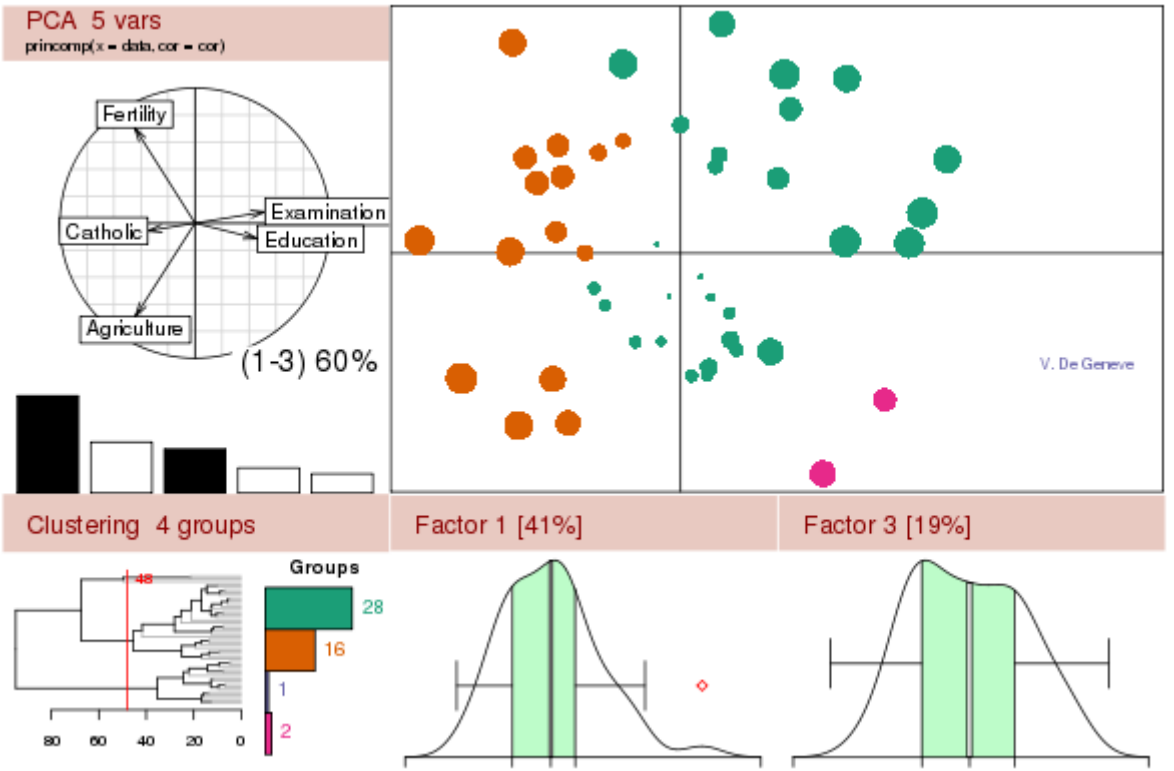
2013 Eric Pitman Summer Workshop in Computational Science



...an introduction to R, statistics, programming, and getting to know datasets


supercomputing 101
Please Do Not Remove Chairs From This Area
What to do

2013 Workshop Staff

- Jeanette Sperhac, Scientific Programmer, CCR
- Ryan Mraz, RIT
- Sam Steffan (workshop alumnus), UNC
- Brian Narby, Pitt
- Steve Gallo, Lead Software Engineer, CCR
- Adrian Levesque, Multimedia Specialist, CCR
- Jake Brubaker, additional photography, CCR


B1-152
EXIT
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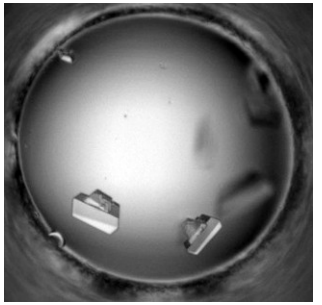
The 2013 Workshop



- Introduce the R language
- Do some programming
- Examine, model, and visualize datasets
- Project: explore and characterize protein crystallization data from HWI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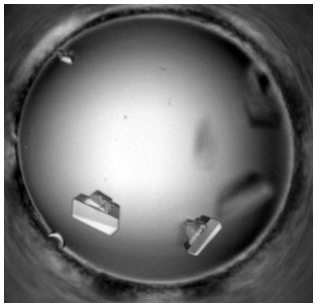
Presentations and Tours



