CONVERGENCE ANALYSIS FOR PRINCIPAL COMPONENT FLOWS†

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A common framework for analyzing the global convergence of several flows for principal component analysis is developed. It is shown that flows proposed by Brockett, Oja, Xu and others are all gradient flows and the global convergence of these flows to single equilibrium points is established. The signature of the Hessian at each critical point is determined.

Keywords: principal component analysis, neural networks, gradient flows, phase portrait, Hessians

1. Introduction

In the theory of neural networks, dynamic systems methods are crucial for the analysis of learning algorithms and conversely, neural network learning algorithms provide interesting examples of dynamical systems that represent challenges for a rigorous mathematical analysis. Although some of these learning algorithms seem to work quite well in practice, their theoretical analysis still lacks a rigorous convergence theory. So far, most results in the literature have focused on local stability issues without addressing the problem of global convergence. In this paper we discuss a special class of learning algorithms for principal component analysis for which a complete phase portrait analysis can be developed.

In principal component analysis (PCA), the main goal is to extract dominant eigenvalues of a covariance matrix A for a sequence of random vectors. A number of neural learning algorithms for principal component or principal subspace analysis (PSA) have been proposed, starting from the early work of Oja (1982), Williams (1985) and Sanger (1989). For a more recent survey, see Baldi and Hornik (1995). In an influential paper, based on ideas from stochastic approximations, Oja and Karhunen

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(1985) demonstrated how to analyze one such algorithm in terms of the phase portrait analysis of an associated differential equation evolving on Euclidean space.

This dynamic system, termed the one-unit Oja flow, is a cubic differential equation

$$\dot{x} = \left(I - xx^\top\right) Ax \tag{1}$$

on $\mathbb{R}^n$. It has the remarkable property that—for any nonzero initial condition $x(0)$—its solutions converge, as $t \to \infty$, to the eigenvectors of the positive definite covariance matrix A.

Oja and Karhunen's work was the precursor for subsequent work on flows for principal component or principal subspace analysis. Oja (1989) considered the matrix generalization of (1)

$$\dot{X} = \left(I - XX^\top\right) AX, \quad X \in \mathbb{R}^{n\times k} \tag{2}$$

for principal subspace analysis and conjectured that solutions $X(t)$ of (2) converge, as $t \to \infty$, to an orthonormal basis matrix X_∞ of an invariant subspace of A. This conjecture was proven by Yan *et al.* (1994), where a phase portrait analysis of (2) was developed. In particular, an explicit description of the domain of attraction for the locally attracting equilibria was given. A characterization of stable manifolds for the other, unstable equilibrium points constitutes, however, an open problem.

The Oja flow is only capable of extracting the principal subspace of A but not the principal eigenvectors. Flows that achieve the principal component analysis were first proposed by Sanger (1989), Oja *et al.* (1992a; 1992b), and Xu (1993). The latter two actually deal with generalizations of the double bracket flow on orthogonal matrices introduced by Brockett (1991), see also (Helmke and Moore, 1994). Although a local stability analysis was developed around the equilibrium points, none of the above three papers really proved global convergence to the equilibrium points (Sanger actually has claimed to achieve this for his equation, but his argument is incomplete at an essential point). In this paper, we focus on Xu's principal component flow

$$\dot{X} = \left(I - XDX^\top\right) AXD \tag{3}$$

and prove the global convergence of (3) to the principal components of A. Moreover, the eigenvalues of the linearization of (3) around the quilibria are determined and thus a local stability analysis is given. The corresponding results for the flows proposed by Oja *et al.* (1992a; 1992b) are obtained as well.

A natural idea to establish the global convergence of (3) to its equilibrium points is to show that the system is the gradient flow of a suitable cost function. This is exactly what we are doing and our main result concerning global convergence is then deduced using an unfamiliar result by Łojasiewicz (1983) on real analytic gradient flows. Of course, this implies that the Oja flows (1), (2) are gradient flows, too. At first sight this seems to be in contradiction to the claim made by Baldi and Hornik (1991) that (1) is not a gradient flow. However, this contradiction is not a real one as Baldi and Hornik use a very restricted notion of the gradient flow. In mathematics, the gradient of a function is defined for an arbitrary Riemannian metric, while Baldi and Hornik consider the gradient only in the special case of the standard Euclidean inner product on $\mathbb{R}^n$. Both Xu's flow (3) and Oja's flow (1), (2) are—as we will show—bona fide gradient flows for some Riemannian metric on Euclidean space, and it is from this fact alone that a complete phase portrait analysis can be developed. A cost function for the Oja flow that serves as a Lyapunov function was also given by Wyatt and Elfadel (1995). However, these authors did not fully realize the connection to gradient flows, nor did they establish any general global convergence results.

