Week 12: Multivariate statistics (Part 1)

ANTH 674: Research Design & Analysis in Anthropology

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Statistics vignette

Are correlations always transitive?

- E.g., if X & Y are correlated and Y & Z are correlated, are X & Z correlated?
- Will prove the answer geometrically, so need to go over the geometric interpretation for correlation

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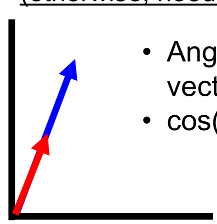
Cosine similarity

= Pearson correlation on centered variables

X	Y
1	2
2	4
3	6
4	8
5	10
⋮	⋮

Looking at first two observations only
(otherwise, need *many* axes)



- Angle between vectors = 0
- cos(0) = 1

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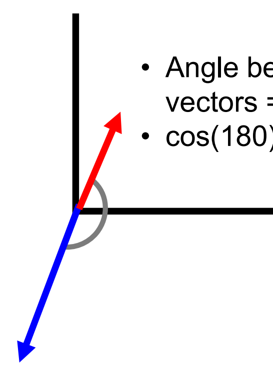
Another example

X	Y
1	-2
2	-4
3	-6
4	-8
5	-10
⋮	⋮

Looking at first two observations only



- Angle between vectors = 180
- cos(180) = -1

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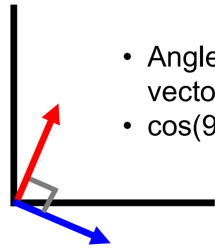
Another example

X	Y
1	2
2	-1
⋮	⋮

Looking at first two observations only



- Angle between vectors = 90
- cos(90) = 0

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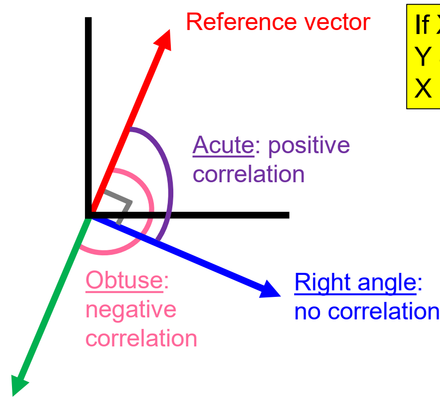
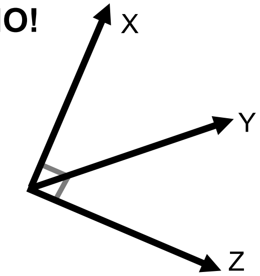
Putting it all together



If X & Y are correlated and Y & Z are correlated, do X & Z have to be correlated?

NO!



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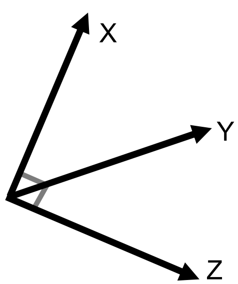
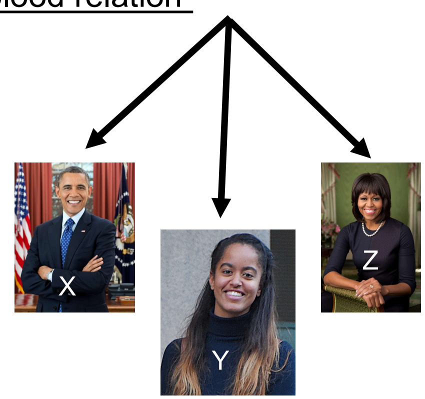
How to think about it



"Blood relation"



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Lecture outline

- Multivariate models
  - What is multivariate data?
  - MV models w/ one categorical IV
    1. Hotelling's T^2
    2. One-way MANOVA
- Introduction to ordination
  - Principal components analysis (PCA)
  - The general mechanics of PCA

