Robust Geometric Metric Learning

EUSIPCO 2022 - Belgrade, Serbia

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Metric learning

Metric learning

Supervised regime with K classes: $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^{n}$.

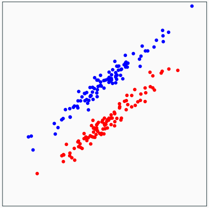
Metric learning

Find a *Mahalanobis* distance

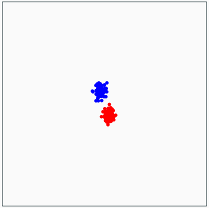
$$d_{\boldsymbol{A}}(\boldsymbol{x}_i, \boldsymbol{x}_j) = \sqrt{(\boldsymbol{x}_i - \boldsymbol{x}_j)^T \boldsymbol{A}^{-1} (\boldsymbol{x}_i - \boldsymbol{x}_j)}$$

relevant for classification problems.

$\boldsymbol{A} \in \mathcal{S}_p^{++}$ the set of $p \times p$ symmetric positive definite matrices.



(a) Raw data



(b) Whitened data

Information-Theoretic Metric Learning (ITML)

Set S: n_S pairs $(\boldsymbol{x}_l, \boldsymbol{x}_q)$ with $y_l = y_q$.
Set D: n_D pairs $(\boldsymbol{x}_l, \boldsymbol{x}_q)$ with $y_l \neq y_q$.

ITML minimization problem

Given $\boldsymbol{A}_0 \in \mathcal{S}_p^{++}$, and $u, v > 0$

$$\begin{aligned} \underset{\boldsymbol{A} \in \mathcal{S}_p^{++}}{\text{minimize}} \quad & \operatorname{Tr}(\boldsymbol{A}^{-1}\boldsymbol{A}_0) + \log|\boldsymbol{A}| \\ \text{subject to} \quad & d_{\boldsymbol{A}}^2(\boldsymbol{x}_l, \boldsymbol{x}_q) \leq u, \quad (\boldsymbol{x}_l, \boldsymbol{x}_q) \in S \\ & d_{\boldsymbol{A}}^2(\boldsymbol{x}_l, \boldsymbol{x}_q) \geq v, \quad (\boldsymbol{x}_l, \boldsymbol{x}_q) \in D \end{aligned}$$

Interpreted as a covariance estimation problem

For $\boldsymbol{A}_0 = \frac{1}{m}\sum_{i=1}^{m} \boldsymbol{x}_i \boldsymbol{x}_i^T$, it is the minimization of the Gaussian negative log-likelihood under constraints.

Geometric Mean Metric Learning (GMML) (1/2)

Minimization problem

$$\underset{\boldsymbol{A} \in \mathcal{S}_p^{++}}{\text{minimize}} \frac{1}{n_S} \sum_{(\boldsymbol{x}_l, \boldsymbol{x}_q) \in S} d^2_{\boldsymbol{A}}(\boldsymbol{x}_l, \boldsymbol{x}_q) + \frac{1}{n_D} \sum_{(\boldsymbol{x}_l, \boldsymbol{x}_q) \in D} d^2_{\boldsymbol{A}^{-1}}(\boldsymbol{x}_l, \boldsymbol{x}_q)$$

GMML Algorithm

$$\boldsymbol{A}^{-1} = \boldsymbol{S}^{-1} \#_t \boldsymbol{D} = \boldsymbol{S}^{-\frac{1}{2}} \left(\boldsymbol{S}^{\frac{1}{2}} \boldsymbol{D} \boldsymbol{S}^{\frac{1}{2}} \right)^t \boldsymbol{S}^{-\frac{1}{2}} \text{ with } t \in [0, 1]$$

$\boldsymbol{S} = \frac{1}{n_S} \sum_{(\boldsymbol{x}_l, \boldsymbol{x}_q) \in S} (\boldsymbol{x}_l - \boldsymbol{x}_q)(\boldsymbol{x}_l - \boldsymbol{x}_q)^T$
$\boldsymbol{D} = \frac{1}{n_D} \sum_{(\boldsymbol{x}_l, \boldsymbol{x}_q) \in D} (\boldsymbol{x}_l - \boldsymbol{x}_q)(\boldsymbol{x}_l - \boldsymbol{x}_q)^T$.

