SAMPLING TECHNIQUE ANALYSIS OF NYSTRÖM APPROXIMATION IN PIXEL-WISE AFFINITY MATRIX

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ABSTRACT

Spectral graph methods are widely employed in image segmentation, and they exhibit excellent performance. However, for high-resolution images, it is impractical to directly calculate the eigenvectors of the affinity matrix owing to the high computational requirements. The Nyström method provides an efficient way to approximate the large-scale affinity matrix by low-rank approximation. In the machine learning field, previous studies have mainly focused on less data points with high dimensional features. To the best of our knowledge, this is the first study to discuss the performance of sampling methods for Nyström approximation, in which we focus on the pixel-wise affinity matrix for a single image. In this paper, we propose a mean-shift segmentation-based Nyström sampling technique for image analysis. The experimental results show that for images with simple compositions and backgrounds, k-means sampling performs better, whereas for images with more complicated compositions and backgrounds, the proposed method can perform better.

Index Terms— Nyström approximation, spectral graph theory, image segmentation, mean-shift, diffusion map

1. INTRODUCTION

Spectral properties (eigenvectors and eigenvalues) play an important role in image analysis, especially in image segmentation and partitioning. Several studies have employed a pixelwise affinity matrix to implement image segmentation[1][2]; however, for a high-resolution image, finding eigenvectors becomes a computation-intensive task because the size of the affinity matrix is large. Therefore, Fowlkes *et al.* [3] used the solution of an integral eigenvalue problem known as the Nyström method to approximate the eigenvectors for a largescale affinity matrix. The Nyström method is a low-rank matrix approximation technique that samples only a small subset of pixels, and then, extends the solution of the subset to the entire image. This method can effectively reduce the computation and memory requirements, thereby facilitating the computation for a large-scale image.

The pre-processing procedure, which selects the sampling points, may have a significant effect on the performance of the approximation. Fowlkes *et al.* [3] used random sampling to accelerate spectral clustering. In [3], a cross-validation study verified the repeatability of 4 leading eigenvectors. However, high repeatability does not guarantee that the error resulting from approximation will be small. The errors occurring in the of Nyström method for an affinity matrix require further investigation. Zhang *et al.* [4] showed that k-means clustering is an effective sampling method because it can result in a smaller error upper bound. Kumar *et al.* [5] suggested that uniform sampling without replacement produces more effective approximations. In this paper, we show a further comparison of different sampling methods for a pixel-wise affinity matrix.

Image segmentation is a typical application of a pixelwise affinity matrix and spectral graph analysis. Shi et al. [1] used a generalized eigenvalue system to find the solution of a normalized cut problem. Cour et al. [2] constructed a graph encoding pairwise pixel affinity, and they partitioned the graph for image segmentation. The segmentation works in different scales simultaneously, which ensures consistency between scales and provides high-quality segmentations. In [6], Lafon and Lee showed that the diffusion distance can be measured by the coordinates of weighted eigenvectors of the graph Laplacian. Farbman et al. [7] replaced the Euclidean distances with diffusion distances in several algorithms, which are approximated using diffusion maps. The diffusion maps are a set of dominant eigenvectors of a largescale affinity matrix, and they can be efficiently computed by the Nyström method. The performance of different sampling methods can be evaluated by measuring the performance of diffusion map applications.

The system flow for finding approximated eigenvectors by the Nyström method is shown in Fig.1. In this paper, a mean-



Fig. 1: System flow for generating approximated eigenvectors for a large-scale affinity matrix by Nyström method.

shift segmentation-based sampling technique is proposed, and it performs better than other sampling methods in certain cases. We also focus on the error analysis of the approximated eigenvectors, which constitute the final part of the system flow.

The main contributions of this work are listed below.

