Lecture 5

Scalable PCA Dimensionality Reduction & Factor Analysis

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https://github.com/haipinglu/ScalableML

COM6012 Scalable Machine Learning Spring 2019

Week 5 Contents / Objectives

• PCA - Dimensionality Reduction

• SVD – Factor Analysis

Scalable PCA in Spark

More on Scala

Week 5 Contents / Objectives

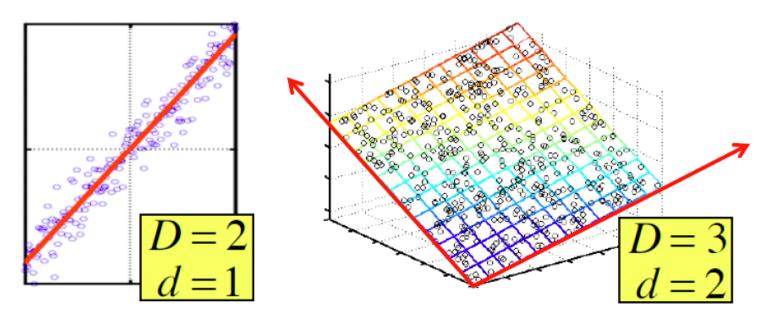
• PCA - Dimensionality Reduction

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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

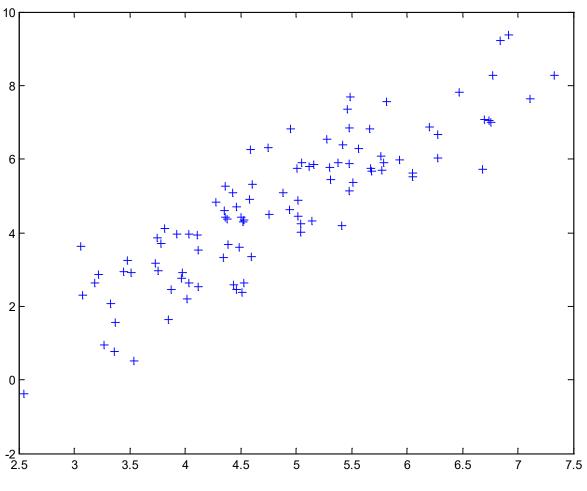
• Goal: Find a 'better' representation for data

- How do we define 'better'?
- For example
 - Minimise reconstruction error
 - Maximise variance
 - They give the same solution \rightarrow PCA!

PCA Algorithm

- Input: N data points, each \rightarrow D-dimensional vector
- PCA algorithm
 - 1. $X_0 \leftarrow$ Form $N \times D$ data matrix, with one row vector \mathbf{x}_n per data point
 - 2. **X**: subtract mean **x** from each row vector \mathbf{x}_n in \mathbf{X}_0
 - 3. $\Sigma \leftarrow X^TX$ Gramian (scatter) matrix for X
 - Find eigenvectors and eigenvalues of Σ
 - PCs U $(D \times d)$ \leftarrow the d eigenvectors with largest eigenvalues
- PCA feature for y D-dim: U^Ty (d-dimensional)
 - Zero correlations, ordered by variance

