Developments in optimization tools for R

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Background

- BIG subject
- Good overview in CRAN Task View: Optimization and Mathematical Programming (Stefan Theussl)
- Many (most?) statistics problems have at least a formal statement as an optimization problem
- For the novice (or not so novice) – too many choices

Attempts to help user

- Package **optimx**
  - Initially to unify a number of tools under a single calling syntax (JSS paper forthcoming with RV)
  - Opportunities for improvements led to
    - Optimality tests (Kuhn Karush Tucker)
    - Scaling tests
    - Bounds checking
    - Inadmissible user-function wrapper
- In-development package **dfoptim** for derivative free methods (some overlap with optimx)

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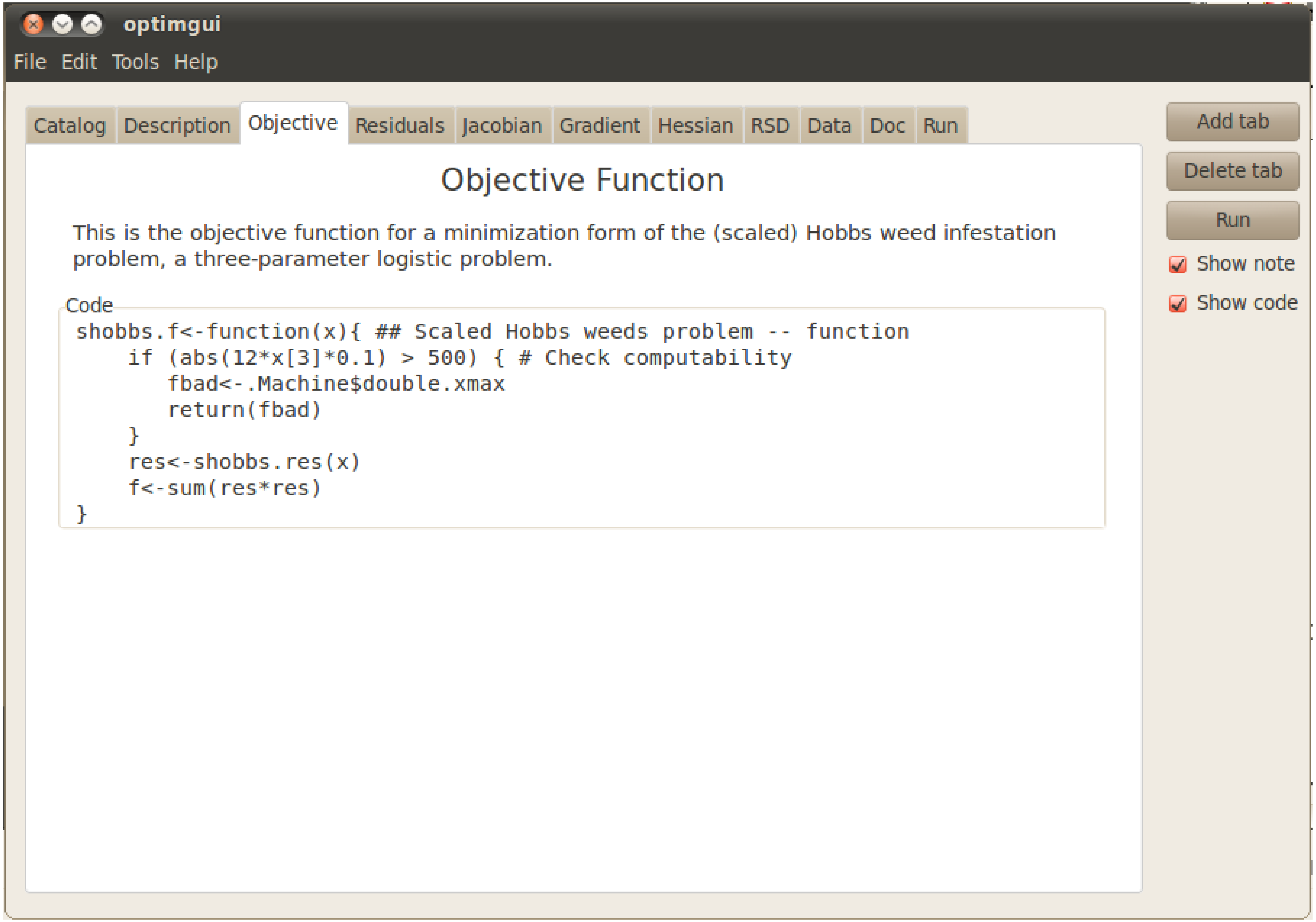
Attempts to help user (2)

