We describe a Lagrange-Newton framework for the derivation of learning rules with desirable convergence properties and apply it to the case of principal component analysis (PCA). In this framework, a Newton descent is applied to an extended variable vector which also includes Lagrange multipliers introduced with constraints. The Newton descent guarantees equal convergence speed from all directions, but is also required to produce stable fixed points in the system with the extended state vector. The framework produces “coupled” PCA learning rules which simultaneously estimate an eigenvector and the corresponding eigenvalue in cross-coupled differential equations. We demonstrate the feasibility of this approach for two PCA learning rules, one for the estimation of the principal, the other for the estimate of an arbitrary eigenvector-eigenvalue pair (eigenpair).
# Contents

1. Introduction 3
2. Notation 4
3. Lagrange-Newton Approach 6
4. Criterion and Constraint 7
5. Derivation of the General Hessian 8
6. Stability Analysis for Exact Hessians 9
7. Principal Eigenpair 15
   7.1. Inverse Hessian 15
   7.2. Newton Descent 17
   7.3. Stability Analysis 18
   7.4. Deflation 19
8. Arbitrary Eigenpair 21
   8.1. Inverse Hessian 21
   8.2. Newton Descent 23
   8.3. Stability Analysis 24
      8.3.1. Stability Analysis via Jacobian 24
      8.3.2. Stability Analysis via Perturbation 32
   8.4. Learning Rule System 38
   8.5. Simulations 38
   8.6. Relation to Deflation 39
9. Conclusions and Future Work 40

References 41

A. Lemmata 41
   A.1. Lagrange Multiplier Method 41
      A.1.1. Bordered Hessian 42
   A.2. Derivatives 45
   A.3. Triangular Matrices 45
1. Introduction

There is a plethora of neural network algorithms for principal component analysis (PCA) (recent textbook: Kong et al., 2017). Particularly the online forms of these algorithms are attractive since they avoid the construction of the potentially very large covariance matrix. Instead, eigenvectors and eigenvalues are directly estimated from a data stream, reducing computational effort and memory demand.

Our main contribution to this field are “coupled” learning rules for PCA (Möller and Könies, 2004). These rules simultaneously estimate eigenvectors and eigenvalues in a coupled system of equations, i.e. the eigenvalue estimates affect the eigenvector update and vice versa. Coupled learning rules mitigate the speed-stability problem which affects other learning rules and make the rules independent on the range of eigenvalues. In our original publication, the rules were derived by applying Newton’s method to an information criterion related to the normalized Mahalanobis distance. Newton’s method ensures approximately equal convergence speed from all directions, at least in the vicinity of the fixed points. Moreover, by choosing the Hessian matrix for a desired fixed point, this fixed point can be turned into an attractor.

The weak point of this approach is the information criterion (Möller, 2020a). While there is considerable freedom in designing the criterion — it just needs to exhibit fixed points in the eigenvector and eigenvalues, but these don’t have to be attractors — there is no systematic way to design such a criterion. Moreover, the criterion has limited explanatory value, since it is not related to an optimization problem. We therefore suggested to derive coupled learning rules from a Newton zero-finding framework (Möller, 2020a). In this approach, an equation derived from the optimum of an objective function is combined with a constraint on the eigenvector estimates (“weight vectors”). This joint vector is set to zero, and the equation is solved by applying Newton’s method as a zero finder. We managed to derive PCA and SVD (singular value decomposition) learning rules from this framework, for both Euclidean and constant-sum constraints of the eigenvector estimates. However, the framework is not entirely satisfactory since the approach may fail if the constraints do not intersect the solution derived from the unconstrained optimum.

Where therefore already indicated in our previous work that switching to a Lagrange-Newton framework may be a more universal approach (Möller, 2020a). The present paper is devoted to exploring this alternative. In the Lagrange-Newton framework, an objective function is linked to constraints through Lagrange multipliers, and Newton’s method is applied to the resulting extended objective function by including both the original variables (eigenvector estimates) and the Lagrange multipliers in the variable vector. It turns out that the Lagrange multipliers coincide with eigenvalues in the fixed points. Here Newton’s method serves an additional purpose: Solutions of the extended objective functions are saddle points if the Lagrange multipliers are included (Kalman, 2009; Baker, 1992; Walsh, 1975); see also section A.1.1. Only through the application of Newton’s method can saddle points be turned into attractors.

We restrict our present investigation to PCA methods and e.g. exclude SVD methods (coupled methods: Kaiser et al., 2010; Möller, 2020a) for the time being. Moreover, we only study
single-component learning rules which estimate a single eigenvector / eigenvalue pair (in short “eigenpair”). We describe two approaches how these single-component rules can be combined for the estimation of multiple eigenpairs. The first approach is the classical deflation operation; the second approach results immediately from the estimation of an arbitrary (rather than just the principal) eigenpair, as described below.

In this paper, we only derive learning rules in averaged form operating on the covariance matrix. Online rules can always be obtained by replacing the covariance matrix by the outer product of the current data vector with itself and introducing a cooling scheme for the learning rates (see e.g. Möller and Körner, 2004).

We derive coupled PCA learning rules for two cases: estimation of the principal eigenpair and estimation of an arbitrary eigenpair. The first case leads to the learning rules known from our previous work (Möller and Körner, 2004); these can be integrated into a deflation scheme to derive multiple eigenpairs. For the second case we derived a multi-component learning rule where each state relies on the eigenpair estimates of all previous stages. The terms relating to deflation in the first case or to the multi-stage scheme in the second case differ from each other. For both cases, we provide a stability analysis.

After introducing the notation in section 2, we outline the Lagrange-Newton approach in section 3. The specific criterion and constraint for the PCA case is introduced in section 4. Then we derive a general Hessian covering both cases studied later in section 5. In section 6 we explore the stability of fixed points under the assumption that the Hessian is known exactly. The case of estimating the principal eigenpair is covered in section 7, the case of estimating an arbitrary eigenpair in section 8. Conclusions and future work are presented in section 9.

2. Notation

Dimensions:

\( n \): data dimension, \( 4 \leq n \)

\( m \): number of eigenpair estimates, \( 4 \leq m \leq n \)

\( p \): eigenpair index, typically index related to desired fixed point, \( 3 \leq p \leq m - 1 \)

\( q \): eigenpair index, typically index related to some fixed point, \( 1 \leq q \leq m \)

Note that the range restrictions of the dimensions are necessary to avoid invalid matrix dimensions in some derivation steps.

Matrices:

\( C \): covariance matrix, symmetric, \( n \times n \)
$\mathcal{C}_{p-1}$: $p - 1$-fold deflated covariance matrix, symmetric, $n \times n$

$V$: true eigenvectors of $C$, orthogonal, $n \times n$

$\Lambda$: true eigenvalues of $C$, distinct, sorted in descending order, diagonal, $n \times n$

$\Lambda_{p-1}$: upper left block of $\Lambda$, diagonal, $(p - 1) \times (p - 1)$

$\Lambda_{n-p}$: lower right block of $\Lambda$, diagonal, $(n - p) \times (n - p)$

$w$: weight vector, eigenvector estimate, arbitrary, $n \times 1$

$l$: Lagrange multiplier, eigenvalue estimate, scalar, $1 \times 1$

$W$: weight vector matrix, arbitrary, $n \times m$

$w_i$: weight vector, arbitrary, $n \times 1$, column vector of $W$

$L$: eigenvalue estimates, diagonal, $m \times m$

$l_i$: eigenvalue estimate, scalar, $1 \times 1$, diagonal element of $L$

$J$: Lagrange criterion, scalar, $1 \times 1$

$T$: transformation matrix, orthogonal, $(n + 1) \times (n + 1)$

$P_{1,n+1}$: elementary permutation matrix between 1 and $n + 1$, permutation, $(n + 1) \times (n + 1)$

$P_{p,n+1}$: elementary permutation matrix between $p$ and $n + 1$, permutation, $(n + 1) \times (n + 1)$

$H$: Hessian matrix, square, $(n + 1) \times (n + 1)$

$H^*$: transformed Hessian matrix, square, $(n + 1) \times (n + 1)$

$E$: identity matrix, unit, $n \times n$

$e_i$: unit vector with element 1 at position $i$, arbitrary, $n \times 1$, column vector of $E$

**Operators:**

$\text{tr}\{A\}$: trace of square matrix $A$

$\text{diag}\{A\}$: diagonal matrix with diagonal elements from square matrix $A$

$\text{sut}\{A\}$: strict upper triangular matrix with elements from square matrix $A$

$\text{det}\{A\}$: determinant of square matrix $A$
3. Lagrange-Newton Approach

While in the original paper (Möller and Könies, 2004) the derivation started from an “information criterion”, we now use a Lagrange-multiplier approach. We will first present the general approach, but already refer to the specific PCA problem.

Starting point is an **unconstrained criterion** which depends on the selected variables. In the PCA case, the criterion is the expectation of the projected variance; the variables are the eigenvector estimates (weight vectors); see section 4.

We define an **equality constraint** on the variables. Here we assume that the constraint is fulfilled if it becomes zero. In the PCA case, this is the case if the weight vector has unit Euclidean length; see section 4.

Criterion and equality constraint are combined in a modified **Lagrange criterion**. This introduces Lagrange multiplier variables for each component of the constraint; see section 4. For single-unit PCA, we have a single Lagrange multiplier; see section 5. From this point on, we operate on an extended variable vector which includes both the original variables and the Lagrange multipliers.

The **set of fixed points** is determined from the zero points of the first-order derivatives of the Lagrange criterion with respect to the extended variable vector. In the PCA case, the original variables have solutions in the eigenvectors, the Lagrange multiplier in the corresponding eigenvalues of the covariance matrix; see section 5.

In the Lagrange-Newton framework, we derive the update equation from a **Newton descent** on the extended variable vector. As mentioned above, Newton’s method turns the selected saddle point of the Lagrange function into an attractor. In addition, the convergence speed is approximately \(-1\) from all directions; see section 6.

For the Newton descent, we **select the desired fixed point**. This is accomplished by **computing the Hessian for this fixed point**. In this work, we explore PCA solutions for the **principal eigenpair** (section 7) and for **arbitrary eigenpairs** (section 8).

A crucial step in the computation of the Hessian for the desired fixed point are **approximations**. Currently, this is the least formal step of the method. We can identity three aspects:

- Since we need to invert the Hessian, we have to transform it to a **simple form**. In the PCA case, we apply an orthogonal similarity transformation which diagonalizes a sub-matrix; see section 5. For this step, **substitutions** are required: The extended variable vector is temporarily substituted by the corresponding fixed-point vector since this enables some simplifications. This rests on the assumption that the Newton descent has moved the estimate of the extended variable vector to the vicinity of the desired fixed point. After the inversion of the Hessian, all fixed-point quantities are substituted back to the variable quantities — the fixed-point quantities are unknown, whereas the variable quantities are determined in the Newton descent.
• For further simplification, we apply knowledge on the fixed points of the extended variable vector. In the PCA case, we assume an ordered set of eigenvalues where preceding eigenvalues are much larger than following eigenvalues. This leads to some approximations which further simplify the Hessian. We noticed that this step is critical in the PCA case: Approximations are required to eliminate unknown estimates (following eigenpairs), but may lead to undesired fixed points if also applied to known estimates (preceding eigenpairs). We therefore recommend to only use approximations to eliminate unknown quantities.

• We have to eliminate unknown fixed-point variables. To determine the principal eigenpair in the PCA case (section 7), we assume that all non-principal eigenpairs are unknown. To determine an arbitrary eigenpair, we assume that there are learning rules which estimate all previous eigenpairs, but that all following eigenpairs are unknown; all fixed-point quantities relating to the following eigenpairs need to be eliminated. It may not always be obvious how to achieve this, since the matrix used in the orthogonal similarity transformation also contains unknown quantities; the transformed Hessian needs to be brought into a form where the unknown quantities disappear in the inverse transformation.

Finally, we invert the approximated Hessian and perform the back-substitution mentioned above. We then combine the inverted approximated Hessian with the gradient to obtain the Newton descent in the form of an ordinary differential equation over the extended variable vector. In the context of neural networks, this equation can be called a “learning rule”.

Note that usually the Newton descent does not change the set of fixed points as expressed by the gradient. If the inverse Hessian $H^{-1}$ is defined, the fixed-point equation of the Newton descent could be multiplied from the left by $H$ which is obviously non-singular, leading to the original fixed-point equation. However, for the case of arbitrary eigenpairs explored in section 8, the Hessian is singular and thus the inverse Hessian not defined in some of the original fixed points. This also introduces an additional set of fixed points.

### 4. Criterion and Constraint

As the objective function for PCA we use the variance of the projection onto the weight vector $w$; this objective function is maximized. This leads to Rayleigh quotient (see e.g. Möller, 2020a, for the derivation):

$$J = \frac{1}{2} w^T C w.$$  \hspace{1cm} (1)

Instead of normalizing the weight vectors within the Rayleigh quotient, we can use the numerator of the Rayleigh quotient as objective function and force the weight vector to L2 unit length by an equality constraint.\footnote{We don’t address the problem of using different constraints, e.g. the constant sum of elements (Möller, 2020a). If a constraint other than the L2 unit length is used, the modified objective function should combine it with the}

\textbf{The constraint is integrated into the modified objective function with}
the Lagrange multiplier $l$:

$$J = \frac{1}{2} w^T C w - \frac{1}{2} l (w^T w - 1).$$

(2)

Note that the sign of the constraint term is arbitrary. A negative sign is used here such that the Lagrange parameter in the fixed points coincides with an eigenvalue (see below) rather than a negative eigenvalue.

