UWEO StatR201 Lecture 11

Clustering; Parallel and Efficient Computing

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Tonight's Menu

■ Tips for final project

"Unsupervised Learning"

- Conceptual Overview
- Hierarchical clustering
- *k*-Means clustering
- "Model-Based" clustering

Then: Computing Performance Enhancement

- Parallel processing and manipulation using foreach and %dopar%
- Fast data manipulation with data.table

Then: (temporary?) Parting Words: summary of class and a look towards Spring, with some last-minute R tricks mixed in.

But first, before we get tired, one long-overdue R trick/annoyance.

Date and Time in R: as.Date and as.POSIX1t

This might have been shown before, but worth (re?) visiting before you graduate 2/3 of the program. What to do about dates?

```
trux = read.csv("../Datasets/summer trucks.csv", as.is = TRUE)
head(trux, 3)
         id
                 date stagnant Caline1.5 caline3
## 1 1313326 2012-8-18
                         52
                                 0.4124 0.4736
## 2 1313326 2012-9-1
                         42
                                 0.5132 0.5700
## 3 1313326 2012-9-15
                       113 0.5640 0.6386
summary(trux$date)
     Length
                Class
                          Mode
##
        513 character character
```

trux\$date is a string vector right now (if not for as.is=TRUE it would have been a factor). Can R speak date? Naturally.

```
trux$date = as.Date(trux$date)

## Min. 1st Qu. Median Mean 3rd Qu.

## "2012-08-18" "2012-09-15" "2012-10-13" "2012-11-10"

## Max.

## "2012-12-08"
```

Note the capital D in as.Date. This class allows addition/substraction (with the unit being days) and other operations. For some functions (e.g., smooth.spline) you will need to convert Date objects to integers via as.numeric.

The date format in trux is the R default. Hence, we can actually read.csv the data directly as Date:

Converting other Date Strings

The format used by R is the ISO 8601 international date standard; its origin (Day 1) is 1970-01-01. Note (as in the example) that R does **not** auto-interpret any string that might look like a Date as such; rather, it needs to be specifically told so via as.Date().

Now... what about importing dates from US-style or other formats?

```
morenox = read.csv("../Datasets/LRnox.csv", as.is = TRUE)
head(morenox, 3)
            on date air nox siteid
       92 7/1/2009
                       13.6 LR001
       91 6/17/2009
                       13.6 LR001
       90 6/3/2009
                       13.6 LR001
morenox$on date = as.Date(morenox$on date, "%m/%d/%Y")
head(morenox, 3)
             on date air nox siteid
     event
       92 2009-07-01
                        13.6 LR001
       91 2009-06-17
                        13.6 LR001
        90 2009-06-03
                       13.6 LR001
summary(morenox$on_date)
          Min.
                    1st Qu.
                                  Median
                                                            3rd Qu.
## "2005-11-23" "2006-09-27" "2007-09-05" "2007-09-11" "2008-08-16"
##
## "2009-07-01"
```

A more detailed standard time class is as.POSIX1t, which includes time as well as several useful utilities (e.g., wday). Date objects can be converted to and from that class.

Final Project Tips, Q&A

Here are my nanny-style tips:

- The basics still apply, regardless of problem type, method and level of sophistication.
- Use plenty of descriptives, even automated ones (with large p). You don't have to present all of them but for yourself.
- Regarding outliers/improbables: if using a repository dataset, do NOT exclude observations without consulting
 me. If using your own dataset, still exercise caution and good judgment.
- Do not forget transformations/alignment/scaling
- Filtering (for information content, correlation, etc.) pays back in multiple ways: improving performance, improving clarity, saving CPU time
- Account for the dataset's "natural" grouping, if there is one.

When choosing/tuning a method, think about:

- Would weighting the features matter for some of your methods? If so, what weighting would be sensible?
- Do you have a basic grasp of what makes the method tick? If not sure, test it out by some deliberately wild tuning.
- Do you need to pre-treat categorical covariates to make them work?
- Do some back-and-forth on the training data from tuning back to descriptives, diagnosing misclassified/outlying observations and seeing whether you have missed something
- Don't be afraid to ask questions. When writing up, remember it is 20 pages max.

"Supervised" vs. "Unsupervised" "Learning"

Personally, I think the importance of these terms is exaggerated, but it is very standard. Here it is in a nutshell.

Classification and regression are both called Supervised Learning. Symbolically, continuous-y regression can be written as

$$E[y] = f(\mathbf{X}),$$

whereas classification (or, equivalently, categorical-outcome regression) is

$$\Pr(y = c) = f_c(\mathbf{X}), \ c = 1, \dots, C.$$

On the other hand,

With "Unsupervised Learning", we have this:

 \mathbf{X}

What Can One Do?

With

 \mathbf{X} ?

