S&DS 265 / 565

Introductory Machine Learning

Unsupervised Learning: PCA

Tuesday, October 12

Yale

Checkpoint

- Assn 3 due Thursday; Assn 4 out
- Quiz 2 available from 12:01pm today for 24 hours
- Midterm one week from today, in class
- Practice midterm posted on Canvas
- Review sessions scheduled
- Questions?

Unsupervised Learning

Supervised learning is about being able to predict a Y using predictors $X_1, X_2, \ldots, X_p$

Unsupervised learning deals with data that do not have labels Y

We are not trying to predict anything. So what else might we hope to do?

Unsupervised Learning

Supervised learning is about being able to predict a Y using predictors $X_1, X_2, \ldots, X_p$

Unsupervised learning deals with data that do not have labels Y

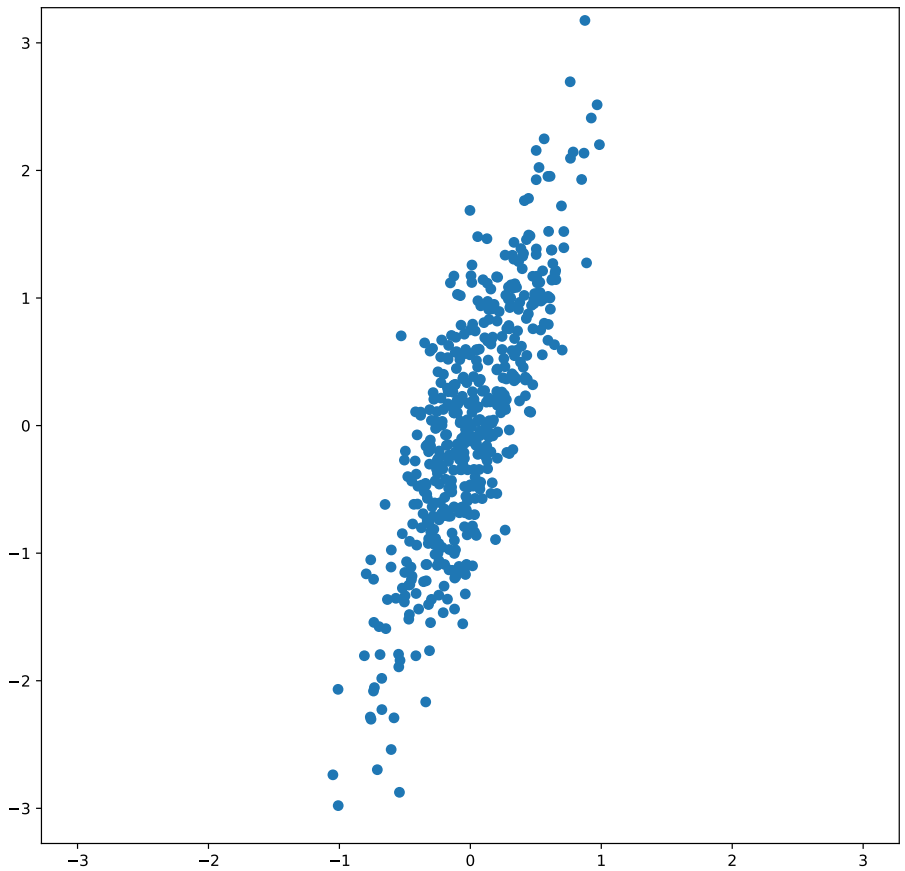
We are not trying to predict anything. So what else might we hope to do?

Consider:

- Are there interesting ways to visualize/summarize the data?
- Are there natural subgroups in the data?
- What are the important types of variation in the data?

Principal Component Analysis (PCA)

PCA finds the directions of greatest variability in the data.