- Previous studies on the Nyström method focused on data sets of smaller data points (few thousands) and higher dimension (tens to hundreds). To the best of our knowledge, this study is the first to compare the performance of different pre-processing methods for a large-scale pixel-wise affinity matrix (large number of data points of low-dimension data) of an image.
- 2. A fast improved Nyström approximation method is proposed for a pixel-wise affinity matrix of an image, which uses mean-shift [8] over-segmentation as the pre-processing technique for selecting suitable sampling points.
- 3. From the experimental result, for images with simple compositions and backgrounds, a suggestion of K-means sampling is made for the selection of preprocessing methods for the Nyström approximation. For the others, mean-shift segmentation-based sampling is a better solution due to its computation efficiency.

The remainder of this paper is organized as follows. First, an overview of the Nyström method is provided in Section 2. In Section 3, we describe the details of the sampling methods for the Nyström approximation. In Section 4, we analyze the performance of different sampling techniques. Finally, in Section 5, we conclude the paper and discuss the scope for future work.

2. NYSTRÖM METHOD

The Nyström method is a numerical approximation technique for the integral equation

$$\int_{a}^{b} W(x,y)\phi(y)\,\mathrm{d}y = \lambda\phi(x). \tag{1}$$

The integral equation can be evaluated by a set of evenly spaced points $\xi_1, \xi_2, ..., \xi_n$ in the interval [a, b],

$$\frac{(b-a)}{n}\sum_{j=1}^{n}W(x,\xi_j)\hat{\phi}(\xi_j) = \lambda\hat{\phi}(x),$$
(2)

where $\hat{\phi}(x)$ is the approximation of $\phi(x)$. Substituting x by ξ_j , the system can be considered as the matrix eigenvalue problem

$$A\hat{\Phi} = n\hat{\Phi}\Lambda,\tag{3}$$

where $A_{ij} = W(\xi_i, \xi_j)$, and Φ and Λ are the eigenvectors and eigenvalues of A, respectively. The *Nyström extension* of $\hat{\phi}_i$ is given by

$$\hat{\phi}_i(x) = \frac{1}{n\lambda_i} \sum_{j=1}^n W(x,\xi_j) \hat{\phi}_i(\xi_j). \tag{4}$$

Thus, the Nyström method can approximate the eigenvectors of the system by extending the eigenvectors of a small set of sample points.

3. SAMPLING METHODS OF NYSTRÖM METHOD

3.1. Completion in Affinity Matrix

For an image of N pixels, an N-by-N affinity matrix can be defined as

$$W_{ij} = \exp(-\frac{\|X_i - X_j\|^2}{\sigma_s} - \frac{\|I_i - I_j\|^2}{\sigma_c}), \qquad (5)$$

where X_i and I_i denote the location and color of pixel *i*, $\|.\|$ is the Euclidean distance, and σ_s and σ_c are pre-defined parameters that control the impact of spatial difference and color difference. After the affinity matrix is constructed, the diffusion map can be calculated by finding the eigenvectors of the affinity matrix W. Since the dimension of W is too high, it is impossible to find the eigenvectors directly. Therefore, the Nyström method is applied to solve this problem. Suppose that n pixels are sampled, and that these sample points can define an n-by-n affinity matrix A. The n-by-m affinity matrix of n sampling points and the remaining m pixels is defined as B, where m is N - n. The original affinity matrix W can be rewritten as $W = [A \ B; B^T \ C]$, where C is the affinity matrix of N - n unsampled points. Usually, the selected n is much smaller than N for computation efficiency. Using the Nyström extension, the eigenvectors can be approximated as $\overline{U} = [U; B^T U \Lambda^{-1}]$ where U denotes the eigenvectors of A, and Λ is the diagonal matrix of the eigenvalues of A. In other words, the diagonalization of the n-by-n affinity matrix A is given by $A = U\Lambda U^T$. Using the approximation eigenvectors \overline{U} , the total affinity matrix W can be approximated as

$$\hat{W} = \bar{U}\Lambda\bar{U}^T = \begin{bmatrix} A & B\\ B^T & B^TA^{-1}B \end{bmatrix}.$$
 (6)

Comparing W and (6), it is evident that the approximation error results from the difference between C and $B^T A^{-1}B$. In order to evaluate approximation performance, the approximation error is defined as $E = ||W - \hat{W}||_F$, where $||.||_F$ denotes the Frobenius norm of a matrix. Throughout this paper, the approximation error is used to check the performance



Fig. 2: The image on the left is the input image. After meanshift over-segmentation, the original image is separated into K regions, as shown on the right. In each region, the point that is closest to the center of mass of that region will be sampled. The centers of the blue crosses in the image on the right are the sampling points for Nyström approximation.

of different pre-processing methods for the Nyström method because a lower error results in more precise approximation.

