# Principal components analysis

Reference: Introduction to Statistical Learning Chapter 10.1-10.2

# Outline

1. Introduction to PCA
2. Brief reminder of some linear algebra notation
3. PCA as a projection
4. PCA as an optimization problem
5. PCA as a regression on latent variables

# Introduction to PCA

The goal of PCA is to find low-dimensional summaries of high-dimensional data sets.

This is useful for compression, for denoising, for plotting, and for making sense of data sets that initially seem too complicated to understand.

It differs from clustering:

- Clustering assumes that each data point is a member of one, and only one, cluster. (Clusters are mutually exclusive.)
- PCA assumes that each data point is like a combination of multiple basic "ingredients." (Ingredients are not mutually exclusive.)

# Think about recipes:

Nestle Toll House Chocolate-chip cookies: 280 grams flour, 150 grams white sugar, 165 grams brown sugar, 225 grams butter, 2 eggs, 0 grams water…

Mary Berry's Victoria sponge cake: 225 grams flour, 225 grams white sugar, 0 grams brown sugar, 225 grams butter, 4 eggs, 0 grams water…

seriouseats.com old fashioned flaky pie dough: 225 grams flour, 15 grams white sugar, 0 grams brown sugar, 225 grams butter, 0 eggs, 115 grams water…

# Think about recipes:

Each baked good is constructed by following a recipe: a combination of the same basic ingredients.

- Each data point $x_i$ is like a baked good.
- In PCA, the **principal components** are like the ingredients.

The amounts of each ingredient differ from one baked good to the next:

- E.g. 225g sugar for sponge cake versus 15 grams sugar for pie dough.
- In PCA, the **scores** are like the amounts of each ingredient in a given baked good.

# Think about recipes:

Our goal is to reverse-engineer both the **ingredients** and the **amounts/recipes** from an observed set of "baked goods" (i.e. original data points).

# The result of PCA

You get summary features for each observation.

Before: raw survey data on a bunch of TV shows

| | Entertaining | Engaged | Original | Confusing | Funny |
|---|---|---|---|---|---|
| 30 Rock | 4.2 | 3.7 | 4.0 | 2.2 | 3.7 |
| America's Next Top Model | 4.2 | 3.8 | 3.8 | 2.0 | 3.5 |
| American Chopper | 4.2 | 3.6 | 3.9 | 2.1 | 3.5 |
| Bones | 4.3 | 4.1 | 3.8 | 1.9 | 3.4 |
| Close to Home | 4.1 | 3.8 | 3.8 | 1.9 | 2.9 |
| Cold Case | 4.2 | 3.9 | 4.0 | 1.9 | 3.0 |

plus 16 more columns.

# The result of PCA

You get summary features for each observation.

After: survey data on a bunch of TV shows run through PCA

| | PC1 | PC2 |
|---|---|---|
| 30 Rock | -2.64 | 0.12 |
| America's Next Top Model | -0.78 | -0.19 |
| American Chopper | -2.31 | 0.68 |
| Bones | 3.24 | 2.22 |
| Close to Home | -0.63 | 2.86 |
| Cold Case | 1.62 | 2.88 |

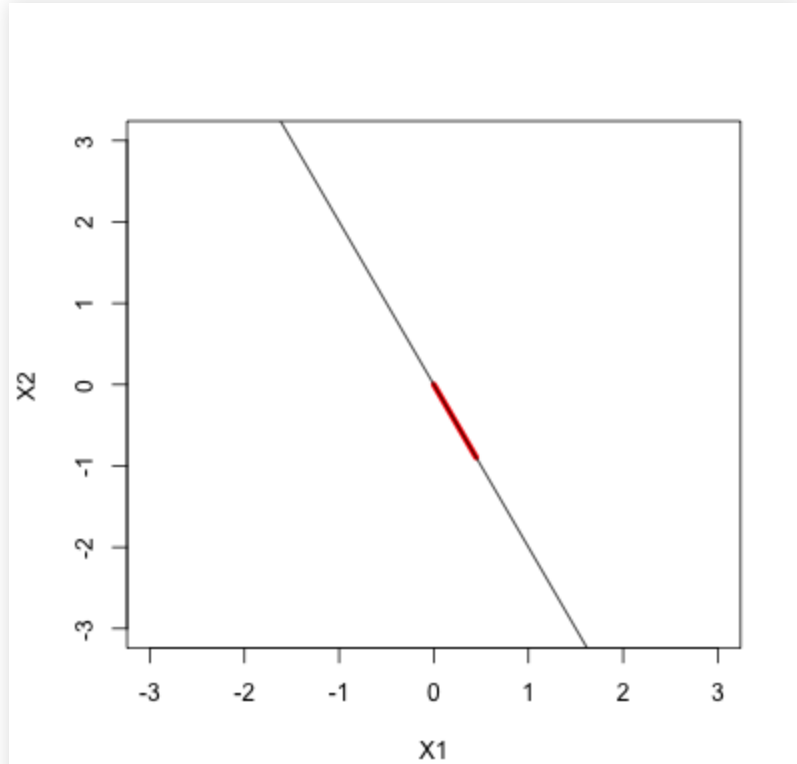
From 20 raw variables to 2 summaries. PC1 and PC2 are like "ingredients." The numbers are "amounts" of each "ingredient."

