Introduction to Machine Learning

Lecture 10
Unsupervised Learning I

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Types of learning problems

Supervised learning

Learning from supervision (i.e., teacher)

Given inputs and **outputs**, learn a function that maps input → output

Examples:

- Recognizing faces
- Predicting the sales for a product
- Learning to rank search results

Unsupervised learning

Learning with no supervision

Given only inputs, extract some pattern from the data.

Examples:

- Clustering (market segmentation)
- Dimensionality reduction (visualization)
- Generating celebrity faces

Reinforcement learning

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.

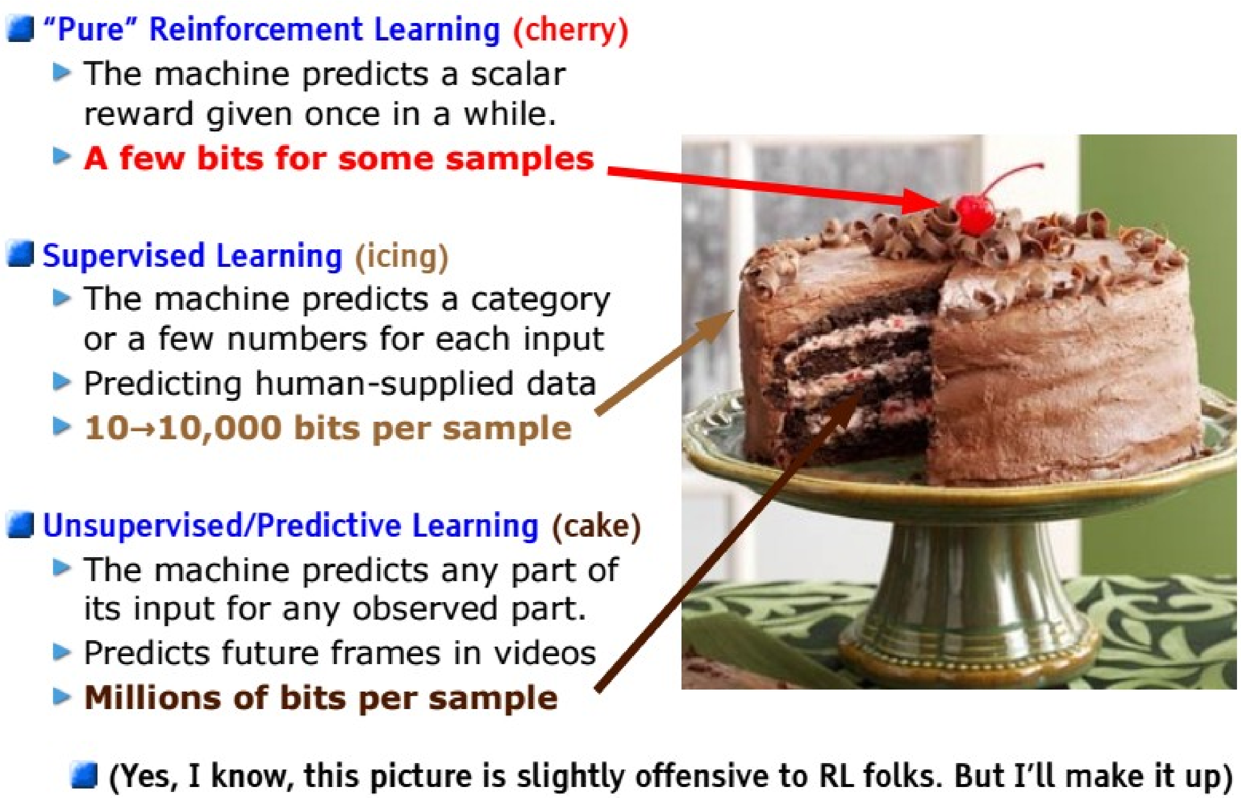
Needs to learn a *policy* to maximize reward.

