R packages rlibkriging and dolka

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rlibkriging is an R package providing an interface to the *libKriging* library (Cpp Armadillo).

It allows

- to use kriging "à la *DiceKriging*", and also
- to write R code that is quite similar to the Python and Matlab/Octave code for the two other interfaces to the library.

These are two different goals!

For the first goal, an R interface quite similar to *DiceKriging* is provided.

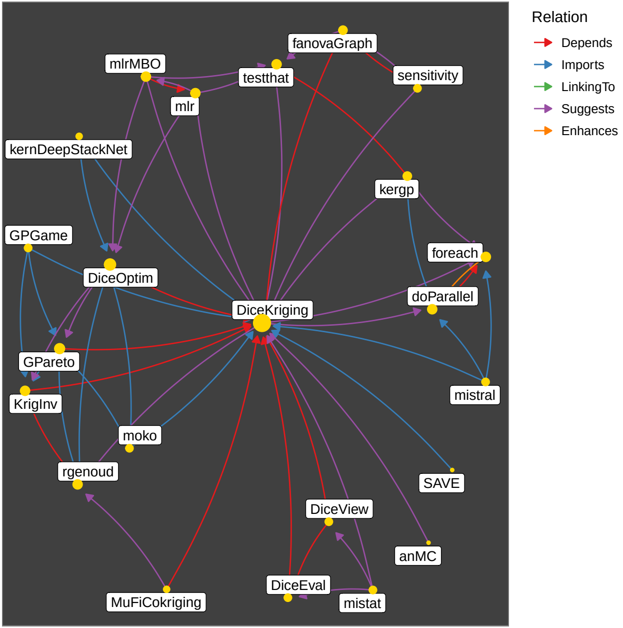
For the second goal there are/will be functionalities with no equivalent in *DiceKriging*, but some from other packages in R, Python or Matlab.

→ Use priors on correlation range as in *RobusGaSP*. Other references: *DACE*, *GPML*, *GPflow*, ...

Target use

Ideally, all R packages relying on *DiceKriging* for usual kriging steps could be made working with *libKriging* via its R interface *rlibkriging*. However, this requires a substantial amount of work and may take some time...

→ See package *dolka* later.


fanovaGraph
mlrMBO
testthat
sensitivity
mlr
kernDeepStackNet
kergp
GPGame
foreach
DiceOptim
doParallel
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mistral
KrigInv
moko
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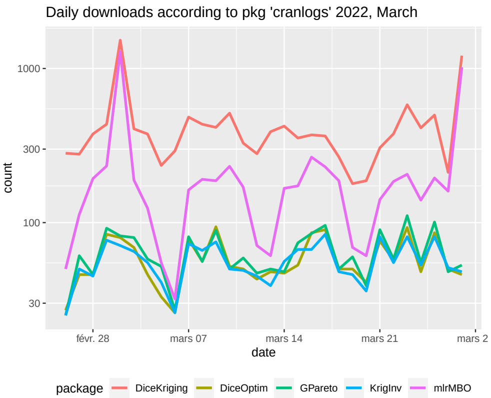


Doing Bayes optimization is the main motivation to download *DiceKriging*!

R Interface Limitations

Due to the multi-language target of *libKriging*

- *rlibkriging* does not use formula or data frames.
- The designs **X** are numeric matrices.

  → Designs provided as data frames (as produced by `expand.grid`) are coerced into numeric matrices.
- The colnames of the designs are not used, so only the number of columns and the position are meaningful.

R pitfalls

Remind that R is not intended to be a matrix programming language, although it embeds matrix algebra.

If you are only an occasional R user, it may be better not to use data frames and stick to numeric vectors, matrices, arrays.

```
## bind the rows of two matrices
mat1 <- cbind(Before = c(1, 2), After = c(10, 11))
mat2 <- cbind(After = c(3, 4), Before = c(12, 13))
(mat <- rbind(mat1, mat2))

##      Before After
## [1,]      1    10
## [2,]      2    11
## [3,]      3    12
## [4,]      4    13

## bind the (coerced) data frames
df1 <- as.data.frame(mat1); df2 <- as.data.frame(mat2)
(df <- rbind(df1, df2))

##   Before After
## 1      1    10
## 2      2    11
## 3     12     3
## 4     13     4

c(mat = class(mat[2, ]), df = class(df[2, ]))

##          mat           df
##    "numeric" "data.frame"
```

data frame $\neq$ *matrix*

A data frame is a frame enclosing objects that are coped with by using their name. In most R packages, the columns of a data frame are not expected to be in a particular order. Moreover, a data frame contains usually more columns (variables) than we need.