This paper is based on the minicourse *Computation and Control—A Dynamical Systems Perspective* which was presented by the second author at the MTNS 2000 in Perpignan. Space limitations do not allow us to present here the material of the minicourse in any detail. We therefore decided to present the basic idea of computation via gradient flows through one example of the current research, i.e., that of a convergence analysis for neural networks. For further background and details on optimization via dynamic systems, we refer the reader to (Helmke and Moore, 1994).

2. Phase Portrait of the Oja-Brockett Flow

For $1 \leq k \leq n$ let $A \in \mathbb{R}^{n\times n}$ and $D \in \mathbb{R}^{k\times k}$ be positive definite matrices with $A = A^\top > 0$, $D = D^\top > 0$. Let $X \in \mathbb{R}^{n\times k}$. We consider the matrix differential equation on $\mathbb{R}^{n\times k}$

$$\dot{X} = AXD - XDX^\top AX. \tag{4}$$

We refer to (4) as the *Oja-Brockett system* as it is a natural generalization of both Oja's flow (2) for principal subspace analysis (for $D = I_k$) and Brockett's flow (Brockett, 1991)

$$\dot{X} = AXDX^\top X - XDX^\top AX$$

on orthogonal matrices for symmetric matrix diagonalization (for $k = n$ and $X \in \mathbb{R}^{n\times n}$ a real orthogonal matrix). The unconstrained flow (4) was first analyzed by Xu (1993), but the full analysis given here appears to be new.

Our first main result on the Oja-Brockett flow (4) on $\mathbb{R}^{n\times k}$ is that it is actually a gradient flow. Consider the real analytic function $f : \mathbb{R}^{n\times k} \to \mathbb{R}$ defined by

$$\begin{aligned} f(X) &:= \frac{1}{4}\mathrm{tr}(AXDX^\top)^2 - \frac{1}{2}\mathrm{tr}(A^2XD^2X^\top) \\ &= \frac{1}{4}\|(A^{\frac{1}{2}}XDX^\top)A^{\frac{1}{2}}\|^2 - \frac{1}{2}\|AXD\|^2, \end{aligned} \tag{5}$$

where $\|X\|^2 = \mathrm{tr}(XX^\top)$ denotes the Frobenius norm.

Lemma 1. $f : \mathbb{R}^{n\times k} \to \mathbb{R}$ *is a lower bounded function with compact sublevel sets.*

Proof. Let $L := A^{1/2}XD^{1/2}$. Then

$$\begin{aligned} f(X) &= \frac{1}{4}\|LL^\top\|^2 - \frac{1}{2}\|A^{\frac{1}{2}}LD^{\frac{1}{2}}\|^2 \\ &\geq \frac{1}{4}\|LL^\top\|^2 - \frac{1}{2}\|A^{\frac{1}{2}}\|^2 \ \|D^{\frac{1}{2}}\|^2 \ \|L\|^2 =: F(L). \end{aligned}$$

It therefore suffices to prove the result for the smooth function $L \mapsto F(L)$ on $\mathbb{R}^{n\times k}$. Using the singular value decomposition

$$L = U\Sigma U^\top, \quad \Sigma = \mathrm{diag}(\sigma_1, \dots, \sigma_l),$$

$\sigma_1 \geq \cdots \geq \sigma_l > 0,\ l \leq k$, we obtain

$$\begin{aligned} F(L) &= \frac{1}{4}\|\Sigma\Sigma^\top\|^2 - \frac{1}{2}\|A^{\frac{1}{2}}\|^2\|D^{\frac{1}{2}}\|^2\|\Sigma\|^2 \\ &= \frac{1}{4}\sum_{i=1}^{l}\sigma_i^4 - \frac{\gamma}{2}\sum_{i=1}^{l}\sigma_i^2, \end{aligned}$$

$\gamma := \|A^{1/2}\|^2\|D^{1/2}\|^2 > 0$. Obviously, the right hand side defines a smooth function in $(\sigma_1, \dots, \sigma_l)$ with compact sublevel sets. The minimum value is attained for $\sigma_1 = \cdots = \sigma_l = \sqrt{\gamma}$ and thus for all $L \in \mathbb{R}^{n\times k}$

$$F(L) \geq \frac{l}{4}\gamma^2 - \frac{l}{2}\gamma^2 = -\frac{l}{4}\gamma^2 \geq -\frac{k}{4}(\mathrm{tr}\ A)^2(\mathrm{tr}\ D)^2$$

is lower bounded with compact sublevel sets. ■

In the sequel, we endow $\mathbb{R}^{n\times k}$ with the Riemannian metric

$$\langle \Omega_1, \Omega_2\rangle_{A,D} := \mathrm{tr}(A\Omega_1 D\Omega_2^\top), \quad \Omega_i \in \mathbb{R}^{n\times k} \tag{6}$$

and the corresponding norm square

$$\|\Omega\|_{A,D}^2 := \mathrm{tr}(A\Omega D\Omega^\top).$$

Note that (6) defines a positive definite inner product on $\mathbb{R}^{n\times k}$, as A, D are assumed to be positive definite. If A, D were only positive semidefinite, then (6) would define a sub Riemannian metric. In order to avoid technical difficulties, we therefore assume the positive definiteness of A and D.