Why, of course:

- Descriptives
- Nicer Descriptives
- Even Nicer Descriptives
- Something Really Grand (let's call it SRG).
- One SRG we've already learned (sort-of), is **SVD/principal-components.**
- "invent" a y, usually a categorical one, and assign it to the observations. This is known as Clustering.
- Another famous SRG is "picking winners" in a high-dimensional dataset: in other words, inventing a continuous y and finding its optimum. That's what Google's PageRank algorithm does (Section 14.10), but it involves material beyond our current reach.

Examples for Clustering Applications

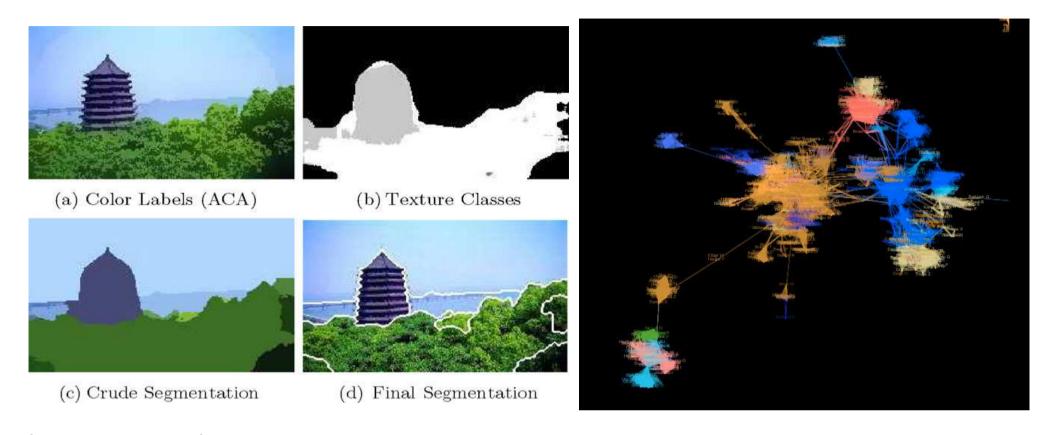
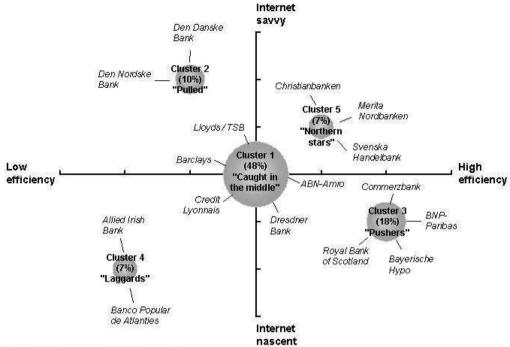


Image segmentation

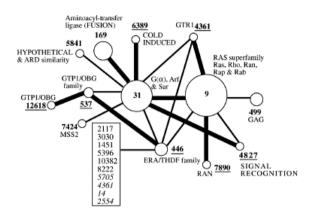
Social networks

CLUSTER ANALYSIS



Source: Bank names are illustrative examples

BS Economics



Molecular biology ("-Omics")

Clustering Basics

Most clustering algorithms are based on D, a pairwise **dissimilarity** or "distance" matrix between the observations, calculated from their features.

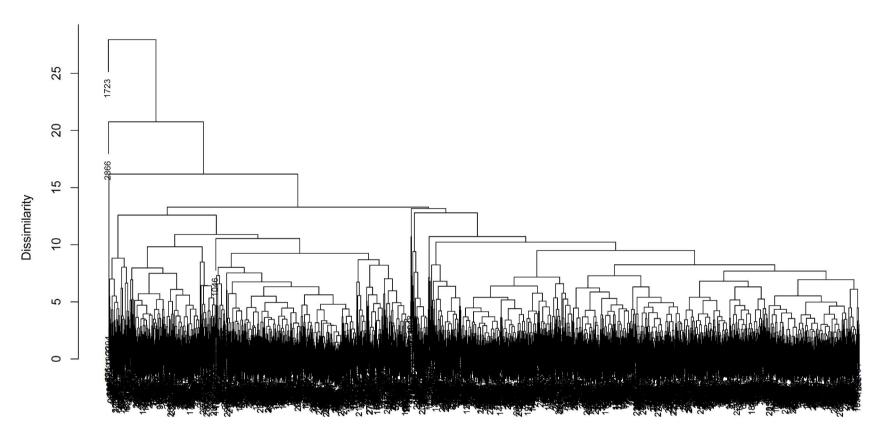
D can be a genuine distance matrix, or any measure deemed appropriate for the context (as usual, categorical variables make this harder).

