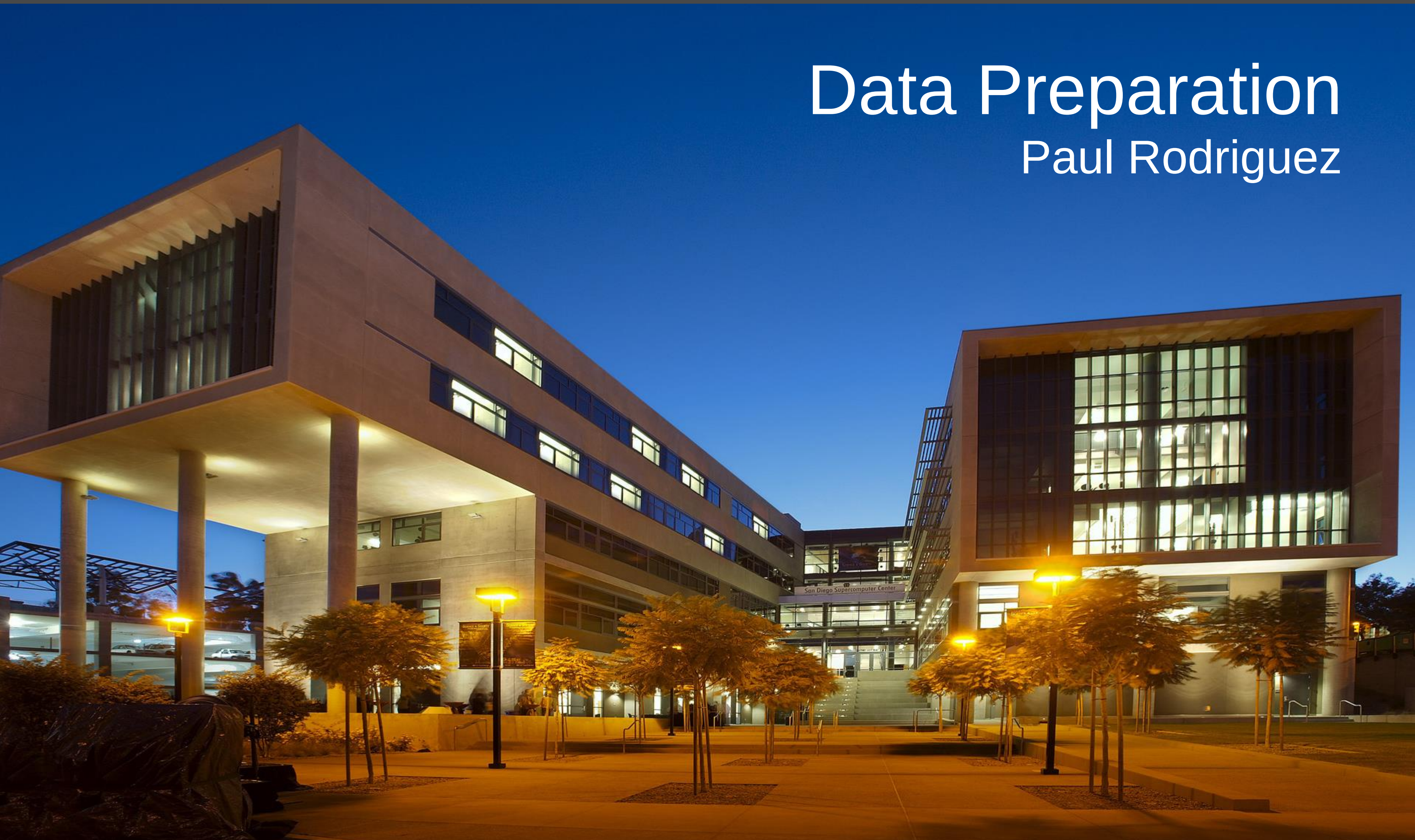
# Data Preparation

Paul Rodriguez



# On the Importance of Data Prep

- “Garbage in, garbage out”
- Sometimes takes 60-80% of the whole data mining effort

# Working definition

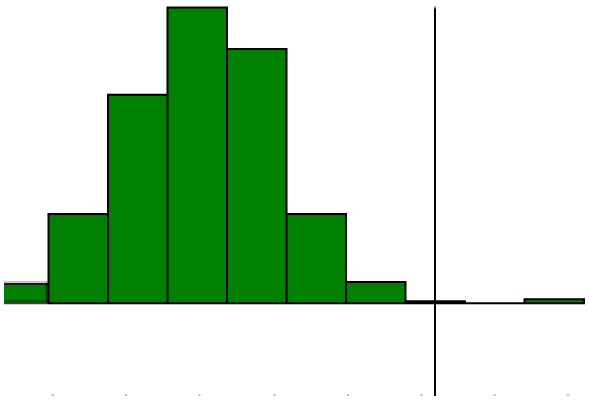
- **Data Preparation:**
  - Cleaning
  - Filtering
  - Transforming
  - Organizing the data matrix (aka ‘data wrangling’ or ‘data munging’)
  - Variable Selection/Dimension Reduction

*In a nutshell, know your variables and prepare data for modeling*

# Statistical Noise:

- Outliers

e.g. remove them,

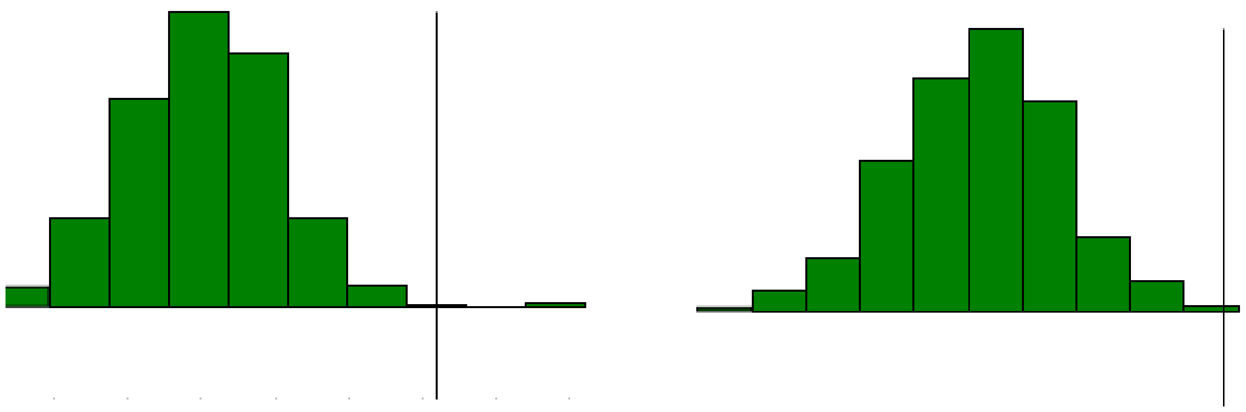


***mean + 3*std-dev***

# Statistical Noise:

- Outliers

e.g. remove them, but cutoff sometimes seems arbitrary



***mean + 3*std-dev***

# Cleaning Noise

- Entity Resolution and Record Linkage

e.g. Are these equal?

***West Main Street*** ***W Main St***

**Strategy:**
***use dictionaries and search possible matches***

# Missing Data (NA vs NULL)

- **Not applicable - NA**

  e.g. spouse name depends on marital status

- **Not available - NULL**

  unknown

  not entered

- **In R:**

  NA is logically missing (ie the value is not available – null)

  NULL is object not yet defined (ie the object is not available)

# Missing Data

- **What are frequency counts of missing variables?**

  Are entries missing completely at random or contingent on some other variable?

# Quick Approaches

- Delete instances

and/or

- Delete attributes with high missing-ness

# Quick Approaches

- Leave as missing
  - Some algorithms implementation handle missing values (ie Decision Trees)

# Simple Imputation

- Use the attribute mean
- Use the attribute mean for each class label

# Complicated Imputation

- **Use a model (based on other attributes) to infer missing value**

# Complicated Imputation

- **Use a model (based on other attributes) to infer missing value**

***Best strategy depends on***

***time vs accuracy tradeoffs***

# R and missing data

- **Several packages, such as 'mice' , 'amelia'**
- **Produces multiple data sets**
- **Iterates over missing data estimates and linear model estimates**
    - Mice uses Gibbs sampling (slower)
    - Amelia uses Expectation Maximization (faster)
- **Beware of correlation in variables**
    - Matrices not invertible

# R and missing data

- **'Amelia' package example**
  - 50 attributes from UN voting data
  - 1K-100K entries missing per col for about 20 cols
  - 300K rows ~ 1 hour on Gordon compute node (not run on the user's PC)

*time variable for time series models*

*cross section to select temporal periods*

*ignore 'id' variables*

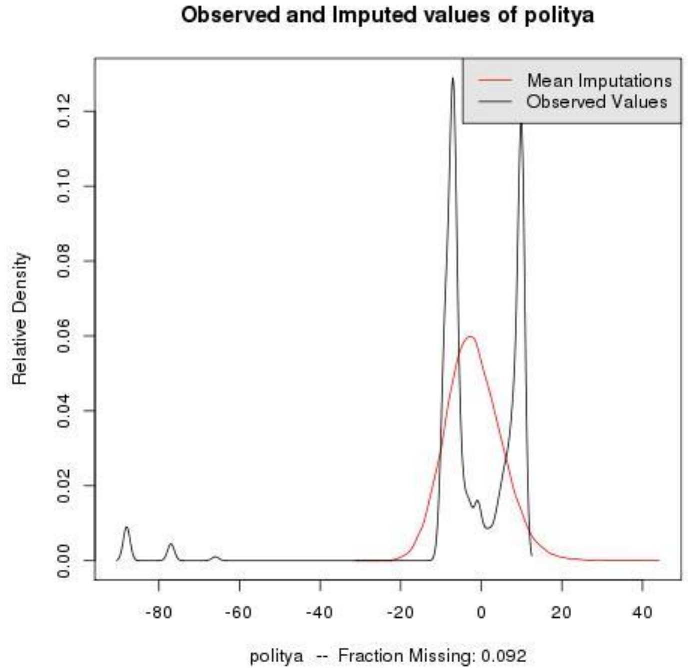
```
# run the imputation
library('amelia')
 a.out <- amelia(data, ts = "year", cs = "dyadid",
              idvars = c("dyadidyr", "cntryera", "statea", "stateb"),
              intercs=FALSE, p2s = 2, m=10, parallel = "multicore")
```