Examples:

- 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



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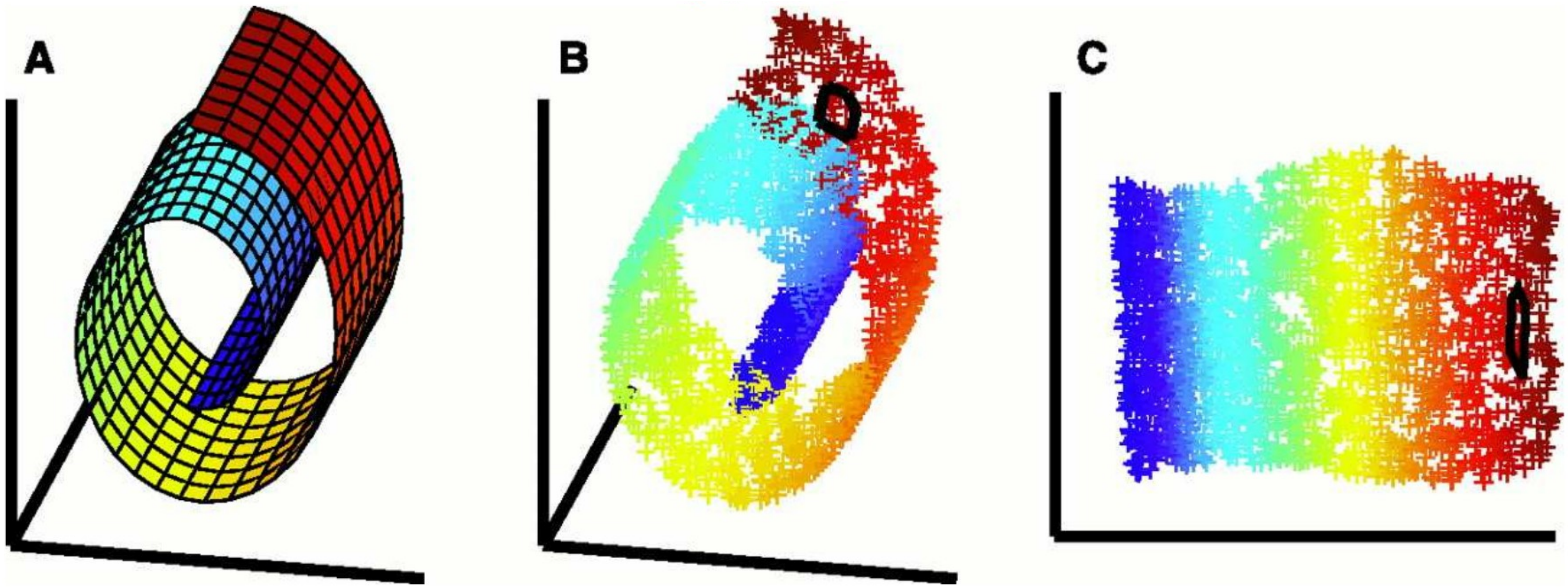
Dimensionality reduction

- 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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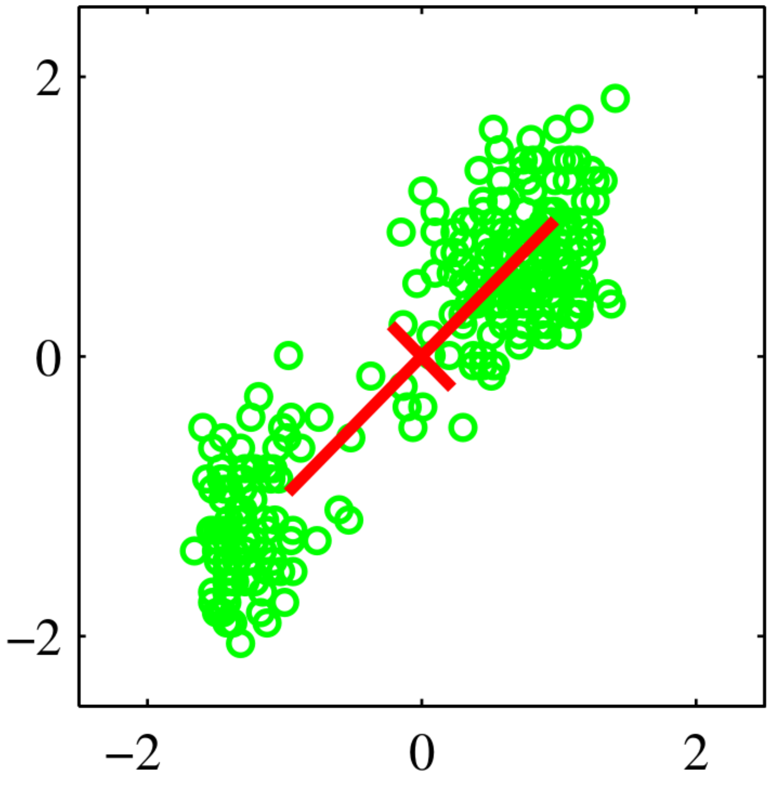
Principal components analysis (PCA)

