

C++ Functions in Maxliklib Library

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Abstract

The functions in the maxliklib repository are described. Arguments and their definitions are specified, and dependencies of functions are stated.

Keywords: Maximization procedures, quadrature procedures, maximum likelihood

The maxliklib repository consists of C++ functions helpful in estimation related to maximum likelihood. The functions should be appropriate for C++11. They rely on the Armadillo library (Sanderson & Curtin, 2016, 2018) at <http://arma.sourceforge.net>. Unless otherwise noted, for the library members considered, it is assumed that users have verified that function arguments are valid. The following functions are found in the library.

- `adapt.cpp`
- `adaptv.cpp`
- `berresp.cpp`
- `conjgrad.cpp`
- `contresp.cpp`
- `cumresp.cpp`
- `genfact.cpp`
- `genprods.cpp`
- `genresp.cpp`

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- `genresplik.cpp`
- `genresplikl.cpp`
- `genrespmle.cpp`
- `genrespmle1.cpp`
- `genrespmleg.cpp`
- `genrespmlel.cpp`
- `gradascent.cpp`
- `gradresp.cpp`
- `gumbel.cpp`
- `hermcoeff.cpp`
- `hermpoly.cpp`
- `hermpw.cpp`
- `logistic.cpp`
- `loglog.cpp`
- `logit.cpp`
- `logmean.cpp`
- `lw.cpp`
- `lwm.cpp`
- `maxberresp.cpp`
- `maxf2vvar.cpp`
- `maxlinq2.cpp`
- `maxquad.cpp`
- `multlogit.cpp`
- `modit.cpp`
- `normal.cpp`

- normalv.cpp
- nrv.cpp
- pack.cpp
- probit.cpp
- ranklogit.cpp
- rebound.cpp
- truncresp.cpp
- unpack.cpp

Distributions of Sums of Independent Multinomial Variables

The functions in this section implement a modified and generalized version of the Lord-Wingsky algorithm (Lord & Wingsky, 1984; Thissen et al., 1995). The numerical procedures and their rationale are discussed in lw.pdf.

lw.cpp

The function lw.cpp finds the probability mass function of the sum S of mutually independent Bernoulli random variables X_j , $0 \leq j < n$. The function declaration is

vec lw(const double & c, const vec & p).

The vector p has dimension n and has positive elements that are less than 1. For $0 \leq j < n$, the probability that $X_j = 1$ is element j of p . The variable c is normally a small positive number used as in lw.pdf to remove very small probabilities from consideration in order to speed computation. If c is not positive, then the modified Lord-Wingsky algorithm used by lw.cpp reduces to the conventional algorithm. The probability mass function is provided by lw , a vector with $n + 1$ elements. For $0 \leq k \leq n$, element k of lw is the probability that $S = k$.

lwm.cpp

The function lwm.cpp finds the probability mass function of the sum S of n mutually independent random variables X_j , $0 \leq j < n$ with integer values from 0 to $I_j - 1$ for an integer $I_j > 1$. The function declaration is

vec lwm(const double & c, const vector<vec> & p).

Here p has n members. For $0 \leq j < n$, member j of p is the vector $p[j]$ with I_j nonnegative elements. The sum of these elements is 1, and element k , $0 \leq k < I_j$, of $p[j]$ is the probability that $X_j = k$. The probability mass function is provided by lwm , a vector with $K = 1 + \sum_{j=1}^n (I_j - 1)$ elements. Element k of lwm , $0 \leq k < K$, is the probability that $S = k$. The variable c is normally a small positive number used as in `lw.pdf` to remove very small probabilities from consideration in order to speed computation. If c is not positive, then the modified algorithm used by `lwm.cpp` reduces to the conventional generalization of the Lord-Wingersky algorithm to sums of independent multinomial variables.

