# Nonlinear PCA for Source Optimization in Optical Lithography

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***Abstract* - In this paper, we propose a Kernel PCA (KPCA) based light source optimization method for computation of the aerial image. The proposed approach is more general in nature and considers both continuous as well as discontinuous intensity distribution from different types of lithography light sources. We have compared both the PCA and KPCA approach, on four different light sources (conventional, annular, dipole, and quadruple light sources) used in optical lithography. Our simulation results clearly indicate that the KPCA performance in variance coverage among discrete data sets is better than the PCA for all the four types of light sources. Thus using KPCA, we can reduce the number of kernels (pixels) for different shapes of light sources using lesser number of principal components (PCs) compared to the PCA based linear approaches. This will help in reducing the computational complexity during the simulation of aerial image formation.**

***Index Terms* - *Resolution enhancement techniques, kernel PCA, lithography simulation, and source optimization.***

## I. INTRODUCTION

The simulation of aerial image formation is a critical step for the development of resolution enhancement techniques (RETs) used in optical lithography. These simulations consider the effect of light sources, optical lenses, mask and the refractive index of the immersion medium and are always computationally expensive. For example, the simulation of a $1\text{cm}^2$ image with a resolution of 1nm requires the computation of $10^{14}$ image pixels [1].

The various steps involved in the aerial image formation process are shown in the Fig. 1. As can be seen, the very first step in the aerial image formation is the use of light source. During the aerial image simulation, the light source is generally discretized into point sources and the aerial image is computed by summing up the contributions from all these discrete point sources. Different techniques are generally used to select the appropriate number of discrete point sources (called kernels) for a given light source. The techniques like Abbe's approach and Hopkin's theory have already been discussed in the literatures for the aerial image simulation. The sum of coherent systems solves the Hopkins partially coherent imaging equation by using the SVD algorithm [2]. The Abbe-PCA [1] utilizes the PCA (a method based on the eigenvalue decomposition of the source covariance matrix) for optimizing the light sources. The PCA assumes that the light intensity measured at various points in the field of interest is linearly related. However this assumption is not true for the light sources used in advanced lithography systems. The conventional laser light source has a continuous and normally distributed beam intensity profile [3], in which the light intensity at various discrete points are linearly related, whereas the other light sources, shown in Fig. 2, shows the discontinuity in their intensity distribution pattern. The annular, dipole and quadruple light source's intensity patterns are non-linear filtered versions (e.g filtering using a signum function like profile) of conventional light source. The SVD and PCA techniques are not adequate to capture the discontinuous intensity patterns for advanced light sources.

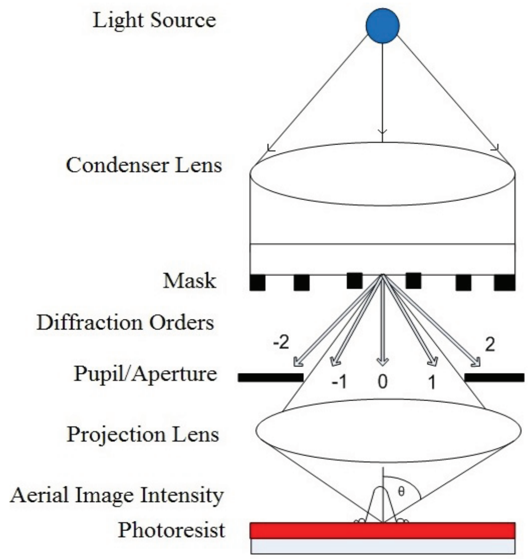


Fig. 1. The block diagram of a projection lithography system

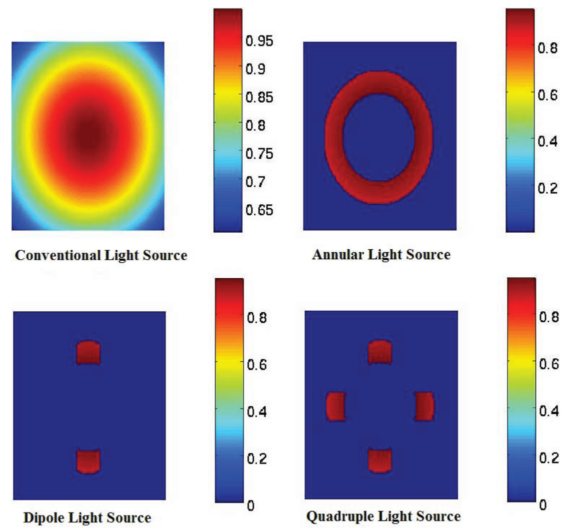


Fig. 2. Four different type of light sources generally used in advanced lithography systems


