Lecture 8

Scalable PCA/SVD

Dimensionality Reduction & Factor Analysis

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COM6012 Scalable Machine Learning

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Week 8 Contents

- **Unsupervised Learning**

- PCA - Dimensionality Reduction

- SVD – Factor Analysis

- Scalable PCA in Spark

Unsupervised Learning

Supervised methods

Unsupervised methods

$y = f(X)$

$f(X)$

predict
our data

as a function of
other data

find structure in the data on its own

Three Topics

- Principal component analysis (PCA) & SVD
  - Dimensionality reduction & factor analysis
- K-means
  - Clustering
- Matrix factorisation (with missing information)
  - Collaborative filtering →Recommender system

- **Scale these algorithms for big data**

Week 8 Contents

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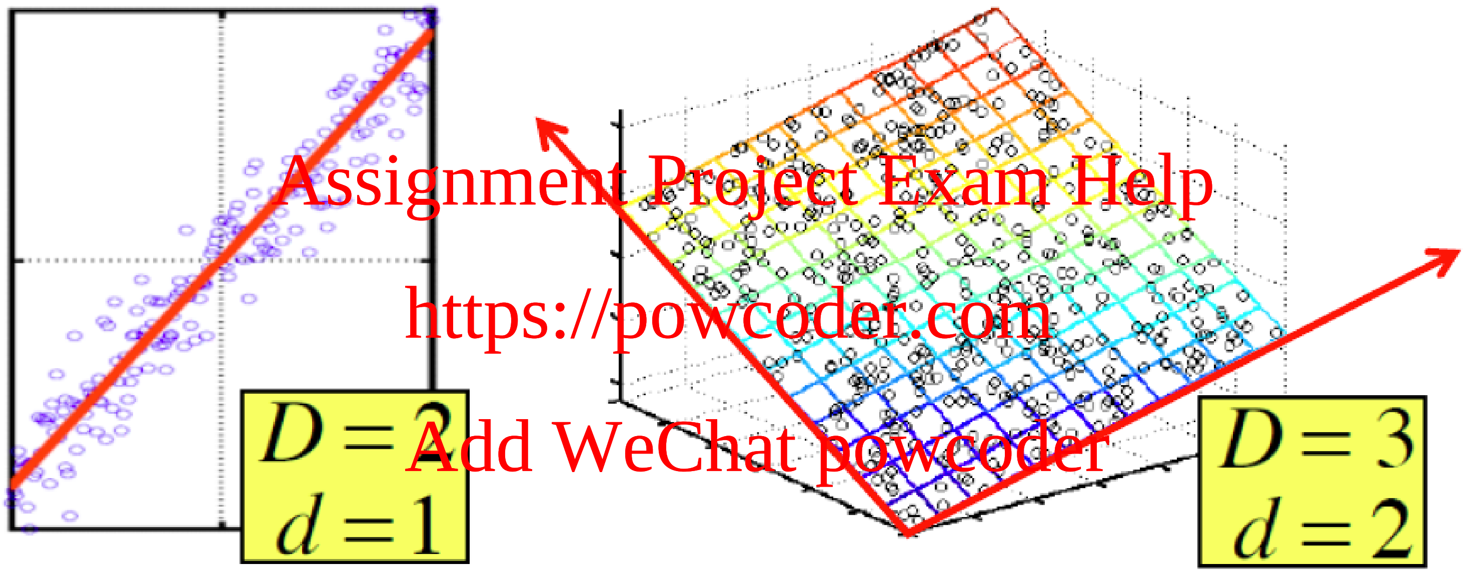
- SVD – Factor Analysis
- Scalable PCA in Spark

Dimensionality Reduction



- **Assumption:** Data lies on or near a low d-dimensional subspace
- Axes of this subspace are effective representation of the data

Why Reduce Dimensions?

Why reduce dimensions?

- Discover hidden correlations/topics
  - Words that occur commonly together
- Remove redundant and noisy features
  - Not all words are useful
- Interpretation and visualization
- Easier storage and processing of the data

Dimensionality Reduction

- Raw data is complex and high-dimensional

- Dimensionality reduction describes the data using a simpler, more compact representation

- This representation may make interesting patterns in the data clearer or easier to see

Dimensionality Reduction

- Goal: Find a 'better' representation for data

- How do we define 'better'?

