Principal Components and Factor Analysis: a tale of two dimension reduction techniques

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Parkinsons example

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- Data was also collected on a control group of 64 healthy patients (23 men and 41 women).
- Each subject was recorded three times.
- The variables of interest consist of 754 auditory measurements for each patient.

Parkinsons example

- The data can be expressed in the following table:

ID	gender	status	PPE	DFA	RPDE	...
1	M	$+$	0.852	0.718	0.572	...
2	M	$+$	0.767	0.695	0.540	...
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	...	

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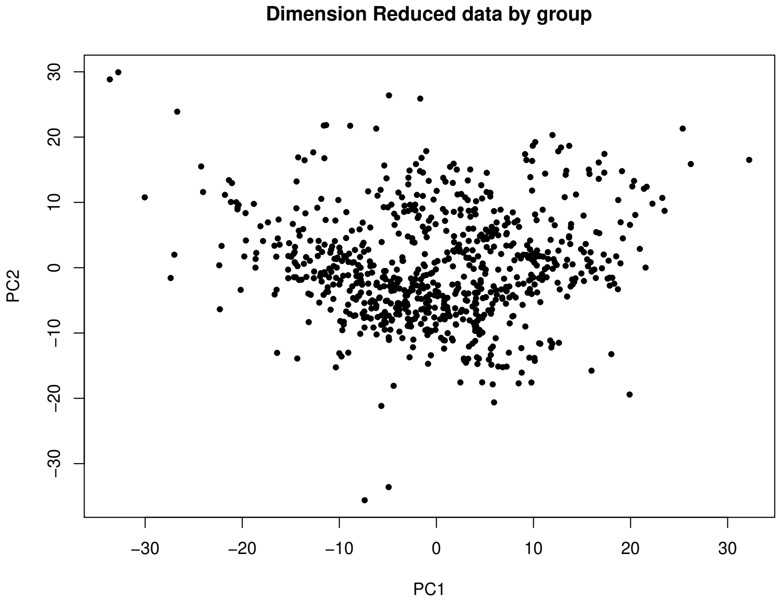
- Time to plot the data ...
- With Principal components analysis (PCA), we can obtain the following *two*-dimensional plot of the data.

Parkinsons example



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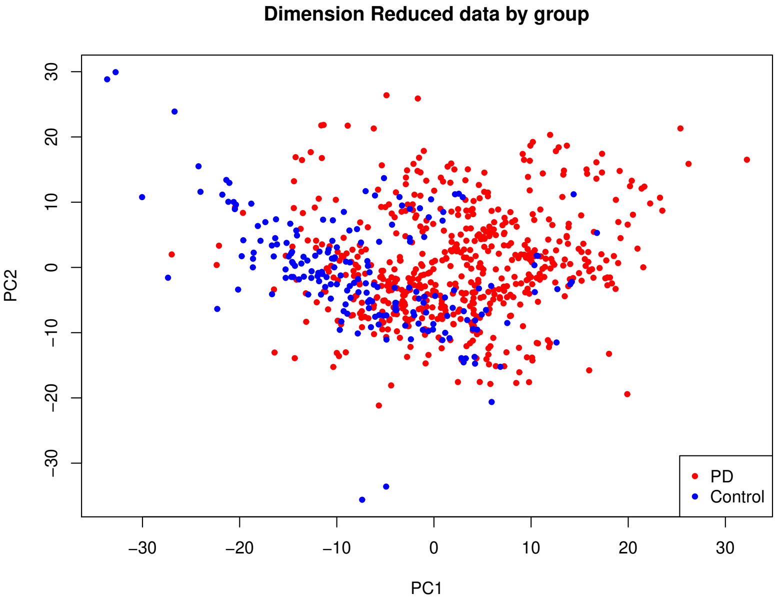

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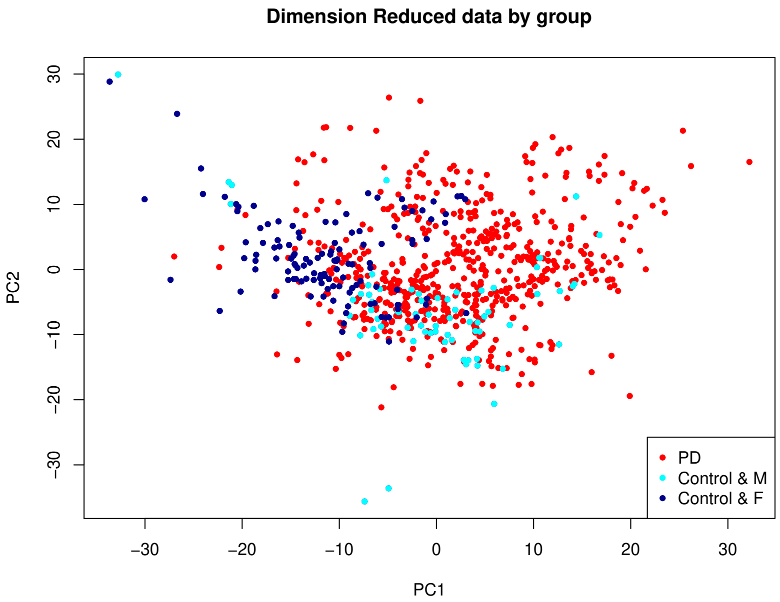

