BatchJobs and BatchExperiments

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(note to myself: Never do meetup talks on my birthday!)

Motivation

- Long-running, independent jobs
- Very often these are benchmarking / comparison experiments
- These types of experiments can get complex very quickly
  - Some jobs can fail
  - Heterogeneous runtimes
  - Very often want to add / remove some experiments later, when partial results are there
  - We often learn about problems during / after calculations

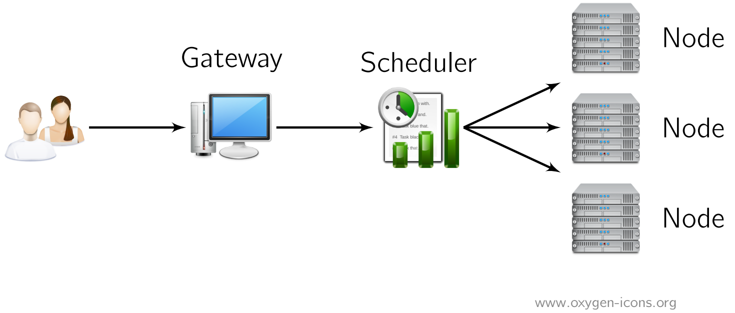
Naive batch computing

Computing on multicore machines (non-cluster)

- Prepare standalone script(s) that run your jobs, save results at end
- Parameters must be hard coded or retrieved through commandline
- Login on a machine per SSH
- Start job(s) with `R CMD BATCH myscript1.R`, combine this with nohup, screen or tmux
- Start remaining jobs when resources get available (argh...)
- Check manually for completion / errors (argh again...)
- Write script to collect results

No automation, no resource management or fair share,
neither extensible nor scalable.
— Don't do it this way —

High Performance Computing (HPC) clusters



- User log onto the gateway server (master or head node)
- Network of multiple computing nodes, managed by the scheduler
- Scheduler orchestrates the computation and organizes queues to fairly distribute compuation times among users
- Nodes either share a file system or support for file staging

Manual working on a batch system

- You have to specify
  - (a) Resource specifications (number CPUs, expected runtime and memory)
  - (b) Where to redirect the output streams
  - (c) Command to execute (e.g. `R CMD BATCH <myscript.R>`)
- Specs passed to CLI tools either directly as arguments or encoded in a shell script
- Check status of jobs via CLI tools (e.g. `qstatus`) or wait for mails
- Write script to collect results

Example Job Description File

Portable Batch System (PBS) syntax:

```
#PBS -N jobname
#PBS -j oe
#PBS -o job.output
#PBS -M lang@statistik.tu-dortmund.de
#PBS -l nodes=1,walltime=500,vmem=1024MB
#PBS -q short_eth

### commands to run
module add R
cd $HOME/my_experiments
R CMD BATCH myjob.R /dev/stdout
```

Submit from a shell:

```
> qsub myjob.pbs
```

Usual workflow on a batch system

- **Unroll** your R **loop(s)** so that your script computes a single iteration
- Write a **script that writes** R **scripts** for each iteration setting the iteration counter(s) at the beginning
- Write a **script that writes job description files** for each R script
- Write a **script that submits** your job description files
- **Crawl** through file system checking for existence of results or log files
- Write a **script that combines** your scattered result files
- Found a bug in your code? Write a **script that kills** all running jobs, fix the bug, submit everything again
- Some jobs have hit the wall time? Write a **script that finds** out which jobs you need to resubmit with weaker constraints
- Want to try your model on another data set or using other parameters? Eventually **start from scratch**, it might get ugly

Synchronous vs. asynchronous computation

Why not simply ask for 100 cores, then use the parallel package?

- You are now basically circumventing the scheduler
- How long are you willing to wait in queue? Infinitely?
- What if some jobs crash?
- What if you later want to add jobs?
- **One independent, embarrassingly parallel job should be submitted as such!**

Pros and Cons of Batch Systems

- + They are pretty fast!
- + Many statistical tasks are embarrassingly parallel
- - Job description files needed
- - We cannot control when jobs are started.
- - Jobs cannot really communicate, except by writing stuff on disk (or we have to allocate multiple cores and use something like MPI)
- - Requesting many nodes at once increases time spend in queue
- - Auxiliary scripts to create files and submit jobs necessary
- - Functions to collect results can get complicated and lengthy
- - If some jobs fail (e. g., singularities), debugging is awful

Packages

BatchJobs

- Basic infrastructure to communicate with a high performance cluster
- Tailored around Map-Reduce paradigm
- Can be incorporated into other packages
- Supported via `parallelMap` and `BiocParallel`

BatchExperiments

- Builds on top of BatchJobs
- Abstraction for “applying algorithms on problems”
- Assists the user in conducting comprehensive computer experiments

BatchJobs – Features

- Basic infrastructure to communicate with batch systems
- Complete control over the batch system from within R: submit, supervise, kill
- Implementation of higher order functions
  Map, **Reduce** and **Filter**
  to define jobs and collect results
- Persistent state of computation for experiments
- R code independent from the underlying batch system
- Reproducibility in distributed environments, even if the architecture changes
- Convenient result collection capabilities
- Debugging tools
- Configurable integrated status mailer

