Anomaly Detection

Dimensionality reduction: PCA, robust PCA

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Outline

- eigenvalue and singular value decomposition
- Principal Component Analysis
- Robust PCA
- Matrix Factorization

The course references are Aggarwal 2017, Ch.3 with papers for Robust PCA by Candès et al. 2011 and Netrapalli et al. 2014.

For a thorough recap of eigen and singular values see Golub and Van Loan 2013.

Preliminaries

Eigenvalues and Eigenvalue Decomposition (EVD)

Given square matrix $A \in \mathbb{R}^{n \times n}$ then its eigenvalues λ and associated eigenvectors $\boldsymbol{v}$ follow:

$$\boldsymbol{A}\boldsymbol{v} = \lambda \boldsymbol{v} \tag{1}$$

which can be obtained through $(\boldsymbol{A} - \lambda \boldsymbol{I}_n)\boldsymbol{v} = 0$ or the factorization of the polynomial $\det(\boldsymbol{A} - \lambda \boldsymbol{I}_n) = 0$

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There are n eigenvalues and eigenvectors, thus we can write the eigenvalue decomposition (EVD):

$$\boldsymbol{A}\boldsymbol{V} = \boldsymbol{V}\Lambda \iff \Lambda = \boldsymbol{V}^{-1}\boldsymbol{A}\boldsymbol{V} \tag{2}$$

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Remark: For symmetric matrices $\boldsymbol{A}^\top = \boldsymbol{A}$ we have $V^{-1} = V^\top$ such that $\boldsymbol{A} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^\top$.

Singular Values and Singular Value Decomposition (SVD)

Given rectangular matrix $A \in \mathbb{R}^{n \times m}$ the singular values σ, the associated left-hand side singular vectors $\boldsymbol{u}$, and associated right-hand side singular vectors $\boldsymbol{v}$

$$\boldsymbol{A}\boldsymbol{v} = \sigma \boldsymbol{v} \boldsymbol{A}^\top \boldsymbol{u} = \sigma \boldsymbol{u} \tag{3}$$

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There are $\min(n, m)$ singular values, n left singular vectors, and m right singular vectors, thus we can write the singular value decomposition (SVD):

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Theorem: The optimal low-rank matrix $\boldsymbol{L} \in \mathbb{R}^{n\ timesm}$ with rank k that approximates $\boldsymbol{A}$ is $\sum_{i=1}^{k} \sigma_i \boldsymbol{u}_i \boldsymbol{v}_i^\top$

Least Squares (LS)

Given data $\boldsymbol{X} \in \mathbb{R}^{N \times d}$, where d is the data dimension and N the number of samples, the least-squares problem solves the following:

$$\min_{\beta} \|\mathbf{X}\beta - \mathbf{y}\|_F^2 \tag{5}$$

- when $N = d$ we have $\beta^\star = \mathbf{X}^{-1}\mathbf{y}$
- when $N > d$ we have $\beta^\star = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$
- when $N < d$ we have $\beta^\star = \mathbf{X}^T(\mathbf{X}\mathbf{X}^T)^{-1}\mathbf{y}$

See Lecture 2 for more details.

LS: line fit

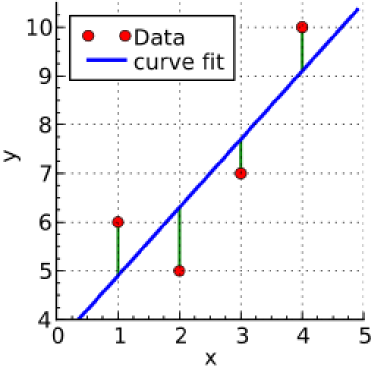

Figure: LS fits 2D points on a line

Source: https://en.wikipedia.org/wiki/Linear_least_squares

LS: projection

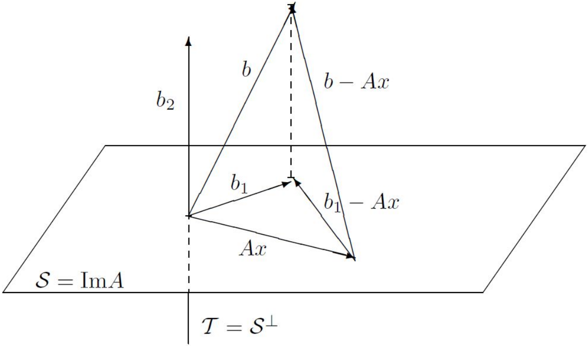

Figure: LS projects vectors on ImA

LS: remarks

Least-squares properties:

- finds $d - 1$ subspace or hyperplane
- the hyperplane is an optimum fit to data
- anomaly score: based on length on orthogonal direction

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Generalization:

- what is the $k < d$ subspace or hyperplane?
- what is the anomaly score then?
- what is an optimum fit on any k-dimensional subspace?

