Introduction to Machine Learning

Lecture 11
Unsupervised Learning I
Dimensionality Reduction

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26 – 30 November 2018
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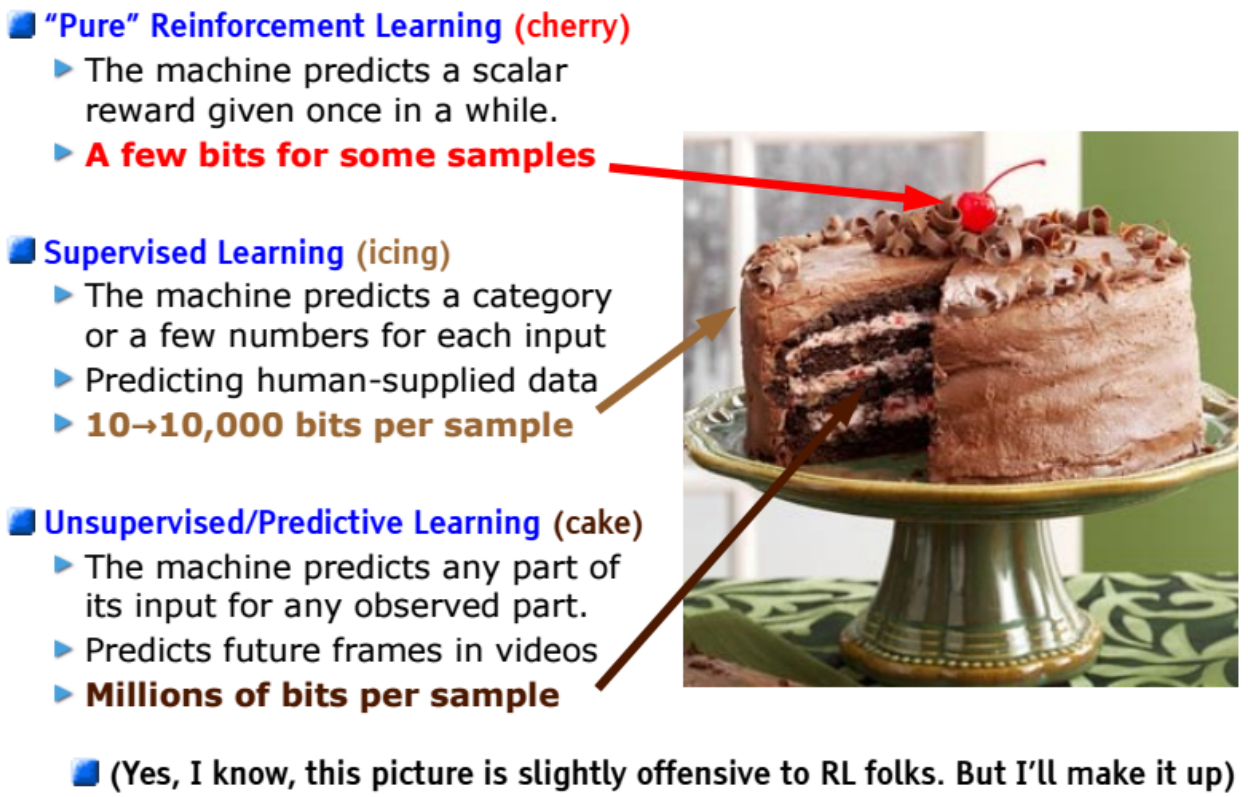
Types of learning problems

Supervised learning	Unsupervised learning	Reinforcement learning
Learning from supervision (i.e., teacher) Given inputs and **outputs**, learn a function that maps input → output	Learning with no supervision Given only inputs, extract some pattern from the data.	Learning from rewards and punishments. Inspired by (operant) conditioning in psychology. The agent acts in an environment over some **time**. It gets reward/punishment from time to time. Needs to learn a *policy* to maximize reward.
Examples: - Recognizing faces - Predicting the sales for a product - Learning to rank search results	Examples: - Clustering (market segmentation) - Dimensionality reduction (visualization) - Generating celebrity faces	Examples: - Most robotics applications (e.g. learning to move around) - Playing games (e.g., AlphaGo)

Unsupervised learning

- Unsupervised learning is difficult but important
  - No clear objective
  - Hard to assess/validate results
  - Most of our learning is unsupervised

