Emerging Directions in Deep Learning

Examples of ML techniques on particular manifolds

Mihai-Sorin Stupariu, 2024-2025

Once again: CNN in the 2D-framework

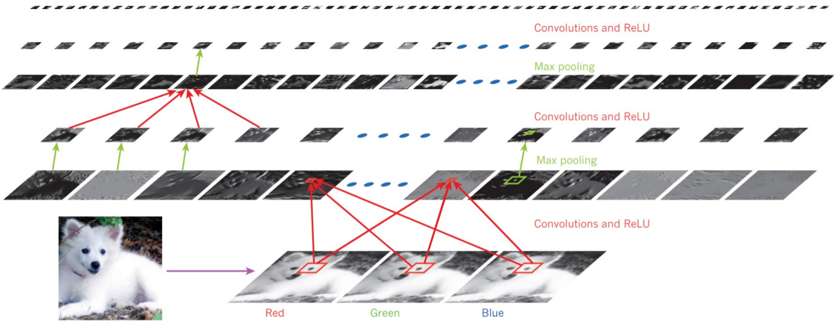
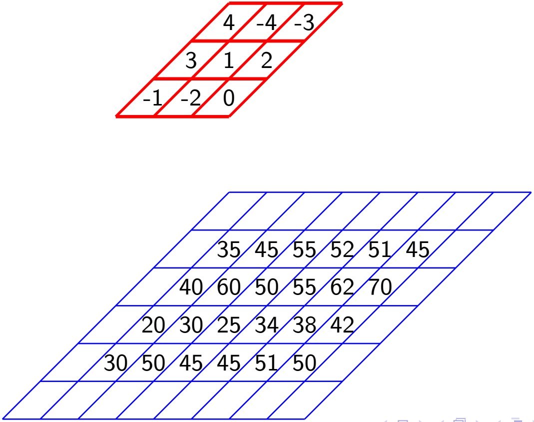


Figure 2 | Inside a convolutional network. The outputs (not the filters) of each layer (horizontally) of a typical convolutional network architecture applied to the image of a Samoyed dog (bottom left; and RGB (red, green, blue) inputs, bottom right). Each rectangular image is a feature map corresponding to the output for one of the learned features, detected at each of the image positions. Information flows bottom up, with lower-level features acting as oriented edge detectors, and a score is computed for each image class in output. ReLU, rectified linear unit.

[LeCun et al., 2015]

Seek for generalizations...

- **Aim:** To extend to other categories of geometric objects techniques that work in the 2D-framework.
- Main operations for a CNN: the grid (regular) structure, the convolution operation).



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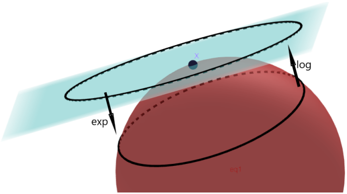

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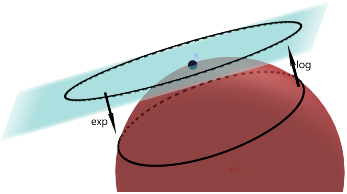

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- How do we relate the manifold set-up to a ML pipeline (in terms of operations to be performed)?

This lecture...

Two examples of manifolds used in ML pipelines. They have a particular structure, which enables specific computations. Both of them are implemented in Geomstats.

(1) Lie groups

(2) Symmetric-positive-definite (SPD) matrices

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- Actually: as examples, consider some natural transformations groups, such as translations, rotations.
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- Let e denote the neutral element of G. The tangent space T_eG of G at e naturally has the structure of a **Lie algebra** (usually denoted by $\mathfrak{g}$ - the Lie algebra of G). The Lie algebra $\mathfrak{g}$ is a vector space endowed with an operation called the Lie bracket $[\ ] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$.

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- For every $a \in G$, the differentials of the maps L_a, R_a above yield natural maps from $\mathfrak{g}$ to the tangent space T_aG.

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- The special orthogonal group $(\mathrm{SO}(n), \cdot)$ - this example is detailed later.

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- The special orthogonal group $(\mathrm{SO}(n), \cdot)$ - this example is detailed later.
- etc.

The group $(\mathrm{SO}(n), \cdot)$

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- For $n = 2$ one has the following fact: a matrix 2×2, say A, is an element of $\mathrm{SO}(2)$ if and only if A has the form
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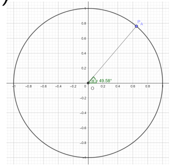
- Actually A corresponds, in a natural manner, to the rotation of angle α. Thus, the group $\mathrm{SO}(2)$ can be identified, in a natural manner, with the group $(S^1, \cdot)$ (the circle S^1 regarded as the multiplicative group of complex numbers with absolute value 1).