$\boldsymbol{A}^{-1}$ is the Riemannian interpolation on $\mathcal{S}_p^{++}$ between $\boldsymbol{S}^{-1}$ and $\boldsymbol{D}$.

In practice, works well for t small, *i.e.* $\boldsymbol{A} \approx \boldsymbol{S}$.

Geometric Mean Metric Learning (GMML) (2/2)

Assumption

Data points of each class are realizations of independent random vectors with class-dependent first and second order moments

$$\boldsymbol{x}_{kl} \stackrel{d}{=} \boldsymbol{\mu}_k + \boldsymbol{\Sigma}_k^{\frac{1}{2}} \boldsymbol{u}_{kl} \, ,$$

with $\boldsymbol{\mu}_k \in \mathbb{R}^p$, $\boldsymbol{\Sigma}_k \in \mathcal{S}_p^{++}$, $\mathbb{E}[\boldsymbol{u}_{kl}] = \boldsymbol{0}$ *and* $\mathbb{E}[\boldsymbol{u}_{kl}\boldsymbol{u}_{kq}^T] = \boldsymbol{I}$ *if* $kl = kq$, $\boldsymbol{0}_p$ *otherwise.*

Interpreted as a covariance estimation problem

$$\mathbb{E}[\boldsymbol{S}] = 2 \sum_{k=1}^{K} \pi_k \boldsymbol{\Sigma}_k$$

where $\{\pi_k\}$ are the classes proportions.

Thus, in practice

$$\mathbb{E}[\boldsymbol{A}] \approx 2 \sum_{k=1}^{K} \pi_k \boldsymbol{\Sigma}_k .$$

Robust Geometric Metric Learning

Robust Geometric Metric Learning (RGML)

Proposed feneral formulation

$$\underset{(\boldsymbol{A},\{\boldsymbol{A}_k\})\in\left(\mathcal{S}_p^{++}\right)^{K+1}}{\text{minimize}} \quad \underbrace{\sum_{k=1}^{K} \pi_k \mathcal{L}_k(\boldsymbol{A}_k)}_{\text{negative log-likelihood}} \; + \lambda \underbrace{\sum_{k=1}^{K} \pi_k d^2_{\mathcal{S}_p^{++}}(\boldsymbol{A}, \boldsymbol{A}_k)}_{\substack{\text{cost function to compute} \\ \text{the center of mass of } \{\boldsymbol{A}_k\}}}$$

where $d_{\mathcal{S}_p^{++}}$ is the Riemannian distance on $\mathcal{S}_p^{++}$

$$d^2_{\mathcal{S}_p^{++}}\left(\boldsymbol{A}, \boldsymbol{A}_k\right) = \left\|\operatorname{logm}\left(\boldsymbol{A}^{-\frac{1}{2}} \boldsymbol{A}_k \boldsymbol{A}^{-\frac{1}{2}}\right)\right\|_F^2 .$$

Robust Geometric Metric Learning (RGML)

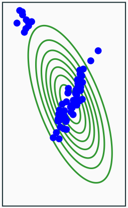
Set S_k: n_k pairs $(\boldsymbol{x}_l, \boldsymbol{x}_q)$ with $y_l = y_q = k$.

Gaussian negative log-likelihood

$$\mathcal{L}_{G,k}(\boldsymbol{A}_k) = \frac{1}{n_k} \sum_{(\boldsymbol{x}_l, \boldsymbol{x}_q) \in S_k} (\boldsymbol{x}_l - \boldsymbol{x}_q)^T \boldsymbol{A}_k^{-1} (\boldsymbol{x}_l - \boldsymbol{x}_q) + \log |\boldsymbol{A}_k|$$

minimized for

$$\boldsymbol{A}_k = \frac{1}{n_k} \sum_{(\boldsymbol{x}_l, \boldsymbol{x}_q) \in S_k} (\boldsymbol{x}_l - \boldsymbol{x}_q)(\boldsymbol{x}_l - \boldsymbol{x}_q)^T$$