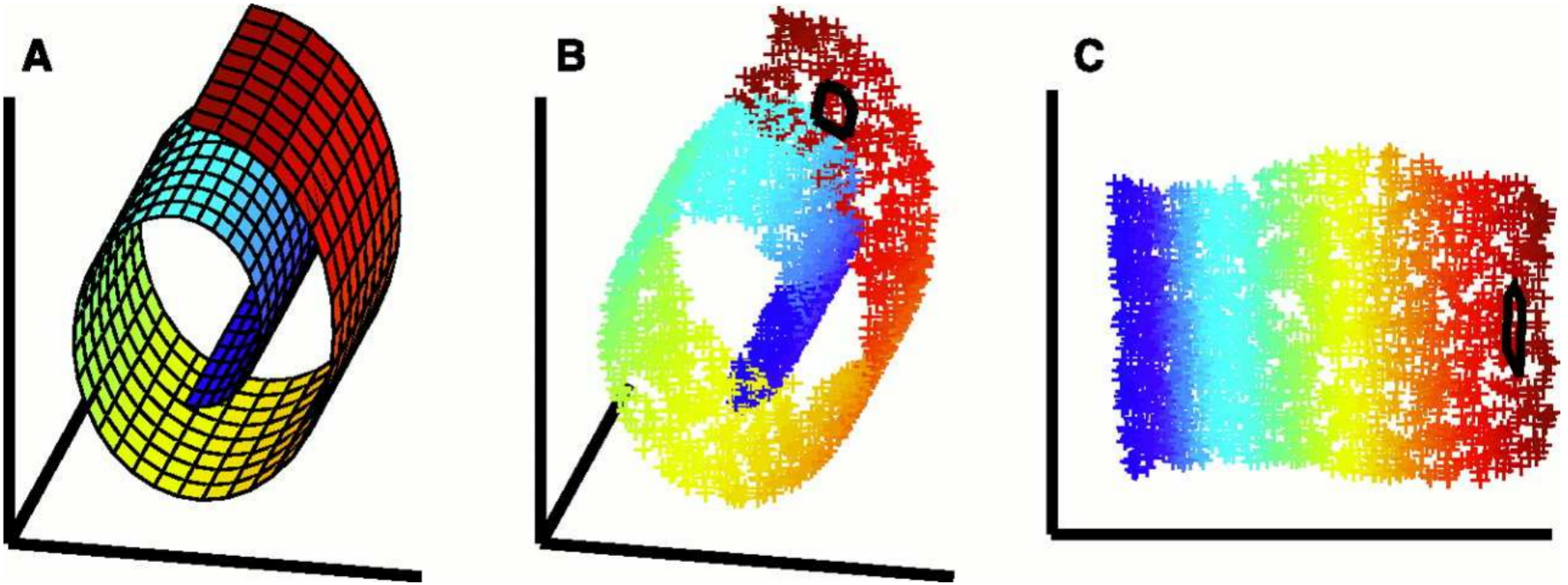


Dimensionality reduction

- Given a dataset of N samples with D features, X_{NxD}
  - Find a low dimensional M < D representation
  - Capture as much of the information as possible
    - Need to define what we mean by information

- Why should this work?
  - Most data is redundant (e.g., images)
    - Correlated features
  - Intrinsic dimensionality

- Useful for
  - Visualization
  - Compression
  - Supervised learning



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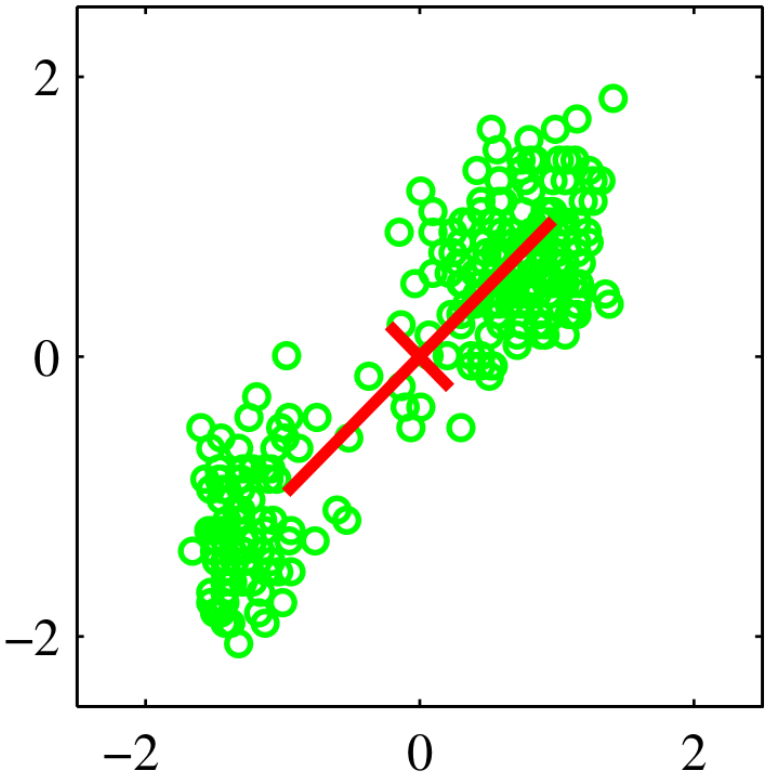
Principal components analysis (PCA)

- Popular technique for dimensionality reduction
  - Linear
  - Objective: Find direction(s) that maximize variance



