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

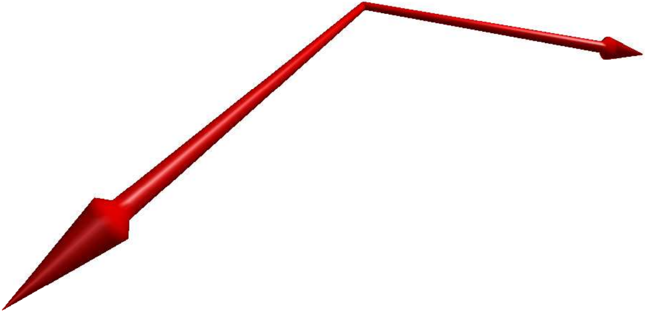
The (compact) Stiefel manifold $V_{n,p}$ is the set of all p-tuples $(x_1, \ldots, x_p)$ of orthonormal vectors in $\mathbb{R}^n$.
If we turn p-tuples into $n \times p$ matrices as follows

$$(x_1, \ldots, x_p) \mapsto \begin{bmatrix} x_1 & \cdots & x_p \end{bmatrix},$$

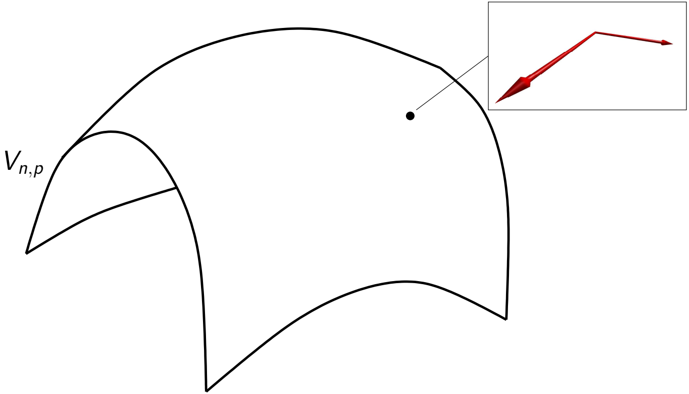
the definition becomes

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

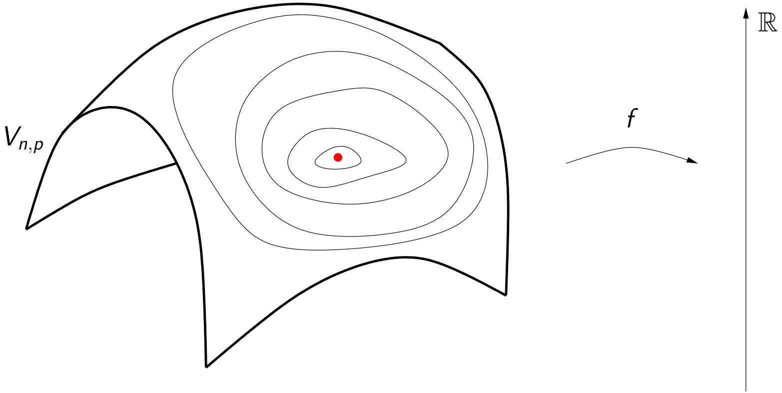
Visualization: an element of $V_{3,2}$



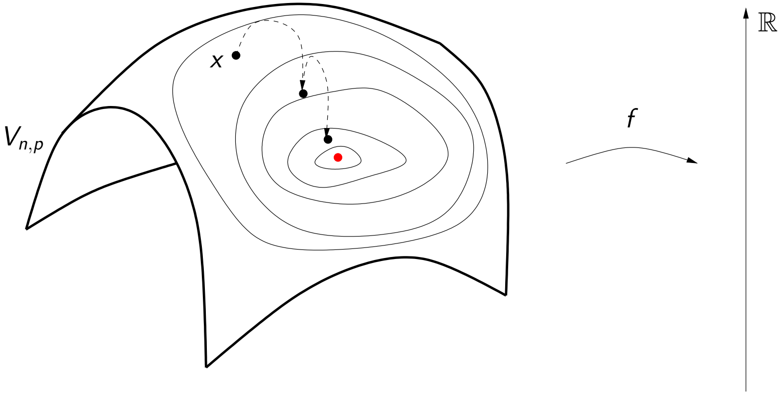
Stiefel manifold: (very unfaithful) artist view