978-1-4673-5736-4/13/$31.00 

In this paper, we have used KPCA for optimization of the advanced light sources used in current technology nodes. We have clearly shown that the KPCA performance in variance coverage among discrete data sets is better than the PCA for all the four types of light sources shown in Fig. 2 and this new approach reduces the computational complexity during aerial image simulation.

## II. PCA AND KERNEL PCA TECHNIQUES

PCA is the eigenvector based multivariate data analysis technique used for the dimensionality reduction of high dimensional data sets [4]. It is an orthogonal basis transformation technique that extracts the eigenvectors from the covariance matrix of original data set with decreasing order of their eigenvalues. In essence, PCA explains most of the variance in the data using less number of orthogonal vectors with the eigenvalues indicating the amount of variance captured by that particular eigenvector (eigenvector corresponding to larger eigenvalue explains the larger variance in the data set). The eigenvectors, generally smaller than the original set of variables, are then used to map the original data set. Principal components (PCs) mapping of original data set is shown in Fig. 3.

KPCA is a non-linear form of PCA and it transforms the data to a feature space, as shown in Fig. 4 [5]. This feature space is basically a higher dimensional space, where the observations (data from source) are related linearly and therefore PCA can be performed in the feature space. Unlike PCA which exploits only the linear relationships in the high dimensional data sets, KPCA find the principal components for data sets that has nonlinear relationships among its variables using appropriate nonlinear mapping ($\Phi(x)$). One of the key feature of KPCA is that the knowledge of nonlinear mapping is not essential for computation and only its inner product k(x,y) (Kernel) $= \Phi(x).\Phi(y)$ is required for obtaining the feature space. The inner product can be computed from the original data points using the kernel function like Gaussian kernel [Eq. (1)] or polynomial kernels [Eq. (2)] which are commonly used in KPCA.

$$k(x,y) = \exp\left(-\frac{||x-y||^2}{2\sigma^2}\right) \tag{1}$$

$$k(x,y) = (x.y)^n \tag{2}$$

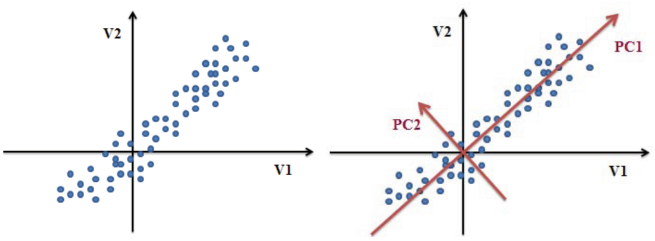


Fig. 3. The principal component mapping using PCA. (a) Original data distribution (b) PCA mapping

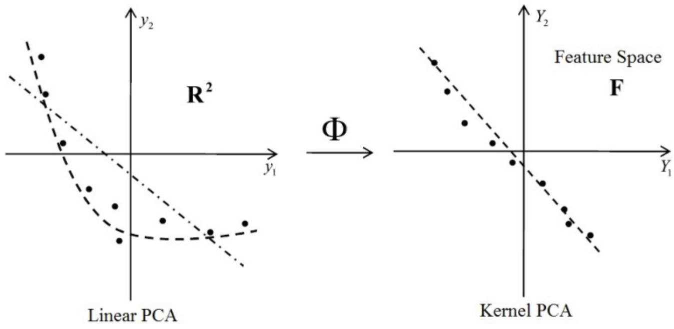


Fig. 4. The feature space mapping using Kernel PCA (KPCA).

The advantages of the KPCA method in lithography source optimization are: (i) It accounts for the nonlinear relationship present among the various discrete intensity distribution points in different light sources, and (ii) the reduction in the number of principal components (small number of kernels can explain the entire variance present in the whole data set in the transformed space) used in the computation of aerial images.