Recall that for any Riemannian metric $\langle\cdot,\cdot\rangle$ on $\mathbb{R}^{n\times k}$ an asociated gradient vector field $\mathrm{grad}\, f(X)$ is defined by the characterizing property

$$\mathrm{df}(X)\Omega = \langle \mathrm{grad}\, f(X), \Omega\rangle \qquad \forall\ X, \Omega \in \mathbb{R}^{n\times k}.$$

We now compute the gradient of our cost function f with respect to the above Riemannian metric.

Proposition 1. *The gradient of the cost function* (5) *with respect to the Riemannian metric* (6) *is the real analytic vector field* $\mathrm{grad}\, f : \mathbb{R}^{n\times k} \to \mathbb{R}^{n\times k}$ *given by*

$$\mathrm{grad}\, f(X) = XDX^\top AX - AXD.$$

In particular, the Oja-Brockett flow (4) *is just the negative gradient flow*

$$\dot{X} = -\mathrm{grad}\, f(X)$$

of the cost function (5).

Proof. The Fréchet derivative of $f : \mathbb{R}^{n\times k} \to \mathbb{R}$ at $X \in \mathbb{R}^{n\times k}$ is the linear functional $\mathrm{df}(X) : \mathbb{R}^{n\times k} \to \mathbb{R}$ given by

$$\begin{aligned}\mathrm{df}(X)\Omega &= \mathrm{tr}\left[\left(AXDX^\top AXD - A^2XD^2\Omega^\top\right)\right]\\ &= \langle XDX^\top AX - AXD, \Omega\rangle_{A,D}.\end{aligned}$$

Thus the gradient associated with the Riemannian metric $\langle\cdot,\cdot\rangle_{A,D}$ is seen as $\mathrm{grad}\, f(X) = XDX^\top AX - AXD$. ■

Choosing other Riemannian metrics on $\mathbb{R}^{n\times k}$, different gradients of the same function $f : \mathbb{R}^{n\times k} \to \mathbb{R}$ are obtained. Using the above proposition, we can now prove our main convergence result for the Oja-Brockett flow.

Theorem 1. *(i) The solutions $X(t) \in \mathbb{R}^{n\times k}$ of the Oja-Brockett flow* (4) *exist for all $t \geq 0$ and, as $t \to +\infty$, every solution of* (4) *converges to a single equilibrium point $X_\infty = \lim_{t\to\infty} X(t)$.*
(ii) The equilibrium points of (4) *are characterized by*

$$AX_\infty D = X_\infty DX_\infty^\top AX_\infty. \tag{7}$$

Moreover, every equilibrium point X_∞ satisfies the additional matrix equation

$$X_\infty^\top AX_\infty(X_\infty^\top X_\infty - I_k) = 0. \tag{8}$$

Proof. By Proposition 1, the Oja-Brockett flow is a real analytic gradient system for the real analytic cost function $f : \mathbb{R}^{n\times k} \to \mathbb{R}$. Since f has compact sublevel sets,

$$\left\{X \in \mathbb{R}^{n\times k};\quad f(X) \leq f(X_0)\right\}$$

is compact for all $X_0 \in \mathbb{R}^{n\times k}$ and thus the solutions $X(t)$ of $\dot{X} = -\mathrm{grad}\, f(X)$ stay in the compact set

$$X(t) \in \left\{X \in \mathbb{R}^{n\times k};\quad f(X) \leq f(X_0)\right\}$$

for all $t \geq 0$. Therefore the solutions $X(t)$ exist for all $t \geq 0$. Since $-\mathrm{grad}\, f(X)$ is real analytic in X, a result by Łojasiewicz (1983) implies that every solution $X(t)$ of (4) converges to a single equilibrium point X_∞ with $0 = -\mathrm{grad}\, f(X_\infty) = AX_\infty D - X_\infty DX_\infty^\top AX_\infty$. This proves (i).

In order to derive (8), we give an argument based on LaSalle's invariance principle. For this purpose, we consider the Lyapunov-type function $V : \mathbb{R}^{n\times k} \to \mathbb{R}$, $V(X) = (1/2)\|X^\top X - I_k\|^2$. A straightforward computation of the Lie derivative $\mathrm{L_F}V$ of V with respect to the gradient vector field $F := -\mathrm{grad}\, f$ yields

$$\begin{aligned}\dot{V}(X) &:= \mathrm{L_F}V(X) := \mathrm{tr}\nabla V(X)F(X)\\ &= -\mathrm{tr}\left[(X^\top X - I)(X^\top AXD + DX^\top AX)(X^\top X - I)\right] \leq 0\end{aligned}$$

since $X^\top AXD + DX^\top AX \geq 0$. Moreover,

$$\begin{aligned}\mathrm{L_F}V(X) = 0 \quad &\Longleftrightarrow \quad (X^\top AXD + DX^\top AX)^{\frac{1}{2}}(X^\top X - I) = 0\\ &\Longleftrightarrow \quad (X^\top AXD + DX^\top AX)(X^\top X - I) = 0.\end{aligned}$$