Generally speaking, clusters are groups of **relatively** less dissimilar points. However, the completely open challenge of *"tell me how many clusters there are, and which points go into which cluster"* is usually too ill-defined to answer without imposing further constraints. Ways out of this morass include:

- Specify how many clusters there are, then let the algorithm define them, as in k-Means Clustering;
- Specify a nested hierarchy of probability (density) models for the general cluster structure, then compare the various maximum-likelihood solutions via nested hypotheses or AIC/BIC, as in Model-Based Clustering;
- Describe the entire cascade of grouping (ungrouping) into (out of) clusters, from a single point to all n (or vice versa) and let the user decide where to make the cut, as in **Hierarchical Clustering**, which is where we start.

Hierarchical Clustering in R

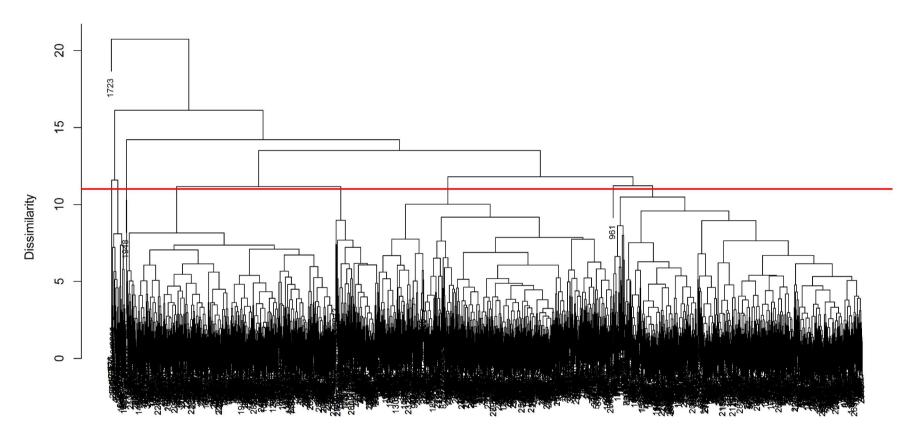
```
par(mar = c(2, 5, 1, 1))
plot(hclust(dist(scale(wine[, -12]))), cex = 0.7, xlab = "", ylab = "Dissimilarity",
    main = "")
```



Hierarchical clustering modestly aims to serve mostly as a powerful descriptive. Here, for example, the asymmetry and gross outliers remind us that perhaps residual.sugar and free.sulfur.dioxide should be log-transformed (the two singletons correspond to the highest values in each feature).

Hierarchical Clustering in R

```
par(mar = c(2, 5, 1, 1))
wine$logsugar = log10(wine$residual.sugar)
wine$logfree = log10(wine$free.sulfur.dioxide)
winedist = dist(scale(wine[, -c(4, 6, 12)]))
plot(hclust(winedist), cex = 0.7, xlab = "", ylab = "Dissimilarity", main = "")
abline(h = 11, lwd = 2, col = 2)
```



The sugar high is still lonely, but there is more structure visible overall, and the tree is less skewed. I am **Not** suggesting to force the tree into symmetric form no matter what, but with Euclidean distance (the default of dist) the skewness of a couple of features might reflect itself in the tree. **So how many clusters?** depends on where we draw the line... at a distance of 11 (=1 SD per feature, marked by red line) there are about 10 clusters, including at least a couple of singetons.

How helust Works

hclust is an Agglomerating Clustering Algorithm:

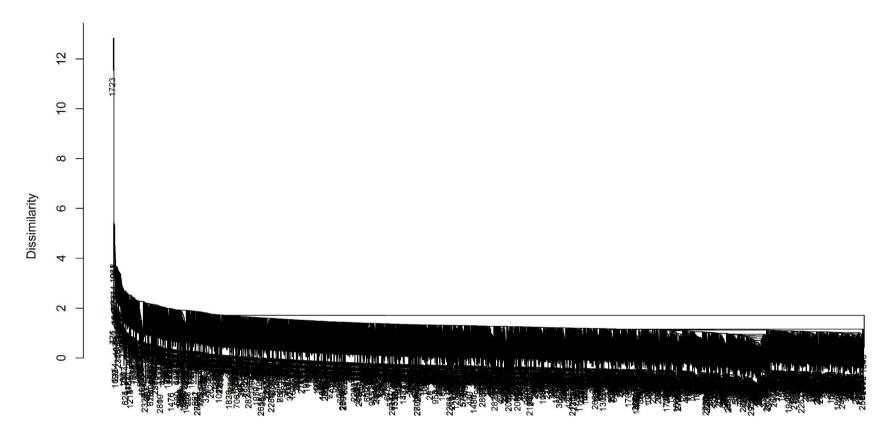
- 0. Calculate (or receive as input) all pairwise D values, and define a **cluster-dissimilarity metric** \tilde{d} that is a function of D.
- 1. Start with each observation in its own cluster.
- 2. At each step, join together the two least-dissimilar clusters, according to the between-cluster metric defined in Step 0.
- 3. Record the recently-joined pair's \tilde{d} value.
- 4. Continue until all observations have been joined to a single cluster (this will take exactly n-1 steps).
- 5. Draw the tree according to the join hierarchy, with heights corresponding to each joining's $ilde{d}$ value.