- For example
  - Minimise reconstruction error
  - Maximise variance
  - **They give the same solution → PCA!**

PCA Algorithm

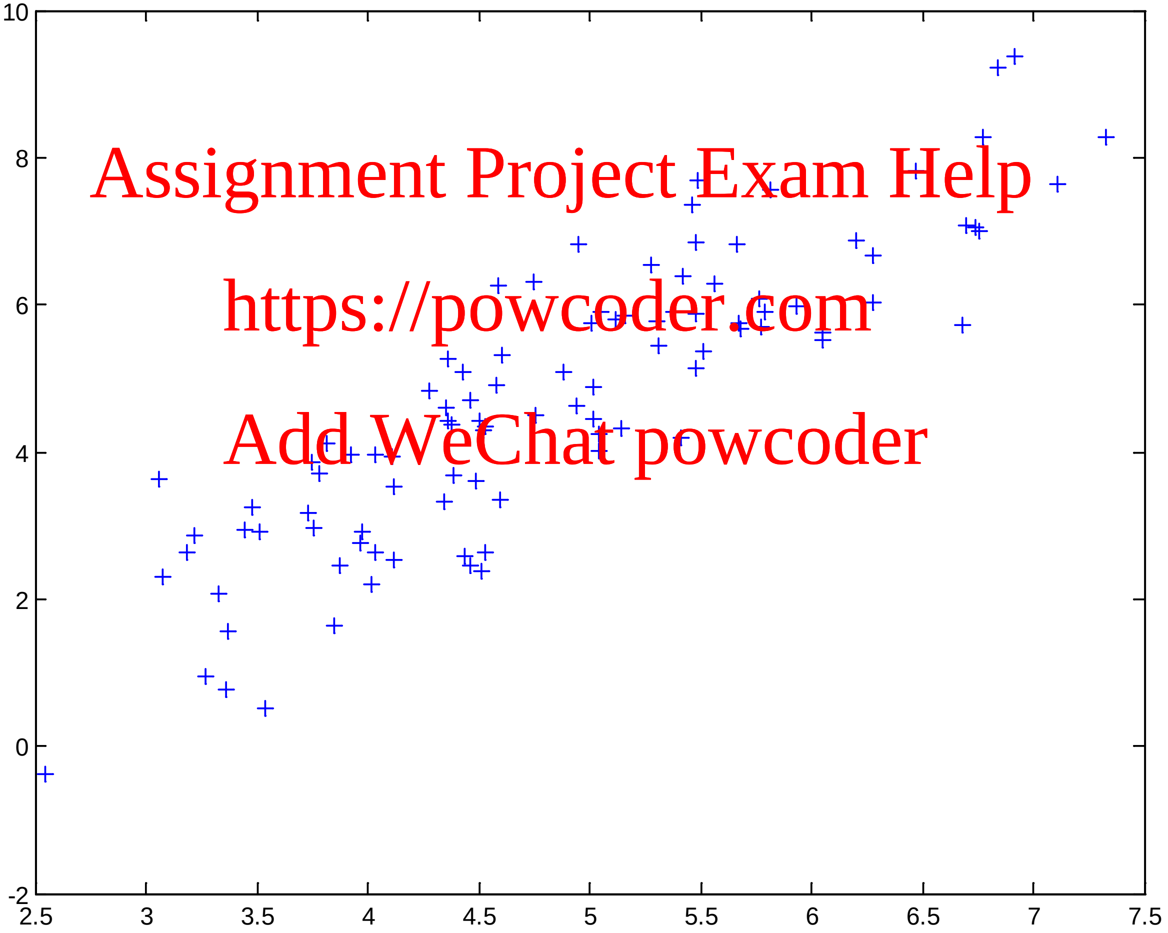
- Input: N data points, each → D-dimensional vector
- PCA algorithm

  - 1. $\mathbf{X_0}$ ← Form $N \times D$ data matrix, with one row vector $\mathbf{x}_n$ per data point

  - 2. $\mathbf{X}$: subtract mean $\mathbf{x}$ from each row vector $\mathbf{x}_n$ in $\mathbf{X_0}$