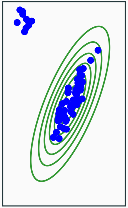


Tyler cost function

$$\mathcal{L}_{T,k}(\boldsymbol{A}_k) = \frac{p}{n_k} \sum_{(\boldsymbol{x}_l, \boldsymbol{x}_q) \in S_k} \log \left((\boldsymbol{x}_l - \boldsymbol{x}_q)^T \boldsymbol{A}_k^{-1} (\boldsymbol{x}_l - \boldsymbol{x}_q) \right) + \log |\boldsymbol{A}_k|$$

minimized for

$$\boldsymbol{A}_k = \frac{1}{n_k} \sum_{(\boldsymbol{x}_l, \boldsymbol{x}_q) \in S_k} \underbrace{\frac{p}{(\boldsymbol{x}_l - \boldsymbol{x}_q)^T \boldsymbol{A}_k^{-1} (\boldsymbol{x}_l - \boldsymbol{x}_q)}}_{\text{weight of } (\boldsymbol{x}_l - \boldsymbol{x}_q)} (\boldsymbol{x}_l - \boldsymbol{x}_q)(\boldsymbol{x}_l - \boldsymbol{x}_q)^T$$



Robust Geometric Metric Learning (RGML)

Gaussian RGML

$$\underset{(\boldsymbol{A},\{\boldsymbol{A}_k\})\in\left(\mathcal{S}_p^{++}\right)^{K+1}}{\text{minimize}}\; h_G\left(\boldsymbol{A},\{\boldsymbol{A}_k\}\right) = \underbrace{\sum_{k=1}^{K}\pi_k\mathcal{L}_{G,k}(\boldsymbol{A}_k)}_{\text{Gaussian negative log-likelihood}} + \lambda\sum_{k=1}^{K}\pi_k d^2_{\mathcal{S}_p^{++}}(\boldsymbol{A},\boldsymbol{A}_k)$$

Tyler RGML

$$\underset{(\boldsymbol{A},\{\boldsymbol{A}_k\})\in\left(\mathcal{SS}_p^{++}\right)^{K+1}}{\text{minimize}}\; h_T\left(\boldsymbol{A},\{\boldsymbol{A}_k\}\right) = \underbrace{\sum_{k=1}^{K}\pi_k\mathcal{L}_{T,k}(\boldsymbol{A}_k)}_{\text{Tyler cost function}} + \lambda\sum_{k=1}^{K}\pi_k d^2_{\mathcal{S}_p^{++}}(\boldsymbol{A},\boldsymbol{A}_k)$$

where $\mathcal{SS}_p^{++} = \left\{\boldsymbol{\Sigma}\in\mathcal{S}_p^{++} : |\boldsymbol{\Sigma}| = 1\right\}$

Riemannian geometry and optimization

What is a Riemannian manifold ?

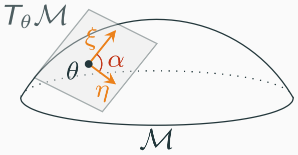


Figure 2: A Riemannian manifold.

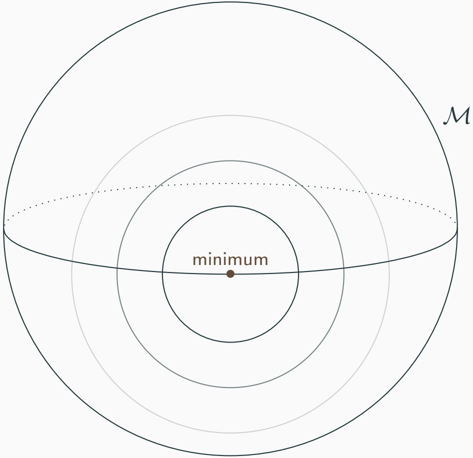
Curvature induced by:

- constraints, *e.g.* the sphere: $\|\boldsymbol{x}\| = 1$,
- the Riemannian metric, *e.g.* on $\mathcal{S}_p^{++}$: $\langle \boldsymbol{\xi}, \boldsymbol{\eta} \rangle_{\boldsymbol{\Sigma}}^{\mathcal{M}} = \mathrm{Tr}(\boldsymbol{\Sigma}^{-1}\boldsymbol{\xi}\boldsymbol{\Sigma}^{-1}\boldsymbol{\eta})$.

