3. The object system(s)

Thomas Lumley
Ken Rice

Universities of Washington and Auckland

Seattle, June 2011
Generics and methods

Many functions in R are generic. This means that the function itself (eg plot, summary, mean) doesn’t do anything. The work is done by methods that know how to plot, summarize or average particular types of information.

If you call summary on a data.frame, R works out that the correct function to do the work is summary.data.frame and calls that instead. If there is no specialized method to summarize the information, R will call summary.default

You can find out all the types of data that R knows how to summarize with two functions...
Generics and methods

> methods("summary")

[1] summary.Date       summary.POSIXct       summary.POSIXlt
[7] summary.data.frame summary.default      summary.ecdf*
[10] summary.factor     summary.glm         summary.infl
[13] summary.lm         summary.loess*       summary.manova
[16] summary.matrix     summary.mlm         summary.nls*
[19] summary.packageStatus* summary.ppr* summary.prcomp*
[22] summary.princomp*  summary.stepfun     summary.stl*
[25] summary.table      summary.tukeysmooth*

Non-visible functions are asterisked

> getMethods("summary")

NULL

There are two functions because S has two object systems, for historical reasons.
Methods

The class and method system makes it easy to add new types of information (e.g. survey designs) and have them work just like the built-in ones.

Some standard methods are

- **print, summary**: everything should have these
- **plot or image**: if you can work out an obvious way to plot the thing, one of these functions should do it.
- **coef, vcov**: Anything that estimates parameters and corresponding covariance matrices should have these.
- **anova, logLik, AIC**: models fitted by maximum likelihood should have these.
- **residuals**: anything that has residuals should have this.

[Informal analogue of Java interfaces]
New classes: S3

Creating a new class is easy

class(x) <- "duck"

R will now automatically look for the `print.duck` method, the `summary.duck` method, and so on.

There is no formal registration or documentation of the structure of the object. You need to make sure that anything of class `duck` can `look.duck`, `walk.duck`, `quack.duck`.

Yes, this is different from Java and C++.
Generic functions: S3

A generic function has a call to `UseMethod()`, which does the method dispatching.

```r
> print
function (x, ...)
UseMethod("print")
```

By default, method dispatch is on the first argument. It can be on any (single) argument.

```r
> svymean
function (x, design, na.rm = FALSE, ...)
{
    UseMethod("svymean", design)
}
```
Example: ROC curves

The Receiver Operating Characteristic (ROC) curve describes the ability of an ordinal variable $T$ to predict a binary variable $D$.

The ROC curve graphs $P(T > c | D = 1)$ against $P(T > c | D = 0)$ for every cutpoint $c$;

![Outcome (D) vs predictor (T)](image)

![ROC curve (color-coded)](image)
Example: ROC curves

Here's a simple way to code it:

ROC <- function(test, disease){
  #test = e.g. levels of a biomarker
  # where is the curve going to change?
  cutpoints <- c(-Inf, sort(unique(test)), Inf)

  # what values will it take when it does change?
  sensitivity <- sapply(cutpoints,
    function(result) mean(test>result & disease)/mean(disease))
  specificity <- sapply(cutpoints,
    function(result) mean(test<=result & !disease)/mean(!disease))

  # plot the curve, return the coordinates
  plot(sensitivity, 1-specificity, type="l")
  abline(0,1,lty=2)

  return(list(sens=sensitivity, spec=specificity))
}

3.7
Example: ROC curve

Here's a more efficient version of the calculation;

drawROC<-function(T,D){
  DD <- table(-T,D)
  tpr <- cumsum(DD[,2])/sum(DD[,2])
  fpr <- cumsum(DD[,1])/sum(DD[,1])
  plot(fpr, tpr, type="l")
}

Note that we use the vectorized \texttt{cumsum()} rather than the implied loop of \texttt{sapply()}.

