Learning From Data
Lecture 27
Learning Aides

Input Preprocessing
Dimensionality Reduction and Feature Selection
Principal Components Analysis (PCA)
Hints, Data Cleaning, Validation, ...

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CSCI 4100/6100

Learning Aides

Additional tools that can be applied to all techniques

Preprocess data to account for arbitrary choices during data collection (input normalization)

Remove irrelevant dimensions that can mislead learning (PCA)

Incorporate known properties of the target function (hints and invariances)

Remove detrimental data (deterministic and stochastic noise)

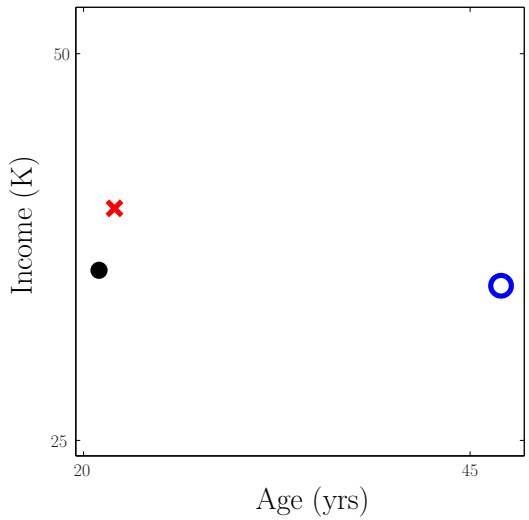
Better ways to validate (estimate E_{out}) for model selection

Nearest Neighbor

Mr. Good and Mr. Bad were both given credit cards by the Bank of Learning (BoL).

	Mr. Good	Mr. Bad
(Age in years, Income in $\$ \times 1,000$)	(47,35)	(22,40)

Mr. Unknown who has "coordinates" (21yrs,\$36K) applies for credit. Should the BoL give him credit, according to the nearest neighbor algorithm?

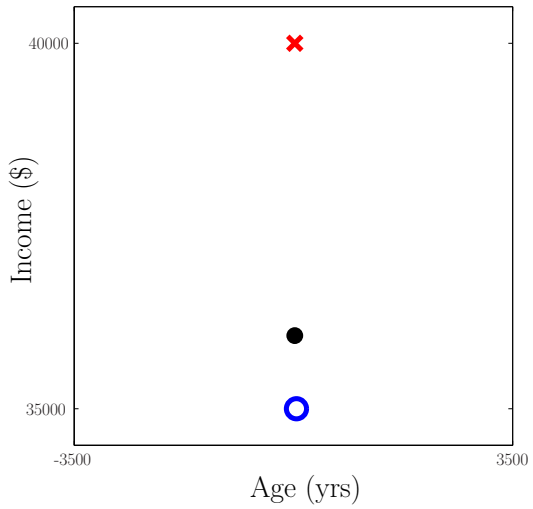


Nearest Neighbor Uses Euclidean Distance

Mr. Good and Mr. Bad were both given credit cards by the Bank of Learning (BoL).

	Mr. Good	Mr. Bad
(Age in years, Income in $)	(47,35000)	(22,40000)

Mr. Unknown who has "coordinates" (21yrs,$36000) applies for credit. Should the BoL give him credit, according to the nearest neighbor algorithm?
What if, income is measured in dollars instead of "K" (thousands of dollars)?



Uniform Treatment of Dimensions

Most learning algorithms treat each dimension equally

Nearear neighbor: $d(\mathbf{x}, \mathbf{x}') = \| \mathbf{x} - \mathbf{x}' \|$

Weight Decay: $\Omega(\mathbf{w}) = \lambda \mathbf{w}^{\mathrm{T}} \mathbf{w}$

SVM: margin defined using Euclidean distance

RBF: bump function decays with Euclidean distance

Input Preprocessing

Unless you want to emphasize certain dimensions, the data should be *preprocessed* to present each dimension on an equal footing

