GENERAL ASSEMBLY

INTRO TO DATA SCIENCE

LECTURE 12: DIMENSIONALITY REDUCTION

I. DIMENSIONALITY REDUCTION
II. PRINCIPAL COMPONENTS ANALYSIS (PCA)
III. SINGULAR VALUE DECOMPOSITION
IV. KERNEL METHODS IN PCA

EXERCISE:
IV. DIMENSIONALITY REDUCTION IN SCIKIT-LEARN

I. DIMENSIONALITY REDUCTION

Problem: Consider this.

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Dimensionality reduction is frequently performed as a pre-processing step before another learning algorithm is applied.

Q: What are the motivations for dimensionality reduction?

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The number of features in our dataset can be difficult to manage, or even misleading (eg, if the relationships are actually simpler than they appear).

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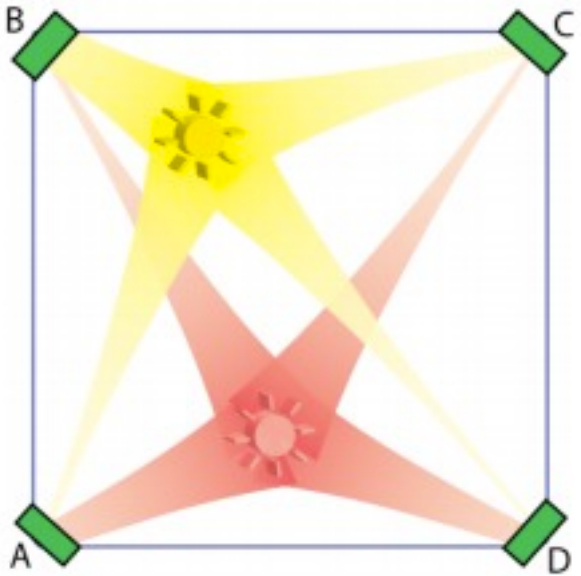
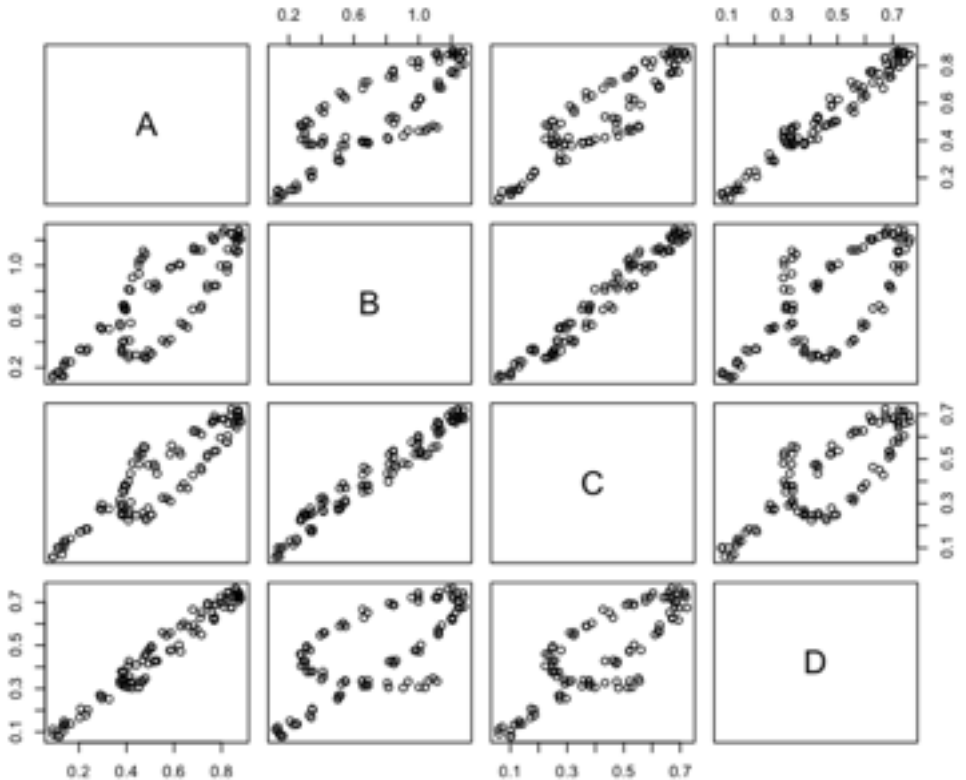
If these relationships are linear, then we can use well-established techniques like PCA/SVD.