From (i) we already know that every solution $X(t)$ of (4) is bounded on $[0,\infty)$ and converges to a single equilibrium point X_∞ as $t \to +\infty$. Thus $\{X_\infty\}$ is the ω-limit set of $X(t)$. LaSalle's invariance principle then implies that $X_\infty \in (\mathrm{L_F}V)^{-1}(0)$, i.e., X_∞ satisfies

(a) $AX_\infty D = X_\infty D X_\infty^\top A X_\infty$,

(b) $(X_\infty^\top A X_\infty D + D X_\infty^\top A X_\infty)(X_\infty^\top X_\infty - I_k) = 0$.

Substituting (a) into (b) yields

$$\left(X_\infty^\top X_\infty D X_\infty^\top A X_\infty + D X_\infty^\top A X_\infty\right)\left(X_\infty^\top X_\infty - I_k\right) = 0,$$

i.e.,

$$\left(I_k + X_\infty^\top X_\infty\right) D X_\infty^\top A X_\infty \left(X_\infty^\top X_\infty - I_k\right) = 0.$$

Since D and $I_k + X_\infty^\top X_\infty$ are invertible, this implies (8). ■

We now derive an explicit description of the equilibrium points of (4) in terms of the eigenspace decomposition of A, D. For simplicity, we assume that D is in diagonal form, i.e.,

$$D = \operatorname{diag}(\mu_1, \ldots, \mu_1, \ldots, \mu_s, \ldots, \mu_s) \tag{9}$$

with $\mu_1 > \cdots > \mu_s > 0$ and μ_i occuring with multiplicity k_i, $k_1 + \cdots + k_s = k$.

Theorem 2. *Let $\Phi_0 \in \mathrm{SO}(n)$ be a basis matrix of eigenvectors of $A = A^\top > 0$ and let D be a diagonal form (9). Then $X_\infty \in \mathbb{R}^{n\times k}$ is an equilibrium point of the Oja-Brockett flow (4) if and only if*

$$X_\infty = \Phi_0 \pi \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} PS, \tag{10}$$

where $0 \le r \le k \le n$, P and π are $k\times k$ and $n \times n$ permutation matrices, respectively, and $S \in \mathrm{O}(k)$ with $S = \operatorname{diag}(S_1, \ldots, S_s)$, $S_i \in \mathrm{O}(k_i)$. Equivalently,

$$X_\infty = \Phi_0 \pi \begin{bmatrix} \Gamma \\ 0 \end{bmatrix} S, \tag{11}$$

where π is an $n\times n$ permutation matrix, $\Gamma = \operatorname{diag}(\epsilon_1, \ldots, \epsilon_k)$, $\epsilon_i \in \{0,1\}$ and $S = \operatorname{diag}(S_1, \ldots, S_s)$, $S_i \in \mathrm{O}(k_i)$, $i = 1, \ldots, s$.

Proof. Let $X \in \mathbb{R}^{n\times k}$ be an equilibrium point of (4) with $\operatorname{rank} X = r$, $0 \le r \le k \le n$. Let

$$X = \Psi \begin{bmatrix} \Sigma & 0 \\ 0 & 0 \end{bmatrix} \Phi$$

be the singular value decomposition, with $\Psi \in \mathrm{SO}(n)$, $\Phi \in \mathrm{O}(k)$ and $\Sigma = \operatorname{diag}(\sigma_1, \ldots, \sigma_r)$, $\sigma_1 \geq \cdots \geq \sigma_r > 0$. Let $\Delta := \left[\begin{smallmatrix} \Sigma & 0 \\ 0 & 0 \end{smallmatrix}\right]$. Substituting this into (8), we obtain

$$\Phi^\top \Delta^\top \Psi^\top A \Psi \Delta \Phi (\Phi^\top \Delta^\top \Delta \Phi - I_k) = 0, \quad \Delta^\top \Psi^\top A \Psi \Delta (\Delta^\top \Delta - I_k) = 0.$$

Decomposing $\Psi^\top A \Psi$ as

$$\Psi^\top A \Psi = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix},$$

we obtain

$$\begin{bmatrix} \Sigma A_{11} \Sigma & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \Sigma^2 - I & 0 \\ 0 & -I \end{bmatrix} = \begin{bmatrix} \Sigma A_{11} \Sigma (\Sigma^2 - I) & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix},$$

i.e., $\Sigma A_{11} \Sigma (\Sigma^2 - I) = 0$. Since $\Sigma > 0$ and $A_{11} > 0$ (by the positivity of A), we conclude that $\Sigma^2 = I$, i.e., $\Sigma = I_r$. Thus the singular values of X are all 1 and

$$X = \Psi \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} = \Phi. \tag{12}$$