PCA formulation

- Given N samples with D features, X_{NxD}
  - Map each sample to a single number (1D)

$$z_n = \sum_u u_i X_{ni}$$

$$z = Xu$$

Terminology:
u: loading vector
z: principal component

  - Find direction (u) that maximizes variance

$$\max_u \sum_n z_n^2$$

$$\max_u \ (Xu)^T Xu$$

  - Need to constrain u

$$||u||_2^2 = 1$$

$$u^T u = 1$$

PCA formulation

$$\max_u \ (Xu)^T Xu$$

$$\text{s.t. } u^T u = 1$$

- Solution:

$$X^T X u = \lambda u \qquad \lambda \in \mathbb{R}$$

- Known as an eigenvector problem
  - Note $X^T X$ is the covariance matrix of X

$$(X^T X)_{ij} = \mathbb{E}[X_{.i} X_{.j}]$$

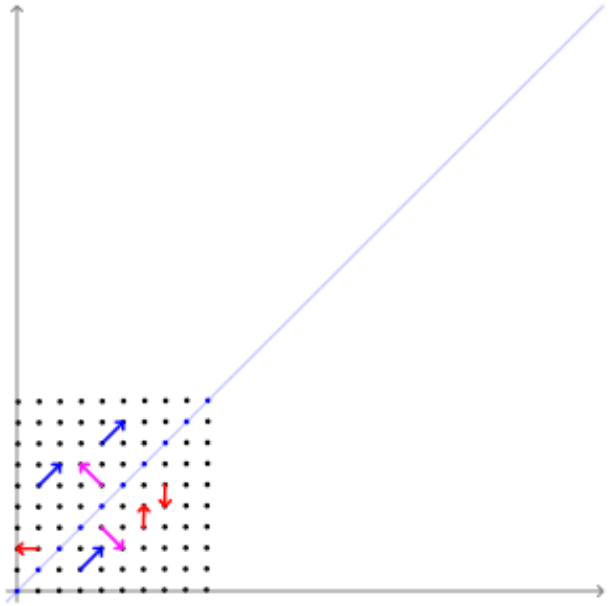
  - u is an eigenvector of $X^T X$
  - λ is the eigenvalue associated with u

- Assumption: X is zero mean. $\frac{1}{N} \sum_n X_{ni} = 0, \ \ \forall i$

Eigenvectors

- Linear transformation A doesn't change direction of v

$$Av = \lambda v$$



- Eigendecomposition (for real symmetric matrices)

$$A = U\Lambda U^T$$

U : orthonormal $\qquad$ Λ : diagonal

Back to PCA

$$X^T X u = \lambda u$$

- Which eigenvector u?

$$\mathrm{Var}(z) = (Xu)^T Xu$$

$$= \lambda$$

- Pick u with largest eigenvalue

- How do you pick the next principal components?
  - Find direction that maximizes variance
  - But uncorrelated with u
  - Pick u_2 orthogonal to u_1

    u_2 = eigenvector with second largest eigenvalue

  - Similarly for u_3, u_4, ...

Finding principal components

PCA

- Given input X_{NxD}
- Zero-mean and scale X (standardize)
- Reduce to M < D dimensions (U_{DxM})

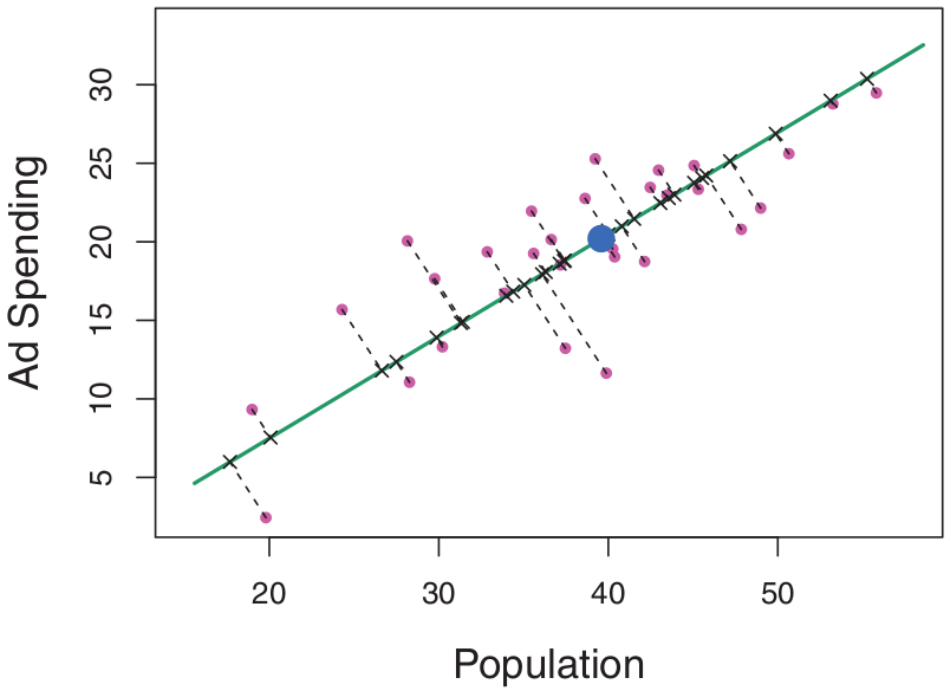
$$Z = XU$$

- Find eigenvectors of $X^T X$
- Pick the eigenvectors with largest M eigenvalues

- More efficient algorithms available
  - No need to calculate the full eigendecomposition
    - Only calculate M
  - If D >> N, calculate using XX^T

An alternative perspective on PCA

- Maximizing variance = Minimizing reconstruction error
  - Find a low dimensional surface that is closest to samples
    - In terms of squared error
    - i.e., for 1D, find the line that minimizes error



