SDSC Summer Institute 2020

ML3 - Data Preparation
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08/05/20
Location: Breakout Room
Gitter (session support): Breakout Room
Gitter (general system support): Help Desk

Overview

- Highlights of data prep
- Variable Selection and Reduction

The Importance of Data Prep

- **“Garbage in, garbage out”**
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But also heuristics

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  - Cleaning – outliers, missing data

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In a nutshell, prepare data for modeling

Missing Data – explore them

- **Get frequency counts and indices of missing variables**

Are the missing entries missing-at-random?

Quick Approaches

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```
foo      = function(x){sum(is.na(x))}      #a count of 'na' in x
sapply(X_data,foo)                         #apply foo to each column
X_data = subset(X_data,select=-c(your_col_name))  #delete a column
```

Imputation

- **Simple: Replace missing values with the mean**

Imputation

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- **Complicated but most accurate:**

  Use a model (based on other attributes) to infer missing values

R and imputation

- **Several packages, such as ‘mice’ , ‘amelia’**

- **Iteratively estimate missing data in one column using data in other columns**

  Mice uses Gibbs sampling (slower)

  Amelia uses Expectation Maximization (faster)

R and imputation

- **‘Amelia’ package example**

  300K+ rows and 50 attributes from UN voting data
  1K-100K entries missing per col for about 20 cols

  Not run on user’s laptop; took about 1 hour on a Comet compute node

R and imputation

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Identify the 'id' variables

```
library('amelia')
 a.out <- amelia(data,
                 idvars = …c("country-id"),
                 m=10, parallel = "multicore")
```

Run 10 models in parallel

Variable Transformations

- Normalize or Scale data (if needed)
- Engineer new features (if it helps)
- Combine attributes (e.g. rates and ratios)
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If variables are on different scales

Use prior knowledge

Normalizing or scaling

- **Mean center** $x_{new} = x - \text{mean}(x)$
- **z-score** $score = \frac{x - \text{mean}(x)}{\text{std}(x)}$
- **Scale to [0…1]** $x_{new} = \frac{x - \min(x)}{\max(x) - \min(x)}$
- **log scaling** $x_{new} = \log(x)$

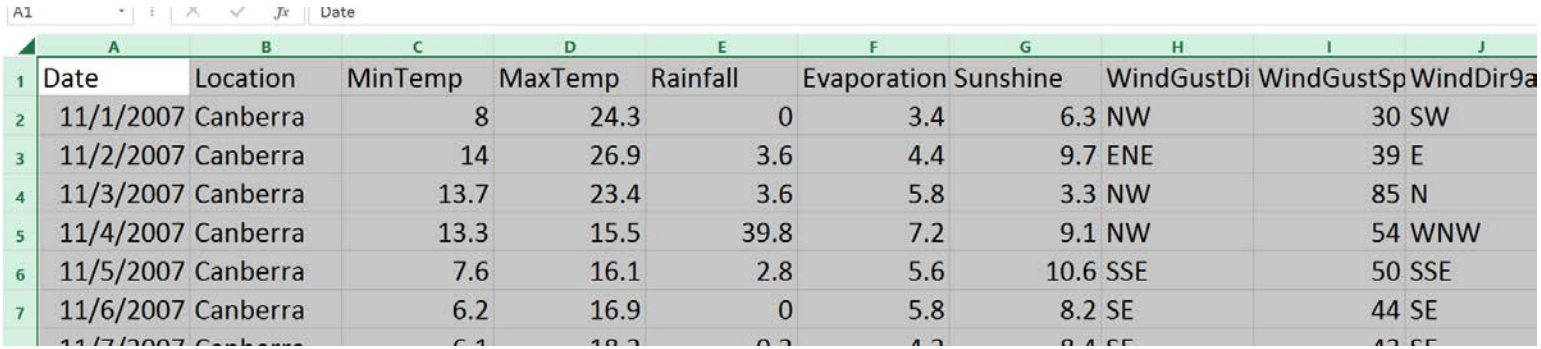
Data Wrangling

- **Organizing data for modeling**

lots of R packages and functions for date strings, matching, selecting, grouping, gathering, reading, etc…

We'll look at a couple of examples

Data Wrangling - Long to Wide transformation



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date, location and the rest identify the row

WindGustDir and WindGustSpeed are repeatedly measured and measurements are on different rows

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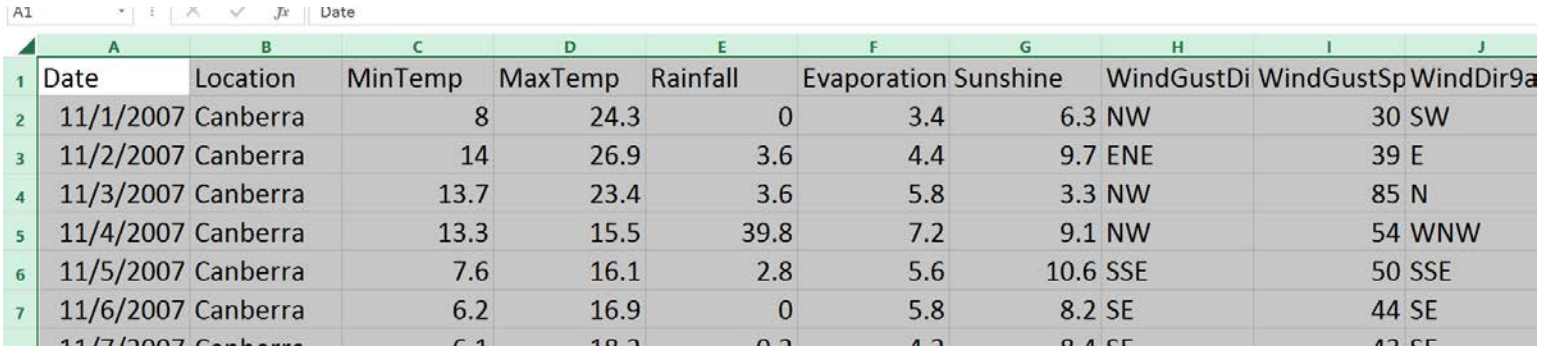

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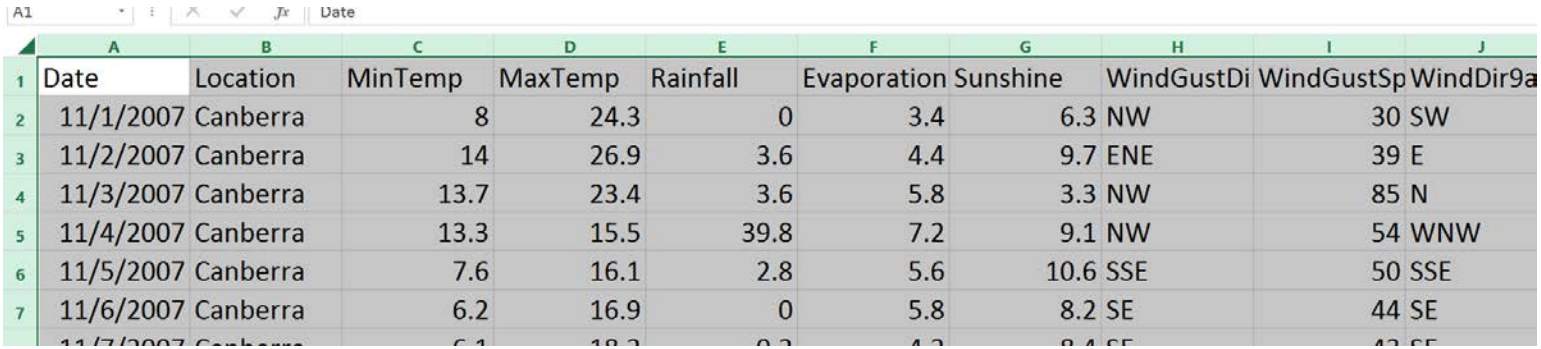

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```
library(reshape2)
W_long   =dcast(W_df,
          formula=Date+Location+ ...~
```