So far we have only used the necessary condition (8) for an equilibrium point. Using (7), we show that Ψ and Φ are of the form as stated in the theorem. Inserting (12) into (7) yields for $\tilde{A} := \Psi^\top A \Psi$ and $\tilde{D} := \Phi A \Phi^\top$ that

$$\tilde{A} \begin{bmatrix} I & 0 \\ 0 & 0 \end{bmatrix} \tilde{D} = \begin{bmatrix} I & 0 \\ 0 & 0 \end{bmatrix} \tilde{D} \begin{bmatrix} I & 0 \\ 0 & 0 \end{bmatrix} \tilde{A} \begin{bmatrix} I & 0 \\ 0 & 0 \end{bmatrix},$$

i.e., for

$$\tilde{A} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \quad \tilde{D} = \begin{bmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{bmatrix}$$

the equivalent relations

(a) $A_{21} = A_{12}^\top = 0$, $D_{21} = D_{12}^\top = 0$,

(b) $D_{11} A_{11} = A_{11} D_{11}$.

Note that the orthogonal matrices Φ and Ψ can be changed by arbitrary block diagonal factors of the form (U, V, W orthogonal)

$$\Phi \to \begin{bmatrix} U & 0 \\ 0 & V \end{bmatrix} \Phi, \quad \Psi \to \Psi \begin{bmatrix} U^\top & 0 \\ 0 & W \end{bmatrix}$$

without changing $X = \Psi \left[\begin{smallmatrix} I & 0 \\ 0 & 0 \end{smallmatrix}\right] \Phi$. Thus we can assume without loss of generality that $\tilde{D}$ is diagonal, i.e., $\tilde{D} = \Phi D \Phi^\top = P D P^\top$ for a $k \times k$ permutation matrix P. Thus

$S := P^\top \Phi$ is orthogonal with $SDS^\top = D$. Therefore $S = \operatorname{diag}(S_1, \ldots, S_s)$, $S_i \in \mathrm{O}(k_i)$, $i = 1, \ldots, s$ and $\Phi = PS$. Moreover, from (b) and the diagonal form of D_{11} we conclude that A_{11} is block diagonal. Using the degree of freedom in specifying Φ by orthogonal transformations U and W (where $UD_{11}U^\top = D_{11}$), we conclude that—without loss of generality—Ψ is such that $\Psi^\top A \Psi = \operatorname{diag}(\lambda_1, \ldots, \lambda_r, \lambda_{r+1}, \ldots, \lambda_n)$, where $\lambda_1 \geq \cdots \geq \lambda_r$, $\lambda_{r+1} \geq \cdots \geq \lambda_n$. Thus there exists a permutation matrix π such that $\Psi = \Psi_0 \pi$. The result (10) follows. Formula (11) follows from (10) via the following claim:

Claim: *For any $n \times n$ permutation matrix π and $\Gamma = \operatorname{diag}(\epsilon_1, \ldots, \epsilon_k)$, $\epsilon_i \in \{0, 1\}$ there exists an $n \times n$ permutation matrix π' and a $k \times k$ permutation matrix P, $0 \leq r \leq k$, such that*

$$\pi \begin{bmatrix} \Gamma \\ 0 \end{bmatrix} = \pi' \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} P. \tag{13}$$

The converse holds, too.

For the necessity in the claim, choose $r = \operatorname{rank} \Gamma$ and a permutation matrix P such that

$$P \Gamma P^\top = \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} \quad k \in \mathbb{R}^{k \times k}.$$

Then

$$\pi' := \pi \begin{bmatrix} P^\top & 0 \\ 0 & I \end{bmatrix}$$

as required.

For the converse, let π', r, P be given. Choose

$$\Gamma := P^\top \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} P \quad \text{and} \quad \pi = \pi' \begin{bmatrix} P^\top & 0 \\ 0 & I \end{bmatrix}.$$

Then (13) holds and the proof of Theorem 2 is complete. ∎

Remark 1. Formula (11) in the above theorem generalizes a result of Xu (1993), who derived the equivalent representation

$$X_\infty = \Psi_0 \pi \begin{bmatrix} S \\ 0 \end{bmatrix},$$

where $S = \operatorname{diag}(\delta_1, \ldots, \delta_k)$, $\delta_i \in \{0, 1, -1\}$, $i = 1, \ldots, k$ for the generic case, where $D = \operatorname{diag}(\mu_1, \ldots, \mu_k)$, $\mu_1 > \cdots > \mu_k > 0$. Our representation also applies to the nongeneric case, and thus in particular to Oja's flow where $D = I_k$.

