

https://www.kdnuggets.com/wp-content/uploads/curse-dimensionality-2.png

# Lecture 5: Scalable PCA - Dimensionality Reduction & Factor Analysis

Haiping Lu - Scalable ML 2020

### Thank You for Your Help!

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### Week 5 Contents / Objectives

• PCA - Dimensionality Reduction

• SVD – Factor Analysis

Scalable PCA in Spark

More on Scala (optional, not to be assessed)

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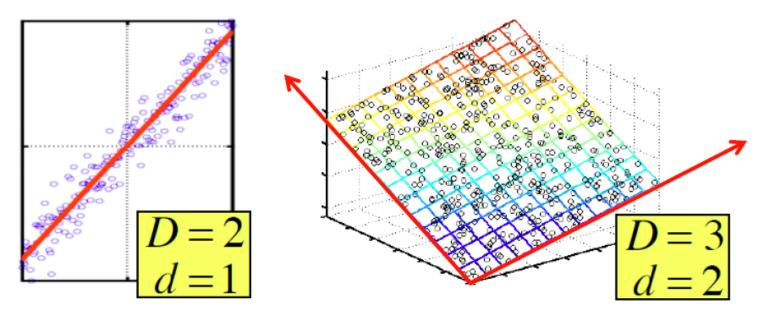
• PCA - Dimensionality Reduction

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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
  - Representation learning
- 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  $\rightarrow$  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  $\Sigma$
  - 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

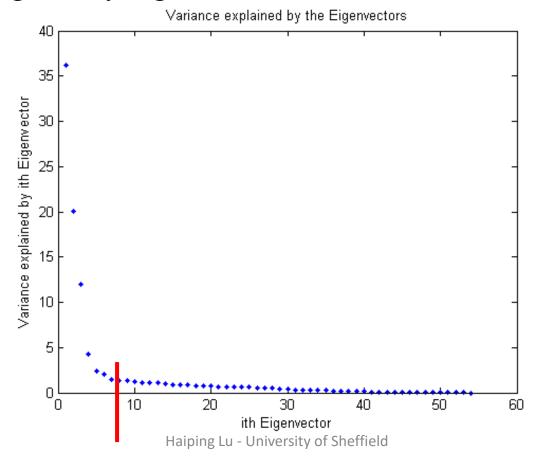
### How Many Components?

• Check the distribution of eigen-values

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



11/03/2020



10

### 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<sup>4</sup>= 100 x 100)
- Problem:
  - Gramian matrix  $\Sigma$  is size (D<sup>2</sup>)
  - D=10<sup>4</sup>  $\rightarrow$  | $\Sigma$ | = 10<sup>8</sup>
- Singular Value Decomposition (SVD)!
  - Efficient algorithms available
  - Some implementations find just top d eigenvectors

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### 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
$\mathbf{MED}\text{-}\mathbf{TR1}$	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)
- $\Lambda$ :  $r \times r$  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 non-negative, 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 ( $\mathbf{U}^{\mathrm{T}}\mathbf{U}=\mathbf{I}$ ),
    - $\Lambda$ ,  $\Sigma$  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  $\Lambda$  V<sup>T</sup>  $\leftarrow$  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  $\Lambda$  are equal to the square roots of the eigenvalues of  $\mathbf{X}^T\mathbf{X}$

### SVD - Properties

'spectral decomposition' of the matrix:

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

### SVD - Interpretation

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

- U: document-to-concept similarity matrix
- V: term-to-concept similarity matrix
- $\Lambda$ : 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

$\mathbf{term}$	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
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MED-TR1	0	0	0	2	2
${f MED-TR2}$	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
$\stackrel{\perp}{\mathrm{MD}}$	0	0	0	3	3
\ \ \	0	0	0	1	1

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

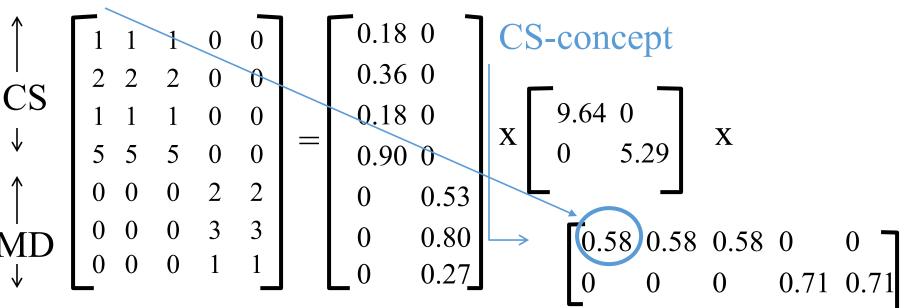
retrieval

$$\frac{\inf_{\text{data}} \text{ inf.}}{\text{ brain}} \text{ lung} \quad \text{ 'strength' of CS-concept}$$