Learning rules are derived from a Newton descent in $J$ over the extended variable vector $(w^T \quad l)^T$ for a selected fixed point.

5. Derivation of the General Hessian

For the Newton descent, we have to determine the Hessian $H$ and the gradient of $J$. The first-order derivatives of $J$ are

$$\left( \frac{\partial J}{\partial w} \right)^T = Cw - lw$$

(3)

$$\left( \frac{\partial J}{\partial l} \right)^T = -\frac{1}{2} (w^T w - 1).$$

(4)

We see that equation (3) is the eigen equation; together with (4) we obtain the fixed points $w = v_i$ and $l = \lambda_i$, with $w^T w = 1$. We see that the Lagrange multiplier coincides with the eigenvalues in the fixed points.

The second-order derivatives are

$$\frac{\partial}{\partial w} \left( \frac{\partial J}{\partial w} \right)^T = C - lI_n$$

(5)

$$\frac{\partial}{\partial l} \left( \frac{\partial J}{\partial w} \right)^T = -w$$

(6)

$$\frac{\partial}{\partial w} \left( \frac{\partial J}{\partial l} \right)^T = -w^T$$

(7)

$$\frac{\partial}{\partial l} \left( \frac{\partial J}{\partial l} \right)^T = 0,$$

(8)

which gives the Hessian

$$H = \begin{pmatrix} C - lI_n & -w \\ -w^T & 0 \end{pmatrix}.$$
In both our original and the novel framework, learning rules are derived by evaluating the Hessian at a chosen fixed point. This step is performed by applying an orthogonal similarity transformation to the Hessian, deriving approximations, inverting the matrix (as required for the Newton descent), and transforming back. We choose the orthogonal transformation matrix

\[ T = \begin{pmatrix} V & 0_n \\ 0_n^T & 1 \end{pmatrix} \]  

and obtain the transformed Hessian

\[ H^* = T^T H T \]

\[ = \begin{pmatrix} V & 0_n \\ 0_n^T & 1 \end{pmatrix}^T \begin{pmatrix} C - l I_n & -w \\ -w^T & 0 \end{pmatrix} \begin{pmatrix} V & 0_n \\ 0_n^T & 1 \end{pmatrix} \]

\[ = \begin{pmatrix} V^T C V - V^T l V & -V^T w \\ (-w^T) V & 0 \end{pmatrix} \]

\[ = \begin{pmatrix} \Lambda - l I_n & V^T (-w) \\ (-w^T) V & 0 \end{pmatrix}. \]

In the following, we choose the Hessian for the principal eigenpair (section 7) and for an arbitrary eigenpair (section 8). This involves assumptions on the relationships between eigenvalues. The Hessians are finally inverted as required for the Newton descent. In the derivation, we approximate the true but unknown eigenpair with the estimated eigenpair. Note that this makes it difficult to predict the behavior of the Newton descent far from the desired fixed point.

### 6. Stability Analysis for Exact Hessians

In the following we analyze the effect of the approximations used in the derivation of the inverse Hessian. We study the stability of fixed points in a Newton descent for an exact inverse Hessian, for both the desired fixed point and the undesired fixed points. Note that the exact inverse Hessian wouldn’t be available in an application. We perform this analysis as a baseline since differences in behavior to this case can then be explained as effect of the necessary approximations.

In the following derivation we assume unordered eigenvectors \( \tilde{V} \) and eigenvalues \( \tilde{\Lambda} \), both in arbitrary order of eigenvalues. We assume a Newton descent is performed for the Hessian matrix \( \tilde{H}_i \) obtained at fixed point \( i \) where \( w = \tilde{v}_i \) and \( l = \tilde{\lambda}_i \):

\[ \begin{pmatrix} w \\ i \end{pmatrix} = -\tilde{H}_i^{-1} \begin{pmatrix} \frac{\partial w}{\partial \tilde{l}} \\ \frac{\partial w}{\partial \tilde{\lambda}} \end{pmatrix}^T \].

The Jacobian of this system is evaluated at the fixed point \( j \) where \( w = \tilde{v}_j \) and \( l = \tilde{\lambda}_j \):

\[ \tilde{J} \]
\[
\begin{align*}
\frac{\partial \dot{\mathbf{w}}}{\partial \mathbf{w}} & = \left( \frac{\partial \mathbf{w}}{\partial \dot{\mathbf{w}}} \right) \quad (16) \\
\frac{\partial \dot{\mathbf{w}}}{\partial \mathbf{l}} & = -\mathbf{H}^{-1} \mathbf{j}. \quad (17)
\end{align*}
\]

For \( i = j \), i.e. for the case where the inverse Hessian corresponds to the fixed point under consideration, we get \( \mathbf{J} = -\mathbf{I}_{n+1} \). We see that the system converges with the same speed from all directions and the speed is constant \((-1)\).

For \( i \neq j \), i.e. for the case where the inverse Hessian belongs to a different fixed point, the eigenvalues of the Jacobian determine stability at undesired fixed point.

Since it is probably challenging to obtain a general statement on the stability for an arbitrary criterion and an arbitrary constraint, we only study the case of PCA.

We first apply an orthogonality transformation with matrix

\[
\mathbf{T} = \begin{pmatrix} \mathbf{\tilde{V}} & 0_n \\ 0_n^T & 1 \end{pmatrix}
\]

(18)

to the Jacobian:

\[
\mathbf{\mathbf{\tilde{J}}} = \begin{pmatrix} \mathbf{\tilde{V}} & 0_n \\ 0_n^T & 1 \end{pmatrix}\begin{pmatrix} \mathbf{\tilde{V}} & 0_n \\ 0_n^T & 1 \end{pmatrix}
\]

(19)

\[
\mathbf{\tilde{J}}^* = \mathbf{T}^T \mathbf{\tilde{J}} \mathbf{T}
\]

(20)

\[
\mathbf{\tilde{J}}^* = \begin{pmatrix} \mathbf{\tilde{V}} & 0_n \\ 0_n^T & 1 \end{pmatrix}\begin{pmatrix} \mathbf{\tilde{V}} & 0_n \\ 0_n^T & 1 \end{pmatrix}
\]

(21)

\[
\mathbf{\tilde{J}}^* = \begin{pmatrix} \mathbf{\tilde{V}} & 0_n \\ 0_n^T & 1 \end{pmatrix} \mathbf{\tilde{H}}^{-1} \mathbf{\tilde{H}}^* 
\]

(22)

\[
\mathbf{\tilde{J}}^* = \begin{pmatrix} \mathbf{\tilde{V}} & 0_n \\ 0_n^T & 1 \end{pmatrix} \mathbf{\tilde{H}}^{-1} \mathbf{\tilde{H}}^* 
\]

(23)

The orthogonal similarity transformation of \( \mathbf{\tilde{J}} \) doesn’t its affect eigenvalue spectrum, so we analyze the eigenvalues of transformed Jacobian \( \mathbf{\tilde{J}}^* \) instead:

\[
\mathbf{\tilde{J}}^* = -\mathbf{\tilde{H}}^{-1} \mathbf{\tilde{H}}^*. 
\]

(24)

We start by determining the Hessian for fixed point \( i \) where \( \mathbf{w} = \mathbf{\tilde{V}}_i \) and \( l = \mathbf{\tilde{\lambda}}_i \). We take the general Hessian from \( \text{(9)} \):

\[
\mathbf{H} = \begin{pmatrix} \mathbf{C} - l \mathbf{I}_n & -\mathbf{w} \\ -\mathbf{w}^T & 0 \end{pmatrix}
\]

(25)

determine the Hessian after orthogonal similarity transformation analogous to \( \text{(14)} \):

\[
\mathbf{H}^* = \mathbf{T}^T \mathbf{H} \mathbf{T}
\]

(26)

\[
\mathbf{H}^* = \begin{pmatrix} \mathbf{\tilde{V}} & 0_n \\ 0_n^T & 1 \end{pmatrix} \mathbf{H} \begin{pmatrix} \mathbf{\tilde{V}} & 0_n \\ 0_n^T & 1 \end{pmatrix}
\]

(27)
\[
\begin{align*}
&= \begin{pmatrix} \tilde{V} & 0_n^T \end{pmatrix} \begin{pmatrix} C - I_n & -w \\ -w^T & 0 \end{pmatrix} \begin{pmatrix} \tilde{V} \\ 0_n^T \end{pmatrix} \\
&= \begin{pmatrix} \tilde{\Lambda} - I_n & \tilde{V}^T (-w) \\ -w^T \tilde{V} & 0 \end{pmatrix},
\end{align*}
\]
(28)

and insert fixed point \(i\)

\[
\begin{align*}
\bar{H}_i^* &= \begin{pmatrix} \tilde{\Lambda} - \tilde{\lambda}_i I_n & \tilde{V}^T (-\tilde{v}_i) \\ -\tilde{v}_i^T \tilde{V} & 0 \end{pmatrix} \\
&= \begin{pmatrix} \tilde{\lambda}_1 - \tilde{\lambda}_i & 0 \\ \vdots & \ddots \\ \tilde{\lambda}_i - \tilde{\lambda}_i & -1 \\ 0 & \ddots \\ \tilde{\lambda}_n - \tilde{\lambda}_i & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \end{pmatrix} \\
&= \begin{pmatrix} \tilde{\lambda}_1 - \tilde{\lambda}_i & 0 \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & \tilde{\lambda}_i - \tilde{\lambda}_i \\ 0 & \ddots & \ddots & \ddots & \tilde{\lambda}_n - \tilde{\lambda}_i \\ \tilde{\lambda}_1 - \tilde{\lambda}_i & 0 \\ \vdots & \ddots & \ddots & \ddots & \tilde{\lambda}_i - \tilde{\lambda}_i \\ 0 & \ddots & \ddots & \ddots & \tilde{\lambda}_n - \tilde{\lambda}_i \\ 0 & \ddots & \ddots & \ddots & -1 \end{pmatrix} \mathbf{P}_{i,n+1}.
\end{align*}
\]
(30)

We then invert the transformed Hessian, and exploit the property \(P_{i,n+1}^{-1} = P_{i,n+1}\) of the elementary permutation:

\[
\bar{H}_i^{-1}
\]
\[
\begin{bmatrix}
(\tilde{\lambda}_1 - \tilde{\lambda}_i)^{-1} & 0 & & & \\
& \ddots & \ddots & \ddots & \\
& & \ddots & -1 & 0 \\
& & & 0 & \ddots \\
& & & & \ddots & 0 \\
0 & \cdots & 0 & \cdots & \cdots & 0 & (\tilde{\lambda}_n - \tilde{\lambda}_i)^{-1}
\end{bmatrix}
\]

\(= \mathbf{P}_{i,n+1} \begin{bmatrix}
(\tilde{\lambda}_1 - \tilde{\lambda}_i)^{-1} & 0 & & & \\
& \ddots & \ddots & \ddots & \\
& & \ddots & -1 & 0 \\
& & & 0 & \ddots \\
& & & & \ddots & 0 \\
0 & \cdots & 0 & \cdots & \cdots & 0 & (\tilde{\lambda}_n - \tilde{\lambda}_i)^{-1}
\end{bmatrix} \) \hspace{1cm} (35)

In the next step, we insert the inverse transformed Hessian into (24), replace the diagonal matrices in the upper-left corner by \(A_i\) and \(B_j\), respectively, and assume \(i \neq j\):

\[
\bar{\mathbf{J}}^*
\]

\[
= -\mathbf{H}_i^*^{-1} \mathbf{H}_j^*
\]

\[
= -\begin{bmatrix}
(\tilde{\lambda}_1 - \tilde{\lambda}_i)^{-1} & 0 & & & \\
& \ddots & \ddots & \ddots & \\
& & \ddots & 0 & \ddots \\
& & & 0 & \ddots \\
& & & & \ddots & 0 \\
0 & \cdots & 0 & \cdots & \cdots & 0 & (\tilde{\lambda}_n - \tilde{\lambda}_i)^{-1}
\end{bmatrix}
\]

\[
= -\begin{bmatrix}
(A_i - \mathbf{e}_i^T) & \mathbf{B}_j - \mathbf{e}_j \\
-e_i^T & 0
\end{bmatrix}
\]

\[
= -\begin{bmatrix}
(A_j \mathbf{B}_j + \mathbf{e}_i \mathbf{e}_j^T - A_i \mathbf{e}_j) & -e_i^T \mathbf{B}_j
\end{bmatrix}
\]

\[
= -\begin{bmatrix}
A_j \mathbf{B}_j + \mathbf{e}_i \mathbf{e}_j^T - (\tilde{\lambda}_j - \tilde{\lambda}_i)^{-1} \mathbf{e}_j \\
-e_i^T (\tilde{\lambda}_i - \tilde{\lambda}_j)
\end{bmatrix}
\]

Since any ordering of eigenpairs is possible, we can choose arbitrary indices, \(i = 1, j = 2\):

\[
\bar{\mathbf{J}}^*
\]
We abbreviate $d_{i,j} = \tilde{\lambda}_i - \tilde{\lambda}_j$ and get

$$\tilde{J}^* = \begin{pmatrix}
0 & -1 \\
0 & 0 & -d_{3,1}^{-1}d_{3,2} \\
0 & 0 & 0 & -d_{n,1}^{-1}d_{n,2} \\
-d_{2,1} & 0 & 0 & \cdots & -d_{n,1}^{-1}d_{n,2} & 0 \\
\end{pmatrix}$$

(45)

We determine the eigenvalues $\alpha$ of $\tilde{J}^*$ from

$$\det\{\tilde{J}^* - \alpha I_{n+1}\}$$

$$= \begin{vmatrix}
-\alpha & -1 & 0 & \cdots & 0 \\
0 & -\alpha & d_{2,1}^{-1} & \cdots & d_{n,1}^{-1}d_{n,2} \\
\end{vmatrix}$$

(46)
develop along the upper row,

\[
\begin{vmatrix}
-\alpha & (d_{3,1}^{-1}d_{3,2}) - \alpha & d_{2,1}^{-1} \\
& \ddots & \vdots \\
0 & (d_{3,1}^{-1}d_{n,2}) - \alpha & 0 \\
0 & \ddots & \vdots \\
-d_{2,1} & \ldots & 0
\end{vmatrix}
\]

and finally factor out

\[
= (-\alpha) \cdot (\ldots)
\]

The eigenvalues are \(1, -\frac{1}{2} \pm \frac{\sqrt{3}i}{2}\) as complex solutions of \(\alpha^3 = 1\), and

\[
\alpha_k = -d_{k,1}^{-1}d_{k,2} = -\left(\tilde{\lambda}_k - \tilde{\lambda}_1\right)^{-1}\left(\tilde{\lambda}_k - \tilde{\lambda}_2\right) \text{ for } k = 3, \ldots, n.
\]
The eigenvalues were confirmed in numerical experiments. The eigenvalue of 1 and the two complex eigenvalues with negative real part of $-\frac{1}{2}$ indicate that we have a saddle point if the inverse Hessian doesn’t correspond to the fixed point. Surprisingly, this statement is independent of the eigenvalue spectrum.