The trick to PCA is interpreting the summaries!

# Some linear algebra reminders

Alas, PCA is less delicious than baking, and it uses more linear algebra. Say that $v \in \mathbb{R}^P$ is some vector. This defines a *subspace* of $\mathbb{R}^P$:

$$\mathcal{V} = \{z : z = \alpha_i v, \alpha_i \in \mathbb{R}\}$$



# Some linear algebra reminders

Now let $X$ be our usual $N \times P$ data matrix with rows $x_i^T$.

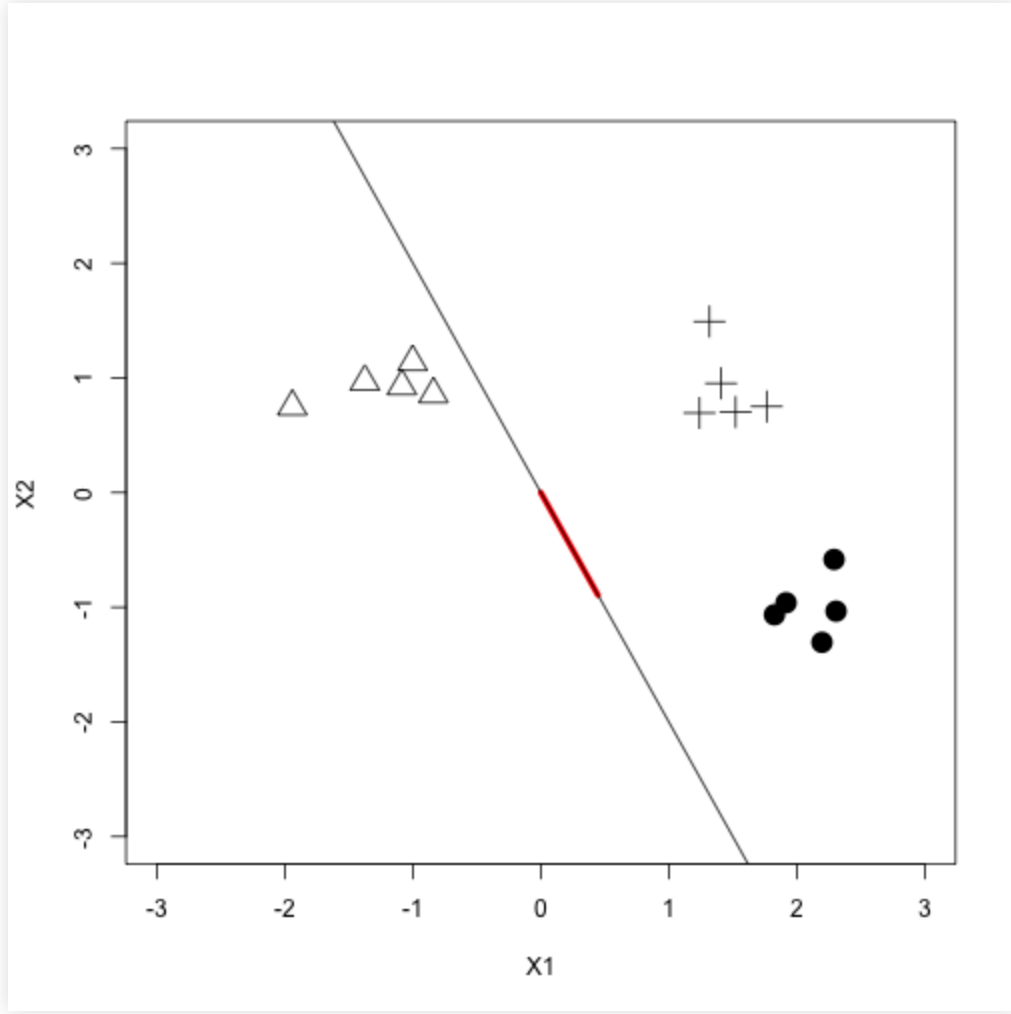
Suppose we *project* each $x_i^T$ in our data matrix onto the subspace $\mathcal{V}$.
The scalar location of this projected point in this subspace $\mathcal{V}$ is