$\rightarrow$ The same data frame can be used to compare models with different covariates

R pitfalls

Be careful

- When using `rbind`, `apply`, ...

  → Are you applying the function on a numeric vector or on a data frame? Will the elements be provided to the function in the right order?
- When preparing and using "new" data as required in `predict`, `simulate`, `update`.

This is especially true when kriging with $d = 4$ inputs or more with no natural order for them e.g. physical variables.

OO programming in R

R has several systems for Object-Oriented (OO) programming.
The S3 and S4 systems are used in *DiceKriging* and *rlibkriging*

In *DiceKriging* we find two main S4 classes.

- Class `"km"` for fitted "kriging" models. The main methods are `predict`, `simulate`, `update`.
- Class `"covStruct"` is for covariance kernels

  → Mainly for experimented users. Most users will only need to choose the name of the kernel: `"gauss"`, `"matern3_2"`, ...

Class "km" of DiceKriging

The methods for the class `"km"` are mainly classical methods as found for classes of "fitted models".

```
library(DiceKriging)
methods(class = "km")

## [1] coef      logLik    plot      predict   show      simulate
## [7] update
## see '?methods' for accessing help and source code
```

There are two creators for the class `"km"`: `km` and `kmData`.

→ The second one is closer to `lm`, because the response and the inputs are assumed to be in the same data frame passed through the `data` argument.

Classes in rlibkriging

The package *rlibkriging* exposes two classes for fitted "kriging models".

- S4 class `"KM"` which inherits from `"km"`.

  → Pretty much the same syntax as `"km"`, so quite R-specific.

- S3 class `"Kriging"`.

  → Intended to be only loosely related to R, in order to increase the inter-language consistency across R, Python and Matlab/Octave.

In both cases, we can use the three main methods `predict`, `simulate` and `update`. Yet the formal arguments and the content of the output differ.

S3 vs S4

- S4 classes are formally defined. Objects haves *slots* such as `myKM@X`.
- S3 objects are mainly list with a `"class"` attribute, they are coped with by “gentleman’s rules”.

  → The method `predict` for the class `"Kriging"` is implemented via the function `predict.Kriging` which is called “internally”.

When a function is ("is registered as") a method, a *dispatch mechanism* is invoked at the call, based on the class of the first argument e.g. `object` for `predict` methods.

→ The name of the formal argument is the same across methods. All `predict` method have (or should have) their first formal argument name `"object"`.

The S3 and S4 systems are widely compatible so you may use methods without even knowing if they are S3 or S4.

→ There are quite technical functions such as `findMethod` to better understand what happens.

```r
library(rlibkriging)
methods(class = "KM")

## [1] predict  show     simulate update
## see '?methods' for accessing help and source code

methods(class = "Kriging")

##  [1] as.km         as.list       coerce        initialize
##  [5] leaveOneOut   logLikelihood logMargPost   predict
##  [9] print         show          simulate      slotsFromS3
## [13] update
## see '?methods' for accessing help and source code
```

In case of doubt, use `getS3method` for a an S3 method or `getMethod` for an S4 method

```
p3 <- getS3method(f = "predict", class = "lm")
p4 <- getMethod(f = predict, signature = "km")
```

We get the functions and we can see their code and know from what package they come.

→ It may happen that, for a given generic function and a given class, the method exist both as S3 and S4. This is the case for `predict` and `"km"`.

Inheriting from `"km"`

Since `"KM"` inherits from `"km"` it inherits all the methods implemented for `"km"` when the package *DiceKriging* is attached.

→ So the class `"KM"` has a `coef` method.

As a general rule do not call S3 methods directly, even when this is possible

good ☺ `predict(object = myObject)`

bad ☹ `predict.km(object = myObject)`

With the second syntax, we "hard code" that `myObject` must have class `"km"`. We also disable the use of possibly inherited method.

As far as possible, use methods to extract a slot or element in an object.

→ E.g. use `logLik(myObj)` method rather than `myObj$logLik` or `myObj@logLik`.

This makes robustness w.r.t. internal changes.

Mind that two different systems of formal arguments and of output names are used for `"KM"` and `"Kriging"`, ...

→ See the help of the two related `predict` methods.

Writing wrappers between the two naming systems is useless since the methods of `"KM"` already are wrappers for methods of `"Kriging"`.

dolka

The *DiceOptim* package is devoted to kriging-based Bayesian Optimization relying on *DiceKriging*. It could be made working with the library *libKriging* via *rlibkriging*.