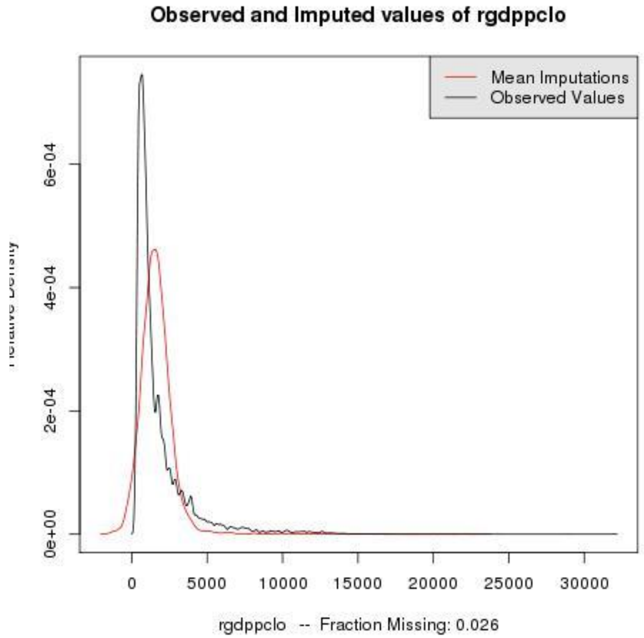
*interactions*

*parallel options*

# R and missing data

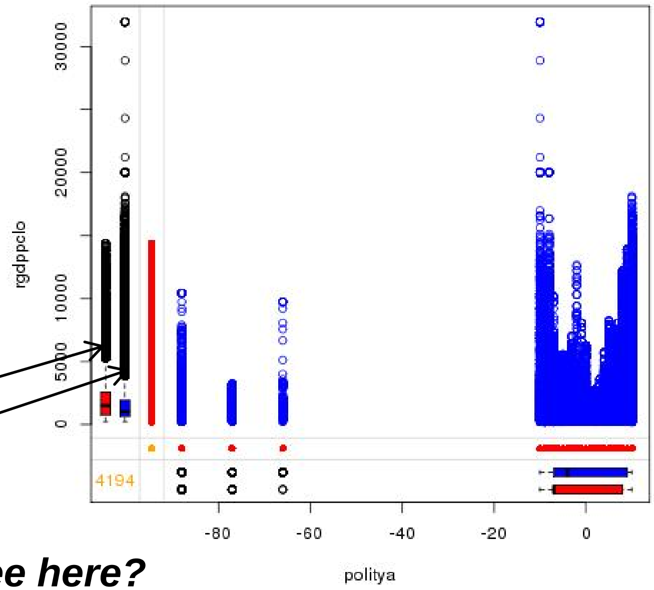
**#QA on missing data by comparing density of imputated & original data**
**compare.density(a.out, var="politya")**
**compare.density(a.out,var='rgdpcontg')**



# R and missing data

```
# Useful library for printing margin plots, to compare histograms
#                         conditional on missing/non-missing data
library('VIM')
marginplot(gart2use[,c('politya', 'rgdppclo')],
  col=c('blue','red','orange')
```




***dist of rgdppclo when***
***politya missing***
***politya present***

***What would you want to see here?***

# Variable Transformations

- **Engineer new features**
- **Combine attributes**
  e.g.  rates and ratios
- **Normalize or Scale data**
- **D**iscretize data
  (perhaps more intuitive to deal with binned data)

# Feature Engineering is Variable Enhancement

- **Use Domain and world knowledge**

- **Example: given date and location of doctor visits**

  a new variable for Number-of-1st-time-visits

  deduce a new variable for Number-of-visits-over-25-miles

  deduce a new variable for Amount-of-time-between-visits

# Re-scaling

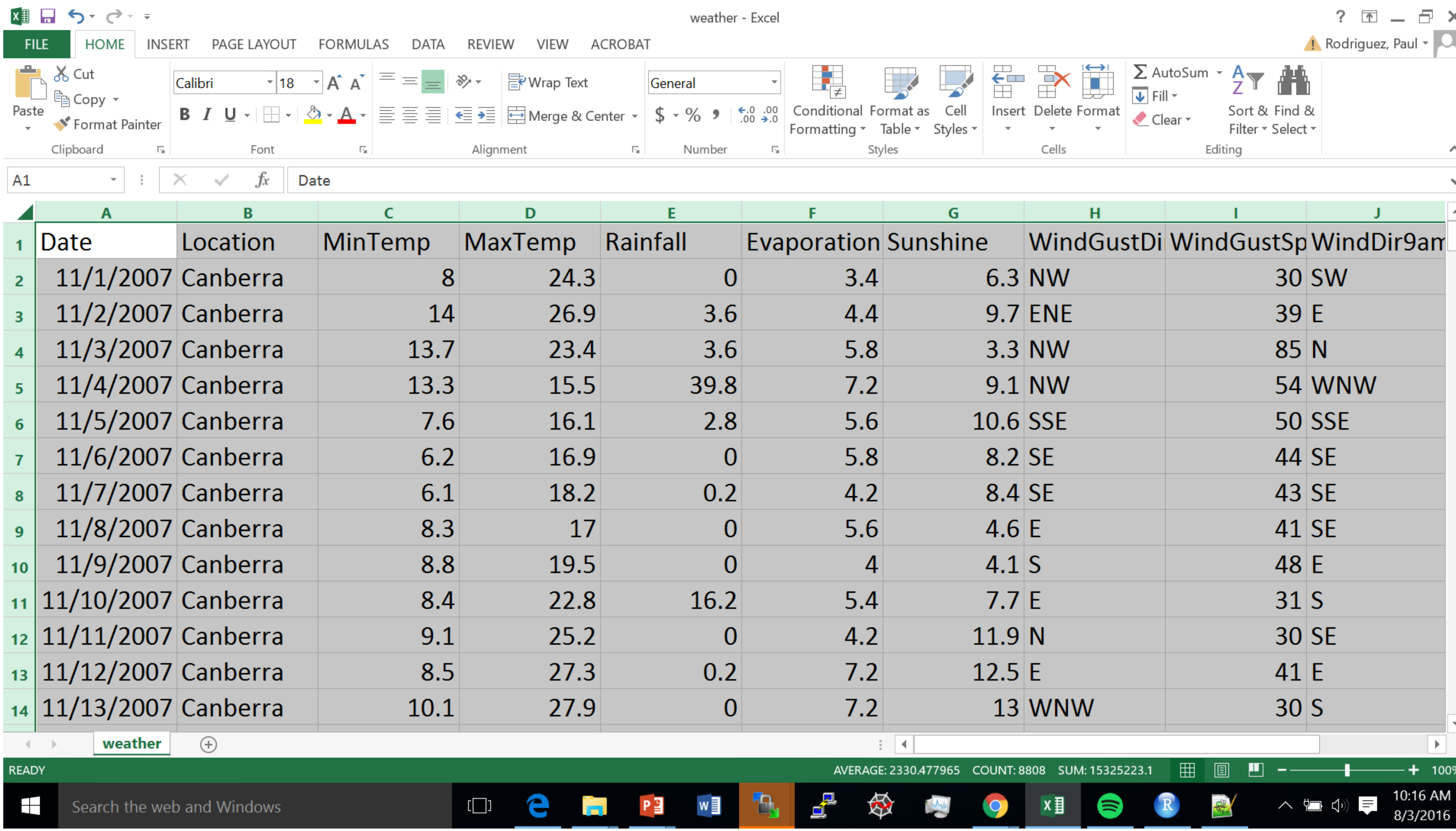
- **Mean center** $$x_{new} = x - \mathrm{mean}(x)$$
- **z-score** $$score = \frac{x - \mathrm{mean}(x)}{\mathrm{std}(x)}$$
- **Scale to [0…1]** $$x_{new} = \frac{x - \min(x)}{\max(x) - \min(x)}$$
- **log scaling** $$x_{new} = \log(x)$$