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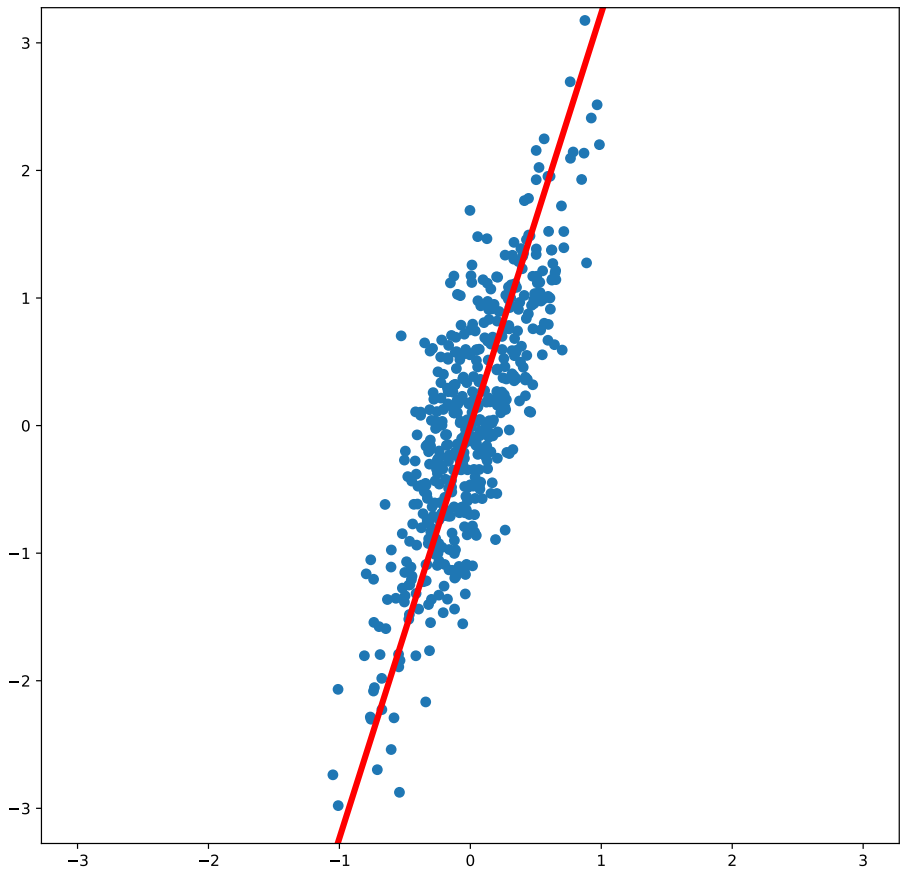
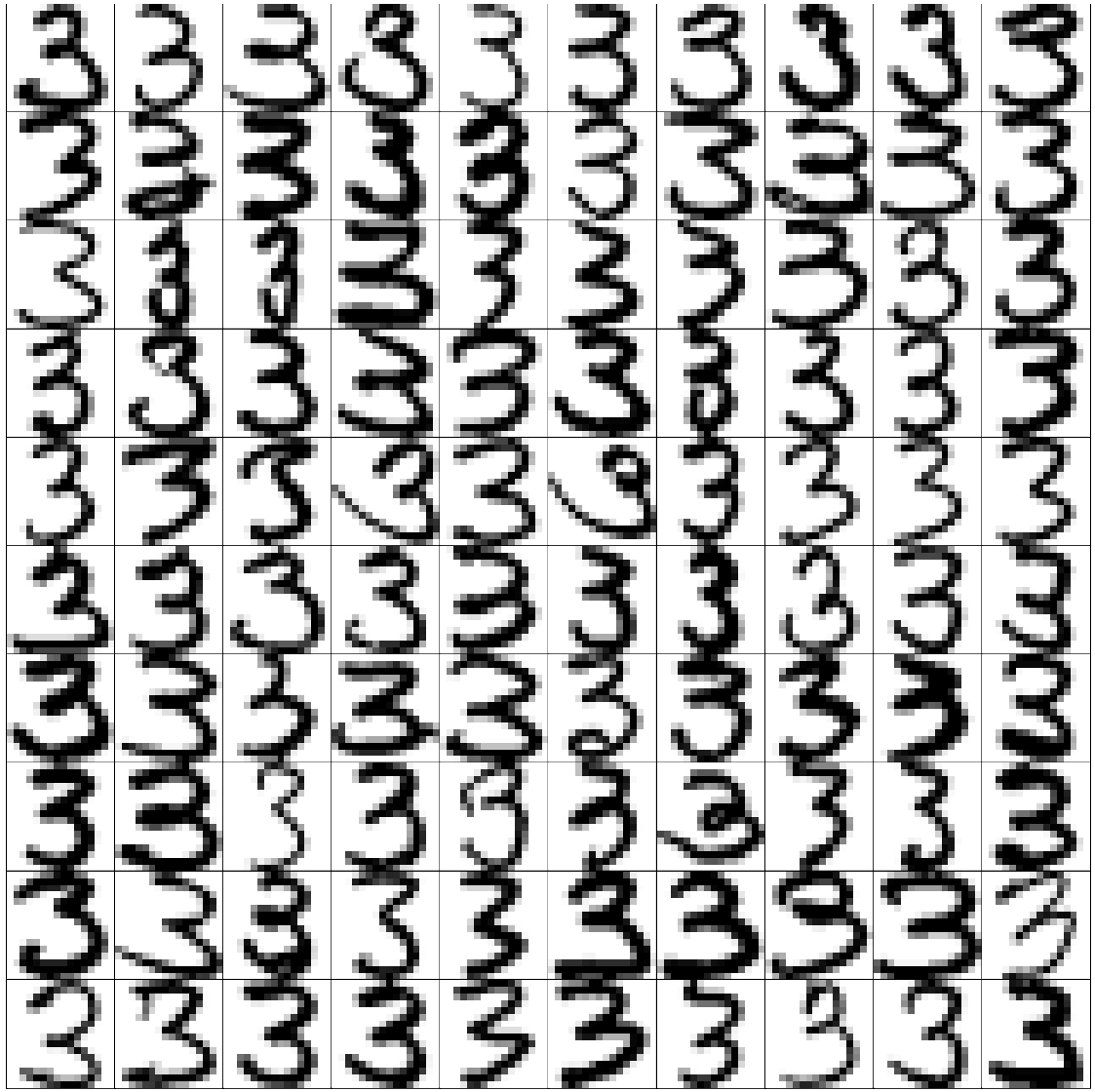
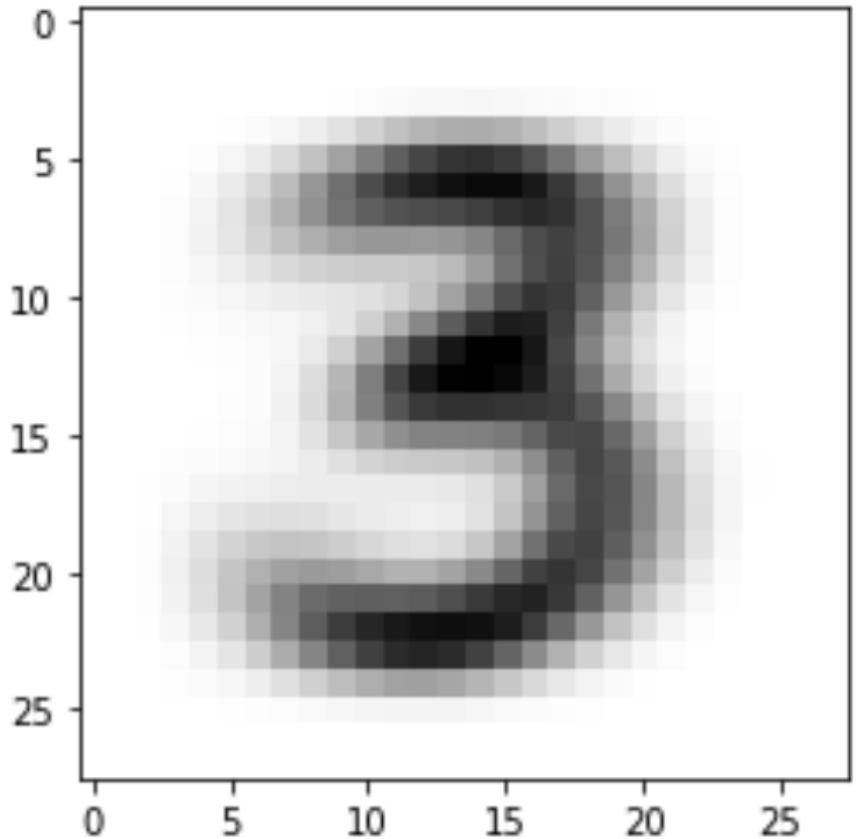


