Fast Multiscale Algorithms for Information Representation and Fusion

Technical Progress Report No. 9

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In the ninth quarter of the work effort, we focused on a) conducting experiments on real-world data sets using the developed algorithms, b) design/implementation of the Multiscale Heat-Kernel Coordinates (MHKC) algorithms and c) packaging for releasing the software as open source. This report documents algorithm designs for the MHKC algorithms. The project is currently on track; in the upcoming quarter, we will continue applying the developed algorithms to various data sets and the design/implementation of the multiscale heat kernel coordinates algorithms. No problems are currently anticipated.
1 Abstract

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

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2 Summary

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

The project is currently on track – in the upcoming quarters, we will continue applying the developed algorithms to various data sets and focus on the design and development of the MHKC algorithms. 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 Error! Reference source not found.. This provides a power tool for discovering the non-linear geometries in any given dataset. This utilizes the fast randomized Singular Value Decomposition (RSVD) algorithms described in the earlier ONR reports [7][8]. Use of the RSVD effectively reduces the computational complexity from $O(m.n.k)$ to $O((m+n).k^2)$ for an $m$ by $n$ matrix of rank $k$. In contrast to the multiscale Singular Value Decomposition (MSVD) algorithms that detect linear structures in data at multiple scales, the MHKC uses heat kernels to discover the non-linear manifold structure in which the data resides at various scales. Similar to the MSVD, the MHKC provides an efficient representation using low-dimensional coordinates corresponding to the original data points.
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 current algorithm design is described below.

Input: A set of $n$ data points in $\mathbb{R}^d$. Assume $n$ is large.

Step 1: The first step comprises constructing the data matrix to be provided as input to the RSVD algorithm. Define the heat kernel as

$$k(x,y) = \exp(-\|x-y\|^2 / t_0)$$

for any two points $x$ and $y$. Here, $t_0$ is a constant (data dependent) representing the kernel window size. The heat kernel matrix is then defined as

$$K = \{k_{ij}\} \text{ where } k_{ij} = k(x_i, x_j)$$

for $i, j = 1, 2, \ldots, n$. The transition probability matrix is $P = D^{-1}K$ where $D$ is the diagonal matrix with the $i$-th entry as sum of the $i$-th row of $K$.

Note that $P$ is not symmetric. There are various techniques to symmetrize $P$ such that the eigenvalues and eigenfunctions are still easy to compute. One way is to define

$$P' = D^{1/2}PD^{1/2}$$

$P'$ is symmetric with the same eigenvalues as $P$. Also, the eigenvectors can easily be obtained using a simple transformation of either $D^{1/2}$ or $D^{1/2}$. The RSVD is used to compute the spectrum of $P'$.

Step 2: Next, the heat kernel coordinates is defined for each of the original data points. Let the eigenvalues of $P$ be defined as $\lambda_j$ and the right-eigenvectors as $v_j$ for $j = 1, 2, \ldots, \text{rank}(P)$.

Each point $x_i$ is then represented as $HKC(x_i) = (\exp(-\lambda_1 t).v_{i1}, \exp(-\lambda_2 t).v_{i2}, \ldots, \exp(-\lambda_r t).v_{ir})$ where $v_{ji}$ is the $i$-th coordinate of the eigenvector $v_j$. Here $t$ is the time/scale parameter that is to be varied to look at the geometries of the data set at various scales.

Note-1: The first eigenvalue/eigenvector of $P$ is trivial and should not be used.

Note-2: A subsequent SVD may be applied to heat-kernel coordinates matrix for mapping the points to the space of their 3 principal components for quick visualization.
4.2 Deliverables / Milestones

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<th>Date</th>
<th>Deliverables / Milestones</th>
<th>Status</th>
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<tr>
<td>Oct 2010</td>
<td>Progress report for period 1, 1st quarter</td>
<td>✔</td>
</tr>
<tr>
<td>Jan 2011</td>
<td>Progress report for period 1, 2nd quarter / complete randomized matrix decompositions task</td>
<td>✔</td>
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<tr>
<td>Apr 2011</td>
<td>Progress report for period 1, 3rd quarter / complete approximate nearest neighbors task</td>
<td>✔</td>
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<tr>
<td>Jul 2011</td>
<td>Progress report for period 1, 4th quarter / complete experiments – part 1</td>
<td>✔</td>
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<tr>
<td>Oct 2011</td>
<td>Progress report for period 2, 1st quarter</td>
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<tr>
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<td>Progress report for period 2, 4th quarter / complete experiments – part 2</td>
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<td>Oct 2012</td>
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<tr>
<td>Apr 2013</td>
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<tr>
<td>Jul 2013</td>
<td>Final project report + software + documentation on CDROM / complete experiments – part 3</td>
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5 Results and Discussion

An important issue with the MHKC algorithm described earlier is to ascertain the right time/scale parameter(s) for any given dataset. The idea is to provide automated techniques to help the analyst determine these parameters. For the representation problem of characterizing the various operational phases of a system, we are investigating metrics that can be used to assess the quality of the clustered representation at various time scales. This may help to quickly narrow down the search for time scales which exhibit the various local geometries in the dataset.
6 Conclusions

The project is on track with design/implementation of the new multiscale heat kernel coordinates algorithms. We will continue with algorithmic improvements and experimentation using the developed algorithms in the next quarter.

No problems are currently anticipated.
7 References