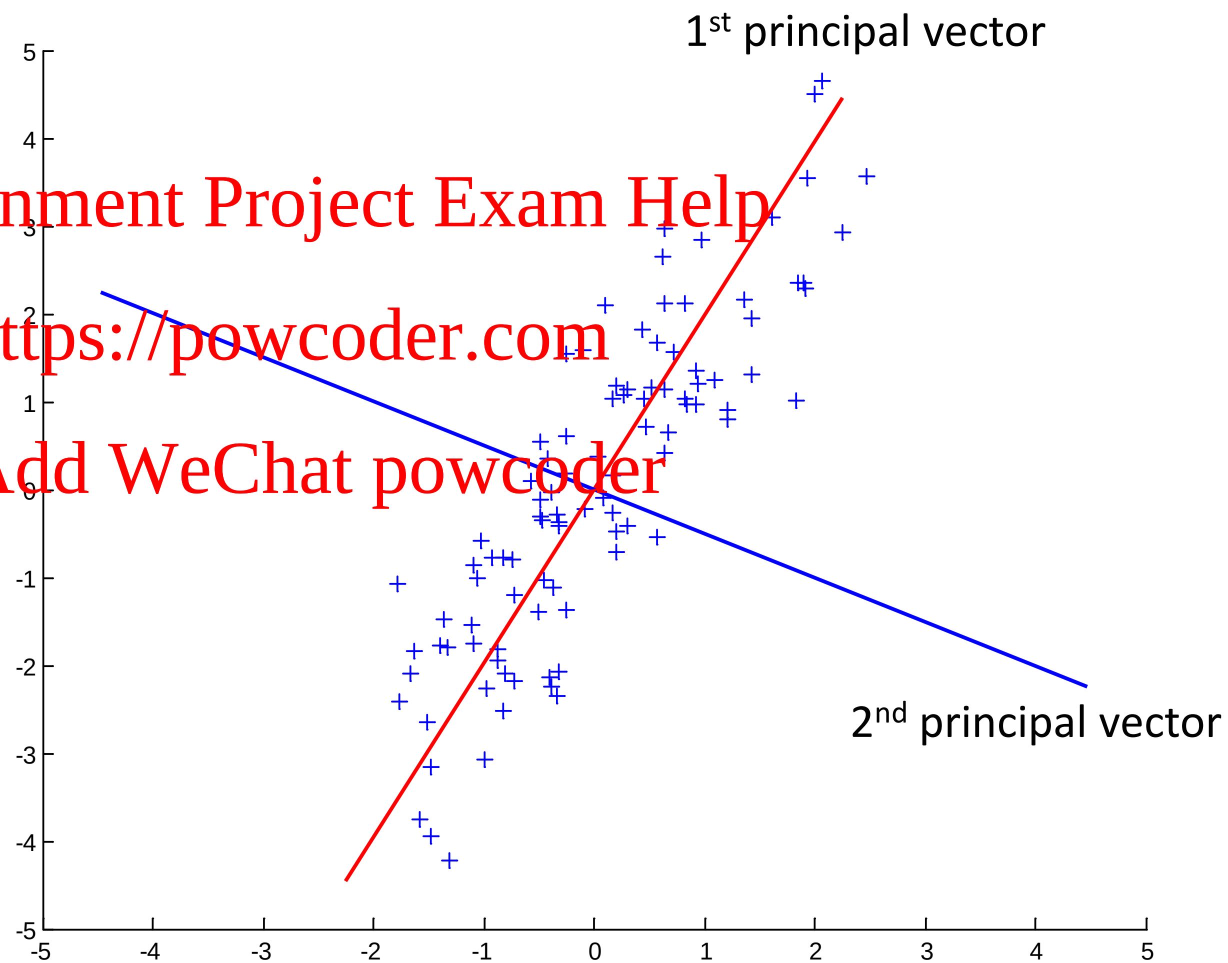
  - 3. $\mathbf{\Sigma}$ ← $\mathbf{X}^T\mathbf{X}$ Gramian (scatter) matrix for $\mathbf{X}$
  - Find eigenvectors and eigenvalues of $\mathbf{\Sigma}$
  - PCs $\mathbf{U}$ ($D \times d$) ← the d eigenvectors with largest eigenvalues
- PCA feature for $\mathbf{y}$ D-dim: $\mathbf{U}^T\mathbf{y}$ (d-dimensional)
  - Zero correlations, ordered by variance