- 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)

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

$$z = Xu$$

  - Find direction (u) that maximizes variance

$$\max_u \sum_n z_n^2$$

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

  - Need to constrain u

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

$$u^T u = 1$$

Terminology:
u: loading vector
z: principal component

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

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

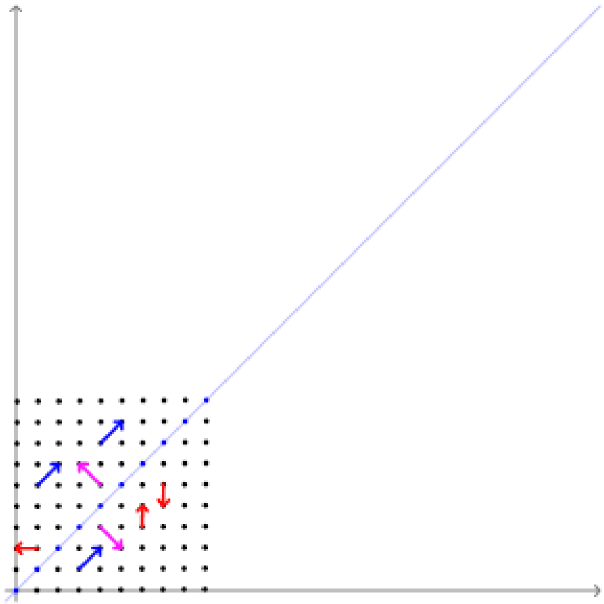
  - u is an eigenvector of $X^T X$
  - λ is the eigenvalue associated with u

- 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)

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

$$U : \text{orthonormal} \qquad \Lambda : \text{diagonal}$$

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

$\boxed{u_2 = \text{eigenvector with second largest eigenvalue}}$

  - 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})