# Generally

- Preparing data is based on statistical principles,

- But also heuristics

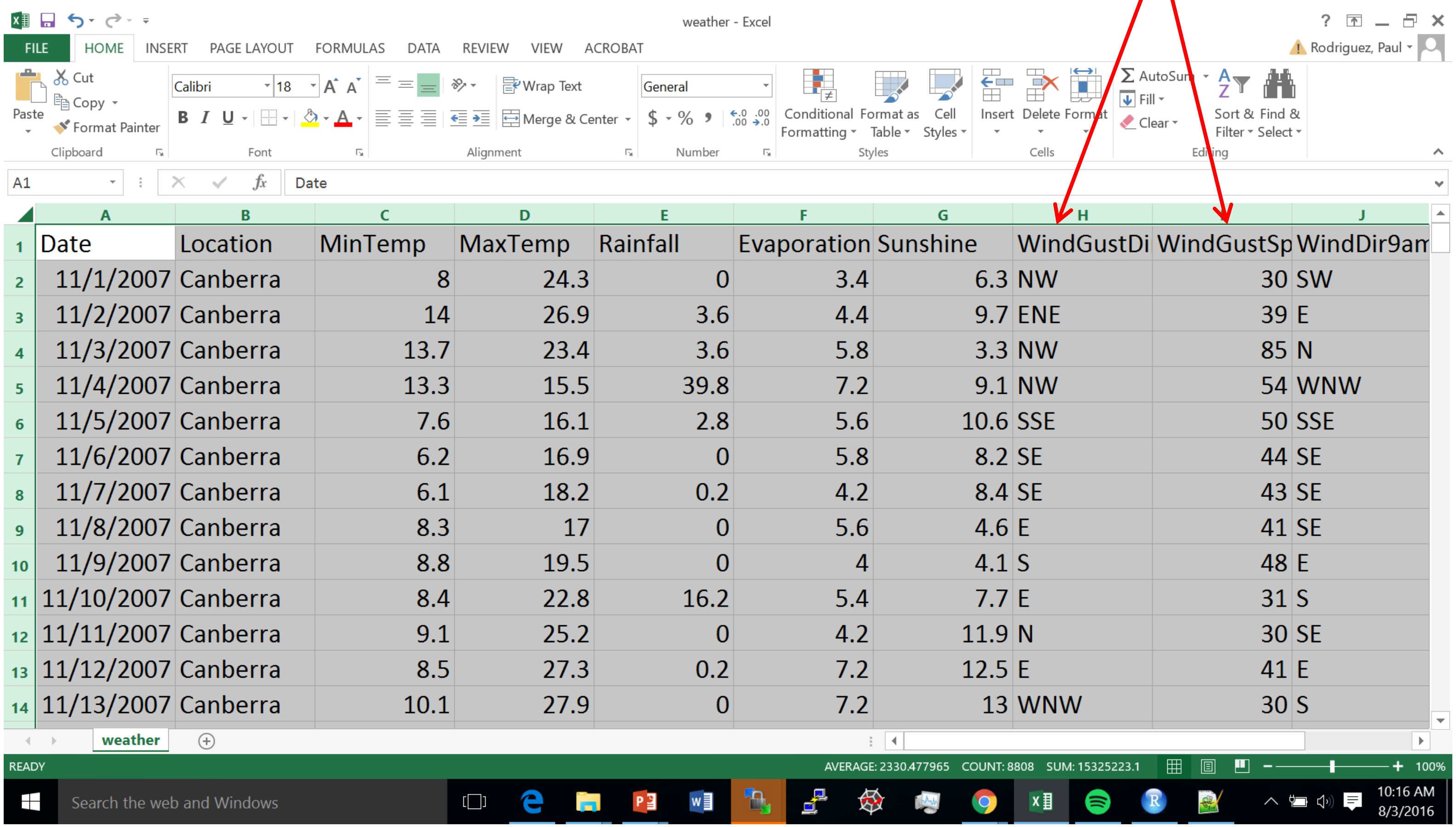
# Data Wrangling Exercise: Weather Data



| Date | Location | MinTemp | MaxTemp | Rainfall | Evaporation | Sunshine | WindGustDi | WindGustSp | WindDir9am |
|---|---|---|---|---|---|---|---|---|---|
| 11/1/2007 | Canberra | 8 | 24.3 | 0 | 3.4 | 6.3 | NW | 30 | SW |
| 11/2/2007 | Canberra | 14 | 26.9 | 3.6 | 4.4 | 9.7 | ENE | 39 | E |
| 11/3/2007 | Canberra | 13.7 | 23.4 | 3.6 | 5.8 | 3.3 | NW | 85 | N |
| 11/4/2007 | Canberra | 13.3 | 15.5 | 39.8 | 7.2 | 9.1 | NW | 54 | WNW |
| 11/5/2007 | Canberra | 7.6 | 16.1 | 2.8 | 5.6 | 10.6 | SSE | 50 | SSE |
| 11/6/2007 | Canberra | 6.2 | 16.9 | 0 | 5.8 | 8.2 | SE | 44 | SE |
| 11/7/2007 | Canberra | 6.1 | 18.2 | 0.2 | 4.2 | 8.4 | SE | 43 | SE |
| 11/8/2007 | Canberra | 8.3 | 17 | 0 | 5.6 | 4.6 | E | 41 | SE |
| 11/9/2007 | Canberra | 8.8 | 19.5 | 0 | 4 | 4.1 | S | 48 | E |
| 11/10/2007 | Canberra | 8.4 | 22.8 | 16.2 | 5.4 | 7.7 | E | 31 | S |
| 11/11/2007 | Canberra | 9.1 | 25.2 | 0 | 4.2 | 11.9 | N | 30 | SE |
| 11/12/2007 | Canberra | 8.5 | 27.3 | 0.2 | 7.2 | 12.5 | E | 41 | E |
| 11/13/2007 | Canberra | 10.1 | 27.9 | 0 | 7.2 | 13 | WNW | 30 | S |

# Transforming Weather Data Matrix

***Let's consider WindGustDir as a repeated measurement***
***Do we want that all in one row? Or in their own row?***
***- depends on the analysis***



| Date | Location | MinTemp | MaxTemp | Rainfall | Evaporation | Sunshine | WindGustDi | WindGustSp | WindDir9am |
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| 11/4/2007 | Canberra | 13.3 | 15.5 | 39.8 | 7.2 | 9.1 | NW | 54 | WNW |
| 11/5/2007 | Canberra | 7.6 | 16.1 | 2.8 | 5.6 | 10.6 | SSE | 50 | SSE |
| 11/6/2007 | Canberra | 6.2 | 16.9 | 0 | 5.8 | 8.2 | SE | 44 | SE |
| 11/7/2007 | Canberra | 6.1 | 18.2 | 0.2 | 4.2 | 8.4 | SE | 43 | SE |
| 11/8/2007 | Canberra | 8.3 | 17 | 0 | 5.6 | 4.6 | E | 41 | SE |
| 11/9/2007 | Canberra | 8.8 | 19.5 | 0 | 4 | 4.1 | S | 48 | E |
| 11/10/2007 | Canberra | 8.4 | 22.8 | 16.2 | 5.4 | 7.7 | E | 31 | S |
| 11/11/2007 | Canberra | 9.1 | 25.2 | 0 | 4.2 | 11.9 | N | 30 | SE |
| 11/12/2007 | Canberra | 8.5 | 27.3 | 0.2 | 7.2 | 12.5 | E | 41 | E |
| 11/13/2007 | Canberra | 10.1 | 27.9 | 0 | 7.2 | 13 | WNW | 30 | S |

# Data Wrangling exercise

```
#Read in data:
W_df = read.table('weather.csv',
                  header=TRUE,
                        sep=",",
                  stringsAsFactors = TRUE)
```

# Long to Wide transform

| Date | Location | MinTemp | MaxTemp | Rainfall | Evaporation | Sunshine | WindGustDi | WindGustSp | WindDir9am |
|---|---|---|---|---|---|---|---|---|---|
| 11/1/2007 | Canberra | 8 | 24.3 | 0 | 3.4 | 6.3 | NW | 30 | SW |
| 11/2/2007 | Canberra | 14 | 26.9 | 3.6 | 4.4 | 9.7 | ENE | 39 | E |
| 11/3/2007 | Canberra | 13.7 | 23.4 | 3.6 | 5.8 | 3.3 | NW | 85 | N |

*date, location and the rest identify the row*

*WindGustDir entries are labels for the repeated measures*

```
install.packages('reshape2')
library(reshape2)
W_wide   =dcast(W_df,
          formula=Date+Location+ ...~ WindGustDir,
          fill=0,
           value.var="WindGustSpeed")
```

*this could be 0 or NA*

*indicate variable that has the repeated measurement values*

# Transformed Data Matrix

***Now: WindGustDir values each have their own column***

| | V | W | X | Y | Z | AA | AB | AC | AD | AE | AF | AG | AH | AI | AJ | AK | AL | AM | AN |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | RISK_M | RainTo | E | ENE | ESE | N | NE | NNE | NNW | NW | S | SE | SSE | SSW | SW | W | WNW | WSW | NA |
| 2 | 3.6 | Yes | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 30 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3 | 3.6 | Yes | 0 | 39 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 4 | 39.8 | Yes | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 85 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | 2.8 | Yes | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 54 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6 | 0 | No | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 50 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7 | 0.2 | No | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 44 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8 | 0 | No | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 43 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 9 | 0 | No | 41 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10 | 16.2 | Yes | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 48 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 11 | 0 | No | 31 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 12 | 0.2 | No | 0 | 0 | 0 | 30 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 13 | 0 | No | 41 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 14 | 0 | No | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 30 | 0 | 0 |
| 15 | 0 | No | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 44 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 16 | 0 | No | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 41 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

Weather_castwide

READY AVERAGE: 1202.530008 COUNT: 14679 SUM: 15392384.1

# Extra to try:

```
# wide to long: ie 'melt' repeated measure into long
#          table
W_melt   =melt(W_cast,
        na.rm=TRUE,
        measure.vars=c(23:39),
        variable.name="WindGustDir_cast")
```

*The repeated measures are now in columns 23 to 30*

# 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 vs Dimensionality Reduction

- **Prior to algorithm, depends on data**
  - For large P, with noise particular to variables, try variable selection
  - For large P, diffuse noise, try dimension reduction by Matrix Factorization