The definition of $ilde{d}$ has a great impact upon the resulting tree. Common options:

- Complete Linkage (the hclust default): the maximum D between the two clusters' individual points;
- Single Linkage: the minimum D between the two clusters' individual points; -Average Linkage: as its name indicates, the average D between the two clusters' individual points;
- hclust allows for 4 more options (see its help page).

hclust with Single Linkage

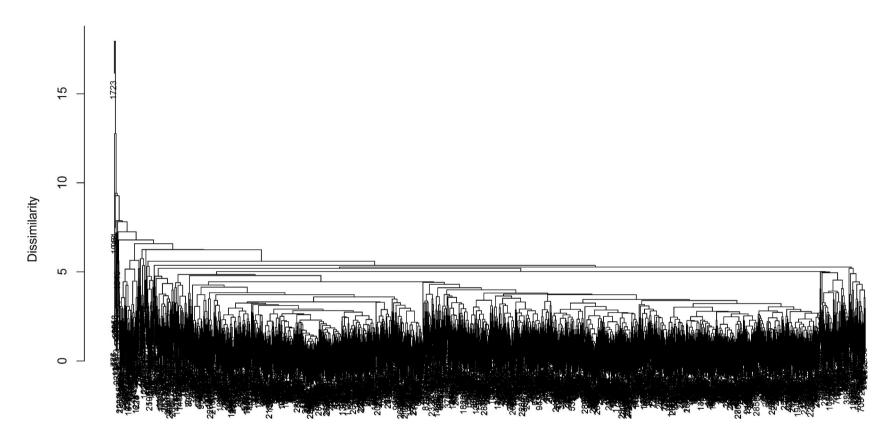
```
par(mar = c(2, 5, 1, 1))
wine$logsugar = log10(wine$residual.sugar)
wine$logfree = log10(wine$free.sulfur.dioxide)
plot(hclust(winedist, method = "single"), cex = 0.7, xlab = "", ylab = "Dissimilarity",
    main = "")
```



Single-linkage downplays dissimilarities; generally not recommended unless you have good content reason.

hclust with Average Linkage

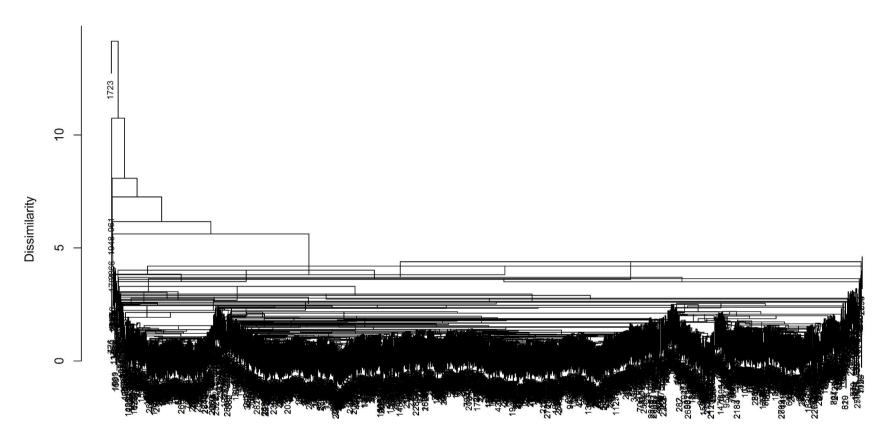
```
par(mar = c(2, 5, 1, 1))
wine$logsugar = log10(wine$residual.sugar)
wine$logfree = log10(wine$free.sulfur.dioxide)
plot(hclust(winedist, method = "average"), cex = 0.7, xlab = "", ylab = "Dissimilarity",
    main = "")
```



If we're going for average, why not the median? It will be more robust to outliers...