## III. IMAGE RECONSTRUCTION

For PCA based image reconstruction of the light source intensity profiles, it is required to first compute the mean for n dimensional intensity distribution data set X (n×n matrix), which is given by the equation (3).

$$m^i = \frac{1}{n}\sum_{i=1}^{n} x^i \tag{3}$$

Here, $m^i$ is mean value for $x^i$ vector ( $i^{th}$ column vector of X). Then, the covariance matrix of X and its n eigenvectors are shown in the equations (4) and (5) respectively.

$$Cov(X) = \frac{1}{n-1}\left[\sum_{i=1}^{n}(x^i - m^i)(x^i - m^i)^T\right] \tag{4}$$

$$E = [EigVec^1 \quad EigVec^2 \quad EigVec^3 \quad \ldots \quad EigVec^n]_{n\times n} \tag{5}$$

After that, the principal component vectors are given by,

$$PC = (\text{zero mean shifted } X)_{n\times n} * (E)_{n\times n} \tag{6}$$

Now, with first p ($\leq$ n) principal component vectors and their corresponding eigenvectors, the pre-image for light source intensity profile is given by,

$$X_{Reconstructed} \approx (PC)_{n\times p} * [\,(E)_{n\times p}]^T + [mean(X)]_{1\times n} \tag{7}$$

The difference between original intensity profile and reconstructed intensity profile depends upon the number of eigenvectors involved in the reconstruction process. Exact original intensity profile can be obtained by including all the eigenvectors of the covariance matrix.

From KPCA intensity profile reconstruction, the exact original profile is difficult to obtain and sometimes it is even impossible to generate the original intensity distribution points [6]. After performing linear PCA in feature space, there can be large number of points in the transformed space, whose pre-image doesn't even exist in the original input space.

For reconstruction of the pre-image in KPCA, we have to consider a projection operator $P_n$ and an approximated pre-image point z, such that,

$$P_n .\Phi(x) \approx \Phi(z) \quad (8)$$

The approximated pre-image can be obtained by minimizing the residual, res(z),

$$res(z) = \|\Phi(z) - P_n\Phi(x)\|^2 \quad (9)$$

For Gaussian kernel function, z, can be approximated as [6]:

$$z_{t+1} = \frac{\sum_{i=1}^{n} \gamma_i \exp(-||z_t - x_i||^2/2\sigma^2)x_i}{\sum_{i=1}^{n} \gamma_i \exp(-||z_t - x_i||^2/2\sigma^2)} \quad (10)$$

where σ represents kernel range, $\gamma_i$ depends upon projection operator and t is iteration variable. The iterative nature of z helps in reducing the residual in equation (9). This iterative pre-image reconstruction process is highly dependent on the initial value of z and the value of σ.

## IV. EXPERIMENTAL DETAILS

Four different light sources (as shown in Fig. 2) have been used for the comparative study of PCA and KPCA techniques. Each light source is represented by a 128×128 matrix dimensions, based on pixel based source representation. Standard PCA algorithm is applied to find the covariance matrix and the eigenvalues of the covariance matrix. For KPCA, Gaussian kernel [5] is used to transform the data into higher dimensions. The implementations of the standard PCA and KPCA algorithms are done using Matlab. The variance coverage from first five principal components (PCs) for all four types of light sources is computed using both linear PCA and KPCA algorithms. For eigenvalue comparison of PCA and KPCA, for different light sources, first 10 eigenvalue indices with descending order of eigenvalues are considered.

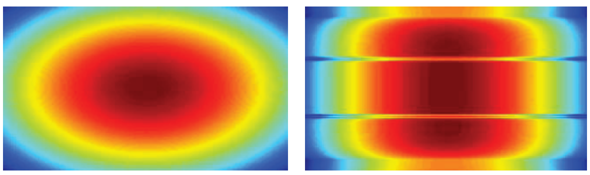

Fig. 5. The reconstructed images of the conventional light source (a) PCA reconstructed image (b) KPCA reconstructed image