Input Preprocessing is a Data Transform

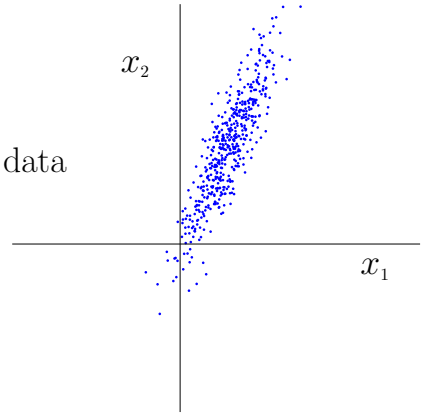
$$\mathrm{X} = \begin{bmatrix} — & \mathbf{x}_1^{\mathrm{T}} & — \\ — & \mathbf{x}_2^{\mathrm{T}} & — \\ & \vdots & \\ — & \mathbf{x}_{\mathrm{N}}^{\mathrm{T}} & — \end{bmatrix} \qquad \mathbf{x}_n \mapsto \mathbf{z}_n$$

$$g(\mathbf{x}) = \tilde{g}(\Phi(\mathbf{x})).$$

Raw $\{\mathbf{x}_n\}$ have (for example) arbitrary scalings in each dimension, and $\{\mathbf{z}_n\}$ will not.

Centering

raw data



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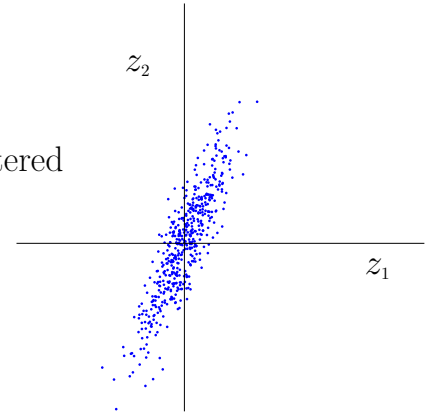
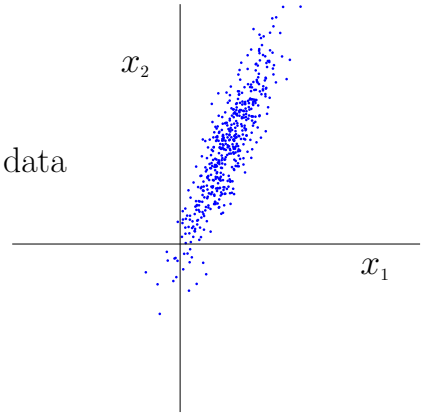


$$\mathbf{z}_n = \mathbf{x}_n - \bar{\mathbf{x}}$$

$$\bar{\mathbf{z}} = \mathbf{0}$$

Normalizing

raw data



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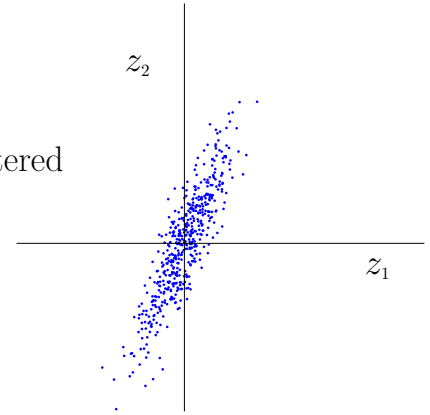
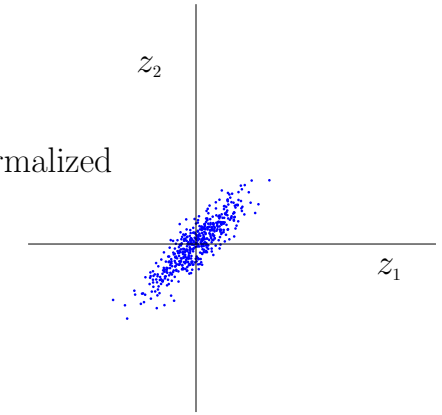