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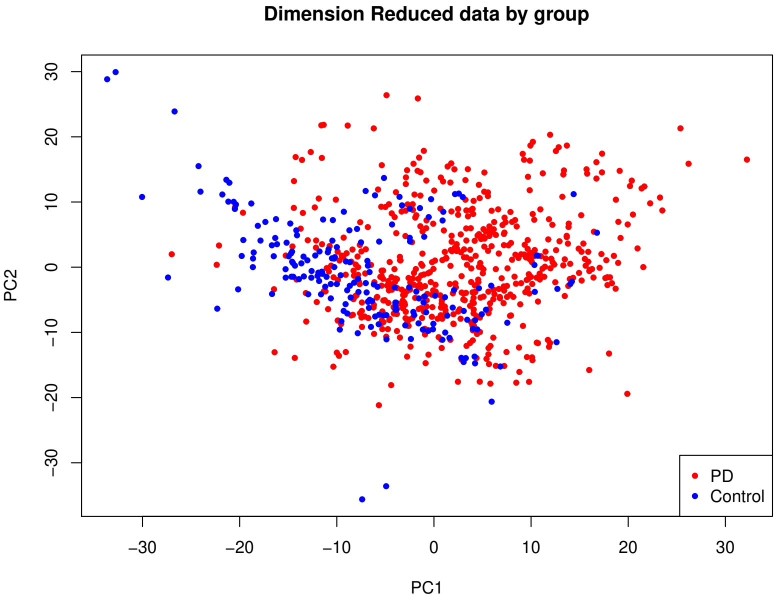

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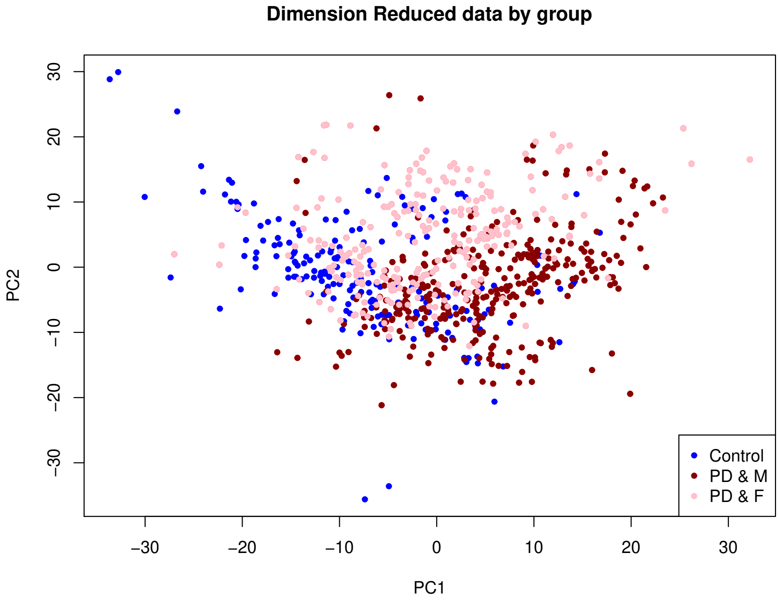

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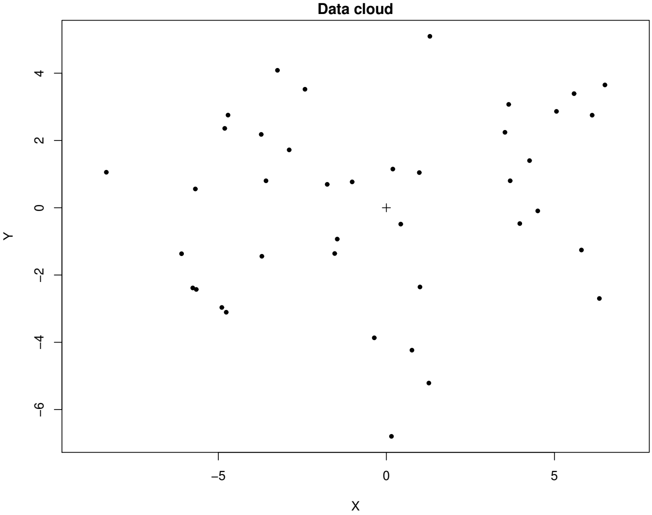
- But how is it carried out? What's going on?
- To get an intuitive sense we'll need to understand:
  - Projecting data into lower dimension
  - and how to maximize the variation of the result

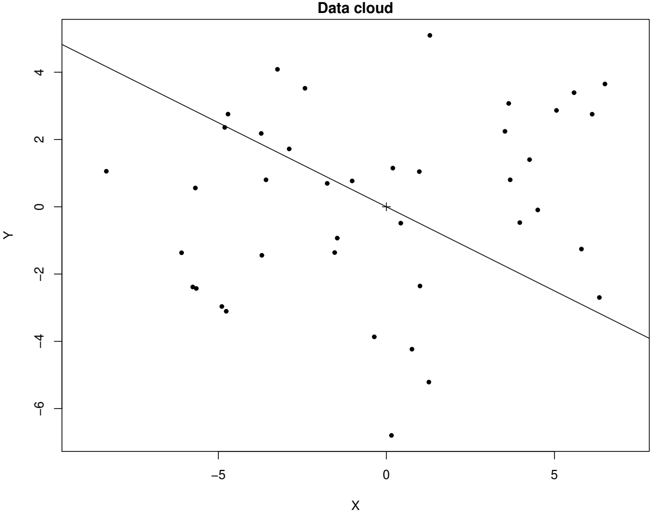
Projections of data

- We have the following (example) data cloud.



