

Master Thesis

An ADMM approach to estimate Sparse Abnormal Subspace for Anomaly Detection and Interpretation

(基于ADMM的PCA异常空间稀疏化方法)

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GOALS

- *ANOMALY DETECTION
- *ANOMALY INTERPRETATION



OUTLINE

- Introduction
- Motivation
- Abnormal Subspace Estimation
- **Experiments**
- *Discussion
- Conclusion
- *References



ANOMALY DETECTION (1/2)

- Most instances have normal trend
 - Very few fit least
 - Termed as anomaly
- Method to detect anomalies
 - Human annotations impossible
- Unlabeled dataset
 - Unsupervised method best choice
- PCA (Principal Component Analysis) can exploit the fact
 - Pioneering tool to find anomalies in high dimensions
 - Known as dimension reduction tool
 - Better visualization support (direction of eigenvectors)
 - Unsupervised
 - Focuses on normal trend of data explaining maximum variance



ANOMALY DETECTION (2/2)

- Downside of PCA
 - Have few zero entries on loadings
 - Non-sparse in nature
 - PCs cannot be interpreted
 - Interpreting PCA can be inherently challenging problem [RSR07]
 - Need sparse PC alongside dimension reduction
- Sparse PCA [ZHT06]
 - Make PCA understandable
 - Returns the most significant sparse PC covering maximum variance
 - Often we need more than one PC to explain required variance
 - No orthogonal guarantee



LITERATURE SHORTCOMINGS

- Cannot use existing methods directly in high dimensions
 - We focus on abnormal subspace
 - Abnormal subspace has more PCs
 - Introduces efficiency issues
 - Mostly focused on significant Principal Components
 - Capturing maximum variance
- Can be used only on Anomaly Detection
 - Anomaly Interpretation is infeasible
- Anomaly Interpretation is ignored on PCA-based model
 - Low sparsity
- Deflation technique
 - Increase in number of PCs increases computation time



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PRIME FOCUS

- Find a sparse Abnormal Subspace
 - Outliers have high projection
- Keep as simple as PCA
 - Keep variance equal
 - Keep PCs similar
 - Can go back to PCA
- Interpret anomalies
 - Using sparse abnormal PCs
- Reduce extravagant SDP computations
 - Introducing SDP formulation for subspace with convex relaxation
- Use efficient and effective optimization tool
 - Alternating Direction Method of Multipliers (ADMM)



ADMM (1/1)

- Popular tool/algorithm to solve convex optimization problem
- Solves optimization problems mostly in the form

$$\min_{x,z} f(x) + g(z)$$
s.t. $Ax + Bz = c$

- fand g are convex
- Two sets of variables with separate objective
- The augmented Lagrangian can be formed as,

$$L_{\rho}(x,z,y) = f(x) + g(z) + y^{T}(Ax + Bz - c) + \left(\frac{\rho}{2}\right) ||Ax + Bz - c||_{2}^{2}$$

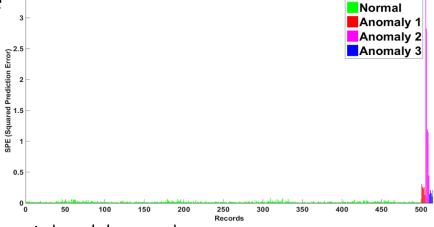
ADMM Steps

```
x^{k+1}:= argmin\ L_{\rho}(x, z^k, y^k) //x-minimization 
 z^{k+1}:= argmin\ L_{\rho}(x^{k+1}, z, y^k) //z- minimization 
 y^{k+1}:= y^k + \rho(x^{k+1} + B\ z^{k+1} - c) //Dual variable update
```



ANOMALY DETECTION (1/1)

- $V_{abnormal} = (v_1, ..., v_d)$ is d-dimensional abnormal subspace
 - Covers minimum variance
- $V_{normal} = (v_{d+1}, v_2, v_3, ..., v_p)$ is the normal subspace
 - Defined by the significant \dot{p} d PCs
 - Complement of abnormal Subspace
 - Covers maximum variance
- For a data point y,
- its residual is
 - $\hat{y} = y V_{normal} V_{normal}^T y$



- The squared length of projection residual length $\widehat{\mathbf{y}}$
 - Metric to indicate whether y is an anomaly
 - Squared Prediction Error (SPE)
 - The higher the SPE, it is more likely instance is an outlier

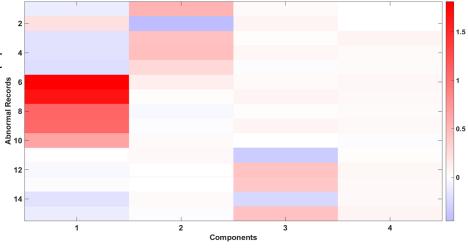


ANOMALY INTERPRETATION (1/1)

- Given V_{normal} and $V_{abnormal}$ subspace[BZS15] $\hat{y} = y V_{normal}V_{normal}^Ty = V_{abnormal}V_{abnormal}^Ty$
- Using orthogonal property [BZS15]

$$SPE = \hat{y}^T \hat{y} = \sum_{i=1}^d (v_i^T y)^2$$

- Squared sum of y's scalar projection on each abnormal PCs
- Abnormal PCs should be
 - Linear combination of important feature variables
 - Strong heatmap projection
 - Responsible for abnormality





