PSY9511: Seminar 5

Unsupervised learning

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Outline

1. Overview of unsupervised learning
2. Clustering
    - K-means
    - Hierarchical
3. Dimensionality reduction
    - Principal component analysis (PCA)
    - Independent component analysis (ICA)
    - Partial least squares (PLS)

Unsupervised learning

Unsupervised learning: Motivation

Supervised learning: Find $\hat{y} = f(X)$

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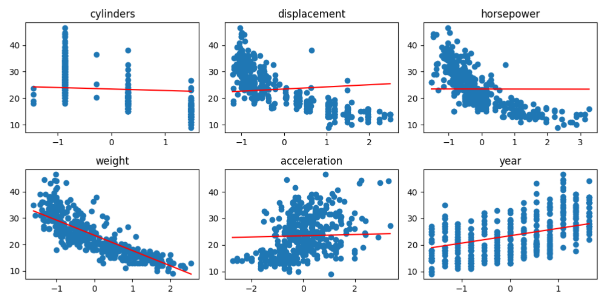
- Descriptive: Understand the relationship between X and y



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- Predictive: Predict y given new X.

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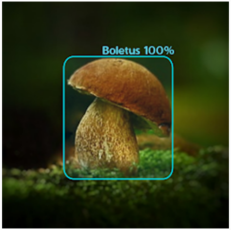

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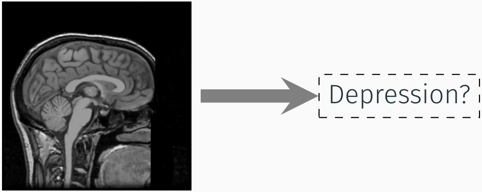

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Unsupervised learning: Are there some interesting patterns in X?

- Can we find subgroups or interesting axes of variability?
- Visualization

Dimensionality reduction

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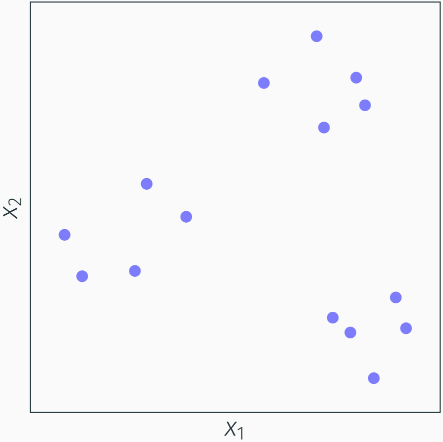

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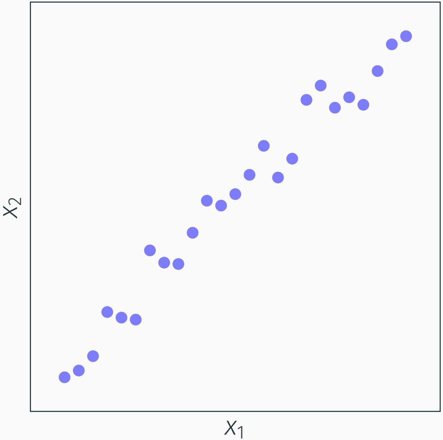

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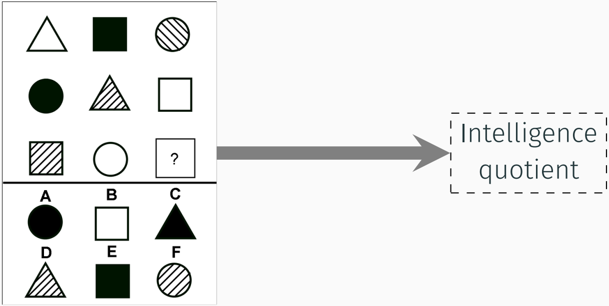

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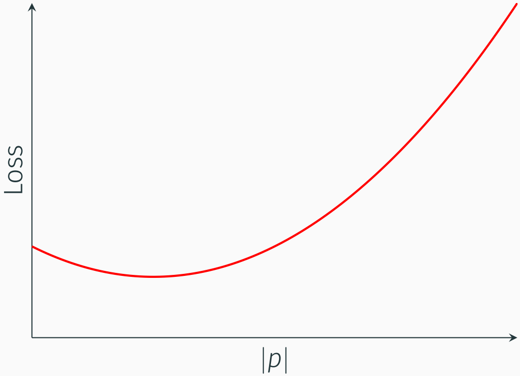