# Variable selection

- **Heuristic methods:**

  remove variables with low correlations to outcome

  (other criteria: information gain, sensitivity, etc…)

- **Step wise: add 1 variable at a time and test algorithm on samples**

# Variable selection

- **Some algorithms are robust to extra noise variables**

**- E.g. Least Angle Regression ($L_1$ penalty),**

penalize small effect sizes (zero them out)

**- E.g. Random Forest outputs 'importance'**

low importance implies non-influence in the model

(other criteria: information gain, sensitivity, etc…)

# Matrix Factorization:

***Given a numeric matrix, can we reduce the number of columns?***

conversely

***Can we find interesting subspaces?***

# Matrix Factorization:

***Given a numeric matrix, can we reduce the number of columns?***

- Yes, if features are constant or redundant

# Matrix Factorization:

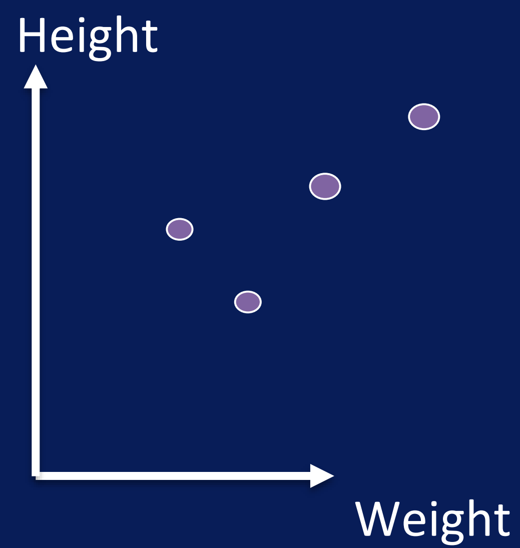
***Given a numeric matrix, can we reduce the number of columns?***

- Yes, if features are constant or redundant
- Yes, if features only contribute noise (conversely, want features that contribute to variations of the data)

# Example: 2D data

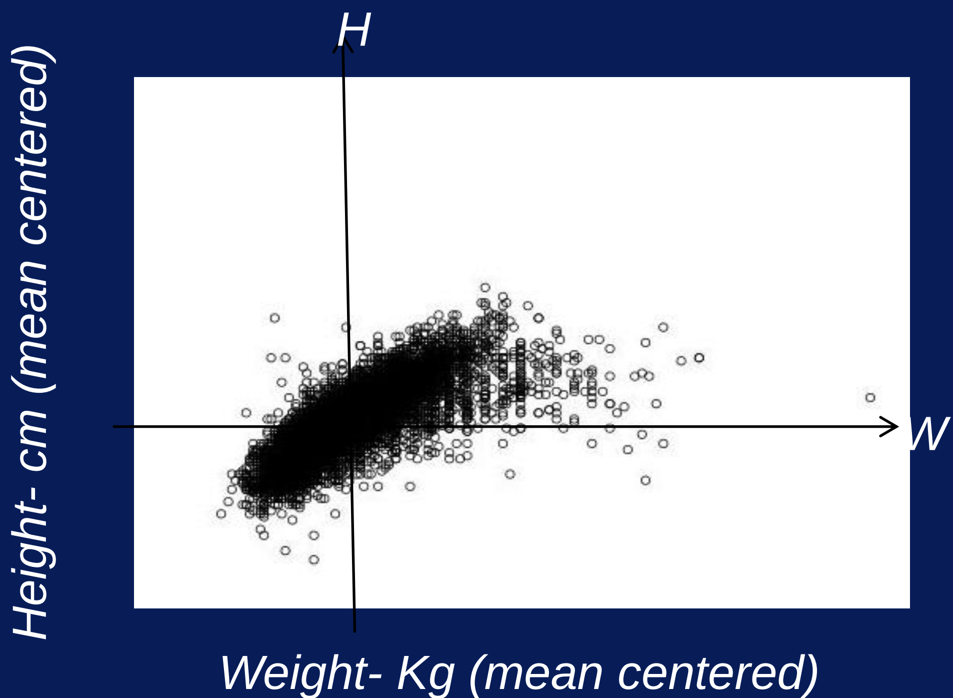
| | Weight | Height |
|---|---|---|
| S1 | 50 | 179 |
| S2 | 66 | 175 |
| S3 | 74 | 180 |
| S4 | 94 | 192 |

PLOT




***this is the input space***

## Example: Athletes' Height by Weight




*Find a line that aligns with the data.*

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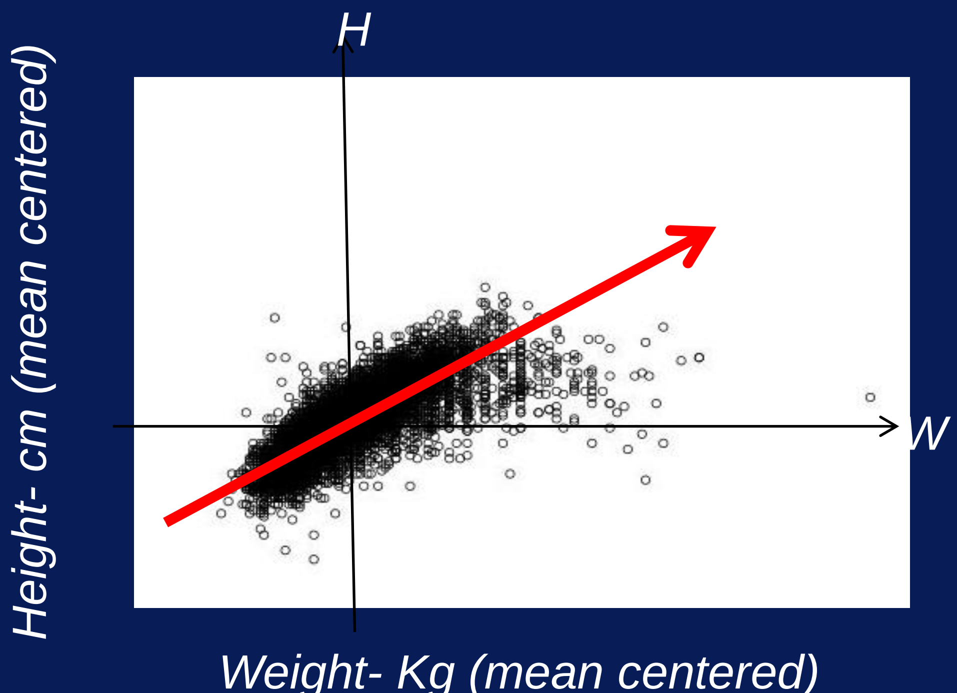
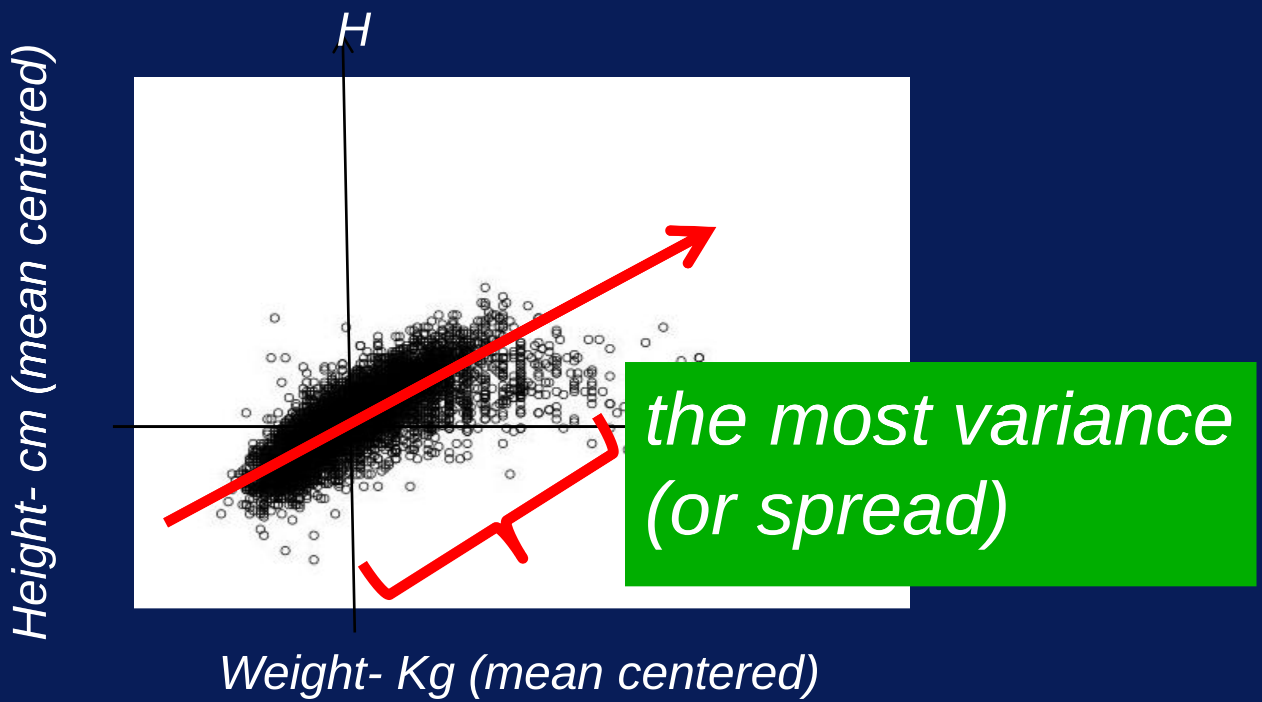