Dr. E. Bruce Pitman – UB Dean of Arts & Sciences

Dr. Thomas Furlani – CCR Director; UB Interim CIO

Dr. Marc Halfon – UB Department of Biochemistry

Dr. Daryl P Nazareth – Roswell Park, Department of Radiation Medicine

Dr. Edward Snell – UB Department of Structural Biology

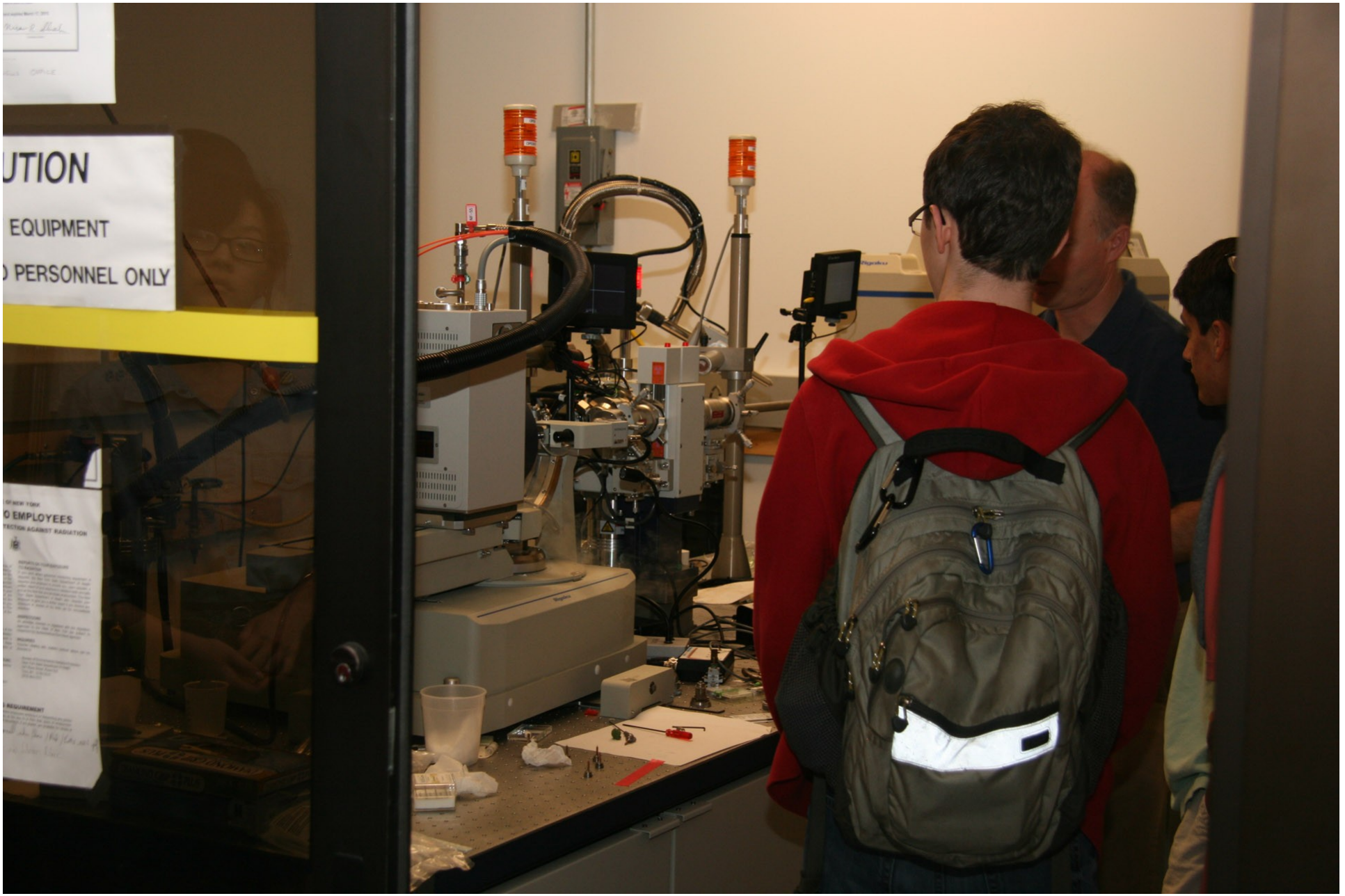
Dr. Norma J. Nowak – UB Department of Biochemistry