In a first stage, a few functions of *DiceOptim* have been re-factored and included into a new package *dolka*.

→ Maybe "DiceOptim with LibKriging Alternative".

dolka

The package *dolka*

- Should work with *DiceKriging* and *rlibkriging* thanks to the use of methods.
- Refactors code from *DiceOptim* in order to make it less dependent on historical artefacts.

  → The Bayes criteria such as `EI` optionally provide the gradient with a straightforward syntax and output structure.
- Is a transitional/temporary package since the job should be done by/with experts in Bayesian Optimization.

Bayesian Optimization

A costly-to-evaluate function $f(\mathbf{x})$ is to be minimised over a domain in $\mathbb{R}^d$, say an hypercube.

Given a number of n evaluations $f(\mathbf{x}_i)$ at n design points $\mathbf{x}_i$ for $i = 1$ to n, we can use kriging to guess one or several "new" inputs $\mathbf{x}^{\text{new}}$ where the function is likely to take a small value. Then the new input(s) can be included in the design is a sequential fashion.

Considering $\{f(\mathbf{x})\}_{\mathbf{x}}$ as a path of a GP, kriging provides us with the distribution of $f(\mathbf{x}^{\text{new}})$ conditional on $\mathbf{f}(\mathbf{x}_{1:n}) := [f(\mathbf{x}_1), \dots, f(\mathbf{x}_n)]^\top$.

The improvement is then the non-negative random variable

$$I(\mathbf{x}) := \left[\min_{1 \leqslant i \leqslant n} f(\mathbf{x}_i) - f(\mathbf{x}) \right]_+$$

where $z_+ := \max\{z, 0\}$ is a positive part of z. Its distribution is the mixture of truncated Gaussian and of a probability mass at zero.

We want to get the largest possible distribution for the improvement $I(\mathbf{x})$ according to some (partial) order on distributions.

→ The distribution being conditional on the known points.

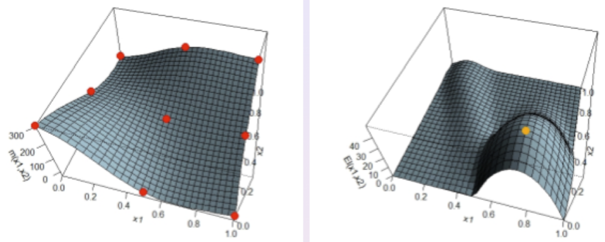
A good choice for $\mathbf{x}^{\text{new}}$ is the/a value maximizing the Expected Improvement

$$\mathrm{EI}(\mathbf{x}) := \mathbb{E}\left\{ I(\mathbf{x}) \,\middle|\, \mathbf{f}(\mathbf{x}_{1:n}) \right\}$$

We could use as well a quantile of the improvement, or some other criterion of improvement to be maximized.

A 2D example (Branin function)

Left: Kriging model surface. Right: EI surface.



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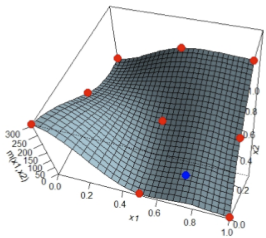

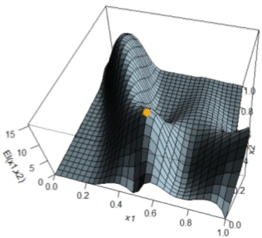

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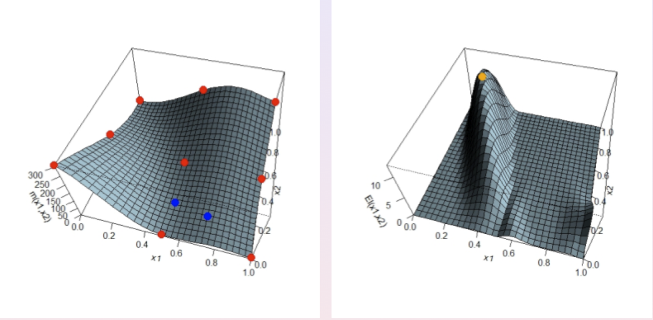

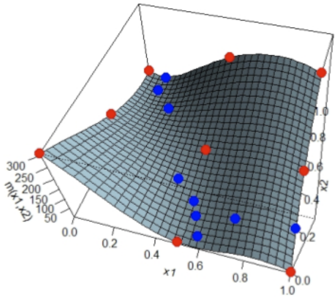

Initial designs (red points) and "new" designs added across iterations (blue points).