Nonlinear PCA

Principal Component Analysis (PCA)

PCA starts from the covariance matrix of the mean-centered data matrix $\boldsymbol{X} \in \mathbb{R}^{N \times d}$

$$\boldsymbol{\Sigma} = \frac{\boldsymbol{X}^T \boldsymbol{X}}{N} \tag{6}$$

such that $\boldsymbol{\Sigma} \in R^{d \times d}$ where element Σ_{ij} is the covariance between data dimension i and j.

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- the normal hyperplane to $\boldsymbol{p}_{min} \in \boldsymbol{P}$ is the LS-hyperplane of dimension $k = d - 1$

PCA as Generalized LS

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- the subspace will be generated by the largest k eigenvectors such that the residual is minimal
- anomalies are the data whose error is high in this new subspace
- anomalies have a large normal component

Example: Principal Eigenvectors

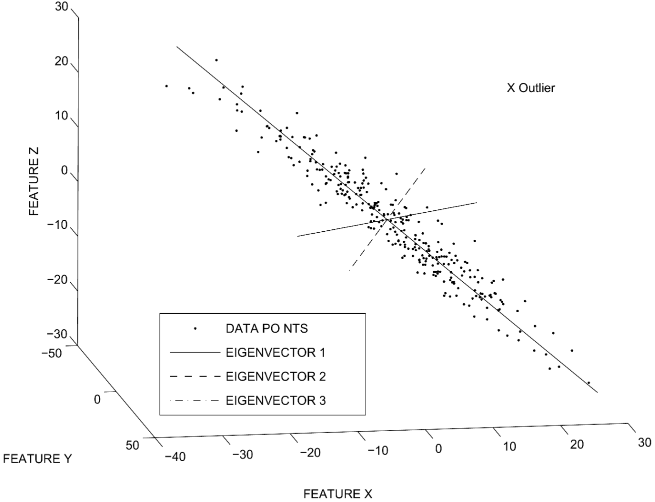

Figure: Distribution along first $k = 3$ eigenvectors (Aggarwal 2017)

PCA as Generalized LS

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- not if we expect anomalies to have higher variance among low variance axis

Example: Eigen Histogram

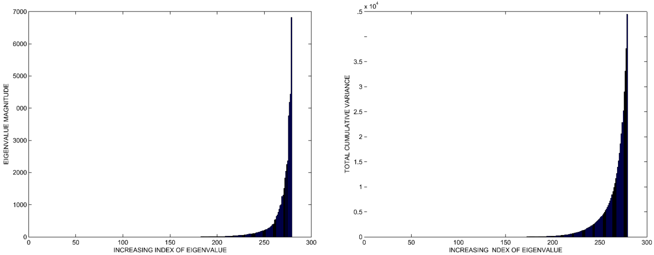
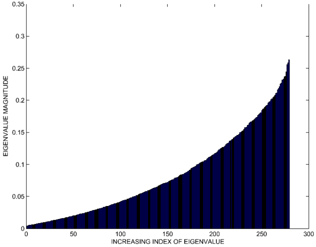


Figure: Eigenvalues magnitude and variance (Aggarwal 2017)

Example: Eigen Histogram Trimmed



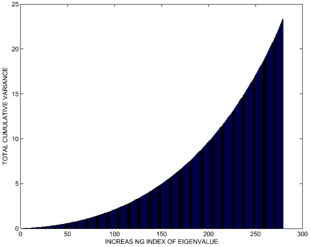


Figure: Eigenvalues magnitude and variance after trimming (Aggarwal 2017)

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- **outlier:** if x'_{ij} has a large deviation compared to other $x'_{\ell j}$ entries

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The approximation through trimming the smallest $d - k$ eigenvectors $\boldsymbol{X}' = \boldsymbol{X}\boldsymbol{P}_k \in \mathbb{R}^{N\times k}$

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will contain in each x'_{ij} with $j \in [k]$

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Hard outlier score: the residuals representing the distance to the rank-k hyperplane described by XP_k.

Soft outlier score: normalize the residuals according to their corresponding variance along the $d-k$ distances.

PCA: Soft Score

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Soft outlier score: normalize the residuals according to their corresponding variance along the $d-k$ distances.

Decompose the sum of squares of the $d-k$ distances and normalize by their corresponding eigenvalue:

$$\text{Score}(\boldsymbol{x}_\ell) = \sum_{j=k+1}^{d} \frac{\left\| x_{\ell j} - \boldsymbol{x}_\ell^\top \boldsymbol{p}_j \right\|^2}{\lambda_j} \tag{10}$$

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Remark: both scores focus on representing data in a low-dimensional space which induces parameter k: selecting the dimensionality

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Mahalanobis performs the normalization across all d directions

$$\text{Score}(\boldsymbol{x}_\ell) = \sum_{j=1}^{d} \frac{\left\| (\boldsymbol{x}_\ell - \boldsymbol{\mu})^\top \boldsymbol{p}_j \right\|^2}{\lambda_j} \tag{11}$$

where $\boldsymbol{\mu} \in \mathbb{R}^d$ is the data centroid (the mean vector along the data dimension).