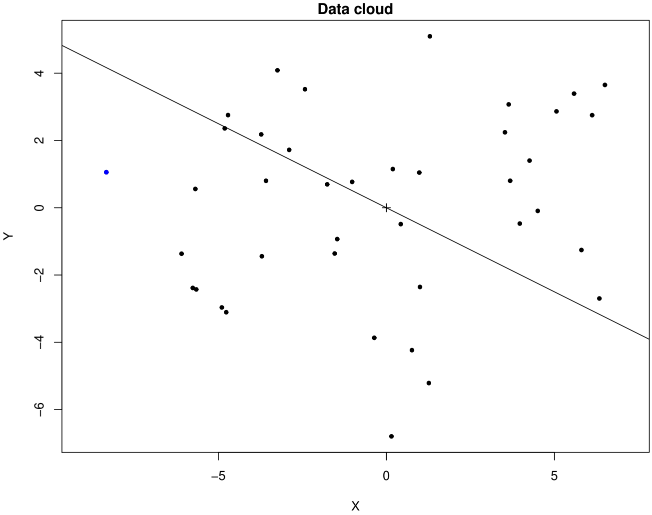
Projections of data

- Suppose we want to *project* our data onto the line.



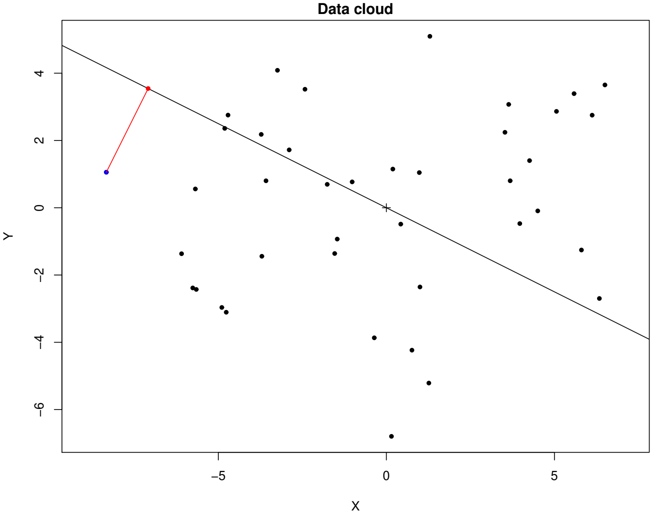
Projections of data

- Let's focus on projecting this point (in blue).



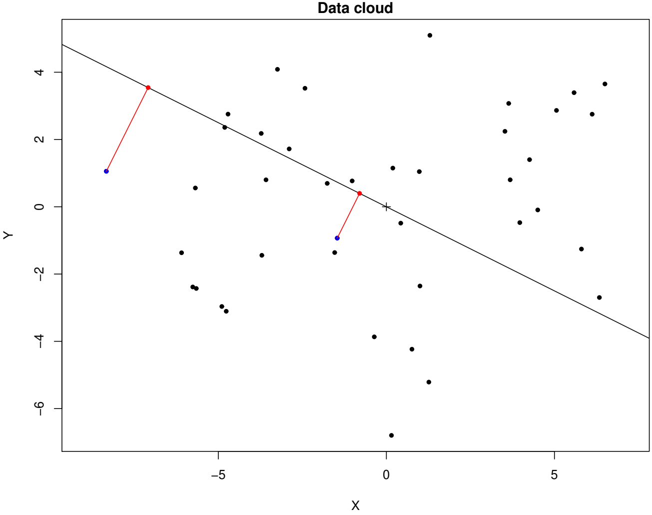
Projections of data

- The red point is nearest to the blue (on the line).



