

Stiefel Manifolds and their Applications

Pierre-Antoine Absil
(UCLouvain)

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Structure

- ▶ Definition and visualization
- ▶ A glimpse of applications
- ▶ Geometry of the Stiefel manifolds
- ▶ Applications

Collaborations

- ▶ Chris Baker (Sandia)
- ▶ Thomas Cason (UCLouvain)
- ▶ Kyle Gallivan (Florida State University)
- ▶ Damien Laurent (UCLouvain)
- ▶ Rob Mahony (Australian National University)
- ▶ Chafik Samir (U Clermont-Ferrand)
- ▶ Rodolphe Sepulchre (U of Liège)
- ▶ Fabian Theis (TU Munich)
- ▶ Paul Van Dooren (UCLouvain)
- ▶ ...

Stiefel manifold: Definition

The (compact) Stiefel manifold $V_{n,p}$ is the set of all p -tuples (x_1, \dots, x_p) of orthonormal vectors in \mathbb{R}^n .

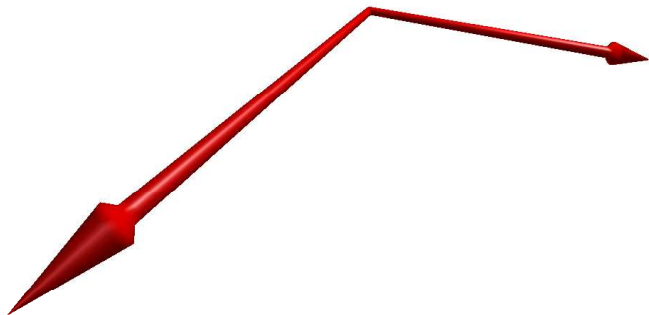
If we turn p -tuples into $n \times p$ matrices as follows