3.2. K-means-based Sampling

In [4], Zhang *et al.* showed that k-means clustering is a good sampling method because it can result in a smaller error upper bound. For an image of N pixels, each pixel is embedded into a 5-D space (R,G,B,X,Y), and then, all the pixels can be divided into K clusters with K centers. For Nyström approximation, these K centers can be used to choose the sampling points(s_k). $s_k = \arg \min_i |Z_i - \mu_k|$, where Z_i is the 5-D data of pixel i and μ_k is the center of cluster k. After all the sampling points S ($S = \{s_1, s_2, ..., s_n\}$) are fully defined, the affinity matrix A can be calculated, and then, the Nyström approximation can be applied.

3.3. Mean-shift segmentation-based Sampling

Mean-shift [8] is a popular technique in feature space analysis, and it is widely employed in image over-segmentation. A mean-shift segmentation-based sampling method is proposed, and the performance of the proposed method will be compared with that of other state-of-the-art sampling methods in Section 4.

An input image I with N pixels can be over-segmented into n regions. In the entire image, there are n points to be sampled. Each region R_k has r_k pixels, and only one landmark point among r_k pixels will be sampled. The sample point (s_k) is defined as the spatially closest point to the center of mass of region R_k , and it given by

$$s_k = \arg\min_i \sum_{j=1}^N Y_j,\tag{7}$$

$$Y_j = \begin{cases} \|X_i - X_j\|^2 & \text{if } i, j \in R_k \\ 0 & \text{otherwise} \end{cases}, \qquad (8)$$

where X_i denotes the location of pixel *i*. The affinity matrix A can be calculated using the set of all sampling points, S.

Table 1: Performance comparison of the proposed meanshift segmentation-based sampling method and other sampling techniques

Datasets	Better than k-means	Better than random	
	sampling	sampling	
MSRC	52% (26/50)	88% (44/50)	
MSRA	55% (55/100)	87% (87/100)	

Fig.2 (right) shows the concept of the proposed mean-shift segmentation-based Nyström approximation. First, the input image is over-segmented into n regions, and then, the centers of the blue crosses are selected as the sampling points of each region. After the affinity matrix of sampling points A is constructed, its eigenvectors (U) and eigenvalues (Λ) can be calculated, and then, the approximated eigenvectors \overline{U} can be derived.

4. SAMPLING TECHNIQUE ANALYSIS

In this section, the performance of different sampling methods is compared on the basis of the approximation error. Furthermore, the effect of the approximation error on a real application, i.e., image segmentation, is discussed.

4.1. Datasets

The two main objectives of this study are to

- 1. Compare the performance of different sampling techniques for Nyström approximation by measuring the reconstruction error of the entire affinity matrix W.
- Discuss the effect of the approximation error in the Nyström method on real applications. Here, we select spectral segmentation as the test application.

In order to discuss the effect on spectral segmentation, the test images must have a clear object. Therefore, two image datasets are used as the test bed. One is the MSRC Grabcut database [9] with 50 images, and the other is the MSRA salient object database [10]. There are 20000 images in the MSRA database; however, owing to time and computation constraints, only 100 images are randomly selected as test images.

4.2. Error Analysis

In this subsection, we compare the approximation errors occurring in different types of sampling methods. Owing to the limitation of physical memory in computing the reconstruction error of \hat{W} , each test image is scaled down such that its longer side has a length of 160 pixels. For mean-shift oversegmentation, the parameters are set as follows: $h_s = 1$, $h_r = 1$, and M = 30. For k-means sampling, we use the default settings of the *kmeans* function in MATLAB. The



(a) Images where k-means sampling has better performance.