The point $P_A = (\cos\alpha, \sin\alpha) = \cos\alpha + i\sin\alpha$ on the circle S^1 corresponds to the matrix A.

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$$\xi = \begin{pmatrix} 0 & -a \\ a & 0 \end{pmatrix},$$

for a suitable a. Actually giving ξ is equivalent to giving the real number a.

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- For $n = 1$ the group reduces to a point, for $n = 2$ one has $\mathrm{SO}(2) \simeq S^1$ (the circle group, the group of 2D rotations). The group $\mathrm{SO}(3)$ is the group of 3D rotations.

A metric on the special orthogonal group

- The Frobenius inner product

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- Try to understand it through examples for $n = 2$ and for $n = 3$!

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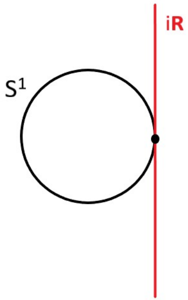
- Fix $A \in \mathrm{SO}(n)$. One has

$$\exp_A(X) = \exp(XA^T), X \in T_A\mathrm{SO}(n)$$

$$\log_A(B) = \log(AB^T), B \in \mathrm{SO}(n) \text{ “close to A”}.$$

Example: the Lie group S^1 and the exponential map

- The group $(S^1, \cdot)$ of complex numbers of absolute value 1 (see also the group $\mathrm{SO}(2)$); the Lie algebra is $i\mathbb{R} \simeq T_1 S^1$



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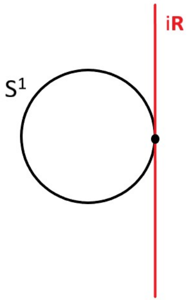

- The exponential map is the usual exponential $i\theta \mapsto e^{i\theta}$.

Application: Lie Group representation for skeletal data

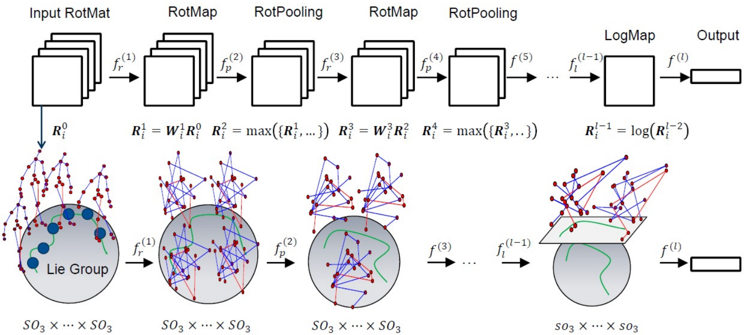

Figure 1. Conceptual illustration of the proposed Lie group Network (LieNet) architecture. In the network structure, the data space of each RotMap/RotPooling layer corresponds to a Lie group, while the weight spaces of the RotMap layers are Lie groups as well.

Source: Huang et al., 2017

Geometry of the space $\mathrm{SPD}(n)$

- Consider the vector space $S(n)$ of symmetric matrices
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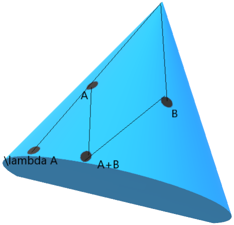
- A matrix $A \in S(n)$ is **positive semi-definite** if $x^T Ax \geq 0$ for all $x \in \mathbb{R}^n$. The set of all positive semi-definite matrices is a convex cone $\mathcal{C}$ in $S(n)$: for any $A, B \in S(n), \lambda > 0$ one has $A + B \in S(n), \lambda A \in S(n)$.