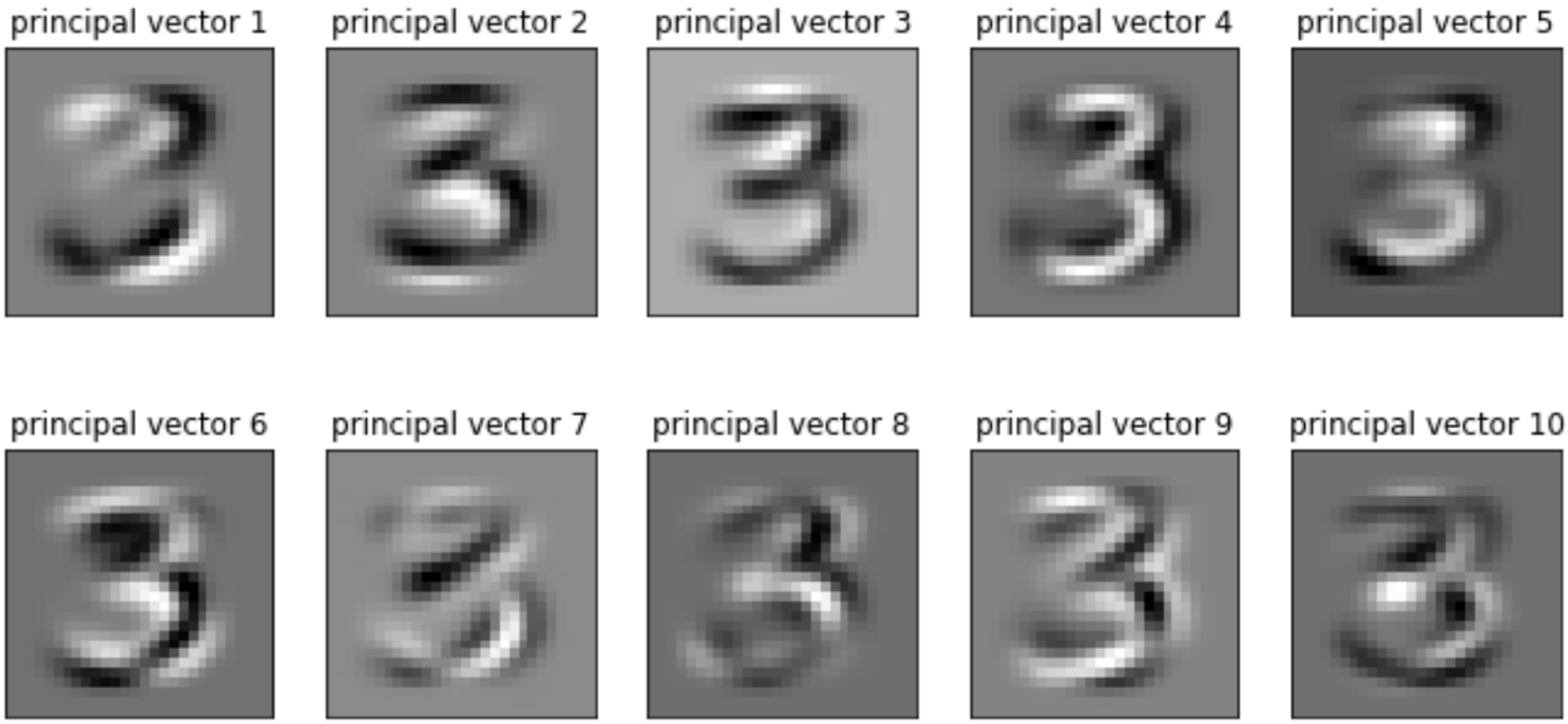
Handwritten Digits (3s)