RELATED WORK (1/2)

FPS[VCLR13]

- Emphasized on the span of eigenvectors called the 'Principal Subspace'
- A novel convex optimization problem to estimate the *d*-dimensional principal subspace
- Captures maximum variance representing normal data
- Represents most significant sparse PC's
- Introduces another issue of interpretation performance

• LFPCA[CL15]

- Focused on sequential estimation of subspace
- SDP with convex relaxation
- Interpretation performance improves computing PCs sequentially
- Enforced orthogonality constraint to be represented as eigenvectors



RELATED WORK (2/2)

- ASPCA-BG[BZS15]
 - Estimates an 'Abnormal Subspace'
 - Represents anomalies with abnormal trend
 - Least significant PCs
 - Covers very minimum variance
 - Interprets anomalies
- Novel to all other mentioned related works in literature
 - All methods emphasizes on PCs with maximum variance
 - ASPCA-BG concerns about the PCs with lowest variance
- Normal data have almost zero length projection on abnormal subspace
- Uses Deflation technique
 - Solves SDP problem iteratively
 - Time consuming



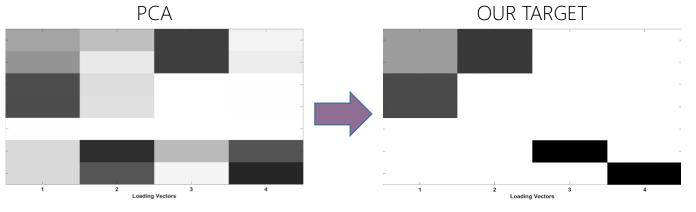
COMPREHENSIVE COMPARISON

TASK	PCA	FPS[VCLR13]	LFPCA[CL15]	ASPCA-BG[BZS15]
ANOMALY DETECTION	✓	✓	✓	✓
SPARSITY	×	✓	✓	✓
anomaly interpretation	×	×	×	✓
LOW TIME CONSUMPTION	✓	✓	✓	×
ABNORMAL SUBSPACE ESTIMATION	×	×	×	✓



CONTRIBUTION

- Estimate d-dimensional abnormal subspace simultaneously
 - Using the connection of PCA
- An ADMM solution of SDP problem with convex relaxation
 - Low rank matrix approximation
 - Sparsity constraint
 - Enforce orthogonality constraint on computed PCs
- Reduce extravagant computation time
- Abnormal Sparse loading vectors representing anomalies





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- ❖Introduction
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- Abnormal Subspace Estimation
 - ➤ Simultaneous Approach
 - ➤ Sequential Approach
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SIMULTANEOUS ESTIMATION (1/4)

- Our focus is to find subspace explaining minimum variance
- The ordinary PCA problem with objective to capture the lowest variance

$$\min_{U \in R^{p \times d}} Tr(U^T S U)$$

$$s. t. U^T U = I_d$$

- Quadratic problem to a linear problem
 - By considering $X = UU^T$, making X positive semidefinite $\min_{X,U} Tr(SX)$ $s.t.X = UU^T$; $U^TU = I_d$
- Or equivalently

$$\min_{X} Tr(SX)$$

s.t.X is a d - dimensional projection matrix



SIMULTANEOUS ESTIMATION (2/4)

- Good News
 - Estimates Subspace
 - Simultaneous extraction of PCs
- Bad News
 - Finding the global minimizer is computationally demanding
- Solution
 - Formulate it with convex relaxation



SIMULTANEOUS ESTIMATION (3/4)

- Tr(SX) is linear in X
 - Equivalent to a convex problem

$$\min_{X} Tr(SX)$$

 $s.t.X \in Convhull(all\ d-dim\ projection\ matrices)$

Add sparsity

$$\min_{X} Tr(SX) + \lambda ||X||_{1,1}$$

 $s.t.X \in Convhull(all\ d-dim\ projection\ matrices)$

- $||X||_{1,1}$ Entrywise l_1 norm
- λ tuning parameter
- The tightest convex relaxation can be Fantope [VCLR13]

$$F_{p_d}(X) := \{ X : X = X^T, 0 \le X \le I \text{ and } Tr(X) = d \}$$

- Is a convex body [Fillmore & Williams 71]
- Comprises with extreme points of convex hulls
- Has non-zero eigenvalues
- Orthonormal matrices with particular dimension



SIMULTANEOUS ESTIMATION (4/4)

Our Abnormal Subspace estimation objective function

$$\min_{X} Tr(SX) + \lambda ||X||_{1,1}$$

$$s.t.X \in F_{p_d}$$

- Solve a linear function over intersection of two convex sets
 - The l_1 ball
 - The Fantope, F_{p_d}
- How to exploit the sparsity constraint and low rank approximation constraint together?
 - Use ADMM
 - We propose ASPCA-ADMM algorithm



ASPCA-ADMM (1/4)