We want to make this return an ROC object that can be plotted and operated on in other ways.
ROC curve object

ROC<-function(T,D){
    DD <- table(-T,D)
    tpr <- cumsum(DD[,2])/sum(DD[,2])
    fpr <- cumsum(DD[,1])/sum(DD[,1])
    rval <- list(tpr=tpr, fpr=fpr,
                 cutpoints=rev(sort(unique(T))),
                 call=sys.call())
    class(rval)<-"ROC"
    rval
}

Instead of plotting the curve we return the data needed for the plot – plus some things that might be useful later; `sys.call()` is a copy of the call.
Methods

We need a `print` method to stop the whole contents of the object being printed

```r
print.ROC<-function(x,...){
    cat("ROC curve: ")
    print(x$call)
}
```
Methods

A plot method

plot.ROC <- function(x, xlab="1-Specificity", ylab="Sensitivity", type="l", ...){
  plot(x$fpr, x$tpr, xlab=xlab, ylab=ylab, type=type, ...)
}

We specify some graphical parameters in order to set defaults for them. Others are automatically included in ....
Methods

We want to be able to add lines to an existing plot

```r
lines.ROC <- function(x, ...){
  lines(x$fpr, x$tpr, ...)
}
```

and also be able to identify cutpoints by clicking on a graph

```r
identify.ROC<-function(x, labels=NULL, ...,digits=1)
{
  if (is.null(labels))
    labels<-round(x$cutpoints,digits)
  identify(x$fpr, x$tpr, labels=labels,...)
}
```
Syntax notes

Methods should have at least the same arguments as the generic, in the same order, with the same defaults (so the first argument to a print method is x, but to a summary method is object).

For inheritance to work, methods must have a ... argument to allow unknown arguments to be ignored.

The language does not enforce these requirements, but the package checking system does.
# Inheritance

The `class` attribute can be a vector, e.g. `c("glm", "lm")`

R will look for a method for each element in turn until it finds one.

Inside a method, use `NextMethod()` to call the next method in the inheritance.

Inheritance is not used much: statisticians extend by generalization, not by specialization. The relationship of `glm` to `lm` should really be delegation, not inheritance.

An exception is data infrastructure (e.g. Bioconductor), which tends to use S4 methods.
S4 classes

Introduced in version 4 of Bell Labs’ S, since extended and refined in R.

Still uses generic functions, with methods belonging to functions rather than to classes.

- Formal declaration of class structure: `setClass()`
- Formal declaration of methods: `setMethod()`
- Multiple dispatch
- Multiple inheritance
Example: ROC curve

Define \texttt{ROC} class

```r
setClass("ROC",
    representation(tpr="numeric", fpr="numeric",
                  cutpoints="numeric", call="call")
)
```

Or we could factor out the 'curve' structure and declare

```r
setClass("xycurve", representation(x="numeric", y="numeric"))
setClass("ROC", contains="xycurve",
    representation(cutpoints="numeric", call="call")
)
```

taking advantage of inheritance
Example: ROC curve

Other options include validity checks at object creation

```
setClass("ROC",
    representation(tpr="numeric",fpr="numeric",
    cutpoints="numeric",call="call")
    validity=function(object){
        if(length(object@tpr)!=length(object@fpr) ||
            length(object@tpr)!=length(object@cutpoints))
            return("length mismatch")
        if(any(object@tpr>1) || any(object@tpr>1) ||
            any(object@tpr<0) || any(object@tpr<0))
            return("outside [0,1]")
        return(TRUE)
    })
```
Example: ROC constructor

Objects are created with `new()`; code is otherwise the same.

```r
ROC <- function(T,D){
  DD <- table(-T,D)
  tpr <- cumsum(DD[,2])/sum(DD[,2])
  fpr <- cumsum(DD[,1])/sum(DD[,1])
  new("ROC",tpr=tpr, fpr=fpr,
       cutpoints=rev(sort(unique(T))),call=sys.call())
}
```
Example: ROC methods

`setMethod` specifies a method for a generic function and an argument `signature` giving the classes of all the arguments used for dispatch.

Use `@` to refer to slots (not `$`), otherwise similar to S3

```r
setMethod("show",signature="ROC",
  function(object){
    cat("S4 ROC curve:")
    print(object@call)
  }
)
```

(Note that S4 uses `show` rather than `print`)

This generic has only one argument, so the signature is a single string.
Example: ROC methods

```
setMethod("plot",signature("ROC","ANY"),
    function(x,y,type="l", xlab="1 - Specificity",
            ylab="Sensitivity",...){
        plot(1-x@spec, x@sens, type=type, xlab=xlab, ylab=ylab ,...)
    }
)
```

This generic, for `plot()`, has two arguments (x, y).