Supported Systems

Real batch systems:

- Torque/PBS based systems
- Sun Grid Engine / Oracle Grid Engine
- Load Sharing Facility (LSF)
- SLURM
- Still missing: Condor

Other modes:

- Interactive: Jobs executed in current interactive `R` session
- Multicore: local multicore execution with spawned processes
- SSH: distributed computing on loosely connected machines which are accessible via SSH (makeshift cluster)

Links and references

- `https://github.com/tudo-r/BatchJobs`
  - Installation infos
  - Intro slides by Henrik Bengtsson
  - R documentation
  - Wiki + FAQ
  - Mailing list + Issue tracker
  - Recent development version in git
- Our tech report:
  Bischl, Lang, Mersmann, Rahnenführer, Weihs:
  "Computing on high performance clusters with R: Packages BatchJobs and BatchExperiments"
  Available on project page
- Shortened version as JSS paper: Cite us!

First Time Configuration

- Specification of scheduling system and template file
- Templates can be downloaded at our website, easy to adept
- Optional mail notifications
- Defaults to interactive mode: no distributed computing, no mails

`BatchJobs.conf`

```
cluster.functions = makeClusterFunctionsTorque("~/lido.tmpl")
mail.to = "<lang@statistik.tu-dortmund.de>"
mail.start = "none"
mail.done = "first+last"
mail.error = "all"
```

Simple brew template for PBS

- One guy for one site has to this once
- Needed for flexibility and specifities of systems
- Talk to your admin for help
- Templates can be downloaded at our website
- Stuck? Put up a issue or email our list

```
#PBS -N <%= job.name %>
## merge standard error and output
#PBS -j oe
## direct streams to our logfile
#PBS -o <%= log.file %>
#PBS -l walltime=<%= resources$walltime %>,
#    nodes=<%= resources$nodes %>,vmem=<%= resources$memory %>M

## Run R:
## we merge R output with stdout from PBS,
## which gets then logged via -o option
R CMD BATCH --no-save --no-restore "<%= rscript %>" /dev/stdout
```

	BatchJobs' functions	Common functions	BatchExperiments' functions
(1) Create Registry	`makeRegistry`		`makeExperimentRegistry`
(2) Define Jobs	`batchMap` `batchReduce` `batchExpandGrid`	`batchMapResults` `batchReduceResults`	`addProblem` `addAlgorithm` `makeDesign` `addExperiments`
(3) Subset Jobs	`findJobs`	`findDone` `findErrors` ...	`findExperiments`
(4) Submit Jobs		`submitJobs`	
(5) Status & Debugging		`showStatus` `testJob` `showLog`	`summarizeExperiments`
(6) Collect Results		`loadResult[s]` `reduceResults` `filterResults` `reduceResults[AggrType]`	`reduceResultsExperiments`

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(1) Create a registry

Registry

- Object used to access and exchange informations: file paths, job parameters, computational events, ...
- Manages SQLite and file system backend
- All information is stored in a single, portable directory
- Initialization of a new registry:

```
library(BatchJobs)
reg = makeRegistry(
  id = "tryout",                  # name of your study
  file.dir = "~/project/bj-files", # accessible on all nodes
  work.dir = "~/project",          # accessible on all nodes
  seed = 1                         # initial seed for first job
)
```

- `loadRegistry(dir)` to resume working with an existing registry

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(2) Define Jobs

batchMap

- Like `lapply` or `mapply`
- $(x_1, x_2) \times (y_1, y_2) \to (f(x_1, y_1), f(x_2, y_2))$
- 10 Jobs to calculate $1 + 9$, $2 + 8$, $\ldots$, $9 + 1$

```r
map = function(i, j) i+j
ids = batchMap(reg, f, i=1:9, j=9:1)
```

- Stores function on file system
- Creates jobs as rows of SQLite database
- Parameters also serialized into the database for fast access
- All jobs get unique positive integers as IDs

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(3) Subset Jobs

- Query job IDs by computational status: `find*` functions `findSubmitted`, `findRunning`, `findDone`, ...
- Query job IDs by parameters: `findJobs(reg, pars)`

```
findJobs(reg, pars = (j==1))
findNotSubmitted(reg)
findDone(reg)
```

- Set operations on ID vectors: `intersect`, `setdiff`, `union`
- Vector of IDs can be passed to basically all functions interacting with the batch system

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(4) Submit Jobs

submitJobs

- Creates R script files and job description files on the fly
- Resources can be provided as named list

```
# 1 hour maximal execution time, about 2 GB of RAM
res = list(walltime=60*60, memory=2000)

# ... and submit
submitJobs(reg, resources=res)
```

- Jobs can be grouped into chunks by providing a list of ID vectors. Each chunk gets executed sequentially as one single batch job

```
chunk(ids, chunk.size = 5)
```