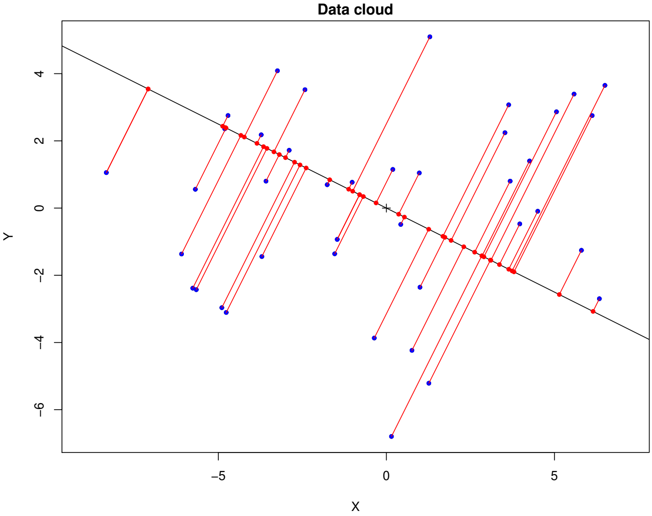
Projections of data

- Similarly for another point



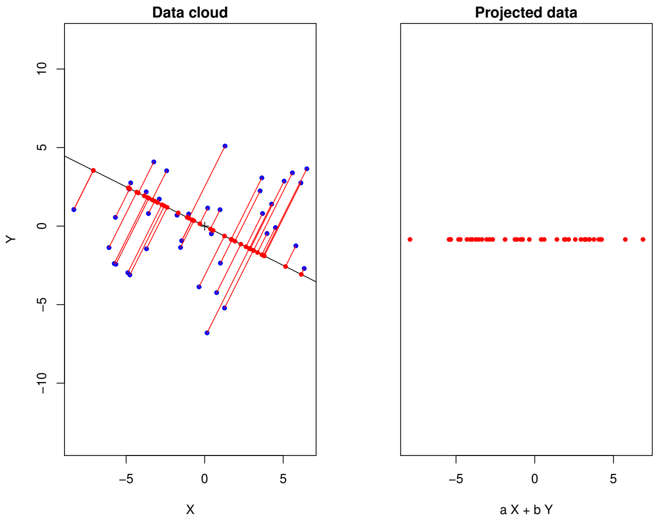
Projections of data

- And finally for all points.



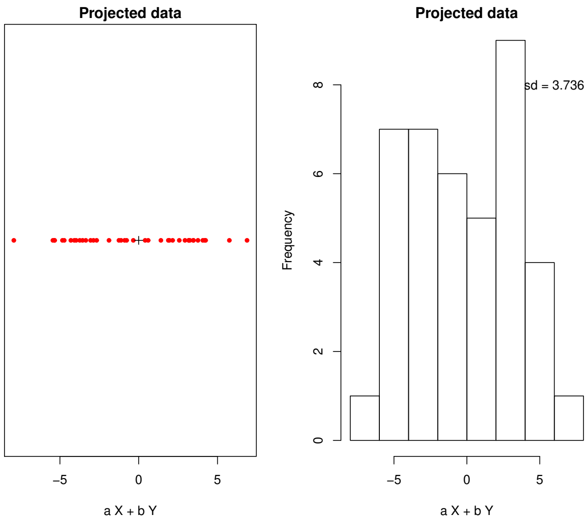
Projections of data

- Data can be treated as univariate while on the line.



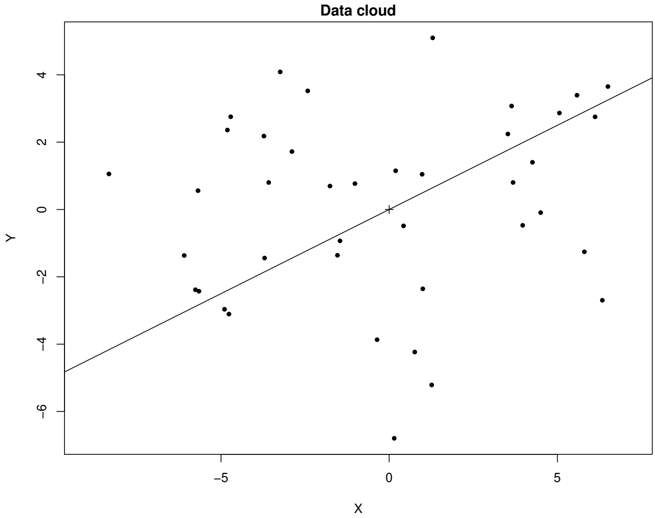
Projections of data

- With histogram



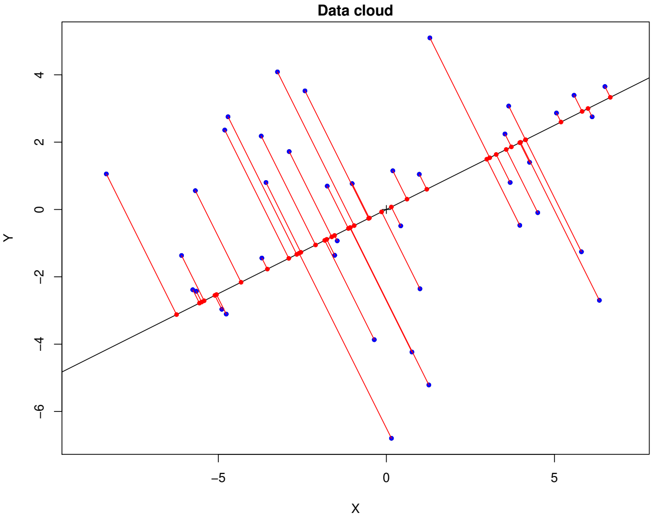
Projections of data

- Let's do this again but with a *new* line



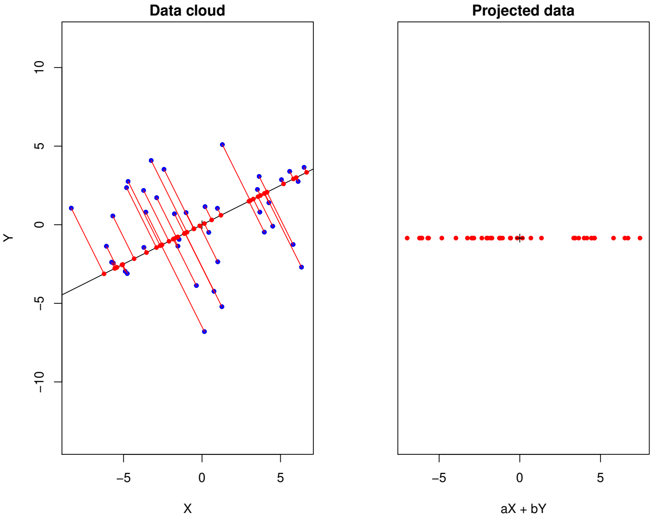
Projections of data

- Results in new *projected* data.