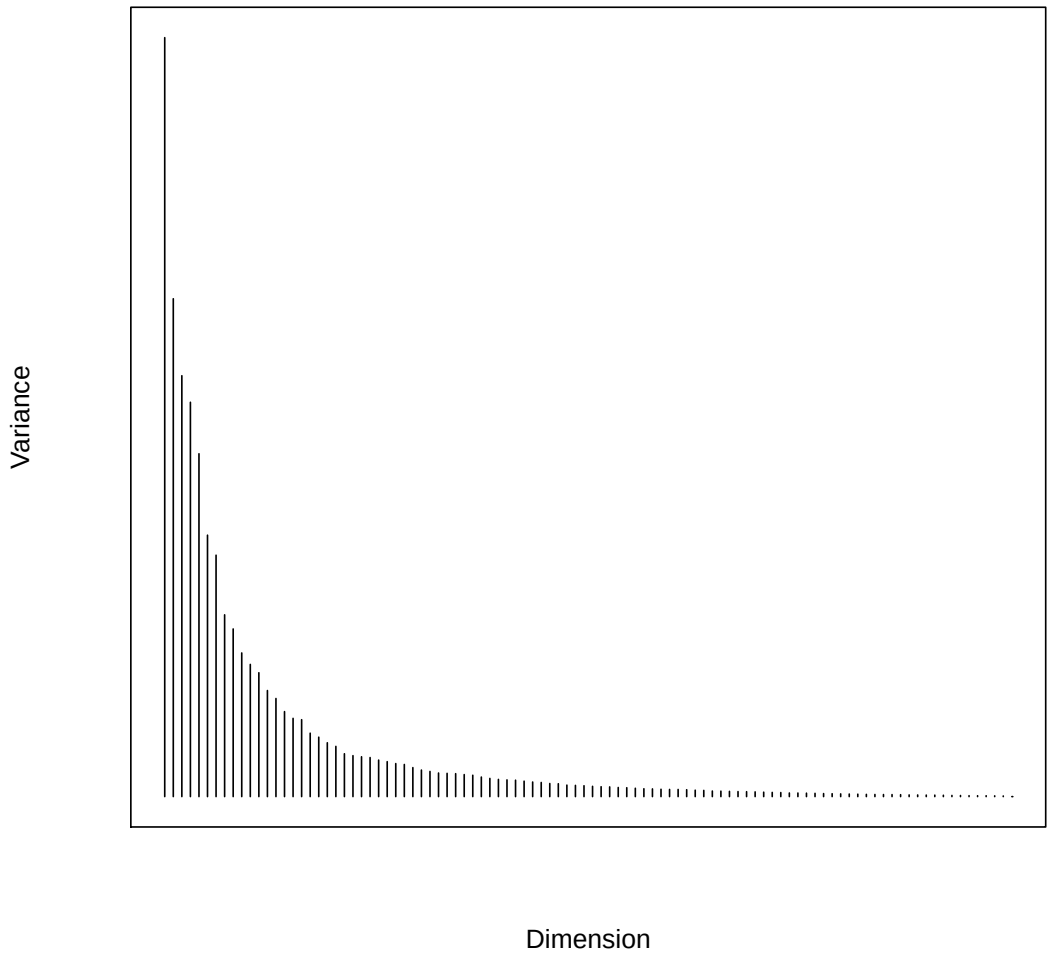
Handwritten Digits (3s) – Average



Handwritten Digits (3s) – Principal vectors



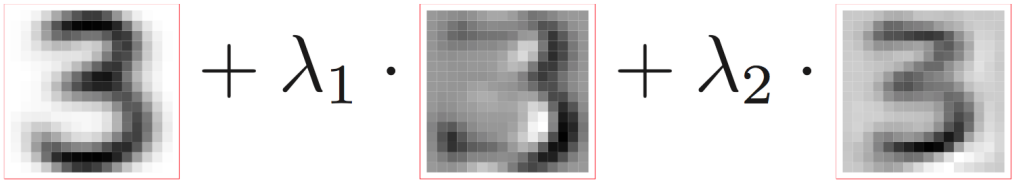
Handwritten Digits (3s) – PCA variance



Handwritten Digits (3s)

$$\hat{f}(\lambda) = \bar{x} + \lambda_1 v_1 + \lambda_2 v_2$$

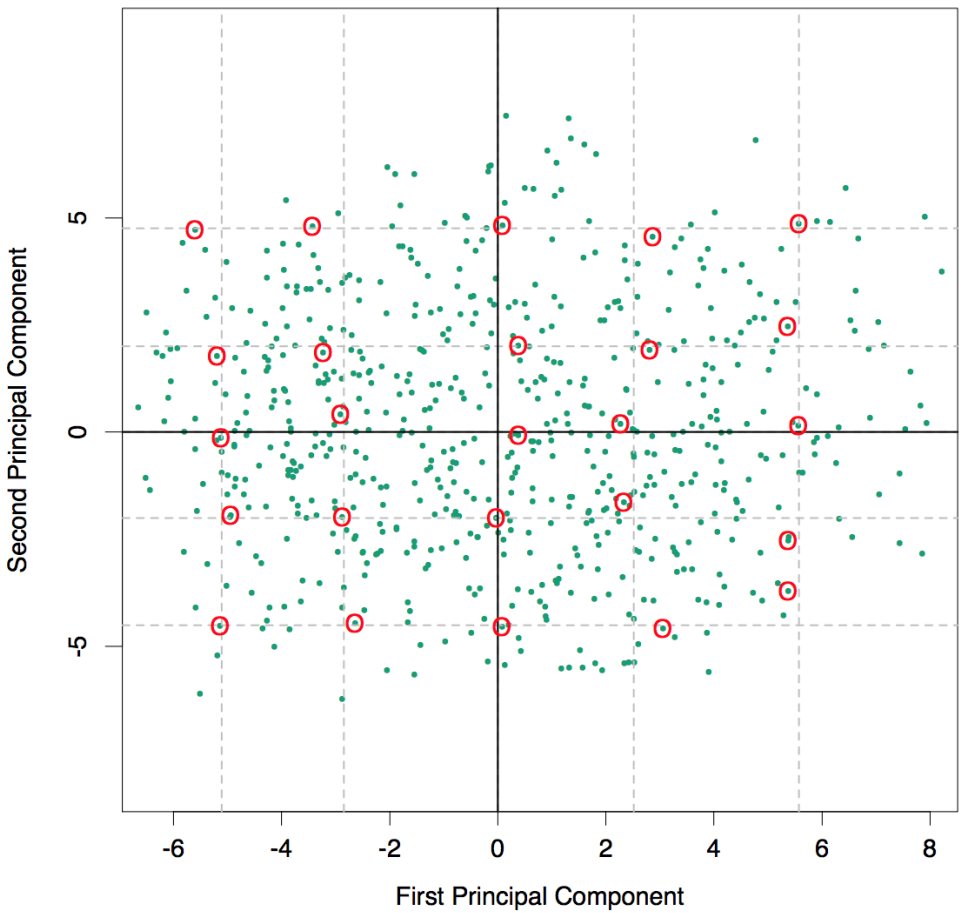
$$= \bar{x} + \lambda_1 \cdot v_1 + \lambda_2 \cdot v_2.$$