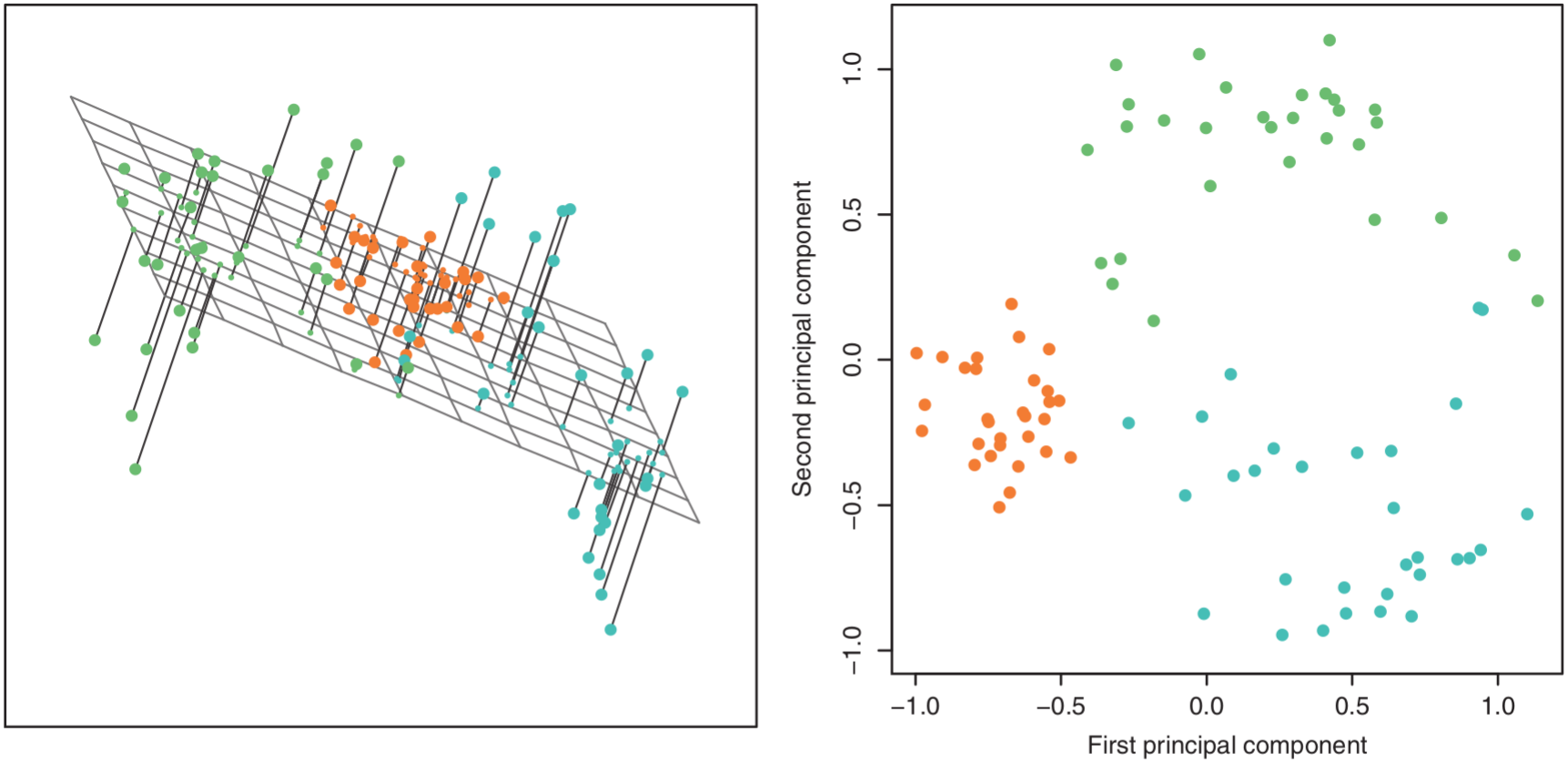


FIGURE 10.2. *Ninety observations simulated in three dimensions.* Left: *the first two principal component directions span the plane that best fits the data. It minimizes the sum of squared distances from each point to the plane.* Right: *the first two principal component score vectors give the coordinates of the projection of the 90 observations onto the plane. The variance in the plane is maximized.*