hclust with Median Linkage

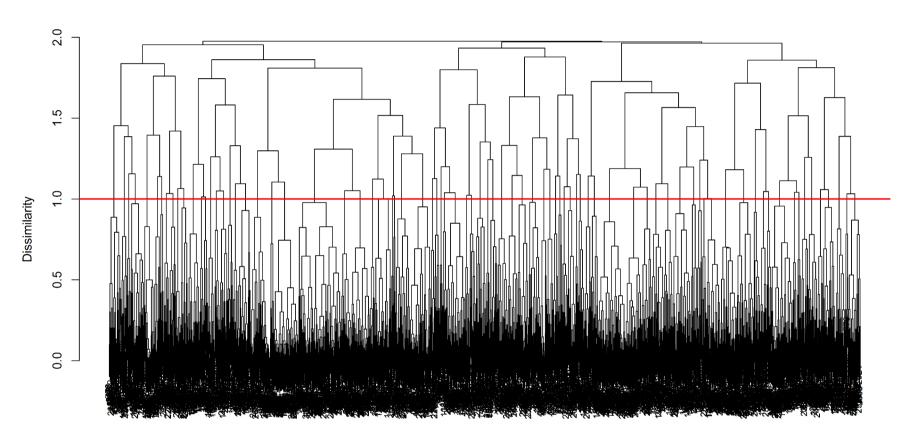
```
par(mar = c(2, 5, 1, 1))
wine$logsugar = log10(wine$residual.sugar)
wine$logfree = log10(wine$free.sulfur.dioxide)
plot(hclust(winedist, method = "median"), cex = 0.7, xlab = "", ylab = "Dissimilarity",
    main = "")
```



Oopsie!... What's going on? Well, some methods (single, complete, average) guarantee **monotonicity** - i.e., that higher joinings always take place at a larger value of \tilde{d} . The median method apparently does **not**.

hclust with Correlation Distance

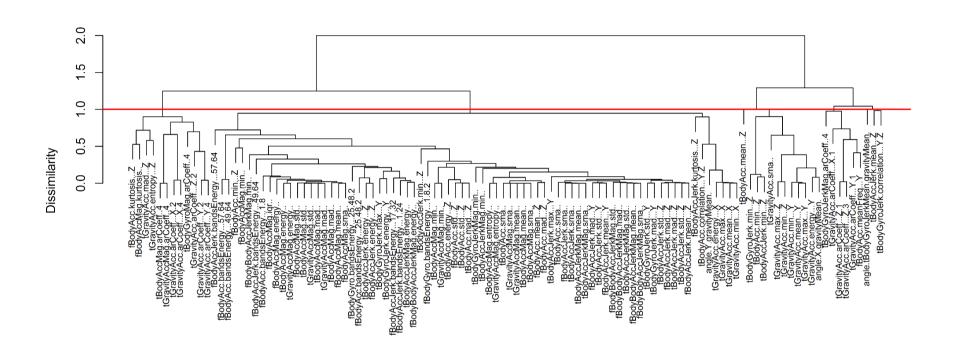
```
par(mar = c(2, 5, 1, 1))
wineRdist = as.dist(1 - cor(t(scale(wine[, -c(4, 6, 12)]))) # note the 't'
plot(hclust(wineRdist), cex = 0.7, xlab = "", ylab = "Dissimilarity", main = "",
    sub = "")
abline(h = 1, lwd = 2, col = 2)
```



Generally, correlation-based dissimilarity is more robust than Euclidean distance. This tree suggests almost no structure: note the high join points (there are > 10 clusters), the **very** symmetric look, and the scarcity of any clusters with strongly positive pairwise correlation (the red line marks r=0).

Clustering the Features

```
plot(hclust(smartRdist), cex = 0.7, xlab = "", ylab = "Dissimilarity", main = "",
    sub = "")
abline(h = 1, lwd = 2, col = 2)
```



More often than not, hclust is more helpful on the **features** than on the observations. Here, with the (between/within filtered) smartphone dataset, we see quite a bit of structure. Clearly, the division into the walking-related and non-walking-related features, as well as quite a few *very* highly correlated pairs (suggesting, for those working on HW6, that correlation-based filtering is probably needed here). But also: some additional structure that is possibly worth investigating. Questions? *Online* questions? Practice this a bit, using the iris dataset (hint: set labels=iris\$Species)

k-Means Clustering

You would *think* that k-Means clustering might be a variant of k-Nearest-Neighbors classification. Ha. k is just the statistician's kneejerk response to the request, "Pick a letter at random…" (my first dissertation paper title: "The k-in-a-row Up-and-Down design, Revisited" - and that k has nothing to do with either of the two:)

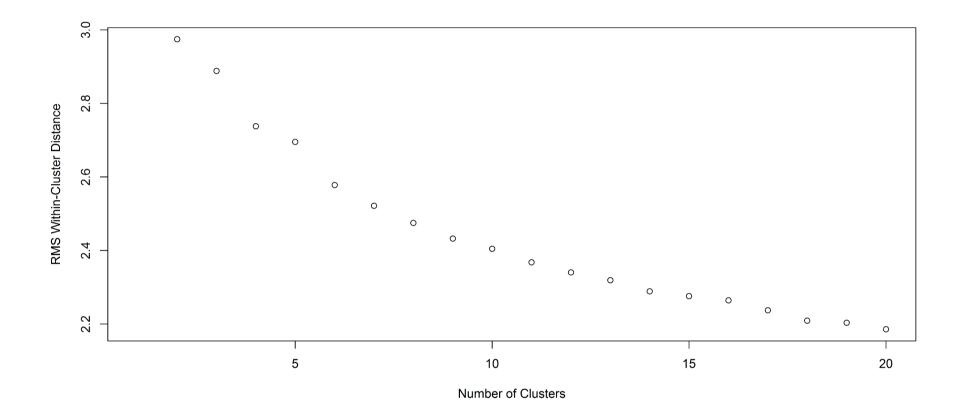
Seriously: k-Means is more closely related to that classification method this class made history by skipping: LDA. Even more closely, as the book says, to **Gaussian mixture modeling** (=density estimation in p dimensions).

