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A Nonlinear Filter for Markov Chains and its Effect on Diffusion Maps

Stefan Steinerberger
Yale University, stefan.steinerberger@yale.edu

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A Nonlinear Filter for Markov Chains and its Effect on Diffusion Maps

YALE DAY OF DATA

Stefan Steinerberger

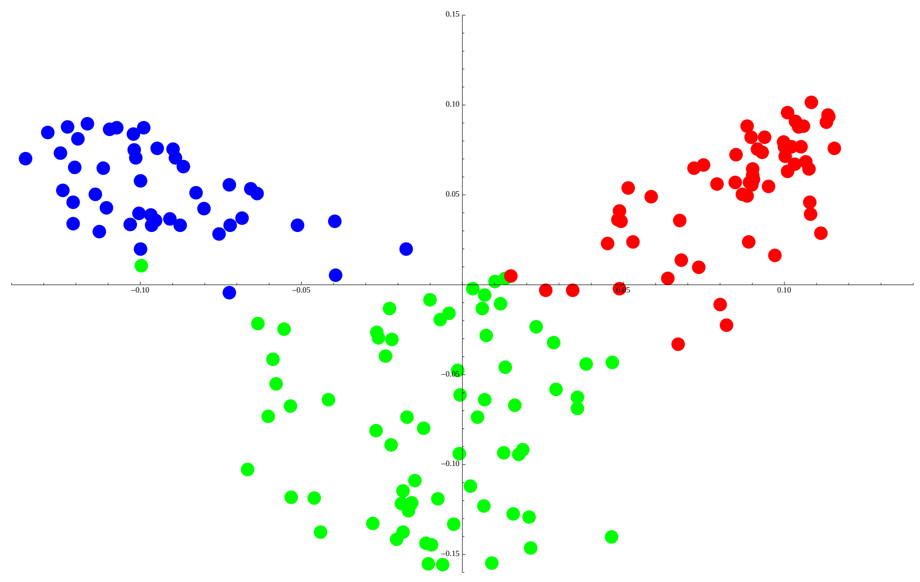
Department of Mathematics

Classical Diffusion Maps

We are interested in the interplay between Markov chains on a high-dimensional data set $\{x_i\}_{i=1}^n \subset \mathbb{R}^d$ and the inner workings of spectral methods. There are many different methods, see e.g. the work of Belkin & Niyogi, Coifman & Lafon, Coifman & Maggioni, Donoho & Grimes. Usually, these techniques proceed by imposing a Markov chain on the data set and analyzing diffusion on the arising graph. A popular and natural choice for the Markov chain is to declare that the probability p_{ij} to move from point x_j to x_i is

$$p_{ij} = \frac{\exp\left(-\frac{1}{\varepsilon}\|x_i - x_j\|^2_{\ell^2(\mathbb{R}^d)}\right)}{\sum_{k=1}^n \exp\left(-\frac{1}{\varepsilon}\|x_k - x_j\|^2_{\ell^2(\mathbb{R}^d)}\right)},$$

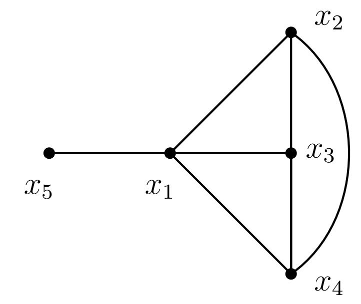
where the value of ε needs to be chosen depending on the given data as it induces a natural length scale $\sim \sqrt{\varepsilon}$ which should match the distance between neighbouring points.



This can work very well: see, for example, the wine data set mapped into two dimensions using a diffusion map (colors were added afterwards).