Dr. Dheerendra Prasad – Roswell Park, Director: Department of Radiation Medicine

Dr. L. Shawn Matott – Computational Scientist, CCR

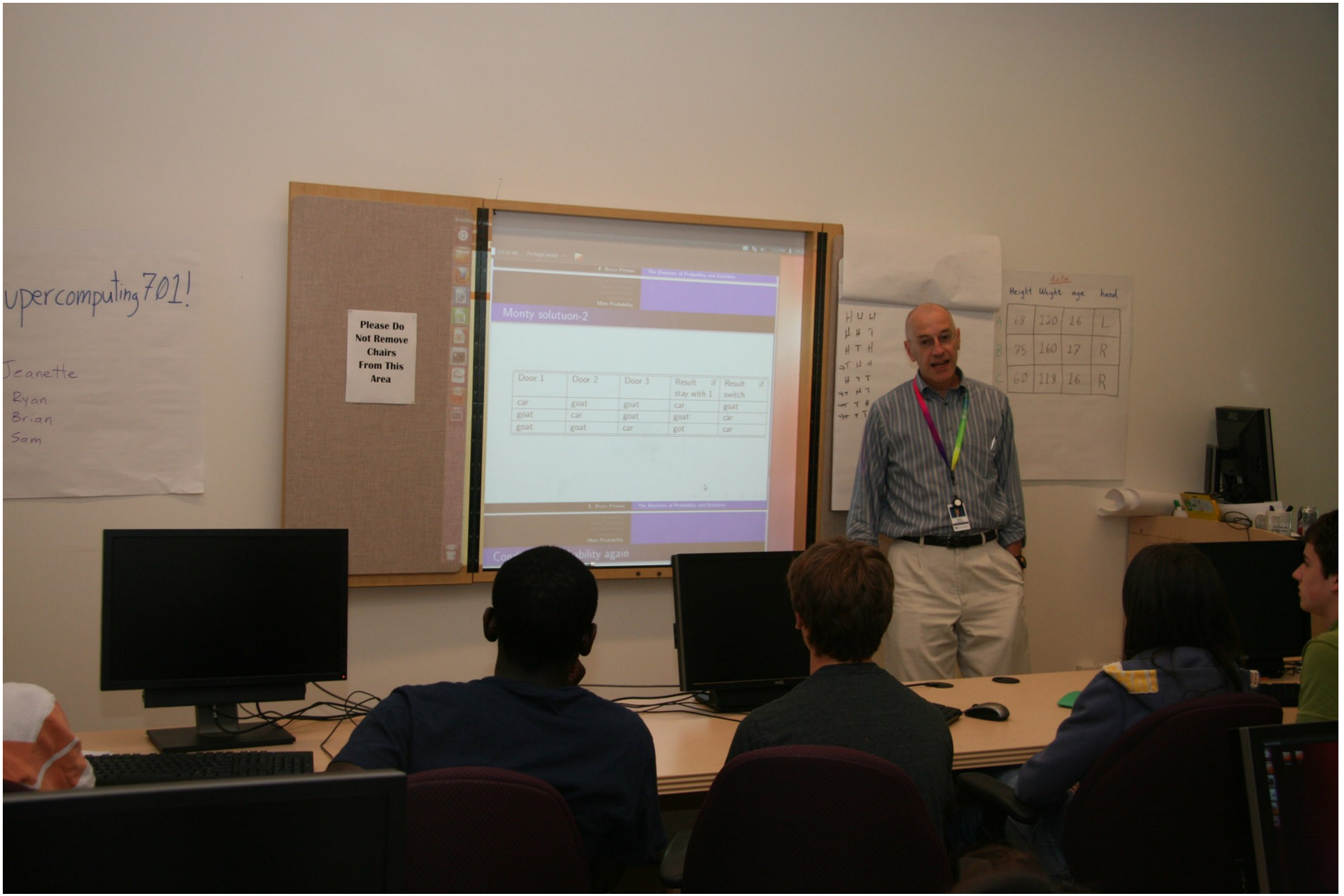
Amanda Ruby – UB Department of Biology and CCR

HWI Protein Crystallization Lab


UTION
EQUIPMENT
PERSONNEL ONLY
EMPLOYEES

Workshop 2013: New Unit Discovered

1 foot = 0.1908 Bhaskar


upercomputing 701!
Jeanette
Ryan
Brian
Sam
Please Do Not Remove Chairs From This Area
Monty solutuon-2
Door 1 | Door 2 | Door 3 | Result if stay with 1 | Result if switch
car | goat | goat | car | goat
goat | car | goat | goat | car
goat | goat | car | got | car
Data
Height Weight age hand
A 68 120 16 L
B 75 160 17 R
C 60 118 16 R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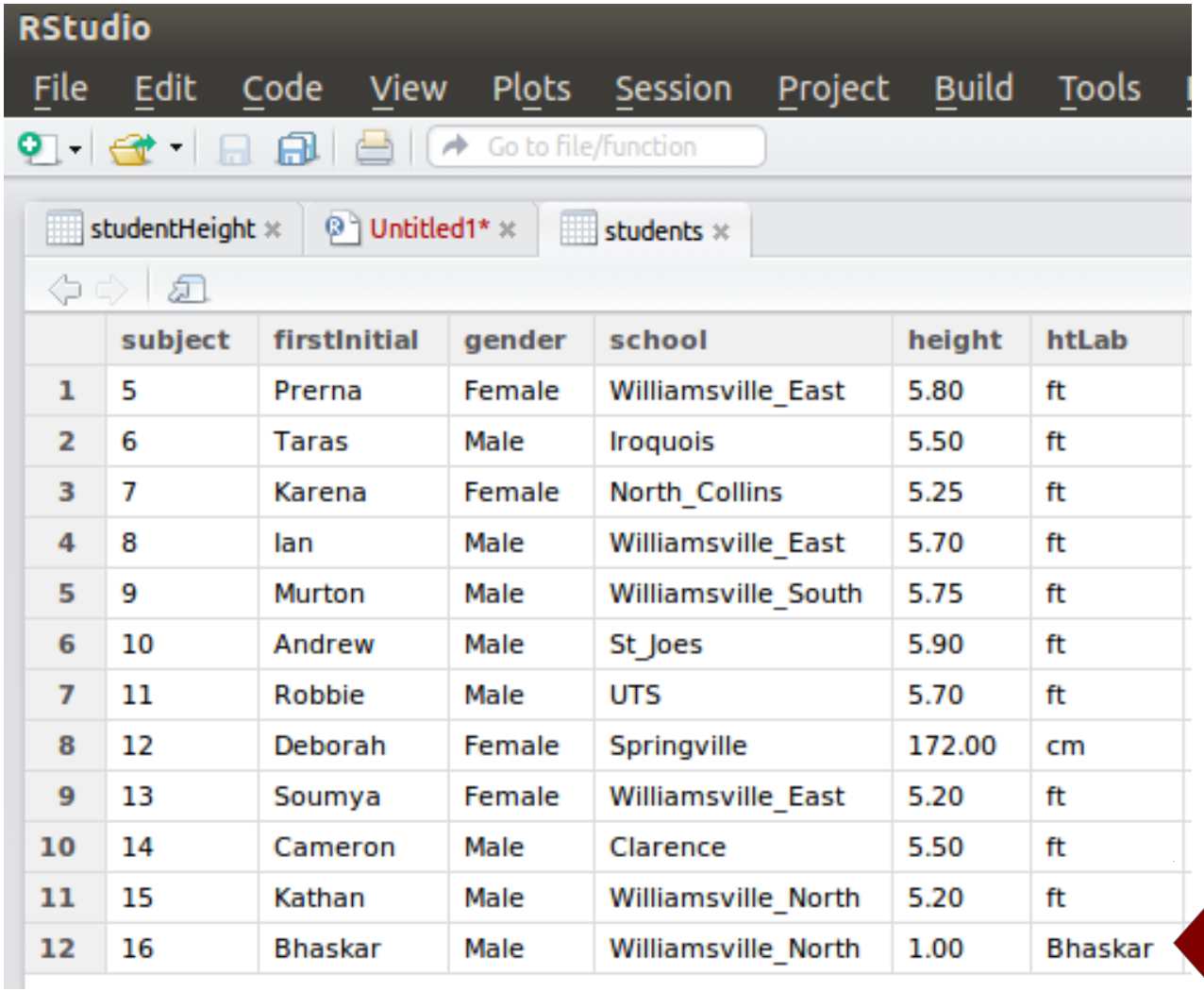
Data Frame in



