Principal Component Analysis

Nate Wells

Math 243: Stat Learning

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Outline

In today's class, we will...

- Discuss Principal Component Analysis as an example of unsupervised learning
- Implement PCA in R and interpret PCA in context

Section 1

Principal Component Analysis

Unsupervised Learning

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- Ex: Finding subgroups of similar Beatles songs.
- Compared to supervised learning, analysis of unsupervised learning methods tend to be more subjective (since we can't assess accuracy using a response variable)
- But unsupervised learning represents an instrumental part of exploratory data analysis (and of pattern recognition, more generally)

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PCA can be used as a means of unsupervised learning and exploratory data analysis.

- PCA finds the consecutive linear combinations of predictors (or features) that have the most variance, once prior linear combinations are taken into account.

PCA

The first principal component of $X_1, \ldots, X_p$ is the normalized linear combination

$$Z_1 = \phi_{11} X_1 + \cdots + \phi_{p1} X_p \qquad \text{with } \sum \phi_{i1}^2 = 1$$

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- The first principal component loading vector solves the optimization problem:

$$\phi_1 = \text{argmax}_{\phi_{11}, \ldots, \phi_{p1}} \left\{ \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{j=1}^{p} \phi_{j1} x_{ij} \right)^2 \right\} \text{ given } \sum_{j=1}^{p} \phi_{ji}^2 = 1$$

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- The vector of loadings $\phi_1 \in \mathbb{R}$ points in the direction in feature space along which the data varies the most.

PCA

The second principal component Z_2 is the linear combination of $X_1, \ldots, X_p$ that has maximal variance among all lin. combos. that are uncorrelated with Z_1, and takes the form

$$Z_2 = \phi_{12} X_1 + \cdots + \phi_{p2} X_p \qquad \text{with } \sum \phi_{i1}^2 = 1 \text{ and } \mathrm{Corr}(Z_1, Z_2) = 0$$

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In general, the kth principal component is a linear combination that has maximal variance among all combos that are uncorrelated with $Z_1, \dots, Z_{k-1}$

$$Z_k = \phi_{1k}X_1 + \cdots + \phi_{pk}X_p \qquad \text{with } \sum \phi_{i1}^2 = 1 \text{ and } \mathrm{Corr}(Z_j, Z_2) = 0,\ 1 \le j \le k-1$$

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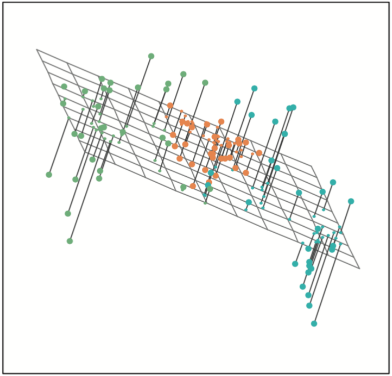
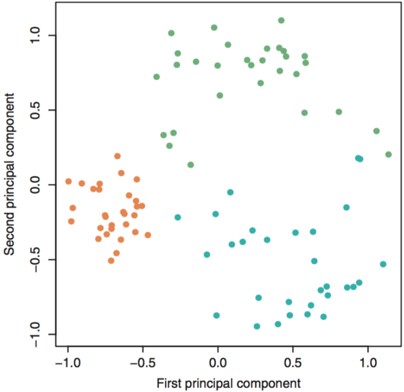
$$x_{ij} \approx \sum_{m=1}^{M} z_{im}\phi_{jm} \qquad \text{where } z_{im} = \phi_{1m}x_{im} + \cdots + \phi_{pm}x_{ip}$$

Visual

Reduction from $p = 3$ to $p = 2$ via principal components.