We conclude that at least if the Hessians would be known exactly (which is not the case when the learning rules are applied), there is only a single stable fixed point at the desired location, whereas all other fixed points are saddle points, thus the system will converge to the desired fixed point.

However, since the derivations of the learning rules below necessarily use approximated Hessians, the stability of each learning rule needs to be studied. Moreover, the learning rules may sometimes converge to an additional set of fixed points which is introduced by Newton’s method.

### 7. Principal Eigenpair

In the following we derive coupled learning rules for the principal eigenpair (the one with largest eigenvalue). The resulting learning rules are the same as in our previous publication (Möller and Könies, 2004), but are now obtained from the Lagrange-Newton approach.

#### 7.1. Inverse Hessian

$\Lambda$ is the matrix of all eigenvalues of $C$, sorted in descending order along the main diagonal. We assume that the eigenvalues are distinct (i.e. pairwise different). The orthogonal matrix $V$ is the matrix of all eigenvectors of $C$; the eigenvectors in its columns appear in the same order as the eigenvalues. We want to determine the principal eigenpair $i = 1$, i.e. the one with the largest eigenvalue. In the vicinity of the desired fixed point for $i = 1$ we have $l \approx \lambda_1$ and $w \approx v_1$, such that (14) turns into:

$$
H^* \approx \begin{pmatrix}
\Lambda - \lambda_1 I_n & V^T (-v_1) \\
(-v_1^T V) & 0
\end{pmatrix}
$$

(53)

$$
= \begin{pmatrix}
\Lambda - \lambda_1 I_n & -e_i \\
-e_i^T & 0
\end{pmatrix}.
$$

(54)

If we look at (52) in addition, we see that positive (instable) eigenvalues are introduced for any $\tilde{\lambda}_k$ lying between $\tilde{\lambda}_1$ and $\tilde{\lambda}_2$. All eigenvalues in (52) are negative if no such $\tilde{\lambda}_k$ can be found. The implications are currently unclear.

It is presently not clear why we obtain eigenvalues of the Jacobian with imaginary part for exact Hessians, but purely real eigenvalues for the approximated Hessians.
We see that element $i$ of the diagonal matrix $\Lambda - \lambda_1 I_n$ is $\lambda_i - \lambda_1$. We assume $\lambda_1 \gg \lambda_i$ for $i > 1$ and therefore $\lambda_i - \lambda_1 \approx -\lambda_1$; the first diagonal element is 0.

\[
H^* \approx \left( \lambda_1 (e_1e_1^T - I_n) - e_1 \right)
\approx \left( l (e_1e_1^T - I_n) - e_1 \right)
= - \begin{pmatrix}
0 & 0^T_{n-1} & 1 \\
0 & l_{n-1} & 0_{n-1} \\
1 & 0^T_{n-1} & 0 \\
0 & 0^T_{n-1} & 1 
\end{pmatrix}
= - \begin{pmatrix}
0 & 0^T_{n-1} & 1 \\
0 & l_{n-1} & 0_{n-1} \\
1 & 0^T_{n-1} & 0 \\
0 & 0^T_{n-1} & 1 
\end{pmatrix} P_{1,n+1}.
\]

In the last step we exchanged column 1 and $n + 1$ by post-multiplying with the corresponding elementary permutation matrix $P_{1,n+1}$. Note that we have $P_{1,n+1} = P_{1,n+1}^{-1}$ since we have an elementary permutation matrix which only exchanges two columns. The resulting matrix is diagonal and therefore easy to invert; this is a more concise derivation than in our previous work (Möller and Könies, 2004; Möller, 2020a). After the inversion we obtain a pre-multiplication by $P_{1,n+1}$ which performs a permutation of rows:

\[
H^{*-1} \approx - P_{1,n+1} \begin{pmatrix}
1 & 0^T_{n-1} & 0 \\
0 & l_{n-1} & 0_{n-1} \\
0 & 0^T_{n-1} & 1 
\end{pmatrix}
= - \begin{pmatrix}
0 & 0^T_{n-1} & 1 \\
0 & l_{n-1} & 0_{n-1} \\
1 & 0^T_{n-1} & 0 \\
0 & 0^T_{n-1} & 1 
\end{pmatrix}.
\]

For the transformation back to $H^{-1}$ we apply

\[
H^* = T^T H T
\]
\[
H^{*-1} = (T^T H T)^{-1}
\]
\[
H^{*-1} = T^T H^{-1} T
\]
\[
H^{-1} = TH^{-1} T^T.
\]

\footnote{This approximation attempts to eliminate the dependency on later eigenpair estimates ($i > 1$) which are unknown from the perspective of the principal-component estimator. However, it may be interesting to explore a derivation where the approximation is not applied.}
We multiply the block matrices

\[
H^{-1} \approx TH^{-1}T^T
\]

\[
= \begin{pmatrix}
V & 0_n \\
0_n^T & 1
\end{pmatrix}
\begin{pmatrix}
l^{-1}(e_1e_1^T - I_n) & -e_1 \\
-e_1^T & 0
\end{pmatrix}
\begin{pmatrix}
V & 0_n \\
0_n^T & 1
\end{pmatrix}^T
\]

\[
= \begin{pmatrix}
Vl^{-1}(e_1e_1^T - I_n)V^T & -Ve_1 \\
-e_1^TV & 0
\end{pmatrix}.
\]

In the vicinity of the fixed point we have \(Ve_1 = v_1\) and \(v_1 \approx w\), so we get

\[
H^{-1} \approx \begin{pmatrix}
l^{-1}(ww^T - I_n) & -w \\
-w^T & 0
\end{pmatrix}.
\]

### 7.2. Newton Descent

Now we insert the inverted Hessian (69) into the Newton descent:

\[
\begin{pmatrix}
\dot{w} \\
\dot{l}
\end{pmatrix}
= -H^{-1}\begin{pmatrix}
\frac{\partial J}{\partial w} \\
\frac{\partial J}{\partial l}
\end{pmatrix}^T
\]

\[
\approx -\begin{pmatrix}
l^{-1}(ww^T - I_n) & -w \\
-w^T & 0
\end{pmatrix}
\begin{pmatrix}
Cw - lw \\
-l\frac{1}{2}(w^Tw - 1)
\end{pmatrix}
\]

\[
= \begin{pmatrix}
l^{-1}ww^T(Cw - lww^T - l^{-1}lww^T w - l^{-1}lw - \frac{1}{2}ww^Tw + \frac{1}{2}w) \\
-w^T(Cw - lw^Tw)
\end{pmatrix}
\]

\[
= \begin{pmatrix}
l^{-1}ww^T(Cw) + l^{-1}Cw + \frac{1}{2}ww^Tw - \frac{1}{2}ww^Tw + \frac{1}{2}w \\
-w^T(Cw - lw^Tw)
\end{pmatrix}
\]

\[
= \begin{pmatrix}
l^{-1}ww^T(Cw) + l^{-1}Cw + \frac{1}{2}ww^Tw - \frac{1}{2}ww^Tw + \frac{1}{2}w \\
-w^T(Cw - lw^Tw)
\end{pmatrix}
\]

\[
= \begin{pmatrix}
l^{-1}(Cw - [w^T(Cw)w]) + \frac{1}{2}(w^Tw - 1)w \\
-w^T(Cw - lw^Tw)
\end{pmatrix}.
\]

These equations are the same as the “nPCA” system derived in our previous work (Möller and König, 2004).

There is one observation to report: Applying the Newton descent introduces additional fixed points which are not present in the original set of fixed points. The differential equation above obviously has a fixed point at \(w = 0_n\) for arbitrary \(l (l \neq 0)\). These additional fixed points probably appear since the Hessian is singular for these values.
7.3. Stability Analysis

We now analyse the stability of the coupled learning rule (76):

\[
\begin{align*}
\dot{w} & = \left( I^{-1} (Cw - [w^TCw]w) + \frac{1}{2} (w^Tw - 1)w \right), \\
\dot{l} & = \left( w^TCw - lw^Tw \right).
\end{align*}
\]  

(77)

Stability at a given fixed point is evident from the eigenvalues of the Jacobian evaluated at this fixed point. We apply derivatives from appendix [A.2] and get the Jacobian

\[
\mathbf{J} = \frac{\partial \dot{w}}{\partial w} \frac{\partial \dot{l}}{\partial l}
\]

(78)

\[
\begin{align*}
\mathbf{J} & = \left( I^{-1} (C - 2ww^TC - [w^TCw]I) + \frac{1}{2} (w^Tw)I - \frac{1}{2} I_n - l^{-2} (Cw - [w^TCw]w) \right), \\
& = \left( \frac{1}{2} (w^Tw)I - \frac{1}{2} I_n \right)
\end{align*}
\]

(79)

Now we insert fixed point \( \bar{q} \) specified by \( (v_q^T, \lambda_q)^T \) with \( v_q^Tv_q = 1 \) and \( Cw_q = \lambda_q v_q \):

\[
\mathbf{\bar{J}} = \mathbf{J}_{w=v_q, l=\lambda_q}
\]

(80)

\[
\begin{align*}
\mathbf{\bar{J}} & = \left( \lambda_q^{-1} (C - 2v_qv_q^TC - [v_q^TCv_q]I_n) + v_qv_q^T + \frac{1}{2} (v_q^Tv_q)I_n - \frac{1}{2} I_n - \lambda_q^{-2} (Cv_q - [v_q^TCv_q]v_q) \right), \\
& = \left( \lambda_q^{-1} (C - 2v_qv_q^T \lambda_q - \lambda_q I_n) + v_qv_q^T \right) 0_n \]
\]

(81)

\[
\begin{align*}
& = \left( \lambda_q^{-1} (C - 2v_qv_q^T \lambda_q - \lambda_q I_n) + v_qv_q^T \right) 0_n \]
\]

(82)

\[
\begin{align*}
& = \left( \lambda_q^{-1} (C - v_qv_q^T \lambda_q - \lambda_q I_n) + v_qv_q^T \right) 0_n \]
\]

(83)

\[
\begin{align*}
& = \left( \lambda_q^{-1} (C - v_qv_q^T \lambda_q - \lambda_q I_n) + v_qv_q^T \right) 0_n \]
\]

(84)

To extract the eigenvalues of \( \mathbf{\bar{J}} \), we apply an orthogonal similarity transformation with \( \mathbf{T} \) from (80). Eigenvalues are invariant under a similarity transformation. We obtain the transformed Jacobian \( \mathbf{\bar{J}}^* \) at the fixed point \( \bar{q} \):

\[
\mathbf{\bar{J}}^* = \left( \begin{array}{cc} \mathbf{V} & 0_n \\ 0_n & 1 \end{array} \right) \mathbf{\bar{J}} \left( \begin{array}{cc} \mathbf{V} & 0_n \\ 0_n & 1 \end{array} \right)^T
\]

(85)

\[
\mathbf{\bar{J}}^* = \left( \begin{array}{cc} \mathbf{V}^T & 0_n \\ 0_n & 1 \end{array} \right) \left( \lambda_q^{-1} (C - v_qv_q^T \lambda_q - \lambda_q I_n) + v_qv_q^T \right) \left( \begin{array}{cc} \mathbf{V} & 0_n \\ 0_n & 1 \end{array} \right)^T
\]

(86)

\[
\mathbf{\bar{J}}^* = \left( \begin{array}{cc} \mathbf{V}^T & 0_n \\ 0_n & 1 \end{array} \right) \left( \lambda_q^{-1} (C - v_qv_q^T \lambda_q - \lambda_q I_n) + v_qv_q^T - \lambda_q^{-2} (Cv_q - [v_q^TCv_q]v_q) \right) \left( \begin{array}{cc} \mathbf{V} & 0_n \\ 0_n & 1 \end{array} \right)^T
\]

(87)

\[
\mathbf{\bar{J}}^* = \left( \begin{array}{cc} \mathbf{V}^T & 0_n \\ 0_n & 1 \end{array} \right) \left( \lambda_q^{-1} (C - v_qv_q^T \lambda_q - \lambda_q I_n) + v_qv_q^T - \lambda_q^{-2} (Cv_q - [v_q^TCv_q]v_q) \right) \left( \begin{array}{cc} \mathbf{V} & 0_n \\ 0_n & 1 \end{array} \right)^T
\]

(88)
\( \hat{J}^* \) is a diagonal matrix, so the eigenvalues can be obtained directly from the main diagonal. We denote these eigenvalues by \( \alpha_k, k = 1, \ldots, n + 1 \), with

\[
\alpha_k = \lambda_q^{-1} \lambda_k - 1 = \lambda_q^{-1} (\lambda_k - \lambda_q) \quad \text{for } k = 1, \ldots, n, \; k \neq q \\
\alpha_q = \lambda_q^{-1} \lambda_q - 1 = -1 < 0 \\
\alpha_{n+1} = -1 < 0.
\] (89) (90) (91)

The first equation shows: Fixed point \( q \) is stable (only negative eigenvalues) if and only if \( \lambda_k < \lambda_q \) for \( k = 1 \ldots, n, \; k \neq q \). Thus the only stable fixed point is found for \( q = 1 \) under the assumption that \( \lambda_1 \) is largest eigenvalue of \( C \). All other fixed points are saddle points: If \( q > 1 \), there exists an index \( k \) (particularly \( k = 1 \)) for which \( \lambda_k > \lambda_q \) and thus \( \alpha_k > 0 \). Since the eigenvalues from the second and third equation are negative, we have a saddle point.