normalized



$$\mathbf{z}_n = \mathbf{x}_n - \bar{\mathbf{x}}$$

$$\mathbf{z}_n = \mathrm{D}\mathbf{x}_n$$

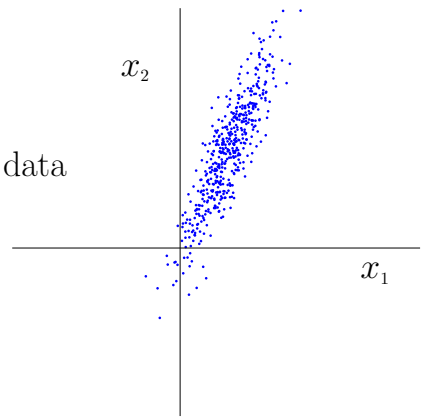
$$D_{ii} = \frac{1}{\sigma_i}$$

$$\bar{\mathbf{z}} = \mathbf{0}$$

$$\tilde{\sigma}_i = 1$$

Whitening

raw data



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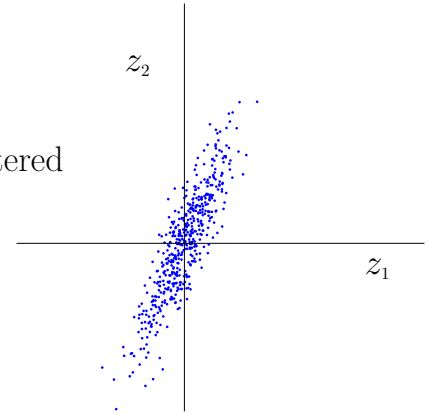
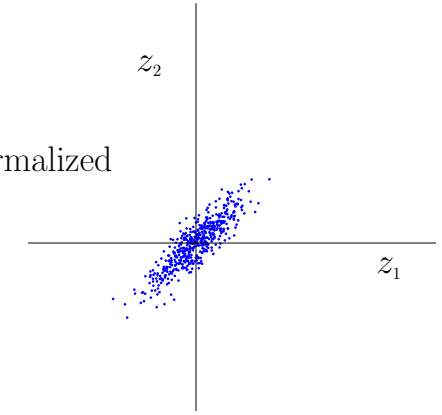
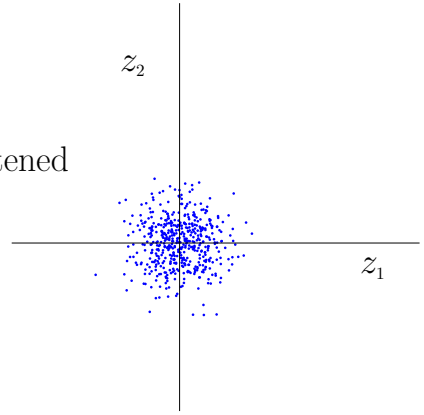


normalized



whitened



$$\mathbf{z}_n = \mathbf{x}_n - \bar{\mathbf{x}} \qquad \mathbf{z}_n = \mathrm{D}\mathbf{x}_n \qquad \mathbf{z}_n = \Sigma^{-\frac{1}{2}}\mathbf{x}_n$$

$$D_{ii} = \frac{1}{\sigma_i} \qquad \Sigma = \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n\mathbf{x}_n^{\mathrm{T}} = \frac{1}{N}\mathrm{X}^{\mathrm{T}}\mathrm{X}$$