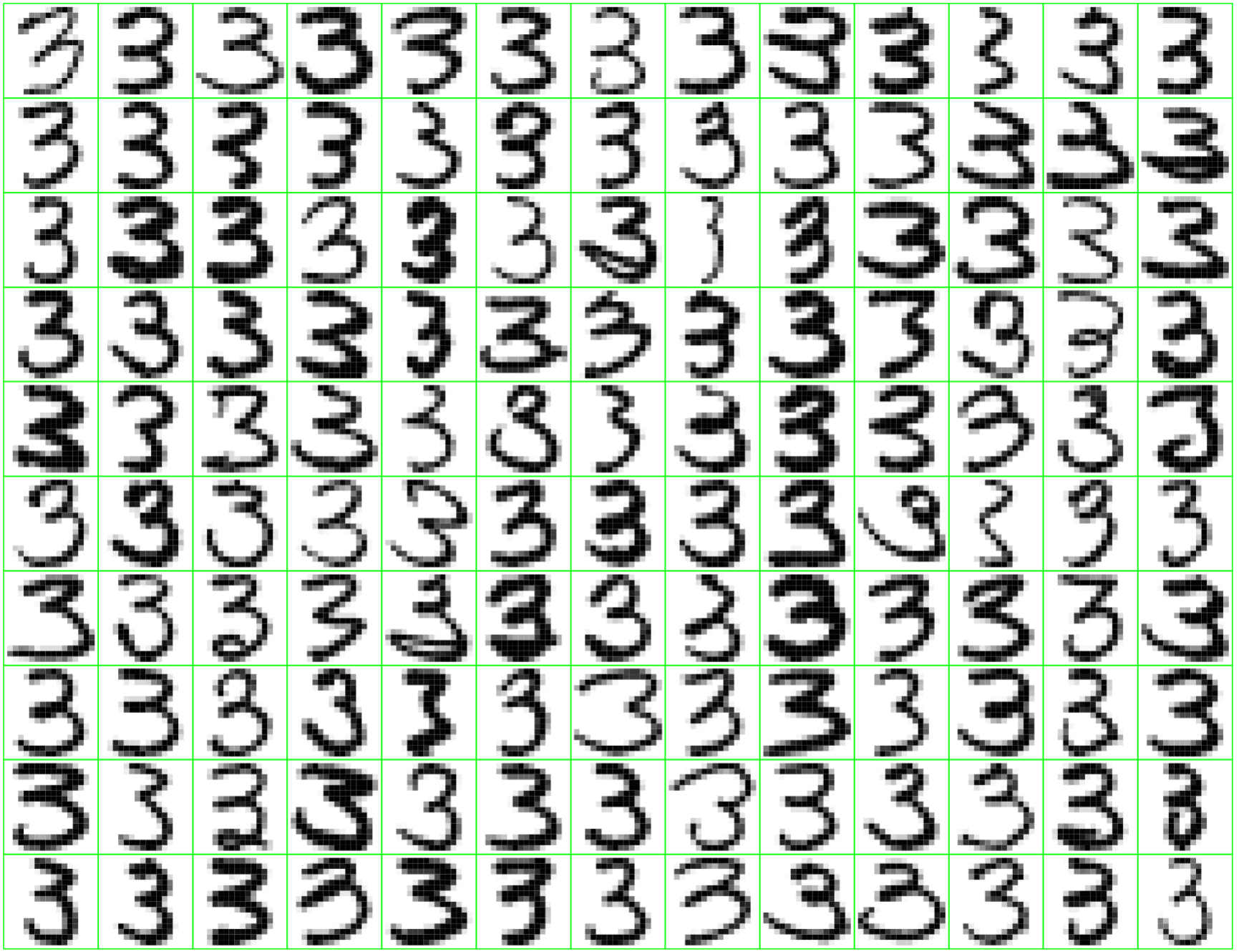


FIGURE 14.22. *A sample of* 130 *handwritten 3's shows a variety of writing styles.*