- Equivalent ADMM formulation
 - Introducing convex Indicator function $1_{F_{p_d}}(X)$

$$\min_{X} Tr(SX) + 1_{F_{p_d}}(X) + \lambda ||X||_{1,1}$$

$$s.t.X \in F_{p_d}$$

Splitting to two variables

$$\min_{X} \infty \cdot 1_{F_{p_d}}(X) + Tr(SX) + \lambda ||Y||_{1,1}$$

$$s \cdot t \cdot X - Y = 0$$

• The augmented Lagrangian associated with it has the form

$$L\rho(X,Y,U) = \infty \cdot 1_{F_{p_d}}(X) + Tr(SX) + \lambda ||Y||_{1,1} + \frac{\rho}{2} (||X - Y - U||_2^2 + ||U||_2^2)$$

- Where $U = (1/\rho)Z$ is the scaled ADMM dual variable [BPC11]
- \bullet ρ is the ADMM penalty parameter



ASPCA-ADMM (2/4)

Iteration scheme is simple

$$X^{new} \leftarrow P_{F^d}(Y^{old} - U^{old} - S/\rho)$$

 $Y^{new} \leftarrow S_{\lambda/\rho}(X^{new} + U^{old})$
 $U^{new} \leftarrow U^{old} + \rho(X^{new} - Y^{new})$

- ¬ Fantope projection
- □ Dual update

- Then
 - $(X^{old}, Y^{old}, U^{old}) \rightarrow (X^{new}, Y^{new}, U^{new})$
 - Repeat until convergence is observed
- Fantope projection ≈ Soft thresholding singular values
- Use common patterns to solve minimization steps
 - Proximal Algorithms [PB14]
- Some algebraic manipulation reduces X and Y updates to
 - Computing Proximal Operators
 - X- update to Euclidean projection onto Fantope
 - Y- update to elementwise soft thresholding



ASPCA-ADMM (3/4)

- Fantope Projection can be computed
 - Euclidean projection onto Fantope and a closed form [VCLR13]

$$P_{F^d}(X) = \sum_i \gamma_i^+(\theta) u_i u_i^T$$

- Where, $\gamma_i^+(\theta) = min(max(\gamma_i \theta, 0), 1)$ and θ satisfies the equation $\sum_i \gamma_i^+(\theta) = d$.
- The second step is called the shrinkage step
 - Defined as Soft Thresholding for any λ/ρ

$$S_{\lambda/\rho}(X) = sign(X) \max(|X| - \lambda/\rho, 0)$$

And we chose to terminate our ADMM when

$$\max(|||X^{(t)} - Y^{(t)}|||_2^2, \rho^2|||Y^{(t)} - Y^{(t-1)}|||_2^2) \le \epsilon$$

Keep the primal and dual residual norms within a constant factor



ASPCA-ADMM (4/4)

Algorithm 1 ASPCA-ADMM

```
Input: D, d, \lambda, \rho, \epsilon

S \leftarrow covariance(D)

Y^{(0)} \leftarrow 0, U^{(0)} \leftarrow 0

repeat t = 0, 1, 2, 3, ...

X^{(t+1)} \leftarrow P_{F^d}(Y^{(t)} - U^{(t)} - \frac{S}{\rho})

Y^{(t+1)} \leftarrow S_{\lambda/\rho}(X^{(t+1)} + U^{(t)})

U^{(t+1)} \leftarrow U^{(t)} + X^{(t+1)} - Y^{(t+1)}

until max(|||X^{(t)} - Y^{(t)}|||_2^2, \rho^2|||Y^{(t)} - Y^{(t-1)}|||_2^2) \leq d\epsilon^2

return Y^{(t)}
```

- ⊲ Covariance matrix
- ⊲ Initialization

- □ Dual update



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SEQUENTIAL APPROACH (1/2)

- Estimate Abnormal Subspace by computing the Abnormal PCs sequentially
 - One by one
- Individual eigenvectors have better interpretability [CL15]
 - Different eigenvectors may have different support
- Required/Guarantee
 - Sparsity
 - Orthogonality



SEQUENTIAL APPROACH (2/2)

- Two major steps
- First step
 - The first least significant eigenvector is simple

•
$$\hat{X}_1 = \min_{X_1 \in P_{F^1}} Tr(SX_1) + \lambda ||X_1||_{1,1}$$

- $\hat{v}_1 = first\ leading\ eigenvector\ of\ \hat{X}_1$
- Second step
 - For $j \geq 2$, let $\hat{V}_{j-1} = (\hat{v}_1, \dots, \hat{v}_{j-1})$
 - Deflated Fantope : $DF_{p_j} = \{X_j \in F_{P_1}; X_j \hat{V}_{j-1} = 0\}$
 - $\hat{X}_j = \min_{X_j \in DF_{p_j}} Tr(SX_j) + \lambda ||X_j||_{1,1}$
 - $\hat{v}_j = first\ leading\ eigenvector\ of\ \hat{X}_j$
- Guarantees orthogonality of estimated eigenvectors
- ASPCA-ADMMSEQ



ASPCA-ADMMSEQ (1/3)