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Put variable that has labels for the repeated measures

```
library(reshape2)
W_wide   =dcast(W_df,
          formula=Date+Location+ ...~ <<<variable-name>>>,
```

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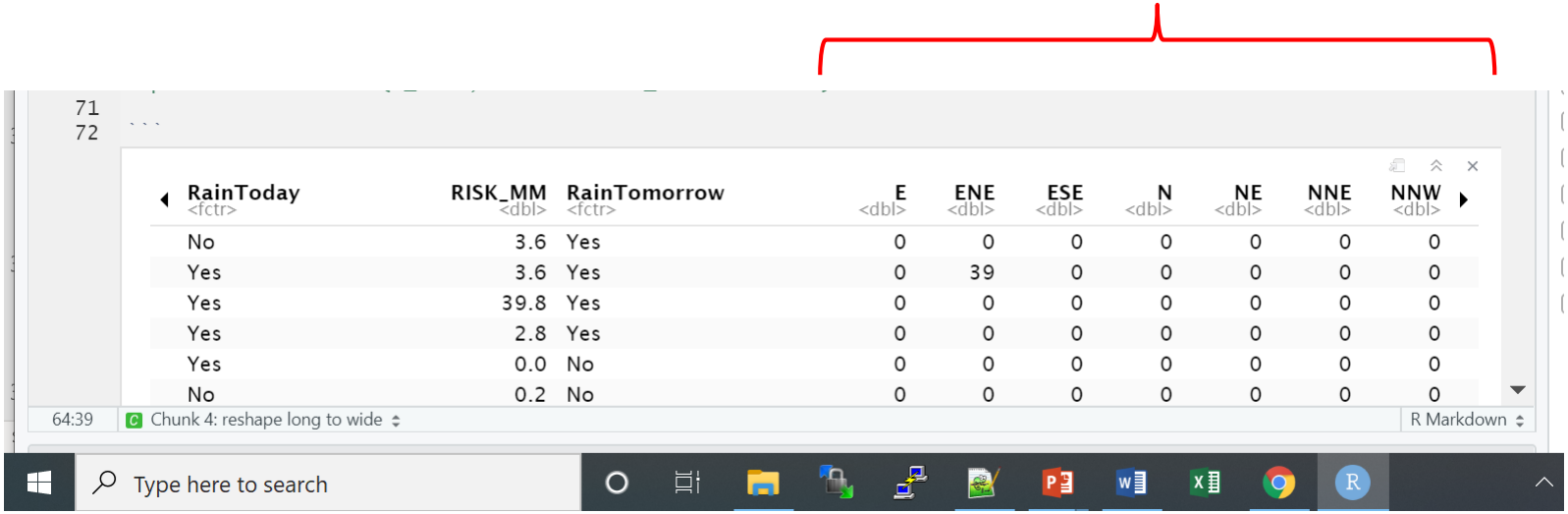
Put variable that has labels for the repeated measures

```
library(reshape2)
W_wide   =dcast(W_df,
          formula=Date+Location+ ...~ <<<variable-name>>>,
          fill=0,
          value.var="<<<variable-name>>>")
```

Indicate variable that has the repeated measurement values

Transformed Data Matrix

After running dcast: WindGustDir category labels are new columns



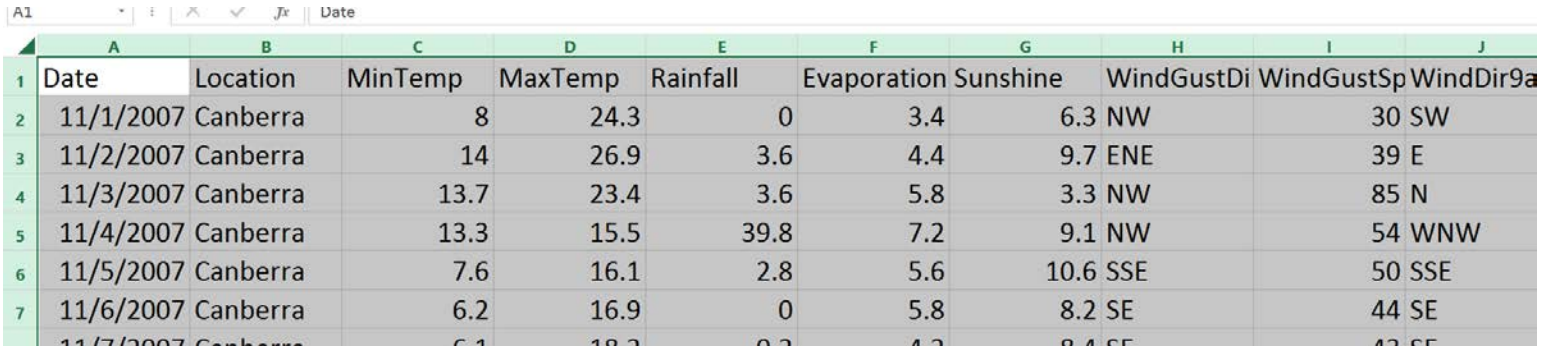
71
72 ```

RainToday <fctr>	RISK_MM <dbl>	RainTomorrow <fctr>	E <dbl>	ENE <dbl>	ESE <dbl>	N <dbl>	NE <dbl>	NNE <dbl>	NNW <dbl>
No	3.6	Yes	0	0	0	0	0	0	0
Yes	3.6	Yes	0	39	0	0	0	0	0
Yes	39.8	Yes	0	0	0	0	0	0	0
Yes	2.8	Yes	0	0	0	0	0	0	0
Yes	0.0	No	0	0	0	0	0	0	0
No	0.2	No	0	0	0	0	0	0	0