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

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

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): $\mathrm{St}(k,n)$ compact Stiefel manifold, $\mathrm{ST}(k,n)$ 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

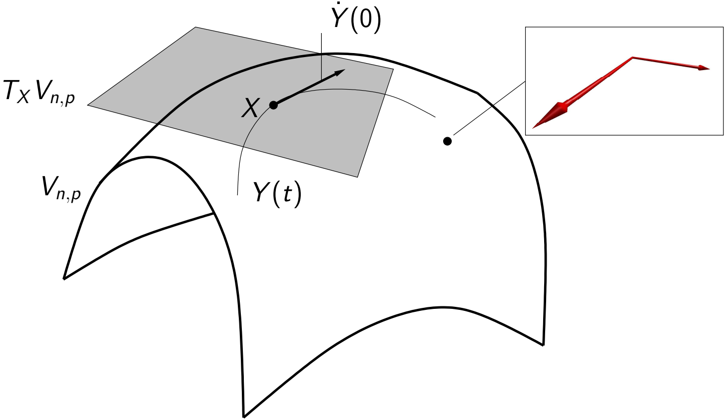
Dimension of $V_{n,p}$:

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



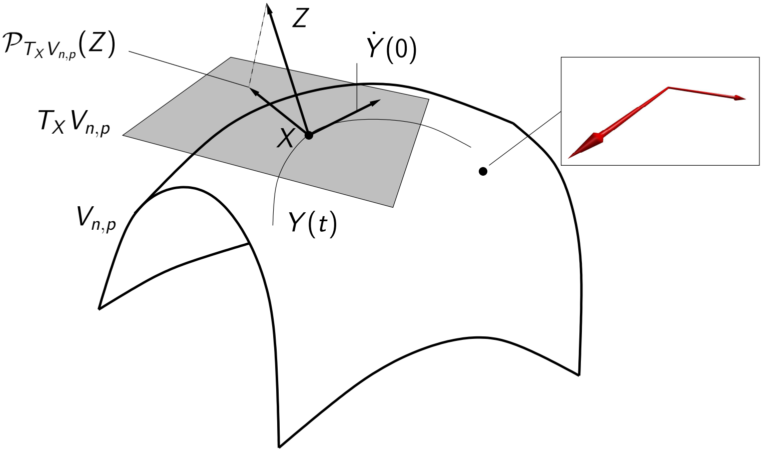
Stiefel manifold: tangent space

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

$$\begin{gathered}
Y(t)^T Y(t) = I_p \quad \text{for all } t \\
\frac{\mathrm{d}}{\mathrm{d}t}(Y(t)^T Y(t)) = 0 \quad \text{for all } t \\
\dot{Y}(0)^T Y(0) + Y(0)^T \dot{Y}(0) = 0 \\
X^T \dot{Y}(0) \text{ is skew} \\
\dot{Y}(0) = X\Omega + X_\perp K,\ \Omega^T = -\Omega.
\end{gathered}$$

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



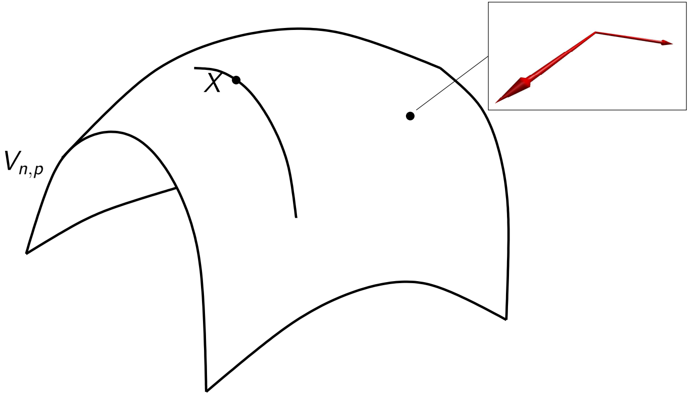
Stiefel manifold: projection onto the tangent space