Problem: Consider this.

Say we have a large room that contains m lights with unique light patterns and n cameras recording them. Using what the cameras record, how do we determine how many lights there are in the room?



EXAMPLE: COMPARING DATA BETWEEN LIGHT CAPTURE CAMERAS



ASIDE: CURSE OF DIMENSIONALITY

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(More precisely, the sample size grows exponentially with $l \leq features$, *the dimension of the manifold embedded in the feature space).*

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Most of the points in the space are "far" from each other.

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The bottom line is that high-dimensional spaces can be problematic.

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More precisely: given an n **x** d *matrix* A *(encoding* n *observations of a* d*-dimensional random variable), we want to find a* k*-dimensional representation of* A *(*$k < d$*) that (approximately) captures the information in the original data, according to some criterion.*

Q: What is the goal of dimensionality reduction?

- *reduce computational expense*
- *reduce susceptibility to overfitting*
- *reduce noise in the dataset*
- *enhance our intuition*

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NOTE

We've already seen one example of feature selection for regression: *backward elimination*.

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feature extraction – *mapping the features to a lower dimensional space*

EXAMPLE: FEATURE SELECTION


```
>>> for i in range(4):
...     print 'P-value for', features[i], ':', feature_selection.f_regression(gas[features].values,
 gas['consumption'].values)[1][i]
...
P-value for tax : 0.00128489067343
P-value for income : 0.0934684297747
P-value for miles : 0.89778460025
P-value for pctlicense : 3.28960494853e-08
```

Feature selection: Removing features with lowest p-values and then refitting model (stepwise regression)

Feature selection is important, but typically when people say dimensionality reduction, they are referring to feature extraction.

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The goal of feature extraction is to create a new set of coordinates (often in lower dimension) that simplify the representation of the data.

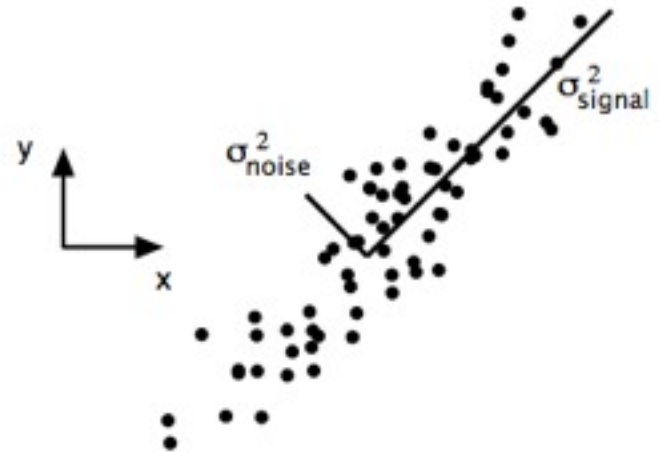

FIG. 2 Simulated data of (x,y) for camera A. The signal and noise variances σ^2_{signal} and σ^2_{noise} are graphically represented by the two lines subtending the cloud of data. Note that the largest direction of variance does not lie along the basis of the recording (x_A, y_A) but rather along the best-fit line.

source: http://www.snl.salk.edu/~shlens/pca.pdf

Q: What are some applications of dimensionality reduction?

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- *topic models (document clustering)*
- *image recognition/computer vision*
- *bioinformatics (microarray analysis)*
- *speech recognition*
- *astronomy (spectral data analysis)*
- *recommender systems*

II. PRINCIPAL COMPONENT ANALYSIS

Principal component analysis is a dimension reduction technique that can be used on a matrix of any dimensions.

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The PCA of a matrix A *boils down to the* **eigenvalue decomposition** *of the* **covariance matrix** *of* A.