*Find a line that aligns with the data.*

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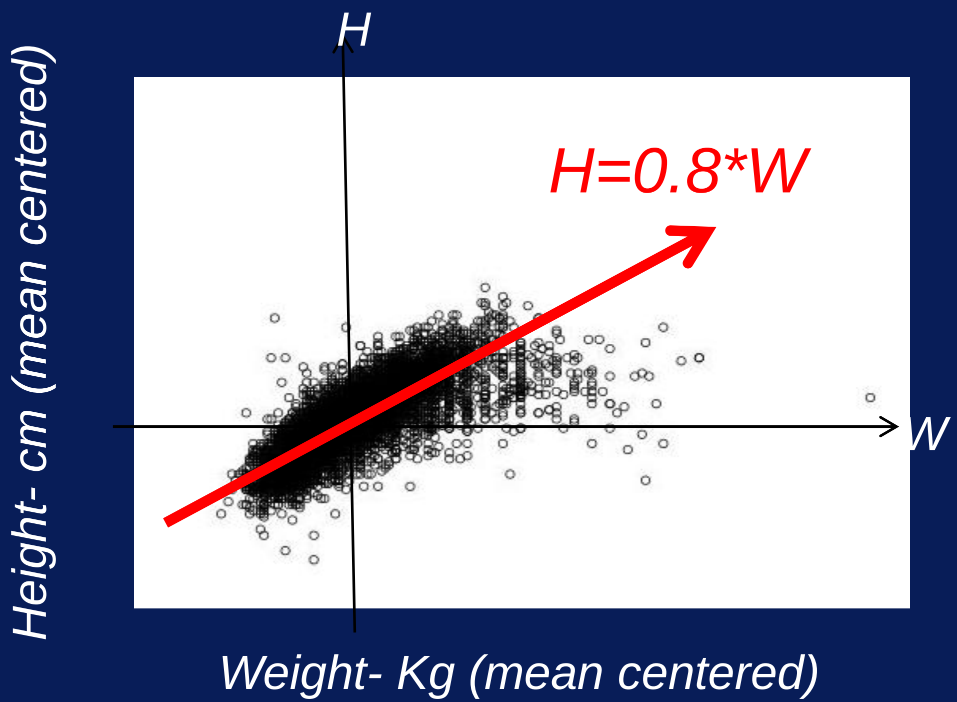
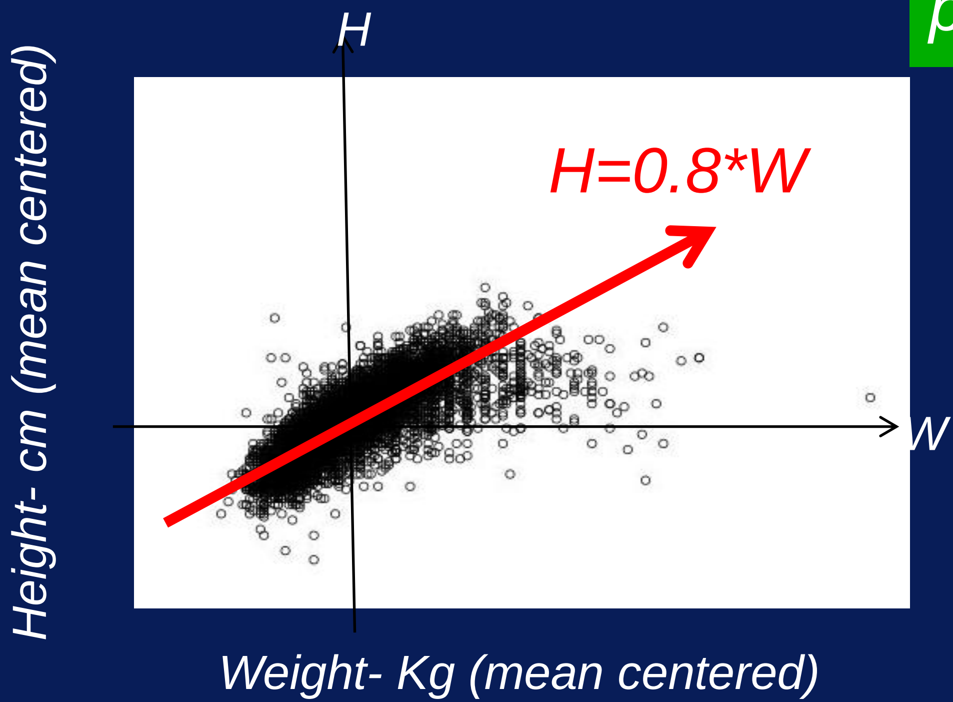



*Find a line that aligns with the data.*

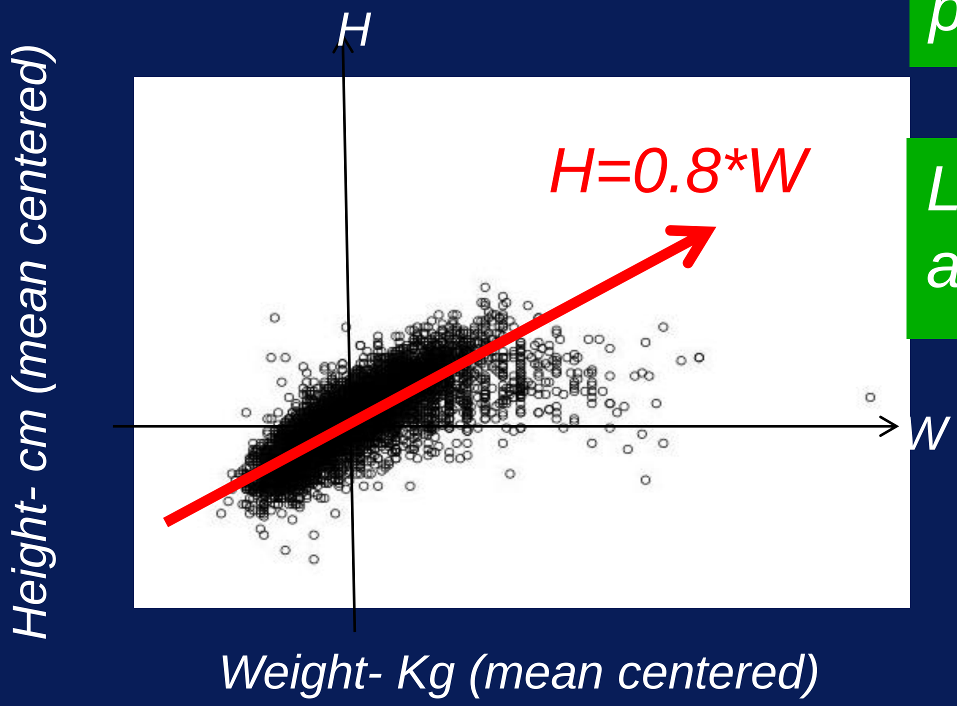
Note that W=1,H=0.8 is a point on the line, for example.




Find a line that aligns with the data.

Note that W=1,H=0.8 is a point on the line, for example.

Let [1 0.8] represent the line, as a combination of W & H.

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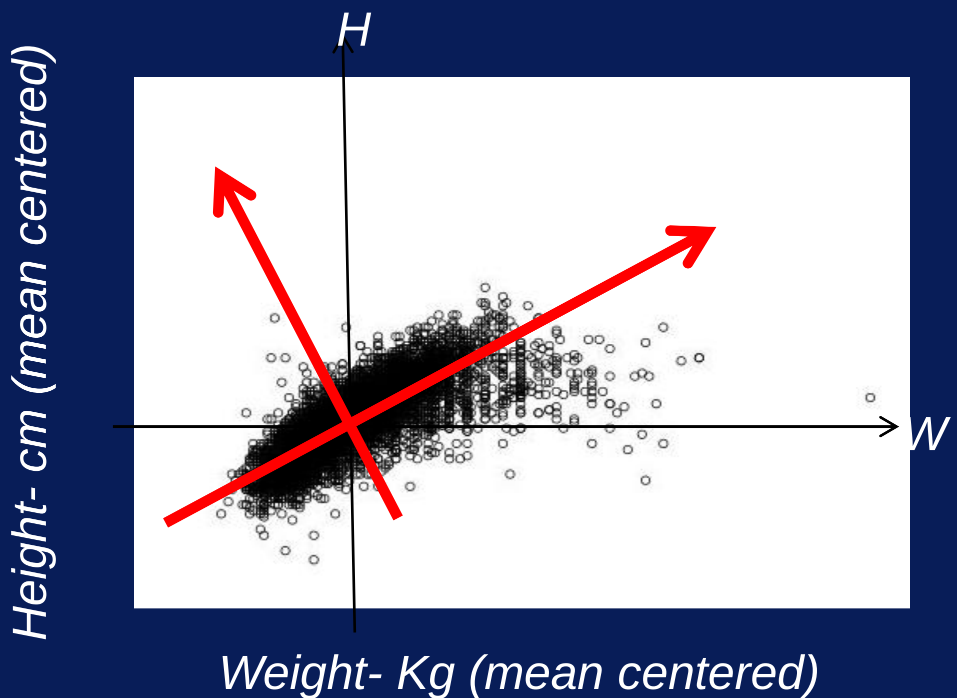
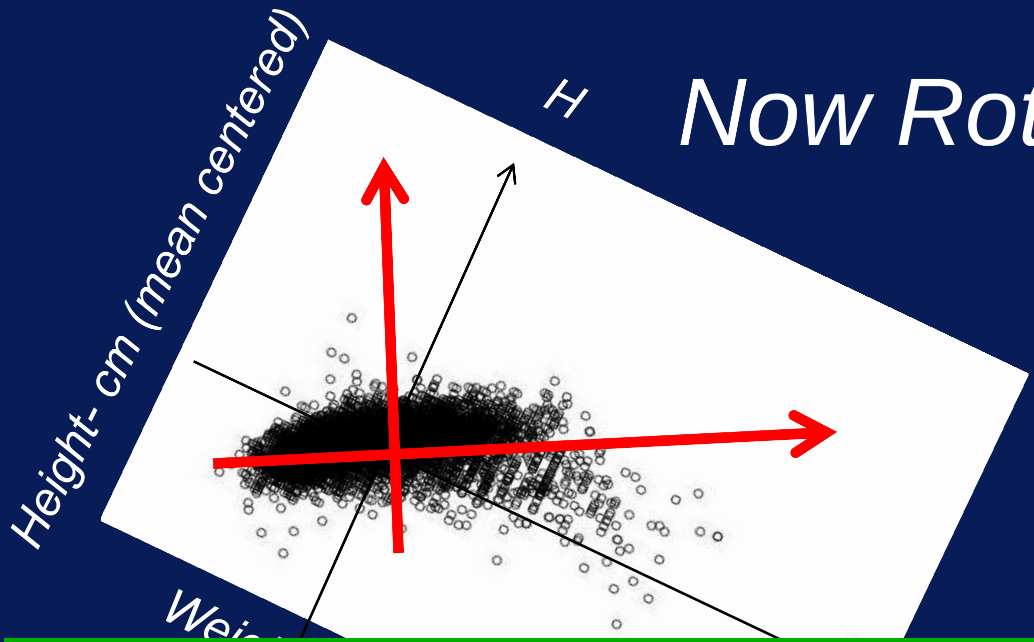