The signature specifies this method when x is ROC and y is ANYthing.
Example: ROC methods

```r
setGeneric("lines")
setMethod("lines",signature("ROC"),
    function(x,...){
        lines(1-x@spec, x@sens,...)
    }
)
```

`lines()` is not an S4 generic.

`setGeneric()` creates an S4 generic that defaults to calling the original `lines()` function.
Multiple dispatch

Generic functions with method choice based on all arguments are strictly more expressive than the Java/C++ model of methods belonging to classes.

Java/C++ style can be translated mechanically: object.method(arg1, arg2) maps to generic(object, arg1, arg2)

The price is slower method lookup, but most of the cost is at installation time, and slower method lookup is inevitable for a system that allows one package to declare methods for another package’s objects.
Multiple dispatch

Generic function style;

- allows symmetric treatment of argument, e.g. matrix multiplication: `multiply(A, B)` not `A.rightmultiply(B)` or `B.leftmultiply(A)`

- allows the programmer to describe whether methods for two objects are actually doing the same thing.

- allows first-class functions, which mathematicians and statisticians like.
Multiple dispatch

`filter()` in the flowCore package for flow cytometry has two arguments: a data set, and an object specifying a subsetting operation. Methods are dispatched based on both arguments.

```r
> showMethods("filter")
Function: filter (package flowCore)
x="flowFrame", filter="filter"
x="flowFrame", filter="filterSet"
x="flowSet", filter="filter"
x="flowSet", filter="filterList"
x="flowSet", filter="filterSet"
x="flowSet", filter="list"
```

The Matrix package has 70 multiplication methods for different combinations of matrix types (`showMethods("%*%")`)
More complex example

Class `AnnDbBimap` is used in the `AnnotationDbi` package in Bioconductor, to provide conversions from one system of identifiers to another (e.g., probe ids, gene ids, gene symbols, GO categories). More details on Wednesday.

Examine the structure and inheritance relationships of the class with `getClass()`
More complex example

> getClass("AnnDbBimap")
Class "AnnDbBimap" [package "AnnotationDbi"]
Slots:
Name:  L2Rchain direction Lkeys Rkeys ifnotfound datacache
Class:  list integer character character list environment
Name:  objName objTarget
Class:  character character

Extends:
Class "Bimap", directly
Class "AnnDbObj", directly
Class "AnnObj", by class "AnnDbObj", distance 2

Known Subclasses:
Class "InpAnnDbBimap", directly
Class "GoAnnDbBimap", directly
Class "GOTermsAnnDbBimap", directly
Class "AnnDbMap", directly
Class "ProbeAnnDbBimap", directly
Class "Go3AnnDbBimap", by class "GoAnnDbBimap", distance 2
Class "IpiAnnDbMap", by class "AnnDbMap", distance 2
Class "AgiAnnDbMap", by class "AnnDbMap", distance 2
Class "ProbeAnnDbMap", by class "AnnDbMap", distance 2  
[..etc..]
More complex example

```r
setClass("AnnDbBimap",
  contains=c("Bimap", "AnnDbObj"),
  representation(
    L2Rchain="list", # list of L2Rlink objects
    direction="integer", # 1L for left-to-right,
    Lkeys="character",
    Rkeys="character",
    ifnotfound="list"
  ),
  prototype(
    direction=1L, # left-to-right by default
    Lkeys=as.character(NA),
    Rkeys=as.character(NA),
    ifnotfound=list() # empty list => raise an error
  )
)
```
More complex example

Multiple inheritance used for 'mix-in' behavior:

- "Bimap" is a **virtual class** that is used only to define a set of methods for its subclasses

- Some implementation is inherited from "AnnDBObj"
is(), as()

- `is(object, "class")` tests whether `object` inherits from "class"

- `as(object, "class")` attempts to convert `object` to "class". This will only work if `object` inherits from "class" or a conversion function has been provided with `setAs()

```r
setAs("ROC", "numeric",
        function(from) cbind(from@fpr, from@tpr, from@cutpoints)
)
```
New generics

When creating a completely new function with methods, you need to specify the arguments to the generic function:

```r
setGeneric("increment",
    function(object, step, ...)
    standardGeneric("increment")
)
```

Methods for `increment` will have a signature specifying classes for `object` and `step`
Some Bioconductor infrastructure

- **eSet**: basic data structure including genomic data, phenotype, metadata; specializes to ExpressionSet, SnpSet, others

- **IRanges**: for manipulating numeric sequences.