64:39 Chunk 4: reshape long to wide R Markdown

Type here to search

Data Wrangling – grouping



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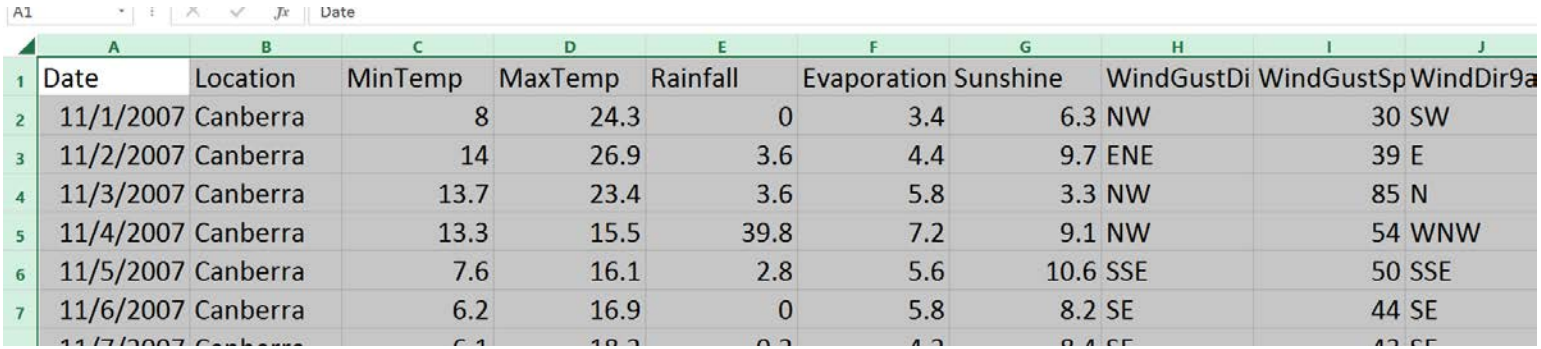

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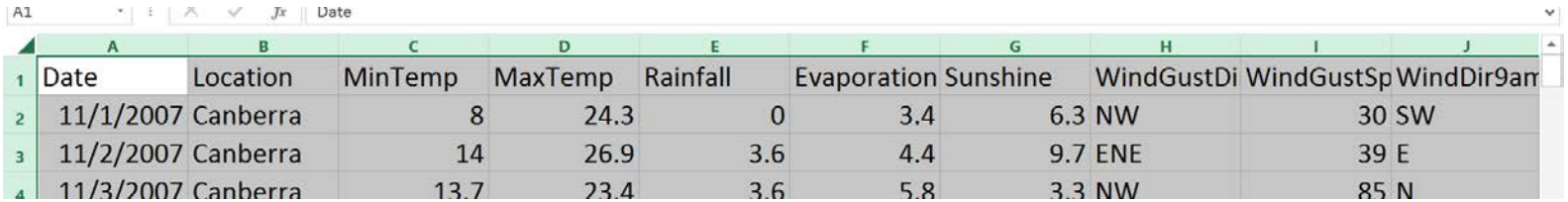

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Identify groups of the values of WindGustDir

```
library(dplyr)

a1 <- group_by(na.omit(W_df), WindGustDir)
```

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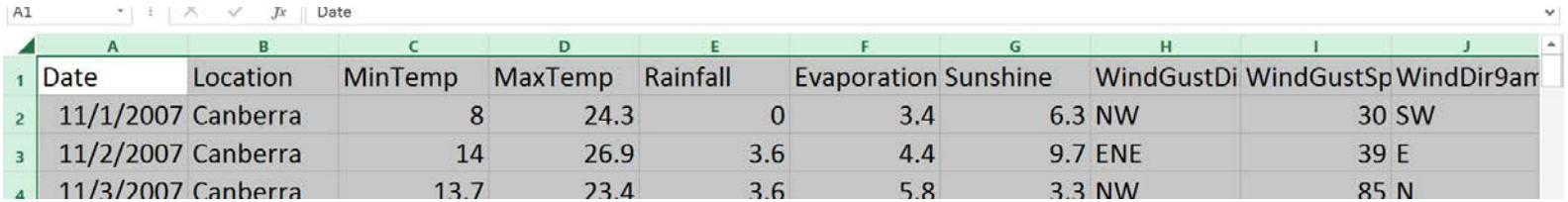

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```
library(dplyr)

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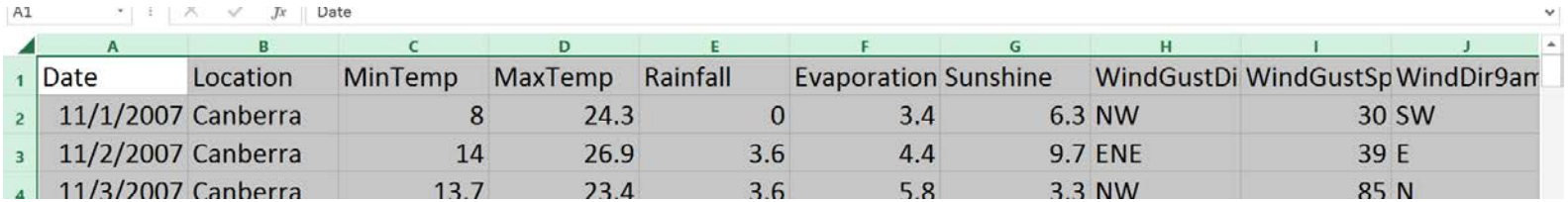