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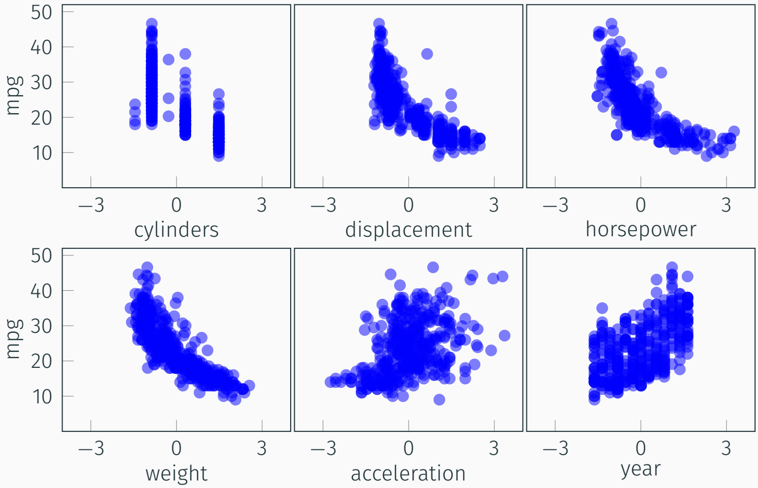

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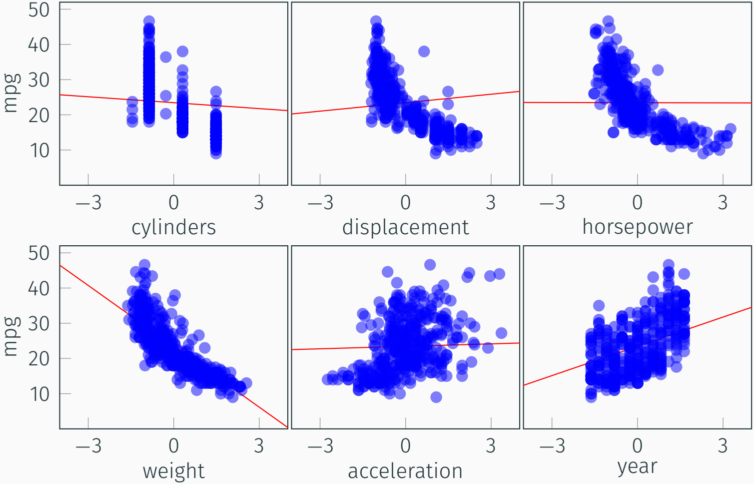

Dimensionality reduction: Motivation

1	0.30	0.86	0.89	0.41	0.93
0.30	1	0.41	0.34	0.29	0.36
0.86	0.41	1	0.84	0.68	0.89
0.89	0.34	0.84	1	0.50	0.95
0.41	0.29	0.68	0.50	1	0.54
0.93	0.36	0.89	0.95	0.54	1

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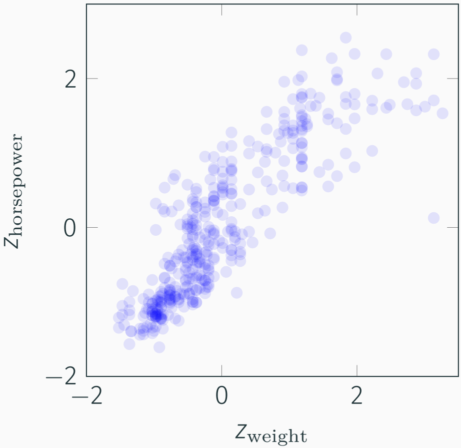
Dimensionality reduction: Principal component analysis