- **Xstring**: stores long strings (specializes to DNAstring, RNAstring, AAString)

- **AnnDbObj, Bimap**: Storage and lookup of annotation data
**eSet**

**assayData** Contains matrices with equal dimensions, and with column number equal to `$\text{nrow(phenodata)}$`. Class: AssayData-class

**phenoData** Contains experimenter-supplied variables describing sample (i.e., columns in assayData) phenotypes. Class: AnnotatedDataFrame-class

**featureData** Contains variables describing features (i.e., rows in assayData) unique to this experiment. Use the annotation slot to efficiently reference feature data common to the annotation package used in the experiment. Class: AnnotatedDataFrame-class

**experimentData** Contains details of experimental methods. Class: MIAME-class

**annotation** Label associated with the annotation package used in the experiment. Class: character

**protocolData** Contains microarray equipment-generated variables describing sample (i.e., columns in assayData) phenotypes. Class: AnnotatedDataFrame-class
eSet

eSet has accessor functions to extract or modify the data; the slots should not be used directly.

eSet is a virtual class that abstracts a set of data properties. Actual objects must be defined using a subclass of eSet, and new("eSet") is an error.

ExpressionSet is a subclass where the assayData slot contains one or more matrices (all the same size) for gene expression data.

SnpSet is a subclass where the assayData slot contains two matrices of the same size, for SNP calls and call probabilities.
Sequences

The **IRanges** package provides an alternative infrastructure to vectors, mostly as virtual classes.

- **Sequence**: virtual class for (potentially large) vectors
- **View**: virtual class for subsequences of a **Sequence**
- **Ranges**: sets of intervals of consecutive integers.
- **IntervalTree**: find overlaps between two **Ranges**
**Biostrings package**

`DNAString` and `RNAString` represent genomic sequences, `AAString` represents an amino-acid sequence

```r
> d <- DNAString("TTGAAAA-CTC-N")
> length(d)
[1] 13
> alphabet(d)  # DNA_ALPHABET
[1] "A" "C" "G" "T" "M" "R" "W" "S" "Y" "K" "V" "H" "D" "B" "N" "-" "+"
> alphabet(d, baseOnly=TRUE)  # DNA_BASES
[1] "A" "C" "G" "T"

> d
13-letter "DNAString" instance
seq: TTGAAAA-CTC-N
> reverseComplement(d)
13-letter "DNAString" instance
seq: N-GAG-TTTTCAA
> RNAString(d)
13-letter "RNAString" instance
seq: UUGAAAA-CUC-N
```

3.35
Efficiency

The underlying sequence is not copied on assignment.

The `subseq()` function (from `IRanges`) makes a view of a subset of the string without copying

