Installing R packages for BART

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BART, R and Operating Systems (OS)

- ► In association with my collaborators, we have created several R packages for BART
- ► GNU R was started by Ross Ihaka and Robert Gentelman as a successor to Bell Labs S that was only available on UNIX
- ▶ 1993: R first released for Apple MacOS (classic), but ports to Microsoft Windows, UNIX and GNU Linux soon followed
- ▶ R does its best to treat the three modern platforms equally: Windows, UNIX/Linux and Apple macOS (OS X)
- ▶ But, there are really just two OS types as far as R is concerned
- ► R> .Platform\$OS.type
 "unix" for UNIX/Linux/macOS and "windows" for Windows
- ► We support BART on all R platforms
- ► However, there are some fundamental differences that R cannot address: in particular, multi-threading
- ► On Windows, multi-threading via *forking* is not available

BART R packages with S3 predict (embedded URLs) Multi-threading Debut Code **CRAN** github 2006 C++**BayesTree** None Java bartMachine 2013 Java 2014 C++ dbarts forking 2014 Message Passing Interface (MPI) BART: Rob, Matt et al. MPI C++Descendents of MPI BART 2017 BART for continuous, categorical & time-to-event outcomes **BART** 2.9.9 BART3 OpenMP/forking 2019 Heteroskedastic BART for continuous outcomes

rbart archived **hbart** OpenMP

OpenMP/forking mBART 2021 NFT BART for time-to-event outcomes

nftbart 2.1 OpenMP Development on github by Rob (remcc) & Rodney (rsparapa).

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Special thanks to Matt Pratola, R Core, Rcpp Core and so many others in the FOSS community!

2021 Monotonic BART for continuous outcomes BART software features: descendents of MPI BART

CRAN Stable	BART	nftbart	rbart	
github Development	BART3		hbart	mBART
github.com user	rsparapa			remcc
predict function	Yes	Yes	Yes	BART
heteroskedastic	No	Yes	Yes	No
monotonic	No	No	No	Yes
continuous	Yes	Yes	Yes	Yes
binary/categorical	Yes	No	No	No
right censoring	Yes	Yes		
left censoring	No	Yes		
competing risks	Yes	No		
recurrent events	Yes	No		
sparse prior	Yes	No	No	No
marginal effects	BART3	Yes	No	No
missing imputation	Yes	Yes	No	No
advanced tree proposals	No	Yes	Yes	No
nonparametric error	No	Yes	No	No
C++ header-only	BART3	No	hbart	No

Skeleton of the BART/BART3 R package

Directory	File Example	Description		
root	configure	To dectect OpenMP for "unix"		
	DESCRIPTION	Dependency on Rcpp and others		
R	gbart.R	Generalized BART function		
	wbart.R	Weighted BART function		
	<pre>predict.pbart.R</pre>	predict for "pbart"/probit type		
	<pre>predict.wbart.R</pre>	<pre>predict for "wbart"/continuous type</pre>		
data	lung.rda	Advanced lung cancer data		
demo	boston.R	Boston housing demo		
	<pre>lung.surv.bart.R</pre>	Advanced lung cancer demo		
man	gbart.Rd	Help pages		
	wbart.Rd			
	<pre>predict.pbart.Rd</pre>			
	<pre>predict.wbart.Rd</pre>			
src	Makevars	Hard-wired settings for "windows"		
	Makevars.in	configure OpenMP template		
		for "unix" Makevars file		
		4/26		

BART and multi-threading

- Multi-threading is supported by software frameworks such as OpenMP and the Message Passing Interface (MPI)
- ▶ MPI can be employed for both simple multi-threading and for distributed computing, e.g., MPI software initially written for a single system could be extended to operate on multiple systems as computational needs expand
- ► For MPI, BART software was re-written with C++ objects simple to modify/maintain for distributed computing: we call this the MPI BART code (Pratola et al. 2014, JCGS)
- ► The BART/BART3 and rbart/hbart/nftbart packages are all descendants of MPI BART and its programmer-friendly objects, but we have moved on from MPI mainly to OpenMP
- ► For a brief primer on R, BART and multi-threading go to slide 21

Testing multi-threading after installing **BART/BART3**

- ▶ parallel::detectCores
- ▶ Returns the number of threads that the computer is capable of
- ► The number of *threads* rather than the number of *cores* since they are not necessarily one-to-one
- ► For example, here I have a single M1 Pro CPU with 10 cores each core capable of one thread so detectCores returns 10
- ► BART::mc.cores.openmp/BART3::mc.cores.openmp
- ► Returns whether OpenMP has been detected 1+ (Yes) vs. 0 (No)