Moreover, for \( \lambda_k < \lambda_q \forall k \neq q \) we have \( \alpha_k \approx -1 \); we also obtained \(-1\) for the remaining eigenvalues, so approximately the same convergence speed is achieved from all directions. This demonstrates that the Newton descent solves the speed-stability problem, at least in the vicinity of the fixed point.

The Hesse matrix was chosen for the desired “principal” fixed point, and the stability analysis confirms that only this fixed point was turned into an attractor, thereby substantiating the proposed design principle.

### 7.4. Deflation

The ordinary differential equation (76) is a single-unit rule which converges towards the principal eigenpair. If multiple principal eigenpairs have to be determined, we can resort to deflation of \( C \). This is based on the removal of preceding eigenpairs from the spectral decomposition of \( C \) (introducing zero eigenvalues). If a learning rule for the principal eigenpair is applied to the deflated matrix, it will converge to the eigenpair with the largest eigenvalue remaining in the deflated matrix. If we want to find the eigenpair \( p \), the deflation substitutes \( C \) with \( \hat{C}_{p-1} \) where the preceding \( p - 1 \) eigenpairs have been removed. The removal sets these eigenvalues to zero, such that a learning rule operating on \( \hat{C}_{p-1} \) converges to the largest remaining eigenpair, the one which corresponds to the \( p \)th largest original eigenvalue. Ultimately, we get a chain of learning rules which in stage \( p \) contains \( p - 1 \) previous estimator units.

The following derivation of matrix deflation \([\text{Diamantaras and Kung, 1996}, \; \text{p.39}]\) uses \( C v_i = \lambda_i v_i \) for further transformations, but we only apply the original equation (92) below:

\[
\hat{C}_{p-1} \\
= C - \sum_{i=1}^{p-1} \lambda_i (v_i v_i^T) \\
= C - \sum_{i=1}^{p-1} C (v_i v_i^T)
\] (92) (93)
\[
I_n - \sum_{i=1}^{p-1} v_i v_i^T \right). \tag{94}
\]

The learning rule for the \( p \)th eigenpair is obtained by inserting \( \tilde{C}_{p-1} \) from (92) instead of \( C \) into (76) and applying (92). We could perform a fully sequential update scheme where we wait until the estimate of the first eigenpair has converged to the true eigenpair, then determine the second eigenpair, and so on. Alternatively, we can run all estimators in parallel. For the parallel scheme, we replace \( w = w_p \) and \( l = l_p \) and substitute true eigenvectors by estimates \( v_i \approx w_i \) and true eigenvalues by estimates \( \lambda_i \approx l_i \) (these would be the converged eigenpair estimates from the previous stages in the sequential scheme), and obtain the ODE for the eigenvector update

\[
\dot{w}_p = l_p^{-1} \left( \tilde{C}_{p-1} w_p - \left[ w_p^T \tilde{C}_{p-1} w_p \right] w_p \right) + \frac{1}{2} \left( w_p^T w_p - 1 \right) w_p \tag{95}
\]

\[
= l_p^{-1} \left( \left[ C - \sum_{i=1}^{p-1} l_i \{ w_i w_i^T \} \right] w_p - \left[ w_p^T \left\{ C - \sum_{i=1}^{p-1} l_i \{ w_i w_i^T \} \right\} \right] w_p \right) + \frac{1}{2} \left( w_p^T w_p - 1 \right) w_p \tag{96}
\]

\[
= \left( Cw_p - \sum_{i=1}^{p-1} w_i l_i w_i^T w_p \right) w_p - \left[ w_p^T Cw_p \right] w_p + \left[ w_p^T \sum_{i=1}^{p-1} w_i l_i w_i^T w_p \right] w_p \right) l_p^{-1} + \frac{1}{2} w_p \left( w_p^T w_p - 1 \right). \tag{97}
\]

The same replacement is performed for the eigenvalue update:

\[
\dot{l}_p = w_p^T \tilde{C}_{p-1} w_p - l_p w_p^T w_p \tag{98}
\]

\[
= w_p^T \left[ C - \sum_{i=1}^{p-1} l_i \{ w_i w_i^T \} \right] w_p - l_p w_p^T w_p \tag{99}
\]

\[
= w_p^T Cw_p - w_p^T \sum_{i=1}^{p-1} w_i l_i w_i^T w_p - l_p w_p^T w_p. \tag{100}
\]

For the simulation, we switch from vector to matrix form, using Lemma 2 for the treatment of the strict upper triangular matrices involved. We use \( m \) eigenpair estimators. We obtain matrix equations for eigenvectors

\[
\dot{W} = \left( CW - WL_{\text{sym}} \{ W^T W \} \right)
- W \text{ diag} \left\{ W^T C W \right\} + W \text{ diag} \left\{ W^T W L_{\text{sym}} \{ W^T W \} \right\}) L^{-1}
+ \frac{1}{2} W \text{ diag} \left\{ W^T W - I_m \right\}
\]

\[5\]The parallel scheme is easier to implement in a simulation, e.g. in Matlab, and may be faster since later stages can already start to converge based on halfway converged estimates from the previous ones. However, the sequential scheme may be more stable and could allow for larger learning rates. There may be a good speed-stability compromise between the two schemes.
and eigenvalues

\[
\dot{L} = \text{diag}\{W^T CW\} - \text{diag}\{W^T WL\} - \text{diag}\{W^T W\} + \text{diag}\{W^T W\}.
\] (102)

8. Arbitrary Eigenpair

We now explore whether we can apply the design principle to derive a learning rule for an arbitrary eigenpair \(p\). We assume that, in each stage \(p\), all previous \(p - 1\) eigenvalues are known, but not the following \(n - p\) eigenvalues.

8.1. Inverse Hessian

We start from the transformed Hessian (14) and approximate in the vicinity of the desired fixed point \(p\) where we have \(l \approx \lambda_p\) and \(w \approx v_p\):

\[
H^* \approx \begin{pmatrix}
\Lambda - \lambda_p I_n & V^T(-w) \\
-w^T & 0
\end{pmatrix}
\] (103)

\[
\approx \begin{pmatrix}
\Lambda - \lambda_p I_n & V^T(-v_p) \\
-v_p^T & 0
\end{pmatrix}
\] (104)

\[
= \begin{pmatrix}
\Lambda - \lambda_p I_n & -e_p \\
-e_p^T & 0
\end{pmatrix}.
\] (105)

The expression in the upper left diagonal matrix of (105) is treated in the following way:

- We look at the preceding \(p - 1\) eigenvalues in \(\Lambda\). These eigenvalues are much larger than \(\lambda_p\), i.e. \(\lambda_i \gg \lambda_p\) for \(i < p\). However, we do not introduce approximations based on this relation, but keep the terms \(\lambda_i - \lambda_p\).

- Element \(p\) of the upper left diagonal matrix is 0.

- We need to eliminate the following \(n - p\) eigenvalues since they are assumed to be unknown for stage \(p\). All following \(n - p\) eigenvalues are much smaller than \(\lambda_p\), i.e. \(\lambda_i \ll \lambda_p\) for \(i > p\), and we can therefore approximate \(\lambda_i - \lambda_p \approx -\lambda_p\).

In the process of analyzing the case of an arbitrary eigenpair, we noticed that the fixed points strongly depend on the terms chosen for the preceding \(p - 1\) eigenvalues. Undesired stable fixed points were introduced if approximations were used (tested for constant and linear Taylor approximation after inversion\(^6\)). In these fixed points, stage \(p\) can converge onto the previous unstable fixed point.

\(^6\)It may be worthwhile to study whether quadratic approximations eliminate the undesired fixed points. Approxi-
estimated eigenpair, such that sequences of the same eigenpair of varying length can appear in the solution (depending on the initial state). We therefore decided not to use an approximation.

We proceed by approximating \( l \approx \lambda_p \) and get:

\[
H^* \\
\approx \begin{pmatrix}
\Lambda_{p-1} - l \mathbf{I}_{p-1} & 0_{p-1} & 0_{p-1,n-p} & 0_{p-1} \\
0_{p-1}^T & 0 & 0_{n-p}^T & -1 \\
0_{p-1,n-p}^T & 0_{n-p} - l \mathbf{I}_{n-p} & 0_{n-p} \\
0_{p-1}^T & -1 & 0_{n-p}^T & 0
\end{pmatrix} \mathbf{P}_{p,n+1}^{-1} \quad (106)
\]

where we exchanged column \( p \) and \( n + 1 \) in the last step to produce a diagonal matrix. The inversion below uses \( \mathbf{P}_{p,n+1} = \mathbf{P}_{p,n+1}^{-1} \) and performs the corresponding row permutation.

We now aim for a learning rule which rests on the assumption that only the preceding eigenvectors for \( i < p \) are known (either given or already estimated). This should lead to a learning rule which exhibits structural similarities to the one derived from deflation in section 7.4. In the following transformation, an explicit dependency on the following eigenvectors for \( i > p \) is avoided by addition of zero on the diagonal and extraction of \( l^{-1} \mathbf{I}_n \). This leads to a zero block \( 0_{n-p,n-p} \) in the lower right corner; the zero diagonal elements of this block eliminate the dependency on \( \mathbf{v}_i \mathbf{v}_i^T \) for \( i > p \) in the back-transformation.

\[
H^{*-1} \\
\approx \mathbf{P}_{p,n+1} \begin{pmatrix}
(\Lambda_{p-1} - l \mathbf{I}_{p-1})^{-1} & 0_{p-1} & 0_{p-1,n-p} & 0_{p-1} \\
0_{p-1}^T & 0 & 0_{n-p}^T & -1 \\
0_{p-1,n-p}^T & 0_{n-p} - l^{-1} \mathbf{I}_{n-p} & 0_{n-p} \\
0_{p-1}^T & -1 & 0_{n-p}^T & 0
\end{pmatrix} \mathbf{P}_{p,n+1}^{-1} \quad (108)
\]

mations might have the advantage that matrix-form learning rule systems could be derived which is not possible in the present form.

\[
\approx \mathbf{P}_{p,n+1} \begin{pmatrix}
(\Lambda_{p-1} - l \mathbf{I}_{p-1})^{-1} & 0_{p-1} & 0_{p-1,n-p} & 0_{p-1} \\
0_{p-1}^T & 0 & 0_{n-p}^T & -1 \\
0_{p-1,n-p}^T & 0_{n-p} - l^{-1} \mathbf{I}_{n-p} & 0_{n-p} \\
0_{p-1}^T & -1 & 0_{n-p}^T & 0
\end{pmatrix}
\]

\[
\approx \begin{pmatrix}
(\Lambda_{p-1} - l \mathbf{I}_{p-1})^{-1} - l^{-1} \mathbf{I}_{p-1} + l^{-1} \mathbf{I}_{p-1} & 0_{p-1} & 0_{p-1,n-p} & 0_{p-1} \\
0_{p-1}^T & 0 & 0_{n-p}^T & -1 \\
0_{p-1,n-p}^T & 0_{n-p} - l^{-1} \mathbf{I}_{n-p} & 0_{n-p} \\
0_{p-1}^T & -1 & 0_{n-p}^T & 0
\end{pmatrix}
\quad (110)
\]

This essentially exploits \( \mathbf{V} \mathbf{V}^T = \mathbf{I}_n \). It may be interesting to explore the derivation of learning rules where each of the \( m \leq n \) eigenpair estimators (index \( p \leq m \)) depends on all \( m \) estimated eigenpairs, not just on the previous ones. The \( m \) eigenpairs could be estimated simultaneously.
We transform back and approximate \( w \approx v_p \) in the last step:

\[
H^{-1} \approx \sum_{i=1}^{p-1} \left[ (\Lambda_i - I)^{-1} V_i V_i^T + l^{-1} V_i v_p^T - l^{-1} I_n - v_p \right] - v_p^T - l^{-1} w^T - l^{-1} I_n - w
\]

\[
8.2. \textbf{Newton Descent}
\]

We insert the approximated inverse Hessian from (116) into the Newton descent:

\[
\dot{w} = -H^{-1} \left( \frac{\partial w}{\partial J} \right)^T
\]

\[
\approx - \sum_{i=1}^{p-1} \left[ (\Lambda_i - I)^{-1} V_i V_i^T + l^{-1} V_i v_p^T - l^{-1} I_n - w \right] \left( \frac{Cw - lw}{-\frac{1}{2}(w^T w - 1)} \right)
\]

\[
= l^{-1}(Cw - [w^T Cw]w) + \frac{1}{2}w(w^T w - 1) - \sum_{i=1}^{p-1} \left[ (\Lambda_i - I)^{-1} V_i v_i^T \right] (Cw - lw)
\]
We see that the first summand of the equation for $\dot{w}$ coincides with the learning rule for the principal eigenpair (76). The second summand depends on the true previous eigenpairs; its second factor disappears in all fixed points but the entire summand can affect their stability. It is interesting to see that the equation for $\dot{l}$ is the same as in (76) (only principal eigenpair estimator), whereas the deflation procedure for the principal eigenpair leads to an additional term in equation (100).