- ADMM iterations
 - Almost same as previous approach
- Fantope Projection can be computed setting d = 1 [VCLR13]

$$P_{F^1}(X) = \sum_{i} \gamma_i^+(\theta) u_i u_i^T$$

- Where, $\gamma_i^+(\theta) = min(max(\gamma_i \theta, 0), 1)$ and θ satisfies the equation $\sum_i \gamma_i^+(\theta) = 1$.
- Deflated Fantope projection can be computed as [CL15]
 - Frobenius norm projection onto Deflated Fantope
 - Let $\widehat{U}_{i-1} \in \mathbb{R}^{p \times p-j+1}$ be an orthonormal complement basis of \widehat{V}_{i-1} , then

$$P_{D_j}(X) = \widehat{U}_{j-1} \left[\sum_{i=1}^{p-j+1} \gamma_i^+(\theta) \eta_i \eta_i^T \right] \widehat{U}_{j-1}^T$$

- Where, (γ_i, η_i) are the Eigen components of $\widehat{U}_{j-1}^T X \widehat{U}_{j-1}$
- $\gamma_i^+(\theta) = min(max(\gamma_i \theta, 0), 1)$
- And θ is chosen such that $\sum_{i=1}^{p-j+1} \gamma_i^+(\theta) = 1$
- The second step is same as previous approach, Soft-thresholding

$$S_{\lambda/\rho}(X) = sign(X) \max(|X| - \lambda/\rho, 0)$$



ASPCA-ADMMSEQ (2/3)

- 2 stopping criterion for 2 loops
- An Outer loop controls required number of Abnormal PCs
 - ullet Terminate sequential computation while d achieved
- An Inner loop controls ADMM convergence for each PC
 - And we chose to terminate our ADMM like previous approach
 - ullet Keep the primal and dual residual norms within a constant factor, $oldsymbol{\epsilon}$



ASPCA-ADMMSEQ (3/3)

Algorithm 2 ASPCA-ADMMSEQ

```
Input: D, d, \lambda, \rho, \epsilon, j = d
S = covariance(D)
P = 0
Y_1^{(0)} \leftarrow 0, U_1^{(0)} \leftarrow 0
repeat t = 0, 1, 2, ...
           X_1^{(t+1)} \leftarrow P_{F_1}(Y_1^{(t)} - U_1^{(t)} - S/\rho)
            Y_1^{(t+1)} \leftarrow S_{\lambda/2} (X_1^{(t+1)} + U_1^{(t)})
            U_1^{(t+1)} \leftarrow U_1^{(t)} + X_1^{(t+1)} - Y_1^{(t+1)}
until \max(||X_1^{(t)} - Y_1^{(t)}||_2^2, \rho^2|||Y_1^{(t)} - Y_1^{(t-1)}|||_2^2) \le d\epsilon^2
P = P \cup Y_1^{(t)}
for j = 2, ..., d
            Y_i^{(0)} \leftarrow 0, U_i^{(0)} \leftarrow 0
            repeat t = 0, 1, 2, ...
                        X_j^{(t+1)} \leftarrow P_{DF_j}(Y_j^{(t)} - U_j^{(t)} - S/\rho)
                        Y_j^{(t+1)} \leftarrow S_{\lambda/\rho} (X_j^{(t+1)} + U_j^{(t)})
                         U_i^{(t+1)} \leftarrow U_i^{(t)} + X_i^{(t+1)} - Y_i^{(t+1)}
            until \max(||X_i^{(t)} - Y_i^{(t)}||_2^2, \rho^2|||Y_i^{(t)} - Y_i^{(t-1)}|||_2^2) \le d\epsilon^2
            P = P \cup Y_i^{(t)}
end
return P
```

- ⊲ Compute covariance matrix
- ¬ Rank-d Projection Matrix
- ⊲ Initialization
- ¬ Rank-1 Fantope projection
- □ Dual update
- Add the first eigenvector
- ⊲ compute d-1 eigenvectors
- ⊲ Initialization
- ⊲ Deflated Fantope projection
- □ Dual update
- Add the jth eigenvector

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EXPERIMENTS

- Explain detection and interpretation process with a Synthetic dataset [BZS15]
 - 500 normal records and 15 anomalies
 - 3 types of anomalies
- Demonstrate performance on Real World benchmark dataset
 - Breast Cancer Dataset
 - 357 benign records (normal), 10 malignant records(abnormal)
 - KDD'99 Network Intrusion Dataset
 - 10% dataset
 - About 97242 normal records
 - 22 classes of attacks (abnormal)
 - Attacks can be classified into four main groups: DoS, Remote- to-local (R2L), User-to-root (U2R), and Probe