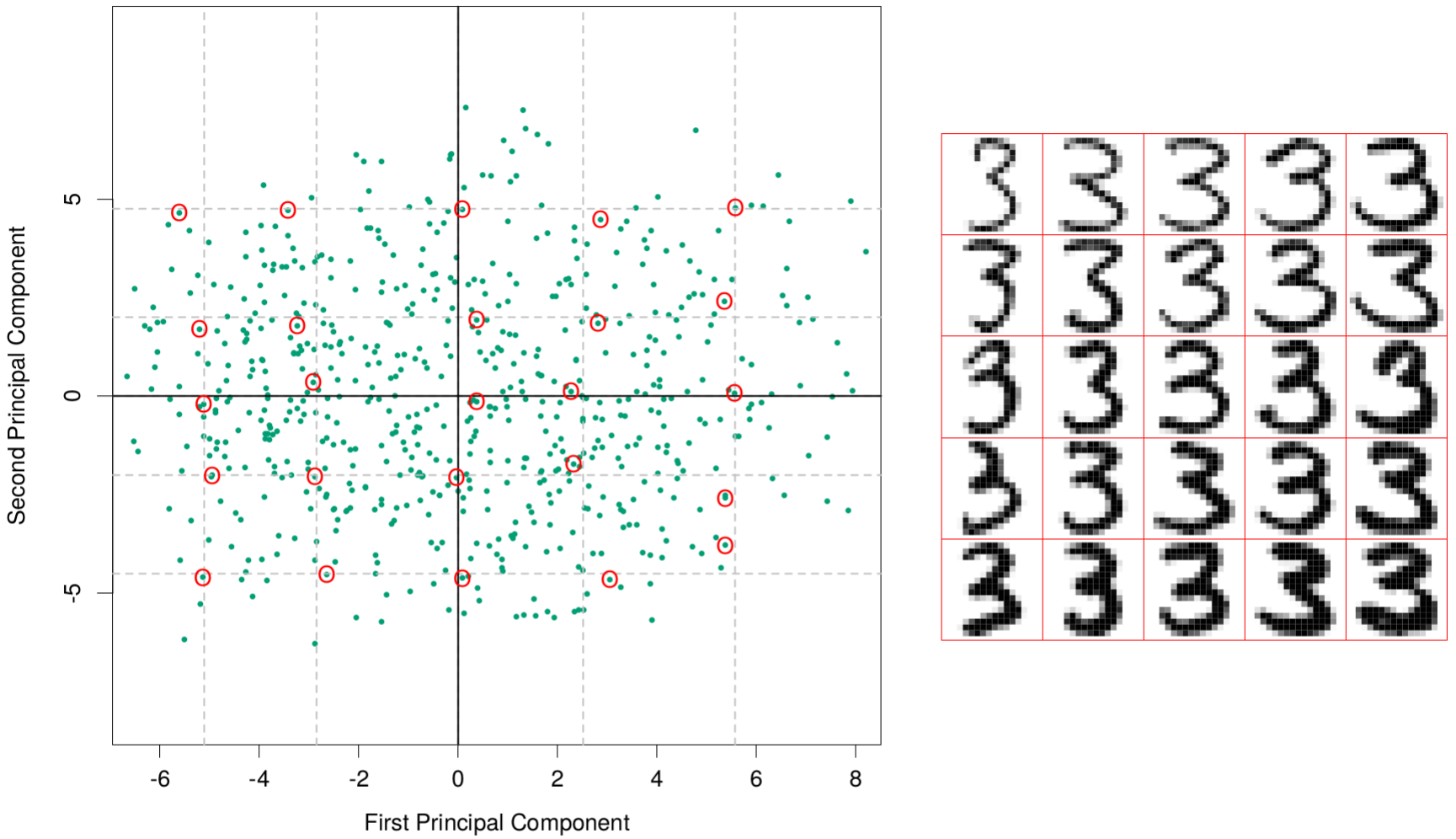


FIGURE 14.23. *(Left panel:) the first two principal components of the handwritten threes. The circled points are the closest projected images to the vertices of a grid, defined by the marginal quantiles of the principal components. (Right panel:) The images corresponding to the circled points. These show the nature of the first two principal components.*

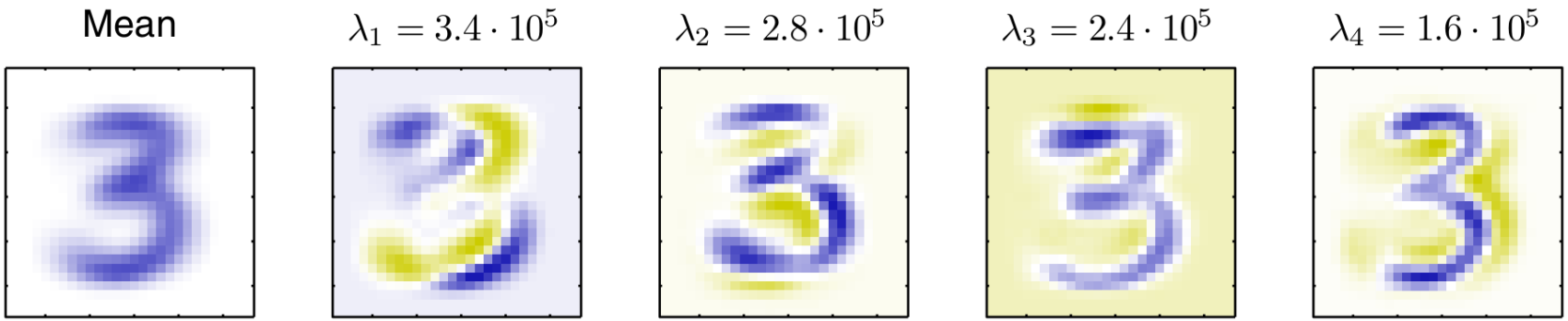


Figure 12.3 The mean vector $\overline{\mathbf{x}}$ along with the first four PCA eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_4$ for the off-line digits data set, together with the corresponding eigenvalues.

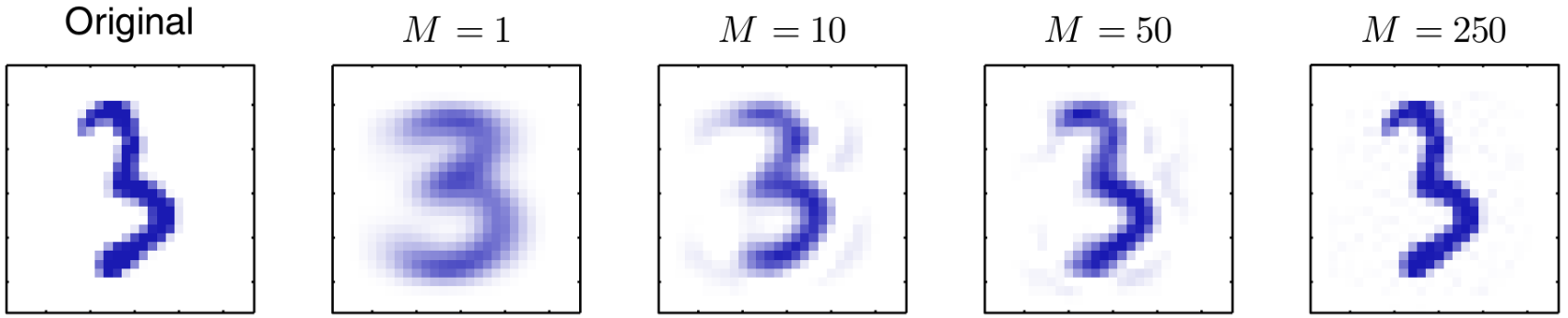


Figure 12.5 An original example from the off-line digits data set together with its PCA reconstructions obtained by retaining M principal components for various values of M. As M increases the reconstruction becomes more accurate and would become perfect when $M = D = 28 \times 28 = 784$.