The covariance matrix C of a matrix A is always symmetric:

$$C = \begin{bmatrix} \mathrm{E}[(X_1 - \mu_1)(X_1 - \mu_1)] & \mathrm{E}[(X_1 - \mu_1)(X_2 - \mu_2)] & \cdots & \mathrm{E}[(X_1 - \mu_1)(X_n - \mu_n)] \\ \mathrm{E}[(X_2 - \mu_2)(X_1 - \mu_1)] & \mathrm{E}[(X_2 - \mu_2)(X_2 - \mu_2)] & \cdots & \mathrm{E}[(X_2 - \mu_2)(X_n - \mu_n)] \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{E}[(X_n - \mu_n)(X_1 - \mu_1)] & \mathrm{E}[(X_n - \mu_n)(X_2 - \mu_2)] & \cdots & \mathrm{E}[(X_n - \mu_n)(X_n - \mu_n)] \end{bmatrix}.$$

off-diagonal elements C_{ij} give the covariance between X_i, X_j $(i \neq j)$

diagonal elements C_{ii} give the variance of X_i

The eigenvalue decomposition of a symmetric matrix A is given by:

$$A = Q \Lambda Q^T$$

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NOTE

This relationship *defines* what it means to be an eigenvector of *A*.

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$$Av = \lambda v$$

The eigenvectors form a basis of the vector space on which A acts (eg, they are orthogonal).

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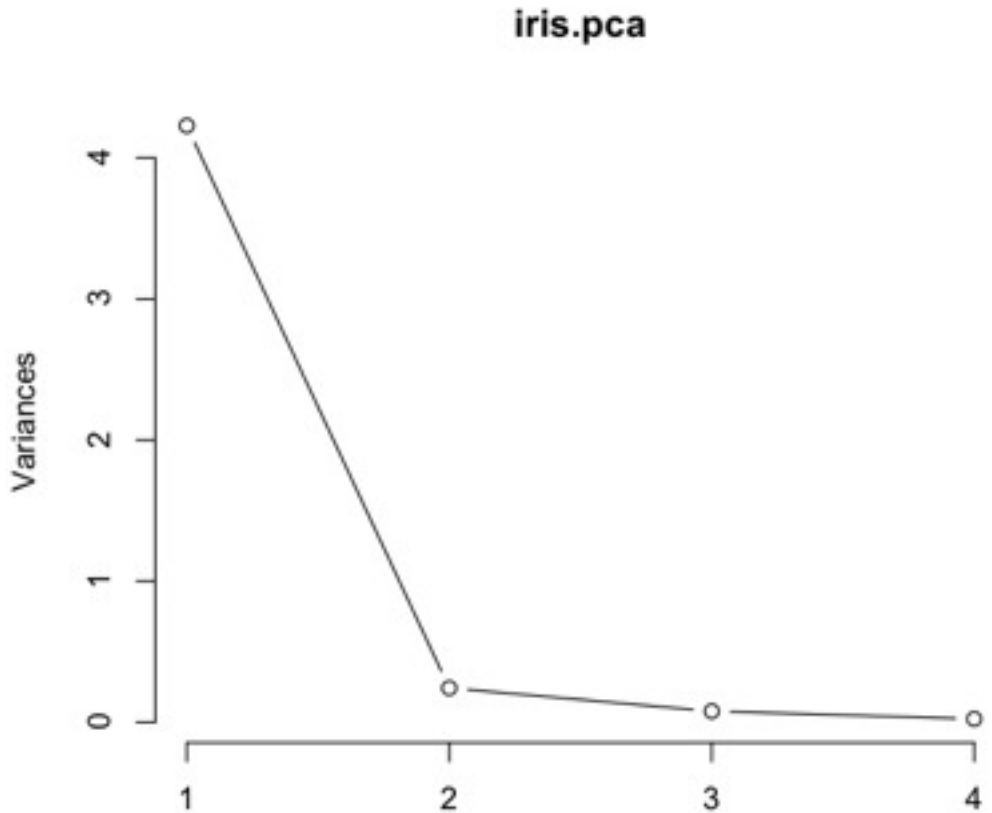
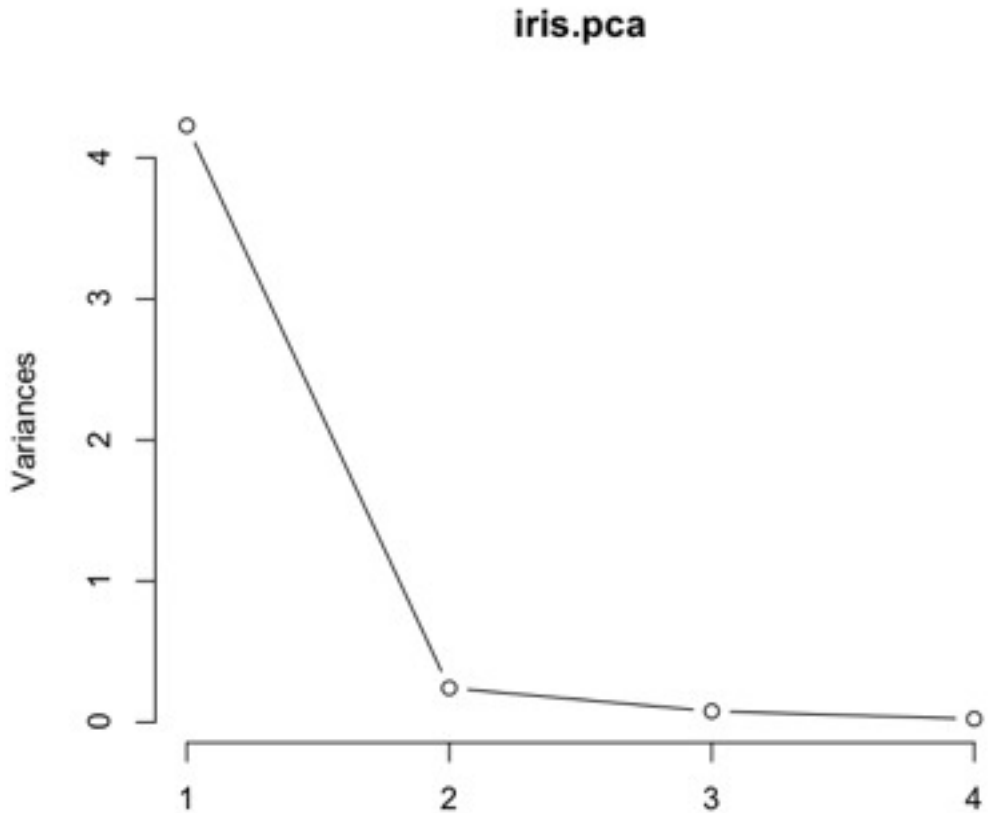
This can be visualized in a **scree plot**, *which shows the amount of variance explained by each basis vector.*