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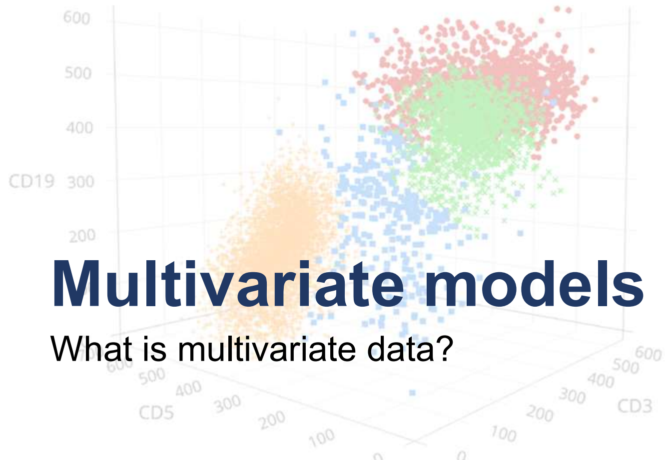

Multivariate models

What is multivariate data?

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What is multivariate data?

- Thus far, we have modeled only univariate DVs ~ one or more IVs
  - E.g., `mtcars$qsec ~ mtcars$hp`
- But many times, we want to simultaneously analyze ≥2 DVs ~ ≥1 IVs
  - E.g., `cbind(iris$Petal.Length, iris$Petal.Width) ~ iris$Species`
  - Looks at overall petal morphology & size ~ species
- Each DV variable can be continuous or categorical (we'll focus on continuous only)

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Independent DVs?

- Because each DV is measured on the same individual, DVs could be non-independent
- E.g., `cbind(iris$Petal.Length, iris$Petal.Width) ~ iris$Species`

Are these two DVs independent?

	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
1	5.1	3.5	1.4	0.2	setosa
2	4.9	3.0	1.4	0.2	setosa
3	4.7	3.2	1.3	0.2	setosa
4	4.6	3.1	1.5	0.2	setosa
5	5.0	3.6	1.4	0.2	setosa
6	5.4	3.9	1.7	0.4	setosa

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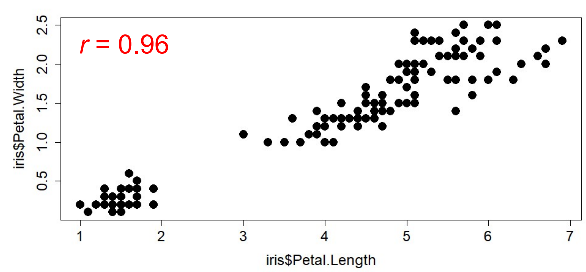
Independent DVs?

- **NO!**
- Individuals w/ larger petal lengths are more likely to have larger petal widths (i.e., size-based)



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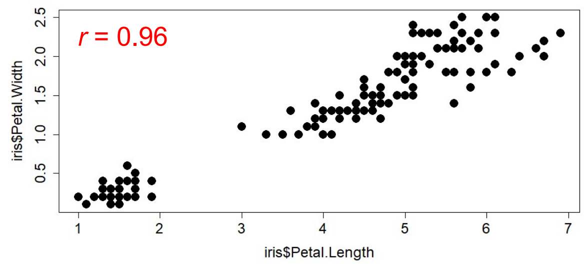
Multivariate models

- Takes into account non-independence (correlation) between DVs



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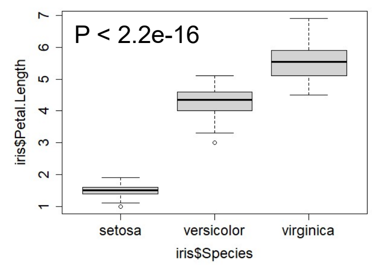
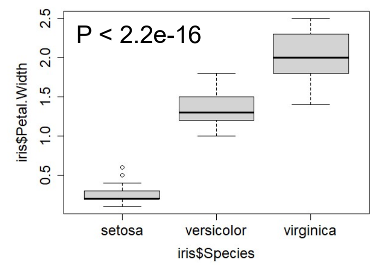
Univariate models

- Can do ANOVAs on DVs separately
- Ignores correlation between `Petal.Length` and `Petal.Width`





