Bayesian manifold estimation

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1. Introduction

In the last twenty years, there are several novel nonlinear dimension reduction procedures appeared, such as Isomap (1) , LLE (2) and its modification (3), Laplacian eigenmaps (4), and t-SNE (5).

Besides its worth mention some recent works using geometric multi retsolution analysis (6), local polynomial estimators (7) and numerical solution of PDE (8).

There are some methods which allows to handle with large noise, based on an optimization problem, such as mean-shift (9) and its variants (10), (11).

We now introduce new method based on tangent space estimation, which is able to handle with large-amplitude noise. All theoretical results are now in process.

2. Background and problem statement

Suppose we have data $\{X_n\}_{n=1}^N \subset \mathbb{R}^D$ sampled from uniform distribution on compact smooth manifold without boundaty $\mathcal{M}$. Let $\mathcal{M}$ have dimension $d < D$. Now let ε be Gaussian unbiased noise, s.t. $\varepsilon \mid X$ has normal distribution and $\mathbb{E}\left(\varepsilon \mid X\right) = 0$. We observe noised sample

$$y_i = X_i + \varepsilon_i$$

The problem of denoising observed sample can be formulated as problem of constructing estimation $\hat{X}$ which is close to X in some way.

3. Purpose and definitions

A presentation of a **topological manifold** is a second countable Hausdorff space that is locally homeomorphic to a vector space, by a collection (called an atlas) of homeomorphisms called charts. The composition of one chart with the inverse of another chart is a function called a transition map, and defines a homeomorphism of an open subset of the linear space onto another open subset of the linear space.

A **differentiable manifold** is a topological manifold equipped with an equivalence class of atlases whose transition maps are all differentiable. More generally, a C^k-manifold is a topological manifold with an atlas whose transition maps are all k-times continuously differentiable.

4. Algorithm

Main idea of our approach is to estimate not only recovered point $\hat{X}$ bat also tangent space to out manifold in point $\hat{X}_i$, which can be represented as projection matrix $\hat{P}_i$ onto tangent subspace.

Algorithm 1 Bayesian manifold estimator

[1] The training sample $_n = (Y_1, \dots, Y_n)$, the number of iterations K, a sequence of bandwidths $\{h_k : 1 \le k \le K\}$ and of regularizers $\{\beta_{k,i} : 1 \le k \le K, 1 \le i \le n\}$ are given. Initialize $\Sigma_i 0 = I_D$, $1 \le i \le n$. **for** k *from* 0 *to* $K-1$ **do**

end

Compute the weights $w_{ij}k$ according to the formula

$$w_{ij}k = \mathrm{K}\left(\frac{(Y_j - Y_i)^T(\Sigma_i k)^{-1}(Y_j - Y_i)}{h_k^2}\right), \quad 1 \le i, j \le n,$$

where $\mathrm{K}(t)$ is a localizing kernel. Compute

$$N_i = \sum_{j=1}^{n} w_{ij}k,$$

$$\mu_i = \frac{1}{N_i}\sum_{j=1}^{n} w_{ij}kY_j,$$

$$\Sigma_i = \frac{1}{N_i}\sum_{j=1}^{n} w_{ij}k(Y_j - \mu_i)(Y_j - \mu_i)^T$$

Sample $\Sigma_i^b \sim IW_p(\beta_{k,i}I_D + N_i\Sigma_i, N_i + D)$. Put $\Sigma_i k + 1 = \Sigma_i, \mu_i k + 1 = \mu_i$. **return** the estimates $\widehat{X}_1 = \mu_1 K, \dots, \widehat{X}_n = \mu_n K$.

5. Numerical experiments

Here are some experiments on deleting noise from artificial data. Figure 1 and 2 illustrate some simple examples. Parameters of algorithm were chosen to be approximately equal to noise amplitude. Also we can see importance of bayesian step for numerical stability. On figure 3 we can see results of two variations of algorithm: with bayesian step and without one.

On Figures 1-3 noise is uniform with different amplitudes A.

	Figure 1	Figure 2	Figure 3
noise amplitude	0.3	1.25	0.1
number of iterations	19	10	10
τ	0.9	4.0	0.4
h_k	0.6*$1.15^{1-k}, k = \overline{1,19}$	$2.5 * 1.1^{1-k}, k = \overline{1,10}$	$0.3 * 1.1^{1-k}, k = \overline{1,10}$

In all experiments ecxept one there there is no bayesian step, loss almost stopped to change after 1-3 iterations.