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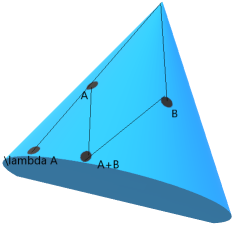
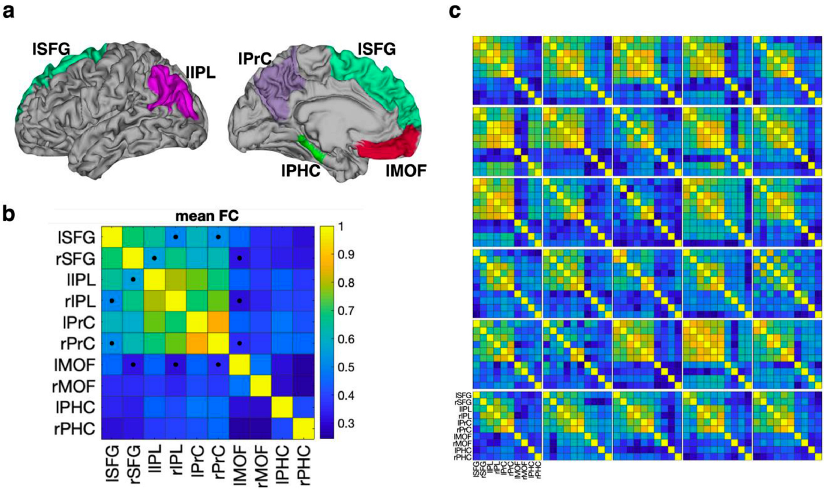


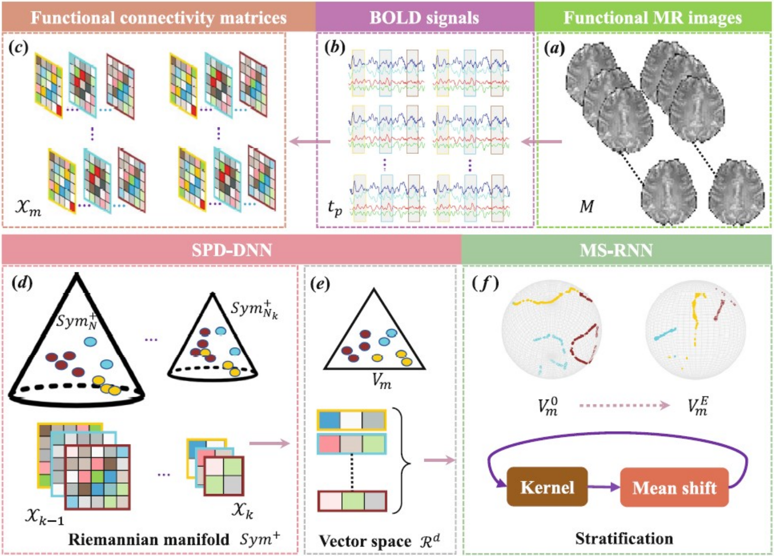
- Consider $\mathrm{SPD}(n)$, the set of **symmetric, positive semi-definite and invertible** matrices (SPD=symmetric positive definite). This is an open set in the cone $\mathcal{C}$. Thus, $\mathrm{SPD}(n)$ has a natural structure of manifold of dimension $\frac{1}{2}n(n+1)$ (e.g. Moakher and Batchelor, 2006). This manifold is actually the interior of a pointed convex cone.

SPD-matrices: brain connectomes



Source: You et al., 2021

SPD-matrices: detection of brain state changes



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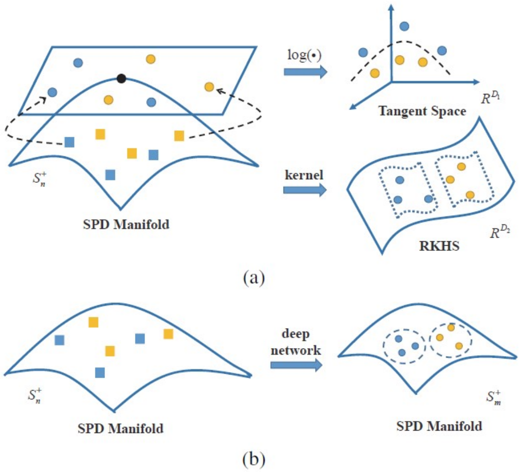
SPD-matrices: application to face recognition



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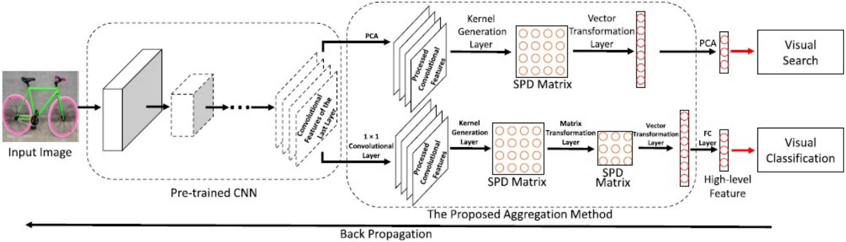
SPD-matrices: CV tasks



Source Gao et al., 2019, see also Gao et al., 2017

Other references of applications involving the manifold $\mathrm{SPD}(n)$

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