This illustration was provided by the authors and contributors of *DiceOptim*.

EGO (Efficient Global Optimization) algorithm

Given an initial design $\mathbf{X}$ and the corresponding vector of responses $\mathbf{f}$, we fit a kriging model .

Then repeat the following steps.

1. Find a design $\mathbf{x}^\star$ that maximizes the criterion.

   → We have to optimize a function of $\mathbf{x}$ which depends on the current model.

2. Evaluate the function $f(\mathbf{x})$ for $\mathbf{x} = \mathbf{x}^\star$.

3. Update the kriging model with the new point.

   → Add the new row $\mathbf{x}^\star$ to $\mathbf{X}$ and the new response $f(\mathbf{x}^\star)$ to the vector $\mathbf{f}$.

Stop if the improvement is small or if our evaluation budget is consumed.

Making things work

Using methods for the specific class of Kriging model that we want to use.

- *In step 1* the criterion function has formal arguments `x` and `model`. It calls the `predict` method.
- *In step 3*, we use the `update` method for the class of kriging models.

We can use `"km"` of *DiceKriging* or `"KM"` from *rlibkriging*. And more...

Optimization of the Criterion of Improvement

The criterion of improvement $C(\mathbf{x}^{\text{new}})$ to be maximized (say) can be computed using the values at $\mathbf{x}^{\text{new}}$ of the kriging mean $m(\mathbf{x})$, and the kriging variance $\sigma^2(\mathbf{x})$.

→ These are the *conditional* expectation and variance.

The criterion to be maximized has often many local maxima.

→ Roughly speaking there are as many local maxima as they are "holes" between the design points.

We want to perform a *global* optimization rather than a *local* one.

→ Genetic algorithms (as in packages *rgenoud*), CMAES as in package *cmaes*, ... or custom methods.

Using derivatives

It can help to use the derivatives of the criterion (gradient w.r.t. $\mathbf{x}$).

Since $m(\mathbf{x})$ and $\sigma^2(\mathbf{x})$ are standard output from the `predict` method, we can simply enhance this method so that it optionally computes the gradients as well.

→ When computed with the other kriging results, the gradients come at a small cost.

Using derivatives in `predict`

For now

- *DiceKriging* and *DiceOptim* do not rely on `predict` to pass the derivatives.

  → This makes *DiceOptim* strongly dependent on *DiceKriging*.

- *dolka* overloads (or "masks") the `predict` method from *DiceKriging* to add the derivatives.

  → This possibly confusing behaviour will no longer be needed it the authors of *DiceKriging* accept a small change in `predict`.

- *rlibkriging* will soon provide suitably enhanced `predict` methods for the classes `"KM"` and `"Kriging"`.

So we can easily switch from one `predict` to another, possibly relying on *libKriging*.

Update

The second key ingredient in kriging-based Bayes optimization is the `update method`.

Once the objective function $f(\mathbf{x})$ is evaluated at $\mathbf{x}^{\text{new}}$ we have to incorporate the new input point in the kriging design, possibly re-estimating the parameters (correlation ranges and variance). The fitted model object then embeds $n+1$ points $\mathbf{x}_i$ with $\mathbf{x}_{n+1} := \mathbf{x}^{\text{new}}$.

Roadmap

- Allow the use of different classes of kriging objects, including `"km"` and `"KM"`.

  → Using methods: `predict` and `update`.

- Allow the use of different optimization functions to maximize the chosen criterion.

  → `stats::optim`, `rgenoud::genoud`. But why not use *nloptr* or other packages?

	DiceOptim	*dolka*
DiceKriging "km"	max_EI max_qEI and much more.	max_EI_genoud, max_EI_cmaes* max_qEI_genoud
rlibkriging "KM"	not available yet requires changes in *DiceOptim*	max_EI_genoud, max_EI_cmaes* max_qEI_genoud

Table: Optimizers for criteria of improvement, available or soon available. Names of optimizers not requiring derivatives are starred $\star$.

Your turn

We will perform a few iterations of the EGO algorithm with EI criterion the `branin` function.

→ Available as `DiceKriging::branin`.

The goal is to a flexible implementation where we can use either *DiceKriging* or *rlibkriging* and we can easily switch from *DiceOptim* to *dolka*.

Your turn

Depending on your experience in Bayesian Optimization, you can find `EGO0.R` (minimal help), `EGO1.R`, ...

The suggested schedule is to write your program from scratch before using any help.

References I