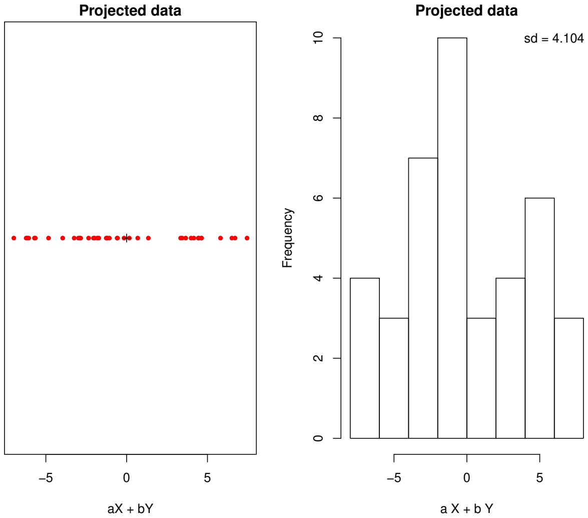
Projections of data

- Which, again, can be considered univariate.



Projections of data

- With a new histogram.



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- The std. dev of this projected data depends on the weights / projection line.

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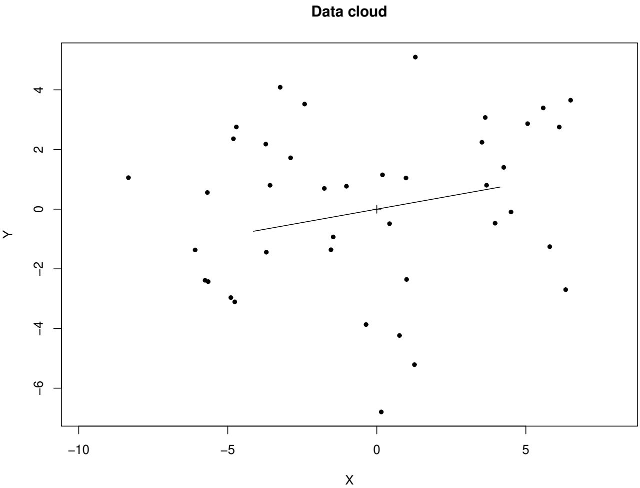
- What projection determines it?

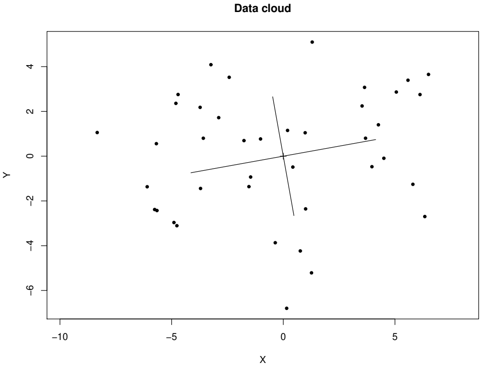
Projections of data

- This projection line *maximizes* the std. dev with sd $= 4.20$ (length $= 2 \times$ sd)



Projections of data

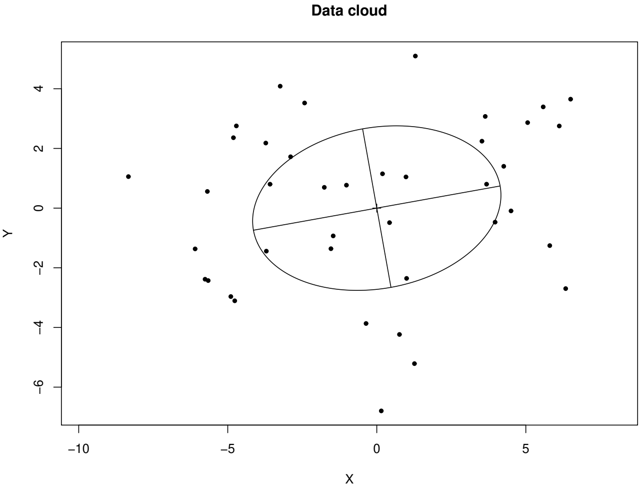
- The additional projection line *minimizes* the std. dev with sd $= 2.69$ (length is $2 \times$ sd)



- Notice that this is orthogonal (perpendicular) to the line for the *maximum*.

Projections of data

- Which motivates the *ellipse*

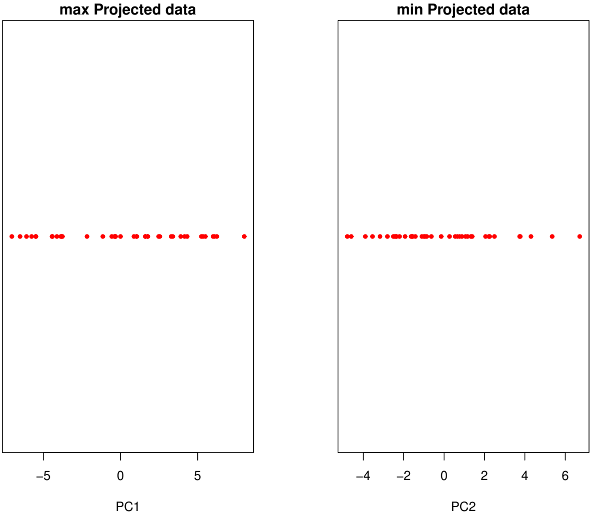


Projections of data

- Now we understand (part of) the sign out front of the building

PCA and Projections

- The maximum and minimum projections give us two sets of univariate data.