BART and multi-threading

- ► Multi-threading is supported in two ways 1) via the parallel package and 2) via OpenMP
- OpenMP takes advantage of modern hardware by performing multi-threading on single machines which often have multiple CPUs each with multiple cores
- ► BART/BART3 only use OpenMP for parallelizing predict function calculations
- ► rbart/hbart/nftbart use OpenMP for fitting and predicting
- ▶ OpenMP support is detected at package installation by the configure script on UNIX/Linux/macOS that defines a C pre-processor macro called _OPENMP if available
- ► But a configure script can't run on Windows
- ► BART/BART3/nftbart hard-wired for Windows OpenMP
- ► In src/Makevars, Windows compiler switches for OpenMP (add to any source package needing OpenMP on Windows)

```
PKG_CXXFLAGS = -fopenmp
PKG_LIBS = -fopenmp
```

Installation resources for R and R packages: BEWARE

- ► The Comprehensive R Archive Network (CRAN)
 http://cran.r-project.org has R binaries for Windows,
 macOS and a few popular Linux distros
- ► CRAN is a wealth of manuals, advice, FAQs, etc.
- ► Avoid the pitfalls: just do it the "CRAN way"!
- ▶ Do NOT use package managers unless CRAN approves
- Extra Packages for Enterprise Linux (EPEL) is approved for Red Hat-flavored Linux
- And, so are Debian-flavored packages at debian.org
- ► But, EPEL and Debian are exceptions
- For example, on macOS, the Homebrew and conda package managers are NOT approved
- Only use CRAN binaries and/or build with CRAN approved tool chains!
- ► Be safe, not sorry

Installation resources for R and R packages

- Windows Rtools 4.5 https://cran.r-project.org/bin/windows/Rtools/rtools45/rtools.html mainly, the GNU Compiler Collection (GCC) v. 14
- macOS tools: https://mac.r-project.org/tools for BART, we need Xcode installed from the App Store with OpenMP installed from https://mac.r-project.org/openmp N.B. R 4.4+ for macOS now ships with OpenMP libraries; however, you still need to install the OpenMP binaries to get the header files like /usr/local/include/omp.h
- ▶ remotes package https://cran.r-project.org/package=remotes
- ► Rcpp package
 https://cran.r-project.org/package=Rcpp

Installing R packages from source

- ▶ Installing R packages from source needs a compiler tool chain that support **Rcpp** and various BART packages therefore, we need ISO standard C++11 (2011) or higher
- ► R 4.4+ now defaults to ISO standard C++17 (2017)
- ► However, by design C++17 is not backwards compatible e.g., nftbart requires ISO C++14 (2014)
- ➤ You can set this in the "DESCRIPTION" file "SystemRequirements: C++14" (or src/Makevars see how it is done in nftbart)

Installing R packages from source

- ► A CRAN compatible C++ compiler is needed there are two common *flavors* used by CRAN the GNU Compiler Collection (GCC) and LLVM Clang Clang maintains compatibility with GCC (but a Fortran compiler is NOT needed for BART)
- ► For Windows, CRAN R Tools provide GCC with OpenMP https://cran.r-project.org/bin/windows/Rtools/rtools45/rtools.html
- ► For macOS, rely on Apple Xcode's Clang from the App Store but you have to install Clang's OpenMP library from CRAN for more details see next slide

Auto-installing OpenMP on macOS with configure

- ► Get the tarball from https://mac.r-project.org/openmp
- ► Make sure you get the version of the OpenMP library compatible with the version of Xcode that you have installed
- ► For example, 17.0.6 is for Xcode 16.0-16.2
- ► Manually install it from the ~/Downloads folder compressed
- \$ sudo bash
- \$ tar fvxz openmp-17.0.6-darwin20-Release.tar.gz -C /
 or uncompressed
- \$ tar fvx openmp-17.0.6-darwin20-Release.tar -C /
 - ► For example, install BART3
 - \$ R CMD INSTALL BART3_5.6.tar.gz
- ► Then you should see the following if OpenMP is auto-detected checking for clang++ ... option to support OpenMP...
- -Xlinker -lomp -Xclang -fopenmp
 - ▶ Due to -lomp which is needed for linking only, you will see a harmless warning when compiling (linking is fine too) clang: warning: -lomp: 'linker' input unused [-Wunused-command-line-argument]