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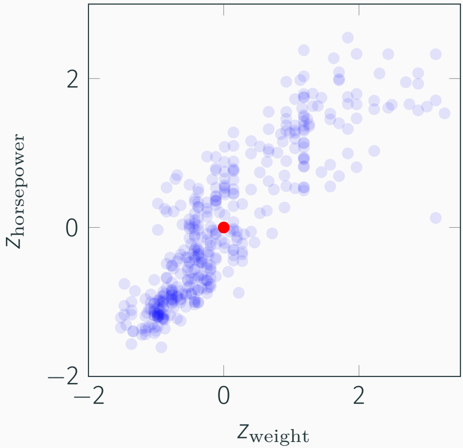
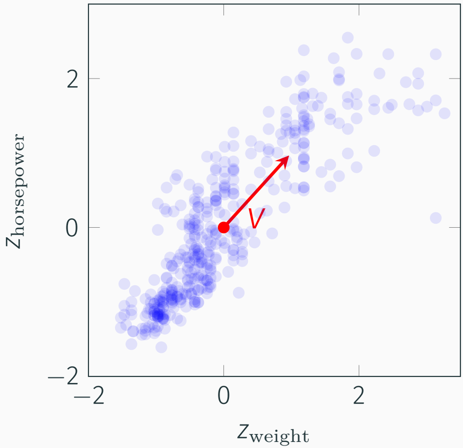


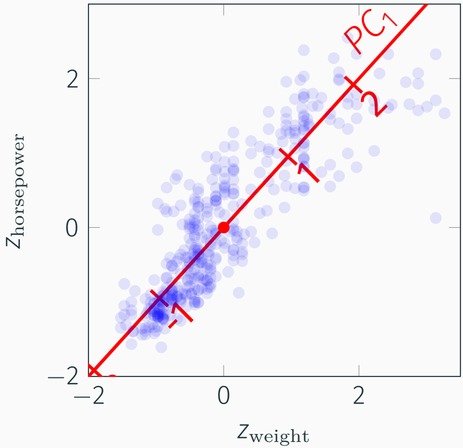
$c \rightarrow$ center of the data

Dimensionality reduction: Principal component analysis



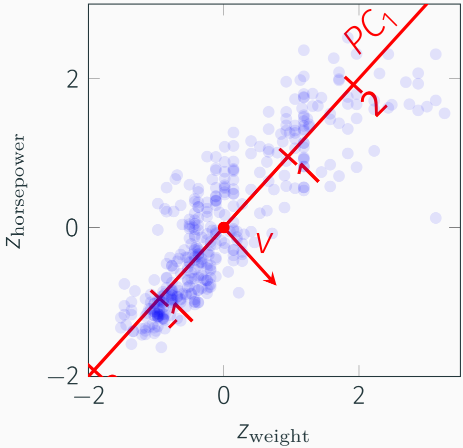
$v \rightarrow$ direction of maximum variance

Dimensionality reduction: Principal component analysis



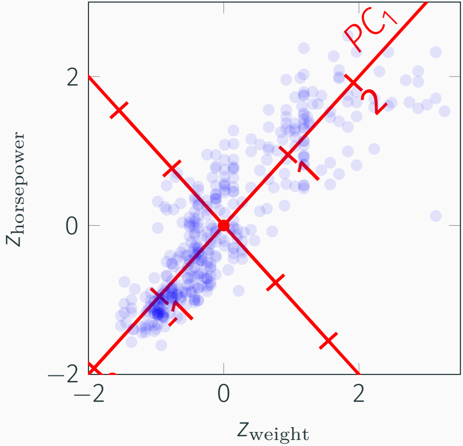
$$PC_1 \rightarrow 0.69 * z_{\text{horsepower}} + 0.71 * z_{\text{weight}}$$

Dimensionality reduction: Principal component analysis



$v \rightarrow$ direction of maximum variance **orthogonal** to PC_1

Dimensionality reduction: Principal component analysis



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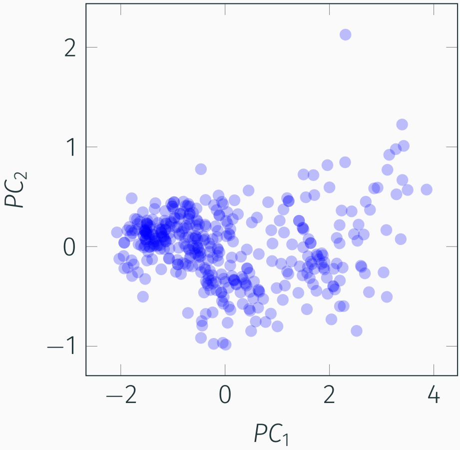