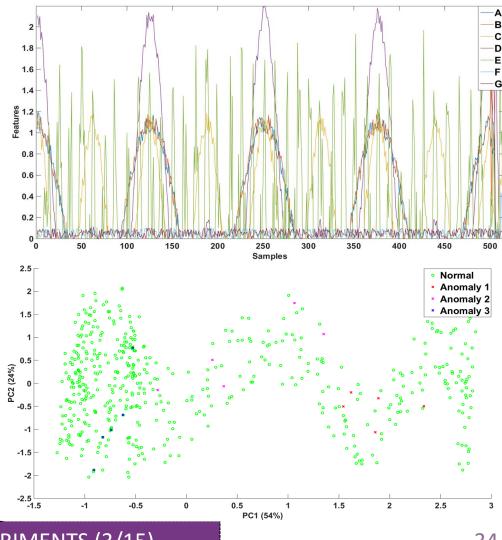
EVALUATION METIRCS

- Anomaly Detection
 - SPE
- Variance
 - Keep close to PCA
- Sparsity of loading vectors
 - Norm 1 (||V||_{1,1})
 - Card_{0.1}
 - Number of entries with absolute value higher than 0.1
 - Card_{0.01}
 - Number of entries with absolute values higher than 0.01
- Anomaly Interpretation
 - Heatmap projection on few Abnormal PCs
 - Need human effort
 - Only ASPCA-ADMMSEQ's performance is illustrated



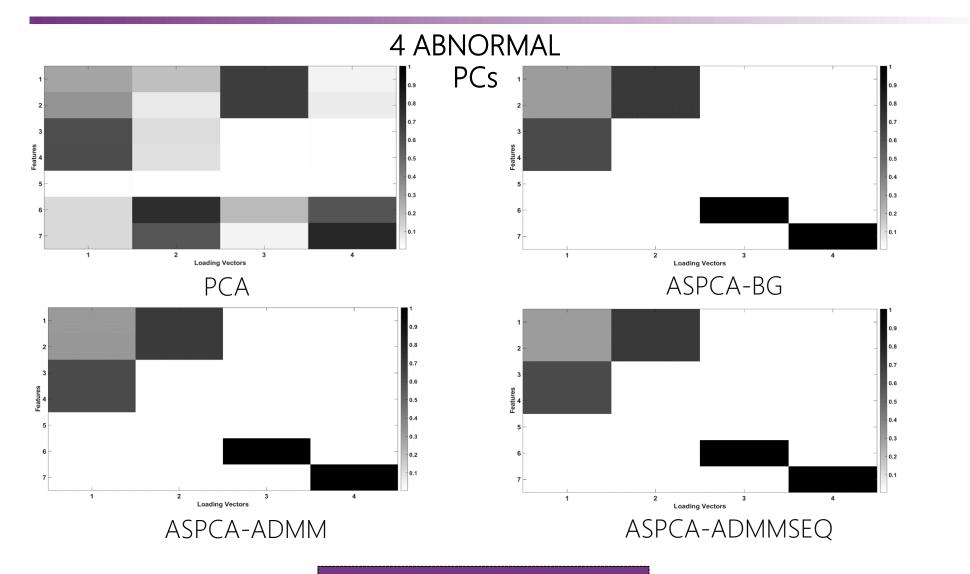
SYNTHETIC DATASET (1/7)

- Samples with Features
 500 normal records and 15 anomalies
 - 3 types of anomalies
- Feature Rules
 - D ≈ C + A
 - A ≈ B
 - F ≈ 0
 - G ≈ 0
- Anomalies break first three rules
- Projection on significant 2 PCs
- Variance captured ≈ 78%
 - PC1 (54%)
 - PC2 (24%)





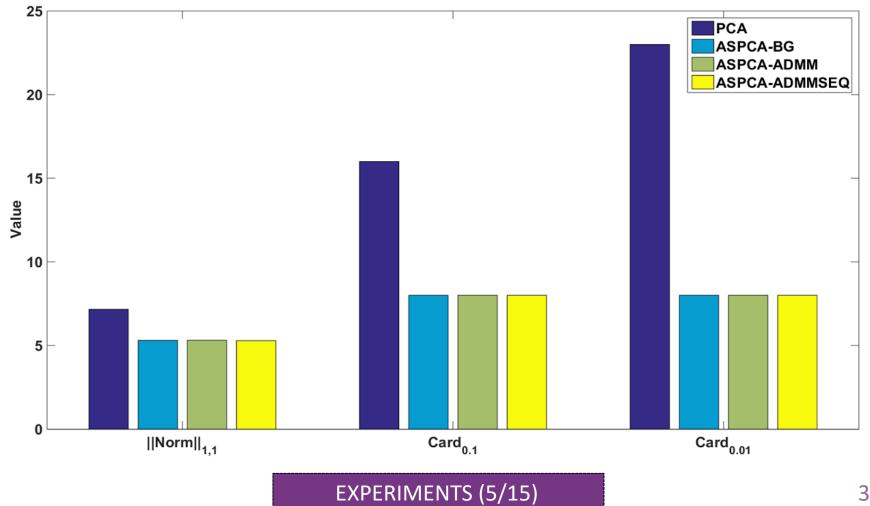
SYNTHETIC DATASET (2/7)





SYNTHETIC DATASET (3/7)