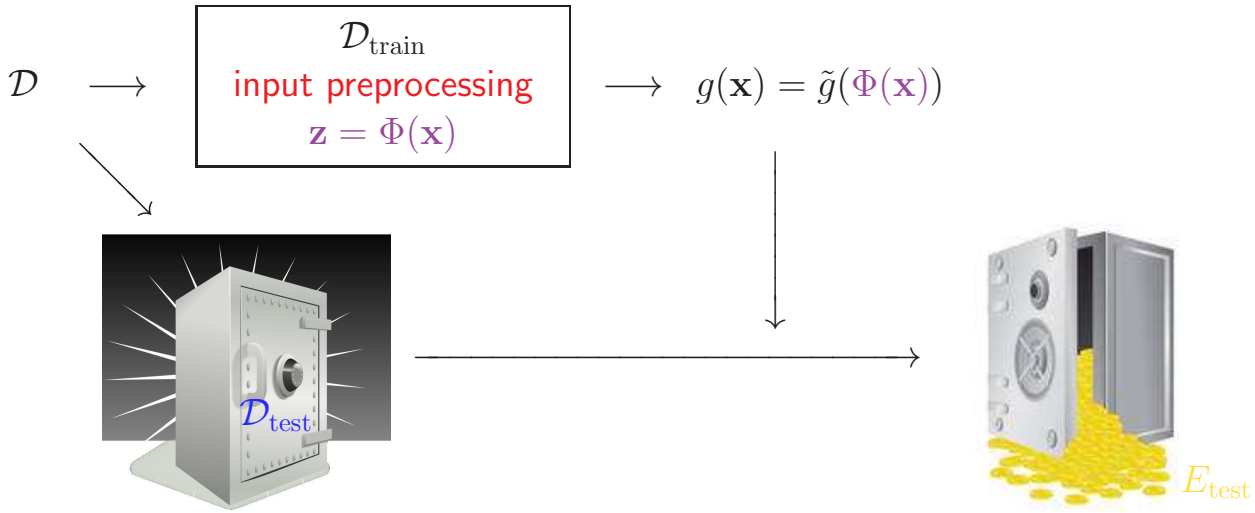
$$\bar{\mathbf{z}} = \mathbf{0} \qquad \tilde{\sigma}_i = 1 \qquad \widetilde{\Sigma} = \frac{1}{N}\mathrm{Z}^{\mathrm{T}}\mathrm{Z} = \mathrm{I}$$

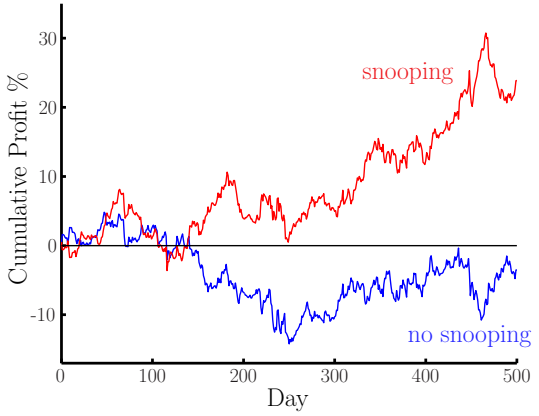
Only Use Training Data For Preprocessing

WARNING!