	subject	firstInitial	gender	school	height	htLab
1	5	Prerna	Female	Williamsville_East	5.80	ft
2	6	Taras	Male	Iroquois	5.50	ft
3	7	Karena	Female	North_Collins	5.25	ft
4	8	Ian	Male	Williamsville_East	5.70	ft
5	9	Murton	Male	Williamsville_South	5.75	ft
6	10	Andrew	Male	St_Joes	5.90	ft
7	11	Robbie	Male	UTS	5.70	ft
8	12	Deborah	Female	Springville	172.00	cm
9	13	Soumya	Female	Williamsville_East	5.20	ft
10	14	Cameron	Male	Clarence	5.50	ft
11	15	Kathan	Male	Williamsville_North	5.20	ft
12	16	Bhaskar	Male	Williamsville_North	1.00	Bhaskar

Workshop student data, reported in various units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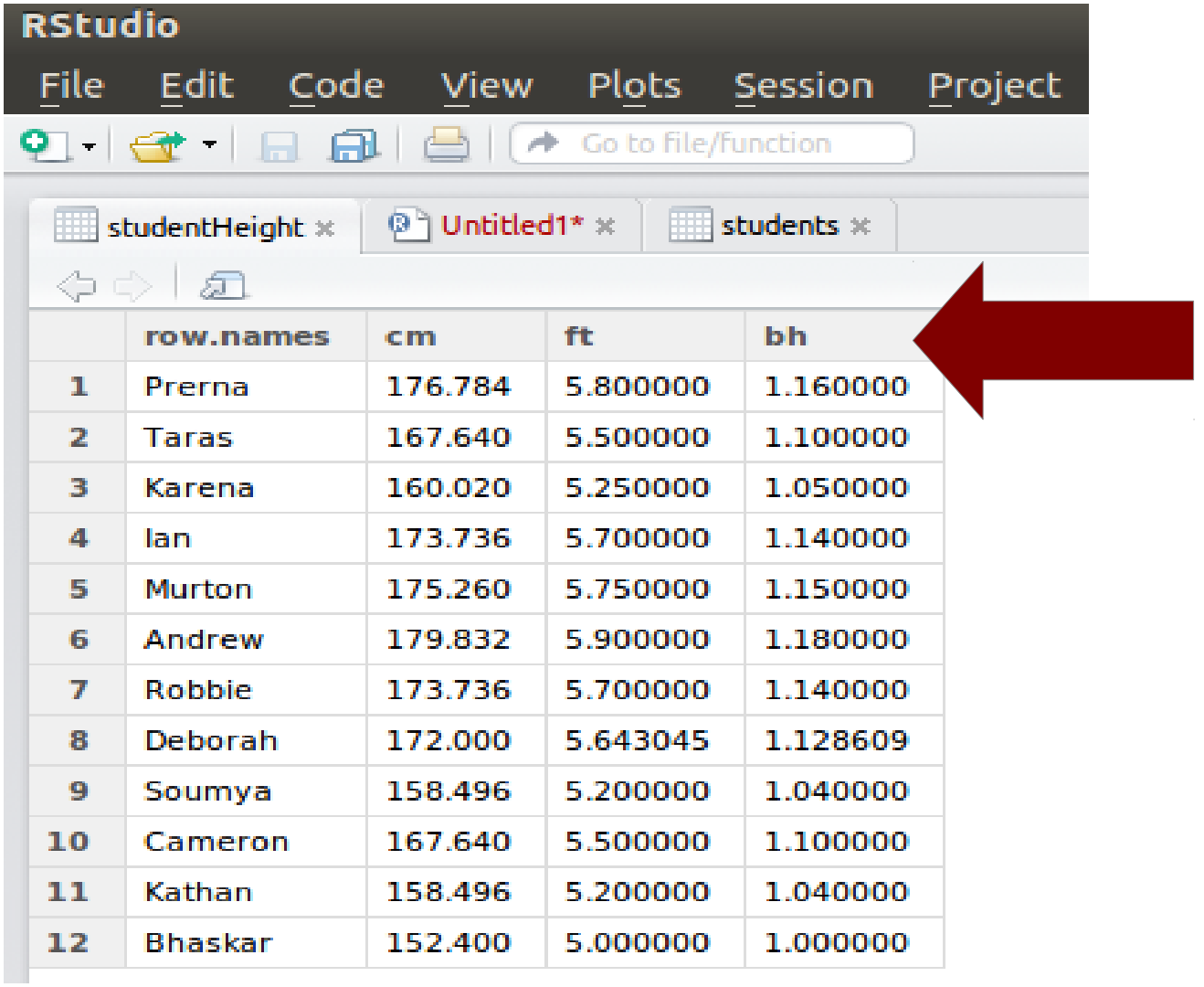
Unit Conversions to Bhaskars