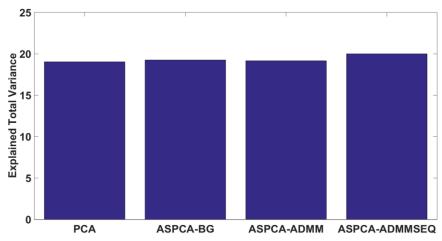
SPARSITY EVALUATION



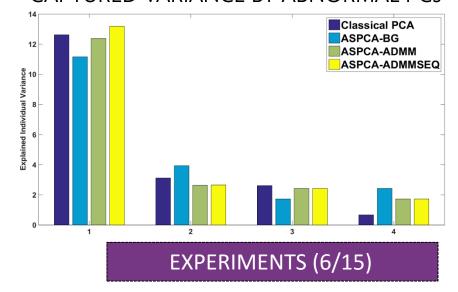


SYNTHETIC DATASET (4/7)

CAPTURED VARIANCE BY ABNORMAL SUBSPACE



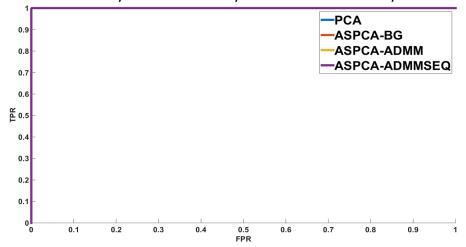
CAPTURED VARIANCE BY ABNORMAL PCs



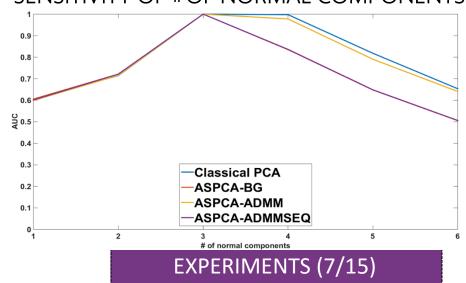


SYNTHETIC DATASET (5/7)

PERFECT AUC FOR PCA, ASPCA-BG, ASPCA-ADMM, ASPCA-ADMMSEQ



SENSITIVITY OF #OF NORMAL COMPONENTS



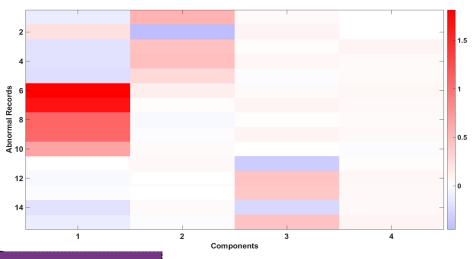


SYNTHETIC DATASET (6/7)

- Both ASPCA-ADMM & ASPCA-ADMMSEQ has same PCs
- Anomalies break rules
 - $D \approx C + A$
 - A ≈ B
 - F ≈ 0
- Heatmap projection
 - Anomalies
 - Abnormal components

ABNORMAL PCs

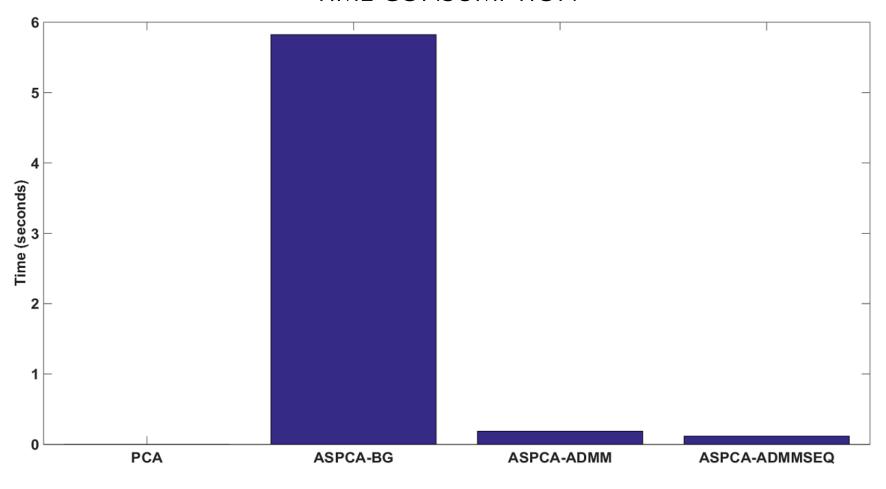
Index	Components	
1	-0.29148 A – 0.291663 B – 0.654865 C + 0.633345 D	
2	-0.70433 A + 0.709883B	
3	1 F	
4	1 G	





SYNTHETIC DATASET (7/7)