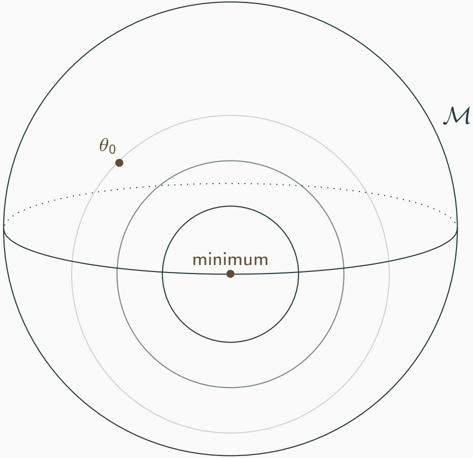
Examples of Riemannian manifolds $\mathcal{M}$:

- linear space (no constraints): $\mathbb{R}^{p\times p}$
- orthogonality constraints: $\mathrm{St}_{p,k} = \{\boldsymbol{U} \in \mathbb{R}^{p\times k} : \boldsymbol{U}^T\boldsymbol{U} = \boldsymbol{I}_k\}$
- positivity constraints: $\mathcal{S}_p^{++} = \{\boldsymbol{\Sigma} \in \mathcal{S}_p : \forall \boldsymbol{x} \neq \boldsymbol{0} \in \mathbb{R}^p,\ \boldsymbol{x}^T\boldsymbol{\Sigma}\boldsymbol{x} > 0\}$
- positivity constraints: $\mathcal{S}\mathcal{S}_p^{++} = \{\boldsymbol{\Sigma} \in \mathcal{S}_p^{++} : |\boldsymbol{\Sigma}| = 1\}$
- rank constraints: $\mathcal{S}_{p,k}^{+} = \{\boldsymbol{\Sigma} \in \mathcal{S}_p^{+} : \mathrm{rank}(\boldsymbol{\Sigma}) = k\}$
- norm constraints: $S^{p^2-1} = \{\boldsymbol{X} \in \mathbb{R}^{p\times p} : \|\boldsymbol{X}\|_F = 1\}$

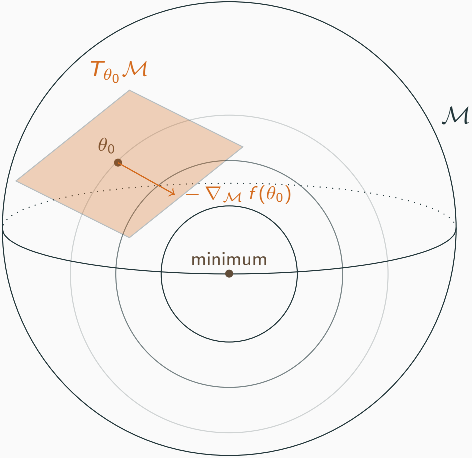
Optimization on a manifold



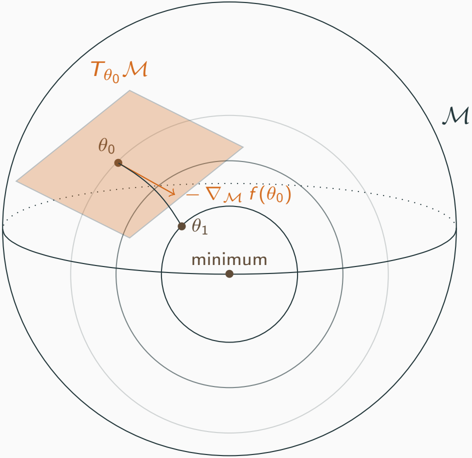
Optimization on a manifold



Optimization on a manifold



Optimization on a manifold



Robust Geometric Metric Learning (RGML)

Riemannian metric

$\forall \xi = (\boldsymbol{\xi}, \{\boldsymbol{\xi}_k\}), \eta = (\boldsymbol{\eta}, \{\boldsymbol{\eta}_k\})$ in the tangent space

$$\langle \xi, \eta \rangle_{(\boldsymbol{A}, \{\boldsymbol{A}_k\})} = \operatorname{Tr}\left(\boldsymbol{A}^{-1}\boldsymbol{\xi}\boldsymbol{A}^{-1}\boldsymbol{\eta}\right) + \sum_{k=1}^{K} \operatorname{Tr}\left(\boldsymbol{A}_k^{-1}\boldsymbol{\xi}_k\boldsymbol{A}_k^{-1}\boldsymbol{\eta}_k\right)$$