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3. Normalize: $\boldsymbol{X}' = \boldsymbol{X}'\Delta^{-1}$

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1. EVD: $\boldsymbol{\Sigma} = \boldsymbol{P\Delta P}^\top$
2. Transform: $\boldsymbol{X}' = \boldsymbol{XP}$
3. Normalize: $\boldsymbol{X}' = \boldsymbol{X}'\Delta^{-1}$
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5. Goto step 1

Example: Outlier Perturbation

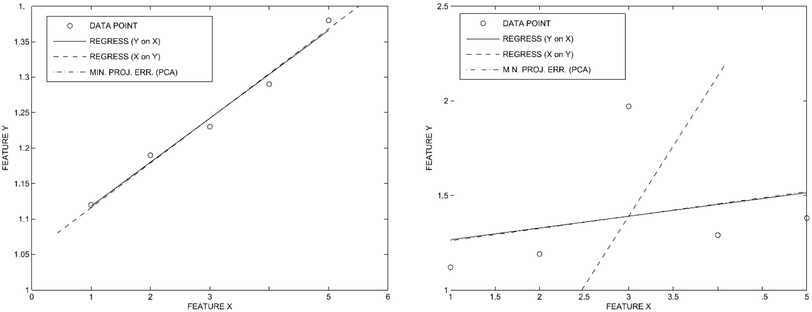

Figure: Sensitivity to outliers (Aggarwal 2017)

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Normalization: original dimensions scales can very widely – normalize to unit variance.

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- alternative: use sub-sampling

Robust PCA

Treat measurement matrix as the super-position of a low-rank matrix with a sparse noise matrix $X = L_0 + S_0$, then recovering L_0 and S_0 involves solving the following optimization problem

$$\arg\min_{L,S} \rho(L) + \lambda \|S\|_0 \quad \text{s.t.} \quad \|X - L - S\|_F^2 = 0 \tag{12}$$

where $\rho(L)$ is the rank function and $\|\cdot\|_0$ is the ℓ_0-norm counting the number of non-zeros.

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Candès et al. 2011 show that the convex relaxation of the above can recover L_0 and S_0 under mild assumpitons

$$\arg\min_{L,S} \|L\|_\star + \lambda \|S\|_1 \quad \text{s.t.} \quad \|X - L - S\|_F^2 = 0 \tag{13}$$

where $\|\cdot\|_\star$ is the nuclear norm summing the singular values.

Escalator Example: PCA versus Robust PCA

Figure: Background separation: truth, PCA and two RPCA implementations (Netrapalli et al. 2014)

Restaurant Example: PCA versus Robust PCA

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Nonlinear PCA

PCA: sample space versus feature space

What if we used $\boldsymbol{S} = \boldsymbol{X}\boldsymbol{X}^\top \in \mathbb{R}^{N \times N}$ instead of $\boldsymbol{\Sigma}$?

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$$\boldsymbol{S} = \boldsymbol{X}\boldsymbol{X}^\top = \boldsymbol{Q}\boldsymbol{\Lambda}^2\boldsymbol{Q}^\top \tag{14}$$

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The transform in the sample space is:

$$\boldsymbol{X}' = \boldsymbol{X}(\boldsymbol{Q}\Lambda)_d \tag{15}$$

where we can easily see that $[\boldsymbol{X}' \ \boldsymbol{O}] = \boldsymbol{X}\boldsymbol{Q}\Lambda = [\boldsymbol{X}(\boldsymbol{Q}\Lambda)_{\boldsymbol{d}} \ \boldsymbol{O}]$.

PCA: sample space uses a similarity matrix

Remark: $\boldsymbol{S} = \boldsymbol{X}\boldsymbol{X}^\top \in \mathbb{R}^{N \times N}$ has s_{ij} as the dot-product between $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ thus acting as a similarity matrix.

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Example: Kernel Space

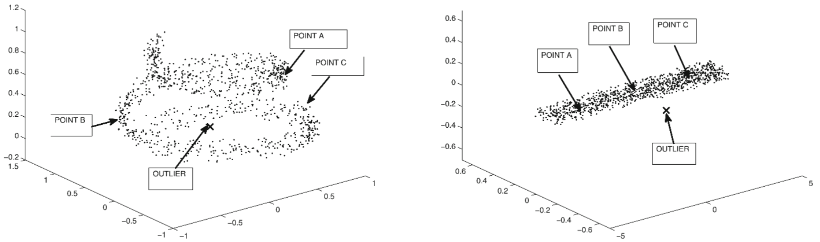

Figure: Sample space to kernel space (Aggarwal 2017)

Nonlinear PCA: Dealing with large sample spaces

Remark: Computing $\boldsymbol{S} = \boldsymbol{Q}\boldsymbol{\Lambda}^2\boldsymbol{Q}^\top \in \mathbb{R}^{N \times N}$ for large N can be prohibitive (e.g. $N = 100,000$).

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8. Complete transform: $[(\boldsymbol{Q}\boldsymbol{\Lambda})_k \ ; \ \boldsymbol{S}_0(\boldsymbol{Q}\boldsymbol{\Lambda}^{-1})_k]^\top$

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