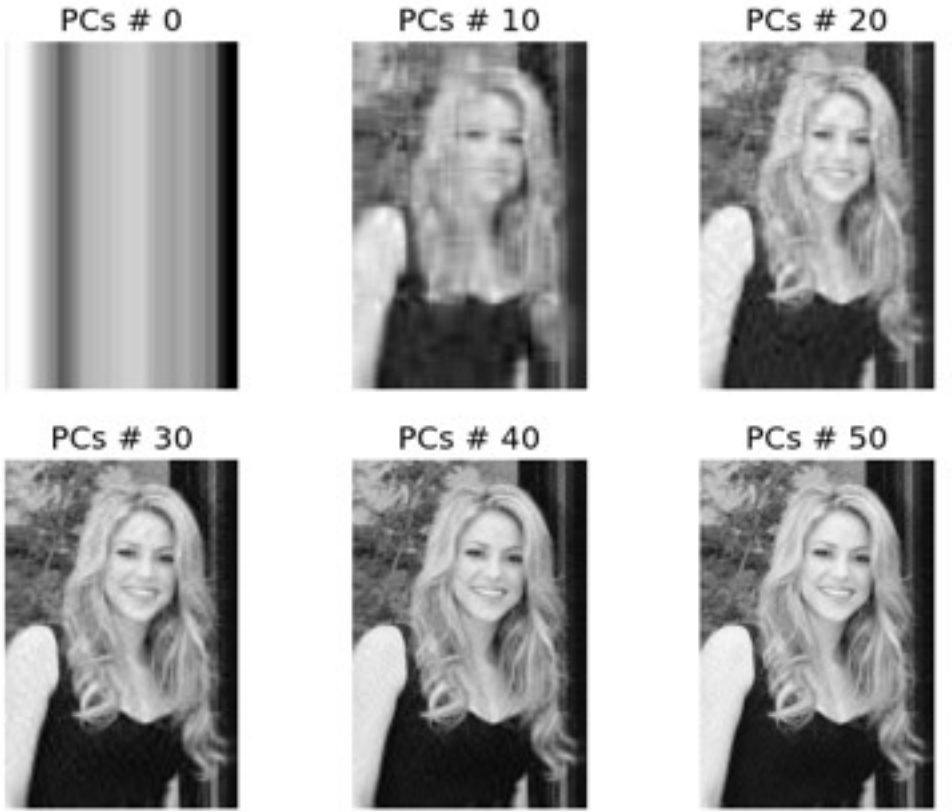

iris.pca
Variances
0
1
2
3
4
1
2
3
4



NOTE

Looking at this plot also gives you an idea of how many principal components to keep.

