The OCE package

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Abstract

The oce package is designed to help Oceanographers in their work, by providing functions for reading a variety of quirky data formats and for summarizing and plotting such data. Some care has been taken to design objects that store both data and meta-information, the latter including not just header data from instruments but also a log of the steps of subsequent processing. In addition to instrument-related functions, oce provides algorithms for computing such things as the equation of state of seawater.

1 Why is the package needed?

Oceanography is still largely in a research phase, with new instruments and new ways of processing data from these instruments appearing frequently. Because measurement techniques change quickly, there are a wide variety of data formats to be dealt with. It is common for meta-information to be stored as headers within data files, and these headers vary from instrument to instrument. This is a problem. In a rush, many (probably most) researchers are tempted to just delete the headers and start working with the data, hoping that the meta-information will stay in memory for long enough to finish the task. This practice leads to errors and to difficulties in sharing and archiving data.

Manufacturers will tell you that they have a solution to this problem. Provided with most instruments is software to read data files and produce standardized graphs or data summaries. However, Oceanography is not a fully-developed field, with the equivalent of laboratory technicians applying standard methods to standard problems. It is a research field, in which practitioners need to invent their own methods for problems not tackled before. The first step in doing this is to get the instrumental data into an analysis system, like R.

The oce package is designed to help with this. It provides functions to read some common data formats and to produce some stock graphs. A series of objects has been created for some of the most common oceanographic instruments. These provide ease of use, with plot, summary, etc. being overloaded for each object. The objects store both meta-information (including processing history) along with the actual data. This frees practitioners to carry out their work with the data, without losing the context.

In addition to the data-handling functions, oce provides functions for working with seawater properties, such as the equation of state. Many of the algorithms derive from the UNESCO formulations, but the design is open-ended, so that new algorithms may be added as they come into use in the literature.

The package is easy to use. For example, the following commands read a CTD file, summarize its contents, and draw a detailed plot of the data:

```
> ctd <- read.ctd("profile001.cnv")
> summary(ctd)
> plot(ctd)
```

It is worth noting that the first line reads a rather complex header that contains information on the sampling location and time, the ship being used, the optional sensors attached to the CTD frame, etc. Of course, read.ctd has many optional arguments to permit setting some of this meta-information, in the (not uncommon) cases in which the data were not properly entered into the data stream at the time of acquisition.

The following sections provide a rough sketch of the oce package, mainly through a examples. This document, like oce itself, is a work in development, as of the second quarter of 2007. Please contact the author if there are sections that are unclear, if there are new topics that should be added here, or if oce is missing a feature that would be useful in your work. (Feel free to request that this package handles new instruments. For example, the author is himself surprised that the word "ADCP" appears just once in this document!)

2 Calculations of seawater properties

oce provides many functions for dealing with seawater properties. Probably the most used is sw.rho(S, t, p), which computes seawater density ρ as a function of salinity S (PSU), in-situ temperature t (°C ... note the use of lower-case to avoid confusion with T, an abbreviation used sometimes in R programs) and pressure p (decibar). The result is a number in the order of 1000kg/m^3 . For many purposes, Oceanographers prefer to use the density anomaly $\sigma = \rho - 1000 \text{kg/m}^3$, and this is provided with sw.sigma(S,t,p), or the related quantity σ_{θ} , provided with sw.sigma.theta(S, t, p).

By now, you've no doubt noticed a pattern in the names. All functions relating to seawater properties start with sw. in their name. This is for two reasons. First, it prevents a confusion with beta, which is used in oceanographic notation to mean the haline contraction coefficient, but which has quite a different meaning in R. The second reason is that oce may eventually get functions for dealing with the properties of air, sediments, etc., and so the prefix sw. will come in handy if these extensions are made.

Most of the functions use the UNESCO formulations of seawater properties, but new formulations may be added as options, as they come into use in the literature.

The seawater functions are: sw.N2, sw.S.C.T.p, sw.S.T.rho, sw.T.S.rho, sw.T.freeze, sw.alpha, sw.alpha.over.beta, sw.beta, sw.conductivity, sw.depth, sw.lapse.rate, sw.rho, sw.sigma, sw.sigma.t, sw.sigma.theta, sw.specific.heat, sw.spice, sw.theta, and sw.viscosity. Oceanographers will probably be able to guess the meaning of each, since the notation is standard.