Installing R packages

- ► The variable .Library contains the location of the default directory for R packages
- ► R> .Library
- ▶ Depending on the OS, this directory may not be writeable
- ► To create an alternative library for your R packages that with write access, use the .libPaths() function put this in your ~/.Rprofile
- ▶ .libPaths("~/RLIB")
 options(repos=c(CRAN="http://lib.stat.cmu.edu/R/CRAN"))
 options(mc.cores=8) ## multi-threading with BART3
- ▶ N.B. you need to create the directory before package installs
- ► terminal\$ mkdir ~/RLIB
- ► And, you can find installed packages by system.file()
- ► R> system.file(package="BART")
- ► For example, to find the demo directory
- ► R> system.file("demo", package="BART")

Installing R packages with CRAN

- ightharpoonup CRAN has 22,411 R packages as of this writing (07/16/25)
- ► In the US, I use the following mirror at Carnegie-Mellon http://lib.stat.cmu.edu/R/CRAN
- ► The mirror in Belgium that I have tried https://ftp.belnet.be/mirror/CRAN
- R> options(repos=c(CRAN="http://lib.stat.cmu.edu/R/CRAN"))
- R> install.packages("remotes", dependencies=TRUE)
- R> install.packages("Rcpp", dependencies=TRUE)
- R> install.packages("BART", dependencies=TRUE)
- R> install.packages("nftbart", dependencies=TRUE)
- To install all CRAN packages (takes hours: I run this over-night)
- R> install.packages(available.packages()[, 1])
- Some of them will fail for missing system dependencies like device drivers, required software, etc., but R will try to install them all

build and INSTALL R packages: command line

- ► For macOS/Linux, use bash
- ► For Windows, use CMD.EXE
- ▶ Build and install R packages from the command line: \$
- ► This works with your own R packages or those of others
- ► If it is your own in the sub-directory PACKAGE, then build it: \$ R CMD build PACKAGE
- ► For others, download the archive of source files either a gzipped TARFILE ending in .tar.gz or .tgz or a PKWARE/Info-ZIP ZIPFILE ending in .zip
- ► Unpack it: \$ tar xzf TARFILE or \$ unzip ZIPFILE which should create the PACKAGE sub-directory
- ► Build the package: \$ R CMD build PACKAGE
- ► Typically the vignettes take a long time or may crash the build \$ R CMD build --no-build-vignettes PACKAGE
- ► So now you have created PACKAGE_VERSION.tar.gz
- ► Install it: \$ R CMD INSTALL PACKAGE_VERSION.tar.gz
- ► And you can remove it later: \$ R CMD REMOVE PACKAGE

build and INSTALL R packages: remotes package

- ➤ You can build and install R packages from anywhere on the internet with the remotes package
- ► For example, former CRAN packages that have been Archived: https://cran.r-project.org/src/contrib/Archive
- ► These can be installed with the install_url function
- ► For example, the sbart package
- R> install.packages("LaplacesDemon")
- R> install.packages("msm", dependencies=TRUE)
- R> install.packages("Rcpp", dependencies=TRUE)
- R> install_url(paste0("https://cran.r-project.org",
- R+ "/src/contrib/Archive/sbart/sbart_0.1.1.tar.gz"))

build and INSTALL R packages: remotes package

- ► More commonly: R packages on https://github.com
- ► These can be installed with the install_github function
- ► However, R 3.6.2 or higher appears to be necessary
- ► For example, the **BART3** package (beta **BART**) at https://github.com/rsparapa/bnptools/
- R> install_github("rsparapa/bnptools/BART3")
- Or the mBART package, monotonic BART, at https://github.com/remcc/mBART_shlib/
- ► R> install_github("remcc/mBART_shlib/mBART")
- ▶ N.B. installing from the command line usually faster

build and INSTALL R packages with git

- ► This is much faster than remotes::install_github
- ► To install either R package: **BART3** or **mBART** first, you have to "clone" the repository

```
$ mkdir DIR
$ cd DIR
$ git clone https://github.com/rsparapa/bnptools.git
$ cd bnptools ## where BART3 is a sub-directory
$ R CMD build --no-build-vignettes BART3
$ R CMD INSTALL BART3_VERSION.tar.gz
$ cd ..
$ git clone https://github.com/remcc/mBART_shlib.git
$ cd mBART_shlib ## where mBART is a sub-directory
$ R CMD build --no-build-vignettes mBART
$ R CMD INSTALL mBART_VERSION.tar.gz
```

Emacs and ESS for R/C++

- ▶ 1975: Emacs "Editor MACroS" by Richard Stallman (RMS) intelligent development environment (IDE) for programmers
- ▶ 1980: US law changes to recognize software Copyright
- ► 1983: RMS founds the GNU project GNU stands for "GNU is Not UNIX" "a complete UNIX-compatible software system"
- ► 1984: RMS releases GNU Emacs as free software re-written in C with Elisp (Emacs Lisp) for modes
- ▶ 1986: emacs FORTRAN-mode: IDE for FORTRAN
- ▶ 1989: the GNU General Public License (GPL) for free software
- ► 1994: Anthony Rossini releases ESS (GPL) containing Emacs modes for statistical software like ESS[R]