- 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:

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

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

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

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

Stiefel manifold: quotient geodesics

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

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

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 $N = \mathrm{diag}(p, p-1, \cdots, 1)$ and solve

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

  The columns of X are the p dominant eigenvectors or A.
- A basic method: Steepest-descent on $V_{n,p}$.
- Let $f : \mathbb{R}^{n\times p} \to \mathbb{R} : X \mapsto \mathrm{tr}(X^T A X N)$.
- We have $\frac{1}{2}\mathrm{grad}\, f(X) = AXN$.
- Thus $\frac{1}{2}\mathrm{grad}\, f|_{V_{n,p}}(X) = \mathcal{P}_{T_X V_{n,p}}(AXN) = AXN - X\mathrm{sym}(X^T AXN)$, where $\mathrm{sym}(Z) := (Z + Z^T)/2$.
- Basic algorithm: Follow $\dot{X} = \mathrm{grad}\, f|_{V_{n,p}}(X)$.

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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 kth principal axis evolves as

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

then λ_k is the kth *Lyapunov exponent* of the system along the nominal trajectory.
The mean Lyapunov exponents are given by

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

Computing Lyapunov exponents: a method on the Stiefel manifold

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- Challenge 1: Compute just a few Lyapunov exponents $\rightsquigarrow$ work with p-frames (noncompact Stiefel manifold).
- Perturbed system:

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

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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

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

Computing Lyapunov exponents: a method on the Stiefel manifold

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Computing Lyapunov exponents: details of method on Stiefel

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- Principle: track $Q(t)$ in $Z(t) = Q(t)R(t)$.
- We have the formula

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

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

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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:
  Consider $f : \mathbb{R}^{n \times p} \to \mathbb{R} : Q \mapsto \|AQ - B\|_F^2$. We have

$$f(Q) = \mathrm{tr}(B^T B) + \mathrm{tr}(Q^T A^T A Q) - 2\mathrm{tr}(Q^T A^T B)$$

$$\mathrm{D}f(Q)[\dot{Q}] = -2\mathrm{tr}(\dot{Q}^T A^T B) + 2\mathrm{tr}(\dot{Q}^T A^T A Q),$$

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$$A^T B = U \Sigma V^T, \qquad Q = UV^T.$$

Procrustes problem on the Stiefel manifold

- *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

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

- First-order optimality condition *à la* manifold:
Consider $f : \mathbb{R}^{n\times p} \to \mathbb{R} : Q \mapsto \|AQ - B\|_F^2$. We have

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- Applications: factor analysis, used notably in psychometrics.
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Joint diagonalization on the Stiefel manifold

- Measurements $X = \begin{bmatrix} x_1(t_1) & x_1(t_2) & \cdots & x_1(t_f) \\ \vdots & \vdots & \ddots & \vdots \\ x_n(t_1) & x_n(t_2) & \cdots & x_n(t_f) \end{bmatrix}$.
- Goal: Find a matrix $W \in \mathbb{R}^{n \times p}$ such that the rows of
$$Y = W^T X$$
look as statistically independent as possible.
- Decompose $W = U \Sigma V^T$. We have
$$Y = V^T \underbrace{\Sigma U^T X}_{=:\tilde{X}}.$$
- Whitening: Choose Σ and U such that $\tilde{X}\tilde{X}^T = I_n$. Then $YY^T = V^T \tilde{X}\tilde{X}^T V = V^T V = I_p$.
- 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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