obvious that exact back-projection keeps $W$ on the Stiefel manifold, and it is also clear that the approximated back-projection almost achieves the same, at least for small learning rates $\gamma = 1/\tau$. Why the rules return to the Stiefel manifold after each learning step without back-projection remains to be explored.
B. Additional Fixed Points of “M2S”

We analyze whether the second factor in equation (37) can become singular:

\[
\tilde{D}'_\alpha = (1 + \alpha) \det\{\tilde{W}^T C \tilde{W}\} - \alpha \tilde{W}^T C \tilde{W} \\
= (1 + \alpha) \det\{\tilde{A}^T V^T C \tilde{A}\} - \alpha \tilde{A}^T V^T C \tilde{A} \\
= (1 + \alpha) \det\{\tilde{A}^T \Lambda \tilde{A}\} - \alpha \tilde{A}^T \Lambda \tilde{A}.
\]

(83) (84) (85)

In a simulation, we generate a random semi-orthogonal \(A\) of size \(n \times m\) (with \(n = 10, m = 4\)) and use eigenvalues \(\{n, n-1, \ldots, 1\}\) to form \(A\). We vary \(\alpha\) and plot \(\det\{\tilde{D}'_\alpha\}\) in steps of 0.1 from 0.0 to 20.0 in figure 3. We often see two zero-crossings as shown in the figure, but curves with other shapes appear as well, depending on the random initialization of \(A\).

C. Fixed-Point Constraints of “M2S”

We describe two attempts at deriving the constraints on matrices \(S\) and \(T\) which lead to the same result.

Figure 3: Determinant \(\det\{\tilde{D}'_\alpha\}\) over \(\alpha\) for a random, semi-orthogonal \(W\) of size \(10 \times 4\) and eigenvalues descending from 10.0 to 1.0 in steps of 1.0.
C.1. Attempt 1

The first attempt starts from (28):

\[
0 = (1 + \alpha) (C \bar{W} D - \bar{W} D W T C \bar{W})
- \alpha (C \bar{W} - \bar{W} W T C \bar{W})(W T C \bar{W})
\]

\[
0 = (1 + \alpha) (C V \bar{A} D - V \bar{A} D A T V T C V \bar{A})
- \alpha (C V \bar{A} - V \bar{A} \bar{A} T V T C V \bar{A})(\bar{A} T V T C V \bar{A})
\]

\[
0 = (1 + \alpha) (C V \bar{A} D - V \bar{A} D A T \bar{A} \bar{A})
- \alpha (C V \bar{A} - V \bar{A} \bar{A} T \bar{A} \bar{A})(\bar{A} T \bar{A} \bar{A})
\]

\[
0 = (1 + \alpha) (V T C V \bar{A} D - V T V \bar{A} D A T \bar{A} \bar{A})
- \alpha (V T C V \bar{A} - V T V \bar{A} \bar{A} T \bar{A} \bar{A})(\bar{A} T \bar{A} \bar{A})
\]

\[
0 = (1 + \alpha) (\bar{A} A D - \bar{A} D A T \bar{A} \bar{A})
- \alpha (\bar{A} A - \bar{A} \bar{A} T \bar{A} \bar{A})(\bar{A} T \bar{A} \bar{A})
\]

\[
0 = (1 + \alpha) \left[ \Lambda Q \begin{pmatrix} I_m \\ 0 \end{pmatrix} D - Q \begin{pmatrix} I_m \\ 0 \end{pmatrix} D (I_m \ 0^T) Q^T \Lambda Q \begin{pmatrix} I_m \\ 0 \end{pmatrix} \right]
- \alpha \left[ Q^T \Lambda Q \begin{pmatrix} I_m \\ 0 \end{pmatrix} - Q \begin{pmatrix} I_m \\ 0 \end{pmatrix} (I_m \ 0^T) Q^T \Lambda Q \begin{pmatrix} I_m \\ 0 \end{pmatrix} \right]
\]

\[
0 = (1 + \alpha) \left[ Q^T \Lambda Q \begin{pmatrix} I_m \\ 0 \end{pmatrix} D - Q^T Q \begin{pmatrix} I_m \\ 0 \end{pmatrix} D (I_m \ 0^T) Q^T \Lambda Q \begin{pmatrix} I_m \\ 0 \end{pmatrix} \right]
- \alpha \left[ Q^T \Lambda Q \begin{pmatrix} I_m \\ 0 \end{pmatrix} - Q^T Q \begin{pmatrix} I_m \\ 0 \end{pmatrix} (I_m \ 0^T) Q^T \Lambda Q \begin{pmatrix} I_m \\ 0 \end{pmatrix} \right]
\]

\[
\cdot \left[ (I_m \ 0^T) Q^T \Lambda Q \begin{pmatrix} I_m \\ 0 \end{pmatrix} \right]
\]

\[
0 = (1 + \alpha) \left[ M \begin{pmatrix} I_m \\ 0 \end{pmatrix} D - \begin{pmatrix} I_m \\ 0 \end{pmatrix} D (I_m \ 0^T) M \begin{pmatrix} I_m \\ 0 \end{pmatrix} \right]
- \alpha \left[ M \begin{pmatrix} I_m \\ 0 \end{pmatrix} - \begin{pmatrix} I_m \\ 0 \end{pmatrix} (I_m \ 0^T) M \begin{pmatrix} I_m \\ 0 \end{pmatrix} \right]
\]

\[
\cdot \left[ (I_m \ 0^T) M \begin{pmatrix} I_m \\ 0 \end{pmatrix} \right]
\]