Proportion of variance explained

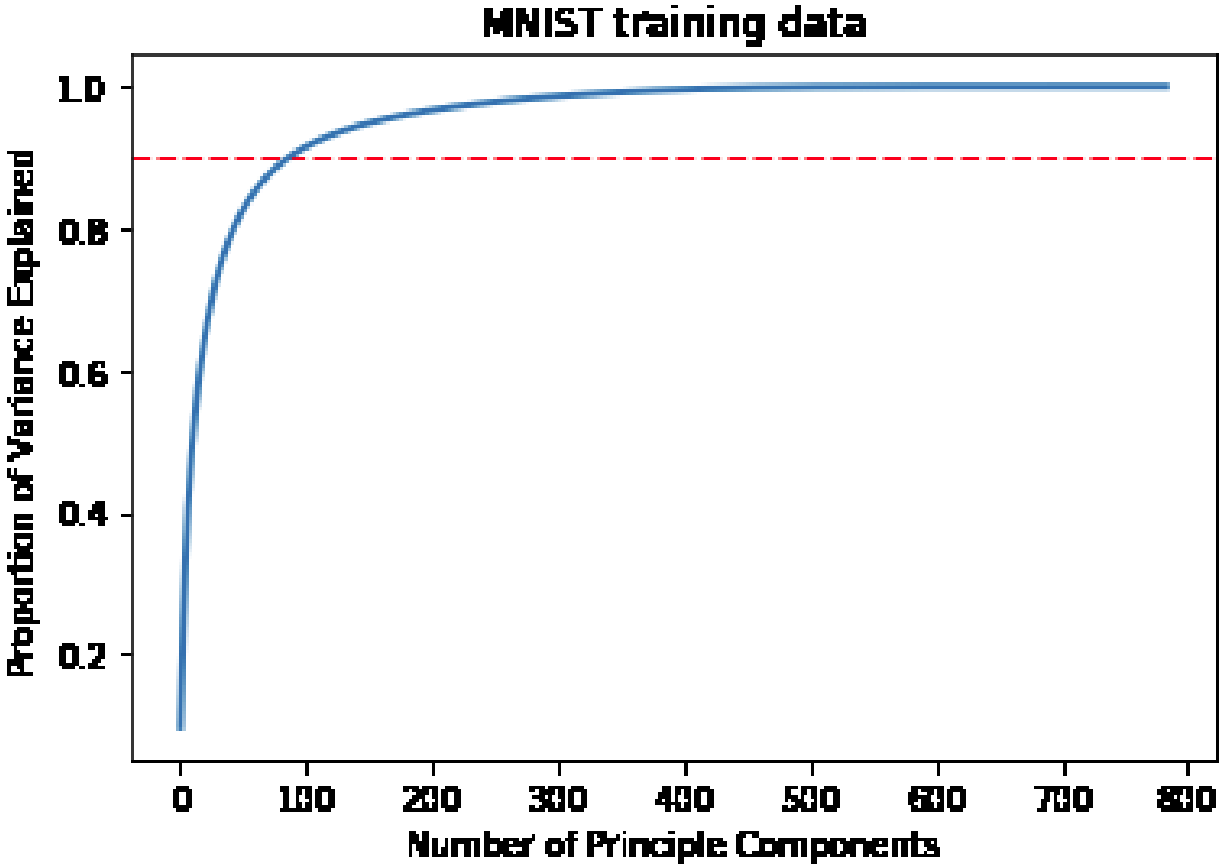
- What should M be?
- Remember

$$\mathrm{Var}(z_m) = \mathrm{Var}((Xu_m^T)Xu_m) = \lambda_m$$

- Total variance: $\sum_{m=1}^{D} \lambda_m$
- Explained variance: $\sum_{m=1}^{M} \lambda_m$

- Proportion of explained variance:

$$\frac{\sum_{m=1}^{M} \lambda_m}{\sum_{m=1}^{D} \lambda_m}$$


MNIST training data
Proportion of Variance Explained
1.0
0.8
0.6
0.4
0.2
0
100
200
300
400
500
600
700
800
Number of Principle Components

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Whitening (sphering)

- Standardize inputs
  - Zero-mean, unit variance
  - But features can be correlated