As for the system in section 7.2 we observe additional fixed points $w = 0$, for arbitrary values of $l$ with the exception of the values of $l$ excluded by the inversions.

### 8.3. Stability Analysis

In the following, we analyze the stability of the coupled learning rule (121) in two different ways: by studying the eigenvalues of the Jacobian (as for the case of the principal eigenpair) and by studying the effect of small perturbations from the fixed points. The first way resulted in difficulties for one of the sub-cases since some terms were undefined (which was not visible any longer after some transformation steps). The second way coincides with the first for two of the sub-cases, but allows to study the critical sub-case.

#### 8.3.1. Stability Analysis via Jacobian

We analyze the stability of the coupled learning rule (121) by studying the eigenvalues of the Jacobian:

$$
\begin{pmatrix}
\dot{w} \\
\dot{l}
\end{pmatrix} = 
\begin{pmatrix}
t^{-1}(Cw - [w^T Cw]w) + \frac{1}{2}w(w^T w - 1) - \sum_{i=1}^{n-1} \left[ \lambda_i - l \right]^{-1} v_i v_i^T (Cw - lw) \\
\end{pmatrix}.
$$

(122)

We determine the Jacobian

$$
J = \begin{pmatrix}
\frac{\partial}{\partial w} \dot{w} & \frac{\partial}{\partial l} \dot{w} \\
\frac{\partial}{\partial w} \dot{l} & \frac{\partial}{\partial l} \dot{l}
\end{pmatrix},
$$

(123)

the Jacobian at the fixed point

$$
\bar{J} = J|_{w = v_q, l = \lambda_q}
$$

(124)

$$
= \begin{pmatrix}
\left( \frac{\partial}{\partial w} \dot{w} \right)|_{w = v_q, l = \lambda_q} & \left( \frac{\partial}{\partial l} \dot{w} \right)|_{w = v_q, l = \lambda_q} \\
\left( \frac{\partial}{\partial w} \dot{l} \right)|_{w = v_q, l = \lambda_q} & \left( \frac{\partial}{\partial l} \dot{l} \right)|_{w = v_q, l = \lambda_q}
\end{pmatrix},
$$

(125)

and the transformed Jacobian at the fixed point

$$
\bar{J}^*.
$$
determine the derivative (using section A.2) block, we first compute the derivative, insert the fixed point. Since the terms are complex, we proceed for the individual blocks of the Jacobian. For each $Cv_q = \lambda_q v_q$, and apply the transformation.

**Upper left block:**

We repeat the differential equation

$$w = l^{-1} (Cw - [w^T Cw] w) + \frac{1}{2} w (w^T w - 1)$$

(129)

$$- \left( \sum_{i=1}^{p-1} [(\lambda_i - l)^{-1} + 1] v_i v_i^T \right) (Cw - lw),$$

determine the derivative (using section A.2)

$$\frac{\partial}{\partial w} \dot{w}$$

$$= l^{-1} (C - 2ww^T C - [w^T Cw] I_2) + ww^T + \frac{1}{2} (w^T w) I_2 - \frac{1}{2} I_2$$

(130)

$$- \left( \sum_{i=1}^{p-1} [(\lambda_i - l)^{-1} + 1] v_i v_i^T \right) (C - lI_2),$$

determine the derivative for the fixed point

$$\left( \frac{\partial}{\partial w} \dot{w} \right)_{w=v_q, l=\lambda_q}$$

$$= \lambda_q^{-1} (C - 2v_q v_q^T C - [v_q^T Cv_q] I_2) + v_q v_q^T + \frac{1}{2} (v_q^T v_q) I_2 - \frac{1}{2} I_2$$

(131)

$$- \left( \sum_{i=1}^{p-1} [(\lambda_i - \lambda_q)^{-1} + \lambda_q^{-1}] v_i v_i^T \right) (C - \lambda_q I_2)$$

$$= \lambda_q^{-1} (C - 2v_q v_q^T \lambda_q - \lambda_q I_2) + v_q v_q^T + \frac{1}{2} I_2 - \frac{1}{2} I_2$$

(132)

$$- \sum_{i=1}^{p-1} [(\lambda_i - \lambda_q)^{-1} + \lambda_q^{-1}] v_i v_i^T (C - \lambda_q I_2)$$

25
We repeat the differential equation, prepared to reveal dependencies on \( l \)

\[
\dot{w} = l^{-1} (Cw - [w^T Cw] w) + \frac{1}{2} w (w^T w - 1)
\]
\[- \left( \sum_{i=1}^{p-1} [\lambda_i - l]^{-1} + l^{-1} \right) v_i v_i^T \right) (Cw - lw) \]

\[= l^{-1} (Cw - [w^T Cw] w) + \frac{1}{2} w (w^T w - 1) \] (144)

\[- \sum_{i=1}^{p-1} (\lambda_i - l)^{-1} v_i v_i^T Cw - \sum_{i=1}^{p-1} l^{-1} v_i v_i^T Cw + \sum_{i=1}^{p-1} (\lambda_i - l)^{-1} v_i v_i^T lw + \sum_{i=1}^{p-1} l^{-1} v_i v_i^T lw \]

\[= l^{-1} (Cw - [w^T Cw] w) + \frac{1}{2} w (w^T w - 1) \] (145)

\[- \sum_{i=1}^{p-1} (\lambda_i - l)^{-1} v_i v_i^T Cw - l^{-1} \sum_{i=1}^{p-1} v_i v_i^T Cw + \sum_{i=1}^{p-1} (\lambda_i - l)^{-1} v_i v_i^T lw + \sum_{i=1}^{p-1} v_i v_i^T lw \]

\[= l^{-1} (Cw - [w^T Cw] w) + \frac{1}{2} w (w^T w - 1) \] (146)

\[- \sum_{i=1}^{p-1} (\lambda_i - l)^{-1} v_i v_i^T \lambda_i w - l^{-1} \sum_{i=1}^{p-1} v_i v_i^T \lambda_i w + \sum_{i=1}^{p-1} (\lambda_i - l)^{-1} v_i v_i^T lw + \sum_{i=1}^{p-1} v_i v_i^T lw \]

\[= l^{-1} (Cw - [w^T Cw] w) + \frac{1}{2} w (w^T w - 1) \] (147)

\[- \sum_{i=1}^{p-1} (\lambda_i - l)^{-1} v_i v_i^T (\lambda_i - l) w - l^{-1} \sum_{i=1}^{p-1} v_i v_i^T \lambda_i w + \sum_{i=1}^{p-1} v_i v_i^T w \]

\[= l^{-1} (Cw - [w^T Cw] w) + \frac{1}{2} w (w^T w - 1) \] (148)

\[- \sum_{i=1}^{p-1} v_i v_i^T w - l^{-1} \sum_{i=1}^{p-1} v_i v_i^T \lambda_i w + \sum_{i=1}^{p-1} v_i v_i^T w \]

\[= l^{-1} (Cw - [w^T Cw] w) + \frac{1}{2} w (w^T w - 1) - l^{-1} \sum_{i=1}^{p-1} v_i v_i^T \lambda_i w \] (149)

(again note the deflation term in the last summand), determine the derivative

\[ \frac{\partial}{\partial l} \dot{w} \]

\[= (-l^{-2} [Cw - \{w^T Cw\} w]) + l^{-2} \sum_{i=1}^{p-1} v_i v_i^T \lambda_i w, \] (150)

determine the derivative for the fixed point

\[ \left( \frac{\partial}{\partial l} \dot{w} \right) \bigg|_{w=v_q, l=\lambda_q} \]

\[= (-\lambda_q^{-2} [Cv_q - \{v_q^T Cv_q\} v_q]) + \lambda_q^{-2} \sum_{i=1}^{p-1} v_i v_i^T \lambda_i v_q \] (151)
\[ (-\lambda_q^{-2} [C\nu_q - \lambda_q \nu_q]) + \lambda_q^{-2} \sum_{i=1}^{p-1} \nu_i \nu_i^T \lambda_i \nu_q \]

\[ = \lambda_q^{-2} \sum_{i=1}^{p-1} \nu_i \nu_i^T \lambda_i \nu_q, \]  

(152)

and transform:

\[ V^T \left( \frac{\partial}{\partial \lambda} \dot{w} \right) \bigg|_{w=v_q, \lambda=\lambda_q} \]

\[ = V^T \left( \lambda_q^{-2} \sum_{i=1}^{p-1} \nu_i \nu_i^T \lambda_i \nu_q \right) \]

\[ = \lambda_q^{-2} \sum_{i=1}^{p-1} \nu_i \nu_i^T \lambda_i \nu_q \]

\[ = \lambda_q^{-2} \sum_{i=1}^{p-1} \nu_i \nu_i^T \lambda_i \nu_q. \]  

(153)

Note that we cannot resolve the sum with the Kronecker delta at this point since \( q \) may be outside the sum’s range.

**Lower left block:**

We repeat the differential equation

\[ \dot{i} = w^T Cw - l w^T w, \]  

(157)

determine the derivative

\[ \frac{\partial \dot{i}}{\partial w} \]

\[ = 2 (w^T C - l w^T), \]  

(158)

determine the derivative at the fixed point

\[ \left( \frac{\partial \dot{i}}{\partial w} \right) \bigg|_{w=v_q, \lambda=\lambda_q} \]

\[ = 2 (\nu_q^T C - \lambda_q \nu_q^T) \]

\[ = 0^T_n, \]  

(159)

and transform:

\[ \left( \frac{\partial \dot{i}}{\partial w} \right) \bigg|_{w=v_q, \lambda=\lambda_q} \quad V \]

\[ = 0^T_n. \]  

(160)
Lower right block:

We repeat the differential equation

\[ \dot{l} = w^T C w - lw^T w, \]  

(162)

determine the derivative

\[ \frac{\partial \dot{l}}{\partial l} = -w^T w, \]  

(163)

and determine the derivative for the fixed point

\[ \left( \frac{\partial \dot{l}}{\partial l} \right) \bigg|_{w = v_q, l = \lambda_q} = -v_q^T v_q \]  

(164)

\[ = -1 \]  

(165)

(note that the transformation is an identity mapping for lower right block).

We combine the results for the 4 blocks and obtain

\[
\begin{align*}
\bar{J}^* &= \\
&= \left( \begin{array}{ccc}
0_{p-1,p-1} & 0_{p-1} & 0_{p-1,n-p} \\
0_{p-1} & \lambda_q^{-1} \Lambda_p & 0_{n-p} \\
0_{p-1,n-p} & 0_{n-p} & \lambda_q^{-1} \Lambda_{n-p}
\end{array} \right) - e_q e_q^T - \mathbf{I}_n - \lambda_q^{-2} \sum_{i=1}^{p-1} e_i \lambda_i \delta_{i,q} \\
&\quad - e_p e_p^T - 1
\end{align*}
\]  

(166)

Since the analysis of the eigenvalues is complex, we distinguish between 3 different cases.

For the first case, we look at the desired fixed point \( q = p \). The upper right term disappears (since \( i \neq q \) for \( i = 1, \ldots, p - 1 \)) and we get:

\[
\begin{align*}
\bar{J}^* \bigg|_{q=p} &= \\
&= \left( \begin{array}{ccc}
0_{p-1,p-1} & 0_{p-1} & 0_{p-1,n-p} \\
0_{p-1} & \lambda_q^{-1} \Lambda_p & 0_{n-p} \\
0_{p-1,n-p} & 0_{n-p} & \lambda_q^{-1} \Lambda_{n-p}
\end{array} \right) - e_p e_p^T - \mathbf{I}_n \quad 0_n
\end{align*}
\]  

(167)

\[
\begin{align*}
&= \left( \begin{array}{ccc}
0_{p-1,p-1} & 0_{p-1} & 0_{p-1,n-p} \\
0_{p-1} & 0_{n-p} & \lambda_q^{-1} \Lambda_{n-p}
\end{array} \right) - \mathbf{I}_n \quad 0_n
\end{align*}
\]  

(168)

\[
\begin{align*}
&= \left( \begin{array}{ccc}
-I_{p-1} & 0_{p-1} & 0_{p-1,n-p} \\
0_{p-1} & -1 & 0_{n-p}
\end{array} \right) - \mathbf{I}_n \quad 0_n
\end{align*}
\]  

(169)

29
Since this matrix is diagonal, its eigenvalues $\alpha_k$, $k = 1, \ldots, n + 1$ appear on the diagonal. We get:

\[
\begin{align*}
\alpha_k &= -1 & \text{for } k = 1, \ldots, p - 1 \\
\alpha_p &= -1 \\
\alpha_k &= \lambda_p^{-1} \lambda_k - 1 \approx -1 & \text{for } k = p + 1, \ldots, n, \lambda_k \ll \lambda_p \\
\alpha_{n+1} &= -1.
\end{align*}
\] (170) (171) (172) (173)

We see that fixed point $p$ is an attractor, and the convergence speed is about the same from all directions.

Note that stability only requires relations such as $\lambda_k < \lambda_p$ to ensure negative eigenvalues of the Jacobian, but not $\lambda_k \ll \lambda_p$ which just guarantees that the eigenvalues are close to $-1$. However, the convergence speed depends on the differences between the eigenvalues of $C$.