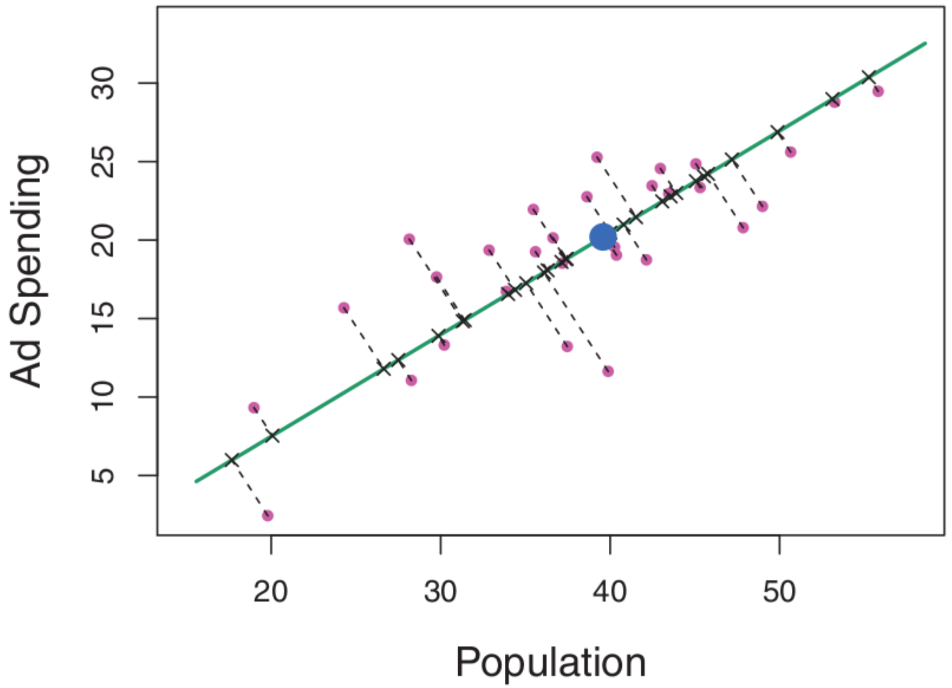
$$Z = XU$$

- 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



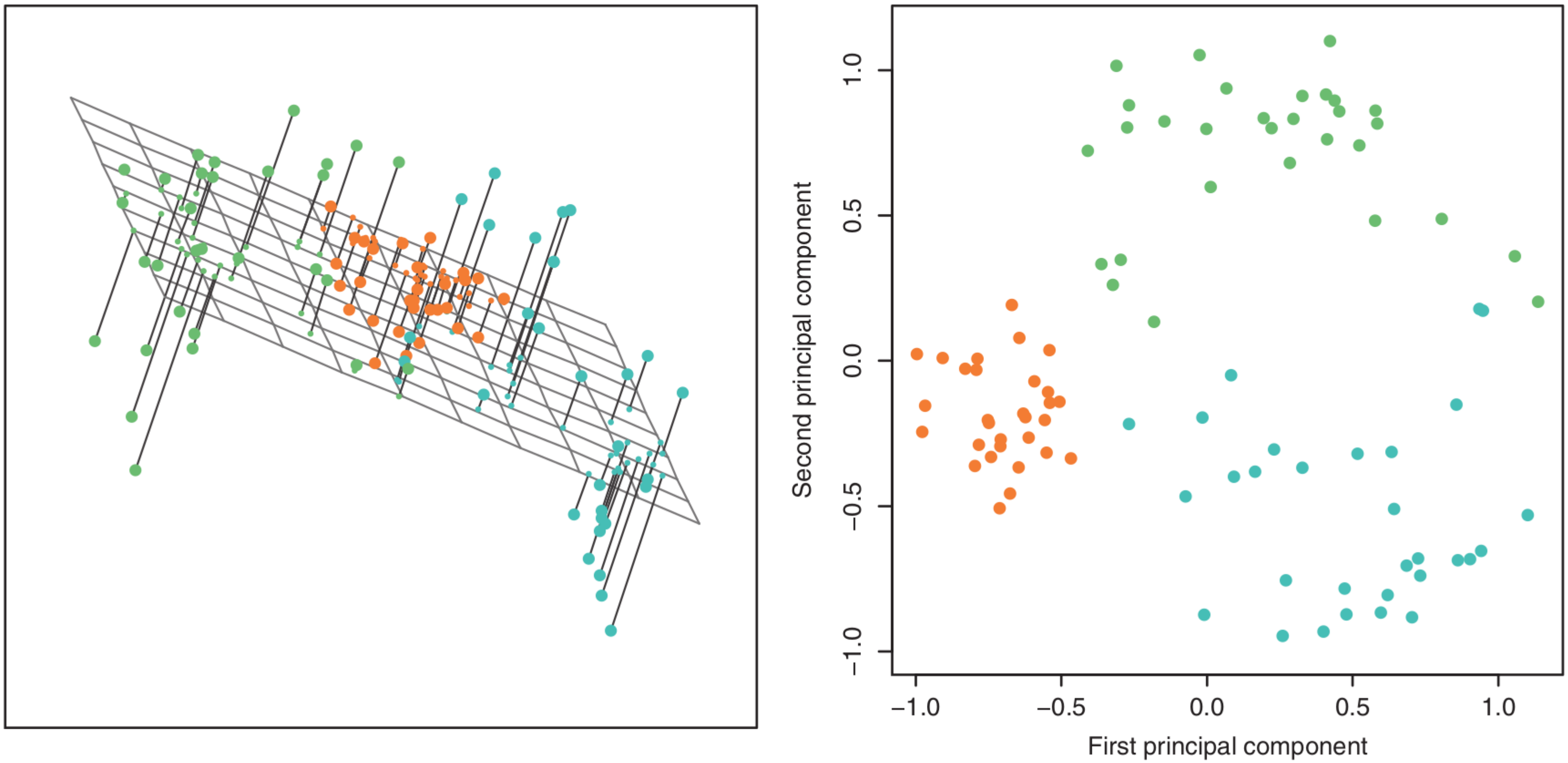


FIGURE 10.2. *Ninety observations simulated in three dimensions.* Left: *the first two principal component directions span the plane that best fits the data. It minimizes the sum of squared distances from each point to the plane.* Right: *the first two principal component score vectors give the coordinates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