2D Data



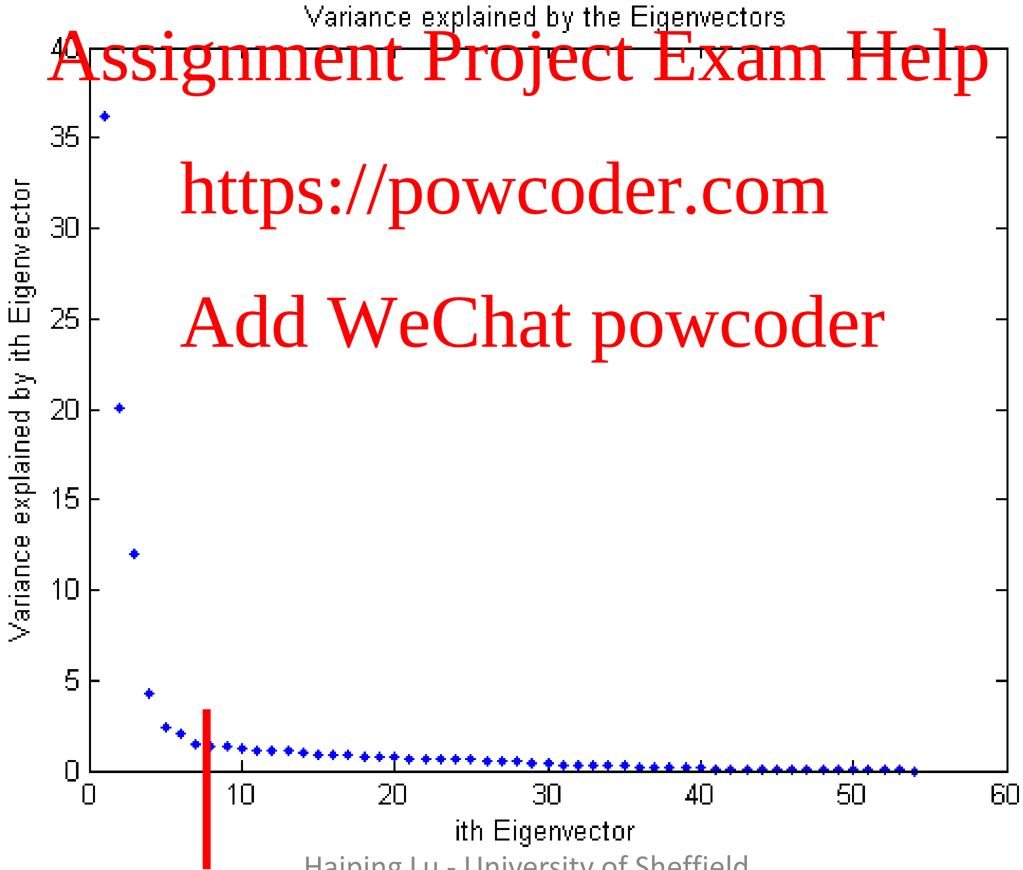
Principal Components

- The best axis to project
- Minimum RMS error
- Principal vectors are orthogonal



How Many Components?

- Check the distribution of eigen-values
- Take enough many eigen-vectors to cover 80-90% of the variance



Other Practical Tips

- PCA assumptions (linearity, orthogonality) not always appropriate
- Various extensions to PCA with different underlying assumptions, e.g., manifold learning, Kernel PCA, ICA

- Centring is crucial, i.e., we must preprocess data so that all features have zero mean before applying PCA
- PCA results dependent on scaling of data
- Data is sometimes rescaled in practice before applying PCA

Problems and Limitations

- What if very large dimensional data?
  - e.g., Images ($D \geq 10^4 = 100 \times 100$)
- Problem:
  - Gramian matrix Σ is size (D^2)
  - $D = 10^4 \rightarrow |\Sigma| = 10^8$
- Singular Value Decomposition (SVD)!
  - Efficient algorithms available
  - Some implementations find just top *d* eigenvectors

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- Unsupervised Learning

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- **SVD – Factor Analysis**
- Scalable PCA in Spark