	row.names	cm	ft	bh
1	Prerna	176.784	5.800000	1.160000
2	Taras	167.640	5.500000	1.100000
3	Karena	160.020	5.250000	1.050000
4	Ian	173.736	5.700000	1.140000
5	Murton	175.260	5.750000	1.150000
6	Andrew	179.832	5.900000	1.180000
7	Robbie	173.736	5.700000	1.140000
8	Deborah	172.000	5.643045	1.128609
9	Soumya	158.496	5.200000	1.040000
10	Cameron	167.640	5.500000	1.100000
11	Kathan	158.496	5.200000	1.040000
12	Bhaskar	152.400	5.000000	1.000000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Chairs
From This
Area


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B1-152

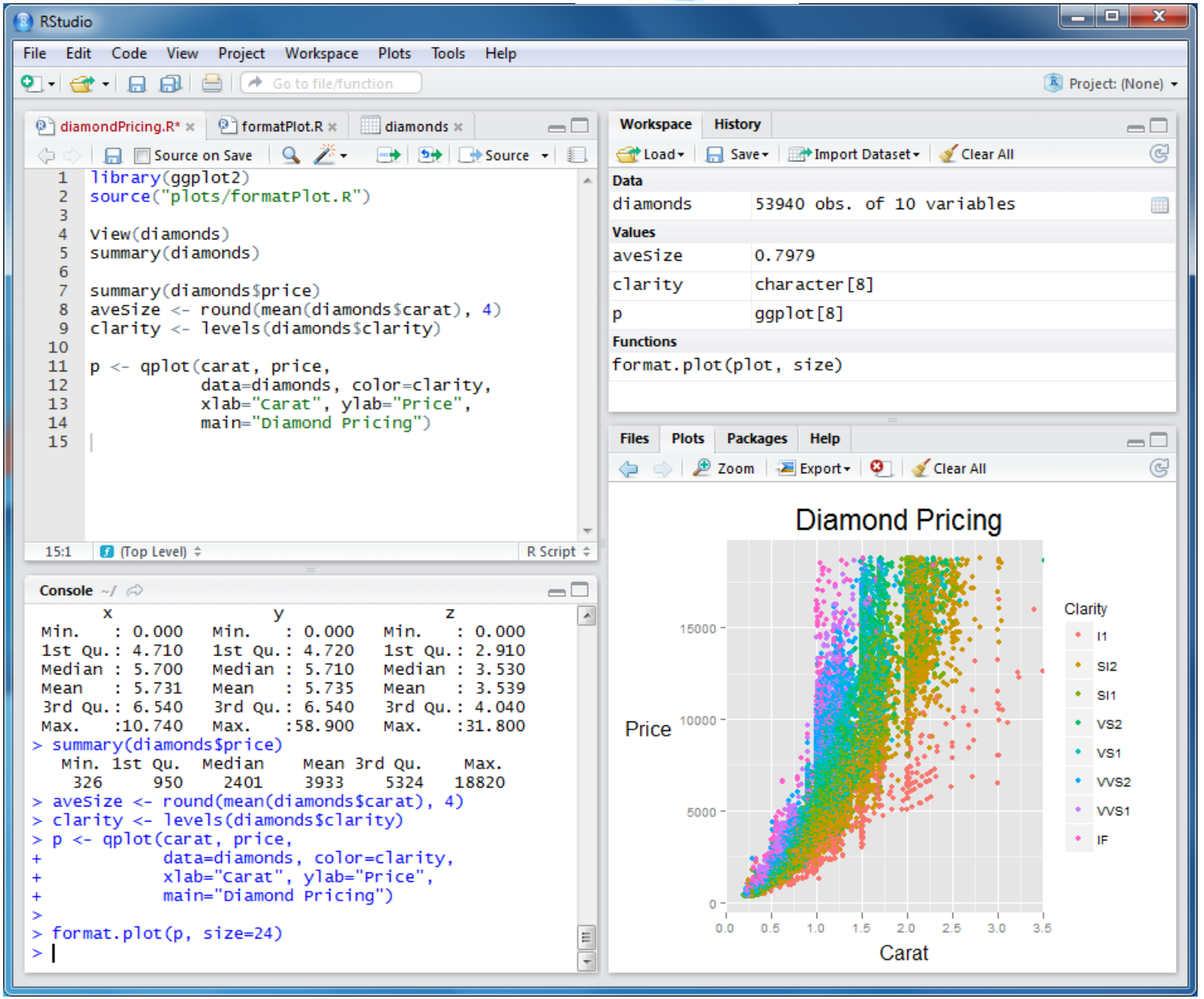
htConvertSimple() function

```
# ---------  writing a simple function to convert heights ----------

# define constants for the conversions
ft.cm.Factor = 30.48 # feet to cm
ft.b.Factor = 0.2 # feet to Bhaskars

# perform height conversion
# input is assumed to be a single value
# input value assumed to be in feet
# (or conversion will be incorrect)
htConvertSimple = function(f) {

  # find equivalent measurement in Bhaskars
  bh = f * ft.b.Factor
  # find equivalent measurement in cm
  ch = f * ft.cm.Factor

  # create vector of the 3 values and return it
  return ( c(f, ch, bh) )
}
```

Dr. Norma Nowak Lab


Worm

Got R ?



