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1 Abstract

In the eleventh quarter of the work effort, we focused on a) conducting experiments on real-world data sets using the developed algorithms, b) continued design/implementation of the Multiscale Heat-Kernel Coordinates (MHKC) algorithms with function estimation and c) packaging for releasing the software as open source. This report documents algorithm designs for the MHKC algorithms for visualization and function estimation.

The project is currently on track – in the upcoming final quarter, we will wrap up all pending work, write the final report and package all the deliverables. No problems are currently anticipated.

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2 Summary

In this quarter, we continued design and implementation of the new multiscale heat kernel coordinates (MHKC) algorithms for visualization and function extension. The design variants for MHKC algorithms are documented in this report.

The project is currently on track – in the upcoming final quarter, we will wrap up all pending work, write the final report and package all the deliverables. No problems are currently anticipated.

3 Introduction

The primary project effort over the last quarter focused on completing design/development of the multiscale heat-kernel coordinates algorithms [1]. An outline of the MHKC algorithms was presented in previous quarterly reports [10][11]. This reports presents the MHKC algorithms for obtaining stable coordinate charts to represent the data in low dimensions. It also describes algorithms for performing function estimation for an arbitrary function defined on the data cloud.

4 Methods, Assumptions and Procedures

4.1 Multiscale Heat Kernel Coordinates

The Multiscale Heat Kernel Coordinates (MHKC) algorithms are based on theoretical results presented in [1]. The basic algorithms was described in [11]. We use the same notation in this report.

Given a set of n data points $\{x_1, x_2, \dots, x_n\}$ in R^d , we

1. Normalize the data by centering the cloud at zero and scaling to fit the data in a ball of unit variance,
2. Compute the transition probability matrix and its SVD

to obtain the eigenvalues $\{\lambda_i\}$ and associated eigenvectors $\{\vec{v}_i\}$. The MHKC embedding in r -dimensions for the point x_i is then given by

$$y_i = (e^{-\lambda_1 t} \cdot v_{i1}, e^{-\lambda_2 t} \cdot v_{i2}, \dots, e^{-\lambda_r t} \cdot v_{ir})$$

The heat kernel function is defined as

$$k(x, y) = \exp\left(-\frac{\|x - y\|_2^2}{\varepsilon}\right)$$

for any two points x and y . Here, ε is a constant (data dependent) representing the kernel window size.

4.1.1 Coordinate Charts

We now describe the algorithm to create canonical coordinate charts in 2 dimensions. This can be easily extended to r dimensions. The first step in to obtain a pair of points for each dimension. Next, we use these pairs as reference points to represent the entire data set. Specifically,

1. Center the 2-dimensional data cloud $\{y_i\}$ at the origin by subtracting the mean value
2. Find a pair of points $\{w_0, w_1\}$ in the dataset such that $(e^{-\lambda_1 t} \cdot v_1(w_0), e^{-\lambda_2 t} \cdot v_2(w_0))$ and $(e^{-\lambda_1 t} \cdot v_1(w_1), e^{-\lambda_2 t} \cdot v_2(w_1))$ are closest to the points $(1, -\frac{1}{4})$ and $(1, \frac{1}{4})$ respectively
3. Repeat step 2 to find another pair of points $\{z_0, z_1\}$ corresponding to the points $(-\frac{1}{4}, 1)$ and $(\frac{1}{4}, 1)$ respectively
4. The coordinate chart for the point x_i is then given by $(\log \frac{k(x_i, w_1)}{k(x_i, w_0)}, \log \frac{k(x_i, z_1)}{k(x_i, z_0)})$
5. Center the new coordinates at zero.

Note: The MSVD algorithm may be subsequently run on the coordinate chart to read off the local changes.

4.1.2 Function Estimation

Assume that we are given the function values $\{f(x_i)\}$ for an arbitrary unknown function f . The objective is to compute the value of $f(x)$ for a new point x that is not in the dataset. The function estimation algorithm is based on the Donoho-Johnstone technique for function estimation in the context of wavelets.

The function estimate at a new point x is given by

$$\hat{f}(x) = \frac{\sum_{i=1}^n k(x, x_i) \cdot f(x_i)}{\sum_{i=1}^n k(x, x_i)}$$

Note-1: The above equation is also a function of the window size ε . To obtain a stable function estimate, we require the estimate value to approximately remain the same across successive values of $\varepsilon = 1, \frac{1}{2}, \frac{1}{4}, \frac{1}{8}, \dots$

Note-2: The above equation corresponds to a single time step in the diffusion process with the constraint that the random walk does not revisit the new point x . For arbitrary time t (keeping the constraint), we simply replace $k(x, x_i)$ by the i -th component of the vector given by

$$(k(x, x_1), k(x, x_2), \dots, k(x, x_n)) \cdot P^{t-1}$$

where P is the Markov transition probability matrix for the original dataset.

4.2 Deliverables / Milestones

Date	Deliverables / Milestones	Status
Oct 2010	Progress report for period 1, 1 st quarter	✓
Jan 2011	Progress report for period 1, 2 nd quarter / complete randomized matrix decompositions task	✓
Apr 2011	Progress report for period 1, 3 rd quarter / complete approximate nearest neighbors task	✓
Jul 2011	Progress report for period 1, 4 th quarter / complete experiments – part 1	✓
Oct 2011	Progress report for period 2, 1 st quarter	✓
Jan 2012	Progress report for period 2, 2 nd quarter / complete multiscale SVD task	✓
Apr 2012	Progress report for period 2, 3 rd quarter	✓
Jul 2012	Progress report for period 2, 4 th quarter / complete experiments – part 2	✓
Oct 2012	Progress report for period 3, 1 st quarter	✓
Jan 2013	Progress report for period 3, 2 nd quarter / complete multiscale Heat Kernel task	✓
Apr 2013	Progress report for period 3, 3 rd quarter	✓
Jul 2013	Final project report + software + documentation on CDROM / complete experiments – part 3	

5 Results and Discussion

We described two additional MHKC algorithms – one to build stable canonical coordinate charts for representing the dataset, and the other to obtain function estimates for an unknown function defined on the dataset. We will experimentally evaluate both these techniques against real-world datasets.

6 Conclusions

The project is on track with design/implementation of the new multiscale heat kernel coordinates algorithms. We will finish up pending work, start writing up the final report and packaging all deliverables in the upcoming final quarter.

No problems are currently anticipated.

7 References

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