3 CTD data

3.1 Example with pre-trimmed data

Most CTD packages place the sensors at the bottom of a large instrument frame, so that they sample ambient water only as the instrument is being lowered. (The upcast data are contaminated by mixing caused by the package, and other effects.) However, the instrument is turned on and off at the surface, which means that data records typically contain upcast data that should be removed. It is also common to discard data acquired for a time during which the instrument is hung just below the water surface to equilibrate, and to discard data acquired when the instrument is near its maximum depth, when it might be held for a time to take a water sample with a bottle.

Different instruments need different handling, and sometimes this is done by technicians, before scientists even see the data. For this reason, the issue of trimming CTD data is deferred to the next section. Here, attention is focussed on a pre-trimmed data set. To get you started, oce provides a sample data set. For example,

- > library(oce)
- > data(ctd)
- > plot(ctd)

produces Figure 1.

The object used to hold CTD data stores not just the data, but also the raw header sequence, and whatever has been discovered about the dataset by parsing the header; use

summary(ctd)

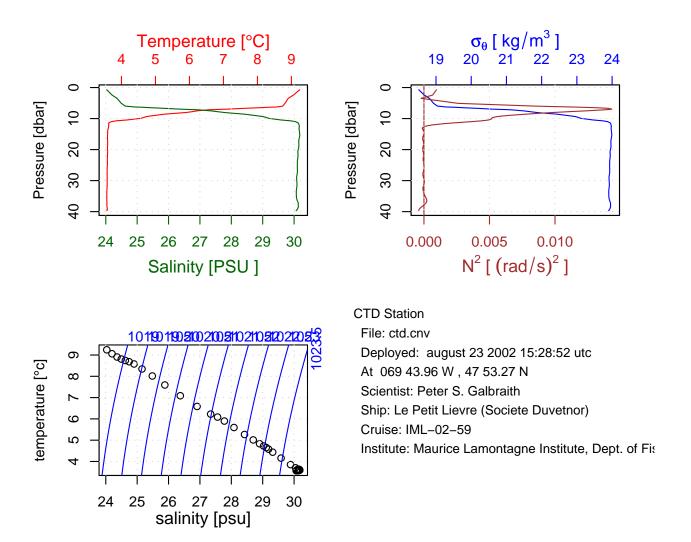


Figure 1: Plot of CTD data with built-in dataset.

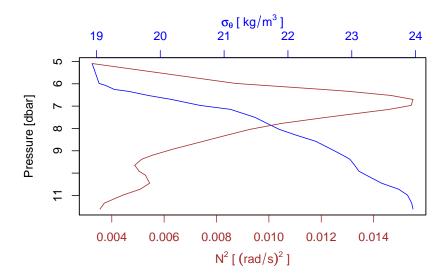


Figure 2: Density and buoyancy-frequency variation within the pycnocline.

to get a scientific overview of the data, and e.g.

```
names(ctd)
names(ctd$header)
names(ctd$data)
```

to learn more about both the ctd object generally, and the instruments that were attached to the CTD frame for the measurement in question.

It is also possible to plot the components individually, either by accessing the data directly (e.g. ctd\$data\$pressure is a vector of pressure; use names(ctd) to discover the names) or by using more specialized functions such as plot.TS and plot.profile. As an example of the latter,

```
> library(oce)
> data(ctd)
> pycnocline <- ctd.trim(ctd, "pressure", c(5, 12))
> plot.profile(pycnocline, type = "sigmatheta+N2")
```

produces Figure 2. Note that the buoyancy frequency is determined by differentiating an approximation to the density profile calculated with a smoothing cubic spline. See the manual for N2() to see how to control the smoothing.

3.2 Example with raw data

The oce library provides ctd.trim() for trimming CTD data. It has a parameter called method to control the method of trimming. For quick and dirty work, method=downcast may be useful, but the method is not perfect, and it is probably best to trim the data by eye. (Spending a few minutes doing this makes sense because the data are so valuable. Do you really want your conclusions to be biased by using untrustworthy data?)