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```
library(dplyr)

a1 <- group_by(na.omit(W_df), WindGustDir)
a2 <- select(a1,WindSpeed9am,Temp9am)
a3 <- summarise(a2,
  avg_speed = mean(WindSpeed9am, na.rm = TRUE),
  avg_temp  = mean(Temp9am, na.rm = TRUE)  )
```

Summarise

R exercise

Use “reshape2” library to

1. “cast” repeated measurements into one row (long to wide): <<< fill-in variable names >>>

[Extra: “melt” row back into repeated measurements]

2. Use “dplyr” library to perform grouping and aggregations: <<< fill-in variable names >>>

and compare that to ‘reshape’ with ‘sum’

pause

Reading Material

- **Data Preparation for Data Mining by Dorian Pyle**
  - http://www.ebook3000.com/Data-Preparation-for-Data-Mining_88909.html
- **Data mining – Practical Machine learning tools and techniques by Witten & Frank**
  - http://books.google.com

Many Variables

- **More variables => more information, but also more noise and more ways of interactions**

- **2 ways to handle many variables**
  - Variable Selection
  - Dimension reduction methods

Variable selection

- **Heuristically, pick off or put in 1 variable at a time (step wise)**

  based on some criteria, like correlation with outcomes

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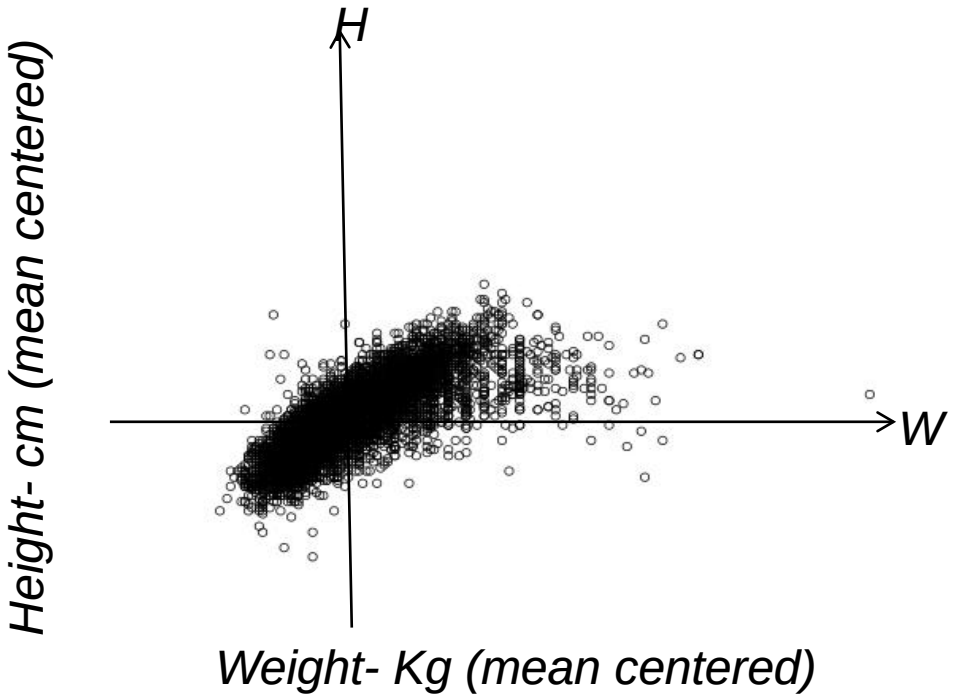
Conversely, want features that contribute to variations of the data

Example: Athletes' Height by Weight



Find a line that aligns with the data.

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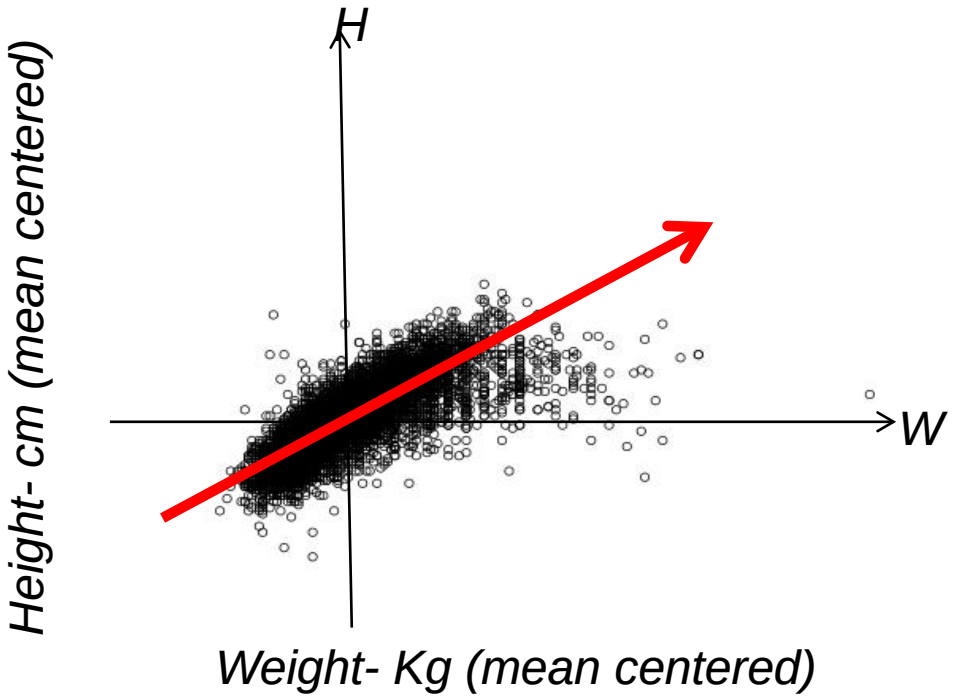