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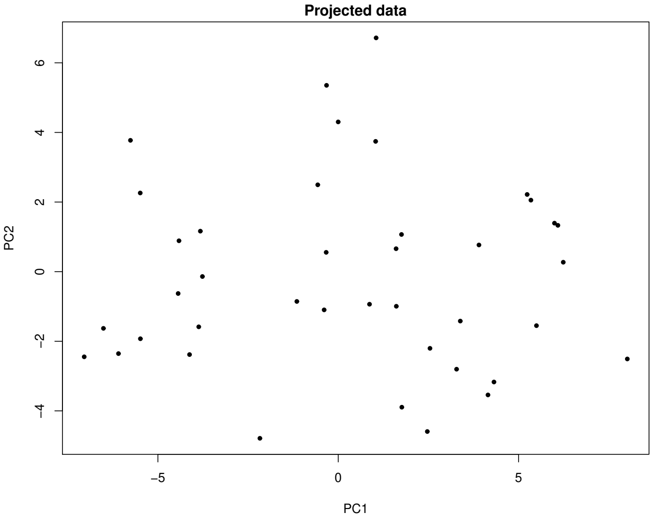
- maximum $\rightarrow$ **first Principal Component** i.e. PC1.
- minimum $\rightarrow$ **second Principal Component** i.e. PC2.
- And remember that each is given by

$$\text{PC1} = a^* X + b^* Y,$$
$$\text{PC2} = c^* X + d^* Y.$$

PCA and Projections

- Plotting both gives



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- Obviously, no dimension reduction happens in this case.

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- Why not use PC2 as our new dataset instead?
- One popular method decides PC1 over PC2.

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$$\text{var}(\text{PC1}) \geq \text{var}(\text{PC2})$$

  from before.

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- This motivates choosing PC1 over PC2.

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- 'Information' depends on context, goals, etc.

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$$a_1 X_1 + \cdots + a_p X_p$$

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- Note that $-a_1, \ldots, -a_p$ also works.

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- We now have PC1 based on some projection line.

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  - and is *orthogonal* to the first projection line.
- This can be found and results in univariate data which is denoted by

$$\mathrm{PC2} := b_1^* X_1 + \cdots + b_p^* X_p$$

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- The process results in p sets of univariate data

$$(\text{PC}1, \ldots, \text{PC}p)$$

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- Decreasing variation

$$\mathrm{var}(\mathrm{PC}1) \geq \cdots \geq \mathrm{var}(\mathrm{PC}p).$$

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- Many subsets are possible, how do we decide?
- The previous method, as in the bivariate case, gives one possibility.

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- The proportion of variability explained by each PC

$$\frac{\text{var(PC1)}}{\text{total variation}} \geq \cdots \geq \frac{\text{var(PC}p\text{)}}{\text{total variation}}$$

- Suppose we want to best explain variability of the original data
- Then the optimal choice for each size is

$$\begin{aligned}
\text{univariate} &\implies \text{PC1} \\
\text{bi-variate} &\implies (\text{PC1}, \text{PC2}) \\
\text{tri-variate} &\implies (\text{PC1}, \text{PC2}, \text{PC3}) \\
&\vdots
\end{aligned}$$

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- So to best account for variation we substitute the original data with $(\mathrm{PC}1, \ldots, \mathrm{PC}q)$, in order, for some q.
- But how do we choose q?
- This depends on what goals we have for the data analysis.

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- Let's show how to do PCA on a simple example
- In R, we an use `princomp()`
- We use the following data

	X1	X2	X3	X4	X5
1	1.43	0.44	-0.08	-0.53	-1.25
2	2.59	1.33	-1.20	-0.66	0.44
3	1.55	0.70	1.05	-0.79	1.54
⋮	⋮	⋮	⋮	⋮	⋮

Example in R

- Using the following code

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X = read.table("example_data.csv")
X_pca = princomp(X)
print( X_pca$loadings, cutoff = 0 )
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- Gives the following output

Example in R

	Comp.1	Comp.2	Comp.3	Comp.4	Comp.5
X1	0.89	0.40	0.03	0.22	0.00
X2	0.42	-0.78	-0.38	-0.24	0.09
X3	-0.13	0.39	-0.91	-0.06	-0.01
X4	-0.05	0.05	0.01	0.11	0.99
X5	-0.10	-0.28	-0.17	0.94	-0.10
Proportion of Var	0.43	0.25	0.17	0.09	0.06
Cumulative Var	0.43	0.68	0.85	0.94	1.00

Example in R

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X2	0.42	-0.78	-0.38	-0.24	0.09
X3	-0.13	0.39	-0.91	-0.06	-0.01
X4	-0.05	0.05	0.01	0.11	0.99
X5	-0.10	-0.28	-0.17	0.94	-0.10
Proportion of Var	0.43	0.25	0.17	0.09	0.06
Cumulative Var	0.43	0.68	0.85	0.94	1.00

- then PC1 is given by

$$\mathrm{PC1} := 0.89X_1 + 0.42X_2 - 0.13X_3 - 0.05X_4 - 0.10X_5$$

Example in R

	Comp.1	Comp.2	Comp.3	Comp.4	Comp.5
X1	0.89	0.40	0.03	0.22	0.00
X2	0.42	-0.78	-0.38	-0.24	0.09
X3	-0.13	0.39	-0.91	-0.06	-0.01
X4	-0.05	0.05	0.01	0.11	0.99
X5	-0.10	-0.28	-0.17	0.94	-0.10
Proportion of Var	0.43	0.25	0.17	0.09	0.06
Cumulative Var	0.43	0.68	0.85	0.94	1.00

- then PC1 is given by

$$PC1 := 0.89X_1 + 0.42X_2 - 0.13X_3 - 0.05X_4 - 0.10X_5$$

- which accounts for 43% of the variation in the data.