$$\alpha_i = x_i \cdot v = x_i^T v$$

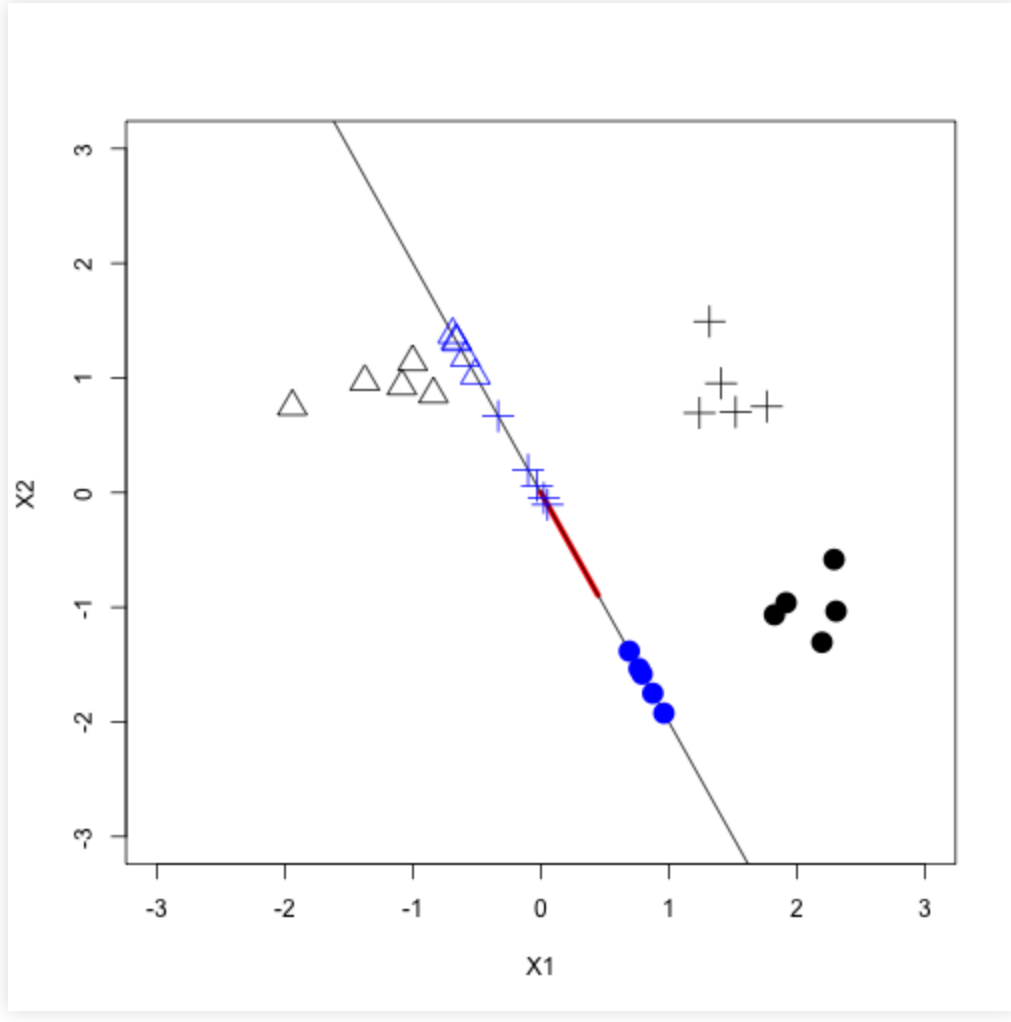
This is a one-number summary of our original point $x_i$. A different choice of $v$ gives a different summary.

