McTorch, a manifold optimization library for deep learning

Mayank Meghwanshi[⋆]
Pratik Jawanpuria[⋆]
Anoop Kunchukuttan[⋆]
Hiroyuki Kasai[†]
Bamdev Mishra[⋆]

[⋆] Microsoft, India
[†] The University of Electro-Communications, Japan

Our interest is the optimization problem of the form

$$\begin{array}{ll} \min\limits_{x \in \mathbb{R}^n} & f(x) \\ \text{subject to} & x^\top x = 1. \end{array}$$

Assume that f is differentiable.

Manifold optimization generalizes unconstrained optimization to manifolds

Solving

$$\min_{x \in \mathcal{M}} \quad f(x),$$

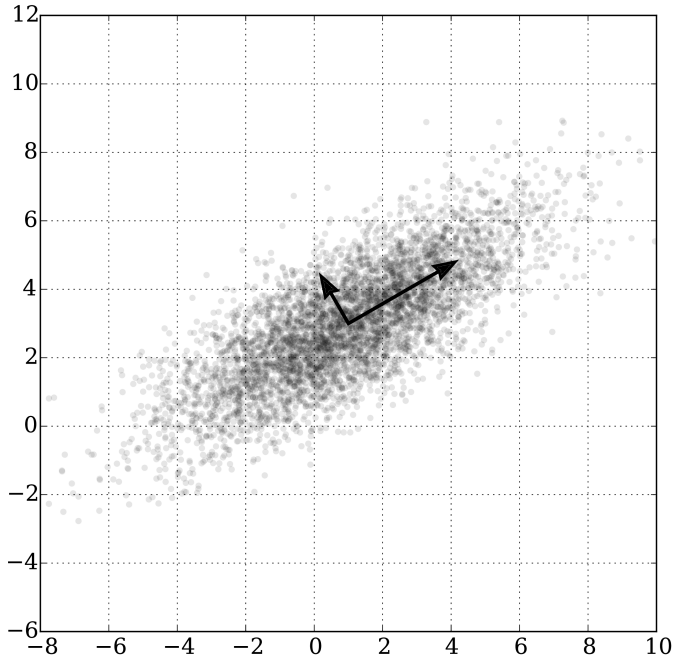
where $\mathcal{M} =: \{x \in \mathbb{R}^n : x^\top x = 1\}$

is equivalent to

Unconstrained optimization over the (nonlinear) manifold $\mathcal{M}$.

Applications

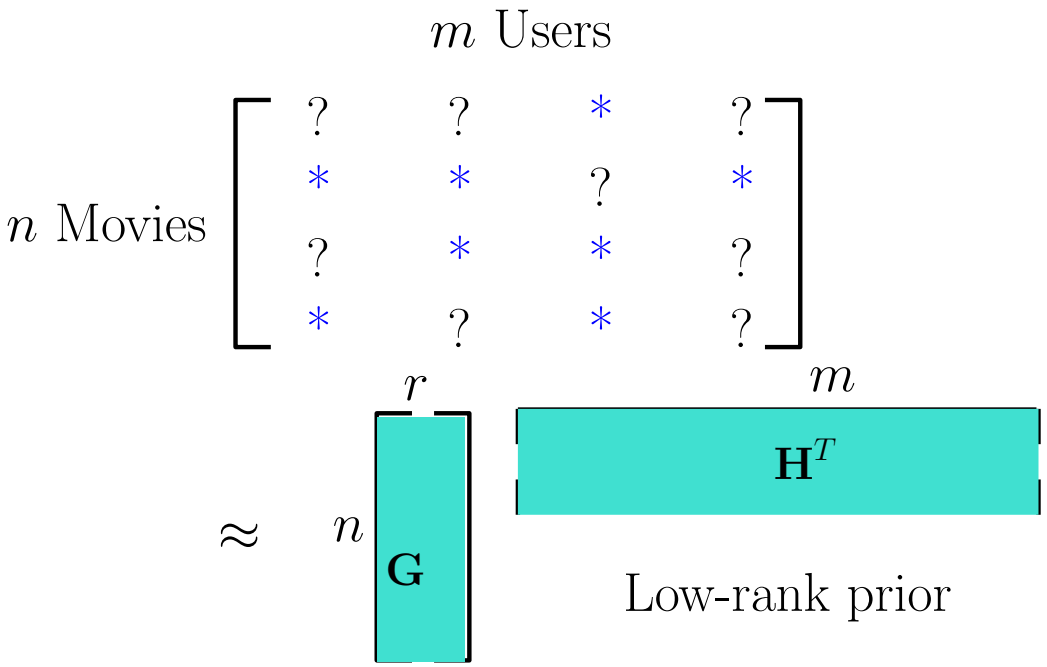
Principal components analysis (PCA) is on manifold of orthogonal matrices



Stiefel manifold models such orthogonal constraints

Figure from Wikipedia.org.