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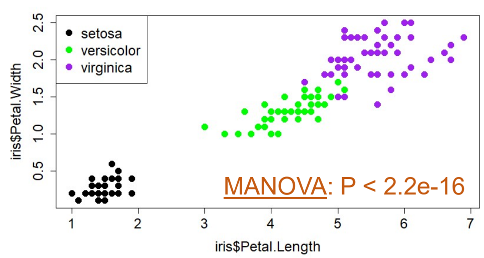
Multivariate models

- Takes into account correlation between `Petal.Length` and `Petal.Width`
- Are means of `Petal.Length` & `Petal.Width` point clouds different across species? (different question!)



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Questions?

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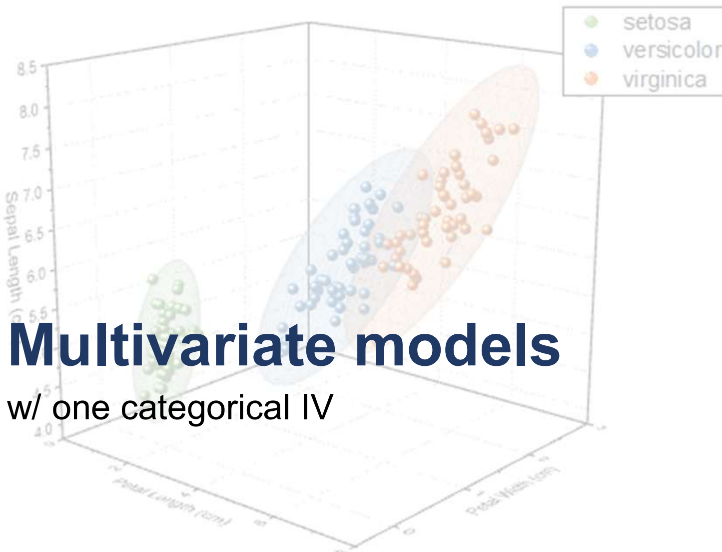

Multivariate models

w/ one categorical IV

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Multivariate models

- Models two or more DVs ~ one or more IVs
- We will look at models w/ one categorical IV only
- <u>Which test?</u> Univariate DV ~ one binomial IV?
  - t-test → Hotelling's T^2 (multivariate)
- <u>Which test?</u> Univariate DV ~ one multinomial IV?
  - One-way ANOVA → One-way MANOVA (multivariate)

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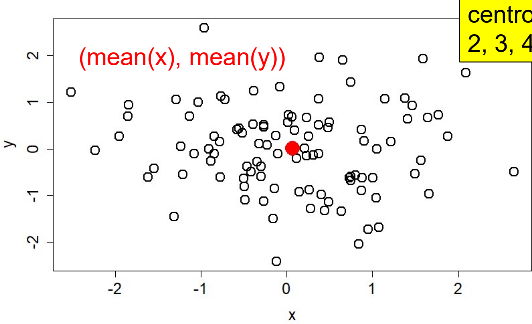
MV models w/ 1 categorical IV

- Asks if **<u>centroids</u>** of point clouds between groups are significantly different

Can calculate centroids for 2, 3, 4,…, *n* DVs



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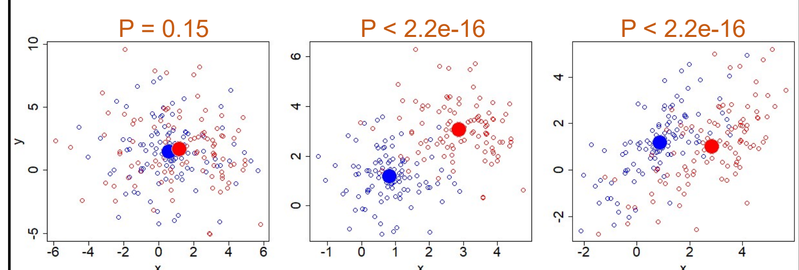
Hotelling's T^2

- Tests if two groups' centroids are significantly different, given how much DVs vary & covary
- E.g., simulated example w/ 2 DVs