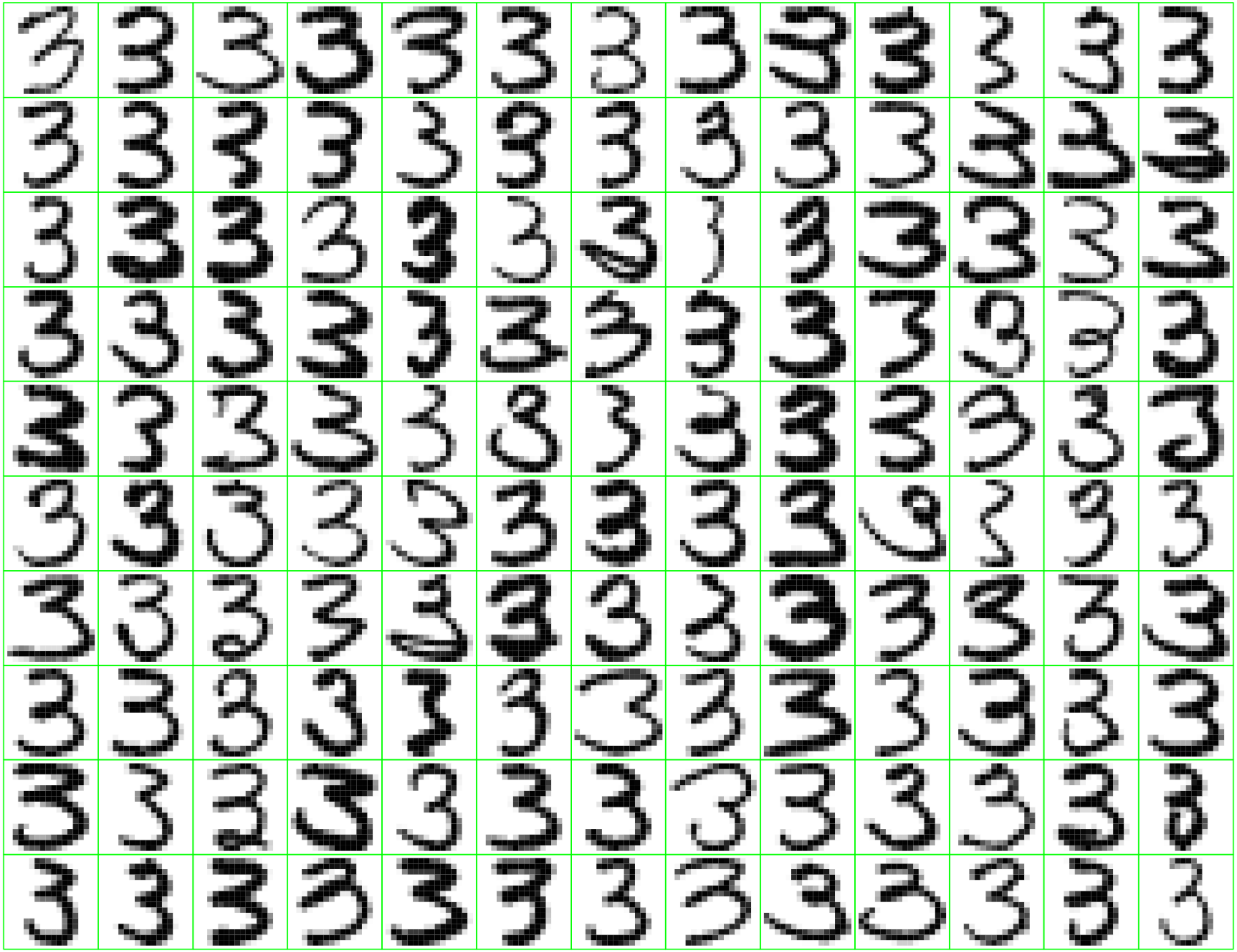


FIGURE 14.22. *A sample of* 130 *handwritten 3's shows a variety of writing styles.*

