

Using LIKELTD

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NULL

1 Code usage

Computing a likelihood model takes place in three-parts: (i) creation of the hypothesis, (ii) creation of the model itself from the hypothesis, (iii) maximizing the likelihood function over the set of nuisance parameters.

1.1 Creating a hypothesis

A hypothesis consists of all the parameters are used to describe the model, e. g. the known profiles to include, the number of unprofiled contributors, and whether to include dropin. A proper description of the hypothesis should be independent of other information, including neither information about the maximization of the likelihood nor any information which needs to be computed.

```
> require(likeLTD)
> require(DEoptim)
> # Case we are going to be looking at.
> caseName = 'hammer'
> datapath = file.path(system.file("extdata", package="likeLTD"),
+                       caseName)
> args = list(
+   databaseFile = NULL,
+   cspFile      = file.path(datapath, 'hammer-CSP.csv'),
+   refFile      = file.path(datapath, 'hammer-reference.csv'),
+   nUnknowns   = 0,
+   doDropin    = TRUE,
+   ethnic      = "EA1",
+   adj         = 1.0,
+   fst         = 0.02,
+   relatedness = c(0, 0)/4
+ )
> # Create hypothesis for defence and prosecution.
> defenceHyp = do.call(defence.hypothesis, args)
> prosecuHyp = do.call(prosecution.hypothesis, args)
```

Two methods are provided to facilitate the creation of a hypothesis from a common minimal set of input parameters, `defence.hypothesis` for the defence

and `prosecution.hypothesis` for the prosecution. These two methods read the allele database, the known profiles, and the crime-scene profile from file. They also automate sensible default decisions about the input, (determining which known profiles need be subject to dropout; in the defence hypothesis the queried individual is replaced by an unprofiled contributor; in the prosecution case, relatedness is set to zero.) These default choices may be further modified by the user at this point. These methods return lists with all the input needed for model execution.

```
> defenceModel <- create.likelihood(defenceHyp)
> prosecuModel <- create.likelihood(prosecuHyp)
```

`create.likelihood` returns a method which takes as arguments the nuisance parameters and computes the full weight of evidence, e. g. the product of the likelihoods and penalties associated with each locus.

```
> defenceModel(rcont=c(1, 1e-8, 1.63),
+             degradation=c(10^-2.27, 10^-2.74, 10^-2.47),
+             locusAdjustment=list(D3=0.983, vWA=1.010, D16=1.028,
+                                 D2=1.072, D8=1.020, D21=0.930,
+                                 D18=0.850, D19=0.932,
+                                 TH01=1.041, FGA=0.916),
+             dropout=c(0.5072, 1e-8),
+             dropin=1.0216,
+             power=-4.4462)
```

The function above returns a scalar which represents the weight of evidence for the given values of the nuisance parameters. One could then use `defenceModel` to perform an optimisation or to create a plot with respect to various arguments. For instance, the following leads to Fig. 1:

```
> require(ggplot2)
> require(scales)
> # Function that winnows down to a single value
> scalarWoE <- function(x) {
+   defenceModel(locusAdjustment=list(D3=0.983, vWA=1.010,
+                                     D16=1.028, D2=1.072,
+                                     D8=1.020, D21=0.930,
+                                     D18=0.850, D19=0.932,
+                                     TH01=1.041, FGA=0.916),
+               dropout=c(0.5072, 1e-8),
+               degradation=c(10^-2.27, 10^-2.74, 10^-2.47),
+               rcont=c(x, 1e-8, 1),
+               dropin=1.0216,
+               power=-4.4462)
+ }
> x = 0:30/30 * 3e0
> data = data.frame(x=x, y=sapply(x, scalarWoE))
> plots <- ggplot(data, aes(x=x, y=y))
+   geom_line()
+   xlab("Relative contribution of Victim 1") +
```

```

+           ylab("Weight of Evidence")           +
+           scale_y_log10(
+             labels=trans_format("log10", math_format(10^.x)))
> print(plots)