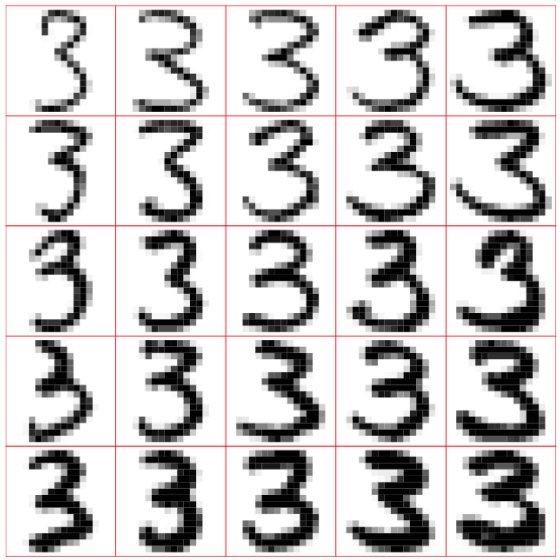


Handwritten Digits (3s) – Top 2 components

$$\hat{f}(\lambda) = \bar{x} + \lambda_1 v_1 + \lambda_2 v_2$$

$$= \bar{x} + \lambda_1 \cdot v_1 + \lambda_2 \cdot v_2 .$$



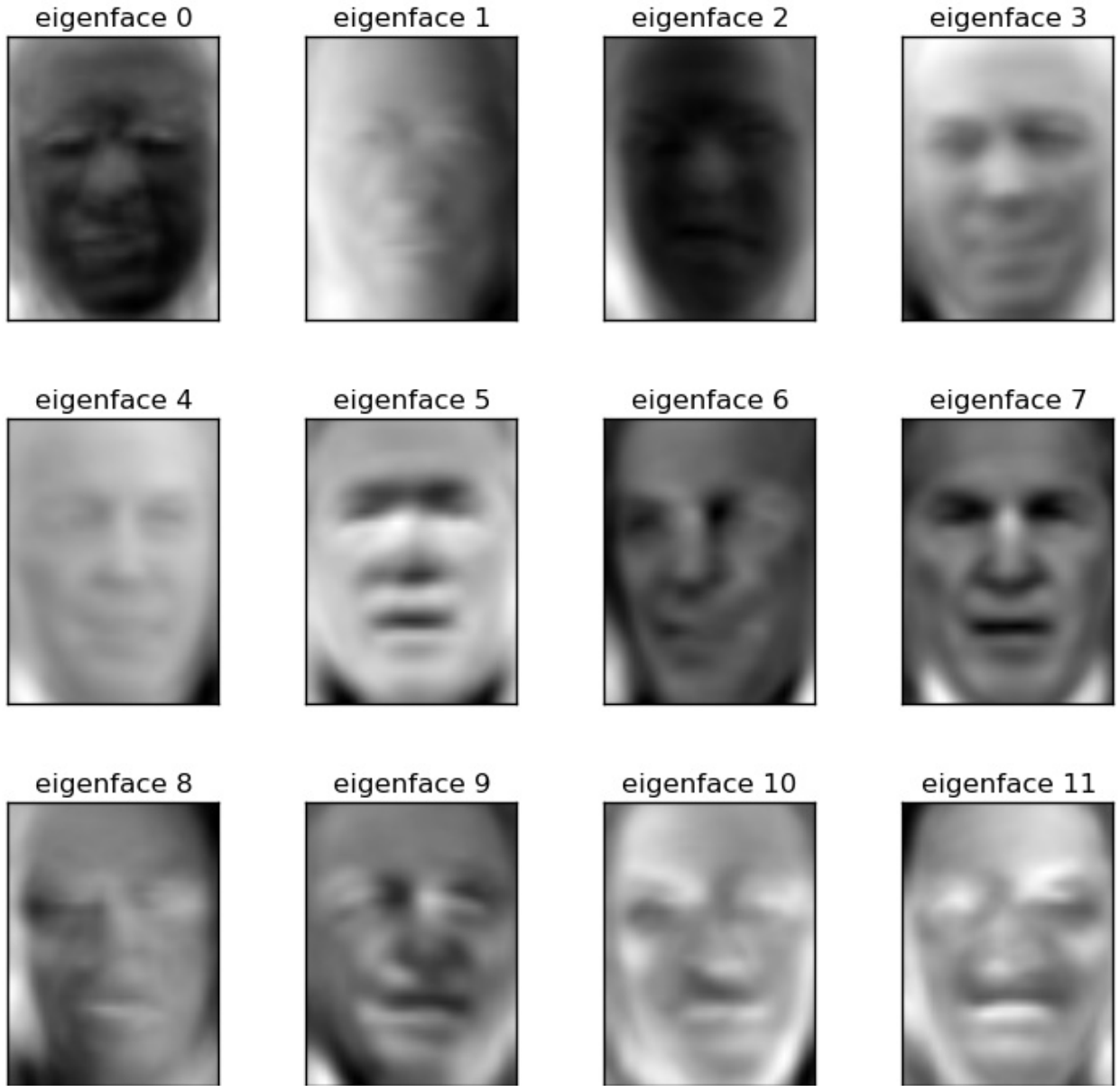


Handwritten Digits (3s) – PCA reconstruction

Faces


test face 0
test face 1
test face 2
test face 3
test face 4
test face 5
test face 6
test face 7
test face 8
test face 9
test face 10
test face 11

Eigenfaces (principal vectors)



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Genes mirror geography within Europe

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Abstract

Go to:

Understanding the genetic structure of human populations is of fundamental interest to medical, forensic and anthropological sciences. Advances in high-throughput genotyping technology have markedly improved our understanding of global patterns of human genetic variation and suggest the potential to use large samples to uncover variation among closely spaced populations[1–5]. Here we characterize genetic variation in a sample of 3,000 European individuals genotyped at over half a million variable DNA sites in the human genome. Despite low average levels of genetic differentiation among Europeans, we find a close correspondence between genetic and geographic distances; indeed, a geographical map of Europe arises naturally as an efficient two-dimensional summary of genetic variation in Europeans. The results emphasize that when mapping the genetic basis of a disease phenotype, spurious associations can arise if genetic structure is not properly accounted for. In addition, the results are relevant to the prospects of genetic ancestry testing[6]; an individual's DNA can be used to infer their geographic origin with surprising accuracy—often to within a few hundred kilometres.