1. Editor

2. Workspace (Variables) and History

3. Plots, etc.

4. Console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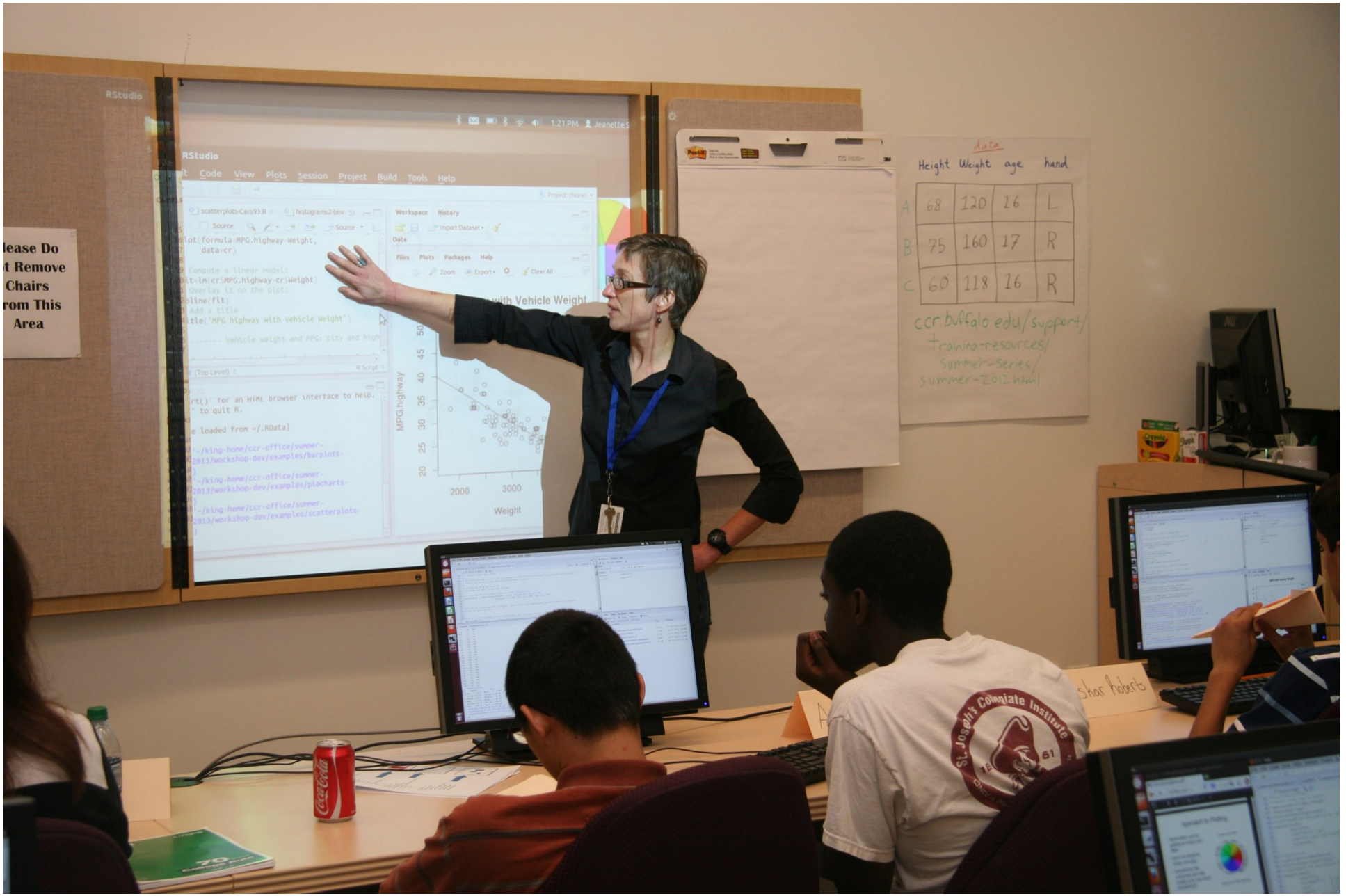
RStudio
Please Do Not Remove Chairs From This Area
RStudio
File Edit Code View Plots Session Project Build Tools Help
Workspace History
Import Dataset
Files Plots Packages Help
Zoom Export Clear All
MPG.highway
Weight
2000
3000
20
25
30
35
40
45
50
Data
Height Weight age hand
A 68 120 16 L
B 75 160 17 R
C 60 118 16 R
ccr.buffalo.edu/support/training-resources/summer-series/summer-2012.html
Coca-Cola
St. Joseph's Collegiate Institute