$$(x_1, \dots, x_p) \mapsto [x_1 \ \cdots \ x_p],$$

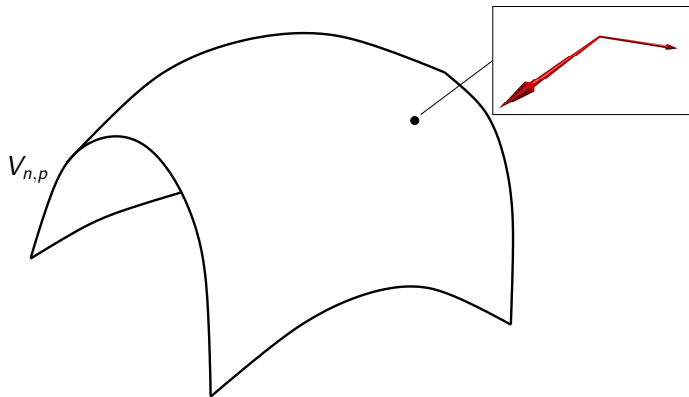
the definition becomes

$$V_{n,p} = \{X \in \mathbb{R}^{n \times p} : X^T X = I_p\}.$$

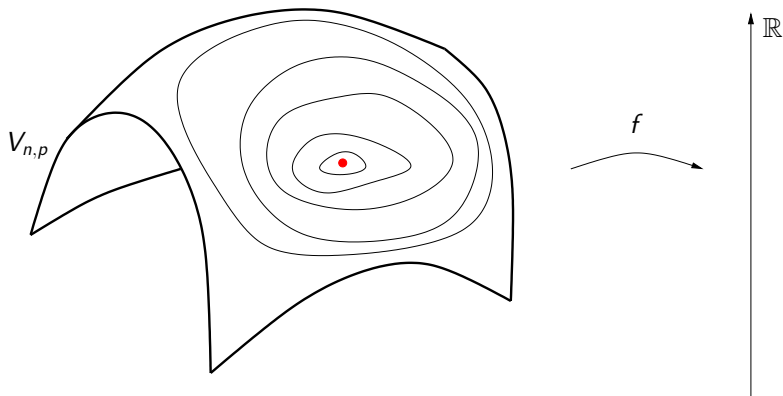
Visualization: an element of $V_{3,2}$



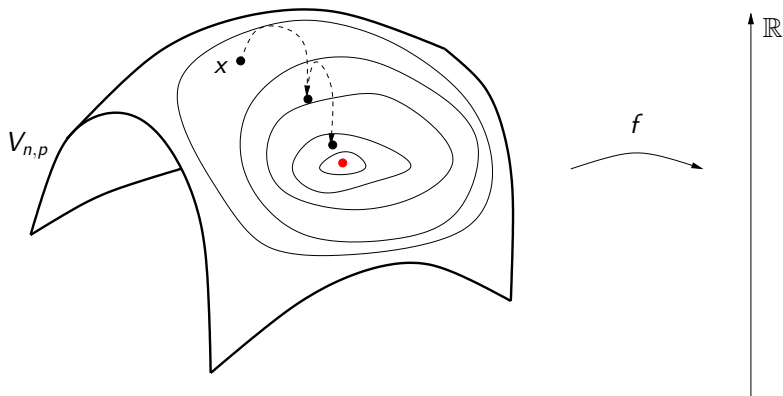
Stiefel manifold: (very unfaithful) artist view



Stiefel manifold: optimization problems



Stiefel manifold: optimization algorithms



Stiefel manifold: Extensions

- ▶ Recall: Real case:

$$V_p(\mathbb{R}^n) = \{X \in \mathbb{R}^{n \times p} : X^T X = I_p\} =: V_{n,p}.$$

- ▶ Complex case:

$$V_p(\mathbb{C}^n) = \{X \in \mathbb{C}^{n \times p} : X^H X = I_p\}.$$

- ▶ Quaternion case:

$$V_p(\mathbb{H}^n) = \{X \in \mathbb{H}^{n \times p} : X^* X = I_p\}.$$

- ▶ If M is a Riemannian manifold, one can define

$$V_p(TM) = \{(\xi_1, \dots, \xi_p) \mid \exists x \in M : \xi_i \in T_x M, \langle \xi_i, \xi_j \rangle = \delta_{ij}\}.$$

Stiefel manifold: Particular cases

- ▶ Recall: Real case:

$$V_p(\mathbb{R}^n) = \{X \in \mathbb{R}^{n \times p} : X^T X = I_p\} =: V_{n,p}.$$

- ▶ $p = 1$: the sphere

$$V_{n,1} = \{x \in \mathbb{R}^n : x^T x = 1\}.$$

- ▶ $p = n$: the orthogonal group

$$V_{n,n} = O_n = \{X \in \mathbb{R}^{n \times n} : X^T X = I_n\}.$$

Notation

- ▶ E. Stiefel (1935): $V_{n,m}$ (compact), $V_{n,m}^*$ (noncompact).
- ▶ I. M. James (1976): $O_{n,k}$ (compact) Stiefel manifold, $O_{n,k}^*$ noncompact Stiefel manifold, $V_{n,k}$ in the real case, $W_{n,k}$ in the complex case, $X_{n,k}$ in the quaternion case.
- ▶ Helmke & Moore (1994): $St(k, n)$ compact Stiefel manifold, $ST(k, n)$ noncompact Stiefel manifold.
- ▶ Edelman, Arias, & Smith (1998): $V_{n,p}$.
- ▶ Bridges & Reich (2001): $V_k(\mathbb{R}^n)$.
- ▶ Bloch *et al.* (2006): $V(n, N) = \{Q \in \mathbb{R}^{nN}; QQ^T = I_n\}$.

