Principal components analysis

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Reference: Introduction to Statistical Learning Chapter 10.1-10.2

Outline

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.)

You can fiddle with ingredients continuously, but cluster membership only discretely.

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
- ...

Think about recipes

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
- ...

Think about recipes

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.

In our analogy of baking with data:

- 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 between baked goods:

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

Think about recipes

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In PCA, 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

Let's see a before and after to start building some intuition for what PCA does.

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
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

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

```
                   PC1   PC2
30 Rock          -2.64  0.12
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
```

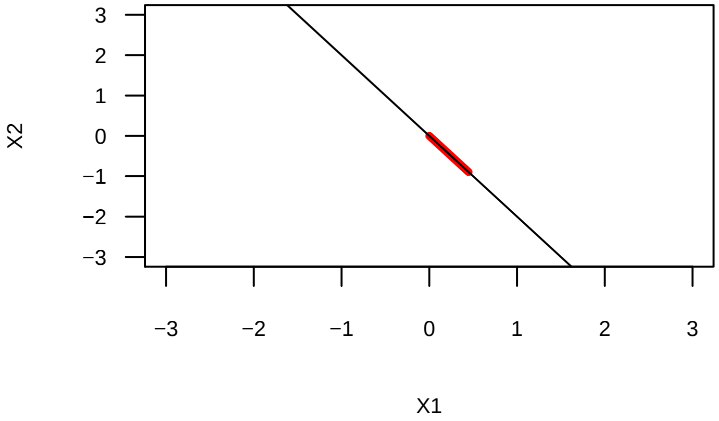
From 20 raw variables to 2 summaries. PC1 and PC2 are like “ingredients.” The numbers are “amounts” of each “ingredient.”

The trick to PCA is interpreting the summaries!

Some linear algebra reminders

Alas, PCA is less tasty than baking, and 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 ${x_i}^T$.

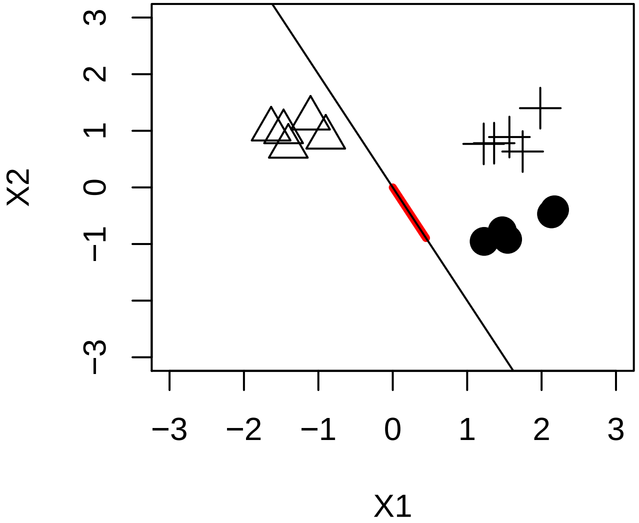
Suppose we *project* each ${x_i}^T$ in our data matrix onto the subspace $\mathcal{V}$. The scalar location of this projected point in this subspace $\mathcal{V}$ is

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

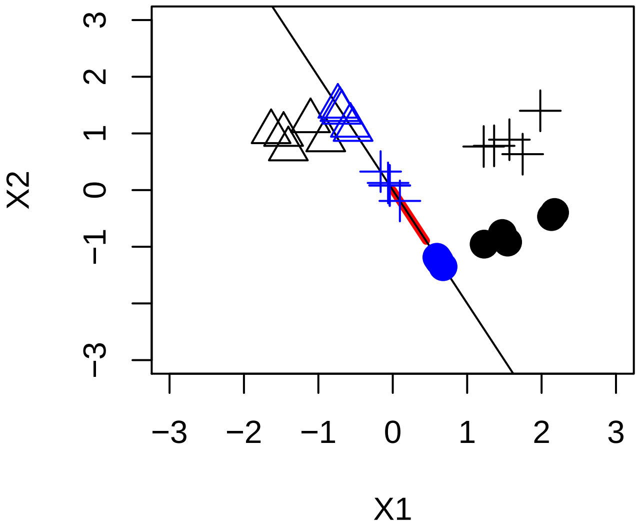
This is a one-number summary of our original point x_i. A different choice of v gives a different summary.

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 original data points.
- But what does "best" actually mean?

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 the scores (α_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 a unit-length vector of dimension P.
- is called the first principal component (synonyms: loading, rotation.)
- represents, via the set of its scalar multiples $\{\alpha v_1 : \alpha \in \mathcal{R}\}$, 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 α_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 PCs 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 $M - 1$.

Notes:

- In practice we often stop with far fewer than P principal components.
- This process is a thought experiment that serves to **define** the PCs; it isn't how they're actually calculated in practice.

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?