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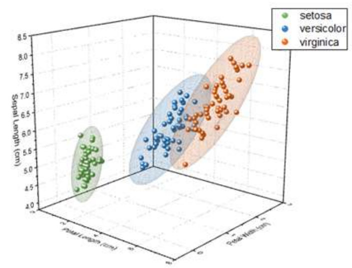
One-way MANOVA

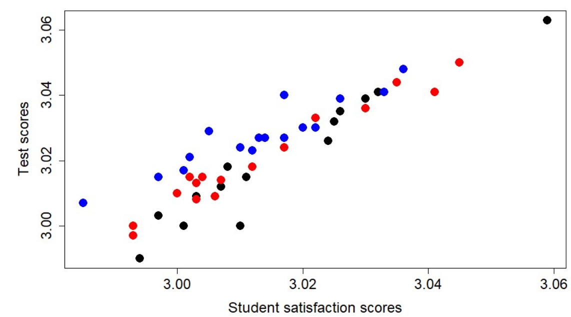
- Multivariate ANOVA → MANOVA
- Tests if ≥ 3 groups' centroids are significantly different, given how much DVs vary & covary



https://statisticsbyjim.com/anova/multivariate-anova-manova-benefits-use/

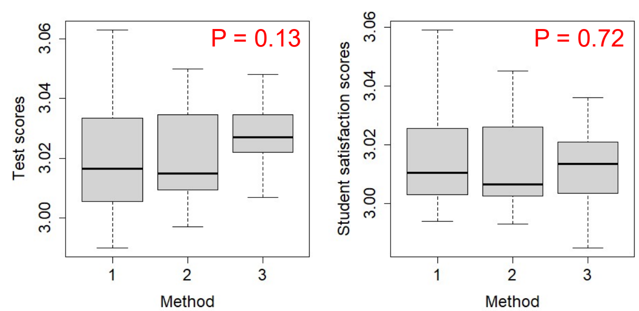
E.g., teaching scores

- We have two DVs (student satisfaction & test scores) ~ three different teaching methods



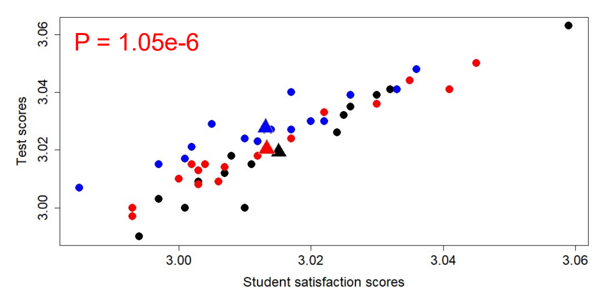
Univariate approach

- Two one-way ANOVAs (one per DV)
- Ignores correlation btw test & satisfaction scores



Multivariate approach

- Takes into account correlation between DVs
- Overlap between groups in X- or Y-dimension, but not when looking at X & Y together



MV model advantages

- Greater statistical power
  - When DVs are correlated, MV models can detect smaller effects than w/ ANOVAs
- Detect IV affecting relationship between DVs
- Limit the number of tests run (e.g., multiple ANOVAs)

https://statisticsbyjim.com/anova/multivariate-anova-manova-benefits-use/

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Assumptions

1. Observations are independent and randomly sampled from population
2. W/in each group, DVs are multivariate normally distributed (cf., each DV is normally distributed w/in each group)
   - ANOSIM relaxes this assumption (nonparametric)
3. Variances of DVs and how they're correlated w/ each other are the same for each group (cf. homoscedasticity)

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Questions?