- Forthcoming package **optimgui** to provide a template for building and running optimization tasks (Yixuan Qiu, Google Summer of Code 2011)
  - Catalog of existing problems that can be modified
  - Problem files combine data, objective, gradient etc. with documentation
  - Linkage to a decision tree to suggest methods
  - Google Summer of Code: student Yixuan Qui


optimgui
File Edit Tools Help
Catalog Description Objective Residuals Jacobian Gradient Hessian RSD Data Doc Run
Add tab
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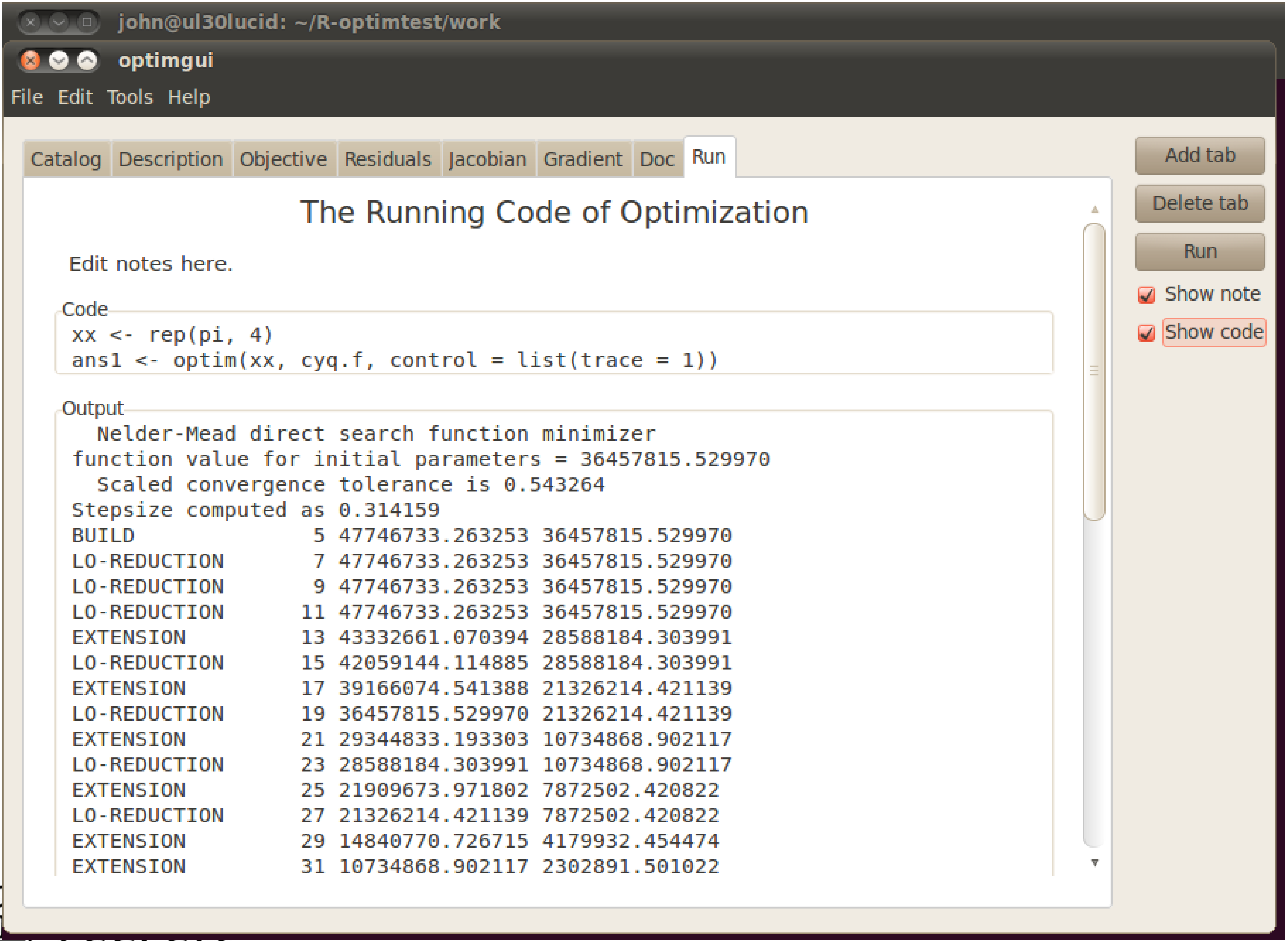
Run
Show note
Show code