k-Means tries to define k clusters (with k given) that optimize the between/within sum-of-squares ratio. As the book explains, this deceptively simple task is actually a combinatorial explosion. So instead, the algorithm iterates between

- Finding the centers-of-mass of the *k* clusters (=the "Means")
- Re-assigning points to the closest "Mean"

This algorithm is actually lightning-quick.

k-Means Clustering



Ok, let's give k-Means a road test. Do the same drill above, for iris (don't need to go all the way to k=20; 6-7 should suffice). Also possibly for the **features** of smartscale.

Questions? Online questions?

Model-Based Clustering with mclust

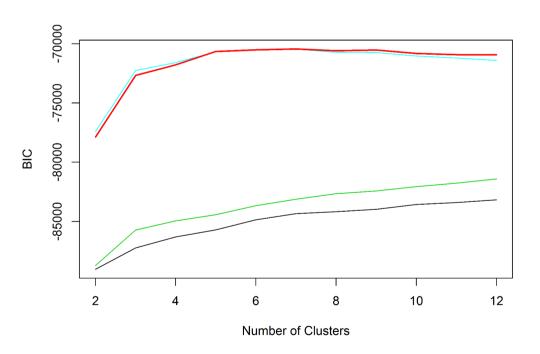
The RMS-within vs. k plot almost begs the question "where to draw the line?". By now you might have guessed that the within-distance is pretty much guaranteed to go down as we add clusters.

You might have also realized, that (hyper-)spherical clusters in feature space are analogous to a very specific **probability** model: Normal. In fact, independent, equal-variance Normal.

Adrian Raftery and many others right here at the UW stats department, decided to combine these two nuggets and turn the cluster-finding exercise in Euclidean space, into nested-hypothesis model selection.

```
library(mclust)
mout = Mclust(scale(wine[, -c(4, 6, 12)]), G = 2:12)
c(mout$G, mout$modelName, mout$df)

## [1] "7" "VEV" "485"
```



Model-Based Clustering, Mixture Models and LDA

Model-based clustering assumes the features follow a Gaussian mixture distribution:

$$egin{aligned} \Pr(\mathbf{X}) &= \sum_k \Pr(\mathbf{X} \in \operatorname{Cluster} k) \Pr(\mathbf{X} \mid \mathbf{X} \in k) \ &= \sum_k \pi_k I(\mathbf{X} \in k) \operatorname{Normal}ig(\mu_k, \Sigma_kig), \end{aligned}$$

where $I(\cdot)$ is the indicator function, and μ_k, Σ_k are the mean and covariance matrix of cluster k in p-dimensional feature space.

Linear Discriminant Analysis (LDA) and its direct extensions such as Quadratic Discriminant Analysis, make essentially the same assumption. However, with LDA/QDA, both the number of classes and their (training-set) assignments are fully known.

LDA/QDA are not good classifiers, because they constrain class boundaries to be *very* smooth. OTOH, when it comes to cluster discovery, the exact boundaries might concern us less than identifying high-density centers of mass.

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Model-Based Clustering: Specification

A multivariate Gaussian can be more or less constrained, for example with respect to each single cluster:

- Equal variance and i.i.d. features? 'Spherical'
- Unequal variance, but i.i.d. features? 'Diagonal'
- Unequal variance and correlated features? 'Ellipsoidal'

And also, between-cluster constraints:

- Are they all the same size?
- Are they all the same shape?
- Are they all the same orientation?

Some constraints are associated with a whole bunch of degrees of freedom (e.g., going from "Diagonal" to "Ellipsoidal", or allowing each cluster to have its own shape or orientation).

Since Mclust criterion is BIC, the fit has to be *much* better to justify these moves. Oftentimes, it is easier for the model to retain the constraints, and just add a couple more clusters.

If we have time, we will explore ellipsoids interactively with rgl.

Questions? Online questions?

foreach and %do%: Yet Another Flavor of Xapply?

We will now learn the basics of parallel processing, using the packages provided by Revolution Analytics. This private company attempts to establish R community "street cred" by providing performance-enhancing packages.

As infrastructure for parallel processing, Revolution developed foreach, with the namesake command paired with %do.

randomForest has a built-in combine functionality, that allows to break up a single "Forest" into pieces and put it together again for the final calculations.