Rewarding Self-Consistency

We were motivated by the following example: suppose we are given



The standard diffusion paradigm proceeds by defining a random walk. However, given this local structure one would certainly believe that x_1, x_2, x_3, x_4 are well connected while x_5 seems to be an outlier. Consider a random walk starting in x_1. A simple computation yields

probability of being in	x_1	x_2	x_3	x_4	x_5
after 1 step	0	1/4	1/4	1/4	1/4
after 2 steps	1/2	1/6	1/6	1/6	0
minimum	0	1/6	1/6	1/6	0

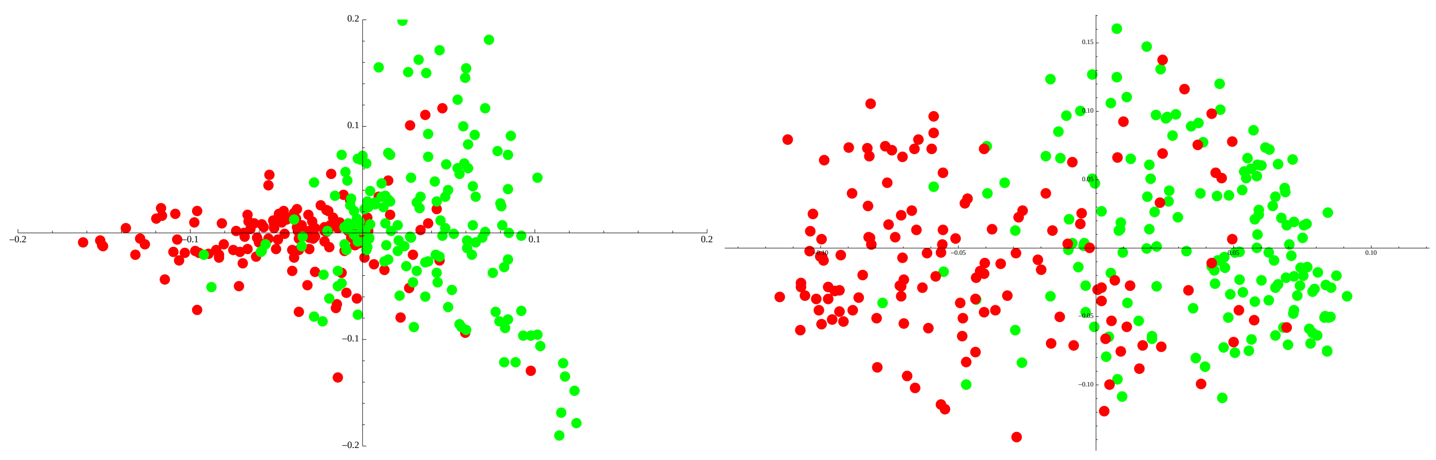
The minimum automatically detects unlikely outliers. Formally, assume we are given $\{x_i\}_{i=1}^n \subset \mathbb{R}^d$ and an associated Markov chain described by the matrix $P = (p_{ij})_{i,j=1}^n$. We propose using another matrix Q instead: we obtain the matrix P^* by setting $p_{ii} = 0$ and rescaling every column of P so that to we are once again given a transition matrix. Q is then given by

$$q_{ij} = \frac{\min((P^*)_{ij}, ((P^*)^2)_{ij}, \dots, ((P^*)^k)_{ij})}{\sum_{m=1}^n \min((P^*)_{mj}, ((P^*)^2)_{mj}, \dots, ((P^*)^k)_{mj})}.$$

We may then proceed with an analysis of the data set using Q instead of P. It seems that $k = 2$ is most effective in practice but there are certainly cases where a larger k may prove advantageous.