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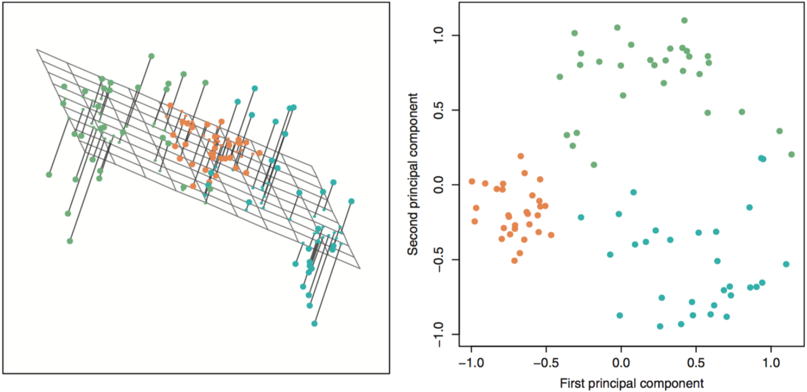

How does this differ from least squares regression?

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- Thus, the *Proportion of Variance Explained* by the mth principal component PVE_m is

$$\mathrm{PVE}_m = \frac{V_m}{TV} = \frac{\sum_{i=1}^{n} \left(\sum_{j=1}^{p} \phi_{jm} x_{ij} \right)^2}{\sum_{j=1}^{p} \sum_{i=1}^{n} x_{ij}^2}$$

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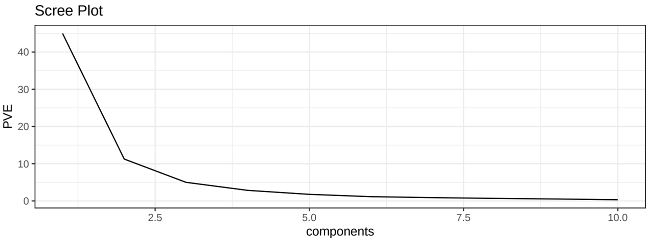

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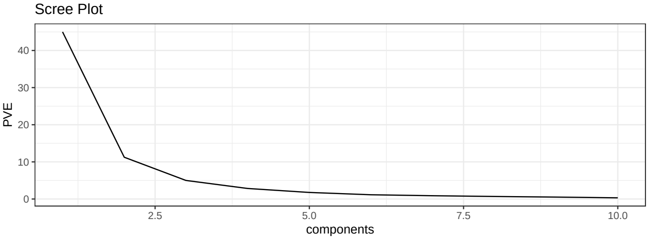

An alternative is to investigate the data structure present in the first several principal components, and then continue adding further components until the structures of interest no longer change substantially

Section 2

PCA in R

PCA Example

12 perfumers were asked to rate 12 perfumes on 11 scent adjectives

```
##  [1] "spicy"    "heady"    "fruity"   "green"    "vanilla"  "floral"
##  [7] "woody"    "citrus"   "marine"   "greedy"   "oriental"
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```

Each was rated on a scale of 1-10, and ratings for each perfume were averaged across experts.

```
head(experts)
```

```
## # A tibble: 6 x 12
##   perfume      spicy heady fruity green vanilla floral woody citrus marine greedy
##   <fct>        <dbl> <dbl>  <dbl> <dbl>   <dbl>  <dbl> <dbl>  <dbl>  <dbl>  <dbl>
## 1 "Angel"      3.22  8.26   1.9   0.133   7.75    2.09 1.05   0.142 0.125    8.28
## 2 "Aromatics~ 7.41  8.17   0.575 0.35    1.75    3.71 3.39   0.375 0.0583   0.258
## 3 "Chanel N5" 3.93  8.42   1.18  0.5     1.73    4.66 1.02   0.6   0.05     0.458
## 4 "Cin\xe9ma" 0.983 2.07   5.2   0.267   4.18    5.32 1.25   0.775 1.02     3.66
## 5 "Coco Made~ 0.925 0.717  4.58  1.2     2.02    7.31 1.13   1.17  1.14     2.72
## 6 "J'adore E~ 0.108 1.03   6.85  1.62    0.183   8.51 0.925  2.13  1.91     1.47
## # ... with 1 more variable: oriental <dbl>
```

Fitting the PCA

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The rotation value contains the principal component loadings