At first glance, foreach ... %do% looks like just another way to do loop. However,

- 1. You can have multiple arguments inside foreach, including lists etc. The %do% will cycle over all of them element-wise, just like mapply.
- 2. Replace %do% with %dopar%, add some syntax... and Voila!

Parallel

Processing with foreach and %dopar%

```
library(doSNOW); library(randomForest); options(width=80)
cl <- makeCluster(3, type = "SOCK")</pre>
registerDoSNOW(cl)
system.time(rf1 <-</pre>
    foreach(ntree=rep(667,3), .combine=combine,.packages='randomForest')
            %dopar% randomForest(factor(quality)~.,data=wine,ntree=ntree))
      user system elapsed
      5.25
              0.49 10.20
stopCluster(cl)
cl <- makeCluster(6, type = "SOCK")</pre>
registerDoSNOW(cl)
system.time(rf2 <-</pre>
    foreach(ntree=rep(333,6), .combine=combine,.packages='randomForest')
            %dopar% randomForest(factor(quality)~.,data=wine,ntree=ntree))
      user system elapsed
      3.45
              0.76
                       7.23
```

Notes:

■ Until not long ago, users had to

```
stopCluster(cl)
```

specify every variable passed to parallel processes. foreach ... %dopar% make it far more convenient, "fishing out" any needed variable out of the current environment.

- If you use functions from additional packages, the package names need to be passed down via .packages.
- This was a toy example, also to demonstrate one of parallel processing's futility bounds: sending jobs that are too small, is not worth the overhead.
- Our main use for foreach ... %dopar% is in tuning, where each job is a complete run.

Parallel Processing with foreach and %dopar%

```
options(width = 130)
source("../Code/foreachRF.r")
serial = rfTune0(factor(quality) ~ ., data = wine, mvals = 1:6, nodevals = 1:5)  # %do% with no parallel overhead
c13 = rfTune(factor(quality) ~ ., data = wine, mvals = 1:6, nodevals = 1:5, nclust = 3)
c16 = rfTune(factor(quality) ~ ., data = wine, mvals = 1:6, nodevals = 1:5, nclust = 6)
c(serial$times[3], c13$times[3], c16$times[3])
## elapsed elapsed elapsed
## 31.26 12.46 8.46
```

Run it, and look at the main dataset returned by rfTune0, rfTune (that would be the performance component), to see if they give the same tuning answer!

Please, **try and write**, **RIGHT NOW**, **an analogous parallel-tuning function** for a classifier/regression you plan to use in your project. Questions? *Online* questions?

Cool R Trick 1: expand.grid

Did you note this in the foreachRF function?

This wonderful little base R utility generates a data frame including all level combinations.

Data Manipulation 4.1.1: Yet Another Xapply?

Last week, we got a quick tasting of plyr and its ddply functions, that can carry out manipulations that under the standard Xapplys are either cumbersome or impossible.

Nice. But ddply et al. do not improve efficiency. For this and other purposes, a new package called data.table has been developed. It is a closer analogue of SQL than the others. The package defines a new class data.table, which inherits from data.frame - meaning that you can convert data frames to data.table with (nearly?) no adverse impace on the ability to work with them using other functions (plotting, modeling, etc.)

```
library(data.table)
smartrain = read.csv("../Datasets/smarTrain.csv", as.is = TRUE)
smartrain = data.table(smartrain)
```

Test-Running data.table vs. plyr

```
library(plyr)
system.time(smartscale1 <- ddply(smartrain, "Subject", function(x) data.frame(cbind(scale(x[, 2:562]), class = x$Class))))

## user system elapsed
## 1.68 0.08 1.76

smartscale2 = copy(smartrain)
scalenames = names(smartscale2)[2:562]
system.time(smartscale2[, `:=`(eval(scalenames), as.data.table(scale(.SD))), .SDcols = scalenames, by = Subject])

## user system elapsed
## 0.61 0.00 0.61</pre>
```

Ok... a time-savings of 3x to 5x. Not bad for a fairly short task; data.table authors demonstrate much larger savings on heavier tasks. It often helps to define a **key** variable via setkey (yes, like with SQL, upon which data.table draws heavily). But did we get the same results in this little exercise?

```
table(smartscale1 == data.frame(smartscale2))

##
## TRUE
## 4139176
```

We have to "notch down" the data.table back to a data.frame for the comparison. Also, note that doing e.g., smartscale2[,2:562] will try to run a function rather than just return the specified columns. You need to do smartscale2[,2:562,with=FALSE] to get the latter.

Learn more about data.table: http://cran.r-project.org/web/packages/data.table/vignettes/datatable-intro.pdf, http://datatable.r-forge.r-project.org/datatable-faq.pdf.

R Trick 2: What Shall We Do to Fill those Empty Spaces?