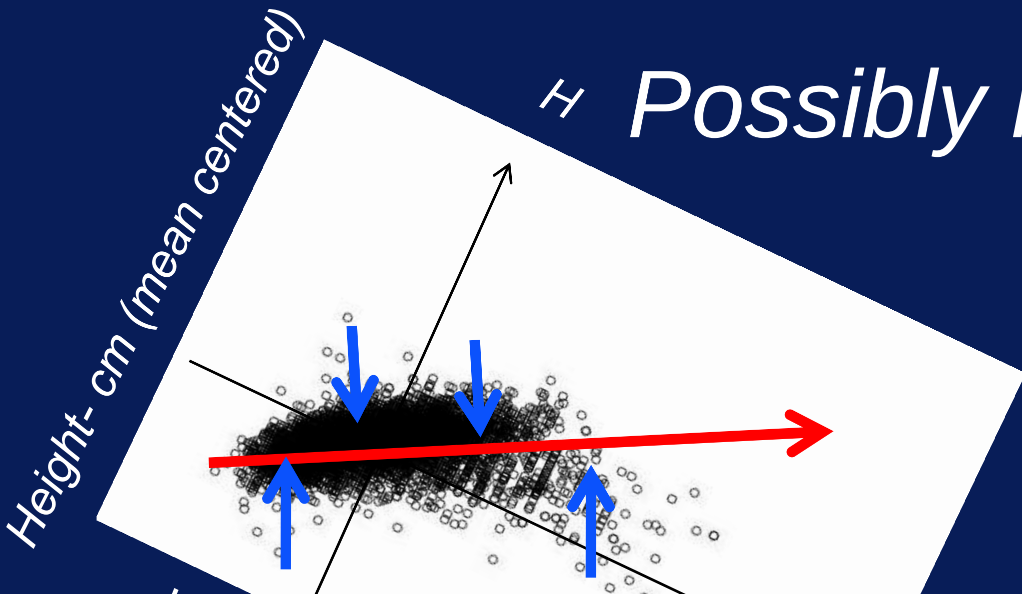

*The next direction of most variance.*

# Now Rotate Axis




*New axis (AKA features) defined as combinations of old features*

# Possibly reduce dimensions

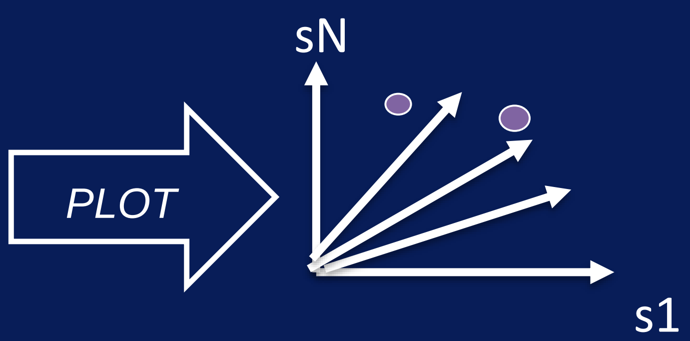



*Project all points to one axis*

*(defined by the [1  0.8] 2D vector)*

# 2D data transposed to 2 points in high dimensional space

| | s1 | s2 | s3 | … |
|---|---|---|---|---|
| Height | 179 | 175 | 180 | … |
| Weight | 50 | 66 | 74 | … |



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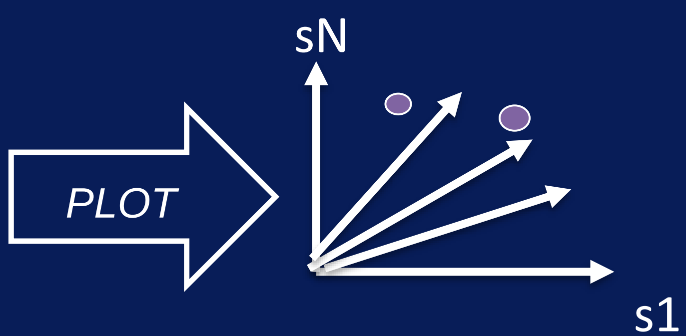
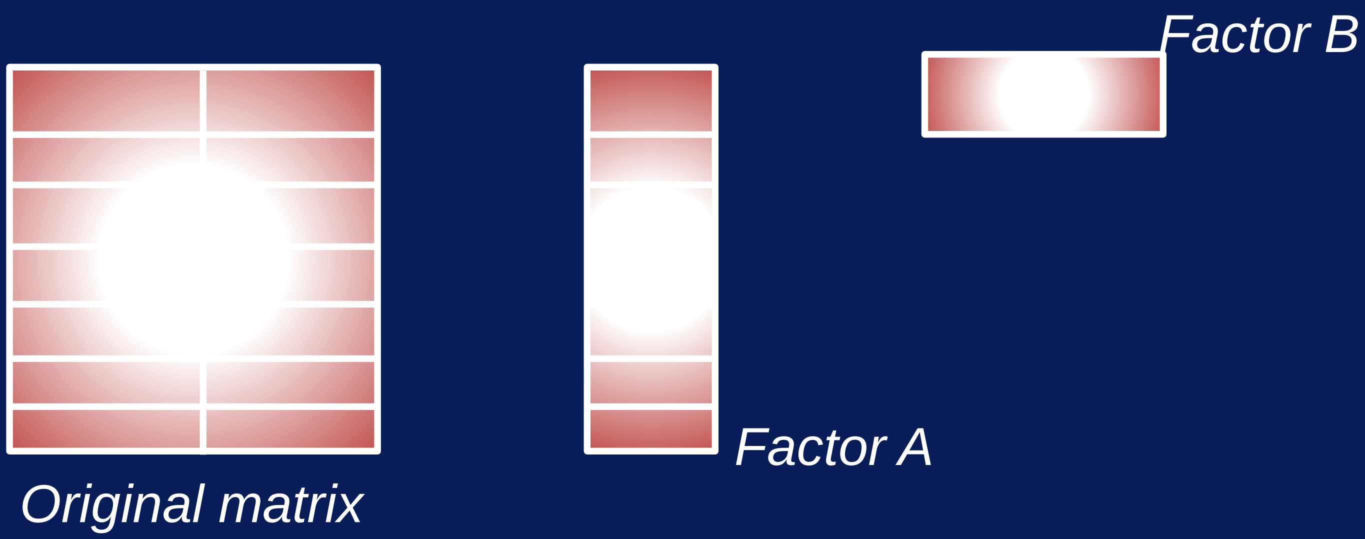