The dataset ctd.raw is an example of an untrimmed file. The code

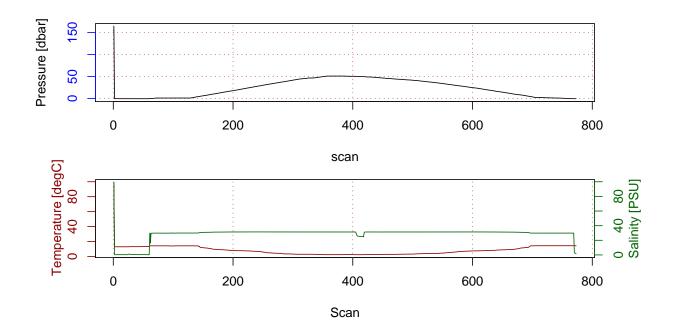


Figure 3: Scanwise plot of raw CTD data.

```
> library(oce)
> data(ctd.raw)
> plot.ctd.scan(ctd.raw)
```

will create a two-panel plot (Figure 3) that is often used in the trimming of CTD data. The bottom panel shows temperature in red and salinity in green. Oceanographers will see in an instant that this dataset needs trimming, to isolate the downcast. A rough trimming job can be accomplished by

```
ctd.trimmed <- ctd.trim(ctd.raw)
and checked by
plot.ctd.scan(ctd.trimmed)</pre>
```

A more precise trimming job really requires an expert's eye, though. This work is made easy by commands such as

```
plot.ctd.scan(ctd.trim(ctd.raw, "scan", c(150,250))
```

in which the numbers are altered a bit at a time.

4 Coastline data

```
The commands
```

```
> library(oce)
> data(coastline)
> plot(coastline, col = "darkred")
> hfx.lat <- 44 + 39/60
> hfx.lon <- -(63 + 34/60)
> points(hfx.lon, hfx.lat, col = "blue", cex = 3, pch = 20)
> text(hfx.lon, hfx.lat, "Halifax", col = "blue", pos = 4, cex = 1.3)
```

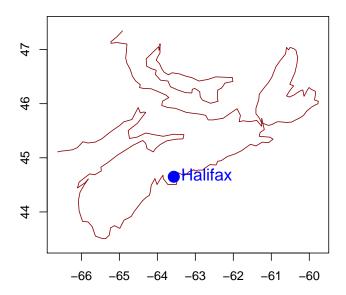


Figure 4: Coastline of eastern Canada, showing Prince Edward Island, New Brunswick, and Nova Scotia. (Halifax is the home of the author.)

produce a map of the coastline of Eastern Canada (Figure 4). Such coastline data are available from a variety of sources. The NOAA site http://www.ngdc.noaa.gov/mgg_coastline/ is particularly popular, and it has the advantage of providing data in Splus format.

5 Sea-level data

The commands

- > library(oce)
- > data(sealevel)
- > plot(sealevel)

load and graph a build-in dataset of sea-level timeseries. The result, shown in Figure 5, is a four-panel plot. The top panel is a timeseries view that provides an overview of the entire data set. The second panel is narrowed to the most recent month, which should reveal spring-neap cycles if the tide is mixed. The third panel is a spectrum, with a few tidal constituents indicated. At the bottom is a cumulative spectrum, which makes these narrow-banded constituents quite visible.

Of course, it is possible to work directly with the data, e.g.

```
> spectrum(sealevel$eta, spans = 48)
```

> abline(v = 1/12.42)

> mtext("M2", at = 1/12.42, side = 3)