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...is free

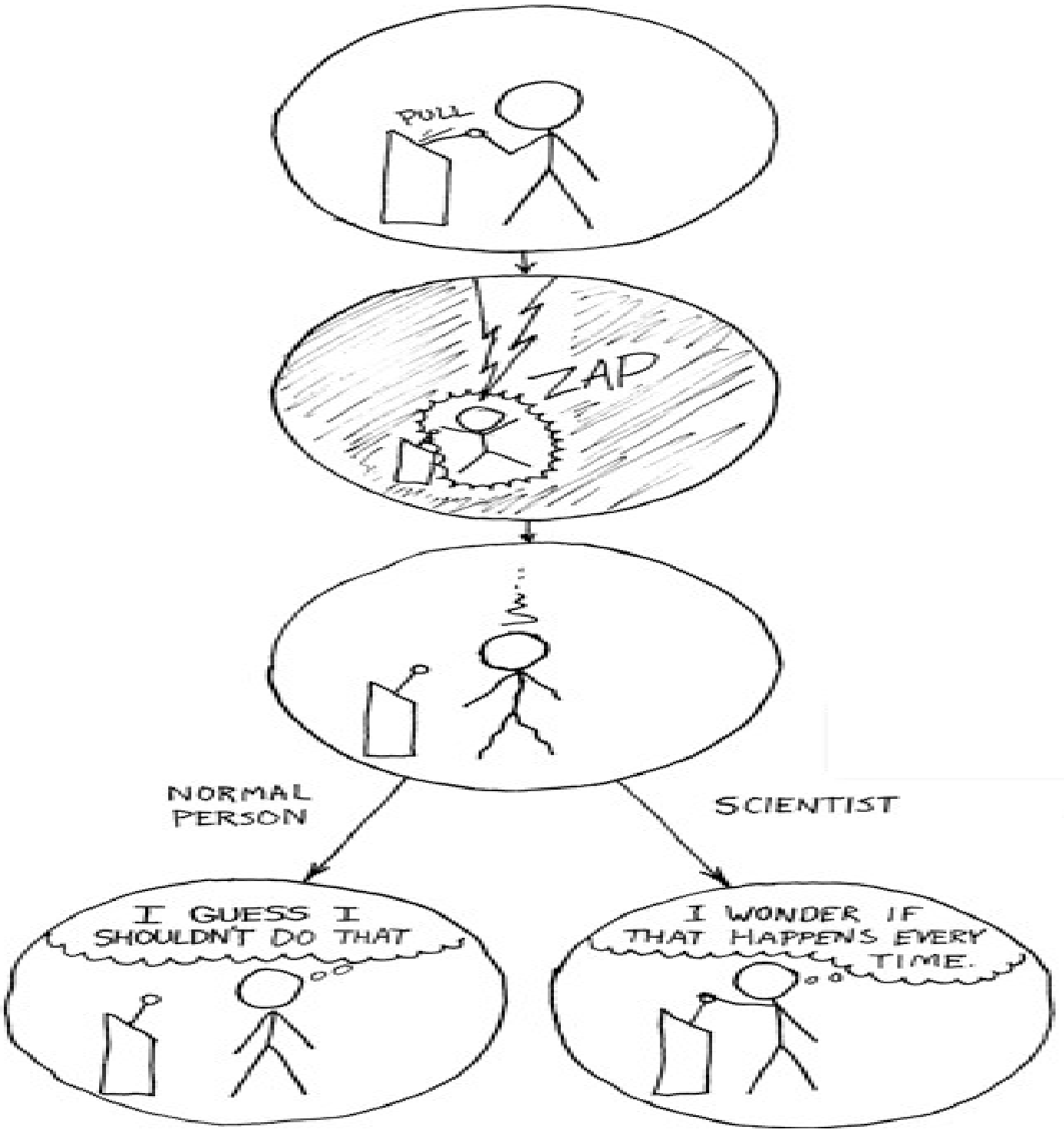
To experiment further with R and RStudio, you can install them on your favorite hardware at home.

First, install R:

http://cran.r-project.org/

Then, install the RStudio IDE:

http://www.rstudio.com/ide/


PULL
ZAP
NORMAL PERSON
SCIENTIST
I GUESS I SHOULDN'T DO THAT
I WONDER IF THAT HAPPENS EVERY TIME.