Corollary 1. *Let* $\Psi_0 \in \mathrm{SO}(n)$ *be a basis matrix of the eigenvectors of* $A = A^\top > 0$ *and let* D *be in the diagonal form* (9). *For any equilibrium point* X_∞ *of* (4) *we have*

$$X_\infty X_\infty^\top = \Psi_0 \mathrm{diag}\,(\epsilon_1, \ldots, \epsilon_n)\Psi_0^\top,$$

$\epsilon_i \in \{0,1\},\ \epsilon_1 + \cdots + \epsilon_n = \mathrm{rank}\, X_\infty$ *and*

$$X_\infty^\top X_\infty = S^\top \mathrm{diag}\,(\delta_1, \ldots, \delta_k) S,$$

$\delta_i \in \{0,1\},\ \delta_1 + \cdots + \delta_k = \mathrm{rank}\, X_\infty,\ S = \mathrm{diag}\,(S_1, \ldots, S_s),\ S_i \in O(k_i)$. *In particular, if* $\mathrm{rank}\, X_\infty = k$, *then* $X_\infty^\top X_\infty = I_k$.

3. The Weighted Subspace Flow

Another flow that achieves PCA is the *weighted subspace flow* introduced by Oja *et al.* (1992a; 1992b). This is given as the matrix differential equation on $\mathbb{R}^{n\times k}$

$$\dot{X} = AX - XX^\top AXD, \tag{14}$$

where $A = A^\top > 0$ and $D = D^\top > 0$. (Actually, Oja *et al.* only consider the case where $D = \mathrm{diag}\,(\mu_1, \ldots, \mu_k)$, $\mu_1 > \cdots > \mu_k > 0$.) We show that (14) admits a similar convergence analysis as (4). We just state the relevant results; the proofs are similar to those for (4) and therefore they are omitted.

Proposition 2. *The gradient of the function* $g : \mathbb{R}^{n\times k} \to \mathbb{R}$

$$g(X) := \frac{1}{4}\mathrm{tr}(X^\top AX)^2 - \frac{1}{2}\mathrm{tr}(A^2 X D^{-1} X^\top) \tag{15}$$

with respect to the Riemannian metric (6) *is the real analytic vector field* $\mathrm{grad}\, g : \mathbb{R}^{n\times k} \to \mathbb{R}^{n\times k}$ *given by*

$$\mathrm{grad}\, g(X) = XX^\top AXD - AX.$$

In particular, the weighted subspace flow (14) *is the negative gradient flow* $\dot{X} = -\mathrm{grad}\, g(X)$ *of* (5).

Theorem 3. *(i) The cost function* (15) *on* $\mathbb{R}^{n\times k}$ *has compact sublevel sets and is lower bounded. The solutions* $X(t) \in \mathbb{R}^{n\times k}$ *of the weighted subspace flow* (14) *exist for all* $t \geq 0$ *and, as* $t \to +\infty$, *every solution* $X(t)$ *converges to a single equilibrium point* $X_\infty = \lim_{t\to\infty} X(t)$.
(ii) Equilibrium points of (14) *are characterized by*

$$AX_\infty = X_\infty X_\infty^\top AX_\infty D.$$

There is a close connection between the solutions of the Oja-Brockett flow and the weighted subspace flow. This becomes particularly transparent if D is assumed to be diagonal:

$$D = \mathrm{diag}\,(\mu_1, \ldots, \mu_k), \quad \mu_1 > \cdots > \mu_k > 0. \tag{16}$$

Lemma 2. *Let* $A = A^\top > 0$ *and* D *satisfy* (16). *Then* $X(t) = (x_1(t), \ldots, x_k(t)) \in \mathbb{R}^{n\times k}$ *is a solution of* (14) *if and only if*

$$Y(t) := (\sqrt{\mu_1}x_1(\frac{t}{\mu_1}), \ldots, \sqrt{\mu_k}x_k(\frac{t}{\mu_k}))$$

is a solution of

$$\dot{Y} = AYD^{-1} - YD^{-1}Y^\top AY. \tag{17}$$

Proof. It is straightforward. ∎

Corollary 1. *Let* D *satisfy* (16).
(i) X_∞ *is an equilibrium point of* (14) *if and only if* $Y_\infty = X_\infty D^{\frac{1}{2}}$ *is an equilibrium point of* (17). *In particular, the equilibria points of* (14) *are given by*

$$X_\infty = \Psi_0 \pi \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} P D^{\frac{1}{2}} S,$$

where $0 \le r \le k \le n$, P *and* π *are* $k \times k$ *and* $n \times n$ *permutation matrices, respectively, and* $S \in \mathrm{O}(k)$ *satisfies* $SDS^\top = D$.
(ii) If $\mu_1 > \cdots > \mu_k > 0$, *then the equilibria of* (14) *are given by*

$$X_\infty = \Psi_0 \pi \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} P D^{\frac{1}{2}} S$$

with $S = \mathrm{diag}\,(\epsilon_1, \ldots, \epsilon_n)$, $\epsilon_i \in \{-1, 1\}$.