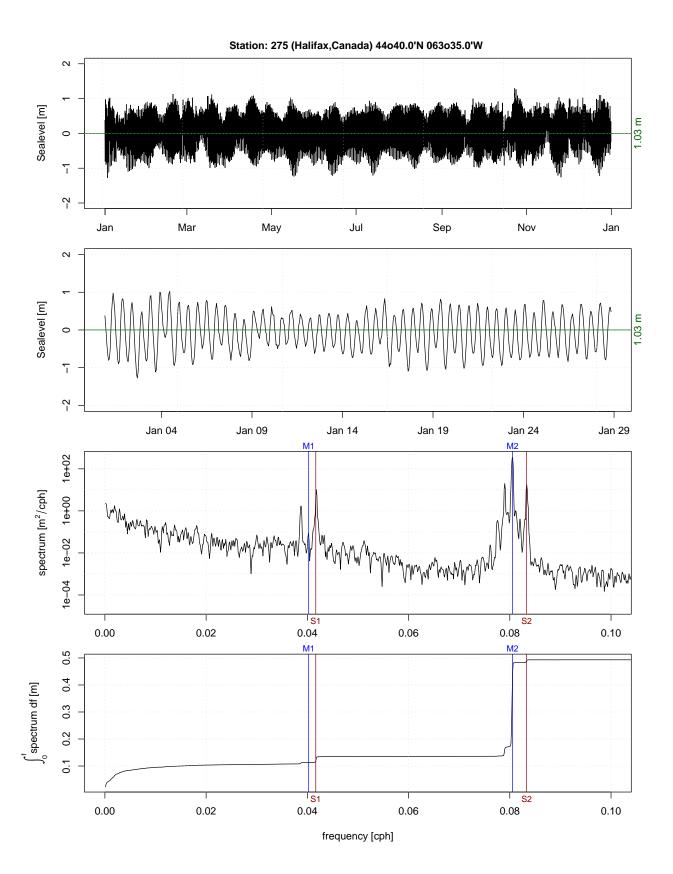


Figure 5: Plot of sealevel time series measured at Halifax, Nova Scotia. $\stackrel{7}{}$

6 Lobo data

The commands

```
> library(oce)
> data(lobo)
> plot(lobo)
```

produce a plot (Figure 6) of lobo data from the Northwest Arm of Halifax Harbour. As usual, oce provides access to the raw data. Try the following, to see a TS diagram with dots colour-coded by time:

```
> a <- as.numeric(lobo$time - lobo$time[1])
> hue <- 0.5 * a/max(a)
> plot.TS(as.CTD(lobo$S, lobo$T, 0), col.data = hsv(hue, 1, 1),
+ pch = 20, cex = 2)
```

(Here, note the use of coercion to a CTD object, to get a TS diagram with density lines.)

Appendix A: bugs

- 1. read.lobo makes overly strong assumptions about which sensors will be deployed in a LOBO instrument
- 2. read.ctd only handles data from SeaBird instruments

Appendix B: plans

- 1. WOCE exchange formats should be handled.
- 2. There should be a way to combine profile sequences into sections.
- 3. ADCP data should be handled.
- 4. Microstructure data should be handled.
- 5. Levitus-atlas data should be handled.
- 6. Air-sea flux formulae should be provided.

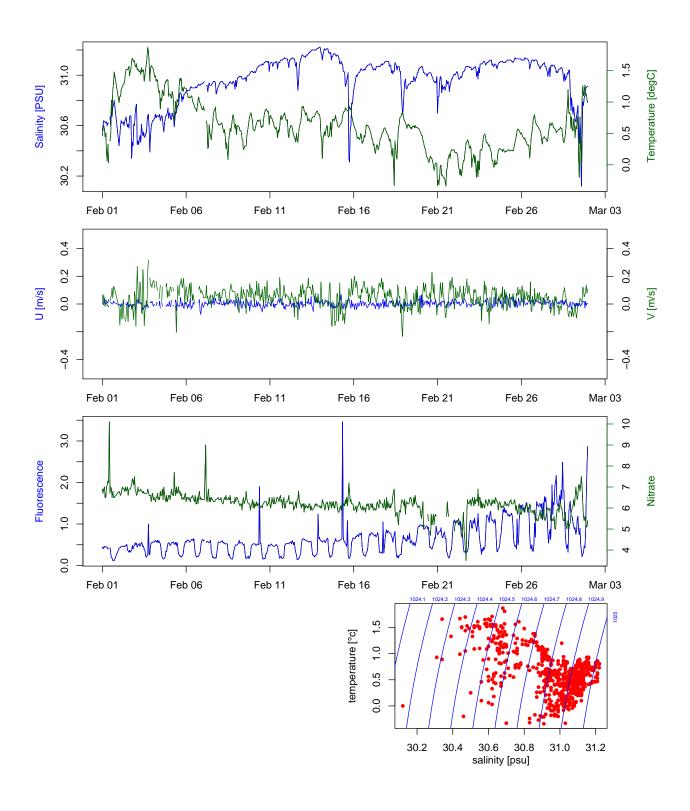


Figure 6: Plot of lobo data obtained in Northwest Arm of Halifax Harbour, just before the Spring bloom of 2007.