A glimpse of applications

- ▶ Principal component analysis
- ▶ Lyapunov exponents of a dynamical system
- ▶ Procrustes problem
- ▶ Blind Source Separation - soft dimension reduction

Geometry

- ▶ Dimension
- ▶ Tangent spaces
- ▶ Projection onto tangent spaces
- ▶ Geodesics

Stiefel manifold: dimension

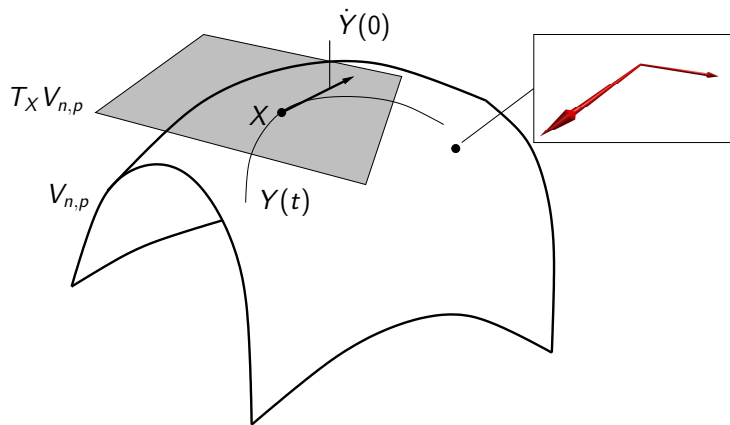
Dimension of $V_{n,p}$:

- ▶ 1st vector: one unit-norm constraint: $n - 1$ DOF.
- ▶ 2nd vector: unit-norm and orthogonal to 1st: $n - 2$ DOF.
- ▶ ...
- ▶ p th vector: $n - p$ DOF.

Total:

$$\begin{aligned}\dim(V_{n,p}) &= pn - (1 + 2 + \cdots + p) \\ &= pn - p(p + 1)/2 \\ &= p(n - p) + p(p - 1)/2.\end{aligned}$$

Stiefel manifold: tangent space



Stiefel manifold: tangent space

Let $X \in V_{n,p}$ and let $Y(t)$ be a curve on $V_{n,p}$ with $Y(0) = X$.

Then $\dot{Y}(0)$ is a *tangent vector* to $V_{n,p}$ at X .

The set of all such vectors is the *tangent space* to $V_{n,p}$ at X .

We have

$$Y(t)^T Y(t) = I_p \quad \text{for all } t$$

$$\frac{d}{dt}(Y(t)^T Y(t)) = 0 \quad \text{for all } t$$

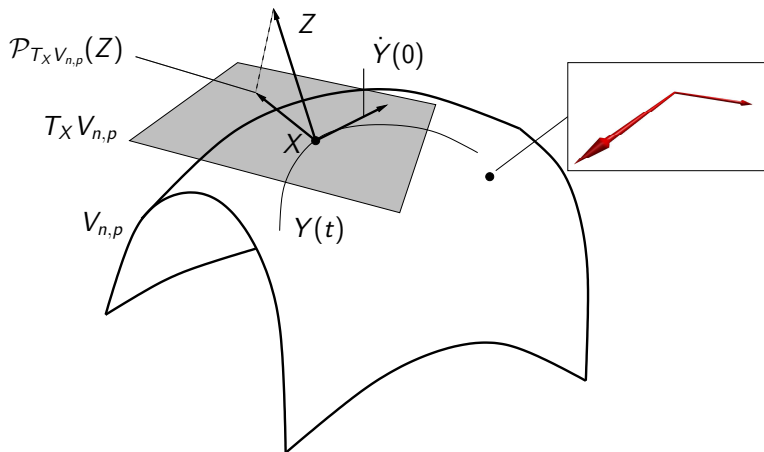
$$\dot{Y}(0)^T Y(0) + Y(0)^T \dot{Y}(0) = 0$$

$$X^T \dot{Y}(0) \text{ is skew}$$

$$\dot{Y}(0) = X\Omega + X_{\perp}K, \quad \Omega^T = -\Omega.$$

Hence $T_X V_{n,p} = \{X\Omega + X_{\perp}K : \Omega^T = -\Omega, K \in \mathbb{R}^{(n-p) \times p}\}$.