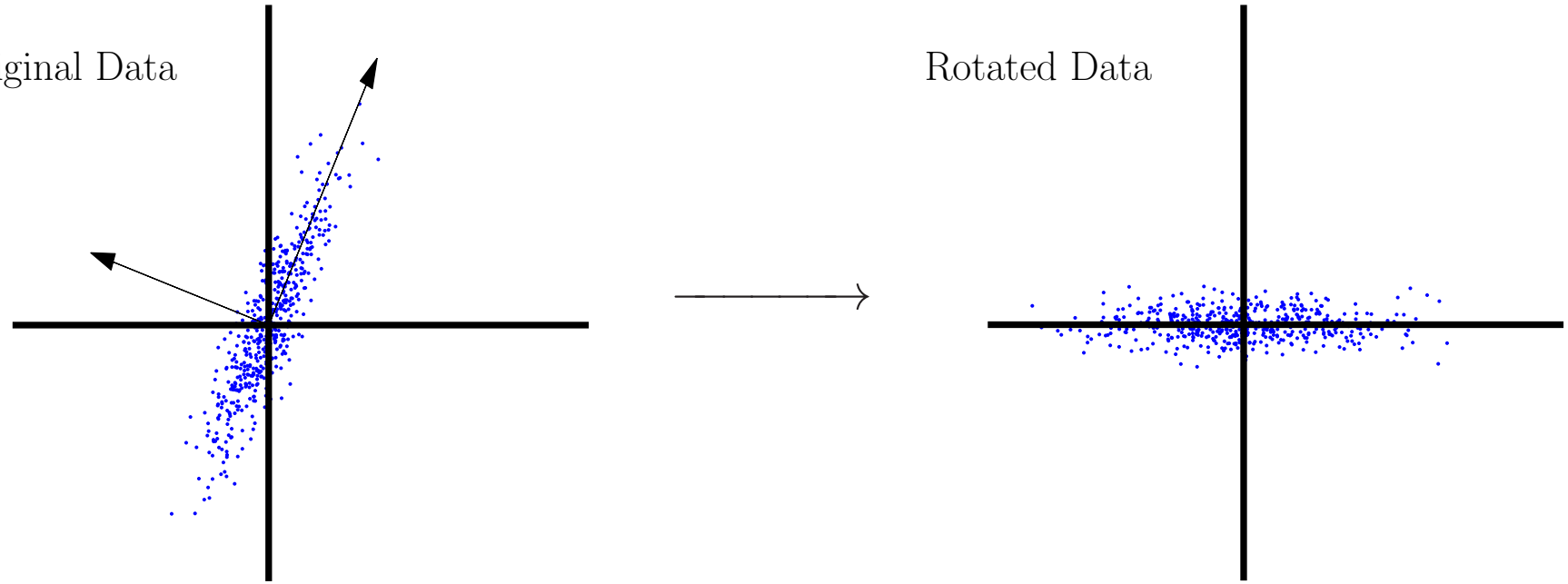
Transforming data into a more convenient format has a hidden trap which leads to data snooping.

When using a test set, determine the input transformation from training data *only*.
Rule: lock away the test data until you have your final hypothesis.





Principal Components Analysis



Rotate the data so that it is easy to

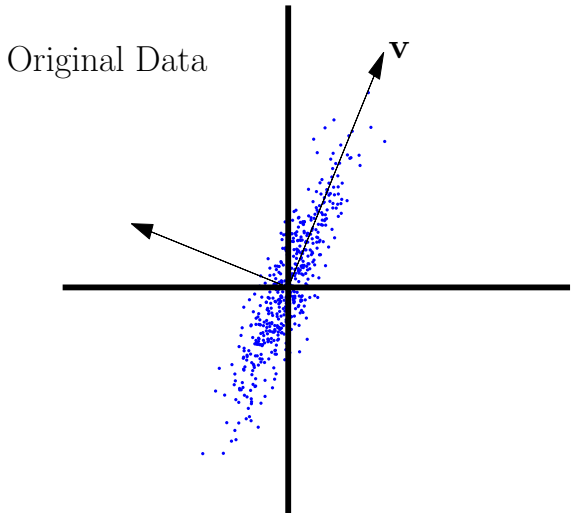
- Identify the dominant directions (information)
- Throw away the smaller dimensions (noise)

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \rightarrow \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} \rightarrow \begin{bmatrix} z_1 \end{bmatrix}$$

Projecting the Data to Maximize Variance

(Always center the data first)