```

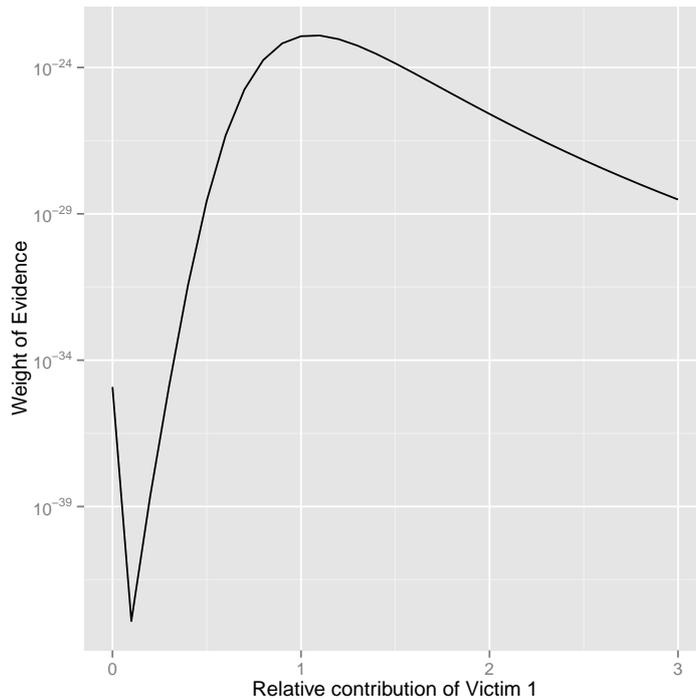


Figure 1: Logarithmic plot of the weight of evidence versus the relative contribution from "Victim 1". The likelihood is for the Hammer case, with one unprofiled contributor ("X"), and including dropin. The fixed parameters are given in Tab. 1.

1.2 Maximizing the likelihood

Once we have a likelihood method, it is possible to use the `stats` package to maximize it. However, the likelihood method takes several arguments (`rcont`, `degradation`, etc), whereas `DEoptim::DEoptim` expects a methods which takes only a vector as argument. Hence, we need to transform our method into the form the optimisation method expects:

```

> skeleton = initial.arguments(defenceHyp)
> vector.model <- function(x) {
+   args <- relist(x, skeleton)
+   args[["degradation"]] = 10^args[["degradation"]]
+   result <- do.call(defenceModel, args)
+   log10(result)

```

```

+ }
> # Call vector.model with vector argument.
> arguments = skeleton
> arguments[["degradation"]] = log10(arguments[["degradation"]])
> vector.model( as.vector(unlist(arguments)) )

```

The new method `vectorModel` achieves three objectives: (i) it recreates the list of arguments for `defenceModel`, (ii) it transforms the degradation parameter from an exponential form, (iii) it takes the logarithm of the weight of evidence. The last two points make optimisation somewhat easier. We can now apply the optimisation methods on `vectorModel`.

```

> require(stats)
> # define upper and lower bounds for constrained maximization
> nloci = ncol(defenceHyp$cspProfile)
> upper = list(locusAdjustment = rep(1.5, nloci),
+             dropout          = c(1-1e-3, 1-1e-3),
+             degradation      = rep(-1e-3, 3),
+             rcont            = rep(100, 2),
+             dropin           = 1,
+             power            = -2 ) [names(arguments)]
> lower = list(locusAdjustment = rep(0.5, nloci),
+             dropout          = c(1e-3, 1e-3),
+             degradation      = rep(-20, 3),
+             rcont            = rep(1e-3, 2),
+             dropin           = 1e-3,
+             power            = -6 ) [names(arguments)]
> # perform maximization
> result <- DEoptim(fn = vector.model,
+                 upper = unlist(upper),
+                 lower = unlist(lower),
+                 control = list(strategy=3, itermax=500)
+                 )
> opti = relist(result$optim$bestmem, skeleton)
> cat(sprintf("Resulting Weight of Evidence: 10^%f\n",
+           -result$optim$bestval))

```

```
[1] -37.31798
```

```
Resulting Weight of Evidence: 10^Inf
```

The above calculates the maximum of the likelihood using a differential evolution (DE) algorithm to to perform evolutionary global optimization. The particular flavor of DE algorithm used here allows the user to set upper and lower bounds for parameters. Upon convergence, it returns a list with the optimum and its location. Please see the `DEoptim` package for description.