Stiefel manifold: projection onto the tangent space



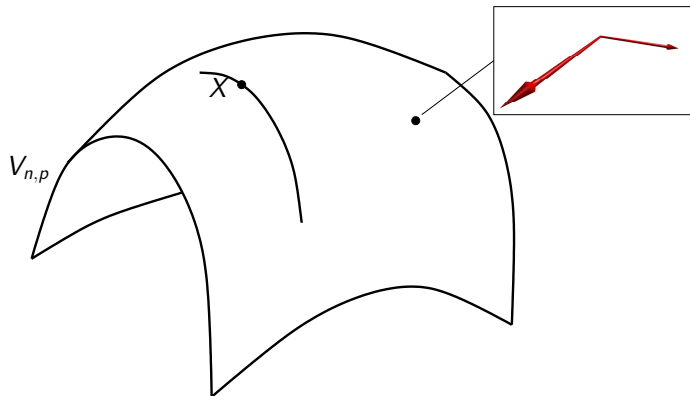
Stiefel manifold: projection onto the tangent space

- ▶ Tangent space: $T_X V_{n,p} = \{X\Omega + X_\perp K : \Omega^T = -\Omega, K \in \mathbb{R}^{(n-p) \times p}\}$.
- ▶ Normal space: $N_X V_{n,p} = \{XS : S^T = S\}$.
- ▶ Projection onto the tangent space:

$$\begin{aligned} \mathcal{P}_{T_X V_{n,p}}(Z) &= Z - X \text{sym}(X^T Z) \\ &= (I - XX^T)Z + X \text{skew}(X^T Z), \end{aligned}$$

where $\text{sym}(M) = \frac{1}{2}(M + M^T)$ and $\text{skew}(M) = \frac{1}{2}(M - M^T)$.

Stiefel manifold: geodesics



Stiefel manifold: geodesics

A curve $X(t)$ on $V_{n,p}$ is a *geodesic* if, for all t ,

$$\ddot{X}(t) \in N_{X(t)} V_{n,p}.$$

Ross Lippert showed that

$$X(t) = [X(0) \quad \dot{X}(0)] \exp t \begin{bmatrix} X(0)^T \dot{X}(0) & -\dot{X}(0)^T \dot{X}(0) \\ I & X(0)^T \dot{X}(0) \end{bmatrix} I_{2p,p} e^{-tX(0)^T \dot{X}(0)}.$$

Stiefel manifold: quotient geodesics

Bijection between $V_{n,p}$ and O_n/O_{n-p} :

$$V_{n,p} \ni X \leftrightarrow \left\{ \overbrace{\begin{bmatrix} X & X_{\perp} \end{bmatrix}}^U : U^T U = I_n \right\} \in O_n/O_{n-p}$$

Quotient geodesics: If

$$U(t) = U(0) \exp t \begin{bmatrix} A & -B^T \\ B & 0 \end{bmatrix}.$$

then $U_{:,1:p}(t) \in V_{n,p}$ follows a *quotient geodesic*.

Applications

- ▶ Principal component analysis
- ▶ Lyapunov exponents of a dynamical system
- ▶ Procrustes problem
- ▶ Blind Source Separation - soft dimension reduction

Principal component analysis

- ▶ Let $A = A^T \in \mathbb{R}^{n \times n}$.
- ▶ Goal: Compute the p dominant eigenvectors of A .
- ▶ Principle: Let $N = \text{diag}(p, p-1, \dots, 1)$ and solve

$$\max_{X^T X = I_p} \text{tr}(X^T A X N).$$

The columns of X are the p dominant eigenvectors of A .

- ▶ A basic method: Steepest-descent on $V_{n,p}$.
- ▶ Let $f : \mathbb{R}^{n \times p} \rightarrow \mathbb{R} : X \mapsto \text{tr}(X^T A X N)$.
- ▶ We have $\frac{1}{2} \text{grad} f(X) = A X N$.
- ▶ Thus $\frac{1}{2} \text{grad} f|_{V_{n,p}}(X) = \mathcal{P}_{T_X V_{n,p}}(A X N) = A X N - X \text{sym}(X^T A X N)$,
where $\text{sym}(Z) := (Z + Z^T)/2$.
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Computing Lyapunov exponents: a method on the Stiefel manifold