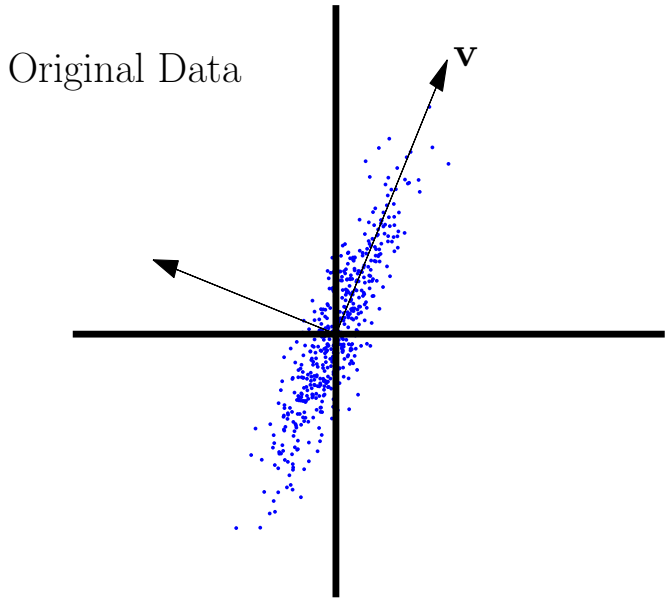
$$z = \mathbf{x}_n^{\mathrm{T}}\mathbf{v}$$



Find $\mathbf{v}$ to maximize the variance of z

Maximizing the Variance

$$
\begin{aligned}
\mathsf{var}[z] &= \frac{1}{N}\sum_{n=1}^{N} z_n^2 \\
&= \frac{1}{N}\sum_{n=1}^{N} \mathbf{v}^{\mathrm{T}}\mathbf{x}_n\mathbf{x}_n^{\mathrm{T}}\mathbf{v} \\
&= \mathbf{v}^{\mathrm{T}}\left(\frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n\mathbf{x}_n^{\mathrm{T}}\right)\mathbf{v} \\
&= \mathbf{v}^{\mathrm{T}}\Sigma\mathbf{v}.
\end{aligned}
$$



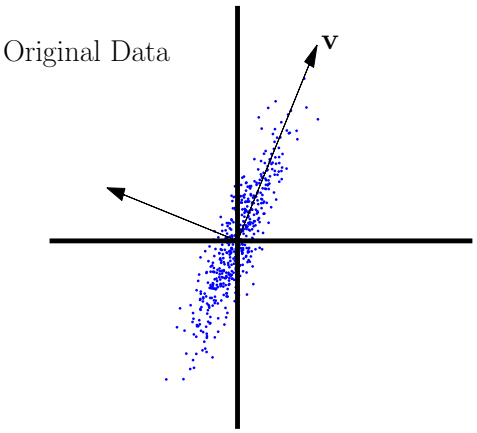
Choose $\mathbf{v}$ as $\mathbf{v}_1$, the top eigenvector of Σ — the top principal component (PCA)

The Principal Components

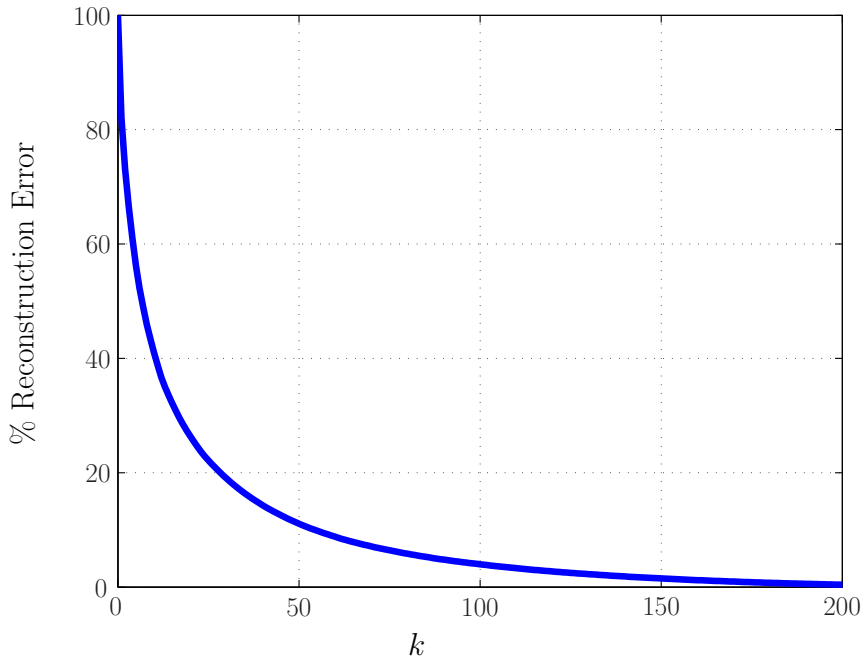
$$
\begin{aligned}
z_1 &= \mathbf{x}^{\mathrm{T}}\mathbf{v}_1 \\
z_2 &= \mathbf{x}^{\mathrm{T}}\mathbf{v}_2 \\
z_3 &= \mathbf{x}^{\mathrm{T}}\mathbf{v}_3 \\
&\vdots
\end{aligned}
$$