Singular Value Decomposition

- Factorization (decomposition) problem
  - #1: Find concepts/topics/genres → Factor Analysis
  - #2: Reduce dimensionality

term / document	data	information	retrieval	brain	lung
CS-TR1	1	1	1	0	0
CS-TR2	2	2	2	0	0
CS-TR3	1	1	1	0	0
CS-TR4	5	5	5	0	0
MED-TR1	0	0	0	2	2
MED-TR2	0	0	0	3	3
MED-TR3	0	0	0	1	1

The above matrix is actually "2-dimensional." All rows can be reconstructed by scaling [1 1 1 0 0] or [0 0 0 1 1]: D=5→d=2

SVD - Definition

$$\mathbf{A}_{[\mathbf{n} \times \mathbf{m}]} = \mathbf{U}_{[\mathbf{n} \times \mathbf{r}]} \boldsymbol{\Lambda}_{[\mathbf{r} \times \mathbf{r}]} (\mathbf{V}_{[\mathbf{m} \times \mathbf{r}]})^T$$

- **A**: $n \times m$ matrix (e.g., n documents, m terms)
- **U**: $n \times r$ matrix (n documents, r concepts)

- **Λ**: $r \times r$ diagonal matrix (strength of each 'concept') (r: rank of the matrix)
- **V**: $m \times r$ matrix (m terms, r concepts)

SVD - Properties

Always possible to decompose matrix **A** into $\mathbf{A} = \mathbf{U}\,\mathbf{\Lambda}\,\mathbf{V}^T$, where

- **U, Λ, V**: unique (*)

- **U**, **V**: column orthonormal (i.e., columns are unit vectors, orthogonal to each other)

  - $\mathbf{U}^T\mathbf{U} = \mathbf{I}$; $\mathbf{V}^T\mathbf{V} = \mathbf{I}$ (**I:** identity matrix)
- **Λ:** singular value are positive, and sorted in decreasing order

SVD ←→ Eigen-decomposition

- SVD gives us:
  - $\mathbf{A} = \mathbf{U}\,\Lambda\,\mathbf{V}^T$
- Eigen-decomposition:
  - $\mathbf{B} = \mathbf{W}\,\Sigma\,\mathbf{W}^T$
    - $\mathbf{U}$, $\mathbf{V}$, $\mathbf{W}$ are orthonormal ($\mathbf{U}^T\mathbf{U}=\mathbf{I}$);
    - Λ, Σ are diagonal

- Relationship:
  - $\mathbf{AA}^T = \mathbf{U}\,\Lambda\,\mathbf{V}^T(\mathbf{U}\,\Lambda\,\mathbf{V}^T)^T = \mathbf{U}\,\Lambda\,\mathbf{V}^T(\mathbf{V}\,\Lambda^T\mathbf{U}^T) = \mathbf{U}\,\Lambda\,\Lambda^T\,\mathbf{U}^T$
  - $\mathbf{A}^T\mathbf{A} = \mathbf{V}\,\Lambda^T\,\mathbf{U}^T(\mathbf{U}\,\Lambda\,\mathbf{V}^T) = \mathbf{V}\,\Lambda\,\Lambda^T\,\mathbf{V}^T = \mathbf{V}\,\Lambda^2\,\mathbf{V}^T$
  - $\mathbf{B} = \mathbf{A}^T\mathbf{A} = \mathbf{W}\,\Sigma\,\mathbf{W}^T$

SVD for PCA

- PCA by SVD:
  - 1. $\mathbf{X}_0 \leftarrow$ Form $N \times d$ data matrix, with one row vector $\mathbf{x}_n$ per data point
  - 2. $\mathbf{X}$ subtract mean $\mathbf{x}$ from each row vector $\mathbf{x}_n$ in $\mathbf{X}_0$
  - 3. $\mathbf{U}\ \boldsymbol{\Lambda}\ \mathbf{V}^T \leftarrow$ SVD of $\mathbf{X}$
  - The right singular vectors $\mathbf{V}$ of $\mathbf{X}$ are equivalent to the eigenvectors of $\mathbf{X}^T\mathbf{X} \rightarrow$ the PCs
  - The singular values in $\boldsymbol{\Lambda}$ are equal to the square roots of the eigenvalues of $\mathbf{X}^T\mathbf{X}$

SVD - Properties

'spectral decomposition' of the matrix:

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 3 & 3 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix} = \begin{bmatrix} | & | \\ u_1 & u_2 \\ | & | \end{bmatrix} \text{ x } \begin{bmatrix} \lambda_1 & \varnothing \\ \varnothing & \lambda_2 \end{bmatrix} \text{ x } \begin{bmatrix} \text{---} & v_1 & \text{---} \\ \text{---} & v_2 & \text{---} \end{bmatrix}$$

SVD - Interpretation

'documents', 'terms' and 'concepts':

- **U**: document-to-concept similarity matrix
- **V**: term-to-concept similarity matrix
- **Λ**: its diagonal elements: 'strength' of each concept

Projection:

- Best axis to project on: ('best' = min sum of squares of projection errors)

SVD - Example

- $\mathbf{A} = \mathbf{U}\ \mathbf{\Lambda}\ \mathbf{V}^T$ - example:

term / document	data	information	retrieval	brain	lung
CS-TR1	1	1	1	0	0
CS-TR2	2	2	2	0	0
CS-TR3	1	1	1	0	0
CS-TR4	5	5	5	0	0
MED-TR1	0	0	0	2	2
MED-TR2	0	0	0	3	3
MED-TR3	0	0	0	1	1

$$
\begin{array}{c c}
 & \begin{array}{ccccc} \text{data} & \text{inf.} & \text{retrieval} & \text{brain} & \text{lung} \end{array} \\
\begin{array}{c} \text{CS} \\ \\ \\ \\ \text{MD} \\ \\ \\ \end{array} &
\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 3 & 3 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix}
\end{array}
=
\begin{bmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.27 \end{bmatrix}
\times
\begin{bmatrix} 9.64 & 0 \\ 0 & 5.29 \end{bmatrix}
\times
\begin{bmatrix} 0.58 & 0.58 & 0.58 & 0 & 0 \\ 0 & 0 & 0 & 0.71 & 0.71 \end{bmatrix}
$$

SVD - Example

- $\mathbf{A} = \mathbf{U}\, \boldsymbol{\Lambda}\, \mathbf{V}^T$ - example:

doc-to-concept similarity matrix

CS-concept

MD-concept

$$
\begin{array}{c}
\\ \text{CS} \\ \\ \\ \text{MD} \\ \\
\end{array}
\begin{array}{c}
\begin{array}{ccccc} \text{data} & \text{inf.} & \text{retrieval} & \text{brain} & \text{lung} \end{array} \\
\begin{bmatrix}
1 & 1 & 1 & 0 & 0 \\
2 & 2 & 2 & 0 & 0 \\
1 & 1 & 1 & 0 & 0 \\
5 & 5 & 5 & 0 & 0 \\
0 & 0 & 0 & 2 & 2 \\
0 & 0 & 0 & 3 & 3 \\
0 & 0 & 0 & 1 & 1
\end{bmatrix}
\end{array}
=
\begin{bmatrix}
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\end{bmatrix}
\times
\begin{bmatrix}
0.58 & 0.58 & 0.58 & 0 & 0 \\
0 & 0 & 0 & 0.71 & 0.71
\end{bmatrix}
$$

SVD - Example

- $\mathbf{A} = \mathbf{U}\,\mathbf{\Lambda}\,\mathbf{V}^T$ - example:

'strength' of CS-concept

$$
\begin{array}{c}
\\
\text{CS} \\
\\
\text{MD} \\
\\
\end{array}
\begin{array}{c}
\begin{array}{ccccc} \text{data} & \text{inf.} & \text{retrieval} & \text{brain} & \text{lung} \end{array} \\
\begin{bmatrix}
1 & 1 & 1 & 0 & 0 \\
2 & 2 & 2 & 0 & 0 \\
1 & 1 & 1 & 0 & 0 \\
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0.58 & 0.58 & 0.58 & 0 & 0 \\
0 & 0 & 0 & 0.71 & 0.71
\end{bmatrix}
$$