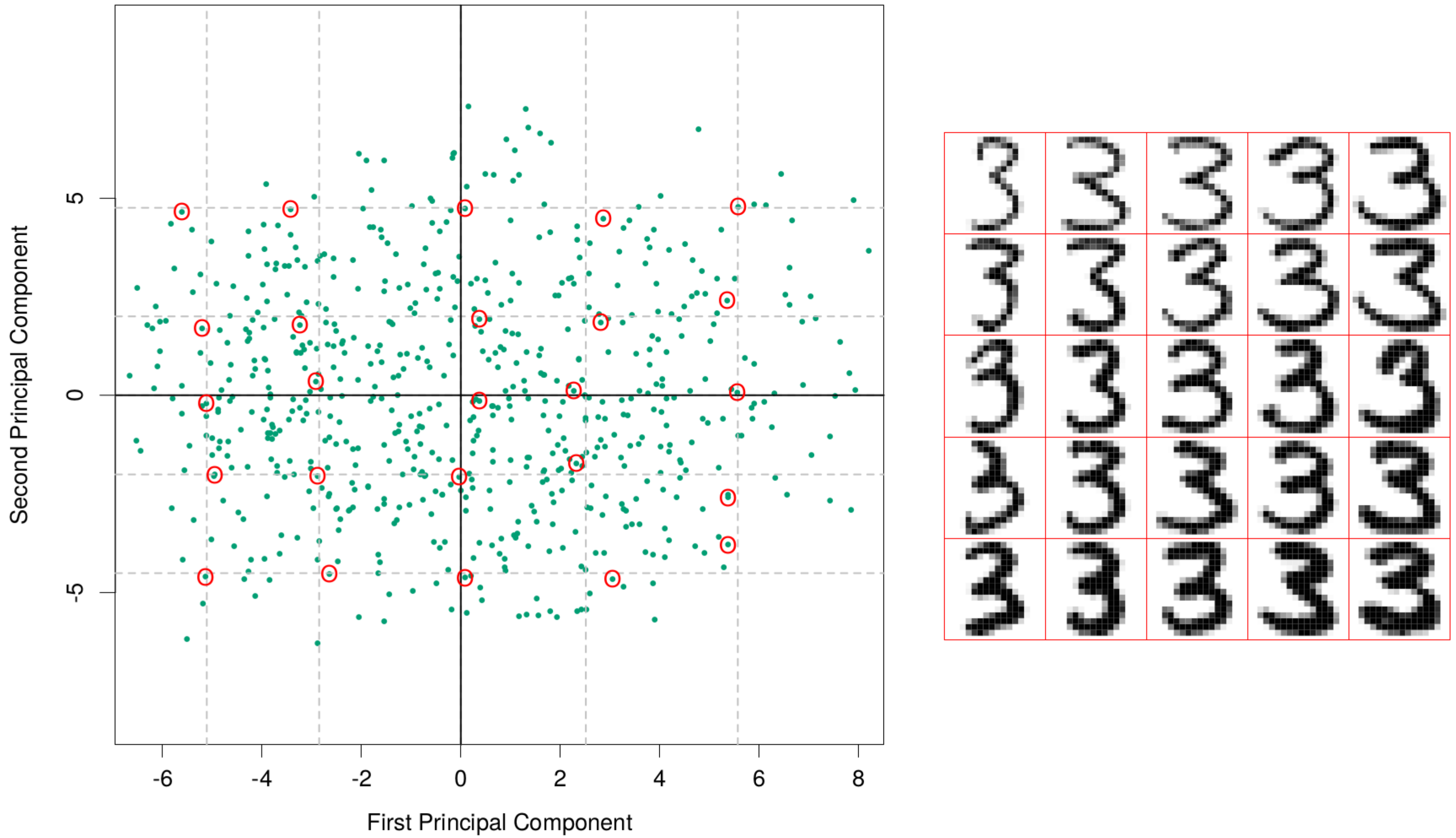


FIGURE 14.23. *(Left panel:) the first two principal components of the handwritten threes. The circled points are the closest projected images to the vertices of a grid, defined by the marginal quantiles of the principal components. (Right panel:) The images corresponding to the circled points. These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

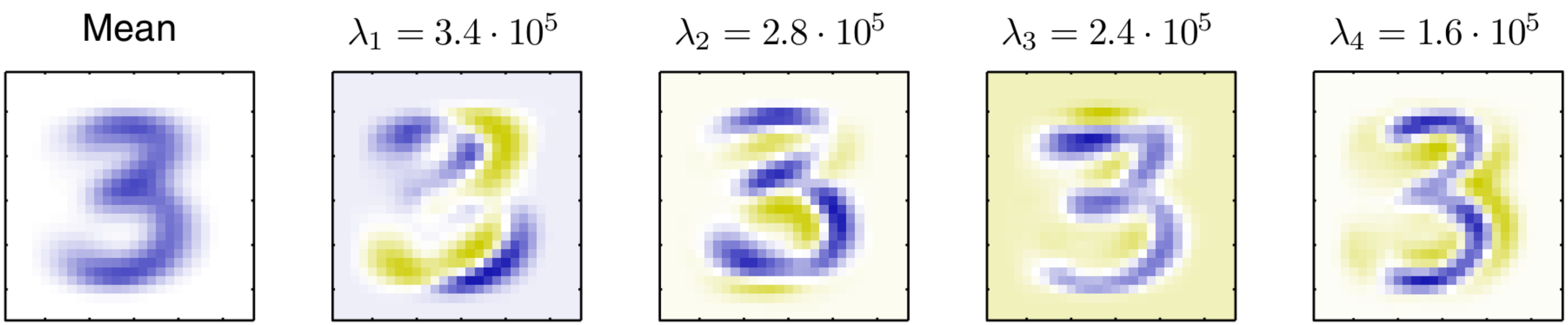


Figure 12.3 The mean vector $\overline{\mathbf{x}}$ along with the first four PCA eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_4$ for the off-line digits data set, together with the corresponding eigenvalues.