Example in R

	Comp.1	Comp.2	Comp.3	Comp.4	Comp.5
X1	0.89	0.40	0.03	0.22	0.00
X2	0.42	-0.78	-0.38	-0.24	0.09
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Proportion of Var	0.43	0.25	0.17	0.09	0.06
Cumulative Var	0.43	0.68	0.85	0.94	1.00

- and PC2 is given by

$$\text{PC2} := 0.40X_1 - 0.78X_2 + 0.39X_3 + 0.05X_4 - 0.28X_5$$

Example in R

	Comp.1	Comp.2	Comp.3	Comp.4	Comp.5
X1	0.89	0.40	0.03	0.22	0.00
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X3	-0.13	0.39	-0.91	-0.06	-0.01
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- and PC2 is given by

$$PC2 := 0.40X_1 - 0.78X_2 + 0.39X_3 + 0.05X_4 - 0.28X_5$$

- which accounts for 25% of the variation in the data.

Example in R

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- The new data from PC's, called **scores**, is also calculated and can be accessed by `X_pca$scores`
- This completes PCA (for calculation).

Using PCA

- Now that we understand the how PCA achieves dimension reduction, how can it be used?

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- Some examples:
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Using PCA

- Now that we understand the how PCA achieves dimension reduction, how can it be used?
- Some examples:
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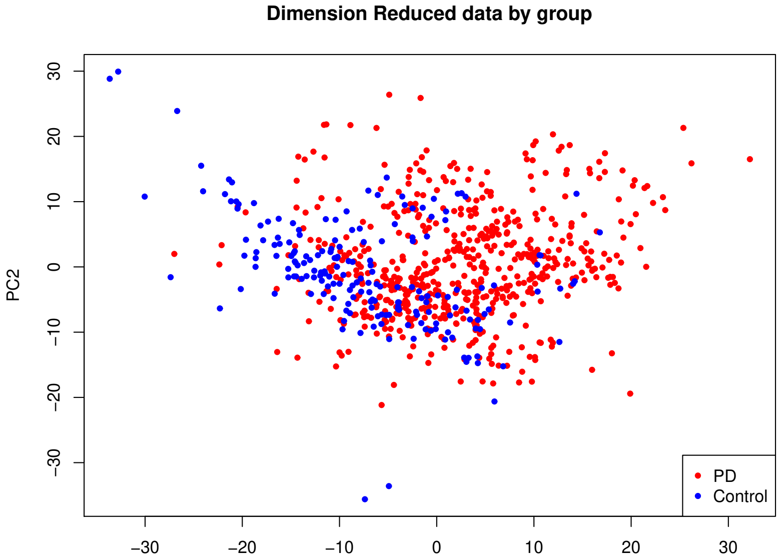
  - PC's for data interpretation
  - Combination with other methods (e.g. Regression)
  - And many more ...

PCA and Data visualization

- We've already seen this at the beginning



PCA and Data visualization

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- How to 'make sense' of the plot will depend on the subject, etc.

PCA for Interpretation

- [Nash et al.1994] gives a dataset of Abalone measurements.

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PCA for Interpretation

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- 2835 Abalone specimen composed of Male and Female (1528 and 1307, resp).
- 7 anatomical measurements
- Let's do PCA and inspect the results.

PCA for Interpretation

Group	Male		Female	
Component	1	2	1	2
length	-0.17	-0.12	0.16	-0.02
diameter	-0.14	-0.14	0.13	-0.06
height	-0.05	-0.09	0.05	-0.08
whole weight	-0.85	-0.14	0.85	-0.15
shucked weight	-0.39	0.76	0.38	0.76
viscera weight	-0.18	-0.02	0.18	0.00
shell weight	-0.22	-0.60	0.23	-0.62
Cumulative	0.97	0.98	0.96	0.98

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- Is this a real effect? Or is something else happening?

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- The sample standard deviations are given in the following table

	length	diameter	height	whole weight	shucked weight	viscera weight	shell weight
M	2.95	2.42	1.00	13.52	6.41	3.01	3.76
F	2.15	1.77	1.00	10.76	4.97	2.44	3.14

- Values have been ‘normalized’ by dividing by the minimum standard deviation.

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- Whole weight **dominates** the others in terms of variation.
- Hence, PC1 considers it as the most important.