SVD - Example

- $\mathbf{A} = \mathbf{U}\,\mathbf{\Lambda}\,\mathbf{V}^T$ - example:

term-to-concept similarity matrix

CS-concept

$$
\begin{array}{c|c}
 & \begin{array}{ccccc} \text{data} & \text{inf.} & \text{retrieval} & \text{brain} & \text{lung} \end{array} \\
\begin{array}{c} \text{CS} \\ \\ \\ \\ \text{MD} \\ \\ \\ \end{array} &
\begin{bmatrix}
1 & 1 & 1 & 0 & 0 \\
2 & 2 & 2 & 0 & 0 \\
1 & 1 & 1 & 0 & 0 \\
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\end{bmatrix}
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0 & 5.29
\end{bmatrix}
\times
\begin{bmatrix}
0.58 & 0.58 & 0.58 & 0 & 0 \\
0 & 0 & 0 & 0.71 & 0.71
\end{bmatrix}
$$

SVD – Dimensionality Reduction

- Q: how exactly is (**further**) dim. reduction done?
- A: set the smallest singular values to zero:
- Note: **3 zero singular values** already removed

$$
\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 3 & 3 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix}
=
\begin{bmatrix} 0.18 & \cancel{0} \\ 0.36 & \cancel{0} \\ 0.18 & \cancel{0} \\ 0.90 & \cancel{0} \\ 0 & \cancel{0.53} \\ 0 & \cancel{0.80} \\ 0 & \cancel{0.27} \end{bmatrix}
\text{x}
\begin{bmatrix} 9.64 & 0 \\ 0 & \cancel{5.29} \end{bmatrix}
\text{x}
\begin{bmatrix} 0.58 & 0.58 & 0.58 & 0 & 0 \\ \cancel{0} & \cancel{0} & \cancel{0} & \cancel{0.71} & \cancel{0.71} \end{bmatrix}
$$

SVD - Dimensionality Reduction

$$
\begin{bmatrix}
1 & 1 & 1 & 0 & 0 \\
2 & 2 & 2 & 0 & 0 \\
1 & 1 & 1 & 0 & 0 \\
5 & 5 & 5 & 0 & 0 \\
0 & 0 & 0 & 2 & 2 \\
0 & 0 & 0 & 3 & 3 \\
0 & 0 & 0 & 1 & 1
\end{bmatrix}
\sim
\begin{bmatrix}
0.18 \\
0.36 \\
0.18 \\
0.90 \\
0 \\
0 \\
0
\end{bmatrix}
\text{x}
\begin{bmatrix}
9.64
\end{bmatrix}
\text{x}
\begin{bmatrix}
0.58 & 0.58 & 0.58 & 0 & 0
\end{bmatrix}
$$

SVD - Dimensionality Reduction

- Best rank-1 approximation

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 3 & 3 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

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- PCA - Dimensionality Reduction
- SVD – Factor Analysis
- **Scalable PCA in Spark**

PCA & SVD in Spark MLlib

- Not scalable: computePrincipalComponents( ) from RowMatrix
- **Scalable**: computeSVD( ) from RowMatrix
- Code: https://github.com/apache/spark/blob/v2.1.0/mllib/src/main/scala/org/apache/spark/mllib/linalg/distributed/RowMatrix.scala
- Documentation: https://spark.apache.org/docs/2.1.0/api/scala/index.html#org.apache.spark.mllib.linalg.distributed.RowMatrix

PCA in Spark MLlib (RDD)

- https://spark.apache.org/docs/2.1.0/mllib-dimensionality-reduction.html


```scala
val mat: RowMatrix = new RowMatrix(dataRDD)

// Compute the top 4 principal components.
// Principal components are stored in a local dense matrix.
val pc: Matrix = mat.computePrincipalComponents(4)
```


- Not scalable, local computation

```scala
val brzSvd.SVD(u: BDM[Double], s: BDV[Double], _) = brzSvd(Cov)
```

- Notebook 8

PCA in Spark ML (DF)

- Now in

  https://spark.apache.org/docs/2.1.0/ml-features.html#pca

- Under features

- Scalable? Not likely


```
val pca = new PCA()
  .setInputCol("features")
  .setOutputCol("pcaFeatures")
  .setK(3)
  .fit(df)
```

SVD in Spark MLlib (RDD)

- https://spark.apache.org/docs/2.1.0/mllib-dimensionality-reduction.html
- With distributed implementations


```
val mat: RowMatrix = new RowMatrix(dataRDD)

// Compute the top 5 singular values and corresponding singular vectors.
val svd: SingularValueDecomposition[RowMatrix, Matrix] = mat.computeSVD(5, computeU = true)
val U: RowMatrix = svd.U  // The U factor is a RowMatrix.
val s: Vector = svd.s  // The singular values are stored in a local dense vector.
val V: Matrix = svd.V  // The V factor is a local dense matrix.
```

SVD in Spark MLlib (RDD)

- An $m \times n$ data matrix **A** with $m > n$ (note different notations)

- For large matrices, usually we don't need the complete factorization but only the top k singular values and its associated singular vectors.