- ▶ Ref: T. Bridges and S. Reich, *Computing Lyapunov exponents on a Stiefel manifold*, Physica D 156, pp. 219–238, 2001.
- ▶ Dynamical system: $\dot{x} = f(x)$.
- ▶ Nominal trajectory: $x_*(t)$.
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- ▶ Principle: Consider the evolution of an infinitesimal ball of perturbed initial conditions. The ball becomes distorted into an infinitesimal ellipsoid. If the length $\delta_k(t)$ of the k th principal axis evolves as

$$\delta_k(t) \approx \delta_k(0)e^{\lambda_k t},$$

then λ_k is the k th *Lyapunov exponent* of the system along the nominal trajectory.

The mean Lyapunov exponents are given by

$$\lambda_k = \lim_{t \rightarrow \infty} \frac{1}{t} \frac{\|\delta_k(t)\|}{\|\delta_k(0)\|}.$$

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- ▶ Dynamical system: $\dot{x} = f(x)$.
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- ▶ Goal: Describe the behavior of nearby trajectories.
- ▶ **Principle:** $\delta_k(t) \approx \delta_k(0)e^{\lambda_k t}$.
- ▶ Challenge 1: Compute just a few Lyapunov exponents \leadsto work with p -frames (noncompact Stiefel manifold).
- ▶ Perturbed system:

$$\dot{Z} = A(t)Z, \quad Z \in \mathbb{R}^{n \times p}, \quad A(t) := Df(x_*(t)). \quad (1)$$

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- ▶ Challenge 2: Perform continuous orthogonalization to prevent the columns of Z from converging to 1st Lyapunov vector $\rightsquigarrow V_{n,p}$.
- ▶ Method: Follow the evolution of $Q(t)$ in the thin QR decomposition

$$Z(t) = Q(t)R(t).$$

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$$\dot{Q} = (I - QQ^T)\dot{Z}R^{-1} + QS, \quad S_{i,j} = \begin{cases} (Q^T \dot{Z} R^{-1})_{i,j}, & i > j \\ 0 & i = j \\ -(Q^T \dot{Z} R^{-1})_{j,i} & i < j. \end{cases}$$

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- ▶ This is a *dynamical system on the Stiefel manifold* $V_{n,p}$. It can be rewritten as

$$\dot{Q} = A(t)Q - QT,$$

where T is upper triangular.

- ▶ For almost all initial $Q(0)$, the p columns of $Q(t)$ converge to the p leading Lyapunov vectors for the given trajectory of the given

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$$\lambda_j = \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t T_{jj}(s) ds, \quad j = 1, \dots, p.$$

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Procrustes problem on the Stiefel manifold

- ▶ Ref: Lars Eldén and Haesun Park, *A Procrustes problem on the Stiefel manifold*, Numer. Math. (1999) 82: 599–619.
- ▶ *Orthogonal Procrustes problem*: given $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{m \times p}$. find $Q \in \mathbb{R}^{n \times p}$ that solves

$$\min_{Q^T Q = I_p} \|AQ - B\|_F^2.$$

- ▶ First-order optimality condition à la manifold:
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- ▶ **Applications: factor analysis**, used notably in psychometrics.
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Joint diagonalization on the Stiefel manifold

▶ Measurements $X = \begin{bmatrix} x_1(t_1) & x_1(t_2) & \cdots & x_1(t_f) \\ \vdots & \vdots & \ddots & \vdots \\ x_n(t_1) & x_n(t_2) & \cdots & x_n(t_f) \end{bmatrix}$.

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- ▶ Independence and dimension reduction: Consider a collection of covariance-like matrix functions $C_i(Y)$ such that $C_i(Y) = V^T C_i(\tilde{X})V$. Choose V to make the $C_i(Y)$'s as diagonal as possible.
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Joint diagonalization on the Stiefel manifold: application

The application is blind source separation.

Two mixed pictures are given as input to a blind source separation algorithm based on a trust-region method on $V_{2,2}$.

Joint diagonalization on the Stiefel manifold: application: input



Joint diagonalization on the Stiefel manifold: application: output



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