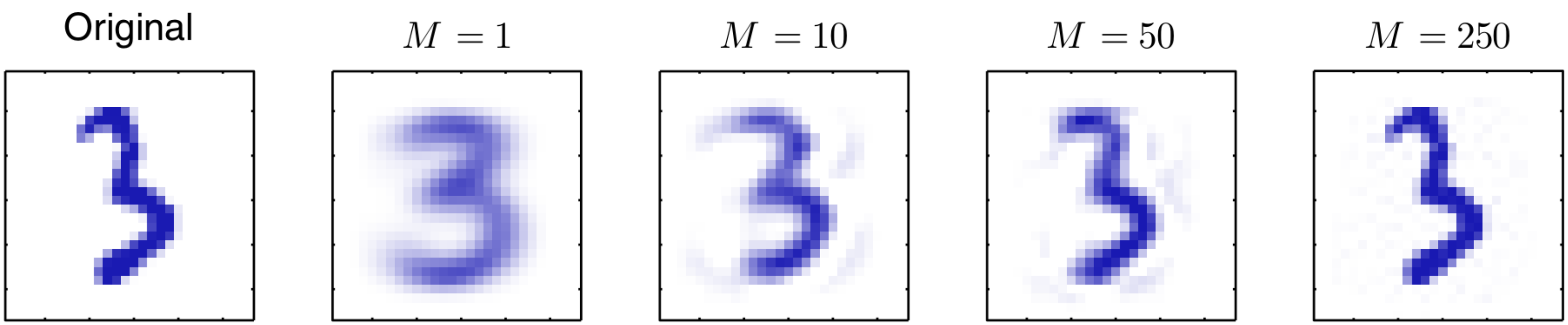


Figure 12.5 An original example from the off-line digits data set together with its PCA reconstructions obtained by retaining M principal components for various values of M. As M increases the reconstruction becomes more accurate and would become perfect when $M = D = 28 \times 28 = 784$.