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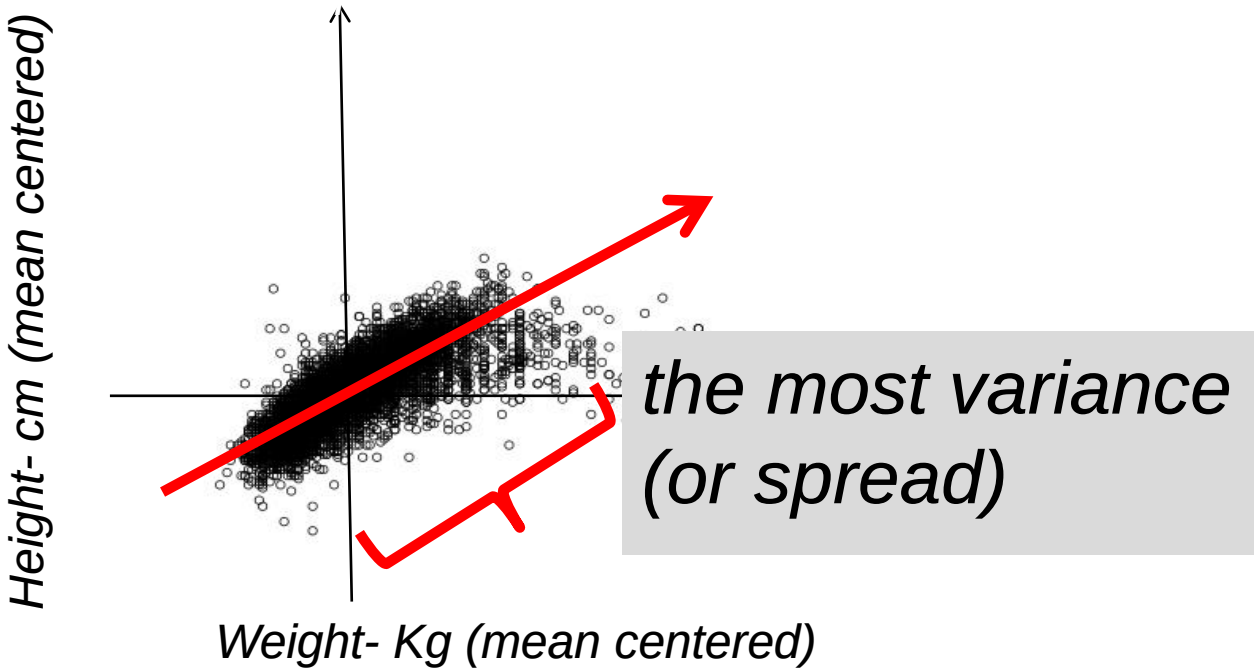

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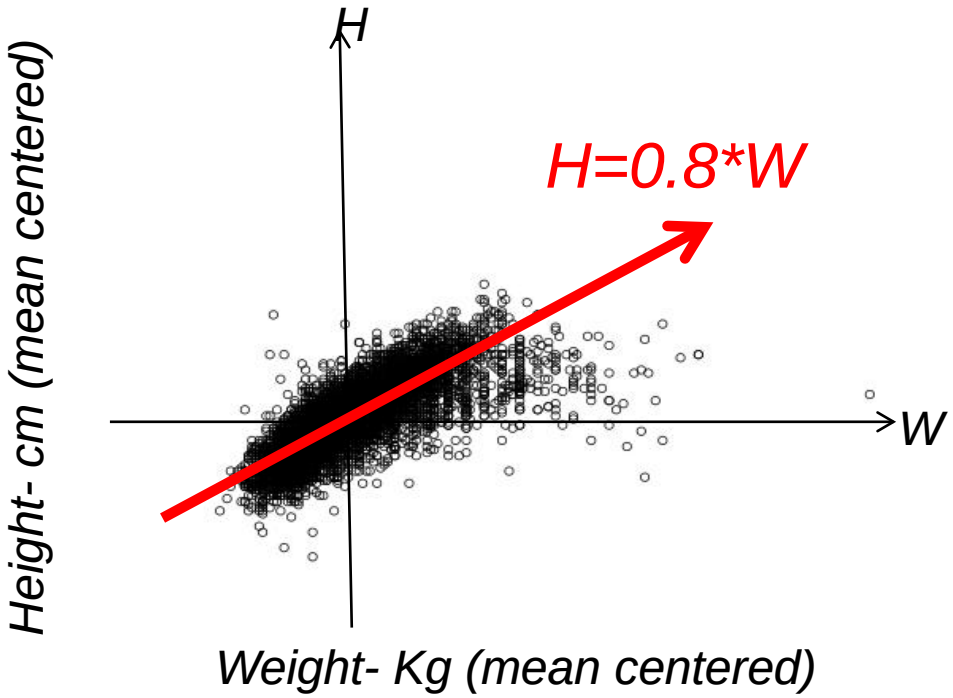
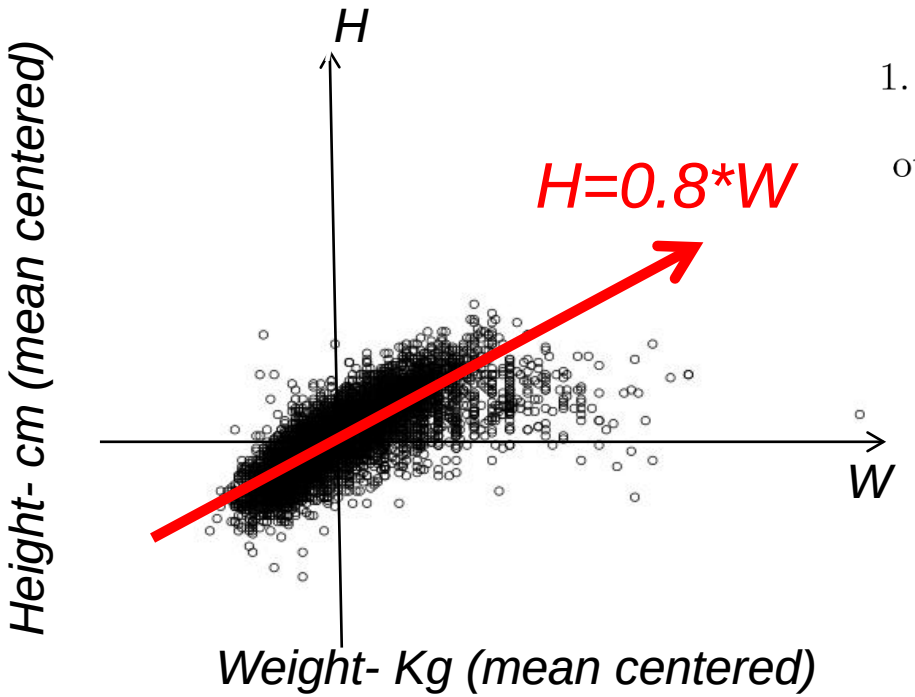


Find a line that aligns with the data.

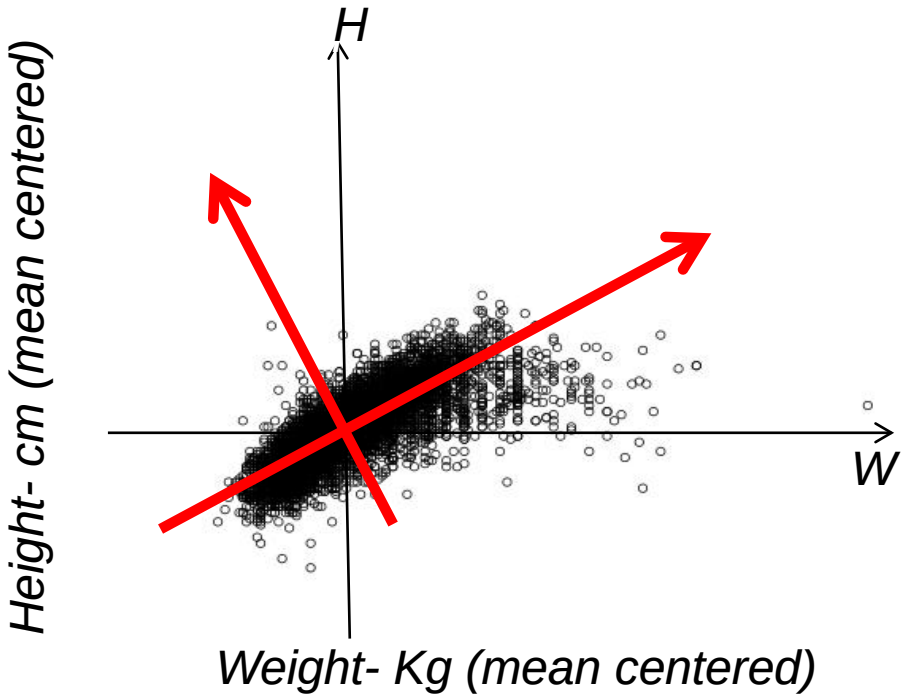
Note that ***(0,0) and (1,0.8) are points on the line that are combinations of H,W***



1. The vector in HxW space: $v = \begin{pmatrix} W = 1 \\ H = 0.8 \end{pmatrix}$

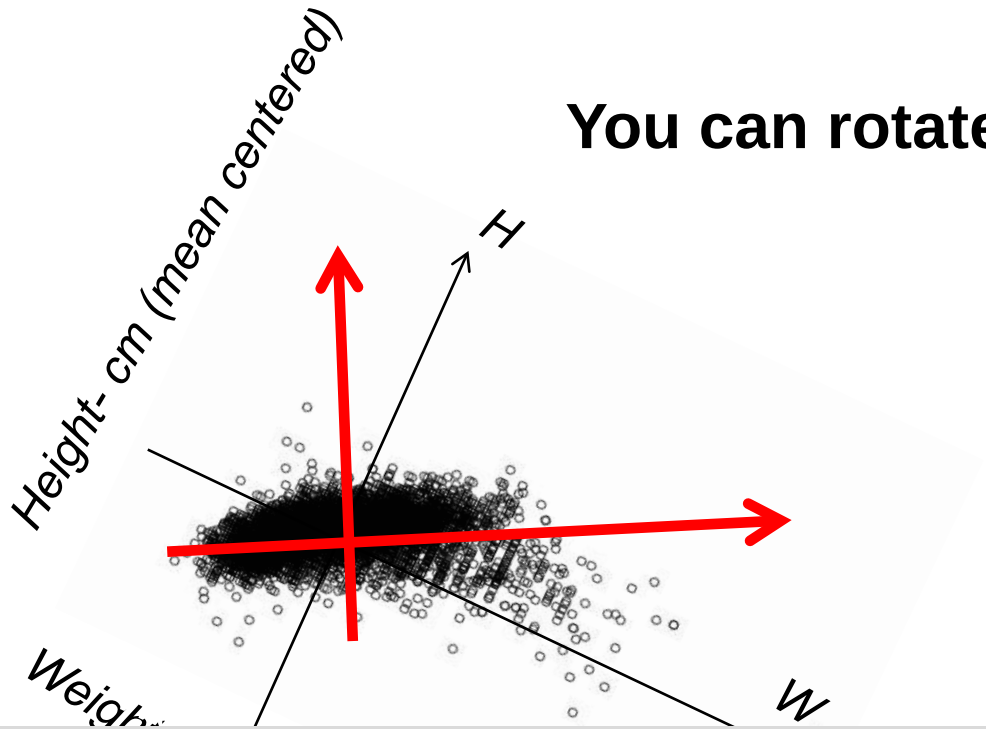
other points also satisfy H=0.8*W : $\alpha * v$

Find a line that aligns with the data.



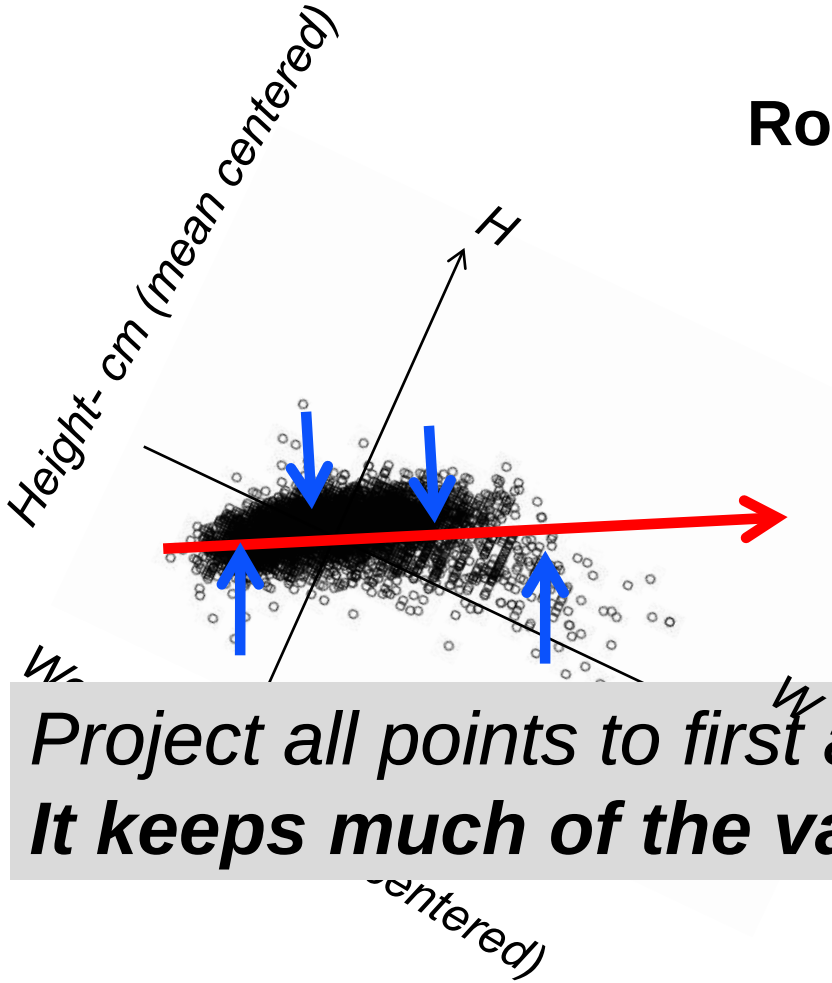
The next direction of most variance.

You can rotate the axes



New axes (i.e., new features or latent factors) are combinations of old axis