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(5) Supervise and debug

- Quick overview of what is going on: `showStatus(reg)`

```
Status for jobs:  10
Submitted:        10 (100.0%)
Started:          10 (100.0%)
Errors:            0 (  0.0%)
Running:           2 ( 20.0%)
Expired:           0 (  0.0%)
Done:              8 ( 80.0%)
Time: min=1.50s avg=5.20s max=8.80s
```

- Display log files with a customizable pager (less, vi, ...): `showLog(reg, findErrors(reg)[1])`
- You can also `grepLogs(reg, pattern)`
- Found a bug? `killJobs(reg, findRunning(reg))`
- Run a job in the current R session: `testJob(reg, id)`

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(6) Collect results

Simple loading

```r
loadResult(reg, id = 1)
loadResults(reg)
loadResults(reg, ids)
```

Reduce

```r
# combine in numeric vector
reduceResults(reg, ids = findDone(reg), init = numeric(0),
  fun = function(aggr, job, res) c(aggr, res))
```

- Convenience wrappers around `reduceResults`: `reduceResults[Vector|Matrix|DataFrame|List]`
- `batchReduceResults` to reduce results on the nodes

Seeding

- Every job has a unique seed
- Registry stores initial seed x_0, all job seeds are defined as $x_0 + \mathrm{ID}$
- In some rare cases you need to manually change seeds, therefore all seeds are stored in DB
- Jobs become reproducible, even on another site
- But note all other ugly problems due to changes in hardware, software, compilers, versions, ...

Configuration again

.BatchJobs.conf

```
cluster.functions = makeClusterFunctionsTorque("~/lido.tmpl")
mail.to = "<lang@statistik.tu-dortmund.de>"
mail.start = "none"
mail.done = "first+last"
mail.error = "all"
default.resources = list(walltime = 3600, memory = 1024)
debug = FALSE
raise.warnings = FALSE
max.concurrent.jobs = 400
```

BatchExperiments

- Builds on top of BatchJobs
- Intended as abstraction for typical statistical tasks:

  Applying algorithms on problems
- More aimed at the end user
- Convenient for simulation studies, comparison and benchmark experiments, sensitivity analysis, . . .
- Workflow differs only in job definition

Scenarios

- Compare machine learning algorithms on many data sets
- Compare one/many estimation procedure(s) on simulated data
- Compare optimizers on objective functions
- ...

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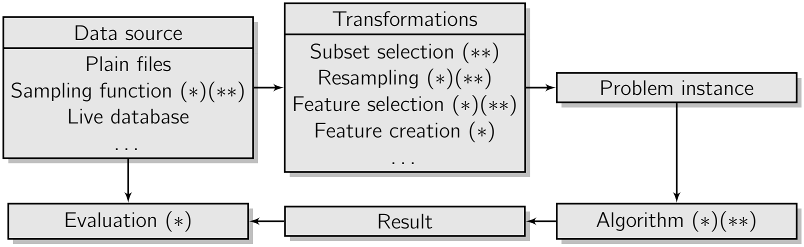
Abstraction of Computer Experiments



- (∗): Parameter requirements
- (∗∗): Stochastic, seeding needed
- Evaluation step often needs raw data
- Efficient and flexible abstraction?

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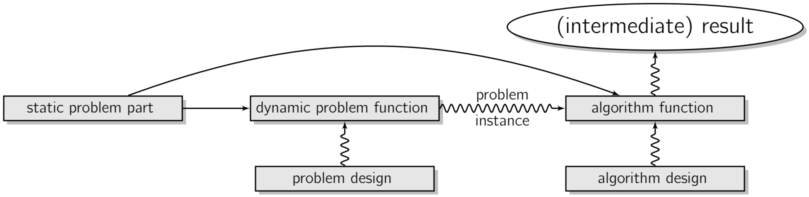

- Problem definition split into static and dynamic part
  - Static: immutable R objects: matrix, data frames, ...
  - Dynamic: Arbitrary R function: transformations of static part, extraction of data from external sources, ...
- Parametrization through specifying experimental designs for both problems and algorithms
- Each step automatically seeded, random seeds stored in a database

Job definition steps in BatchExperiments

1. Add problems to registry: `addProblem`
   - Efficient storage: Separation of static and dynamic problem parts
   - Can be connected with an experimental design
2. Add algorithms to registry: `addAlgorithm`
   - Problem instance gets passed to algorithm
   - Can be connected with an experimental design
   - Return value will be saved on the file system
3. Connect experimental designs: `makeDesign`
4. Add experiments to registry: `addExperiments`
   - Experiment: problem instance + algorithm + algorithm parameters
   - Job: Experiment + replication number

What you get

- Reproducibility: Every computation is seeded, special seeding mechanism for synchronized problem generation
- Portability: Data, algorithms, results and job information reside in a single directory
- Extensibility: Add more problems or algorithms, try different parameters or increase the replication numbers at any computational state
- Exchangeability: Share your file directory to allow others to extend your study with their data sets and algorithms