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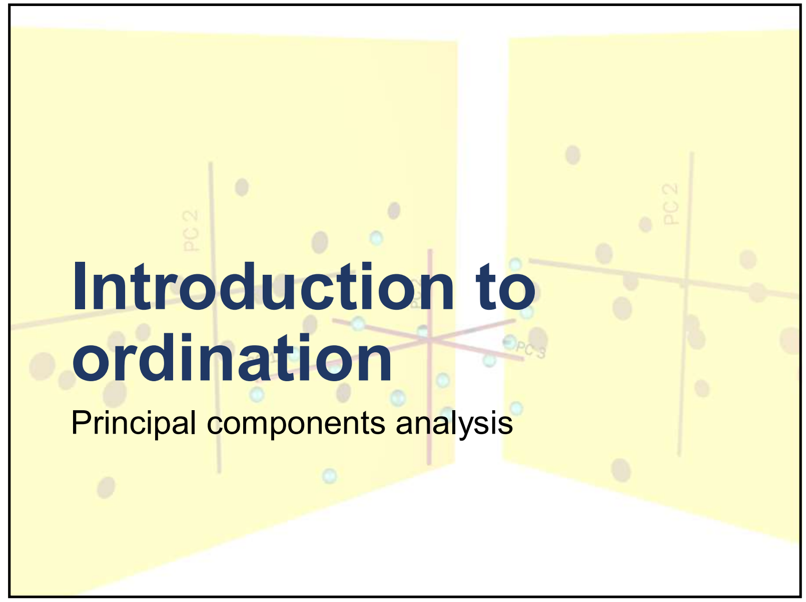

Introduction to ordination

Principal components analysis

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What is ordination?

- A method for ordering multivariate data along newly constructed variables (hence the name, **ordination**)
- Uses correlations among variables to collapse them into fewer composite variables that still explain a lot of variation in the dataset (i.e., it's a data reduction technique)
- E.g., collapse highly correlated `iris$Petal.Length` and `iris$Petal.Width` into one composite variable

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Why do ordination?

- Used primarily to explore MV data, but can also be used for hypothesis testing and prediction
  - Great way to visualize multidimensional MV data on a few axes (e.g., two or three)
- Can distill multiple correlated variables into one → can use as IV or DV in plots & linear models
  - E.g., collapse collinear IVs into one composite IV
- Composite variables produced by ordination are uncorrelated → can be used as IVs in multiple regression (i.e., no collinearity)

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Principal components analysis

- PCA is ordination done on continuous variables
- How it works conceptually:

1. Center variables & fit line through axis of greatest variation in variables

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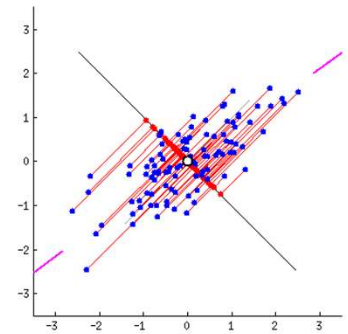
1. Fit line through axis of greatest variation

- Done by minimizing errors in X **AND** Y (i.e., shortest distance from each point to line)



- Must pass through centroid
- *Exactly* the same as major axis regression

https://stats.stackexchange.com/questions/2691/making-sense-of-principal-component-analysis-eigenvectors-eigenvalues/2700

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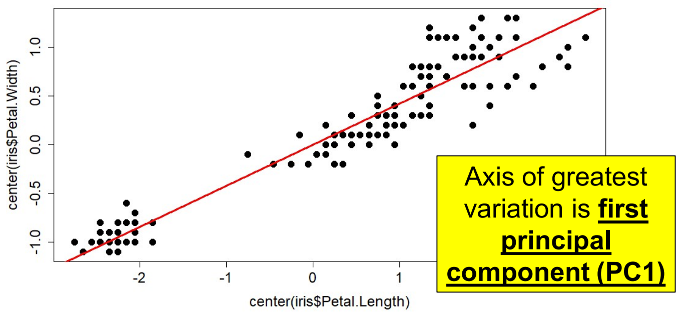
1. Fit line through axis of greatest variation

- E.g., `iris$Petal.Width` & `iris$Petal.Length`



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Principal components analysis

- PCA is ordination done on continuous variables
- How it works conceptually:

1. Center variables & fit line through axis of greatest variation in variables
2. Rotate plot, so PC1 is now on x-axis

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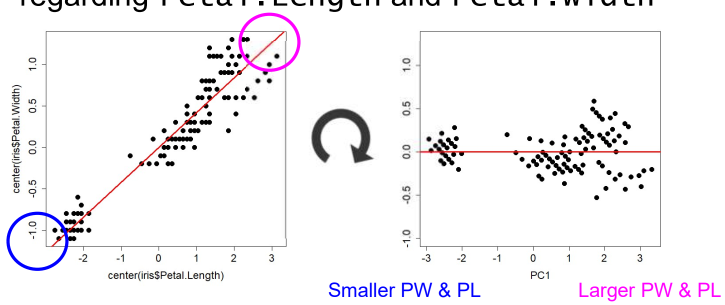
2. Rotate plot

- Larger PC1 scores → larger `Petal.Length` and `Petal.Width`, and vice versa
- Points closer in PCA space are more similar, regarding `Petal.Length` and `Petal.Width`



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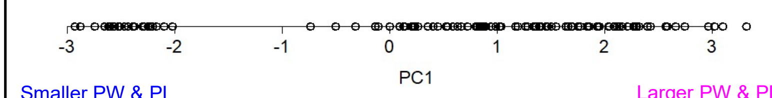
Data reduction

- Distilled two highly correlated variables into one (PC1)!
- Can now represent two variables with one (and thus one axis) that still captures 99% of the variation in the original MV dataset (to be explained later)



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Principal components analysis

- PCA is ordination done on continuous variables
- How it works conceptually:

1. Center variables & fit line through axis of greatest variation in variables
2. Rotate plot, so PC1 is now on x-axis
3. Subsequent PCs (e.g., PC2) are perpendicular to previous ones & explain residual (less) variation from previous PCs
   - Only have as many PCs as you do variables

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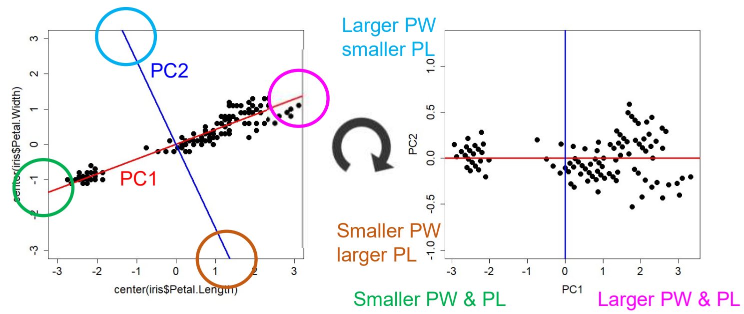
3. Subsequent PCs

- PC2 is perpendicular to (i.e., independent of) PC1
- More variation along PC1 → more variation in data explained by PC1 (99%)



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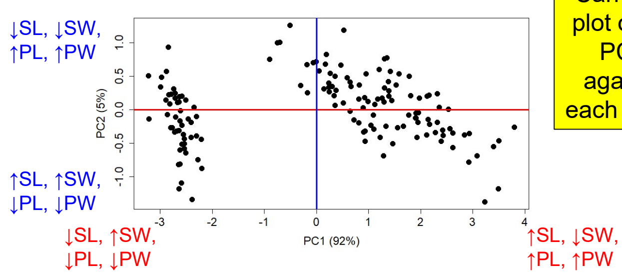
Visualizing many variables

- PCA most useful for visualizing >3 variables, which cannot be plotted (i.e., need >3 axes)
- E.g., `Sepal.Length, Sepal.Width, Petal.Length, Petal.Width`



Can also plot other PCs against each other

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Things to note thus far

- Can only have as many PCs as variables (though the later ones might explain very little variation in variables)
- PCs are perpendicular to and independent of each other (each can be thought of as explaining a different dimension of the data)
- Variation explained by PC1 > variation explained by PC2 > variation explained by PC3, etc.