(b) Images where the proposed method has better performance.

Fig. 3: The MSRC Grabcut database is clustered into two sets. One is the set in which the proposed method has better performance, and the other is the set in which k-means sampling method has better performance. It is evident that the images enclosed in red rectangles in (a) have relatively simple backgrounds. It can be observed that for pictures with simple backgrounds without texture, k-means sampling tends to perform better. In contrast, for images with complicated backgrounds, the proposed method performs better.

average sampling rates for the MSRA and MSRC datasets are 1.10% and 1.14%, respectively.

The experiment is conducted as follows. First, each image is segmented into n regions by mean-shift over-segmentation, and then, the proposed method is applied to find the approximated eigenvectors. Next, n is set to be the number of sampling points of k-means and random sampling. The k-means and random sampling methods are characterized by randomness, which means that the approximation result of every trial is not unique. Therefore, for each image, k-means and random sampling are repeated 30 times; thus, 30 sets of approximated eigenvectors are obtained for every image. Because the proposed method provides only one approximation result given fixed parameters, mean-shift segmentation-based approximation is conducted only once for each image, instead of 30 times. To compare the performance of the proposed method with that of other sampling techniques, the reconstruction error $E = ||W - \hat{W}||_F$ is calculated, and the results are listed in Table 1. Here, we use the average error of 30 trials of k-means and random sampling for comparison with the error of the proposed mean-shift segmentation-based sampling. As seen in Table 1, the performance of the proposed method is slightly better than that of k-means sampling (52% & 55%), and considerably better than that of random sampling (88% & 87%). For further analysis of the characteristics of k-means sampling and the proposed method, the images in the MSRC database are clustered into 2 categories,

as shown in Fig.3. The category on the left contains images in which k-means sampling performs better, whereas that on the right contains images in which the proposed method performs better. The images enclosed in red rectangles have relatively simple backgrounds without texture, and k-means sampling performs better. Therefore, we propose a hypothesis that for images with simple compositions and backgrounds, k-means sampling method performs better, whereas for images with more complicated compositions and backgrounds, the proposed method can perform better.

4.3. Variance in K-means-based Sampling

The obversion in Fig.3 is not sufficiently strong to support our viewpoint. In order to verify our viewpoint, further numerical analysis is required. Fig.4 shows the number of trials in which k-means sampling performs worse than the proposed method. The higher the bar, the better is the performance of the proposed method. The images with simple backgrounds in Fig.3 are represented by vertical red lines. For 6 of the 8 images, the performance is not worse than that of the proposed method in 30 trials. K-means sampling performs worse in only 6.25% of the 240 trials for these 8 images; this proves that "for images with simple compositions and backgrounds, k-means sampling method performs better."

Furthermore, an interesting observation can be made from Fig.4. When comparing the average error, in 52% of the cases, the proposed method performs better; however, when



Fig. 4: Histogram of number of trials in which k-means sampling is worse than the proposed method for each image of the MSRC database. The red vertical lines represent the images enclosed by red rectangles in Fig.3.