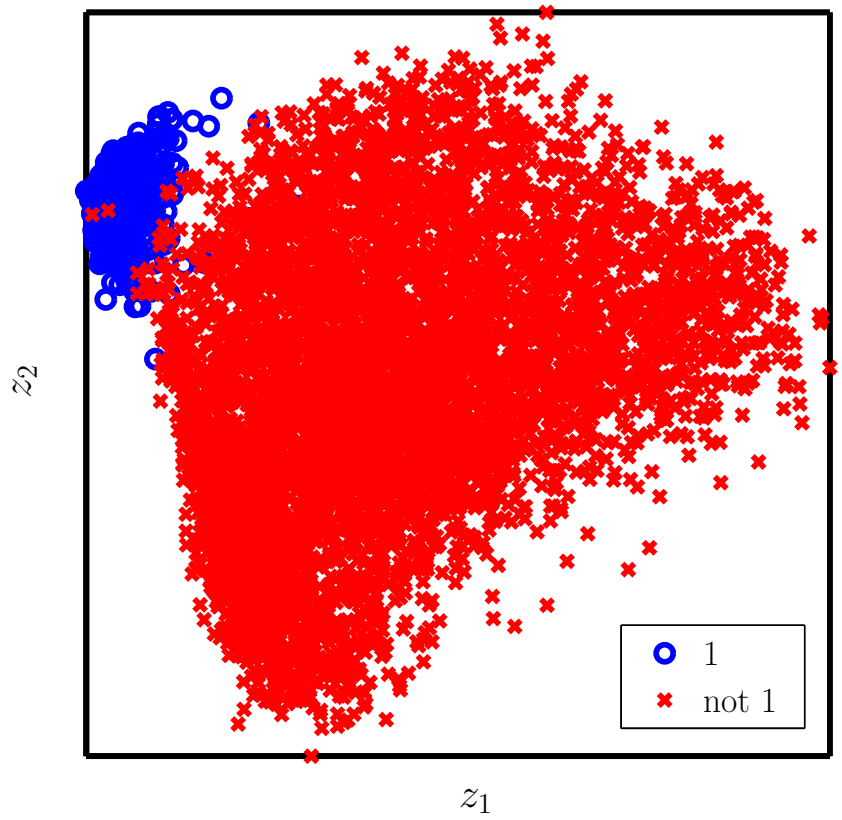
$\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_d$ are the eigenvectors of Σ with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_d$

Theorem [Eckart-Young]. These directions give best reconstruction of data; also capture maximum variance.