https://ghr.nlm.nih.gov/primer/genomicresearch/snp

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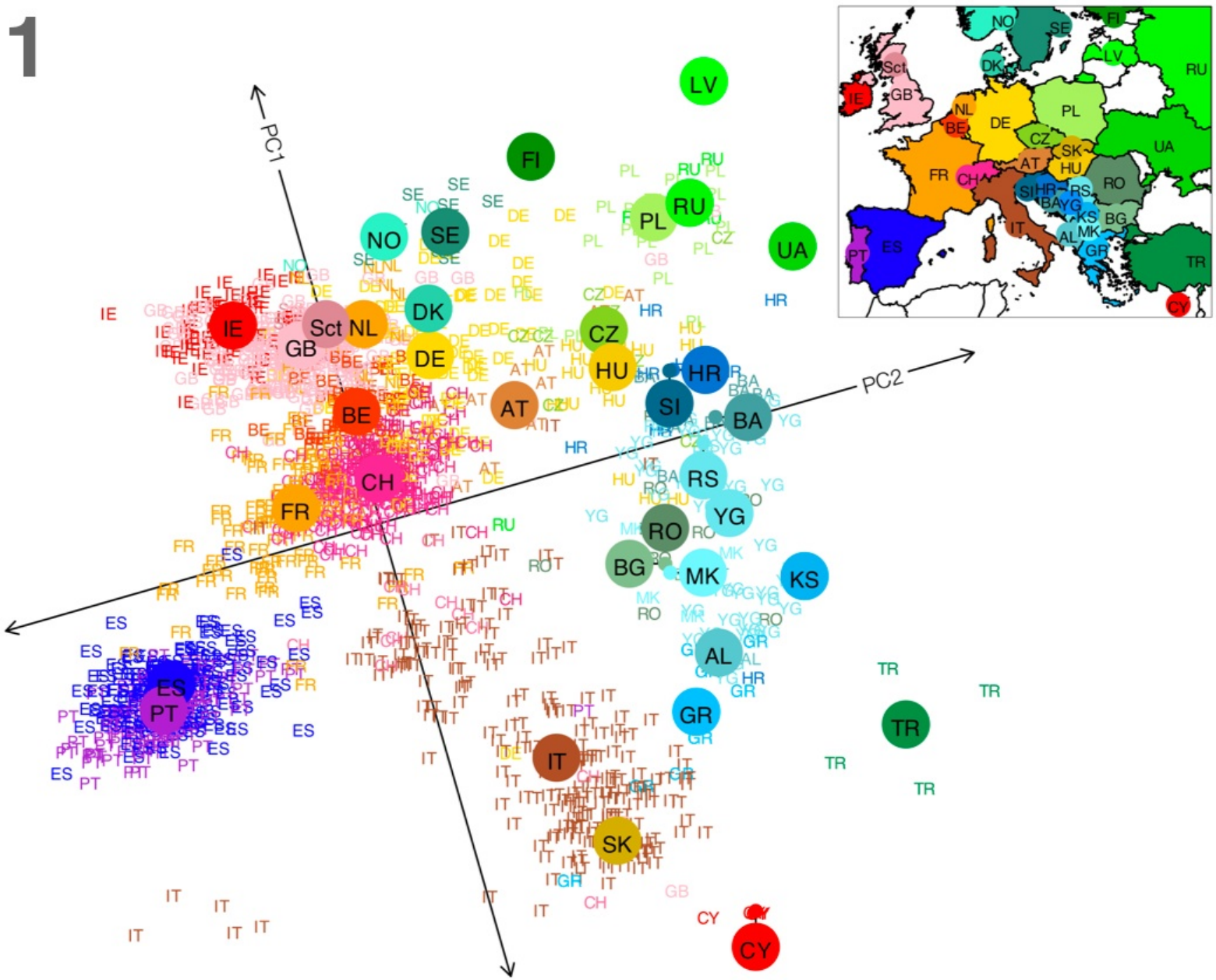
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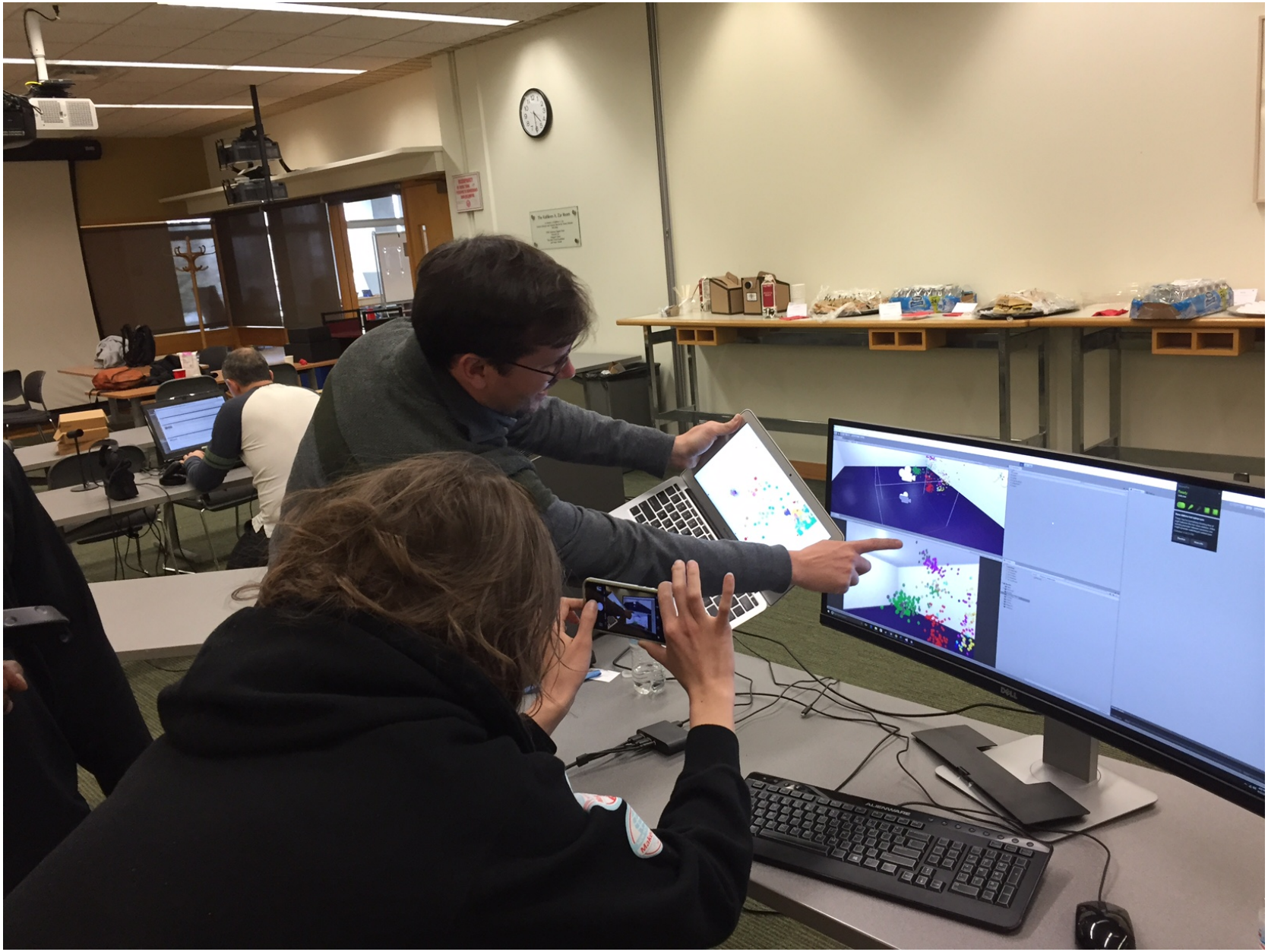
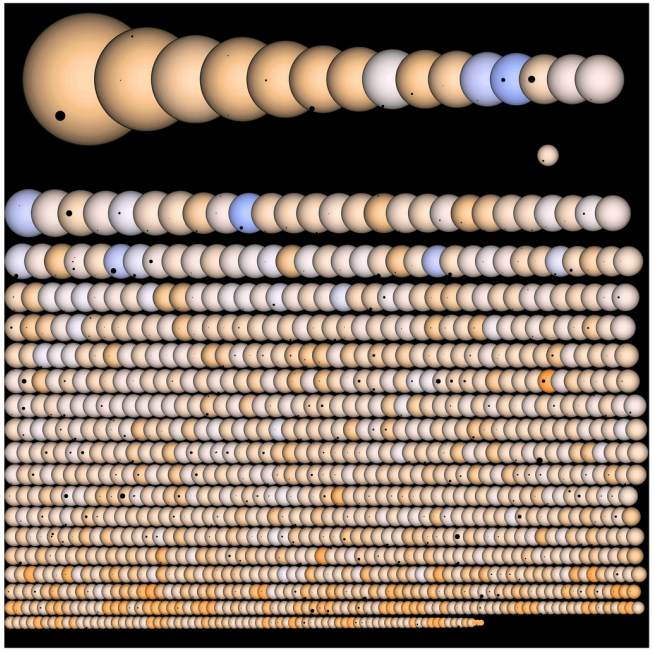