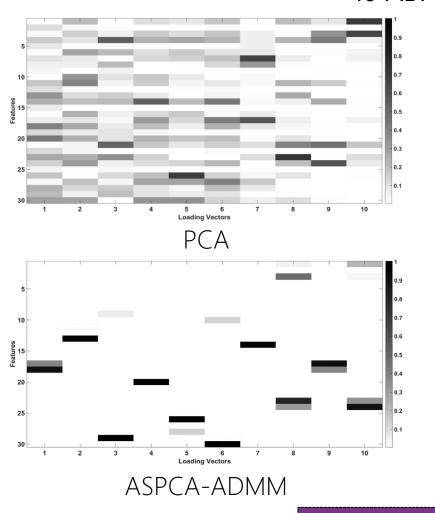
TIME CONSUMPTION

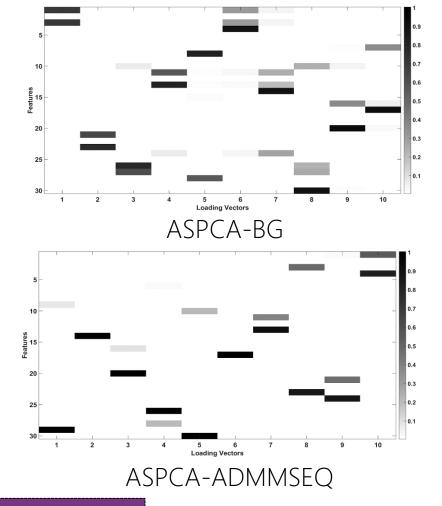




BREAST CANCER DATASET (1/4)

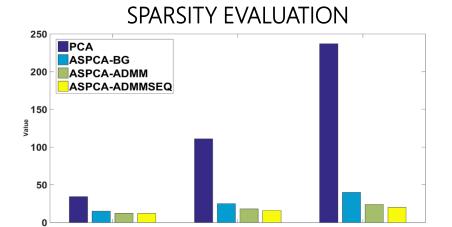
10 ABNORMAL PCs

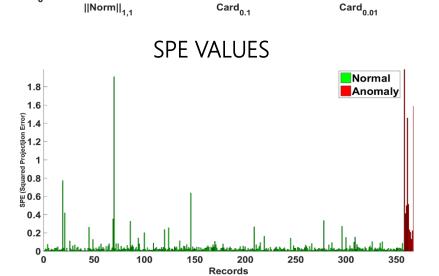




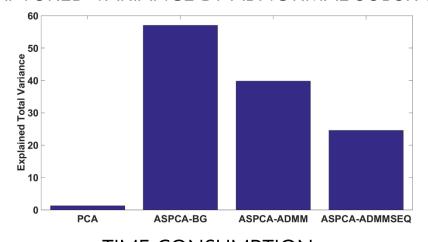


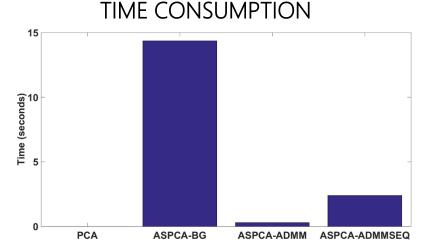
BREAST CANCER DATASET (2/4)





CAPTURED VARIANCE BY ABNORMAL SUBSPACE





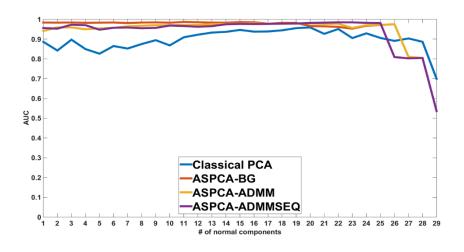


BREAST CANCER DATASET (3/4)

AUC COMPARISON

PCA —ASPCA-BG —ASPCA-ADMM —ASPCA-ADMMSEQ 0.6 0.7 0.8 0.9 1 FPR

SENSITIVITY OF #OF NORMAL COMPONENTS



AUC VALUES

Method	AUC
PCA	0.958
ASPCA-BG	0.965
ASPCA-ADMM	0.978
ASPCA-ADMMSEQ	0.981

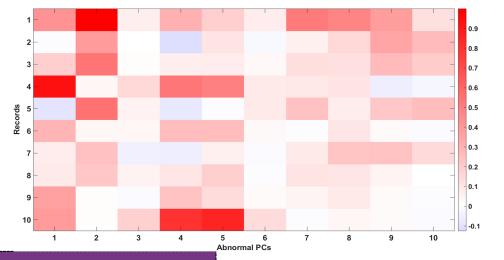


BREAST CANCER DATASET (4/4)

- 2 kinds of malignant records [BZS15] [WSH95]
 - area-se, area-worst, radius-worst
 - symmetry, fractal dimension, compactness
- Heatmap projection
 - Anomalies
 - Abnormal components