Objective Function

This is the objective function for a minimization form of the (scaled) Hobbs weed infestation problem, a three-parameter logistic problem.

Code

```
shobbs.f<-function(x){ ## Scaled Hobbs weeds problem -- function
    if (abs(12*x[3]*0.1) > 500) { # Check computability
       fbad<-.Machine$double.xmax
       return(fbad)
    }
    res<-shobbs.res(x)
    f<-sum(res*res)
}
```


john@ul30lucid: ~/R-optimtest/work
optimgui
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The Running Code of Optimization

Edit notes here.

Code

```
xx <- rep(pi, 4)
ans1 <- optim(xx, cyq.f, control = list(trace = 1))
```

Output

```
  Nelder-Mead direct search function minimizer
function value for initial parameters = 36457815.529970
  Scaled convergence tolerance is 0.543264
Stepsize computed as 0.314159
BUILD              5 47746733.263253 36457815.529970
LO-REDUCTION       7 47746733.263253 36457815.529970
LO-REDUCTION       9 47746733.263253 36457815.529970
LO-REDUCTION      11 47746733.263253 36457815.529970
EXTENSION         13 43332661.070394 28588184.303991
LO-REDUCTION      15 42059144.114885 28588184.303991
EXTENSION         17 39166074.541388 21326214.421139
LO-REDUCTION      19 36457815.529970 21326214.421139
EXTENSION         21 29344833.193303 10734868.902117
LO-REDUCTION      23 28588184.303991 10734868.902117
EXTENSION         25 21909673.971802 7872502.420822
LO-REDUCTION      27 21326214.421139 7872502.420822
EXTENSION         29 14840770.726715 4179932.454474
EXTENSION         31 10734868.902117 2302891.501022
```

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My Active Tasks

- Refactoring of **optimx** / links with **optimgui**
  - Features useful to other optimization tools put in separate packages
  - More optimizers – see also dfoptim
- Under development for **optimx**
  - Axial search around minimum (2*n function evaluations)
  - Grid search to explore “nasty” situations – n^gstep fns – slow!
  - Measures of dispersion – “standard errors”
  - Masks – fixed parameters; need vignettes and examples
  - Extend box constraints to more methods
  - Measures of effort other than timing

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JN: Medium – Long Term

- Automatic or symbolic derivatives
  - Existing tools awkward; “gaps” in function coverage
  - Need good tutorial material
- Linear & nonlinear constraints
  - Tools for penalty and barrier methods (few)
  - Math programming tools (some in R, but …)
- Measures of dispersion at constraint boundary
- “Noisy” functions – RSMIN
- Automated perfomance data gathering ==> R

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Other work

- Non – R (and possibly not cross platform)
  - NLOpt: http://ab-initio.mit.edu/wiki/index.php/NLopt
  - Eigen: http://eigen.tuxfamily.org
- Multiple-minima → messy optimizations often approached by stochastic methods
  - rgenoud, DEoptim, soma, other developments
- Acceleration of iterations (SQUAREM, etc.)
- Many activities about which I should be better informed!

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Collaboration?

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    - Cannot be too strict; need compromise
    - Measures of effort vs. timing – what counts?
    - Making constructing function and gradient easier
    - ALL methods fail sometimes – Why?
- Need help from users
    - Tell us what works and what does not (and why!)
    - Help build vignettes, documentation, "best practice", example problem sets

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