PCA Features for Digits Data



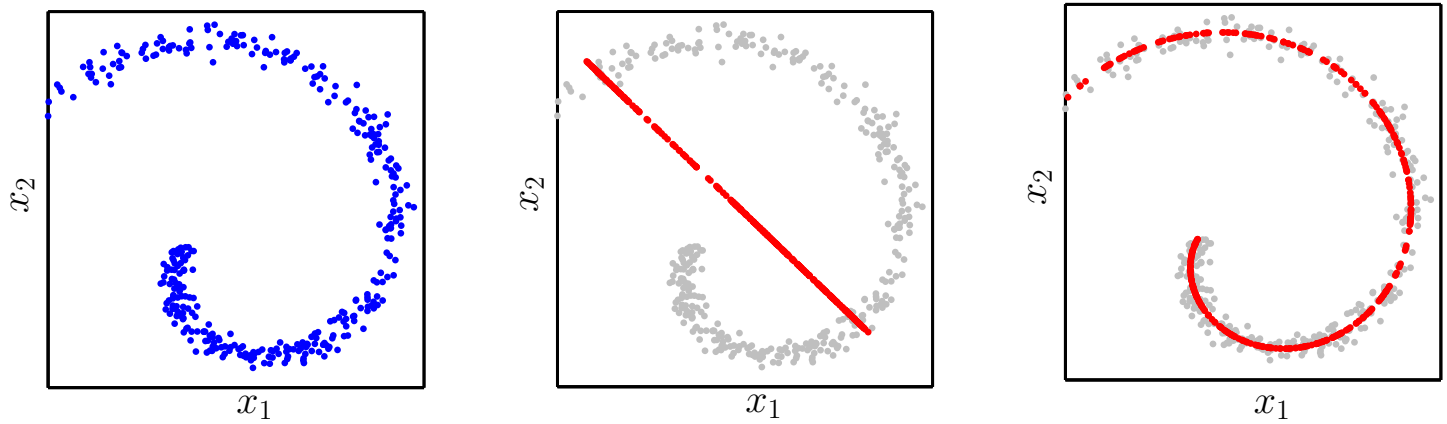


Principal components are **automated**

- Captures dominant directions of the data.
- May not capture dominant dimensions for f.

Other Learning Aides

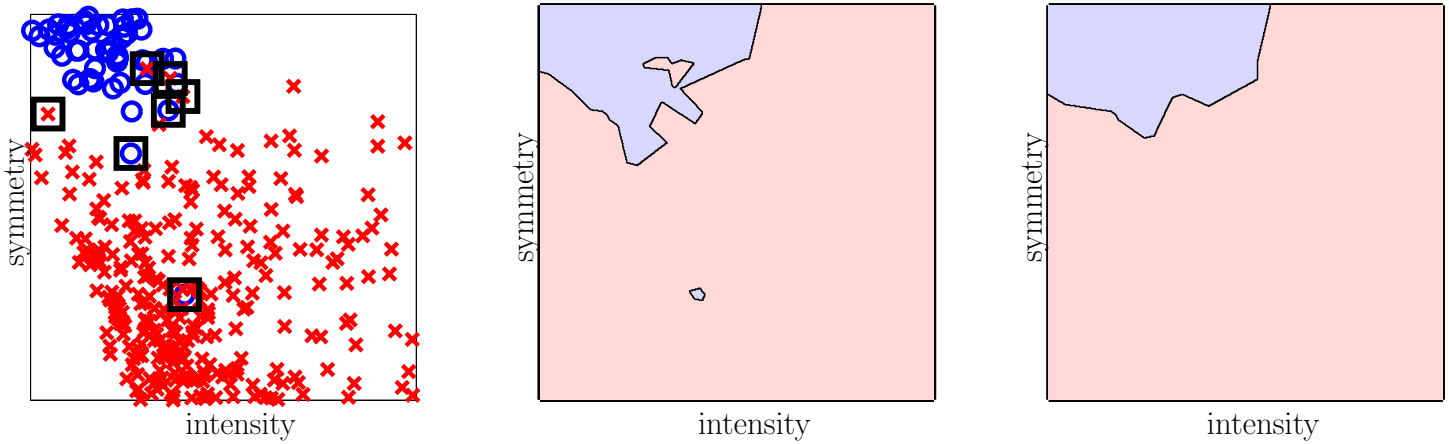
1. **Nonlinear dimension reduction:**



2. **Hints (invariances and prior information):**

   rotational invariance, monotonicity, symmetry, ...

3. **Removing noisy data:**



4. **Advanced validation techniques:** Rademacher and Permutation penalties

   More efficient than CV, more convenient and accurate than VC.