*Same process as before, but now factors are N-dimensional vectors*

# Any Matrix can be approximated by outer product of factors



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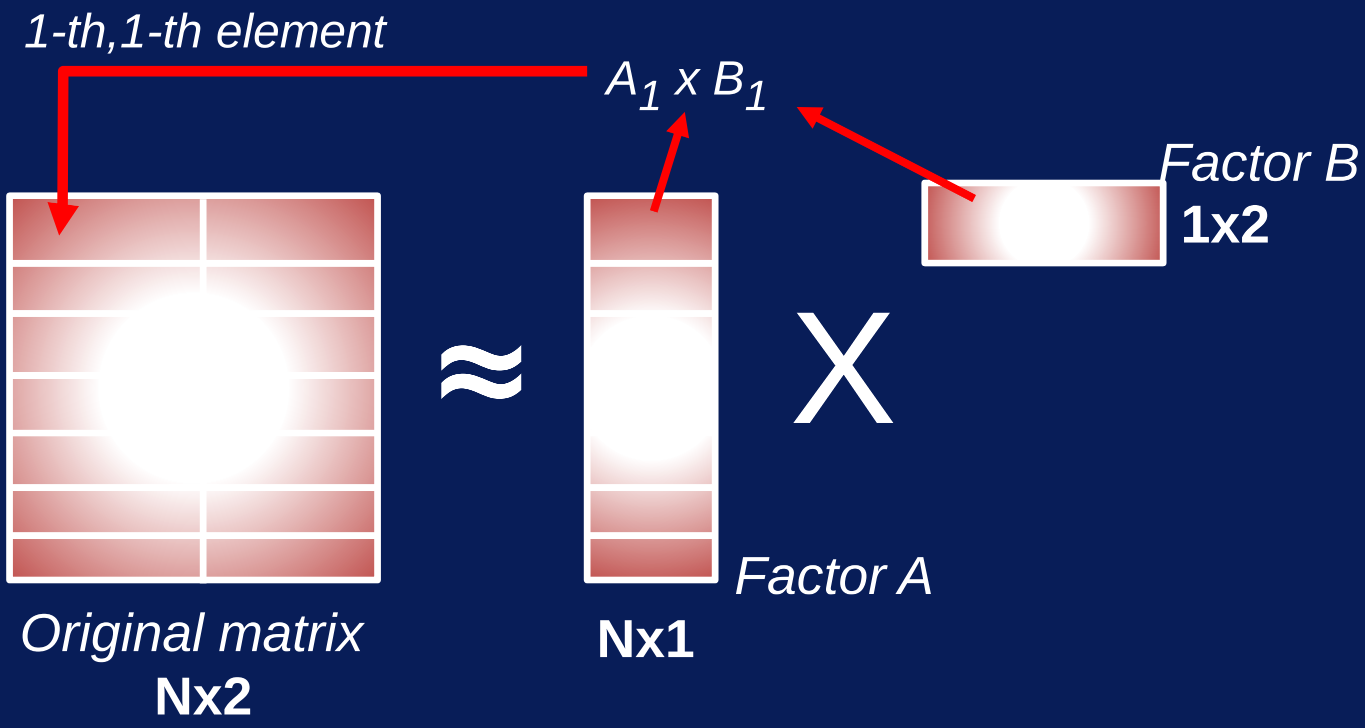

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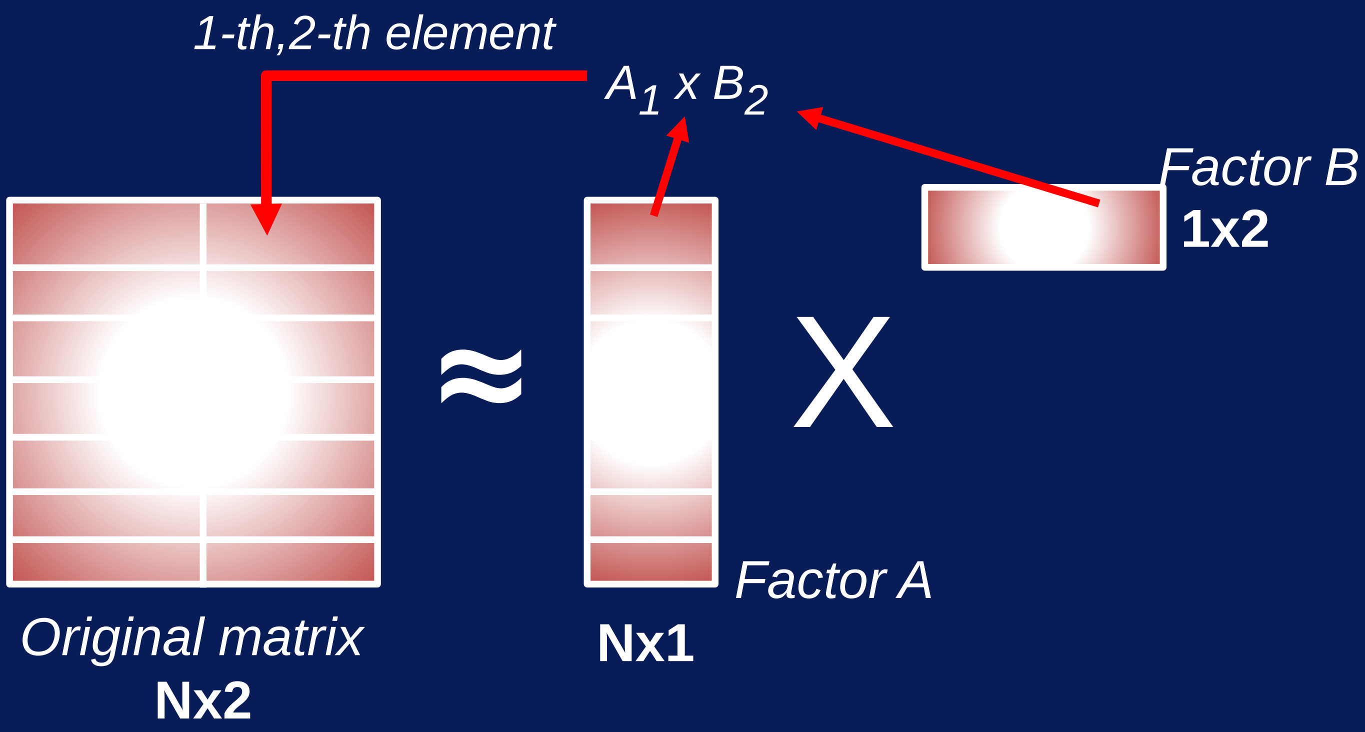
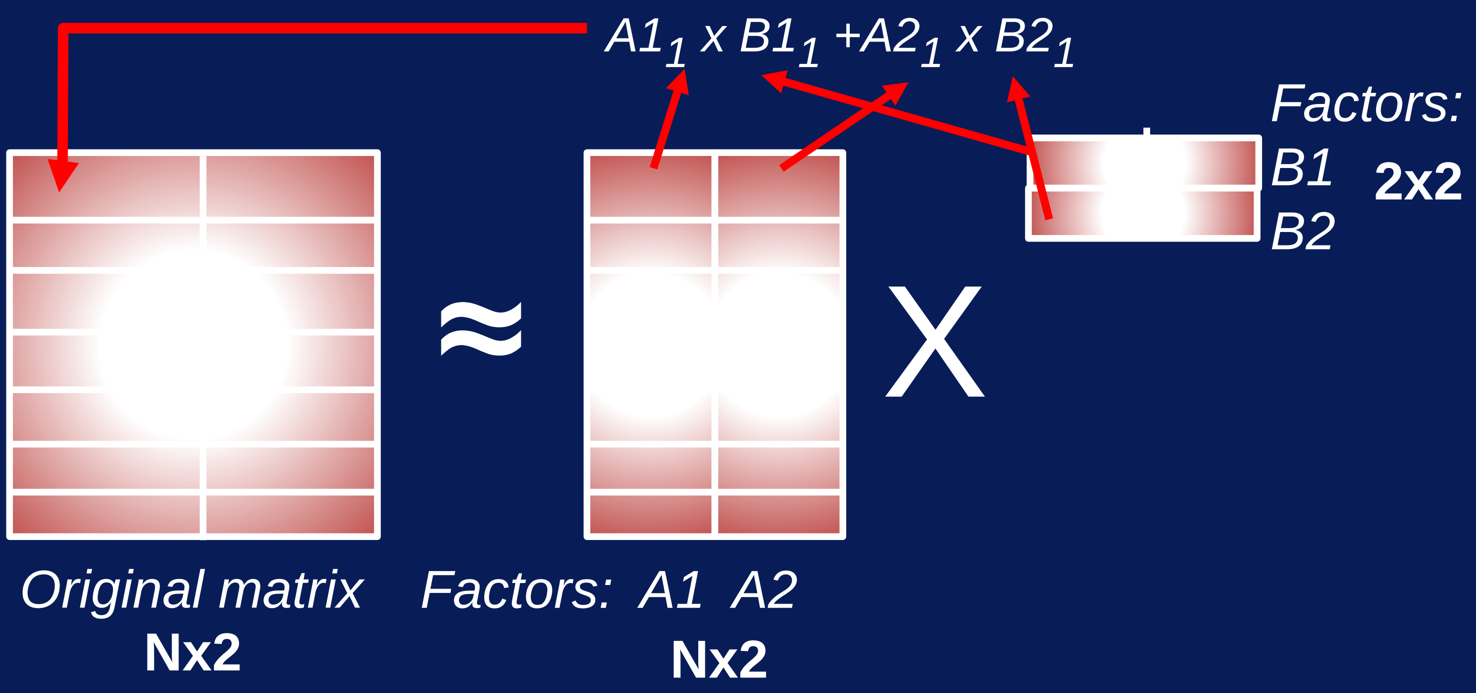


# More factors gives better approximation



- Best Known Factorization Algorithms:
  - SVD (singular value decomposition)
  - PCA (principle component analysis)