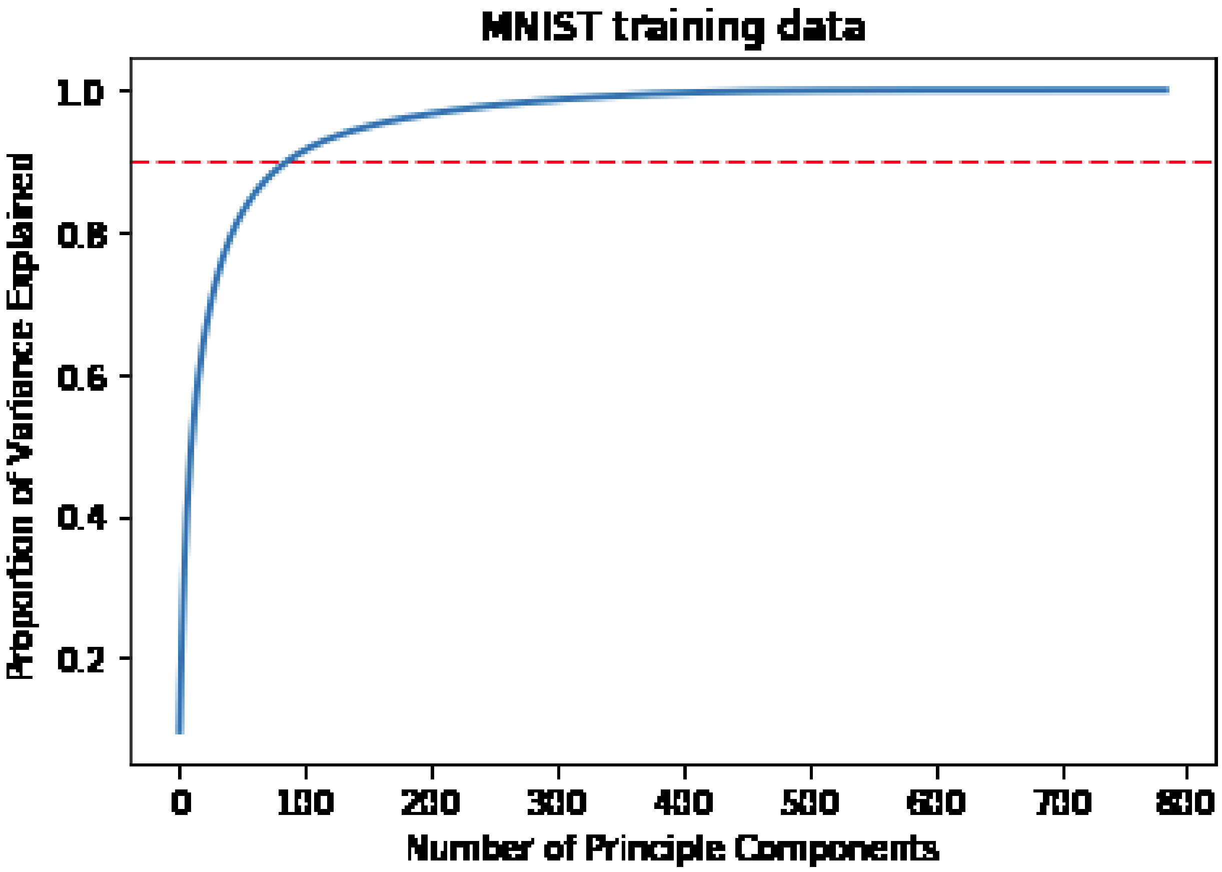
Proportion of variance explained

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

[6]

Whitening (sphering)

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

- Whitening removes correlations
  - De-correlates input data

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

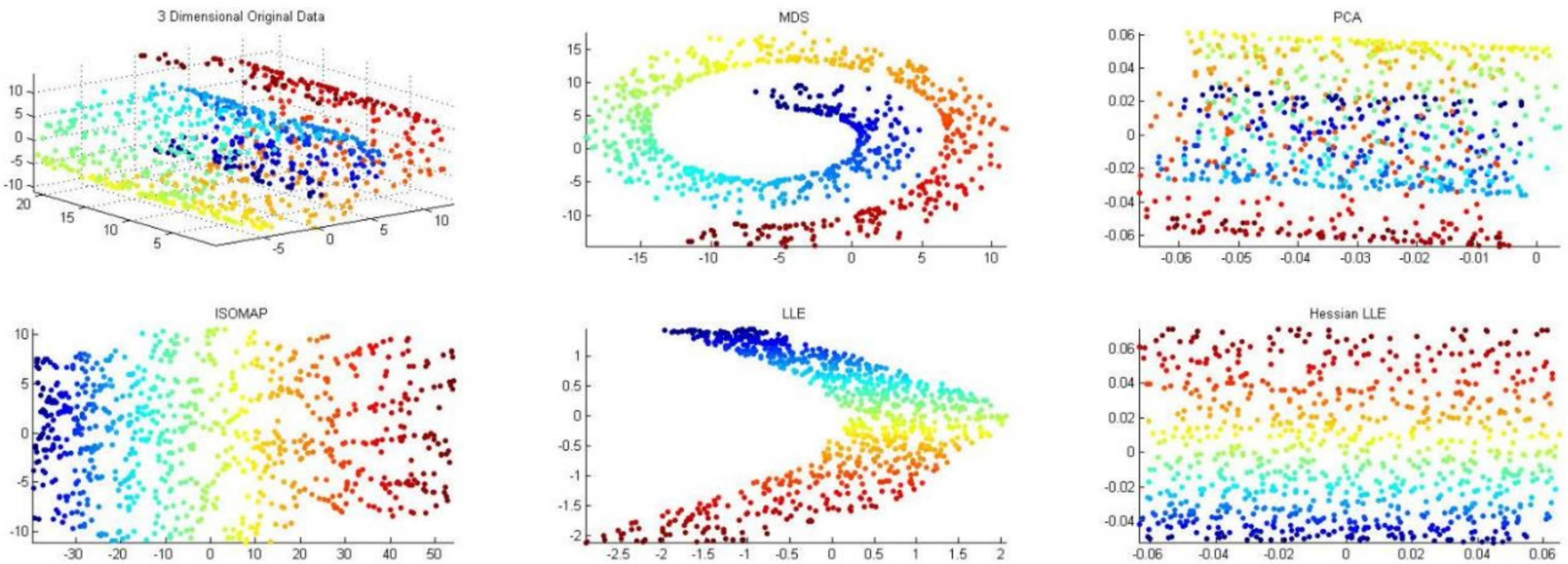
  - Uncorrelated features

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

- 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