Proof. It is an immediate consequence of Lemma 2 and Theorem 2. ∎

One additional interesting feature of the subspace flow in contrast to (4) is that it defines a rank preserving flow.

Proposition 3. *Let* $A = A^\top > 0$ *and* $D = D^\top > 0$. *Then the weighted subspace flow* (14) *is rank preserving, i.e. for every solution* $X(t)$ *of* (14) *we have*

$$\mathrm{rank}\, X(t) = \mathrm{rank}\, X(0) \quad \forall t \ge 0.$$

Proof. By Proposition 2, $X(t)$ exists for all $t \ge 0$. Let $F(t) := A$ and $G(t) := -X(t)^\top AX(t)D$, $t \ge 0$. Then (14) is equivalent to the time-varying system

$$\dot{X}(t) = F(t)X(t) + X(t)G(t), \qquad t \ge 0.$$

By Lemma 1.12, p. 146, in (Helmke and Moore, 1994), the result follows. ∎

4. Hessians and Asymptotic Stability

Finally, we establish local stability properties of the Oja-Brockett flow. This immediately implies the corresponding results for the weighted subspace flow (4), which are not, however, explicitly stated here. Let

$$X_\infty = \Psi_0 \pi \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} PS \in \mathbb{R}^{n\times k}$$

be an equilibrium point of (4). We calculate the signature of the Hessian of the cost function $f : \mathbb{R}^{n\times k} \to \mathbb{R}$, cf. (5), at X_∞ and characterize the asymptotically stable equilibria of (4).

Theorem 4. *Let $D = \operatorname{diag}(\mu_1, \ldots, \mu_k)$ with $\mu_1 > \cdots > \mu_k > 0$ and let $A = A^\top > 0$ have distinct eigenvalues $\lambda_1 > \cdots > \lambda_n > 0$.*
(i) Every critical point of $f : \mathbb{R}^{n\times k} \to \mathbb{R}$ is nondegenerate.
(ii) The signature of the Hessian at the equilibrium points

$$X_\infty = \Psi_0 \pi \begin{bmatrix} I_r & 0 \\ 0 & 0 \end{bmatrix} PS$$

is given by

$$\nu_+ := \dim \operatorname{Eig}_+(\operatorname{Hess} f)(X_\infty) = nk - (n-r)(k-r) - s,$$

$$\nu_- := \dim \operatorname{Eig}_+(\operatorname{Hess} f)(X_\infty) = (n-r)(k-r) + s,$$

where ν_+ and ν_- are the numbers of positive and negative eigenvalues of the Hessian, respectively, and

$$s := \operatorname{card}\left\{(i,j);\ \ 1 \le i < j \le r \ \ \textit{and} \ \ \big(\pi^\top(i) - \pi^\top(j)\big)\big(p(i) - p(j)\big) < 0\right\}.$$

(iii) In particular, the asymptotically stable equilibria are precisely those of the form

$$X_\infty = \Psi_0 \begin{bmatrix} I_k \\ 0 \end{bmatrix} S$$

with $S = \operatorname{diag}(\epsilon_1, \ldots, \epsilon_k)$, $\epsilon_i \in \{-1, 1\}$.

Proof. The Hessian of f at a critical point $X \in \mathbb{R}^{n\times k}$ is computed as the quadratic form in $\Omega \in \mathbb{R}^{n\times k}$ given as

$$\begin{aligned}(\mathrm{D}^2\mathrm{f})(X)(\Omega,\Omega) = \frac{1}{2}\operatorname{tr}\Big[& A\Omega D X^\top A X D \Omega^\top + AXD\Omega^\top AXD\Omega^\top \\ &+ AXDX^\top A\Omega D\Omega^\top - A^2\Omega D^2\Omega^\top\Big]. \end{aligned} \tag{18}$$

Substituting X_∞ into (18) and setting $\tilde{\Omega} = \pi^\top \tilde{N} \Psi_0^\top \Omega H S P^\top$ and $\tilde{N} = \Psi_0^\top N \Psi_0$, we obtain

$$(\mathrm{D}^2\mathrm{f})(X_\infty)(\Omega,\Omega) = \frac{1}{2}\mathrm{tr}\Big[\tilde{\Omega} J^\top \pi^\top \tilde{N} \pi J \tilde{\Omega}^\top \pi^\top \tilde{N}^{-1} \pi + J\tilde{\Omega}^\top J \tilde{\Omega}^\top \\ + JPDP^\top J^\top \tilde{\Omega} P D^{-1} P^\top \tilde{\Omega}^\top - \tilde{\Omega}\tilde{\Omega}^\top\Big]$$