For the second case, we look at fixed point $q$ which corresponds to an eigenpair following $p$, i.e. $q > p$. Again, the upper right term disappears and we get:

\[
\begin{bmatrix}
0_{p-1,p-1} & 0_{p-1} & 0_{p-1,n-p} \\
0_{p-1} & 0_{n-p} & \lambda_q^{-1} \lambda_p \\
0_{p-1,n-p} & 0_{n-p} & 0_{n-p}
\end{bmatrix}
- \begin{bmatrix}
e_q e_q^T - I_n \quad \lambda_q^{-2} \sum_{i=1}^{p-1} e_i \delta_i,q
\end{bmatrix}
\] (174)

\[
= \begin{bmatrix}
0_{p-1,p-1} & 0_{p-1} & 0_{p-1,n-p} \\
0_{p-1} & 0_{n-p} & \lambda_q^{-1} \lambda_p \\
0_{p-1,n-p} & 0_{n-p} & 0_{n-p}
\end{bmatrix}
- \begin{bmatrix}
e_q e_q^T - I_n \\
0_n
\end{bmatrix}
\] (175)

\[
= \begin{bmatrix}
-I_{p-1} & 0_{p-1} & 0_{p-1,n-p} \\
0_{p-1} & \lambda_q^{-1} \lambda_p - 1 & 0_{n-p} \\
0_{p-1,n-p} & 0_{n-p} & \lambda_q^{-1} \Lambda_n - I_{n-p}
\end{bmatrix}
- \begin{bmatrix}
e_q e_q^T \\
0_n
\end{bmatrix}
\] (176)

The eigenvalues $\alpha_k$, $k = 1, \ldots, n + 1$, can again be read out from the diagonal. Index $q$ lies in the lower right block of the inner block matrix, so we get eigenvalues for the upper left block, for the middle block, and for 3 different regions in the lower right block (before, at, and after $q$):

\[
\begin{align*}
\alpha_k &= -1 < 0 & \text{for } k = 1, \ldots, p - 1 \\
\alpha_p &= \lambda_q^{-1} \lambda_p - 1 > 0 & \text{for } p < q, \lambda_p \gg \lambda_q \\
\alpha_k &= \lambda_q^{-1} \lambda_k - 1 > 0 & \text{for } k = p + 1, \ldots, q - 1, \lambda_k \gg \lambda_q \\
\alpha_q &= \lambda_q^{-1} \lambda_q - 2 = -1 < 0 \\
\alpha_k &= \lambda_q^{-1} \lambda_k - 1 < 0 & \text{for } k = q + 1, \ldots, n, \lambda_k \ll \lambda_q \\
\alpha_{n+1} &= -1 < 0
\end{align*}
\] (177) (178) (179) (180) (181) (182)
We conclude that the fixed points following \( p \) are always saddle points.

The **third case** is the critical case and concerns \( q < p \), i.e. fixed points preceding \( p \). Here the upper right term does not disappear. We get

\[
\begin{align*}
\mathbf{J}^+ |_{q < p} &= \begin{pmatrix}
0_{p-1,p-1} & 0_{p-1} & 0_{p-1,n-p} \\
0^T_{p-1} & \lambda_q^{-1} \lambda_p & 0^n_{T,p-1} \\
0^T_{p-1,n-p} & 0_{n-p} & \lambda_q^{-1} \Lambda_{n-p}
\end{pmatrix} - e_q e_q^T - I_n - \lambda_q^{-2} \sum_{i=1}^{p-1} e_i \lambda_i \delta_{i,q} \\
&= \begin{pmatrix}
0_{p-1,p-1} & 0_{p-1} & 0_{p-1,n-p} \\
0^T_{p-1} & \lambda_q^{-1} \lambda_p & 0^n_{T,p-1} \\
0^T_{p-1,n-p} & 0_{n-p} & \lambda_q^{-1} \Lambda_{n-p}
\end{pmatrix} - e_q e_q^T - I_n - \lambda_q^{-1} e_q \\
&= \begin{pmatrix}
-1 & 0_{p-1} & 0_{p-1,n-p} \\
0^T_{p-1} & \lambda_q^{-1} \lambda_p - 1 & 0^n_{T,p-1} \\
0^T_{p-1,n-p} & 0_{n-p} & \lambda_q^{-1} \Lambda_{n-p} - I_{n-p}
\end{pmatrix} - e_q e_q^T - \lambda_q^{-1} e_q
\end{align*}
\]

(183)

(184)

(185)

The single off-diagonal element at row \( q \) of column \( n + 1 \) doesn’t affect eigenvalues, since the matrix is triangular and still all eigenvalues \( \alpha_k, k = 1, \ldots, n+1 \) are found on the main diagonal.

Index \( q \) lies in the upper left block, so we get eigenvalues for 3 different regions in the upper left block (before, at, and after \( q \)), for the middle block, and for the lower right block:

\[
\begin{align*}
\alpha_k &= -1 < 0 \quad \text{for } k = 1, \ldots, q - 1 \\
\alpha_q &= -2 < 0 \\
\alpha_k &= -1 < 0 \quad \text{for } k = q + 1, \ldots, p - 1 \\
\alpha_p &= \lambda_q^{-1} \lambda_p - 1 < 0 \quad \text{for } q < p, \; \lambda_q \gg \lambda_p \\
\alpha_k &= \lambda_q^{-1} \lambda_k - 1 < 0 \quad \text{for } k = p + 1, \ldots, n, \; \lambda_k \ll \lambda_q \\
\alpha_{n+1} &= -1 < 0.
\end{align*}
\]

(186)

(187)

(188)

(189)

(190)

(191)

We would have to conclude from this result that there are additional stable fixed points at undesired indices \( q < p \). However, this stands in conflict with observations from simulations which prompted us to re-examine the stability analysis. The problem is visible in equation (131): For \( q < p \), one term \( (\lambda_i - \lambda_q)^{-1} \) for summation indices \( i = 1 \ldots p - 1 \) is undefined. The other two stability cases are unaffected, since for \( q > p \), the index \( q \) lies outside the summation range. Unfortunately, the problem is no longer visible in (135) since the critical terms have disappeared. Nevertheless, the analysis of the third case above is flawed since the fixed points under consideration don’t even exist any longer after the multiplication with the inverse Hessian in the Newton descent.
8.3.2. Stability Analysis via Perturbation

To avoid the problem with the stability analysis via the eigenvalues of the Jacobian, we re-examine stability by a different method: We introduce small perturbations at the original fixed points of the Lagrange criterion (i.e. including those that become undefined after the inversion of the Hessian in the Newton descent). At the point of the perturbed state, we analyze the scalar product between the perturbation and the direction of movement. If we can show that this scalar product is negative for all perturbations, the point under consideration is approached. If there are perturbations where the scalar product is positive, there are directions where the movement leads away from this point. Since the perturbations are small, we can eliminate all terms of higher order, if terms of lower order exist.

We start from $w = v_q + \mu$ and $l = \lambda_q + \nu$:

\[
\begin{align*}
\dot{w} & = l^{-1}(Cw - [w^T Cw] w) \\
& + \frac{1}{2} w (w^T w - 1) \\
& - \left( \sum_{i=1}^{p-1} \left[ \{\lambda_i - l\}^{-1} + l^{-1} \right] v_i v_i^T \right) (Cw - lw) \\
& = (\lambda_q + \nu)^{-1} \left( C[v_q + \mu] - \left[ \{v_q + \mu\}^T C[v_q + \mu] \right] [v_q + \mu] \right) \\
& + \frac{1}{2} (v_q + \mu) \left( [v_q + \mu]^T [v_q + \mu] - 1 \right) \\
& - \left( \sum_{i=1}^{p-1} \left[ \{\lambda_i - (\lambda_q + \nu)\}^{-1} + (\lambda_q + \nu)^{-1} \right] v_i v_i^T \right) (C[v_q + \mu] - [\lambda_q + \nu][v_q + \mu]) \\
& \approx (\lambda_q + \nu)^{-1} \left( C\mu - 2 [\mu^T \lambda_q v_q] v_q - \lambda_q \mu \right) \\
& + v_q v_q^T \mu \\
& - \left( \sum_{i=1}^{p-1} \left[ \{\lambda_i - (\lambda_q + \nu)\}^{-1} + (\lambda_q + \nu)^{-1} \right] v_i v_i^T \right) (C\mu - \lambda_q \mu - \nu v_q) \\
& \approx \lambda_q^{-1} \left( C\mu - 2 [\mu^T \lambda_q v_q] v_q - \lambda_q \mu \right) \\
& + v_q v_q^T \mu \\
& - \left( \sum_{i=1}^{p-1} \left[ \{\lambda_i - (\lambda_q + \nu)\}^{-1} + \lambda_q^{-1} \right] v_i v_i^T \right) (C\mu - \lambda_q \mu - \nu v_q)
\end{align*}
\]
\[ \frac{d}{dt} \begin{pmatrix} \lambda_q^{-1} C \mu - v_q \dot{v}_q^T \mu - \mu \\ \frac{d}{dt} \hat{\mathbf{w}} \\ \hat{l} \end{pmatrix} = \mu^T \dot{\mathbf{w}} + \nu \dot{l} \]

\[ \approx \lambda_q^{-1} \mu^T C \mu - \mu^T \dot{v}_q \dot{v}_q^T \mu - \mu^T \mu - \nu^2 \]

\[ - \sum_{i=1}^{p-1} ([\lambda_i - \{\lambda_q + \nu\}]^{-1} + \lambda_q^{-1}) \mu^T \dot{v}_i \dot{v}_i^T \mu \approx \lambda_q^{-1} \mu^T C \mu - \mu^T \mu - \nu^2 \]

\[ \approx \lambda_q^{-1} \sum_{i=1}^{n} \mu^T v_i \lambda_i v_i^T \mu - (v_q^T \mu)^2 - \mu^T \mu - \nu^2 \]

\[ - \sum_{i=1}^{p-1} ([\lambda_i - \{\lambda_q + \nu\}]^{-1} + \lambda_q^{-1}) (v_i^T \mu)^2 \]

\[ + \sum_{i=1}^{p-1} ([\lambda_i - \{\lambda_q + \nu\}]^{-1} + \lambda_q^{-1}) \nu \mu^T \dot{v}_i \dot{v}_i^T \mu \approx \sum_{i=1}^{n} \lambda_q^{-1} \lambda_i (v_i^T \mu)^2 - (v_q^T \mu)^2 - \mu^T \mu - \nu^2 \]

where we approximated \((\lambda_q + \nu)^{-1} \approx \lambda_q^{-1} - \nu \lambda_q^{-2}\) and omitted terms of second order and above.

The same perturbation transformation is done for \(\hat{l}\):

\[ \hat{l} = w^T C \hat{w} - l \hat{w}^T w \]

\[ = (v_q + \mu)^T C (v_q + \mu) - (\lambda_q + \nu) (v_q + \mu)^T (v_q + \mu) \]

\[ = v_q^T C v_q + \mu^T C v_q + v_q^T C \mu + \mu^T C \mu \]

\[ - \lambda_q v_q^T v_q - \lambda_q \mu^T v_q - \lambda_q v_q^T \mu - \lambda_q \mu^T \mu - \nu v_q^T v_q - \nu \mu^T v_q - \nu v_q^T \mu - \nu \mu^T \mu \approx -\nu. \]
We start with the critical cases to check whether the results coincide with the former analysis.

We study all three stability cases as before, even though only one is critical; we use the non-critical cases to check whether the results coincide with the former analysis.

We start with the first case \( q = p \):

\[
\sum_{i=1}^{n} (\lambda_i^{-1} \lambda_i - 1) (v_i^T \mu)^2 - (v_q^T \mu)^2 - \nu^2
\]

\[
- \sum_{i=1}^{p-1} ([\lambda_i - \{\lambda_q + \nu\}]^{-1} + \lambda_q^{-1}) (\lambda_i - \lambda_q) (v_i^T \mu)^2
\]

\[
+ \sum_{i=1}^{p-1} ([\lambda_i - \{\lambda_q + \nu\}]^{-1} + \lambda_q^{-1}) \nu \mu^T v_i \delta_{i,q}
\]

We study all three stability cases as before, even though only one is critical; we use the non-critical cases to check whether the results coincide with the former analysis.
We continue with the second case \( q > p \)

\[
\sum_{i=p+1}^{n} (\lambda_q^{-1} \lambda_i - 1) (v_i^T \mu)^2 - (v_q^T \mu)^2 - \nu^2
\]

\[
- \sum_{i=1}^{p-1} ([\lambda_i - \{ \lambda_p + \nu \}]^{-1} + \lambda_q^{-1}) (\lambda_i - \lambda_q) (v_i^T \mu)^2
\]

\[
+ \sum_{i=1}^{p-1} ([\lambda_i - \{ \lambda_q + \nu \}]^{-1} + \lambda_q^{-1}) \nu \mu^T v_i \delta_{i,q}
\]

\[
= \sum_{i=1}^{n} (\lambda_q^{-1} \lambda_i - 1) (v_i^T \mu)^2 - (v_q^T \mu)^2 - \nu^2
\]  

\[
\text{for } q > p; \text{the quadratic terms are independent of each other. We observe that the coefficients}
\]

\[
\text{coincide with the eigenvalue spectrum obtained from the Jacobian.}
\]
In the first term, the coefficients of the squared expression are positive since \( \lambda_q < \lambda_i \) for \( i < q \). Since \( q > p \), there is at least one such term, so we have a saddle point. As before, the quadratic terms are independent of each other. Again we observe the correspondence between the coefficients and the eigenvalues of the Jacobian.