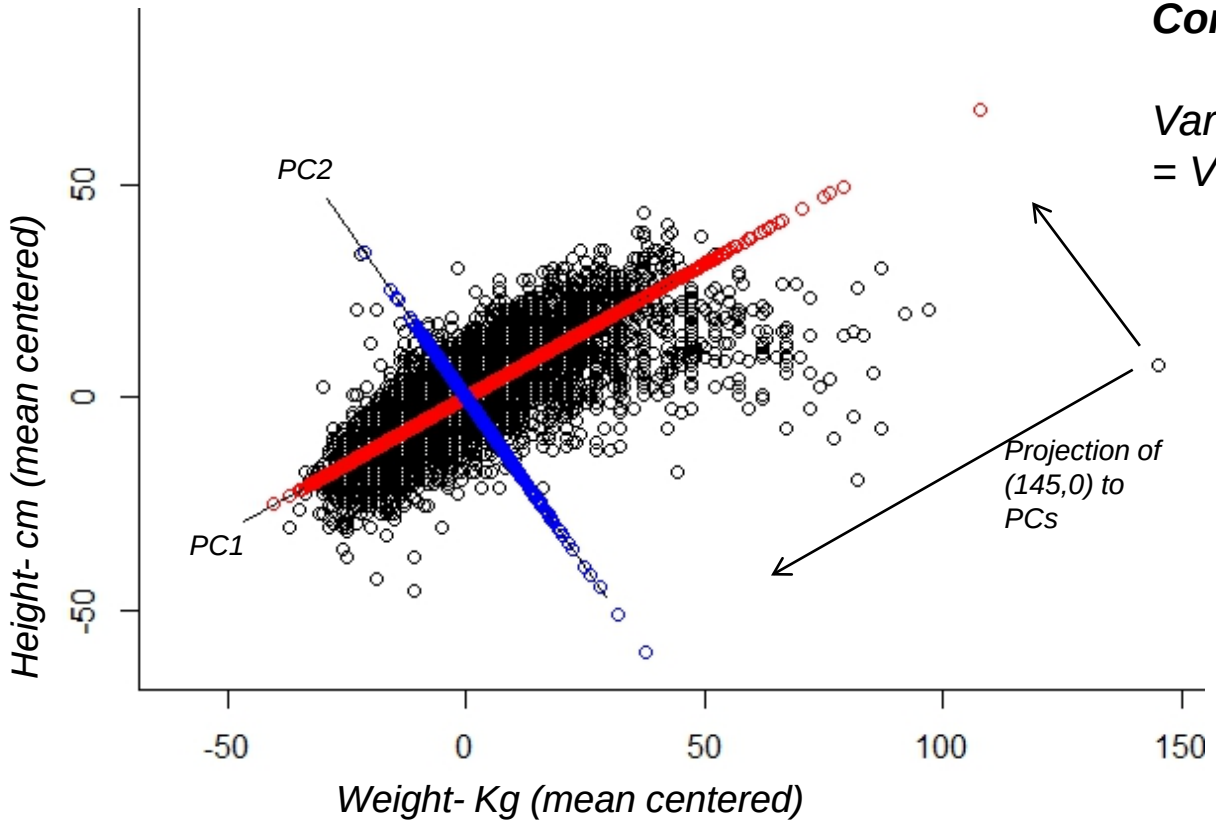
Rotate axis



Project all points to first axis

It keeps much of the variance

Note: this factorization conserves total variance



Total Variance Conserved:

Var in Weight + Var in Height
= Var in PC1 + Var in PC2

Best Known Algorithms

SVD (singular value decomposition)

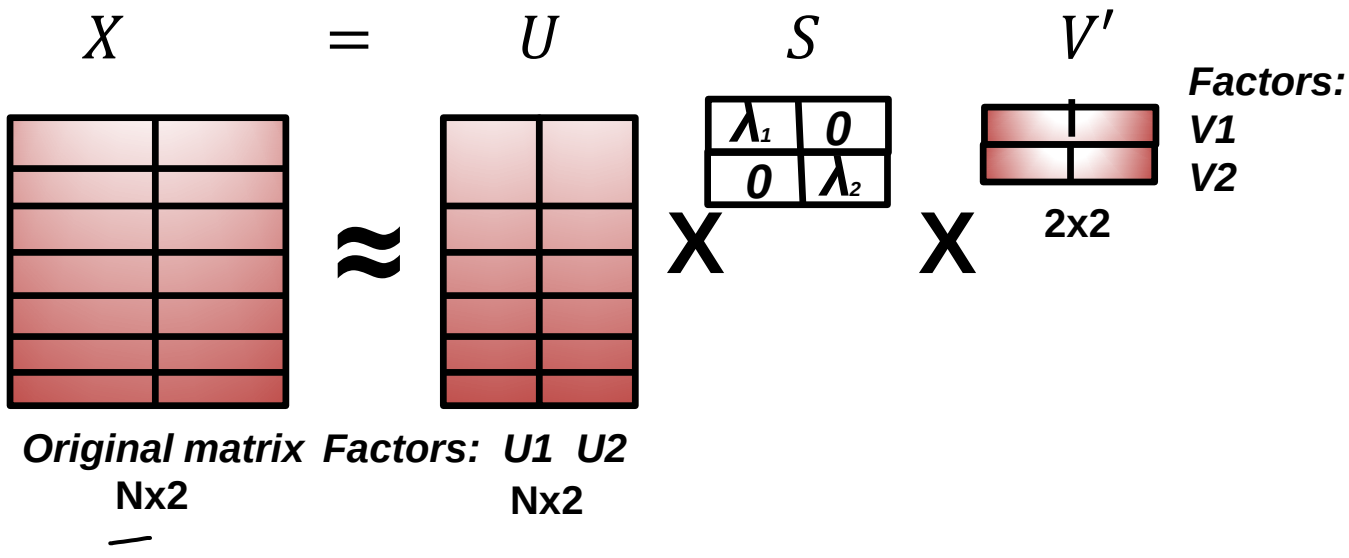
PCA (principle component analysis)

SVD more generally works on non square matrices

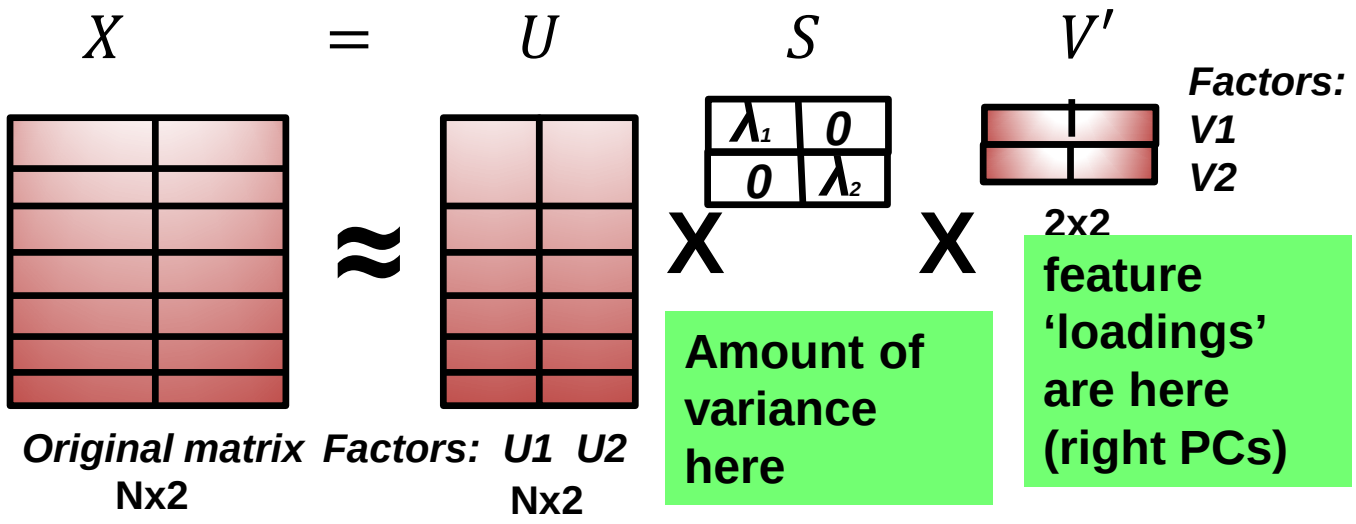
SVD decomposes X matrix into factors (ie column vectors) and 'singular' values

$$X = U S V'$$

SVD decomposes X matrix into factors (ie column vectors) and 'singular' values



SVD decomposes X matrix into factors (ie column vectors) and 'singular' values



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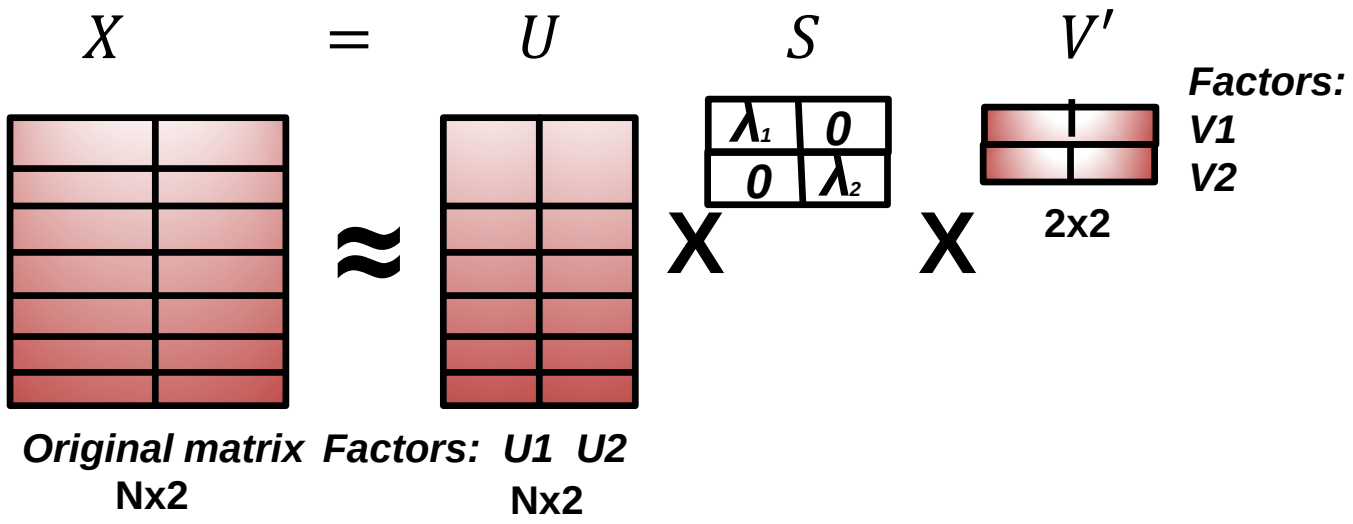

For U,S,V with less than P dimensions it is an approximation $X \sim U\ S\ V'$

The V here is same as in Principle Components (up to a sign change) of cov(X) matrix

Using PCs

- **SVC or PCA:**

  only use numeric columns, center and normalize

Use for dimension reduction, visualization, examine factor scores/loadings

Combine with clustering, regression, classification, etc…

Run the SVD exercise for practice and later it with K-means clustering

Note, the SVD command in R looks like this:

```
> Xsvd=svd(X)

> str(Xsvd)

List of 3
 $ d: num [1:9] 27442.7 231.2 96.4 68.2 44.5 ...
 $ u: num [1:363, 1:9] -0.0524 -0.0521 -0.052 -0.0519 -0.0525 ...
 $ v: num [1:9, 1:9] -0.005042 -0.014276 -0.000969 -0.00314 -0.005491 ...
```

- **end**