\[
0 = (1 + \alpha) \left[ S \begin{pmatrix} T \\ 0 \end{pmatrix} D - \begin{pmatrix} I_m \\ 0 \end{pmatrix} DS \right]
\]
\[
- \alpha \begin{pmatrix} S \\ T \end{pmatrix} - \begin{pmatrix} I_m \\ 0 \end{pmatrix} S
\]

\[
0 = (1 + \alpha) \begin{pmatrix} SD \\ TD \end{pmatrix} - \begin{pmatrix} DS \\ 0 \end{pmatrix}
- \alpha \begin{pmatrix} S^2 \\ TS \end{pmatrix} - \begin{pmatrix} S^2 \\ 0 \end{pmatrix}
\]

\[
0 = \begin{pmatrix} (1 + \alpha)[SD - DS] \\ T[(1 + \alpha)\bar{D} - \alpha S] \end{pmatrix}.
\]

The upper part of equation (96) gives

\[
SD = DS.
\]

Equation (97) coincides with the constraint (247) derived for the fixed points of learning rule “N2S”.

The lower part of equation (96) gives

\[
T[(1 + \alpha)\bar{D} - \alpha S] = 0
\]

which differs from the equation \(TD = 0\) derived for “N2S”.

**C.2. Attempt 2**

The second attempt starts from (30) and proceeds in the same way as in section 7.8 of our previous work (Möller, 2020), from equation (239) onward, except with \(\hat{D}_\alpha\) instead of \(\hat{D}\):

\[
0 = C\hat{D}_\alpha - \hat{W}\hat{D}_\alpha \bar{W}^T C\hat{W}
\]

\[
0 = CV\hat{A}\hat{D}_\alpha - V\hat{A}\hat{D}_\alpha \bar{A}^T V^T CV\bar{A}
\]

\[
0 = V^T CV\hat{A}\hat{D}_\alpha - V^T V\hat{A}\hat{D}_\alpha \bar{A}^T V^T CV\bar{A}
\]

\[
0 = \Lambda\hat{A}\hat{D}_\alpha - \hat{A}\hat{D}_\alpha \bar{A}^T \Lambda \bar{A}
\]

\[
0 = \Lambda Q \begin{pmatrix} I_m \\ 0 \end{pmatrix} \hat{D}_\alpha - Q \begin{pmatrix} I_m \\ 0 \end{pmatrix} \hat{D}_\alpha (I_m \ 0^T) Q^T \Lambda Q \begin{pmatrix} I_m \\ 0 \end{pmatrix}
\]

\[
0 = Q^T \Lambda Q \begin{pmatrix} I_m \\ 0 \end{pmatrix} \hat{D}_\alpha - Q \begin{pmatrix} I_m \\ 0 \end{pmatrix} \hat{D}_\alpha (I_m \ 0^T) Q^T \Lambda Q \begin{pmatrix} I_m \\ 0 \end{pmatrix}
\]

\[
0 = \begin{pmatrix} S & T \\ T & U \end{pmatrix} \begin{pmatrix} I_m \\ 0 \end{pmatrix} \hat{D}_\alpha - \begin{pmatrix} I_m \\ 0 \end{pmatrix} \hat{D}_\alpha (I_m \ 0^T) \begin{pmatrix} S & T^T \\ T & U \end{pmatrix} \begin{pmatrix} I_m \\ 0 \end{pmatrix}
\]

\[
0 = \begin{pmatrix} SD'_\alpha \\ TD'_\alpha \end{pmatrix} - \begin{pmatrix} D'_\alpha S \\ 0 \end{pmatrix}.
\]
To analyze the constraint on $S$ in the upper equation of (106), we look at

$$\tilde{D}'_\alpha = (1 + \alpha)\tilde{D} - \alpha\tilde{W}^T C \tilde{W}$$

(107)

and see that

$$\tilde{W}^T C \tilde{W} = \tilde{A}^T V^T C V \tilde{A}$$

(108)

$$= \tilde{A}^T \Lambda \tilde{A}$$

(109)

$$= (I_m \ 0^T) Q^T M \Lambda Q (I_m \ 0)$$

(110)

$$= (I_m \ 0^T) \begin{pmatrix} S & T^T \\ T & U \end{pmatrix} (I_m \ 0)$$

(111)

$$= S.$$  

(112)

Note that we also have $\tilde{D} = d\{\tilde{W}^T C \tilde{W}\} = d\{S\}$.

We can therefore write $\tilde{D}'_\alpha$ as

$$\tilde{D}'_\alpha = (1 + \alpha)\tilde{D} - \alpha S.$$  

(113)

We proceed with the upper equation of (106):

$$S\tilde{D}'_\alpha = \tilde{D}'_\alpha S$$

(114)

$$S \left[(1 + \alpha)\tilde{D} - \alpha S\right] = \left[(1 + \alpha)\tilde{D} - \alpha S\right] S$$

(115)

$$(1 + \alpha)S\tilde{D} - \alpha S^2 = (1 + \alpha)\tilde{D}S - \alpha S^2$$

(116)

$$S\tilde{D} = \tilde{D}S.$$  

(117)

This constraint is the same as (247) which was derived for the fixed points of the “N2S” learning rule.

We now look at the lower equation of (106):

$$T\tilde{D}'_\alpha = 0$$

(118)

$$T \left[(1 + \alpha)\tilde{D} - \alpha S\right] = 0.$$  

(119)

The corresponding equation for “N2S” was $T\tilde{D} = 0$. 

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