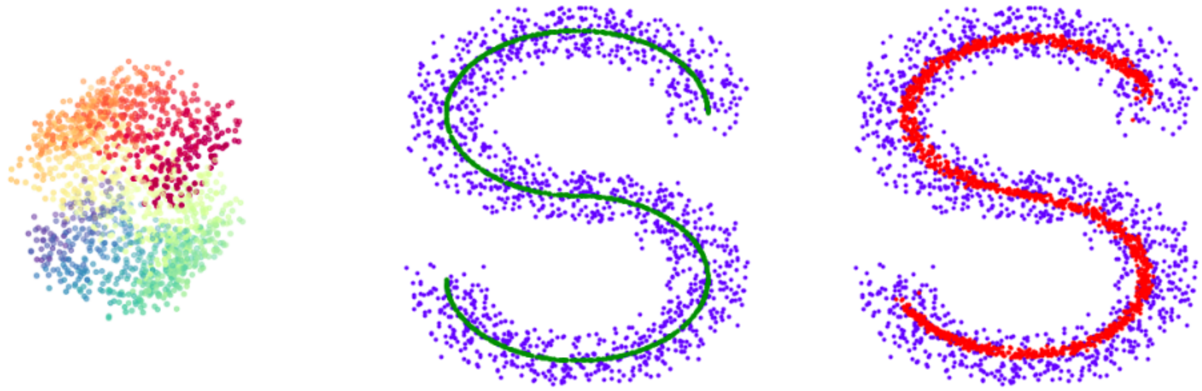

Figure 1: Green points - real data, blue points - noised observations, red points - result of algorithm

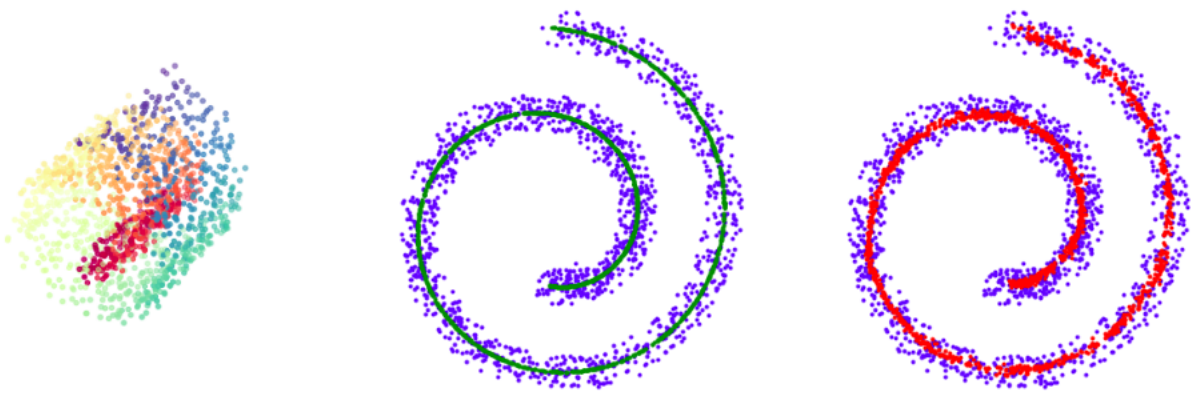

Figure 2: Green points - real data, blue points - noised observations, red points - result of algorithm

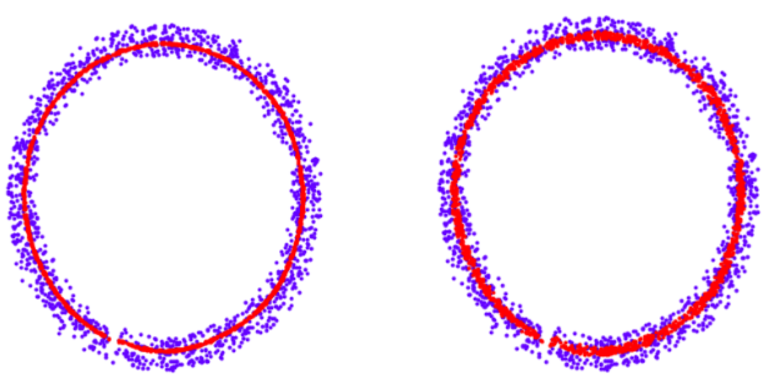

Figure 3: Result of algirithm with bayesian step on the left and without it on the right

6. Discussion of results and plans

New algorithm seems to work well on simple artificial data, so it is time to try it on more complicated examples.

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