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

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

retrieval inf. the brain lung term-to-concept similarity matrix

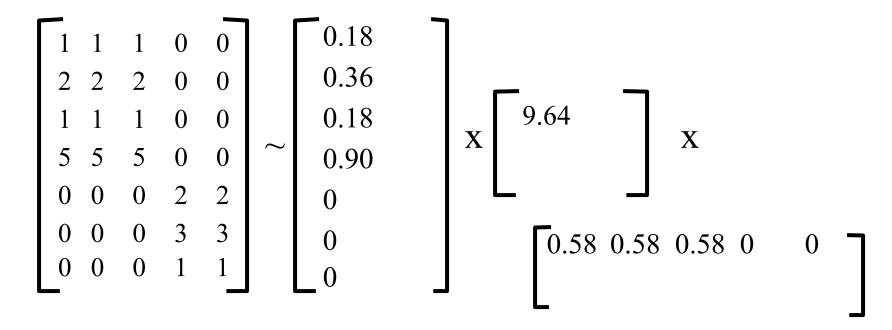


# SVD – Dimensionality Reduction

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

	0	1 5 0	2 1 5	0	0 0 0 0 2 3 1	0.18 0 0.36 0 0.18 0 0.90 0 0 0.50 0 0.80	X X	9.64 0 0 3.29 X 0.58 0.58 0.58 0 0
L	0	0	0	1	1	$\begin{bmatrix} 0 & 0.2 \end{bmatrix}$	Į	0.56 0.56 0.56 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

### SVD - Dimensionality Reduction



# SVD - Dimensionality Reduction

• Best rank-1 approximation

### Week 5 Contents / Objectives

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• Scalable PCA in Spark

More on Scala (optional, not to be assessed)

### 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)

• <a href="https://spark.apache.org/docs/2.3.2/mllib-dimensionality-reduction.html">https://spark.apache.org/docs/2.3.2/mllib-dimensionality-reduction.html</a>

```
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)

- <a href="https://spark.apache.org/docs/2.3.2/mllib-dimensionality-reduction.html">https://spark.apache.org/docs/2.3.2/mllib-dimensionality-reduction.html</a>
- 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  $A^{T}A$  (which is smaller than 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<sup>T</sup>A 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

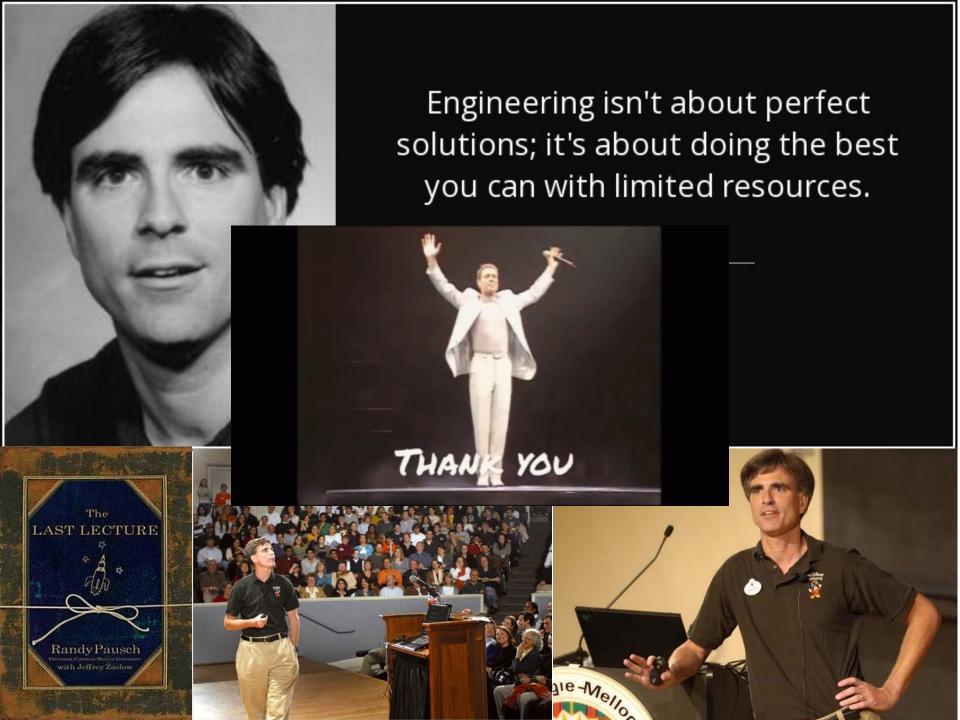
Auto (default)

```
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

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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Scalable PCA in Spark

• More on Scala (optional, not to be assessed)

#### More on Scala

- Useful for deeper understanding of Spark
  - Python source code for Spark is only for interface
  - PySpark still runs on top of Scala code (watch the info/debug info when you run PySpark in terminal)
- Optional: Not to be examined in quiz or assignment
- Please study on your own if interested

# 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;
  public void setName(String name) {      // name setter
   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) => x + foo
```

plusFoo(5) 
$$\rightarrow$$
 6

// Changing foo changes the return value of plusFoo

$$\mathbf{foo} = 5$$

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. <a href="http://www.mmds.org">http://www.mmds.org</a>
- References
  - <a href="http://infolab.stanford.edu/~ullman/mmds/ch11.pdf">http://infolab.stanford.edu/~ullman/mmds/ch11.pdf</a>
  - <a href="http://www.mmds.org">http://www.mmds.org</a>

# Be Scalable for both computing A living