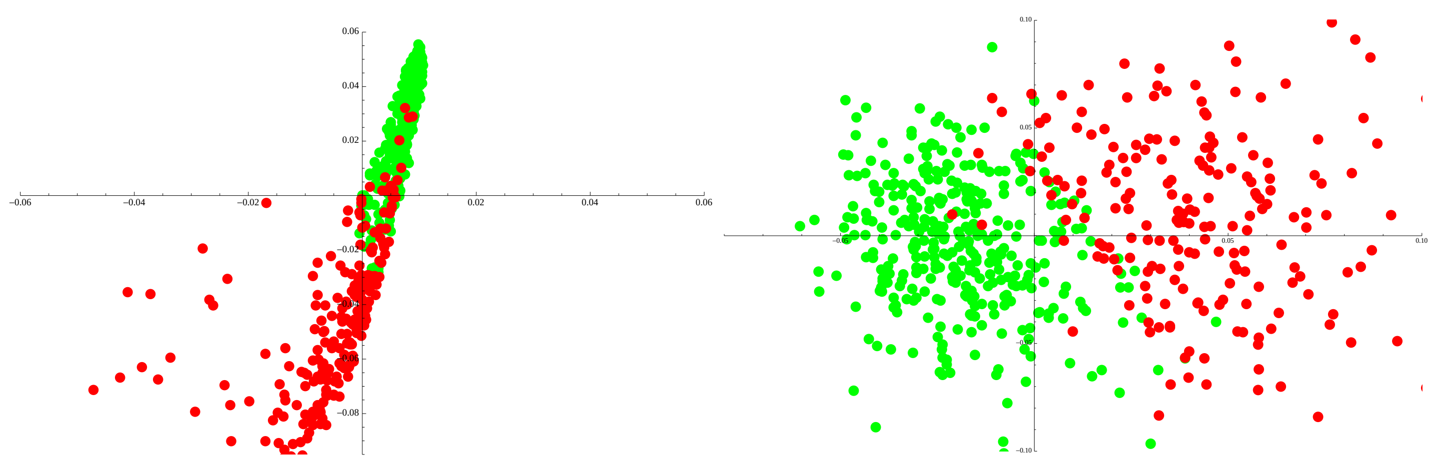
Examples

1 Cleveland Heart Disease Data Set.



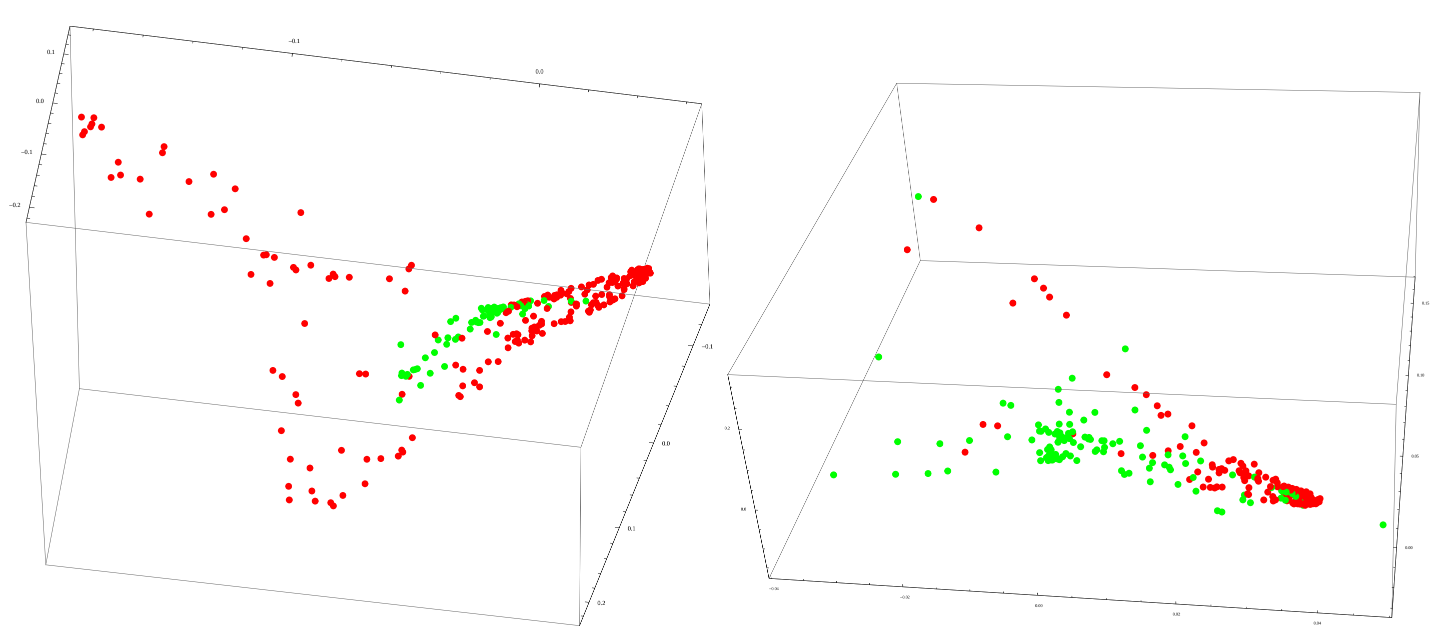
Classical method New method

2 Wisconsin Breast Cancer Data Set.



Classical method New method

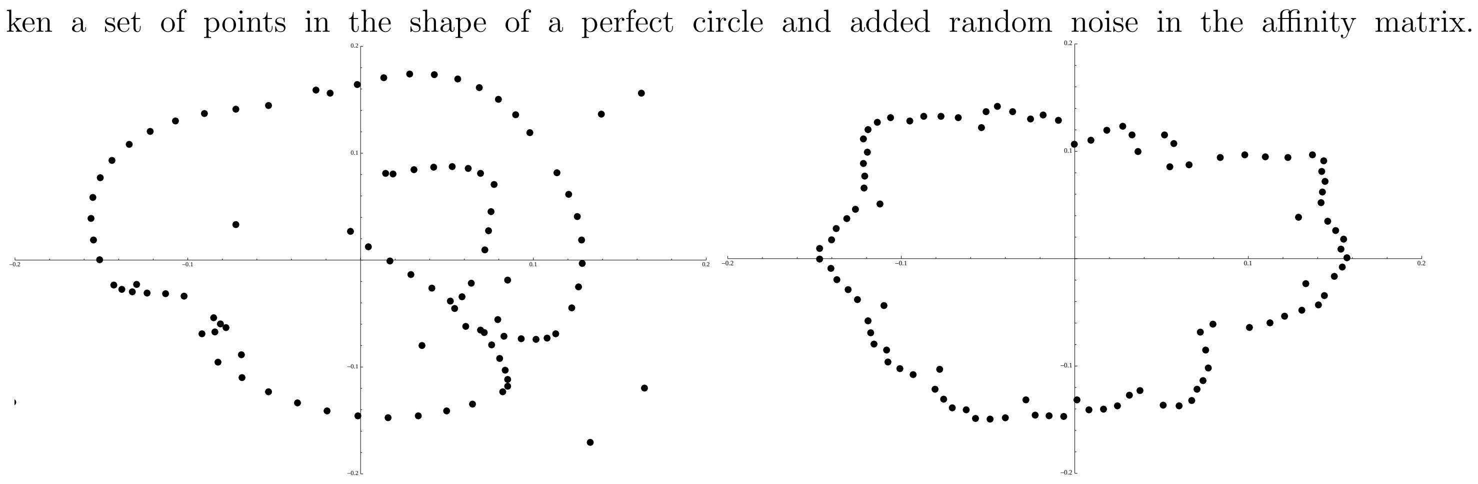
3 Ionosphere data set.



Classical method New method

Error correction

The method can be easily adapt to detect and correct for error. In the following example, we have taken a set of points in the shape of a perfect circle and added random noise in the affinity matrix.



Classical method New method

Theoretical results. Let $G = (V, E)$ be a finite graph with the property that every vertex has at most $c \in \mathbb{N}$ at distance at most 2 with transition matrix P. Construct G_1 by adding every possible edge with probability $0 < p \ll 1$ and let Q be the affinity assigned by the filter applied to the random walk on G_1.

Theorem. *The number N of vertices $(v_i, v_j) \in V \times V$ that are incorrectly thought of as present by the filter*

$$(P)_{i,j} = 0 \qquad \text{and} \qquad Q_{ij} > 0$$

satisfies

$$\mathbb{E}N \le cnp + cn^2p^2 + \frac{1}{2}n^3p^3.$$

This implies that the filter can successfully detect $|V|$ fake edges while only making $\mathcal{O}(1)$ mistakes on average. The trickiest part of the (not very complicated) proof uses the reproducing property of the binomial distribution

$$\mathcal{B}(\mathcal{B}(n,p), q) \sim \mathcal{B}(n, pq)$$

and combines it with a classical theorem of Wald.

Case 1 Case 2 Case 3

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