The functionality of the above code can be achieved more succinctly through a convenience method provided by `LIKELTD optimisation.params`. It returns a list of adequate arguments for `optim` given a hypothesis:

```

> params = optimisation.params(defenceHyp, verbose=FALSE)
> params$control$itermax=50 # Less strict convergence, for demo purposes.

```

```
> results <- do.call(DEoptim, params)
> arguments <- relistArguments(results$optim$bestmem, defenceHyp)
```

Running the above yields the parameters in Tab. 1. The last line transforms the linear vector of arguments returned by `DEoptim` back into a more meaningful list, much as `relist` did earlier. However, it takes care of some specialized problems with the operation, and should be preferred over `relist`.

A method for ensuring proper convergence is provided by `LIKELTD DEoptimLoop`. This calls the external function `DEoptim::DEoptim`, but crucially compares the optimised result every 50 generations with the previous optimised result, and quits once the relative difference is below the given tolerance.

1.3 Testing

`LIKELTD` comes with a fairly extensive suite of tests. The tests can be run as part of the installation process, or using the following commands:

```
> library(svUnit)
> library(likeLTD)
> runTest( svSuite("package:likeLTD") )
> Log()
```

Although not shown here, this snippet will print results for each test. Each should return "OK".

```

Iteration: 1 bestvalit: 60.057348 bestmemit: 1.207931 0.603873 1.265597 0.9116
Iteration: 2 bestvalit: 60.057348 bestmemit: 1.207931 0.603873 1.265597 0.9116
Iteration: 3 bestvalit: 60.057348 bestmemit: 1.207931 0.603873 1.265597 0.9116
Iteration: 4 bestvalit: 60.057348 bestmemit: 1.207931 0.603873 1.265597 0.9116
Iteration: 5 bestvalit: 57.943797 bestmemit: 1.207931 0.603873 1.265597 0.9116
Iteration: 6 bestvalit: 57.943797 bestmemit: 1.207931 0.603873 1.265597 0.9116
Iteration: 7 bestvalit: 57.912302 bestmemit: 1.207931 0.603873 1.265597 0.9116
Iteration: 8 bestvalit: 57.456434 bestmemit: 1.207931 0.603873 1.265597 0.9116
Iteration: 9 bestvalit: 57.456434 bestmemit: 1.207931 0.603873 1.265597 0.9116
Iteration: 10 bestvalit: 57.456434 bestmemit: 1.207931 0.603873 1.265597 0.9116
Iteration: 11 bestvalit: 57.249127 bestmemit: 0.685920 0.603873 1.265597 0.9116
Iteration: 12 bestvalit: 57.249127 bestmemit: 0.685920 0.603873 1.265597 0.9116
Iteration: 13 bestvalit: 52.775465 bestmemit: 0.851930 1.093800 1.196344 0.9116
Iteration: 14 bestvalit: 52.775465 bestmemit: 0.851930 1.093800 1.196344 0.9116
Iteration: 15 bestvalit: 50.661807 bestmemit: 0.649772 0.681851 1.396563 0.793
Iteration: 16 bestvalit: 47.699510 bestmemit: 0.649772 0.897989 0.656130 0.786
Iteration: 17 bestvalit: 46.852793 bestmemit: 0.649772 0.897989 0.656130 0.786