- Save storage, de-noise and recover the low-rank structure of the matrix (dimensionality reduction)

SVD in Spark MLlib (RDD)

- An $m \times n$ data matrix $\mathbf{A}$
- Assume m>n, SVD $\mathbf{A} = \mathbf{U}\,\mathbf{\Lambda}\,\mathbf{V}^{\mathrm{T}}$
- The singular values and the right singular vectors are derived from the eigenvalues and the eigenvectors of $\mathbf{A}^{\mathrm{T}}\mathbf{A}$ (which is smaller than **A)**
- The left singular vectors are computed via matrix multiplication as $\mathbf{U}=\mathbf{AV}\,\mathbf{\Lambda}^{-1}$, if requested by the user via the computeU parameter

Selection of SVD Computation

- Auto
- If n is small (n<100) or k is large compared with n (k>$n/2$), compute $\mathbf{A}^T\mathbf{A}$ first and then compute its top eigenvalues and eigenvectors **locally** on the driver
- Otherwise, compute $\mathbf{A}^T\mathbf{A}\ \mathbf{v}$ in a distributive way and send it to ARPACK to compute the top eigenvalues and eigenvectors on the driver node

Selection of SVD Computation

- Auto (default)

```
if (n < 100 || (k > n / 2 && n <= 15000)) {
  // If n is small or k is large compared with n, we better compute the Gramian matrix first
  // and then compute its eigenvalues locally, instead of making multiple passes.
  if (k < n / 3) {
    SVDMode.LocalARPACK
  } else {
    SVDMode.LocalLAPACK
  }
} else {
  // If k is small compared with n, we use ARPACK with distributed multiplication.
  SVDMode.DistARPACK
}
```

Selection of SVD Computation

- Specify computeMode (private)


```
case "local-svd" => SVDMode.LocalLAPACK
case "local-eigs" => SVDMode.LocalARPACK
case "dist-eigs" => SVDMode.DistARPACK
```

Selection of SVD Computation

- computeMode (note brzSvd.SVD is local)


```
// Compute the eigen-decomposition of A' * A.
val (sigmaSquares: BDV[Double], u: BDM[Double]) = computeMode match {
  case SVDMode.LocalARPACK =>
    require(k < n, s"k must be smaller than n in local-eigs mode but got k=$k and n=$n.")
    val G = computeGramianMatrix().asBreeze.asInstanceOf[BDM[Double]]
    EigenValueDecomposition.symmetricEigs(v => G * v, n, k, tol, maxIter)
  case SVDMode.LocalLAPACK =>
    // breeze (v0.10) svd latent constraint, 7 * n * n + 4 * n < Int.MaxValue
    require(n < 17515, s"$n exceeds the breeze svd capability")
    val G = computeGramianMatrix().asBreeze.asInstanceOf[BDM[Double]]
    val brzSvd.SVD(uFull: BDM[Double], sigmaSquaresFull: BDV[Double], _) = brzSvd(G)
    (sigmaSquaresFull, uFull)
  case SVDMode.DistARPACK =>
    if (rows.getStorageLevel == StorageLevel.NONE) {
      logWarning("The input data is not directly cached, which may hurt performance if its"
        + " parent RDDs are also uncached.")
    }
    require(k < n, s"k must be smaller than n in dist-eigs mode but got k=$k and n=$n.")
    EigenValueDecomposition.symmetricEigs(multiplyGramianMatrixBy, n, k, tol, maxIter)
}
```

Remark

- Acknowledgement
  - Some slides are adapted from slides by Jure Leskovec et al. http://www.mmds.org

- References

  - http://infolab.stanford.edu/~ullman/mmds/ch11.pdf
  - http://www.mmds.org
  - https://en.wikipedia.org/wiki/Principal_component_analysis
  - https://spark.apache.org/docs/2.1.0/mllib-dimensionality-reduction.html