**Let's see a picture.**

# The original points



# With the projected points



# Key ideas

Key idea 1: projection = summary

- Each point's location along the subspace is a **one-number linear summary** of a $P$-dimensional data vector:

$$\alpha_i = x_i \cdot v = x_i^T v$$

- The goal of principal components analysis (PCA) is to find the "best" projection, i.e. the best linear summary of the data points.

# Key ideas

Key idea 2: the "best summary" is the one that preserves as much of the **variance** in the original data points as possible.

- Intuition: we're already trying to crowd these P-dimensional points into 1-D. We should give them "room to breathe" by crowding them on top of each other as little as possible *within* that 1-D space!
- More variance in $\alpha_i$ means more "spread out" summaries in 1-D.
- And the more they're spread out, the more we have preserved differences between the projected points that were present in the original points. **See pca_intro.R**.

# PCA as an optimization problem

Given data points $x_1, \ldots, x_N$, with each $x_i \in \mathbb{R}^P$, and a candidate vector $v_1$, the variance of the projected points is

$$\text{variance} = \frac{1}{n} \sum_{i=1}^{n} [\alpha_i - \bar{\alpha}]^2$$

where $\alpha_i x_i \cdot v_1$.

So we solve:

$$\underset{v_1 \in \mathbb{R},\ \|v\|_2 = 1}{\text{maximize}} \quad \sum_{i=1}^{n} \left[ x_i \cdot v_1 - \left( \frac{1}{n} \sum_{i=1}^{N} x_i \cdot v_1 \right) \right]^2$$

Note: we constrain $v_1$ to have length 1; otherwise we could blow up the variance of the projected points as large as we wanted to.

# PCA as an optimization problem

The solution $v_1$ to this optimization problem:

- is called the first principal component (synonyms: loading, rotation.)
- is the one-dimensional subspace capturing as much of the information in the original data matrix as possible.

The projected points $\alpha_i = x_i \cdot v$ are called the *scores* on the first principal component.

# PCA as regression on latent variables

We can think of the projected location of $x_i$ as an approximation to the original data point: $x_i \approx \hat{x}_i = \alpha_i v$.

Or to make the approximation error explicit:

$$\begin{aligned} x_{ij} &= \hat{x}_{ij} + e_i \\ &= \alpha_i v_j + e_i \end{aligned}$$

This is like a regression problem for the jth feature variable.

- The $\alpha_i$'s are like hidden (latent) features.
- $v_j$ is like a regression coefficient for observed variable $j$.

Thus PCA is like estimating $P$ regression coefficients $v_1 = (v_{11}, \ldots, v_{1P})$ all at once, where the feature variable is hidden.

# PCA as regression on latent variables

We can write the approximation for the whole matrix as follows:

$$
\begin{aligned}
X &\approx \begin{pmatrix}
\alpha_1 v_{11} & \alpha_1 v_{12} & \cdots & \alpha_1 v_{1P} \\
\alpha_2 v_{11} & \alpha_2 v_{12} & \cdots & \alpha_2 v_{1P} \\
\vdots & \vdots & & \vdots \\
\alpha_N v_{11} & \alpha_N v_{12} & \cdots & \alpha_N v_{1P}
\end{pmatrix} \\
&= \alpha v_1^T \quad \text{(outer product of } \alpha \text{ and } v_1\text{)}
\end{aligned}
$$

# PCA as regression on latent variables

And if we explicitly include the error term:

$$X = \alpha v_1^T + E$$

where $E$ is a residual matrix with entries

$$\begin{aligned} E_{ij} &= x_{ij} - \hat{x}_{ij} \\ &= x_{ij} - \alpha_i v_{1j} \end{aligned}$$

# Higher-order principal components

With this in place, we can now define principal components 2 and up!

- PC 2: run PCA on the residual matrix from PC 1.
- PC 3: run PCA on the residual matrix from PCs 1-2.
- …
- PC P: run PCA on the residual matrix from PCs 1-(P-1).

Thus principal component $M$ is defined recursively in terms of the fit from principal components 1 through $M - 1$. In practice we often stop with far fewer than $P$ principal components.

# Higher-order principal components

Let's see the examples in:

- `nbc.R`
- `congress109.R`
- `ercot_PCA.R`

These examples will help us learn to answer the million-dollar question in PCA: what do the summaries mean?