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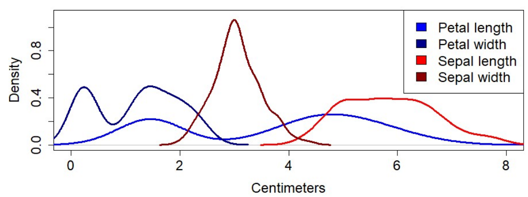
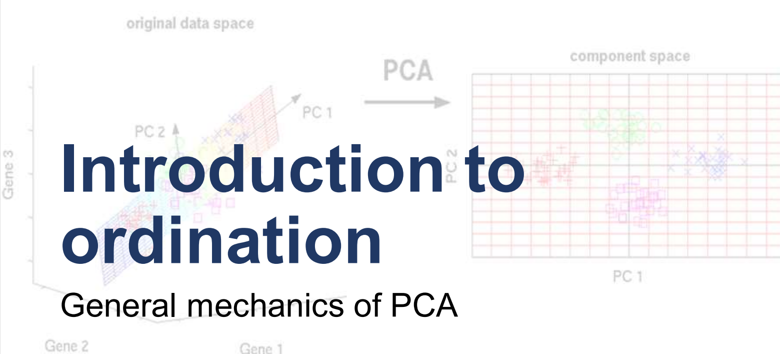
One more thing…

- Because PC1 is fit through axis of greatest variation, PC1 will be dominated by larger variables (which have more variation)
- Thus, it's common practice to scale variables first if they differ in units or orders of magnitude



Doesn't apply to `iris` dataset

Questions?



Introduction to ordination

General mechanics of PCA

PCA steps

1. Center variables & fit line through axis of greatest variation in variables
2. Rotate plot, so PC1 is now on x-axis
3. Subsequent PCs (e.g., PC2) are perpendicular to previous ones & explain residual (less) variation from previous PCs

- What PCA is *actually* doing is **singular value decomposition (SVD)** of the **variance-covariance matrix** of variables (not important)

Eigenvalues & eigenvectors

- SVD produces two main quantities we're interested in:

1. **Eigenvalues**: amount of variance in variables explained by each PC
   - Decreases as you go from PC1 to PC2 to PC3, etc.
2. **Eigenvectors**: direction of, e.g., PC1 given by 1st eigenvector of covariance matrix
   - Tells us how each PC is related to the original variables

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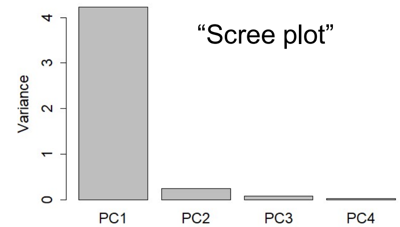
Eigenvalues

- `iris` dataset has four variables → four PCs → four eigenvalues
- Sum of eigenvalues = summed variance of each variable in original dataset

PC1 = 4.23
PC2 = 0.24
PC3 = 0.08
PC4 = 0.02
\- - - - - -
4.57



"Scree plot"

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Eigenvalues

- `iris` dataset has four variables → four PCs → four eigenvalues
- Can rescale to get % variance explained by each PC

PC1 = 100 x 4.23 / 4.57 = 92%
PC2 = 100 x 0.24 / 4.57 = 5%
PC3 = 100 x 0.08 / 4.57 = 1.7%
PC4 = 100 x 0.02 / 4.57 = 0.5%
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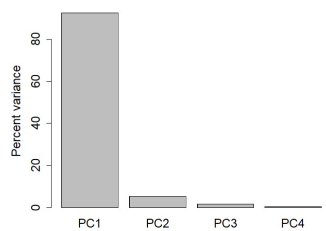
100%



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Eigenvectors

- Each PC is an eigenvector
- **Loadings:** how each original variable is correlated w/ & contributes to each PC
- Ranges from -1 to 1, where sign indicates direction of relationship btw. variable and PC & magnitude indicates strength of "correlation"

	PC1	PC2	PC3	PC4
Sepal.Length	0.36	-0.66	0.58	0.32
Sepal.Width	-0.08	-0.73	-0.60	-0.32
Petal.Length	0.86	0.17	-0.08	-0.48
Petal.Width	0.36	0.08	-0.55	0.75