```
kable(pca1$rotation)
```

	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8	PC9	PC10	PC11
spicy	-0.32	-0.31	0.15	-0.10	0.21	0.00	0.29	-0.17	0.12	-0.77	0.00
heady	-0.35	-0.11	0.25	0.16	-0.21	-0.47	0.36	0.48	0.19	0.22	-0.23
fruity	0.34	0.15	-0.36	-0.17	0.26	-0.49	0.17	-0.21	-0.01	-0.07	-0.57
green	0.30	-0.15	0.62	0.27	0.36	0.31	0.05	-0.06	-0.04	0.14	-0.42
vanilla	-0.19	0.51	0.17	-0.28	-0.09	0.17	-0.29	0.40	-0.26	-0.32	-0.38
floral	0.34	-0.20	-0.27	0.07	-0.17	0.28	-0.13	0.39	0.63	-0.22	-0.18
woody	-0.25	-0.37	-0.14	-0.59	0.48	0.15	-0.10	0.22	0.04	0.35	-0.05
citrus	0.33	-0.18	0.38	-0.18	0.07	-0.54	-0.51	0.14	0.04	-0.17	0.28
marine	0.32	-0.08	0.27	-0.61	-0.51	0.12	0.39	-0.13	-0.02	0.06	0.01
greedy	-0.09	0.58	0.23	-0.16	0.26	-0.02	0.09	-0.17	0.65	0.11	0.20
oriental	-0.35	-0.18	0.08	-0.04	-0.35	-0.05	-0.47	-0.51	0.25	0.12	-0.39

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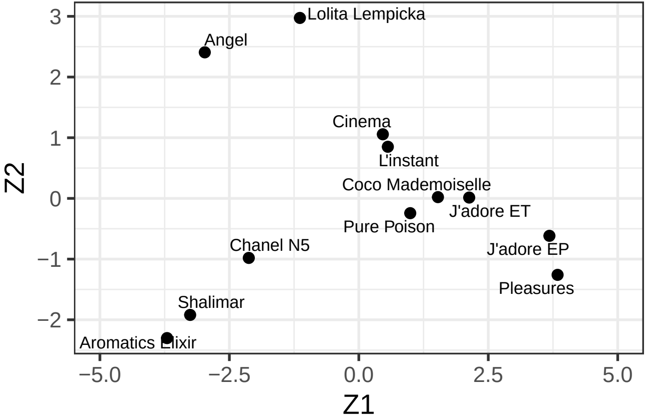
- Representing all pairwise structure requires $\binom{55}{2} = 55$ pairwise scatterplots

We can use principal components to focus our attention on small dimensional representation which describes most of the structure.

Scatterplot



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What does Z_1 represent? (i.e for what values of x is Z_1 large? small?)

```
##    spicy    heady   fruity    green  vanilla   floral    woody   citrus
##   -0.324   -0.352    0.340    0.304   -0.192    0.344   -0.252    0.330
##   marine   greedy oriental
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```
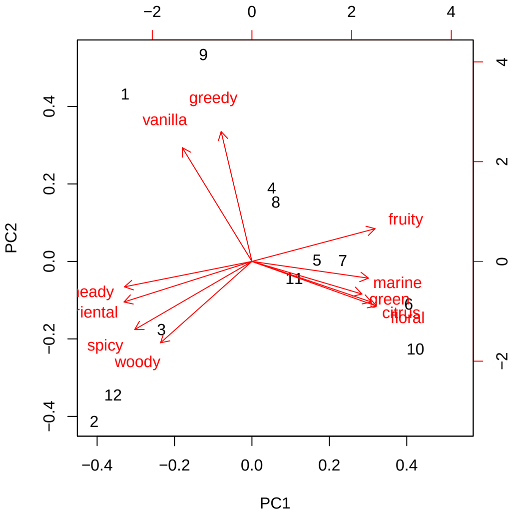

What does Z_2 represent?

```
##    spicy    heady   fruity    green  vanilla   floral    woody   citrus
##   -0.307   -0.114    0.147   -0.147    0.512   -0.201   -0.366   -0.183
##   marine   greedy oriental
##   -0.075    0.584   -0.182
```

Another Visualization

```r
biplot(pca1)
```



Scree Plot

```
d <- data.frame(PC = 1:11, PVE = pca1$sdev^2 / sum(pca1$sdev^2))

ggplot(d, aes(x = PC, y = PVE)) + geom_line() + geom_point() +
  theme_bw(base_size = 18)
```