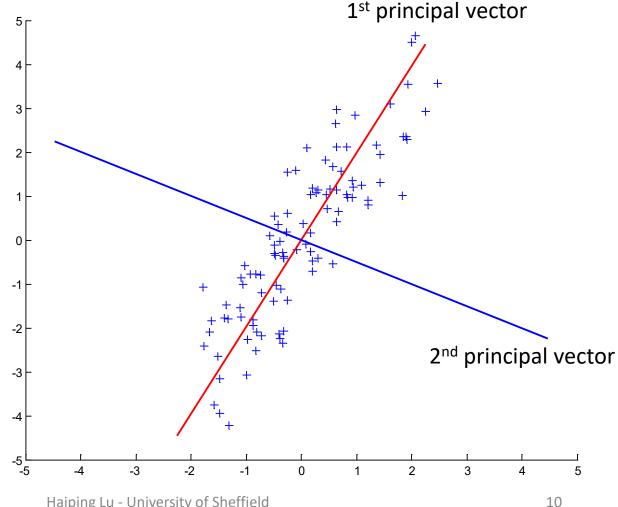
2D Data



17/02/2019

Principal Components

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

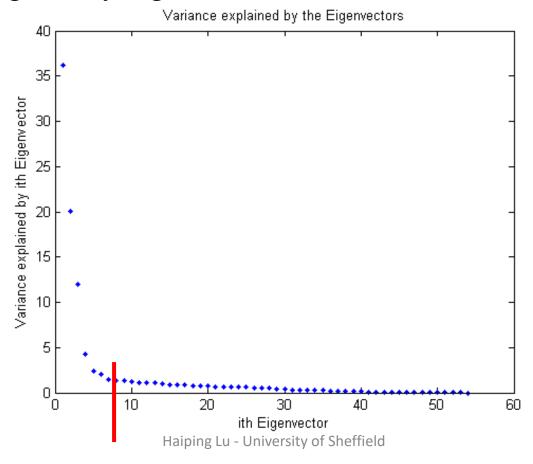


How Many Components?

• Check the distribution of eigen-values

• Take enough many eigen-vectors to cover 80-90% of the





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 10⁴= 100 x 100)
- Problem:
 - Gramian matrix Σ is size (D²)
 - D=10⁴ \rightarrow | Σ | = 10⁸
- Singular Value Decomposition (SVD)!
 - Efficient algorithms available
 - Some implementations find just top d eigenvectors

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Scalable PCA in Spark

More on Scala

Singular Value Decomposition

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

| \mathbf{term} | data | information | retrieval | brain | lung |
|-----------------|------|-------------|-----------|-------|------|
| document | | | | | |
| 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 |
| ${f MED-TR2}$ | 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

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

- 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 \mathbf{A} into $\mathbf{A} = \mathbf{U} \mathbf{\Lambda} \mathbf{V}^{\mathrm{T}}$, where

- **U**, **Λ**, **V**: unique (*)
- U, V: column orthonormal (i.e., columns are unit vectors, orthogonal to each other)
 - $U^TU = I$; $V^TV = I$ (I: identity matrix)
- Λ : singular value are positive, and sorted in decreasing order

SVD ←→Eigen-decomposition

- SVD gives us:
 - $\mathbf{A} = \mathbf{U} \mathbf{\Lambda} \mathbf{V}^{\mathrm{T}}$
- Eigen-decomposition:
 - $\mathbf{B} = \mathbf{W} \mathbf{\Sigma} \mathbf{W}^{\mathrm{T}}$
 - $\mathbf{U}, \mathbf{V}, \mathbf{W}$ are orthonormal ($\mathbf{U}^{\mathrm{T}}\mathbf{U}=\mathbf{I}$),
 - Λ , Σ are diagonal
- Relationship:
 - $AA^T = U \Lambda V^T (U \Lambda V^T)^T = U \Lambda V^T (V \Lambda^T U^T) = U \Lambda \Lambda^T U^T$
 - $A^TA = V \Lambda^T U^T (U \Lambda V^T) = V \Lambda \Lambda^T V^T = V \Lambda^2 V^T$
 - B= $A^TA=W \Sigma W^T$

SVD for PCA

- PCA by SVD:
 - 1. $X_0 \leftarrow$ Form $N \times d$ data matrix, with one row vector \mathbf{x}_n per data point
 - 2. X subtract mean x from each row vector \mathbf{x}_n in \mathbf{X}_0
 - 3. U Λ V^T \leftarrow SVD of X
 - The right singular vectors V of X are equivalent to the eigenvectors of $X^TX \rightarrow$ the PCs
 - The singular values in Λ are equal to the square roots of the eigenvalues of $\mathbf{X}^T\mathbf{X}$

SVD - Properties

'spectral decomposition' of the matrix:

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 3 & 3 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix} = \begin{bmatrix} \begin{vmatrix} 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix} \times \begin{bmatrix} \lambda_1 & \emptyset \\ \lambda_2 & \lambda_2 \end{bmatrix} \times \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & \lambda_2 \end{bmatrix}$$

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:

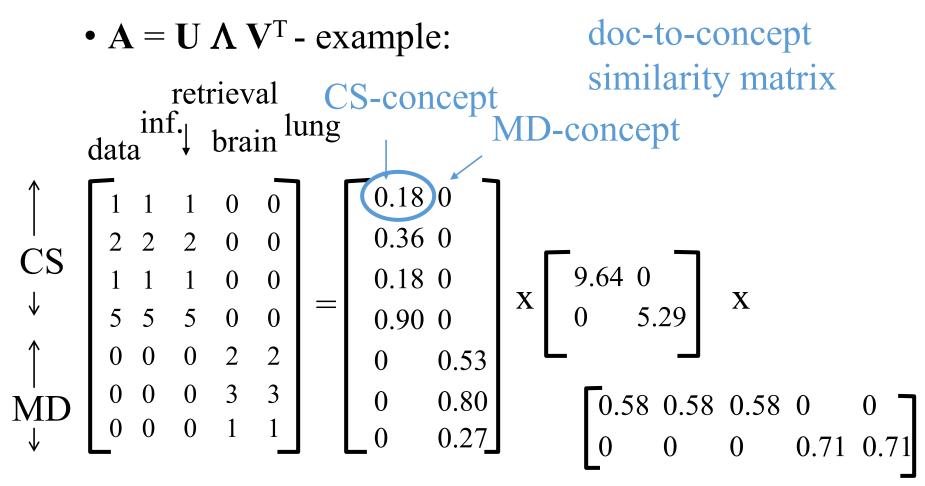
• Best axis to project on: ('best' = min sum of squares of projection errors)

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

retrieval inf.↓ brain ^{lung}

| $_{ m term}$ | data | information | retrieval | brain | lung |
|------------------------------------|------|-------------|-----------|-------|------|
| $\operatorname{document}$ | | | | | |
| 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 |
| $\mathbf{MED}\text{-}\mathbf{TR2}$ | 0 | 0 | 0 | 3 | 3 |
| MED-TR3 | 0 | 0 | 0 | 1 | 1 |

| | 1 | 1 | 1 | 0 | 0 |
|---------------------------------------|---|---|---|---|----|
| | 2 | 2 | 2 | 0 | 0 |
| CS | 1 | 1 | 1 | 0 | 0 |
| \downarrow | 5 | 5 | 5 | 0 | 0 |
| \uparrow | 0 | 0 | 0 | 2 | 2 |
| $\stackrel{\perp}{ m MD}$ | 0 | 0 | 0 | 3 | 3 |
| ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ | 0 | 0 | 0 | 1 | 1_ |



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

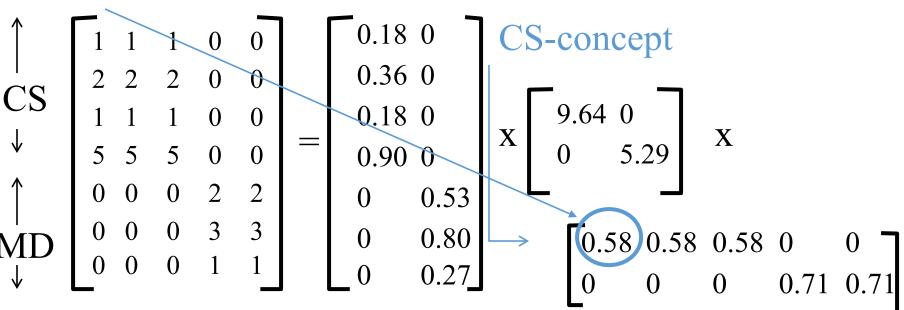
retrieval
$$\inf$$
 brain lung 'strength' of CS-concept