$\implies$ geodesically convexity of the minimization problems

$\theta = (\boldsymbol{A}, \{\boldsymbol{A}_k\})$, α a step size

Iterations of Gaussian RGML: minimization of h_G

$$\theta_{\ell+1} = \underbrace{R_{\theta_\ell}^{\left(\mathcal{S}_p^{++}\right)^{K+1}}}_{\text{retraction on } \left(\mathcal{S}_p^{++}\right)^{K+1}} \left(-\alpha \underbrace{\nabla^{\left(\mathcal{S}_p^{++}\right)^{K+1}} h_G(\theta_\ell)}_{\text{Riemannian gradient of } h_G} \right)$$

Iterations of Tyler RGML: minimization of h_T

$$\theta_{\ell+1} = \underbrace{R_{\theta_\ell}^{\left(\mathcal{SS}_p^{++}\right)^{K+1}}}_{\text{retraction on } \left(\mathcal{SS}_p^{++}\right)^{K+1}} \left(-\alpha \underbrace{\nabla^{\left(\mathcal{SS}_p^{++}\right)^{K+1}} h_T(\theta_\ell)}_{\text{Riemannian gradient of } h_T} \right)$$

Application

Robust Geometric Metric Learning (RGML)

Application to datasets from the UCI Machine Learning Repository

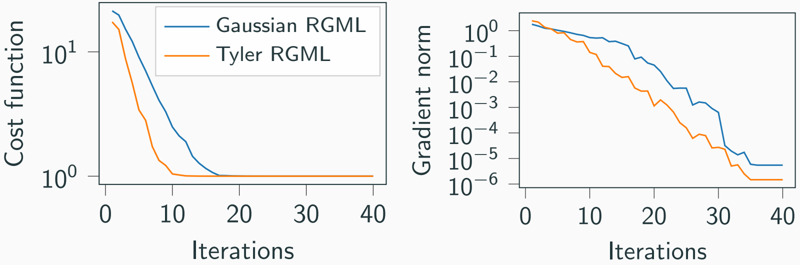


Figure 3: Left: cost function versus the number of iterations. Right: gradient norm versus the number of iterations. The optimization is performed on the *Wine* dataset.

Robust Geometric Metric Learning (RGML)

RGML + *k-NN* on datasets from the UCI Machine Learning Repository

	Wine				Vehicle				Iris			
	$p = 13$, $n = 178$, $K = 3$				$p = 18$, $n = 846$, $K = 4$				$p = 4$, $n = 150$, $K = 3$			
Method	Mislabeling rate				Mislabeling rate				Mislabeling rate			
	0%	5%	10%	15%	0%	5%	10%	15%	0%	5%	10%	15%
Euclidean	30.12	30.40	31.40	32.40	38.27	38.58	39.46	40.35	3.93	4.47	5.31	**6.70**
SCM	10.03	11.62	13.70	17.57	23.59	24.27	25.24	26.51	12.57	13.38	14.93	16.68
ITML - Identity	3.12	4.15	5.40	**7.74**	24.21	23.91	24.77	26.03	3.04	4.47	5.31	**6.70**
ITML - SCM	2.45	4.76	6.71	10.25	23.86	23.82	24.89	26.30	3.05	13.38	14.92	16.67
GMML	2.16	3.58	5.71	9.86	21.43	22.49	23.58	25.11	2.60	5.61	9.30	12.62
LMNN	4.27	6.47	7.83	9.86	20.96	24.23	26.28	28.89	3.53	9.59	11.19	12.22
Proposed - Gaussian	**2.07**	**2.93**	5.15	9.20	**19.76**	21.19	22.52	24.21	**2.47**	5.10	8.90	12.73
Proposed - Tyler	**2.12**	**2.90**	**4.51**	8.31	19.90	**20.96**	**22.11**	**23.58**	**2.48**	**2.96**	**4.65**	7.83

Table 1: Misclassification errors on 3 datasets: Wine, Vehicle and Iris. Mislabeling rate: percentage of labels randomly changed in the training set.

Github: `https://github.com/antoinecollas/robust_metric_learning`

Conclusion

Conclusion

Theoretical contributions:

- new interpretation of GMML algorithm...
- new g-convex optimization problem in *metric learning*: Gaussian RGML and Tyler RGML.

Application to real datasets from the *UCI* repository: RGML is fast, performant and robust to mislabelling.

Publications

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