DELL
ALIENWARE

Robust PCA

Robust PCA (low rank plus sparse) can be used for background subtraction in video.

https://www.youtube.com/watch?v=BTrbow8u4Cw

Kepler telescope



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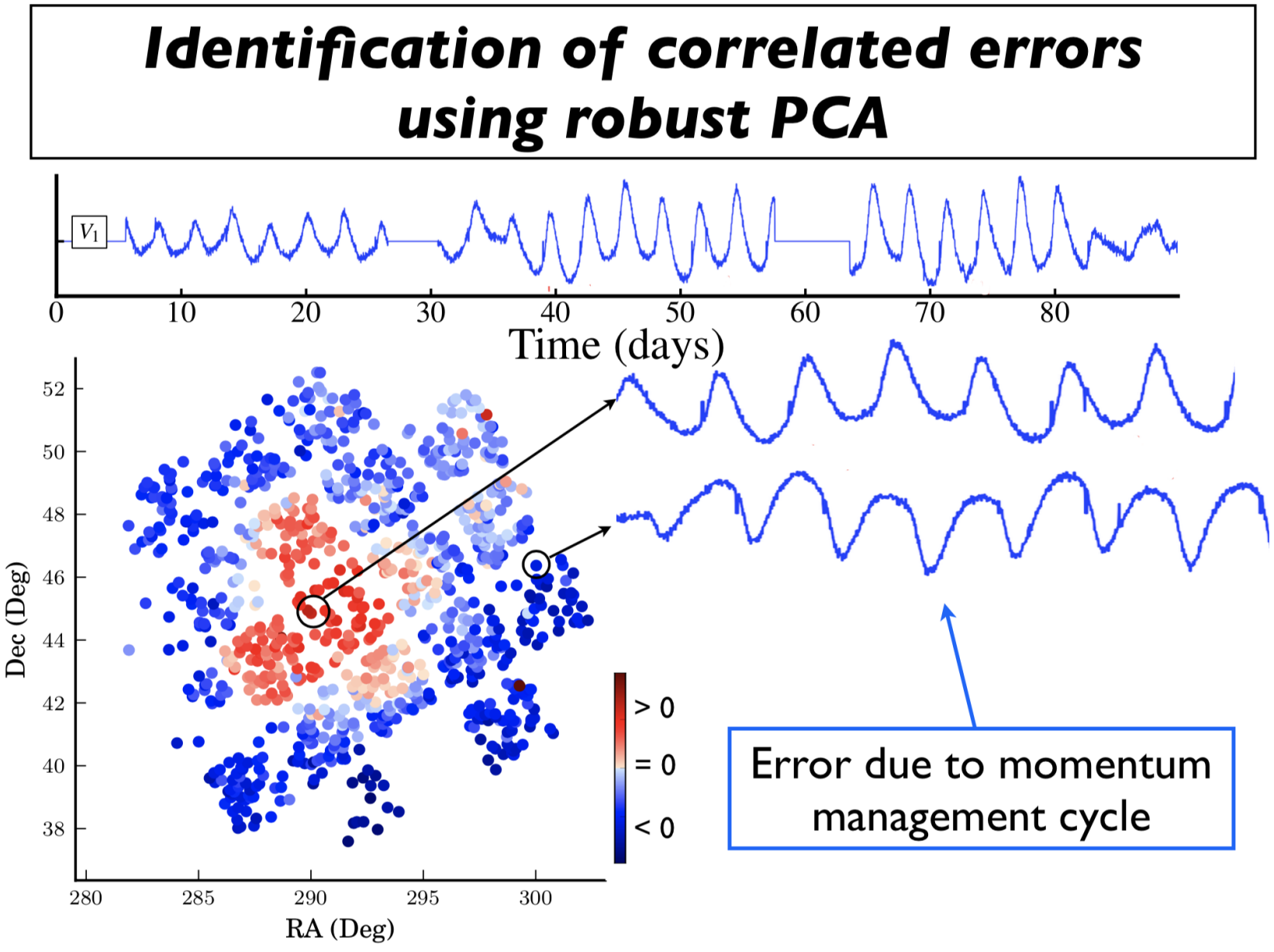
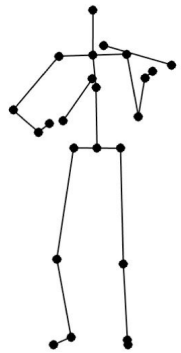
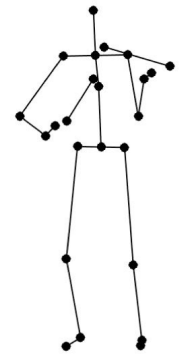