Dimensionality reduction: Principal component analysis

mpg	horsepower	weight	PC1	PC2
18	130	3504	0.908	0.303
15	165	3693	1.709	0.517
18	150	3436	1.219	0.455
16	150	3433	1.217	0.457
17	140	3449	1.046	0.260
15	198	4341	2.856	0.583
14	220	4354	3.272	0.977

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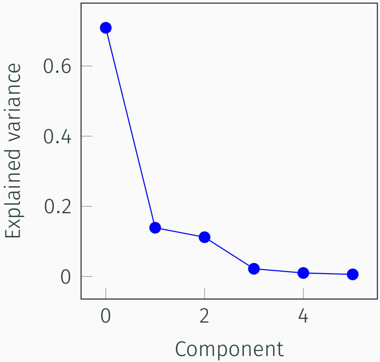
$$PC_1 = 0.69 * z_{\text{horsepower}} + 0.71 * z_{\text{weight}}$$

Dimensionality reduction: Principal component analysis

http://localhost:8888/notebooks/notebooks%2FPCA.ipynb

Dimensionality reduction: Principal component analysis



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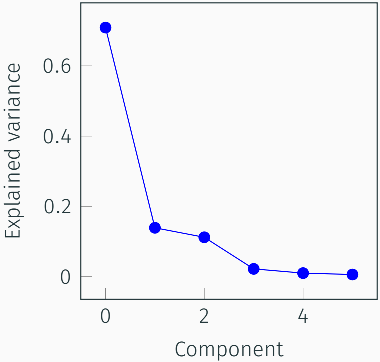
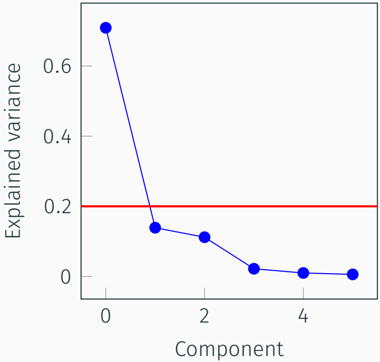


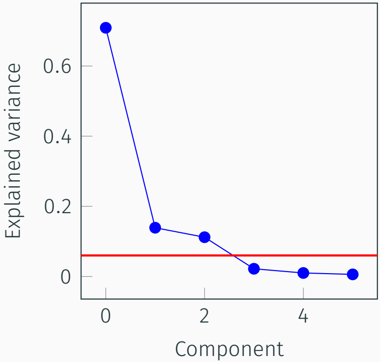
$$\hat{y} = \beta_0 + \sum_{i=0}^{n} \beta_i PC_i$$

Dimensionality reduction: Principal component analysis



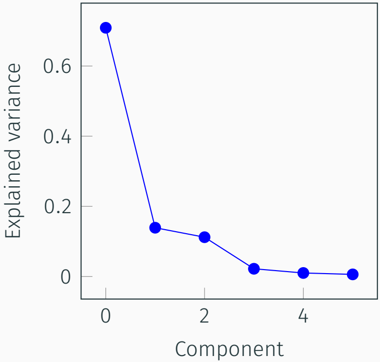
$$\hat{y} = \beta_0 + \sum_{i=1}^{1} \beta_i PC_i$$

Dimensionality reduction: Principal component analysis



$$\hat{y} = \beta_0 + \sum_{i=1}^{3} \beta_i PC_i$$

Dimensionality reduction: Principal component analysis



$$\hat{y} = \beta_0 + \sum_{i=0}^{n} \beta_i PC_i$$

n decided via a validation set, tested in a **held-out test set**

Dimensionality reduction: Principal component analysis

Principal component analysis: Transforms our dataset by computing new *principal components* that replace our original variables.

- Principal components are linear combinations of the original variables
- Principal components are orthogonal to each other, meaning that they capture different signals in our data (in a very strict sense)