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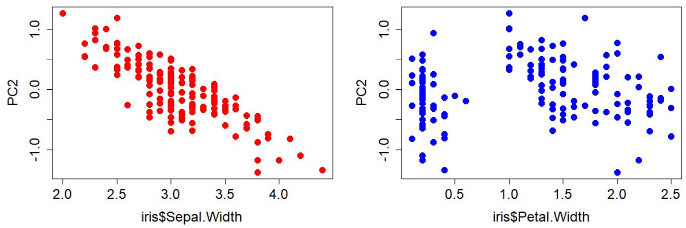
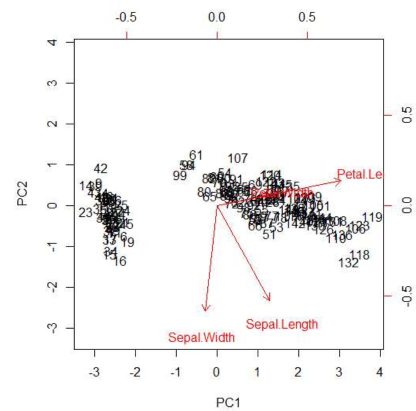
Loadings

	PC1	PC2	PC3	PC4
Sepal.Length	0.36	-0.66	0.58	0.32
Sepal.Width	-0.08	$\boxed{-0.73}$	-0.60	-0.32
Petal.Length	0.86	0.17	-0.08	-0.48
Petal.Width	0.36	$\boxed{0.08}$	-0.55	0.75



Plotting of loadings

	PC1	PC2
Sepal.Length	0.36	-0.66
Sepal.Width	-0.08	-0.73
Petal.Length	0.86	0.17
Petal.Width	0.36	0.08



Loadings

- Also describes how to transform data from original variable coordinate system to PCA space and back
  - **Scores**: coordinates of each data point in PCA space
- E.g., to get PC1 score of Plant #1, multiply plant's measurement for each variable (after centering) by corresponding PC1 loading and then sum everything

Loadings

Plant #1 (after centering)

Sepal.Length	Sepal.Width	Petal.Length	Petal.Width
-0.7	0.4	-2.36	-1.0

Loadings

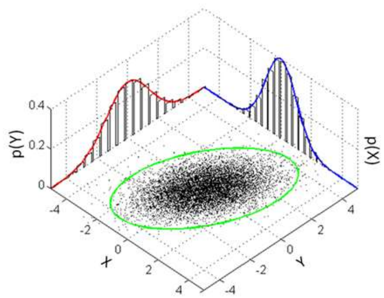
	PC1
Sepal.Length	0.36
Sepal.Width	-0.08
Petal.Length	0.86
Petal.Width	0.36

Plant #1 PC1 score = -0.7 x $\boxed{0.36}$ + 0.4 x $\boxed{-0.08}$ + -2.36 x $\boxed{0.86}$ + -1.0 x $\boxed{0.36}$ = **-2.68**

Loadings act as weights! Quantifies how much each variable linearly contributes to PC score

PCA assumptions

- Variables are multivariate normally distributed



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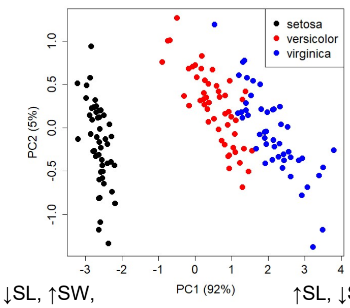
Example of a hypothesis test



↓SL, ↑SW,
↓PL, ↓PW

↑SL, ↓SW,
↑PL, ↑PW

- Does PC1 sig. differ among species?
- ANOVA: $P < 2.2e\text{-}16$
- Or how does PC1 vary ~ N level?

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Questions?

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Summary

- MV models: multiple DVs ~ one or more IVs
  - Takes into account correlation between DVs
- Ordination distills multiple variables into a few important, independent axes (good for visualization!)
- PCA is ordination for continuous variables
  - Eigenvalues: variance explained by each PC
  - Eigenvectors: loadings tell us how much each variable contributes to each PC

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