Iteration: 18 bestvalit: 46.852793 bestmemit: 0.649772 0.897989 0.656130 0.786
Iteration: 19 bestvalit: 46.852793 bestmemit: 0.649772 0.897989 0.656130 0.786
Iteration: 20 bestvalit: 46.852793 bestmemit: 0.649772 0.897989 0.656130 0.786
Iteration: 21 bestvalit: 46.852793 bestmemit: 0.649772 0.897989 0.656130 0.786
Iteration: 22 bestvalit: 46.852793 bestmemit: 0.649772 0.897989 0.656130 0.786
Iteration: 23 bestvalit: 46.852793 bestmemit: 0.649772 0.897989 0.656130 0.786
Iteration: 24 bestvalit: 45.987529 bestmemit: 0.649772 0.897989 0.656130 0.786
Iteration: 25 bestvalit: 45.987529 bestmemit: 0.649772 0.897989 0.656130 0.786
Iteration: 26 bestvalit: 45.987529 bestmemit: 0.649772 0.897989 0.656130 0.786
Iteration: 27 bestvalit: 45.987529 bestmemit: 0.649772 0.897989 0.656130 0.786
Iteration: 28 bestvalit: 45.987529 bestmemit: 0.649772 0.897989 0.656130 0.786
Iteration: 29 bestvalit: 45.987529 bestmemit: 0.649772 0.897989 0.656130 0.786
Iteration: 30 bestvalit: 45.987529 bestmemit: 0.649772 0.897989 0.656130 0.786
Iteration: 31 bestvalit: 45.717450 bestmemit: 0.990146 0.939596 1.281060 0.767
Iteration: 32 bestvalit: 44.682805 bestmemit: 0.990146 0.939596 1.157700 0.871
Iteration: 33 bestvalit: 44.682805 bestmemit: 0.990146 0.939596 1.157700 0.871
Iteration: 34 bestvalit: 44.682805 bestmemit: 0.990146 0.939596 1.157700 0.871
Iteration: 35 bestvalit: 44.654377 bestmemit: 0.990146 1.117104 1.157700 0.871
Iteration: 36 bestvalit: 44.552345 bestmemit: 0.649772 0.798348 0.869659 0.786
Iteration: 37 bestvalit: 44.552345 bestmemit: 0.649772 0.798348 0.869659 0.786
Iteration: 38 bestvalit: 42.758242 bestmemit: 0.891015 1.218903 0.898591 1.020
Iteration: 39 bestvalit: 42.758242 bestmemit: 0.891015 1.218903 0.898591 1.020
Iteration: 40 bestvalit: 42.433448 bestmemit: 0.891015 1.100851 0.898591 1.020
Iteration: 41 bestvalit: 42.433448 bestmemit: 0.891015 1.100851 0.898591 1.020
Iteration: 42 bestvalit: 42.433448 bestmemit: 0.891015 1.100851 0.898591 1.020
Iteration: 43 bestvalit: 42.433448 bestmemit: 0.891015 1.100851 0.898591 1.020
Iteration: 44 bestvalit: 42.420360 bestmemit: 0.891015 1.100851 0.898591 1.020
Iteration: 45 bestvalit: 40.774078 bestmemit: 0.977805 1.126010 1.026108 0.993
Iteration: 46 bestvalit: 40.658252 bestmemit: 0.977805 1.126010 1.026108 0.993
Iteration: 47 bestvalit: 40.593048 bestmemit: 0.977805 1.126010 1.026108 0.993
Iteration: 48 bestvalit: 40.396313 bestmemit: 0.786871 0.939131 1.098478 1.013
Iteration: 49 bestvalit: 40.396313 bestmemit: 0.786871 0.939131 1.098478 1.013
Iteration: 50 bestvalit: 40.396313 bestmemit: 0.786871 0.939131 1.098478 1.013

```

	Victim 1	Victim 2	X
rcont	1.000	14.254	6 0.284
degradation	$10^{0.0407}$	$10^{1.42e-09}$	$10^{0.000299}$

Locus Adjustments for each locus				
D3	vWA	D16	D2	D8
0.787	0.939	1.098	1.013	0.936
D21	D18	D19	TH01	FGA
0.961	0.873	0.587	1.158	1.015