We now analyze the critical third case \( q < p \) for which the analysis via the Jacobian failed:

\[
\sum_{i=1}^{n} (\lambda_i^{-1} \lambda_i - 1) (v_i^T \mu)^2 - (v_q^T \mu)^2 - \nu^2
\]  

\[
- \sum_{i=1}^{p-1} ([\lambda_i - \{\lambda_q + \nu]\}^{-1} + \lambda_q^{-1})(\lambda_i - \lambda_q)(v_i^T \mu)^2
\]  

\[
+ \sum_{i=1}^{p-1} ([\lambda_i - \{\lambda_q + \nu\}]^{-1} + \lambda_q^{-1}) \nu \mu^T v_i \delta_{i,q}
\]  

In the first term, the coefficients of the squared expression are positive since \( \lambda_q < \lambda_i \) for \( i < q \). Since \( q > p \), there is at least one such term, so we have a saddle point. As before, the quadratic terms are independent of each other. Again we observe the correspondence between the coefficients and the eigenvalues of the Jacobian.
\[
\sum_{i=1}^{q-1} (\lambda_i^{-1} \lambda_i - 1)(v_i^T \mu)^2 + (\lambda_q^{-1} \lambda_q - 1)(v_q^T \mu)^2 + \sum_{i=q+1}^{n} (\lambda_i^{-1} \lambda_i - 1)(v_i^T \mu)^2
\]

\[
= \sum_{i=1}^{q-1} (\lambda_i^{-1} \lambda_i - 1)(v_i^T \mu)^2 + \sum_{i=q+1}^{n} (\lambda_i^{-1} \lambda_i - 1)(v_i^T \mu)^2
\]

\[
- (v_q^T \mu)^2 - \nu^2
\]

\[
- \sum_{i=1}^{q-1} (\lambda_i - \{\lambda_q + \nu\})^{-1} + \lambda_i^{-1}(\lambda_i - \lambda_q)(v_i^T \mu)^2
\]

\[
- (\lambda_q - \{\lambda_q + \nu\})^{-1} + \lambda_q^{-1}(\lambda_q - \lambda_q)(v_q^T \mu)^2
\]

\[
+ (\lambda_q - \{\lambda_q + \nu\})^{-1} + \lambda_q^{-1}(\nu \mu^T v_q)
\]

\[
= \sum_{i=1}^{q-1} (\lambda_i^{-1} \lambda_i - 1)(v_i^T \mu)^2 + \sum_{i=q+1}^{n} (\lambda_i^{-1} \lambda_i - 1)(v_i^T \mu)^2
\]

\[
- (v_q^T \mu)^2 - \nu^2
\]

\[
- \sum_{i=1}^{q-1} \lambda_i^{-1} \lambda_i(v_i^T \mu)^2
\]

\[
- \sum_{i=q+1}^{p-1} \lambda_i^{-1} \lambda_i(v_i^T \mu)^2
\]

\[
- \mu^T v_q
\]

\[
= \left( -\sum_{i=1}^{q-1} [v_i^T \mu]^2 \right) + \sum_{i=q+1}^{p-1} (\lambda_i^{-1} \lambda_i - 1)(v_i^T \mu)^2 + \sum_{i=q+1}^{n} (\lambda_i^{-1} \lambda_i - 1)(v_i^T \mu)^2
\]

\[
- (v_q^T \mu)^2 - \nu^2 - \sum_{i=q+1}^{p-1} \lambda_i^{-1} \lambda_i(v_i^T \mu)^2 - \mu^T v_q
\]

\[
= \left( -\sum_{i=1}^{q} [v_i^T \mu]^2 \right) - \sum_{i=q+1}^{p-1} (v_i^T \mu)^2 + \sum_{i=p}^{n} (\lambda_i^{-1} \lambda_i - 1)(v_i^T \mu)^2 - \nu^2 - \mu^T v_q
\]
\[
-w_p \sum_{i=1}^{p-1} \left[ \mathbf{v}_i^T \mathbf{\mu} \right]^2 + \sum_{i=p}^{n} (\lambda_q^{-1} \lambda_i - 1) (\mathbf{v}_i^T \mathbf{\mu})^2 - \nu^2 - \mathbf{\mu}^T \mathbf{v}_q.
\]

We see (incomplete) correspondences between the coefficients of the first three terms (which are all negative) and the eigenvalues of the Jacobian determined above. However, we now have the additional term \(-\mathbf{\mu}^T \mathbf{v}_q\). This term can become positive, e.g. if \(\mathbf{\mu}\) points into the direction \(-\mathbf{v}_q\). If we insert \(\mathbf{\mu} = -\varepsilon \mathbf{v}_q\) with small \(\varepsilon\), only the first and last summand survive, and the term with \(\nu\) has to be preserved since it can’t be zero in this case (as this would result in undefined terms in the differential equation):

\[
\left( -w_p \sum_{i=1}^{p-1} \left[ \mathbf{v}_i^T \mathbf{\mu} \right]^2 \right) + \sum_{i=p}^{n} (\lambda_q^{-1} \lambda_i - 1) (\mathbf{v}_i^T \mathbf{\mu})^2 - \nu^2 - \mathbf{\mu}^T \mathbf{v}_q
\]

\[
= (-\varepsilon^2) + \varepsilon - \nu^2
\]

\[
\approx \varepsilon - \nu^2
\]

which becomes positive for \(\varepsilon > \nu^2\). Therefore the critical points under consideration are saddle points.

Over all three cases, this shows that the system converges to the desired fixed point \(p\).

### 8.4. Learning Rule System

To derive the learning rule system, we continue from (121), replace \(w = w_p\) and \(l = l_p\), replace true eigenvectors by estimates \(\mathbf{v}_i \approx w_i\), and replace true eigenvalues by estimates \(\lambda_i \approx l_i\):

\[
\dot{w}_p = l_p^{-1} (\mathbf{C} w_p - [w_p^T \mathbf{C} w_p] w_p) + \frac{1}{2} w_p (w_p^T w_p - 1)
- \left( \sum_{i=1}^{p-1} \left[ l_i - l_p \right]^{-1} + l_p^{-1} \right) w_i w_i^T (\mathbf{C} w_p - l_p w_p).
\]

For the eigenvalue estimates, this leads to

\[
\dot{l}_p = w_p^T \mathbf{C} w_p - l_p w_p^T w_p.
\]

We see no way how (237) and (238) could be turned into matrix form.

### 8.5. Simulations

For the learning rule system (237) (238) we performed simulations with artificial data using Octave. The problem dimension was chosen as \(n = 10\), the subspace dimension as \(m = 5\). A covariance matrix was determined from a randomly generated orthogonal matrix of true eigenvectors and a log-linear set of true eigenvalues (\(\exp(-i)\) with index \(i\)).
**Stability experiment:** We use the learning rule for the desired fixed point \( p \). The system state is computed by adding a small perturbation to fixed point \( q \). We determine the scalar product between the permutation and the direction vector of the learning rule system. By repeating this computation 100,000 times for different perturbations, we observe instability for \( p \neq q \) (scalar product is sometimes positive) and stability for \( p = q \) (scalar product is never positive), confirming the analytical stability results.

**Numerical solution:** We solve the learning rule system numerically by applying Euler’s method for 100,000 steps with a step width \( \gamma = 10^{-3} \). The previous \( p - 1 \) eigenvector and eigenvalue estimates are set to the true values. We randomly initialize the \( p \)-th eigenvector estimate (normalized to unit length). The behavior differs depending on the initial \( p \)-th eigenvalue estimate. With small initial eigenvalue estimates, the system typically converges to the desired fixed point. If the initial eigenvalue estimates are too small, the system sometimes diverges and delivers “not a number” (NaN) solutions. With large initial eigenvalue estimates, the system sometimes converges to a zero eigenvector estimate with an apparently arbitrary eigenvalue estimate. As pointed out in section 8.2), there is a set of additional fixed points introduced by applying Newton’s method, and the simulations show that these fixed points appear to be semi-stable. We observed that a normalization of the \( p \)-th eigenvector estimates to unit length in each step guarantees convergence to the desired fixed point. We assume that the instabilities are caused by large values obtained in the inverse eigenvalue terms. If we start with random eigenvalue estimates in the vicinity of the eigenvalue in the desired fixed point, the learning rule system converges to the desired fixed point.

In summary, the learning rule system works as expected in the vicinity of the desired fixed point, but has stability problems when started in a larger distance.

### 8.6. Relation to Deflation

We see a structural similarity of the learning rule systems derived for the principal eigenpair (with deflation) and the learning rule system derived for the arbitrary eigenpair. If we compare the deflation-related terms in \( \dot{w}_p \) from (97) (estimate of principal eigenpair and deflation)

\[
\left(- \sum_{i=1}^{p-1} l_i l_p^{-1} w_i w_i^T w_p \right) + \sum_{i=1}^{p-1} l_i l_p^{-1} (w_i^T w_p)^2 w_p
\]

with the related terms in \( \dot{w}_p \) from (237) (arbitrary eigenpair)

\[
\left(- \sum_{i=1}^{p-1} \left[ \{l_i - l_p\}^{-1} + l_p^{-1} \right] w_i w_i^T C w_p \right) + \sum_{i=1}^{p-1} \left(\{l_i - l_p\}^{-1} l_p + 1\right) w_i w_i^T w_p,
\]

we also see similarities, but the mechanisms are clearly different with not obvious mapping between them. There is a further difference in that the deflation-related terms for \( l_p \) in (100) are absent from (238).
It is presently unclear whether there are differences with respect to convergence speed or stabil-
ity for larger learning rates between the two versions.

9. Conclusions and Future Work

This work describes a Lagrange-Newton framework for the derivation of coupled learning rules
which we feel is superior to our earlier two attempts at devising suitable frameworks. For the
example of PCA we could demonstrate for two different cases that learning rule systems with
the desired favorable convergence properties can be derived from this framework. The first case
— a derivation for the principal eigenpair — leads to the same result as the derivations from
our earlier frameworks. The second case — a derivation for an arbitrary eigenpair — leads to
novel learning rules with an interesting alternative to deflation.

A stability analysis for exact Hessians already indicates that — at least for the PCA case — the
framework leads to learning rules which only have stable fixed points at the desired location, i.e.
at those fixed points for which the Hessian was determined; all other locations are saddle points.
However, exact Hessians are unknown when learning rules are applied since they can only be
determined if the eigenpair that needs to be estimated is already known. The usefulness of our
framework is furthermore confirmed by the stability analysis for the two cases mentioned above
which confirms that both learning rules converge to the desired fixed points. However, earlier
attempts revealed that undesired fixed points can appear depending on which approximations
are used in the derivation. Since the effect of approximations on the stability is difficult to
predict, a stability analysis is always required.

Simulations for the second case (the first one has been studied before) are in accordance with
the results of the stability analysis. However, depending on the initial values, the learning rule
system may converge to an additional set of fixed points which is introduced by the multiplica-
tion with the inverse Hessian, since the Hessian is undefined at these points. It is well known
that Newton’s method only works in the vicinity of the fixed point but can diverge in larger
distance. Future work will therefore explore whether the learning rule needs to be modified
in larger distance from the fixed point, e.g. by a Levenberg-Marquardt modification (see e.g.
Chong and Zak [2001]).

We encountered a pitfall in the stability analysis of the second case: for one sub-case, the eigen-
values of the Jacobian indicated a stable undesired fixed point which was in conflict with the
simulation results. The reason was an undefined term which, however, later disappeared from
the derivation. We therefore had to repeat the stability analysis with a perturbation approach
which correctly indicates a saddle point.

In future work we will attempt to apply the Lagrange-Newton framework to symmetric rules as
we have studied before (Möller [2020b,c]).
References

J. Baker. Geometry optimization in cartesian coordinates: Constrained optimization. *Journal of Computational Chemistry*, 13(2):240–253, 1992.

E. K. P. Chong and S. H. Žak. *An Introduction to Optimization*. Wiley, 2nd edition, 2001.

M. P. Deisenroth, A. A. Faisal, and C. S. Ong. *Mathematics for Machine Learning*. Cambridge University Press, 2020.

K. I. Diamantaras and S. Y. Kung. *Principal Component Neural Networks. Theory and Applications*. John Wiley & Sons, 1996.

A. Kaiser, W. Schenck, and R. Möller. Coupled singular value decomposition of a cross covariance matrix. *International Journal of Neural Systems*, 20(4):293–318, 2010.

D. Kalman. Leveling with Lagrange: An alternate view of constrained optimization. *Mathematics Magazine*, 82(3):186–196, 2009.

X. Kong, C. Hu, and Z. Duan. *Principal Component Analysis Networks and Algorithms*. Springer Singapore / Science Press Beijing, 2017.

R. Möller. Derivation of coupled PCA and SVD learning rules from a Newton zero-finding framework. *arXiv:2003.11456*, 2020a.

R. Möller. Derivation of symmetric PCA learning rules from a novel objective function. *arXiv:2005.11689v2*, 2020b.

R. Möller. Improved convergence speed of fully symmetric learning rules for principal component analysis. *arXiv:2007.09426*, 2020c.

R. Möller and A. Könies. Coupled principal component analysis. *IEEE Transactions on Neural Networks*, 15(1):214–222, 2004.