Reading in data from Excel or other point-click software, we sometimes see this: (opening spreadsheet...)

Which, in R, turns into this:

```
missydat = read.csv(".../Datasets/naLOCF.csv", as.is = TRUE)
head(missydat, 10)
       id time1 value1 time2 value2 time3 value3
            500
                   6.0 1800
            700
                        2000
                                      400
            900
                   0.0
                          NA
                                 NA
                                      800
                                               3
           1100
                   2.5
                          NA
                                     1200
           1300
                                     1319
                    NA
                          NA
## 6
             NA
                    NA
                          NA
                                    1600
                    NA
                          NA
                                     2000
## 8
                                     2359
## 9 A266 1300
                   6.0 1630
## 10
           1500
                   6.0 1800
                                      400
```

The empty time and value entries are probably ok - there's no data there. But the id variable needs to be filled down. Turns out, in R it is quite easy:

```
library(zoo)
missydat$id[missydat$id == ""] = NA
missydat$id = na.locf(missydat$id)
head(missydat, 10)
       id time1 value1 time2 value2 time3 value3
  1 A433
                   6.0 1800
            500
     A433
            700
                   8.0
                       2000
                                 8
                                     400
            900
                                     800
     A433
                   0.0
                         NA
                                NA
     A433 1100
                   2.5
                       NA
                                    1200
     A433
           1300
                                    1319
                    NA
     A433
                    NA
                       NA
                                    1600
     A433
             NA
                    NA
                         NA
                                    2000
     A433
             NA
                    NA
                         NA
                                    2359
     A266 1300
                   6.0 1630
```

zoo is a time-series analysis package. It contains fancier, time-series-appropriate ways of filling those empty space (Eli might teach you more tricks from there in Spring).

6.0 1800

400

10 A266 1500

Last Trick... But Not Least: Error Bars, the Simple Way!

So... not for the first time, I needed to plot error bars for an article at work. Previously I made do with the somewhat kludgey solutions plotCI and plotmeans in the gplots package.

But now... I'm an R teacher, ain't I? So I searched far and wide. There are error bars in xYplot (an expansion of lattice functionality, part of Hmisc). Also in the super-hyped ggplot2 - a package with which I still feel ill at ease (Revolution offers a specific ggplot2 class!).

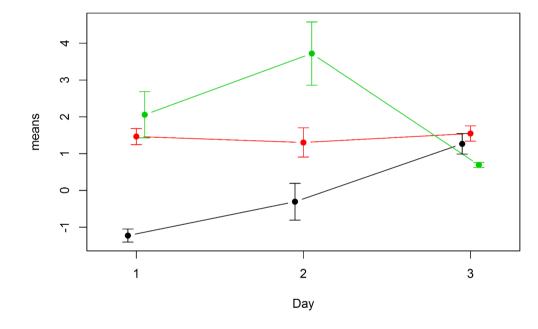
So I fell back to the most primitive solution, courtesy of anthropologist James Holland Jones:

One common frustration that I have heard expressed about R is that there is no automatic way to plot error bars (whiskers really) on bar plots. I just encountered this issue revising a paper for submission and figured I'd share my code. The following simple function will plot reasonable error bars on a bar plot.

```
options(width = 130)
error.bar <- function(x, y, upper, lower = upper, length = 0.1, ...) {
   if (length(x) != length(y) | length(y) != length(lower) | length(lower) != length(upper))
        stop("vectors must be same length")
   arrows(x, y + upper, x, y - lower, angle = 90, code = 3, length = length, ...)
}</pre>
```

Last Trick... But Not Least: Error Bars, the Simple Way!

Fun with Simple Error Bars!



TTFN... and Looking Ahead to Spring

Thank you for investing your time, efforts and resources in this class. I am honored to have taught such a group of people.

I tried to deliver the class from the perspective of an applied statistician, but without losing sight of the theoretical and conceptual angles.

My apologies for the rocky start, and for *still* not coming up with some HW keys... With all that I am satisfied with the breadth and coherence of the statistical material we've covered. It's a lot to digest in a couple of months, but I hope you now have a basic toolset and general mindset to successfully approach modeling problems.

With the rush to get through major regression/classification highlights and examples, the programming angle – as well as some "side" statistical topics – often took a back seat. Items tentatively planned for Winter, now delegated to the Spring wish-list include:

- Direct treatment of publishing via knitr, including LaTex equations;
- More graphics, including the fearsome ggplot2;
- Smoothing splines and Generalized Additive Models (GAM)

More major topics for Spring include

- Simulation inference: permutation and bootstrap
- Bayesian principles and methods
- Hierarchical and mixed models
- Spatial and temporal models
- Package creation and other advanced-programming topics (S3/S4 and other infrastructure, incorporating other languages, "Big Data", etc.)