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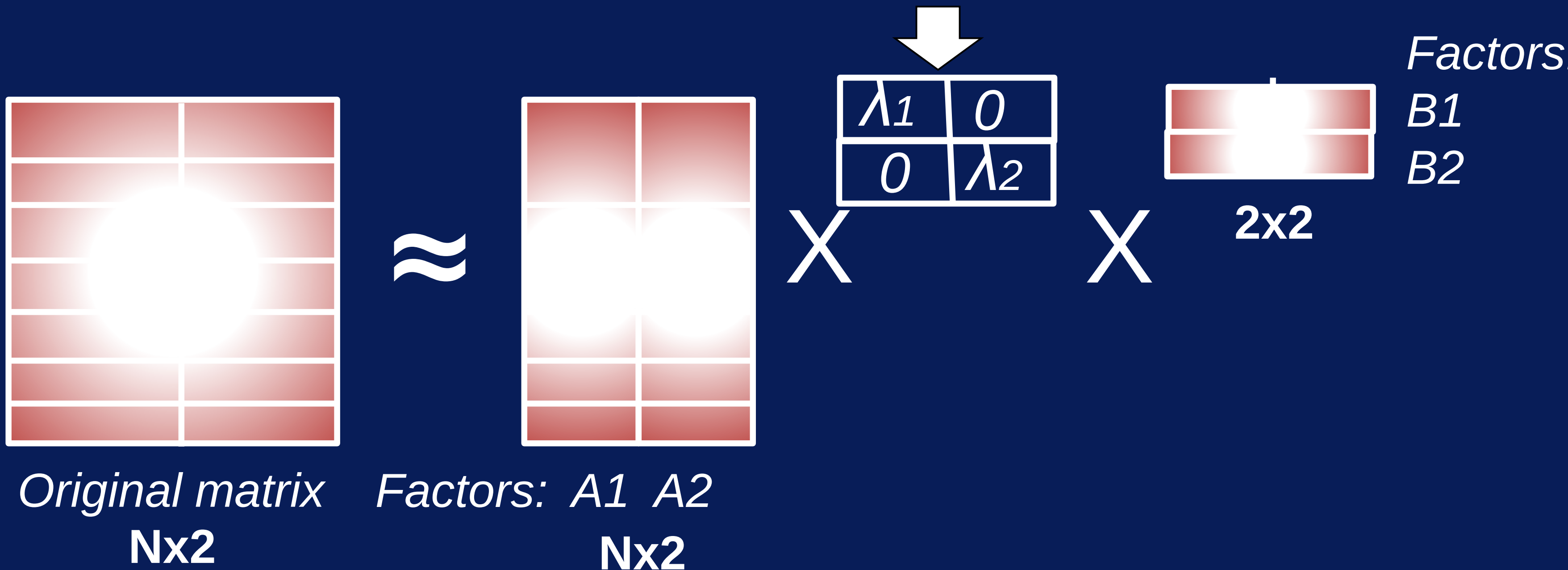
  SVD (singular value decomposition)

  PCA (principle component analysis)

*Find orthogonal factors and*
*scale them down (i.e. normalize)*

# SVD: factors and 'singular' scale values



- More generally:

Factorization Algorithms may vary depending on criterion for how factors ‘align’ with data.

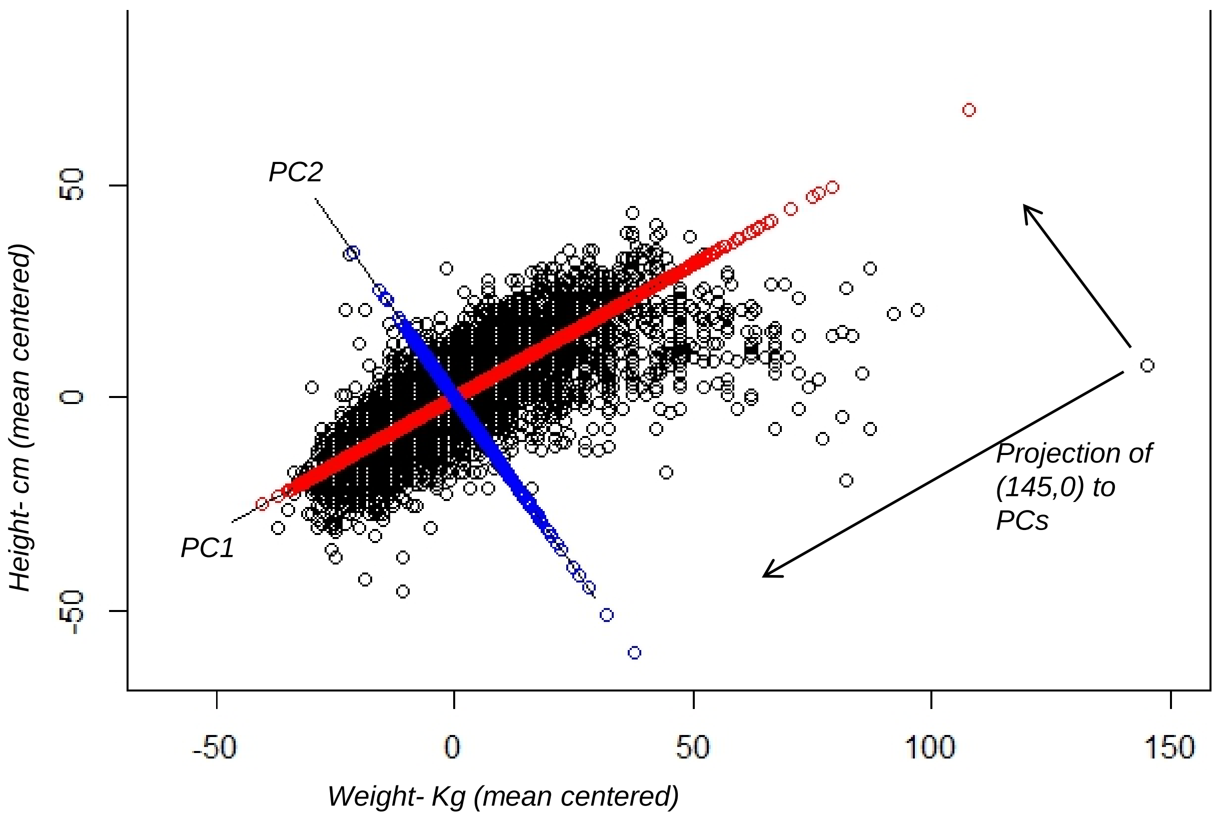
- More generally:

Factorization Algorithms may vary depending on criterion for how factors ‘align’ with data.

- Number of factors to use depends on tradeoff of good approximation vs good dimensional reduction

*Can use cross validation or heuristics to choose.*

# Note: PCA conserves and reorders variance




*Total Variance Conserved:*
*Var in Weight*
*+*
*Var in Height*
*=*
*Var in PC1 +*
*Var in PC2*

*In general:*
*Var in PC1>*
*Var in PC2>*
*Var in PC3…*

# Summary: Principle Components

- **Can choose *k* heuristically as approximation improves,  or choose *k* so that high percent (ie 80-95%) of data variance accounted for**
- **aka Singular Value Decomposition**

  PCA on square matrices only

  SVD gives same vectors on square matrices
- **Works for numeric data only**
- **For higher dimensional data, use factors to visualize 2 factors at a time**

# SVD Exercise

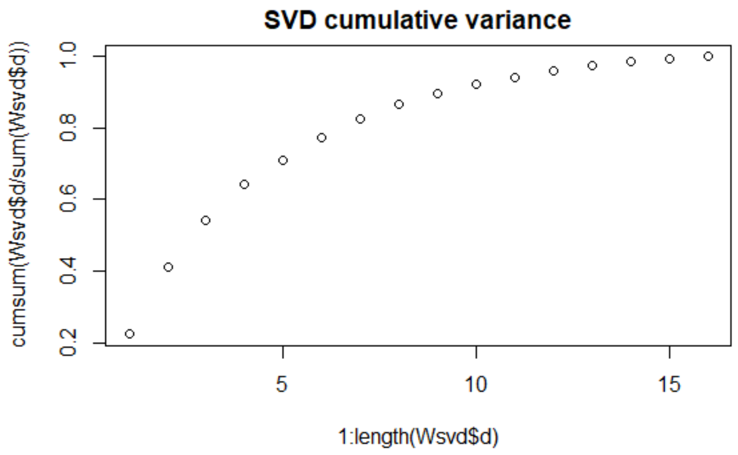
- **Overview**
  - Run on numeric fields of weather data
  - Run SVD and select smaller number of dimensions
  - Run linear model with original and reduced data

# Later, we'll compare SVD components with Clustering

```
#W_num is only numeric or integer fields of Weather data
> Wsvd=svd(W_num)

> str(Wsvd)
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 ...
```

# Exercise highlights




**Compare Linear Model results, using Y = raintomorrow:**

**look for residual standard error values and degree of freedom,**

**look at coefficient estimates**

```
Call:
lm(formula = Ymc ~ W_mncntr)
Coefficients:
                        Estimate Std. Error t value Pr(>|t|)
(Intercept)           -1.124e-15  1.641e-02   0.000 1.000000
W_mncntrMinTemp       -1.368e-02  1.013e-02  -1.350 0.177844
W_mncntrMaxTemp        1.035e-02  2.010e-02   0.515 0.607120
W_mncntrRainfall       4.269e-03  4.471e-03   0.955 0.340442
W_mncntrEvaporation    2.690e-02  1.010e-02   2.663 0.008137 **
W_mncntrSunshine      -3.446e-02  9.898e-03  -3.482 0.000570 ***
W_mncntrPressure9am    6.569e-02  1.325e-02   4.960 1.16e-06 ***
W_mncntrPressure3pm   -8.047e-02  1.337e-02  -6.021 4.89e-09 ***

Residual standard error: 0.2971 on 311 degrees of freedom
```

```
Call:
lm(formula = Ymc ~ W_dfred)
Coefficients: (13 not defined because of singularities)
              Estimate Std. Error t value Pr(>|t|)
(Intercept) -4.874e-16  1.808e-02   0.000 1.000000
W_dfred1     4.519e+00  1.242e+00   3.638 0.000320 ***
W_dfred2     4.650e+00  1.307e+00   3.559 0.000429 ***
W_dfred3     1.580e+00  4.357e-01   3.627 0.000333 ***
W_dfred4            NA         NA      NA       NA
W_dfred5            NA         NA      NA       NA

Residual standard error: 0.3274 on 324 degrees of freedom
```

- **end**