G. R. Walsh. *Methods of Optimization*. John Wiley & Sons, 1975.

A. Lemmata

A.1. Lagrange Multiplier Method

Dimensions:

- \( n \): dimensionality of optimization problem, \( 3 \leq n \)
- \( m \): number of equality constraints, \( 1 \leq m \)
Matrices:

- $x$: arbitrary, $n \times 1$
- $f(x)$: objective function, scalar, $1 \times 1$
- $g(x)$: vector of equality constraints, arbitrary, $m \times 1$
- $g_j(x)$: single equality constraint, scalar, $1 \times 1$, vector element of $g$
- $\lambda$: vector of Lagrange multipliers, arbitrary, $m \times 1$
- $\lambda_j(x)$: single Lagrange multiplier, scalar, $1 \times 1$, vector element of $\lambda$
- $L$: Lagrangian, scalar, $1 \times 1$
- $\bar{H}$: bordered Hessian, symmetric, $(n + m) \times (n + m)$

A.1.1. Bordered Hessian

In the following we explore whether the extended objective function (over an extended variable vector containing the original variables and the Lagrange multipliers) has saddle points at all fixed points. We currently can’t provide a general statement on the eigenvalues, but only analyze the special case of PCA.

We start by deriving the general bordered Hessian. Given an objective function $f(x)$, equality constraints $g(x)$, and Lagrange multipliers $\lambda$, the Lagrangian of the constrained optimization problem is defined as

$$L(x, \lambda) = f(x) + \lambda^T g(x).$$  \hspace{1cm} (241)

The first-order derivatives (gradient of the Lagrangian) are

$$\frac{\partial}{\partial x} L(x, \lambda) = \frac{\partial}{\partial x} f(x) + \lambda^T \left( \frac{\partial}{\partial x} g(x) \right)$$  \hspace{1cm} (242)

$$\frac{\partial}{\partial \lambda} L(x, \lambda) = (g(x))^T.$$  \hspace{1cm} (243)

To form the bordered Hessian

$$\bar{H} = \begin{pmatrix} \frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} L(x, \lambda) \right)^T & \frac{\partial}{\partial x} \left( \frac{\partial}{\partial \lambda} L(x, \lambda) \right)^T \\ \frac{\partial}{\partial \lambda} \left( \frac{\partial}{\partial x} L(x, \lambda) \right)^T & \frac{\partial}{\partial \lambda} \left( \frac{\partial}{\partial \lambda} L(x, \lambda) \right)^T \end{pmatrix}$$  \hspace{1cm} (244)

we need to determine the second-order derivatives in the four blocks. We start with the upper-left block:

$$\frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} L(x, \lambda) \right)^T$$
\[
= \frac{\partial}{\partial x} \left( \frac{\partial f(x)}{\partial x} \right)^T + \frac{\partial}{\partial x} \left( \lambda^T \left[ \frac{\partial g(x)}{\partial x} \right] \right)^T \\
= \frac{\partial}{\partial x} \left( \frac{\partial f(x)}{\partial x} \right)^T + \frac{\partial}{\partial x} \left( \left[ \frac{\partial g(x)}{\partial x} \right]^T \lambda \right). 
\]

(245)

For the second term, we cannot find a closed-form matrix expression, but we can compute the derivative for row \(i\) according to (268)

\[
\left( \frac{\partial}{\partial x} \left[ \left\{ \frac{\partial g(x)}{\partial x} \right\}^T \lambda \right] \right)_{i,*} \\
= \lambda^T \left( \frac{\partial}{\partial x} \left[ \frac{\partial g(x)}{\partial x} \right] \right).
\]

(246)

which in turn can be expressed in single-element form as

\[
\frac{\partial}{\partial x} \left( \left[ \frac{\partial g(x)}{\partial x} \right]^T \lambda \right)_{i,j} = \left( \sum_{k=1}^{m} \lambda_k \left[ \frac{\partial}{\partial x} \left\{ \frac{\partial g_k(x)}{\partial x_i} \right\} \right] \right)_{i,j}^n \times n,
\]

(247)

thus we get

\[
\frac{\partial}{\partial x} \left( \frac{\partial L(x, \lambda)}{\partial x} \right)^T = \frac{\partial}{\partial x} \left( \frac{\partial f(x)}{\partial x} \right)^T + \left( \sum_{k=1}^{m} \lambda_k \left[ \frac{\partial}{\partial x} \left\{ \frac{\partial g_k(x)}{\partial x_i} \right\} \right] \right)_{i,j}^n \times n.
\]

(248)

The other three blocks of the bordered Hessian are easier to determine (note that a Hessian is always symmetric):

\[
\frac{\partial}{\partial x} \left( \frac{\partial L(x, \lambda)}{\partial x} \right)^T = \left( \frac{\partial g(x)}{\partial x} \right)^T 
\]

(250)

\[
\frac{\partial}{\partial x} \left( \frac{\partial L(x, \lambda)}{\partial \lambda} \right)^T = \frac{\partial g(x)}{\partial x} 
\]

(251)

\[
\frac{\partial}{\partial \lambda} \left( \frac{\partial L(x, \lambda)}{\partial \lambda} \right)^T = 0_{m,m}.
\]

(252)

The eigenvalues of the bordered Hessian at a given fixed point determine the stability of this fixed point.

I’m not aware of a general statement on the eigenvalues of the bordered Hessian. In the following, we apply the derivation to the PCA objective function (2) which we can rewrite in this notation as

\[
L(x, \lambda) = \frac{1}{2} x^T C x - \frac{1}{2} \lambda (x^T x - 1)
\]

(253)
thus
\[ f(x) = \frac{1}{2}x^T Cx \]  
(254)
\[ g(x) = -\frac{1}{2}(x^T x - 1). \]  
(255)
The corresponding unconstrained optimization (minimization) problem is
\[ \hat{f}(x) = -\frac{1}{2}x^T Cx \]  
(256)
and the corresponding Hessian is $-C$. Since $C$ is a covariance matrix which is positive semi-definite, all eigenvalues of the Hessian are negative or zero.

The bordered Hessian of the constrained optimization problem (over the extended variable vector) is
\[ \bar{H} = \begin{pmatrix} C - \lambda I_n & -x \\ -x^T & 0 \end{pmatrix}. \]  
(257)
We can proceed as in section 5: At a fixed point $p$, we get a transformed Hessian
\[ \bar{H}^* = \begin{pmatrix} \Lambda - \lambda_p I_n & -e_p \\ -e_p^T & 0 \end{pmatrix}. \]  
(258)
Its eigenvalues $s$ are determined from
\[
\det \left\{ \bar{H}^* - sI_{n+1} \right\} = \begin{vmatrix} (\lambda_1 - \lambda_p) - s & \cdots & (\lambda_{p-1} - \lambda_p) - s \\ \vdots & \ddots & \vdots \\ (\lambda_{p+1} - \lambda_p) - s & \cdots & (\lambda_n - \lambda_p) - s \\ -s & \cdots & -s_{n+1} \end{vmatrix} \]  
(259)
\[ = 0 \]  
(260)
We obtain the eigenvalues $s$ by analyzing under which conditions entire rows become zero, or under which conditions adding multiples of rows to other rows produces zero rows, and obtain:
\[ s_k = \lambda_k - \lambda_p \quad \text{for } k = 1, \ldots, n, \ k \neq p \]  
(261)
\[ s_p = -1 \]  
(262)
\[ s_{n+1} = 1. \]  
(263)
Already $s_p$ and $s_{n+1}$ indicate that all fixed points are saddle points. Moreover, for $p \neq 1$ and $p \neq n$, we have a mix of positive and negative values for $s_k$ (note that we assume descending eigenvalues $\lambda_k$ in $\Lambda$).

Neither following the positive nor following the negative gradient will converge to any fixed point (if we would have only positive or only negative eigenvalues, we would get convergence for either the negative or the positive gradient).
A.2. Derivatives

Derivatives presented in the following without giving a derivation were computed using the tool at [www.matrixcalculus.org]. Note that according to our definition of partial derivatives, the gradient is a row vector (transposed relative to the output of the tool) and the derivative of a vector with respect to a vector produces the standard Jacobian form (same as output of the tool) (overall we use the same convention as in [Deisenroth et al., 2020], p.127).

Given index $n: 1 \leq n$ and matrices $x$: arbitrary, $n \times 1$; $A$: square, $n \times n$; $S$: symmetric, $n \times n$, we have:

$$\frac{\partial}{\partial x} \left( [x^T S x] x \right) = 2xx^T S + (x^T S x) I_n$$  \hspace{1cm} (264)

$$\frac{\partial}{\partial x} \left( [x^T x] x \right) = 2xx^T + (x^T x) I_n$$  \hspace{1cm} (265)

Given indices $n: 1 \leq n$; $m: 1 \leq m$; $i: 1 \leq i \leq n$ and matrices $x$: arbitrary, $n \times 1$; $a$: constant, arbitrary, $m \times 1$; $B(x)$: function of $x$, arbitrary, $m \times n$; $b_i(x)$: function of $x$, arbitrary, $m \times 1$, column vector of $B$, we have

$$\left( \frac{\partial}{\partial x} \left[ \{B(x)\}^T a \right] \right)_{i,*}$$

$$= \frac{\partial}{\partial x} \left[ \{B(x)\}^T a \right]_i$$  \hspace{1cm} (266)

$$= \frac{\partial}{\partial x} \left[ b_i(x)^T a \right]$$  \hspace{1cm} (267)

$$= a^T \left( \frac{\partial}{\partial x} b_i(x) \right).$$  \hspace{1cm} (268)

A.3. Triangular Matrices

**Lemma 1.** Given indices $m: 2 \leq m \leq n$; $p: 2 \leq p \leq m$ and matrix $A$: square, $m \times m$, we have for column $p$ of a strictly upper triangular matrix:

$$(\text{sut} \{A\})_p = \begin{pmatrix} I_{p-1} & 0_{p-1,m-p+1} \\ 0_{m-p+1,p-1} & 0_{p-1,m-p+1} \end{pmatrix} (A)_p$$  \hspace{1cm} (269)

and for the special case $p = 1$

$$(\text{sut} \{A\})_1 = 0_m$$  \hspace{1cm} (270)

**Lemma 2.** Given indices $m: 2 \leq m \leq n$; $p: 2 \leq p \leq m$ and matrices $U$: arbitrary, $n \times m$; $V$: arbitrary, $n \times m$; $W$: arbitrary, $n \times m$, we have with Lemma [1] for column $p$ of the product of a matrix with a strictly upper triangular matrix of a matrix product:

$$(U \text{sut} \{V^T W \})_p$$
\[ = U \left( \sum \{ V^T W \} \right)_p \]  
\[ = U \left( \begin{pmatrix} I_{p-1} & 0_{p-1,m-p+1} \\ 0_{m-p+1,p-1} & 0_{m-p+1,m-p+1} \end{pmatrix} \right) (V^T W)_p \]  
\[ = U \left( \begin{pmatrix} I_{p-1} & 0_{p-1,m-p+1} \\ 0_{m-p+1,p-1} & 0_{m-p+1,m-p+1} \end{pmatrix} \right) [V^T w^]_p \]  
\[ = \left( \begin{pmatrix} I_{p-1} & 0_{p-1,m-p+1} \\ 0_{m-p+1,p-1} & 0_{m-p+1,m-p+1} \end{pmatrix} \right) (V^T w^) \]  
\[ = \sum_{i=1}^{m} \left( U \left( \begin{pmatrix} I_{p-1} & 0_{p-1,m-p+1} \\ 0_{m-p+1,p-1} & 0_{m-p+1,m-p+1} \end{pmatrix} \right) \right) (V^T w^) \]  
\[ = \sum_{i=1}^{m} \sum_{i=1}^{p-1} u_i (v^T w^) \]  
\[ = \sum_{i=1}^{m} u_i v^T w^ \]  

and for the special case \( p = 1 \), the left side is \( 0_m \) and the right side is the empty sum and therefore \( 0_m \) as well.

**Lemma 3.** Given indices \( m: 2 \leq m \leq n; p: 2 \leq p \leq m \) and matrices \( A \): square, \( m \times m \); \( D \): diagonal, \( m \times m \), we have with Lemma[7]

\[ \text{sut}\{AD\} = \text{sut}\{A\}D \]  
\[ (\text{sut}\{AD\})_p = \left( \begin{pmatrix} I_{p-1} & 0_{p-1,m-p+1} \\ 0_{m-p+1,p-1} & 0_{m-p+1,m-p+1} \end{pmatrix} \right) (AD)_p \]  
\[ = \left( \begin{pmatrix} I_{p-1} & 0_{p-1,m-p+1} \\ 0_{m-p+1,p-1} & 0_{m-p+1,m-p+1} \end{pmatrix} \right) A(D)_p \]  
\[ = \left( \begin{pmatrix} I_{p-1} & 0_{p-1,m-p+1} \\ 0_{m-p+1,p-1} & 0_{m-p+1,m-p+1} \end{pmatrix} \right) A \]  
\[ = \sum_{i=1}^{m} \left( \begin{pmatrix} I_{p-1} & 0_{p-1,m-p+1} \\ 0_{m-p+1,p-1} & 0_{m-p+1,m-p+1} \end{pmatrix} \right) \right) \left( \begin{pmatrix} D \end{pmatrix} \right)_i \]  
\[ = \sum_{i=1}^{m} \left( \begin{pmatrix} I_{p-1} & 0_{p-1,m-p+1} \\ 0_{m-p+1,p-1} & 0_{m-p+1,m-p+1} \end{pmatrix} \right) \right) \left( \begin{pmatrix} A \end{pmatrix} \right)_i \left( \begin{pmatrix} D \end{pmatrix} \right)_i \]  
\[ = \sum_{i=1}^{m} \left( \begin{pmatrix} A \end{pmatrix} \right)_i \left( \begin{pmatrix} D \end{pmatrix} \right)_i \]  

\[ = \sum_{i=1}^{m} \left( \begin{pmatrix} A \end{pmatrix} \right)_i \left( \begin{pmatrix} D \end{pmatrix} \right)_i \]
\[ \text{and the special case } p = 1 \text{ is obvious.} \]