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

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

retrieval inf. the brain lung

term-to-concept similarity matrix

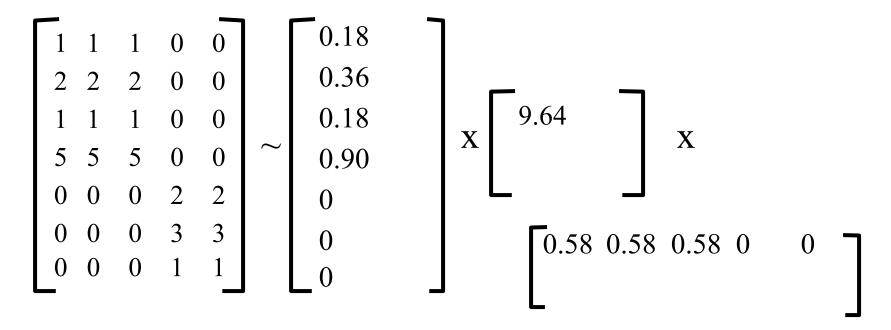


SVD – Dimensionality Reduction

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

| $\begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 2 & 2 & 2 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 5 & 5 & 5 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 3 & 3 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 0.18 & 0 \\ 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \\ 0 & 0.27 \end{bmatrix} \times \begin{bmatrix} 9.64 & 0 \\ 0 & 5.29 \end{bmatrix} \times \begin{bmatrix} 9.64 & 0 \\ 0 & 5.29 \end{bmatrix} \times \begin{bmatrix} 0.58 & 0.58 & 0.58 & 0 \\ 0 & 0 & 6 & 9.71 & 0. \end{bmatrix}$ | $\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 \end{bmatrix} = \begin{bmatrix} 0.36 & 0 \\ 0.18 & 0 \\ 0.90 & 0 \\ 0 & 0.53 \\ 0 & 0.80 \end{bmatrix} \times \begin{bmatrix} 9.64 & 0 \\ 0 & 5.29 \end{bmatrix} \times \begin{bmatrix} 9.64 & 0 \\ 0 $ | 0 0.71 |
|---|---|-----------|
|---|---|-----------|

SVD - Dimensionality Reduction



SVD - Dimensionality Reduction

• Best rank-1 approximation

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• Scalable PCA in Spark

More on Scala

PCA & SVD in Spark MLlib

- Not scalable: computePrincipalComponents() from RowMatrix
- Scalable: computeSVD() from RowMatrix
- Code:

https://github.com/apache/spark/blob/v2.3.2/mllib/src/main/scala/org/apache/spark/mllib/linalg/distributed/RowMatrix.scala

• Documentation:

https://spark.apache.org/docs/2.3.2/api/scala/index.html#org.apache.spark.mllib.linalg.distributed.RowMatrix

PCA in Spark MLlib (RDD)

• https://spark.apache.org/docs/2.3.2/mllib-dimensionality-reduction.html

```
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

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

PCA in Spark ML (DF)

Now in

https://spark.apache.org/docs/2.3.2/ml-features.html#pca

- Under features
- Not scalable

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

SVD in Spark MLlib (RDD)

- https://spark.apache.org/docs/2.3.2/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 A
- Assume m > n, SVD $\mathbf{A} = \mathbf{U} \Lambda \mathbf{V}^{\mathrm{T}}$
- The singular values and the right singular vectors are derived from the eigenvalues and the eigenvectors of $\mathbf{A}^{T}\mathbf{A}$ (which is smaller than \mathbf{A})
- The left singular vectors are computed via matrix multiplication as $\mathbf{U}=\mathbf{A}\mathbf{V}\ \mathbf{\Lambda}^{-1}$, 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 A^TA first and then compute its top eigenvalues and eigenvectors **locally** on the driver
- Otherwise
 - Compute A^TA 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
}</pre>
```

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")</pre>
   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 = n.")
    EigenValueDecomposition.symmetricEigs(multiplyGramianMatrixBy, n, k, tol, maxIter)
```

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More on Scala

Scala (Scalable language)

- A pure object-oriented language. Conceptually, every value is an object and every operation is a method-call.
- A functional language. Supports functions, immutable data structures and preference for immutability over mutation
- Seamlessly integrated with Java
 - Mixed Scala/Java projects
 - Use existing Java libraries
 - Use existing Java tools

Scala Basic Syntax

- When considering a Scala program, it can be defined as a collection of objects that communicate via invoking each other's methods.
- **Object** same as in Java
- Class same as in Java
- **Methods** same as in Java
- **Fields** Each object has its unique set of instant variables, which are called fields. An object's state is created by the values assigned to these fields.
- **Traits** Like Java Interface. A trait encapsulates method and field definitions, which can then be reused by mixing them into classes.
- **Closure** A **closure** is a function, whose return value depends on the value of one or more variables declared outside this function.
 - closure = function + environment

Scala is Statically Typed

- You don't have to specify a type in most cases
- Type Inference