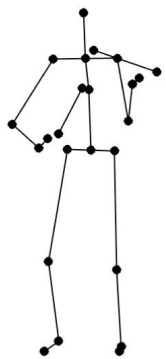
RESULTS: PC VISUALISATION, TECHNICAL VS. NON-TECHNICAL MOTION



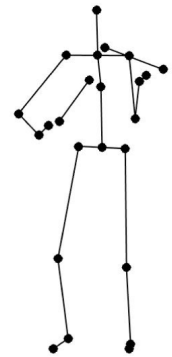
Original



PC1 (45% of variance accounted)
Side-to-side swaying (non-technical)



PC2 (25% of variance accounted)
Right arm string crossing (technical)



PC3 (15% of variance accounted)
Left-right rotation (non-technical)

Aditya Chander

PCA: Algorithm

1. Center the data: $x_i \mapsto x_i - \overline{x}$
2. Compute the $d \times d$ sample covariance $S = \frac{1}{n} \sum_{i=1}^{n} x_i x_i^T$
3. Find the first k eigenvectors of S
4. Project the data onto those k vectors

PCA: Algorithm

1. Center the data: $x_i \mapsto x_i - \frac{1}{n}\sum_{j=1}^{n} x_j = x_i - \overline{x}$

2. Compute the $d \times d$ sample covariance $S = \frac{1}{n}\sum_{i=1}^{n} x_i x_i^T$. Note that

$$\frac{1}{n}\sum_{i} \left(x_{ij} - \overline{x}\right)^2$$

   is the sample variance of jth coordinate of data.

3. Find the first k eigenvectors of S,

$$\phi_1, \ldots, \phi_k \in \mathbb{R}^d, \qquad S\phi_j = \lambda_j \phi_j$$

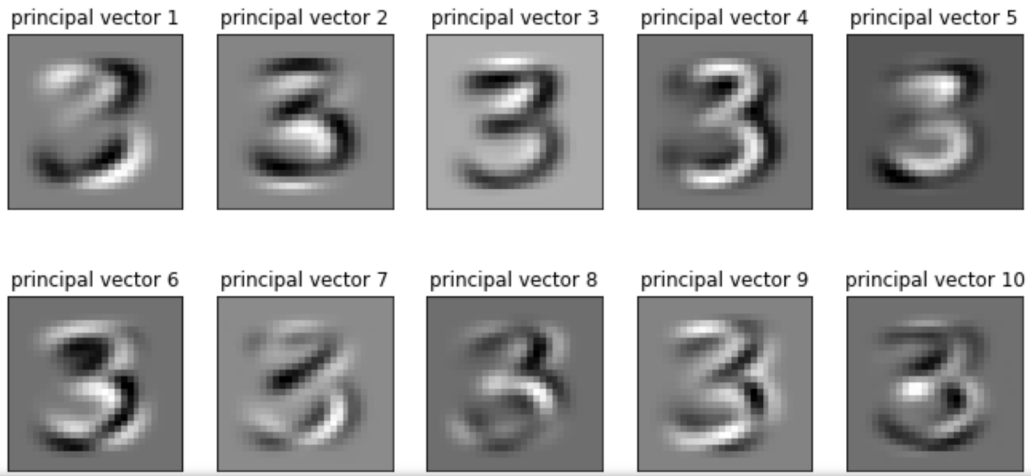
4. Project the data onto those k vectors:

$$x_i \mapsto \overline{x} + (\phi_1^T x_i)\phi_1 + \ldots + (\phi_k^T x_i)\phi_k$$

Let’s go to the notebook

```
pca = PCA(num_components).fit(cimages)
principal_vectors = pca.components_
principal_vectors = principal_vectors.reshape((num_components, height, width))
pcs = pca.fit_transform(cimages)
capprox = pca.inverse_transform(pcs)
labels = ['principal vector %d' % (i+1) for i in np.arange(num_components)]
plot_images(principal_vectors, labels, height, width, int(num_components/5.), 5)
ratio = pca.explained_variance_ratio_.sum()
print('Variance explained by first %d principal vectors: %.2f%%' % (num_components, ratio*100))
```

```
Variance explained by first 25 principal vectors: 72.46%
```



PCA: Summary

- PCA is an unsupervised method
- Finds directions of greatest variation in the data
- The directions are called the *principal vectors*; the weightings on the vectors are called the *principal components*
- The first few vectors may be interpretable
- Orthogonality makes interpretation difficult for the higher components
- Can be used for visualization or dimensionality reduction