...allows manipulation of whole-chromosome sequences.

```r
> data(yeastSEQCHR1)
> yeast1 <- DNAString(yeastSEQCHR1)
> str(yeast1)
Formal class 'DNAString' [package "Biostrings"] with 6 slots
 ..@ shared  :Formal class 'SharedRaw' [package "IRanges"] with 2 slots
    .. ..@ xp :<externalptr>
    .. ..@ .link_to_cached_object:<environment: 0x1cf45fdc>
 ..@ offset  : int 0
 ..@ length   : int 230208
 ..@ elementMetadata: NULL
 ..@ elementType  : chr "ANY"
 ..@ metadata   : list()
```
# Efficiency

```r
> dinucleotideFrequency(yeast1)

<table>
<thead>
<tr>
<th></th>
<th>AA</th>
<th>AC</th>
<th>AG</th>
<th>AT</th>
<th>CA</th>
<th>CC</th>
<th>CG</th>
<th>CT</th>
<th>GA</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>23947</td>
<td>12493</td>
<td>13621</td>
<td>19769</td>
<td>15224</td>
<td>9218</td>
<td>7089</td>
<td>13112</td>
<td>14478</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>GC</th>
<th>GG</th>
<th>GT</th>
<th>TA</th>
<th>TC</th>
<th>TG</th>
<th>TT</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>8910</td>
<td>9438</td>
<td>12938</td>
<td>16181</td>
<td>14021</td>
<td>15617</td>
<td>24151</td>
</tr>
</tbody>
</table>

> trinucleotideFrequency(yeast1)

<table>
<thead>
<tr>
<th></th>
<th>AAA</th>
<th>AAC</th>
<th>AAG</th>
<th>AAT</th>
<th>ACA</th>
<th>ACC</th>
<th>ACG</th>
<th>ACT</th>
<th>AGA</th>
<th>AGC</th>
<th>AGG</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>8576</td>
<td>4105</td>
<td>4960</td>
<td>6306</td>
<td>3924</td>
<td>2849</td>
<td>2186</td>
<td>3534</td>
<td>4537</td>
<td>2680</td>
<td>2707</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>AGT</th>
<th>ATA</th>
<th>ATC</th>
<th>ATG</th>
<th>ATT</th>
<th>CAA</th>
<th>CAC</th>
<th>CAG</th>
<th>CAT</th>
<th>CCA</th>
<th>CCC</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>3697</td>
<td>5242</td>
<td>3849</td>
<td>4294</td>
<td>6384</td>
<td>5147</td>
<td>2722</td>
<td>3091</td>
<td>4264</td>
<td>3696</td>
<td>1622</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>CCG</th>
<th>CCT</th>
<th>CGA</th>
<th>CGC</th>
<th>CGG</th>
<th>CGT</th>
<th>CTA</th>
<th>CTC</th>
<th>CTG</th>
<th>CTT</th>
<th>GAA</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1444</td>
<td>2456</td>
<td>2158</td>
<td>1380</td>
<td>1446</td>
<td>2105</td>
<td>2755</td>
<td>2556</td>
<td>3074</td>
<td>4727</td>
<td>5437</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>GAC</th>
<th>GAG</th>
<th>GAT</th>
<th>GCA</th>
<th>GCC</th>
<th>GCG</th>
<th>GCT</th>
<th>GGA</th>
<th>GGC</th>
<th>GGG</th>
<th>GGT</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2384</td>
<td>2645</td>
<td>4012</td>
<td>2993</td>
<td>1960</td>
<td>1259</td>
<td>2698</td>
<td>2983</td>
<td>1905</td>
<td>1594</td>
<td>2955</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>GTA</th>
<th>GTC</th>
<th>GTG</th>
<th>GTT</th>
<th>TAA</th>
<th>TAC</th>
<th>TAG</th>
<th>TAT</th>
<th>TCA</th>
<th>TCC</th>
<th>TCG</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>3490</td>
<td>2455</td>
<td>2798</td>
<td>4195</td>
<td>4787</td>
<td>3282</td>
<td>2925</td>
<td>5187</td>
<td>4611</td>
<td>2786</td>
<td>2200</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>TCT</th>
<th>TGA</th>
<th>TGC</th>
<th>TGG</th>
<th>TGT</th>
<th>TTA</th>
<th>TTC</th>
<th>TTG</th>
<th>TTT</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>4424</td>
<td>4800</td>
<td>2945</td>
<td>3691</td>
<td>4181</td>
<td>4694</td>
<td>5161</td>
<td>5451</td>
<td>8845</td>
</tr>
</tbody>
</table>
```
## Get the least and most represented 6-mers:

```r
f6 <- oligonucleotideFrequency(yeast1, 6)
f6[f6 == min(f6)]

CCCGGG
   3

f6[f6 == max(f6)]

TTTTTT
   705
```
Comparisons

The S3 system has less overhead, is more widely understood, and is very slightly faster. It is still useful for single-programmer work.

The S4 system is better for multi-person efforts or code that is likely to be reused by others

- Formal definition of class structure, so the contents of an object can be relied on
- Registration of methods means that reflection (looking up what methods are available) is reliable.
- Multiple inheritance is useful for mix-in behavior
- Multiple dispatch is only rarely important, but when you need it you really need it.