Apply the *elbow test*: keep only those pc's that appear to the left of the elbow in the graph.



source: http://glowingpython.blogspot.it/2011/07/pca-and-image-compression-with-numpy.html

III. SINGULAR VALUE DECOMPOSITION

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→ $U^T U = U U^T = I_n$, $V^T V = V V^T = I_d$ → $\Sigma_{ij} = 0 \ (i \neq j)$

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These singular vectors provide **orthonormal bases** *for the spaces* K_n *&* K_d *(columns of* U *&* V*, respectively).*

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NOTE

The number of singular values is equal to the *rank* of A.

The rank of a matrix measures its *non-degeneracy.*

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For a general SVD, the columns of U are the eigenvectors of AA^T, and the columns of V are the eigenvectors of A^TA.

Also, the singular values of A are the square roots of the eigenvalues of AA^T and A^TA.

III. KERNEL PCA

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gaussian (rdf): $exp(-\gamma||x - x'||^2)$

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In particular, KPCA is most often used for image de-noising and pattern recognition (or commonly novelty detection).

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KPCA is particularly useful for extracting nonlinear features, though like standard PCA, the interpretation is not always straightforward!

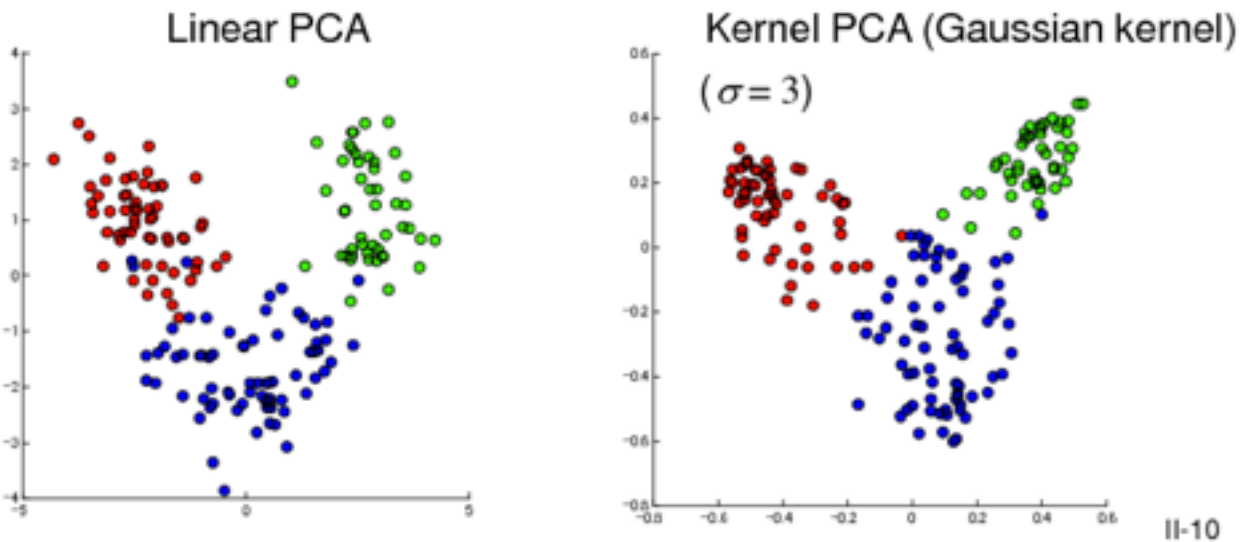
KERNEL PCA - EXAMPLE

- **Wine data** (from UCI repository)

  13 dim. chemical measurements of for three types of wine. 178 data.

  Class labels are NOT used in PCA, but shown in the figures.

  First two principal components:



http://yosinski.com/mlss12/media/slides/MLSS-2012-Fukumizu-Kernel-Methods-for-Statistical-Learning_034.png