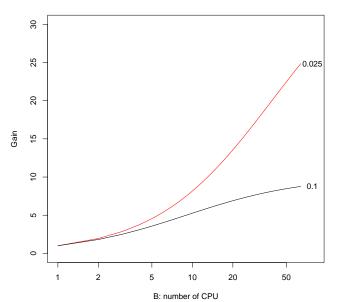
Installing Emacs/ESS for your R IDE

- ➤ Vincent Goulet's *Modified* Emacs installable binaries for both Windows and macOS with ESS and other goodies many modes for programming like C/C++ and markup such as AUCTeX: a LaTeX support mode English, French, German and Spanish dictionaries for Hunspell http://hunspell.github.io
- ▶ Windows: https://emacs-modified.gitlab.io/windows
- ▶ macOS: https://emacs-modified.gitlab.io/macos
- ► Check ESS is working with M-x ess-version

Multi-threading and symmetric multi-processing

- Multi-threading and symmetric multi-processing are advanced technology that are surprisingly easy to use today
- ► Today, most off-the-shelf hardware available features 1 to 4 CPUs each of which is capable of multi-threading
- ► Multi-threading emerged quite early in the digital computer era with the groundwork laid way back in the 1960s
- ► In 1962, Burroughs released the D825 which was the first commercial hardware capable of symmetric multiprocessing (SMP) with CPUs
- ► In 1967, Gene Amdahl derived the theoretical limits for multi-threading which came to be known as Amdahl's law
- ▶ If **B** is the number of CPUs and **b** is the fraction of work that can't be parallelized, then the gain due to multi-threading is $((1-b)/B+b)^{-1}$

Amdahl's law: $((1-b)/B+b)^{-1}$ where $b\in\{0.025,0.1\}$



Multi-threading with parallel package

- ► The mcparallel function uses *forking* to facilitate multi-threading (forking is NOT available on Windows)
- ► Fork is an operation where a process creates a copy of itself
- ► A forked R child process has memory address pointers to all of the objects known to the parent such as loaded packages, function definitions, data frames, etc.
- ▶ But, these *shared* objects are NOT copied into memory for each child: that would be a huge waste of resources!
- ► Each child has a memory address *pointer* to these objects
- ► Furthermore, R has a *copy on write* philosophy
- ► If a child writes to an object owned by the parent, a copy is made for the child while the parent retains the original
- ► This is convenient, but can be dangerous with multiple threads
- ► For example, if this is a big object, now that object has multiple instances which might consume a lot of memory

The mcparallel function and nice

```
R> library(parallel) ## an example of multi-threading
R> library(tools)
R> for(i in 1:mc.cores)
R> mcparallel({psnice(value=19); expr})
R> obj.list = mccollect()
```

expr is processed mc.cores times each in their own threads

Paraphrasing the psnice documentation

Unix schedules processes to execute according to their priority. Priority is assigned values from 0 to 39 with 20 being the normal priority and (counter-intuitively) larger numeric values denoting lower priority. Adding to the complexity, there is a *nice* value: the amount by which the priority exceeds 20. Processes with higher nice values will receive less CPU time than those with normal priority. Generally, processes with nice value 19 are only run when the system would otherwise be idle to enhance system interactivity.

The mccollect function

- ▶ mccollect returns a list of return values from each thread
- ► in my experience, these are returned last in, first out (LIFO) the reverse from what we might have expected
- occasionally, a sporadic failure in one, or more, of the threads failed component(s) are missing from the list of return values
- ▶ if it is sporadic: re-running without any changes can succeed
- ► class(obj)[1]!=type is likely an error message so return it

```
R> obj.list = mccollect() ## last in, first out
R> obj = obj.list[[1]]
R> if(mc.cores==1 | class(obj)[1]!=type) {
R> return(obj)
R> } else {
R> m = length(obj.list)
R> if(mc.cores!=m)
R> warning(pasteO("The number of items is only ", m))
...
R> }
```

The mcparallel function and random number generation

- ► We want each thread to have its own *stream* of random numbers that is reproducible
- ► There is a special random number generator for this purpose
- ► L'Ecuyer's combined multiple-recursive generator (CMRG)

```
R> library(parallel)
R> library(tools)
R> RNGkind("L'Ecuyer-CMRG")
R> set.seed(seed)
R> mc.reset.stream()
R> for(i in 1:mc.cores)
R> mcparallel({psnice(value=19); expr})
```