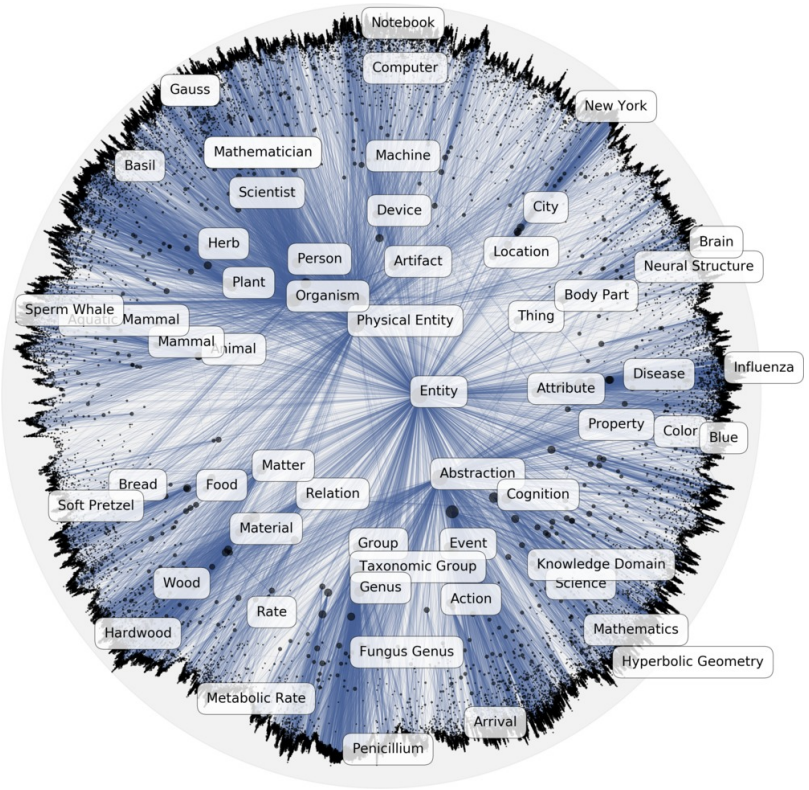
Recommender systems: low-rank matrix / tensor modeling



$$(n + m - r)r,\ r \ll (m, n)$$

Grassmann manifold is used to model such constraints

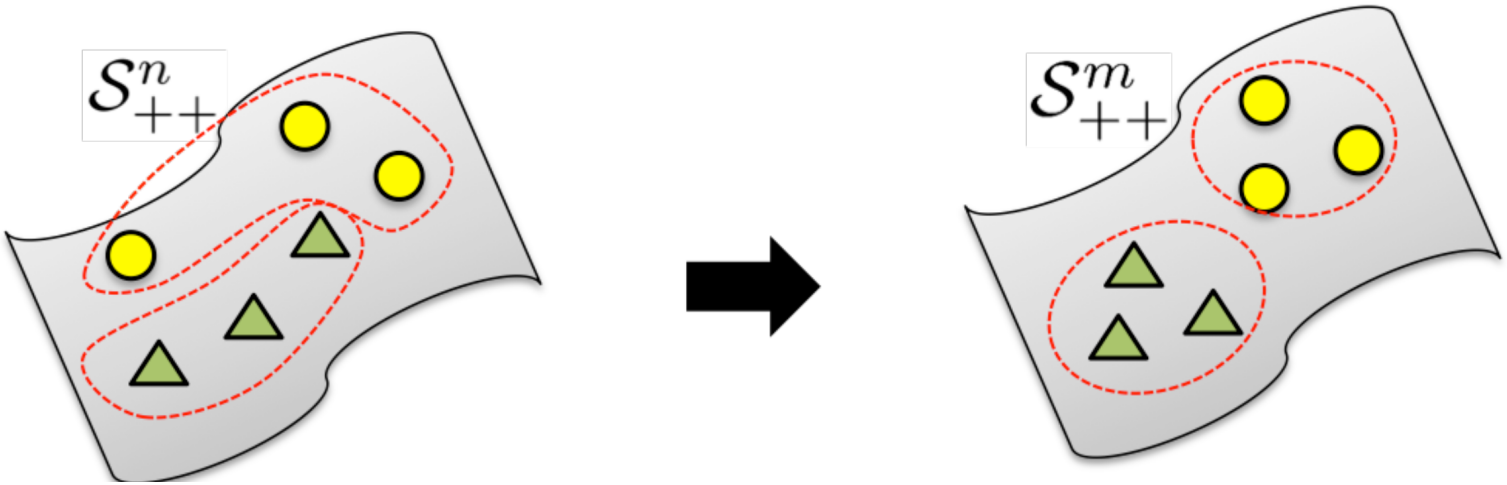
Learning continuous representations of hierarchies



Hyperbolic manifold is used to model hypernymy relationships

Figure from mnick.github.io.

Metric learning



Symmetric positive definite matrices form a manifold

Most Euclidean optimization algorithms generalize well to manifolds

- Conjugate gradients.
- BFGS and Quasi-Newton methods.
- Non-smooth optimization on manifolds.
- Stochastic gradients w/o variance reduction.
- Preconditioning on manifolds.

There exist other independent toolboxes for optimization on manifolds

- Pymanopt: a Python toolbox for manifold optimization.
- ROPTLIB: a C++ Library for optimization on manifolds with Python, R, and Julia wrappers.
- Geomstats: a Python package for computations and statistics on manifolds.
- McTorch: a PyTorch extension to do manifold optimization for deep learning applications painlessly.

To know more about McTorch, visit our demo.

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