comparing the trials individually, the proposed method performs better in only 12.06 trials, on average. This indicates one major problem in the k-means sampling method, i.e., the variance results from randomness. Since the performance of the k-means sampling method is significantly affected by the initial seeds, the randomness may result in a considerable error that destabilizes the approximation result in each trial. In order to check whether the proposed method can provide a more stable solution than k-means sampling, that is, whether the proposed method can handle the images in which k-means sampling has a large variance among different trials, an analysis is conducted, as shown in Fig.5. The X-axis represents the standard deviation of the normalized k-means sampling error (\bar{E}) for 30 trials of one image, where the normalized k-means sampling error \bar{E} is defined as $\bar{E} = \frac{\|W - \hat{W}\|_F}{N}$, where N is the number of pixels in the image. The Y-axis represents the ratio of the mean-shift segmentation-based sampling error to the average of the k-means sampling error for 30 trials. Both these variables are expressed in the log scale in Fig.5. Fig.5 only shows the part where $STD(\bar{E}) > -1.5$ because we focus on the images in which k-means sampling has a large variance. The red line is the regression line for which the correlation coefficient equals -0.7099, which means that these two variables are highly correlated. This proves that when dealing with images in which k-means sampling has a large variance among different trials, the proposed mean-shift segmentationbased sampling method can provide a better solution. The points below the green reference line in Fig.5 represent the images in which the proposed method performs better. Fig.5 shows that the proposed method has a smaller approximation error in 64% (16/25) of the images, which is higher than the value listed in Table 1 (55%). This proves that for images with more complicated compositions and backgrounds, the proposed method can perform better.



Fig. 5: The red line is the regression line of the standard deviation of the k-means-based sampling error (X-axis) and the ratio of the mean-shift segmentation-based sampling error to the k-means-based sampling error (Y-axis); both variables are expressed in the log scale. The points below the green reference line represent the images for which mean-shift segmentation-based sampling performs better than k-means-based sampling. The data is generated from the M-SRA database.

4.4. Computation Time

It is important to consider not only the accuracy but also the computation time when we evaluate the performance of a sampling method. Table 2 lists the average computation time of each sampling method. The second column lists the computation time of the pre-processing step (sampling), the third column lists the computation time for approximation, and the last column lists the total computation time. The MATLAB program is executed on a PC with Core(TM)-i7 2600 (3.40GHz) and 16 GB memory. The proposed method is much faster than K-means sampling. Surprisingly, the proposed method is faster than random sampling mainly because in the approximation procedure, we use a sparse matrix to accelerate the computation. Elements whose values are below the threshold are set to 0. The sampling points in mean-shift segmentation-based and k-means sampling differ considerably, resulting in a more sparse affinity matrix. This explains why the approximation processes of mean-shift segmentation-based and k-means sampling are slightly faster than random sampling.

4.5. Effect in Image Segmentation

In this subsection, we discuss the effect of the approximation error on a segmentation application. A diffusion map is used to implement image segmentation. The red and green lines in Fig. 6 represent the input strokes for identifying the foreground and background. The diffusion distances between each pixel in the image and the labeled pixels are calculated. Every pixel is clustered into the foreground or background, set by the k-nearest neighbor (KNN) algorithm. If a pixel

MSRC	Pre.	Main	Total
Mean-shift	0.1378	1.2862	1.4240
K-means	8.5535	1.3036	9.8571
Random	0.0015	1.5077	1.5092
MSRA	Pre.	Main	Total
MSRA Mean-shift	Pre. 0.1368	Main 1.2148	Total 1.3516
MSRA Mean-shift K-means	Pre. 0.1368 8.1309	Main 1.2148 1.2262	Total 1.3516 9.3571

Table 2: Average computation time of each sampling method in the two datasets (s)

has more KNNs that are identified as foreground pixels, it is clustered into the foreground; otherwise it is regarded as a background pixel. Fig. 6 shows an example of the effect due to the approximation error of different sampling methods.

5. CONCLUSION

In this paper, we compared different sampling methods for Nyström approximation. To the best of our knowledge, this is the first study to focus on a pixel-wise affinity matrix for a single image in order to analyze the performance of sampling methods for Nyström approximation. The proposed meanshift segmentation-based Nyström approximation can handle those images in which k-means sampling does not perform well. Moreover, the proposed method is faster than random sampling, with a lower approximation error.

This work can be potentially extended for further analysis of the relationship between the Nyström approximation error and the error rate of image segmentation. In addition, it can be extended to apply the Nyström approximation with different sampling methods to other applications such as color editing with diffusion maps or spectral clustering.

6. ACKNOWLEDGEMENT

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Fig. 6: Segmentation results of Nyström approximation with different sampling methods.

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