Manifold Optimization for Hyperparameter Estimation in Non-Euclidean Machine Learning

The goal of this internship is to improve the performance of machine learning algorithms by exploiting *manifold optimization techniques* for the estimation of hyperparameters. The problem is motivated by recent work on the estimation of Gaussian process (GP) models with *categorical inputs*, where the structure of the covariance function leads to *non-Euclidean parameter spaces*. In particular, the optimization domain corresponds to a class of *positive definite matrices* (or a specific parameterization thereof), which naturally forms a *Riemannian manifold* rather than an Euclidean space.

Scientific context

In many machine learning models, hyperparameters are typically estimated by maximizing a likelihood or minimizing a loss function. Standard optimization algorithms – such as BFGS or other gradient-based methods – implicitly assume that the parameter space is Euclidean. However, in the context of Gaussian processes with categorical inputs, the structure of the kernel often requires optimizing over families of positive definite matrices. These spaces have *curved geometric structures*, and ignoring this geometry leads to inefficient optimization. In practice, classical optimizers require a large number of multistart initializations to approach a global optimum, and their performance degrades as the dimension grows.

Objectives

The objective of the internship is to *design and implement an optimization algorithm that explicitly accounts for the non-Euclidean geometry of the parameter space*. Techniques from *Riemannian optimization* (e.g., Riemannian gradient descent, trust-region methods, geodesic computations) will be explored and compared against classical Euclidean methods.
A particular focus may be given to the class of *hypersphere kernel matrices*, whose structure induces a meaningful manifold geometry. The intern will investigate how to exploit this geometry to perform efficient hyperparameter optimization and validate his findings with numerical implementations (in R, Python, or Julia).

Expected work plan

- Review of Gaussian process models with categorical inputs and associated kernel structures.
- Study of Riemannian manifolds of symmetric positive definite matrices and related optimization tools.
- Implementation of manifold optimization algorithms, building on libraries such as manopt.
- Application to hyperparameter estimation in GP models, with systematic comparison against classical multistart (gradient-descent type) Euclidean optimizers.
- Numerical experiments, benchmarking, and analysis of convergence properties.
- Optional : exploration of other kernel classes or alternative parameterizations with interesting geometric structures.

Required skills

- Master's degree (Master 2) or engineering school degree in applied mathematics.
- Good background in linear algebra, optimization, and probability.
- Knowledge of machine learning fundamentals.
- Experience in Python or another scientific computing environment.
- (Optional) Familiarity with differential geometry or Gaussian processes is a plus, but not mandatory.

Practical informations

The internship will be hosted at the Institut de Mathématiques de Toulouse (IMT).
The supervising team is composed of F. Iutzeler, expert in optimization, O. Roustant and J. Garnier, experts in GP modeling.
The expected duration is 6 months, typically from March-April to August-September.

Contacts and application

Franck Iutzeler (IMT) : franck.iutzeler@math.univ-toulouse.fr
Olivier Roustant (INSA Toulouse) : roustant@insa-toulouse.fr
Josselin Garnier (Ecole Polytechnique) : josselin.garnier@polytechnique.edu

References

- Carpintero Perez, R., Da Veiga, S. and Garnier, J. (2025), "A reproducible comparative study of categorical kernels for Gaussian process regression, with new clustering-based nested kernels", arXiv preprint 2510.01840.
- Roustant, O., Padonou, E., Deville, Y., Clément, A., Perrin, G., Giorla, J. and Wynn, H. (2020). "Group kernels for Gaussian process metamodels with categorical inputs". SIAM/ASA Journal on Uncertainty Quantification, 8(2), 775-806.
- Boumal, N., An introduction to optimization on smooth manifolds, Cambridge University Press, 2023 : https ://www.nicolasboumal.net/book (freely available online).
- Absil, P.-A., Mahoney, R., and Sepulchre, R., Optimization algorithms on matrix manifolds, Princeton University Press, 2008 : https ://press.princeton.edu/absil (freely available online).
- Manopt, Toolboxes for optimization on manifolds and linear spaces, https ://www.manopt.org/

Keywords

Machine learning, Gaussian process, Optimization on manifolds, Positive definite matrices.