PCA for Interpretation

- To demonstrate the point, suppose we have bi-variate data where

$$\mathrm{sd}(X_1) = 0.991,$$
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$$\mathrm{sd}(X_1) = 0.991,$$
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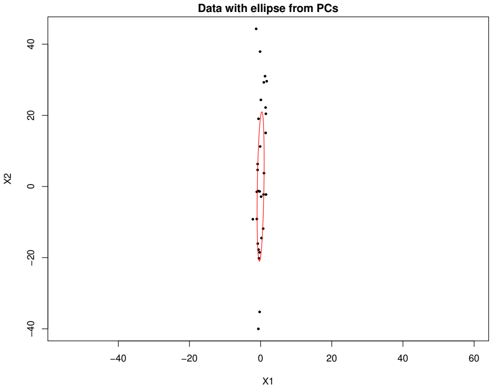
- Then the ellipse based on max / min directions is



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- Examples like this motivate first standardizing your data, then doing PCA.
- Lets re-do PCA on this example but with standardized data.

PCA for Interpretation

	Male		Female	
Component	1	2	1	2
length	-0.38	-0.00	-0.40	0.14
diameter	-0.38	0.07	-0.40	0.12
height	-0.36	0.77	-0.27	-0.96
whole weight	-0.39	-0.22	-0.41	0.10
shucked weight	-0.38	-0.47	-0.39	0.16
viscera weight	-0.38	-0.29	-0.39	0.12
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Cumulative	0.90	0.94	0.84	0.93

Table: PCA on standardized Abalone data

PCA for Interpretation

	Male		Female	
Component	1	2	1	2
length	-0.38	-0.00	-0.40	0.14
diameter	-0.38	0.07	-0.40	0.12
height	-0.36	0.77	-0.27	-0.96
whole weight	-0.39	-0.22	-0.41	0.10
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- The first component can be interpreted as an overall-size component.
- The second component contrasts between different measurements.

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- A popular version is to first do PCA on predictors and then carry out regression.
- By using a smaller number of predictors, via PCA, we may obtain better a regression model (avoid over-fitting).

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- [Hamidieh2018] provides a dataset of physical measurements used to predict superconductor critical temperature.

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- Performed PCA to use only 10 predictors.
- Let's look at the the results of regression.

PCA with regression: an Example

- If we use the first 10 PC's, we obtain the following results

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	34.42	0.15	223.83	0.00
PC1	4.00	0.03	146.22	0.00
PC2	-1.99	0.05	-37.67	0.00
PC3	2.40	0.06	43.38	0.00
PC4	1.25	0.06	20.58	0.00
PC5	-2.57	0.07	-36.42	0.00
PC6	-3.43	0.09	-39.04	0.00
PC7	-0.76	0.09	-8.51	0.00
PC8	0.58	0.10	5.93	0.00
PC9	1.91	0.11	17.18	0.00
PC10	-0.09	0.12	-0.75	0.45

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- and $R^2_{adj} = 0.5714$.

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	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	34.42	0.14	245.57	0.00
PC1	4.00	0.02	160.43	0.00
PC2	-1.99	0.05	-41.33	0.00
PC3	2.40	0.05	47.59	0.00
PC5	-2.57	0.06	-39.96	0.00
PC6	-3.43	0.08	-42.83	0.00
PC23	13.21	0.31	42.95	0.00
PC25	11.53	0.35	32.88	0.00
PC20	8.11	0.25	32.15	0.00
PC11	3.08	0.12	26.72	0.00
PC15	4.01	0.16	25.52	0.00

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PC5	-2.57	0.06	-39.96	0.00
PC6	-3.43	0.08	-42.83	0.00
PC23	13.21	0.31	42.95	0.00
PC25	11.53	0.35	32.88	0.00
PC20	8.11	0.25	32.15	0.00
PC11	3.08	0.12	26.72	0.00
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- and $R^2_{adj} = 0.644$.

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- PCA says nothing about association with some other variable!
- It is possible for later PC's to be better predictors!
- **Lesson**: Always remember PCA only explains variation within a dataset.
- Side note: since the PC dataset are uncorrelated (by construction), dropping variables by t-tests is reasonable.

What is Factor Analysis?

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  - Intelligence (verbal, mathematical, etc.)
  - Personality (extroversion, agreeableness, etc.)
  - Medical diagnoses (depression, anxiety, etc.)
- Researchers collect data with **measurable** quantities that, hopefully, associate with hypothesized **unobservable** quantities.

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Factor Analysis model

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- The Factor model supposes k unobservable and **random** variables, denoted by $(f_1, \dots, f_k)$, explain each variable.
- Specifically, it supposes each variable can be expressed by

$$X_i = a_1^{(i)} f_1 + \cdots + a_k^{(i)} f_k + e_i.$$

Factor Analysis model

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- This method has historically been confused with PCA.
- One possible reason is they can give similar **loadings**

FA and PCA loadings

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$$\mathrm{PC1} := a^{(1)}X_1 + \cdots + a^{(p)}X_p.$$

- Whereas for FA

$$\begin{aligned} X_1 &= a^{(1)}f_1 + e_1, \\ &\vdots \\ X_p &= a^{(p)}f_1 + e_p. \end{aligned}$$

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- The loadings/weights may be similar but their interpretation is not.

How does FA compare to PCA?

- This table summarizes some of the big distinctions between the two

	Method	
Criterion	FA	PCA
Modeling assumption	Very much so	(almost) none
Changing dimension	Major changes	No changes
Estimation	Complex	Simple
Goal	Latent factors	simplify by transformation
Emphasis	Correlation	Variance
Loadings	for Latent factors	for Original variables

Code and Slide materials

- Slides and code used at github
  https://github.com/AndoBlando/PCA_Fa_Talk

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