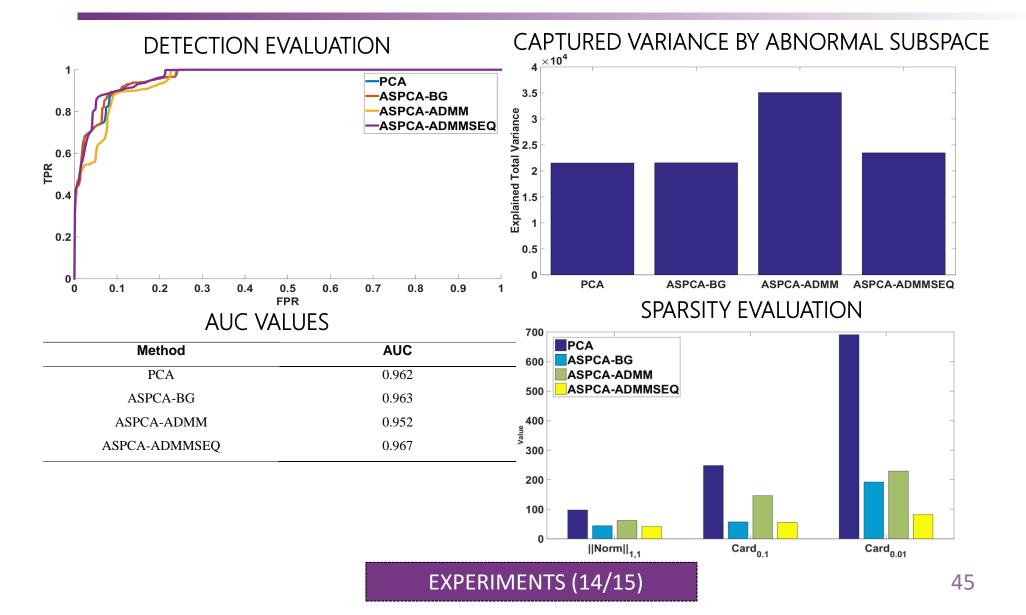
ABNORMAL PCs

Index	Components
1	- 0.08symmetry-mean + 0.996symmetry-worst
2	1area-se
4	$\hbox{-}\ 0.02\ compactness-mean} + 0.97\ compactness-worst \hbox{-}\ 0.20\ concave-points-worst}$
5	- 0.21 fractal dimension-mean + 0.97 fractal dimension-worst
7	- 0.39 radius-se + 0.91 perimeter-se
8	- 0.49 perimeter-mean + 0.86 perimeter-worst
9	- 0.02 radius-mean - 0.47 radius-worst + 0.87 area-worst



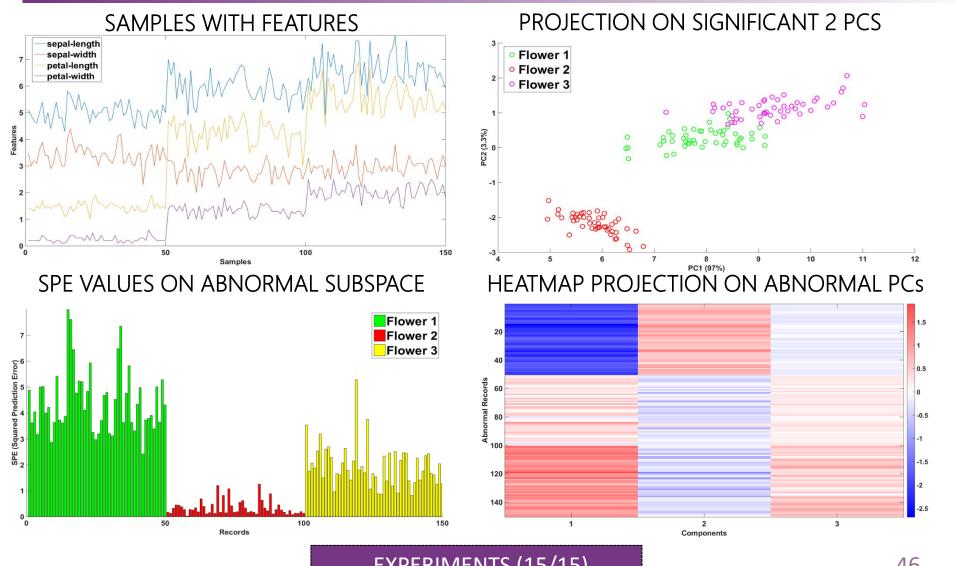


KDD'99 DATASET (1/1)





CLUSTERING PERFORMANCE?





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DISCUSSION (1/1)

- Tradeoff between sparsity, variance, AUC
- Sequential estimation of PCs
 - Has better interpretation performance
 - Keeps most of the correlations of variables
 - Captures variance like PCA
 - Formulate PCA result on certain circumstance
- Simultaneous estimation of PCs
 - Faster
 - Sparsity on subspace rather individual PCs
 - Adds additional variance to make sparse
 - Can not go back to PCA



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SUMMARY (1/1)

- Proposed two models
 - ASPCA-ADMM
 - Simultaneous computation of eigenvectors
 - ASPCA-ADMMSEQ
 - Sequential computation of eigenvectors
- Computation time reduced
- Better Detection performance
 - Individual anomalies
- Better Sparsity performance
 - Understandable Anomaly Interpretation
- ASPCA-ADMMSEQ throws promising competency



FUTURE WORKS (1/1)

- Make Abnormal Subspace size, **d** non-parametric
- Tune other parameters automatically
 - \bullet penalty parameter ρ and regularization parameter λ
- Improve interpretation
 - Make it sparser on high dimensional datasets
- Projection on other convex bodies
 - We only used Fantope
- Make the model more robust and scalable for different big data problems
- Proper understanding of the behavior of data
- Clustering performance on other datasets



OUTLINE

- Introduction
- Motivation
- Abnormal Subspace Estimation
- Experiments
- * Discussion
- Conclusion
- References



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Q&A Thank You ☺