where $J = \left[\begin{smallmatrix} I_r & 0 \\ 0 & 0 \end{smallmatrix}\right] \in \mathbb{R}^{n\times k}$. Note that the corresponding quadratic form in $\tilde{\Omega}$ is isometric to the Hessian $(\mathrm{D}^2\mathrm{f})(X_\infty)(\Omega,\Omega)$ in Ω. Thus both the quadratic forms have the same rank and signature. Choosing Ψ_0 such that $\tilde{N} = \mathrm{diag}(\lambda_1,\ldots,\lambda_n)$, $\lambda_1 > \cdots > \lambda_n$, we have $PDP^\top = \mathrm{diag}(\lambda_{p(1)},\ldots,\lambda_{p(k)})$ and $\pi^\top \tilde{N} \pi = \mathrm{diag}(\lambda_{\pi^\top(1)},\ldots,\lambda_{\pi^\top(n)})$. By setting $\tilde{\Omega} = (\omega_{ij}) \in \mathbb{R}^{n\times k}$, the Hessian, expressed in $\tilde{\Omega}$, decomposes as

$$Q_1 + Q_2 + Q_3 + Q_4,$$

where

$$Q_1 = \frac{1}{2}\sum_{s,t=1}^{r}\left(\frac{\lambda_{\pi^\top(s)}}{\lambda_{\pi^\top(t)}} + \frac{\mu_{p(t)}}{\mu_{p(s)}} - 1\right)\omega_{ts}^2 + \frac{1}{2}\sum_{s,t=1}^{r}\omega_{ts}\omega_{st},$$

$$Q_2 = \frac{1}{2}\sum_{t=r+1}^{n}\sum_{s=1}^{r}\left(\frac{\lambda_{\pi^\top(s)}}{\lambda_{\pi^\top(t)}} - 1\right)\omega_{ts}^2,$$

$$Q_3 = \frac{1}{2}\sum_{t=1}^{r}\sum_{s=r+1}^{k}\left(\frac{\mu_{p(t)}}{\mu_{p(s)}} - 1\right)\omega_{ts}^2,$$

$$Q_4 = -\frac{1}{2}\sum_{t=r+1}^{n}\sum_{s=r+1}^{k}\omega_{ts}^2.$$

The signatures and ranks of Q_2, Q_3 and Q_4 are obvious from their definitions. Thus it remains to determine the signature of the quadratic form Q_1. The form Q_1 can be represented as

$$Q_1 = \frac{1}{2}\sum_{s=1}^{r}\omega_{ss}^2 + \frac{1}{2}\sum_{\substack{s,t=1\\ s<t}}^{r}\omega_{(st)}^\top Q_{(st)}\omega_{(st)},$$

where

$$Q_{(st)} = \begin{bmatrix} \dfrac{\lambda_{\pi^\top(s)}}{\lambda_{\pi^\top(t)}} + \dfrac{\mu_{p(t)}}{\mu_{p(s)}} - 1 & 1 \\ 1 & \dfrac{\lambda_{\pi^\top(t)}}{\lambda_{\pi^\top(s)}} + \dfrac{\mu_{p(s)}}{\mu_{p(t)}} - 1 \end{bmatrix}$$

and $\omega_{(st)}^\top = (\omega_{ts},\omega_{st})$. $Q_{(st)}$ has distinct eigenvalues and this proves (i). Since

$$\det Q_{(st)} = \frac{\lambda_{\pi^\top(t)}}{\lambda_{\pi^\top(s)}}\frac{\mu_{p(s)}}{\mu_{p(t)}}\left(\frac{\lambda_{\pi^\top(s)}}{\lambda_{\pi^\top(t)}} + \frac{\mu_{\pi(t)}}{\mu_{\pi(s)}}\right)\left(\frac{\lambda_{\pi^\top(s)}}{\lambda_{\pi^\top(t)}} - 1\right)\left(1 - \frac{\mu_{p(t)}}{\mu_{p(s)}}\right),$$

it is easily seen that $Q_{(st)}$ is positive definite if and only if

$$\left(\frac{\lambda_{\pi^\top(s)}}{\lambda_{\pi^\top(t)}} - 1\right)\left(1 - \frac{\mu_{p(t)}}{\mu_{p(s)}}\right) > 0,$$

i.e., if and only if

$$\lambda_{\pi^\top(s)} > \lambda_{\pi^\top(t)} \iff \mu_{p(s)} > \mu_{p(t)}.$$

Therefore the positivity of $Q_{(st)}$ for all $s, t = 1, \dots, r$ is in turn equivalent to $\pi^\top(s) = p(s)$ for all $s = 1, \dots, r$. From inspection of Q_2, Q_3 and Q_4 it follows that the Hessian is positive definite if and only if $r = k$ and $\pi^\top(s) = p(s)$ for all $s = 1, \dots, k$. Thus the only asymptotically stable equilibrium point is $X_\infty = \Psi_0[\,{}^{I_k}_{0}\,]S$, $S = \mathrm{diag}(\epsilon_1, \dots, \epsilon_k)$, $\forall \epsilon_i \in \{-1, 1\}$. ■

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