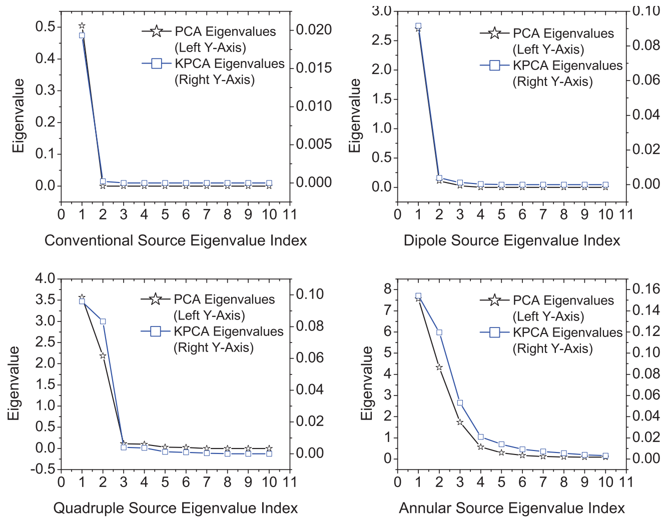


Fig. 6. The eigenvalue plot for different light sources with PCA and KPCA.

TABLE I – Variance coverage results for PCA and KPCA

| Type of light sources | Cumulative variance coverage with principal components ( PC's ) ( %) | | |
|---|---|---|---|
| | PC's | PCA | Kernel PCA |
| Conventional | PC1 | 100 | 99.99 |
| | PC2 | 100 | 100 |
| | PC3 | 100 | 100 |
| | PC4 | 100 | 100 |
| | PC5 | 100 | 100 |
| Annular | PC1 | 48.96 | 57.23 |
| | PC2 | 76.92 | 91.66 |
| | PC3 | 88.14 | 98.49 |
| | PC4 | 91.82 | 99.54 |
| | PC5 | 93.72 | 100 |
| Dipole | PC1 | 95.17 | 99.8 |
| | PC2 | 99.08 | 99.88 |
| | PC3 | 100 | 100 |
| | PC4 | 100 | 100 |
| | PC5 | 100 | 100 |
| Quadrupole | PC1 | 59.35 | 56.85 |
| | PC2 | 95.73 | 99.82 |
| | PC3 | 97.58 | 99.91 |
| | PC4 | 99.17 | 99.99 |
| | PC5 | 99.61 | 100 |

## IV. RESULTS & DISCUSSIONS

Fig. 5 shows the pre-image reconstruction results for the conventional source with both linear PCA and KPCA, using only first principal component. Fig. 6 shows the eigenvalues of all four types of light sources with PCA and KPCA algorithms. The asymptotic nature of these eigenvalue plots represents that first few eigenvalues and their corresponding eigenvectors are more significant compared to the other eigenvectors. The Table 1 shows the variance coverage results from first five principal components of linear PCA and KPCA.

The KPCA variance coverage results show improved performance over linear PCA for all the four types of light sources. At the same time the KPCA pre-image reconstruction results are trailing compared to PCA reconstruction results.

## IV. Conclusions

The simulation study of commonly used lithography light sources based on PCA and KPCA is presented. We have compared the PCA and KPCA approach, on four different types of light sources (conventional, annular, dipole, and quadruple light sources) used in lithography. Our simulation results clearly indicate that the KPCA performance in variance coverage among discrete data sets is better than PCA for all the four types of light sources. Thus using KPCA, we can reduce the number of kernels (pixels) for different shapes of lithography light source using lesser number of principal components compared to PCA based linear approaches. However, there are unresolved issues with pre-image reconstruction in KPCA. We tried to work out the pre-image reconstruction for conventional light source only. The iterative approach used in KPCA pre-image part, seems to be insufficient to reconstruct all the four types of light sources. The KPCA reconstruction problem needs to be resolved with more generalized approach.

## References


[1] Meng Fong Tsai et al., “Abbe-PCA (Abbe-Hopkins): Microlithography Aerial Image Analytical Compact Kernel Generation Based on Principle Component Analysis,” *Proceedings of SPIE,* vol. 7274, 72742D, 2009.

[2] N. Cobb, “Fast Optical and Process Proximity Correction Algorithms for Integrated Circuit Manufacturing,” PhD Dissertation, University of California Berkeley, 1998.

[3] Fred M. Dickey et al., "Laser Beam Shaping Applications," Taylor & Francis Group, 2006.

[4] I. T. Jolliffe, “Principal Component Analysis,” Springer, 2002.

[5] Xiang Ma et al, “Kernel principal component analysis for stochastic input model generation,” *Journal of Computational Physics*, 230, 7311-7331, 2011.

[6] Sebastian Mika et al., "Kernel pca and de-noising in feature spaces," *Advances in Neural Information Processing Systems,* 11, pp. 536-542, MIT Press, 1999.