```
val sum = 1 + 2 + 3
val nums = List(1, 2, 3)
val map = Map("abc" -> List(1,2,3))
```

Explicit Types

```
val sum: Int = 1 + 2 + 3
val nums: List[Int] = List(1, 2, 3)
val map: Map[String, List[Int]] = ...
```

Scala is High level

```
// Java - Check if string has uppercase character
boolean hasUpperCase = false;
for(int i = 0; i < name.length(); i++) {</pre>
    if(Character.isUpperCase(name.charAt(i))) {
        hasUpperCase = true;
        break;
// Scala
val hasUpperCase = name.exists(_.isUpperCase)
```

Scala is Concise // Java

```
public class Person {
 private String name;
 private int age;
 public Person(String name, Int age) {
   this.name = name;
  this.age = age;
 }
 public String getName() {
                                 // name getter
   return name;
 public int getAge() {
                                 // age getter
   return age;
 this.name = name;
 }
 public void setAge(int age) {
                           // age setter
   this.age = age;
```

```
// Scala
class Person(var name: String, private var _age: Int) {
 def age = age
                          // Getter for age
 def age_=(newAge:Int) { // Setter for age
   println("Changing age to: "+newAge)
   _age = newAge
```

Variables and Values

Variables: values stored can be changed

```
var foo = "foo"
foo = "bar" // okay
```

Values: immutable variable

```
val foo = "foo"
foo = "bar" // nope
```

Scala is Functional

- First Class Functions. Functions are treated like objects:
 - passing functions as arguments to other functions
 - returning functions as the values from other functions
 - assigning functions to variables or storing them in data structures

```
// Lightweight anonymous functions
(x:Int) => x + 1

// Calling the anonymous function
val plusOne = (x:Int) => x + 1
plusOne(5) → 6
```

Scala is Functional

• Closures: a function whose return value depends on the value of one or more variables declared outside this function.

// plusFoo can reference any values/variables in scope var foo = 1

val plusFoo =
$$(x:Int) \Rightarrow x + foo$$

plusFoo(5)
$$\rightarrow$$
 6

// Changing foo changes the return value of plusFoo

$$f00 = 5$$

plusFoo(5)
$$\rightarrow$$
 10

Scala is Functional

- Higher Order Functions
 - A function that does at least one of the following:
 - takes one or more functions as arguments
 - returns a function as its result

```
val plusOne = (x:Int) \Rightarrow x + 1
val nums = List(1,2,3)
// map takes a function: Int => T
nums.map(plus0ne) \rightarrow List(2,3,4)
// Inline Anonymous
nums.map(x \Rightarrow x + 1) \rightarrow List(2,3,4)
// Short form
nums.map(_ + 1)
                           \rightarrow List(2,3,4)
```

More Examples on Higher Order Functions

```
val nums = List(1,2,3,4)
// A few more examples for List class
nums.exists(_ == 2)
                                  → true
nums.find(\underline{\phantom{a}} == 2)
                                 \rightarrow Some(2)
nums.indexWhere(\_ == 2) \rightarrow 1
// functions as parameters, apply f to the
 value "1"
def call(f: Int => Int) = f(1)
call(plusOne)
call(x \Rightarrow x + 1) \rightarrow 2
call(_+ 1)
```

The Usage of "_" in Scala

• In anonymous functions, the "_" acts as a placeholder for parameters

```
nums.map(x \Rightarrow x + 1) is equivalent to:

nums.map(_+ 1)

List(1,2,3,4,5).foreach(print(_-)) is equivalent to:

List(1,2,3,4,5).foreach(_- \Rightarrow _-) print(_-)
```

• You can use two or more underscores to refer different parameters.

```
val sum = List(1,2,3,4,5).reduceLeft(\_+\_) is equivalent to:
val sum = List(1,2,3,4,5).reduceLeft((a, b) \Rightarrow a + b)
```

• The reduceLeft method works by applying the function/operation you give it, and applying it to successive elements in the collection

Acknowledgement & References

- 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

Be Scalable for both computing A living