- Whitening removes correlations
  - De-correlates input data

$$\tilde{X} = XU\Lambda^{-1/2}$$

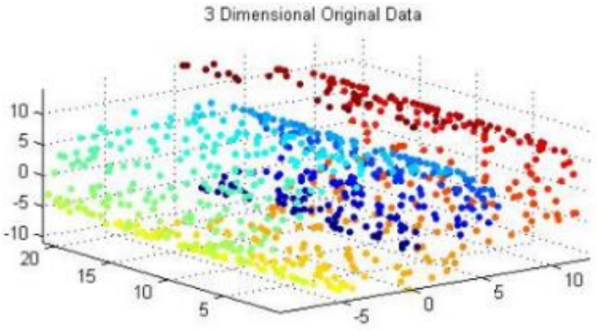
  - Uncorrelated features

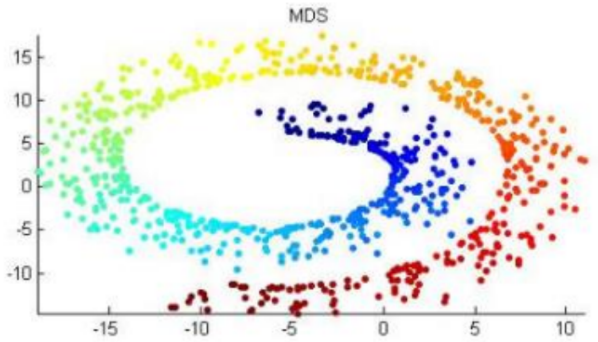
$$\mathrm{Cov}[\tilde{X}] = \mathbf{I}$$

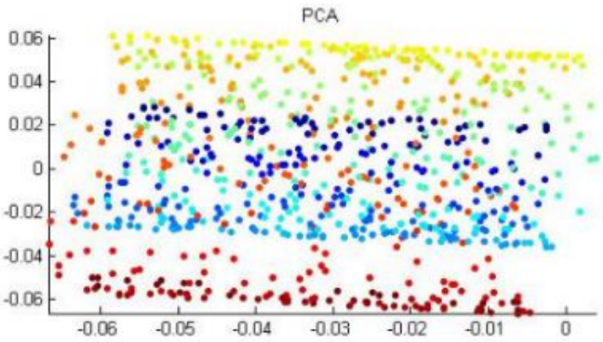
- Feed $\tilde{X}$ instead of X into supervised technique

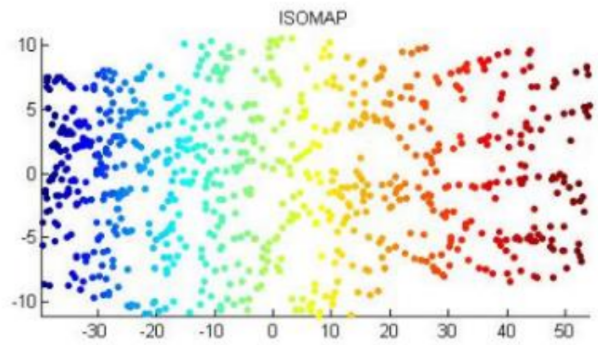
Beyond PCA

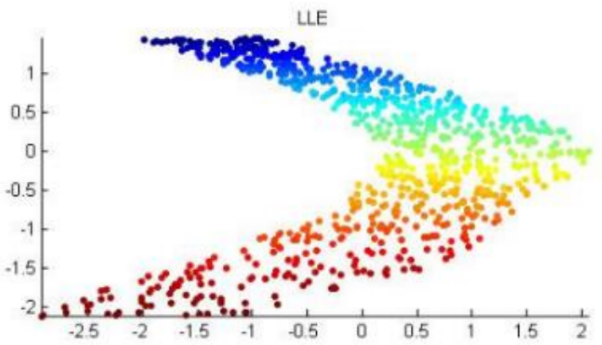
- Many non-linear dimensionality reduction techniques
  - Kernel PCA
  - ISOMAP
  - t-SNE
  - Locally linear embedding
  - Spectral clustering

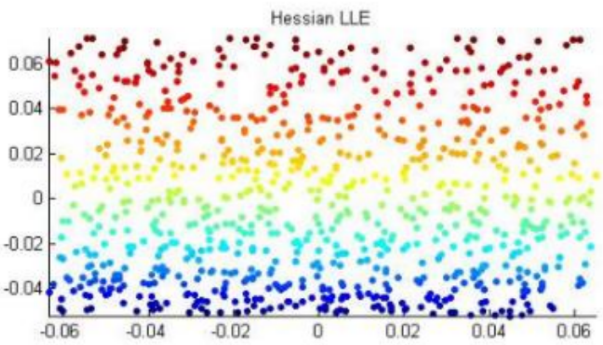












Summary

- Dimensionality reduction
- Principal components analysis
  - Formulation: maximize variance
  - Minimize reconstruction error
  - Proportion of variance explained
- Beyond PCA

- Exercises
  - Show that the direction that maximizes variance is the eigenvector of covariance matrix with largest eigenvalue
  - Do lab 10.4 in ISLR

References

[1]James, Witten, Hastie, and Tibshirani. An Introduction to Statistical Learning with Applications in R. Chapter 10.

[2] Hastie, Tibshirani, and Friedman. The Elements of Statistical Learning. Chapter 14.

[3] Bishop, C. Pattern Recognition and Machine Learning. Chapter 12

[4] LeCun, Y.

[5] http://statweb.stanford.edu/~tibs/sta306bfiles/isomap.pdf

[6] https://www.researchgate.net/figure/PCA-of-MNIST-FIG-4-PCA-of-not-MNIST_fig2_320517142