UB CTRC


Labs
Café
Welcome to Incoming Residents' Week
2012
BUFFALO
ResearchMatch
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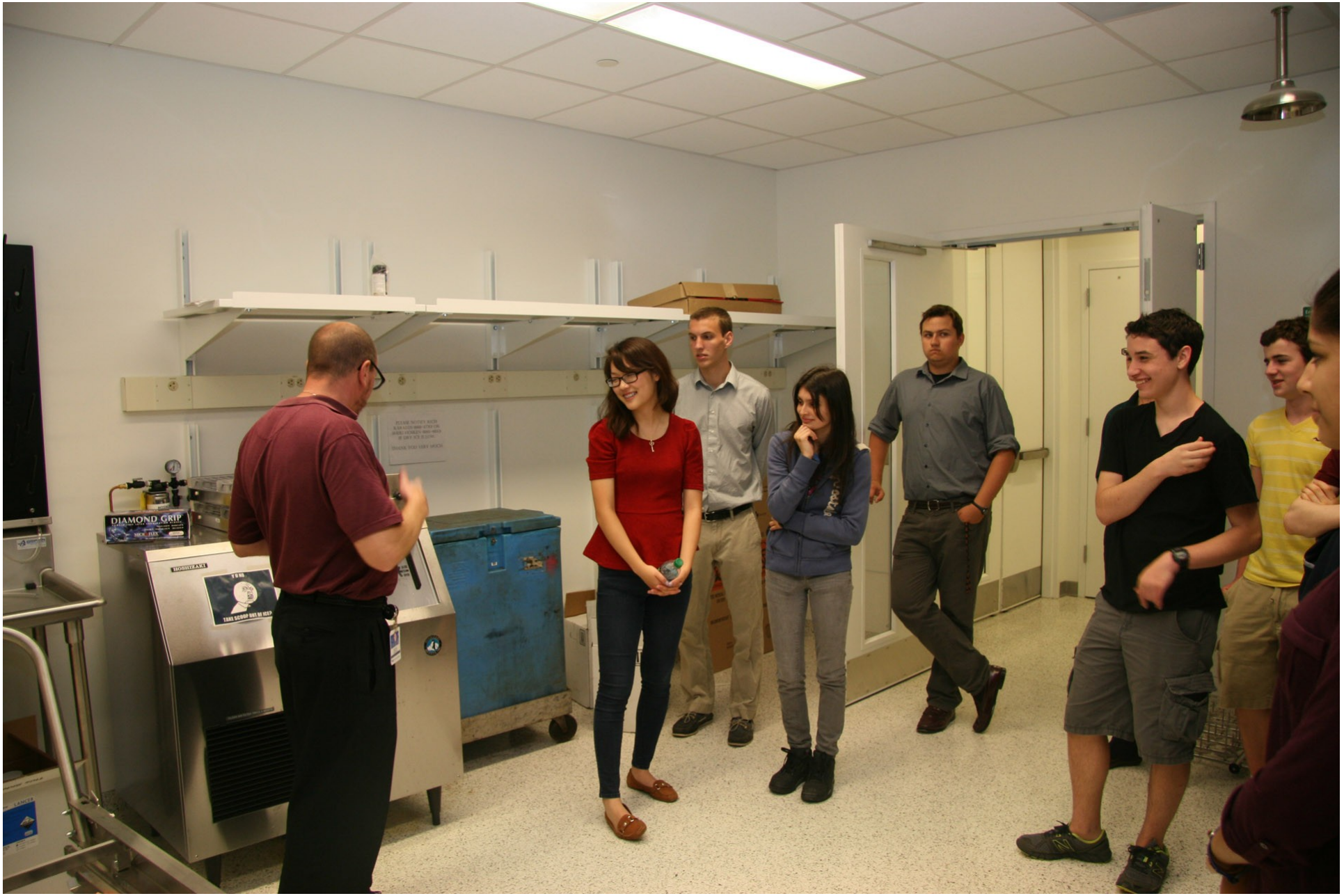
6045


EXIT


OBJET
OBJET


DIAMOND GRIP

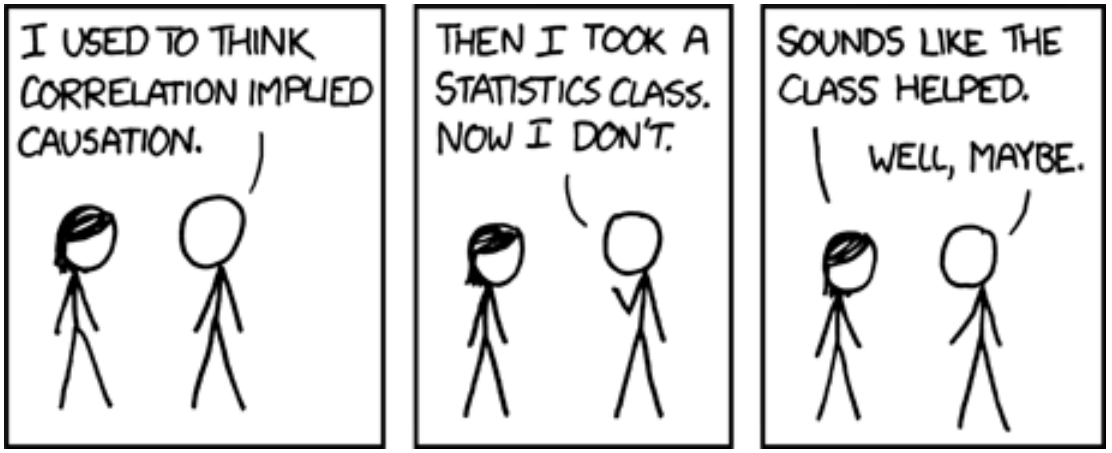
Ryan's Confusion Matrix

What you think you are: \ What you actually are:	Confused	Not Confused
Confused	Extremely Confused	Moderate Crying
Not Confused	Eye-Twitch ↓ Mental Breakdown	0% Confused

N.B.: Type I Error can be overcome, but avoid Type II Error at all costs!!!


TOSHIBA
TOSHIBA

Correlation



$$\rho_{X,Y} = corr(X,Y) = \frac{cov(X,Y)}{\sigma_X \sigma_Y} = \frac{E[(X-\mu_X)(Y-\mu_Y)]}{\sigma_X \sigma_Y}$$

Music credits

Kanto Symphony