Tools for Line Searches

The functions in this section facilitate line searches during function maximization. Throughout discussions in this section and in Functions related to the Newton-Raphson algorithm and Functions Related to Gradient Methods, the theoretical background and the definitions of η , γ_1 , γ_2 , and κ are found in `convergence.pdf`. For some positive integer p and nonempty open convex set O of p -dimensional vectors, a continuously differentiable real function $f.value$ on O is to be maximized by an iterative algorithm with a starting value in O . It is assumed that, for some real a , the set A of members of O at which $f.value$ is at least a is closed and bounded, and the sets A_0 of members of O at which $f.value$ exceeds a is nonempty. The function $f.value$ is assumed to be strictly pseudoconcave on A_0 . The starting values for algorithms are assumed to be in A_0 . The convention is adopted that $f.value$ has value NaN at any p -dimensional vector not in O .

maxlinq2.cpp

The function `maxlinq2.cpp` provides a line search for maximization algorithms. Only function values and gradients are used when `order` is 1, but Hessian matrices are computed if `order` is greater than 1. The function declaration is

```
maxf2v maxlinq2(const int & order, const params & mparams, const vec & v,
const maxf2v & vary0, const std::function<f2v(const int &, const vec &)>f).
```

Here the definition of `maxf2v` is

```
struct maxf2v{vec locmax; double max; vec grad, mat hess;};,
```

`vary0.locmax` is the starting vector for the line search, `vary0.max` is the value of $f.value$ at the starting vector, `maxlinq2.grad` is the gradient of $f.value$ at `vary0.locmax`, `maxlinq2.hess`, if computed, is the gradient of $f.value$ at `vary0.locmax`, and `maxlinq.locmax` is the approximate location of the maximum of $f.value$ on the

half-line that starts at *vary0.locmax* and has direction *v*, *maxlinq2.max* is the approximate maximum of *f.value* on the half-line, *maxlinq2.grad* is the gradient of *f.value* at *maxlinq.locmax*, and *maxlinq2.hess*, if computed, is the Hessian of *f.value* at *vary0.locmax*,

The definition of *params* is

```
struct params{int maxit; int maxits; double eta;
double gamma1; double gamma2; double kappa; double tol;}
```

Here *mparams.maxit* is the number of primary iterations, *mparams.maxits* is the maximum number of uses of *maxquad.cpp* permitted for each primary iteration, *mparams.eta* is η , *mparams.gamma1* is γ_1 , *mparams.gamma2* is γ_2 , and *mparams.kappa* is κ . Iterations cease if the function value changes less than *mparams.tol* after a primary iteration.

The definition of *f2v* is

```
struct f2v{double value; vec grad; vec hess};
```

where *f.value* is the function value, *f.grad* is the gradient of *f.value*, and *f.hess* is the Hessian of *f.value*.

The functions *maxf2vvar.cpp*, *maxquad.cpp*, *modit.cpp*, and *rebound.cpp* are all used.

maxquad.cpp

The function *maxquad.cpp* approximates the maximum of *f.value* along a half-line by use of a quadratic two-point approximation. The function declaration is

```
double maxquad(const double & x0, const double & x1, const double & f0,
const double & f1, const double & g0, const double & stepmax).
```

Here *x0* and *x1* are the points used, *f0* is the function value at *x0*, *f1* is the function value at *x1*, *g0* is the derivative at *x0*, and *stepmax* is the maximum change from *x0* permitted in the estimated location *maxquad* of the function maximum.

modit.cpp

The function *modit.cpp* truncates an iteration to conform to limits on step size and bounds in the case of a real function of one variable with a unique critical point and a limit of $-\infty$ as the absolute value of the function argument approaches ∞ . The function declaration is

```
double modit(const double & eta, const double & alpha0, const double & alpha1,
```

const double & stepmax, const bounds & b),

and the struct *bounds* is defined as

struct bounds {double lower; double upper;}.

Here *eta* corresponds to η , *alpha0* is the previous location, *alpha1* is the proposed new location, *stepmax* is the positive limit on step size, *b.lower* is the lower bound, and *b.upper* is the upper bound. It is assumed that *alpha0* and *alpha1* are different. The function returns a value *modit* that is normally *alpha1*; however, if *alpha1* exceeds *alpha0*, then *modit* is truncated above so that it does not exceed the minimum of *alpha0+stepmax* and *alpha0+eta(b.upper-alpha0)*, while if *alpha1* is less than *alpha0*, then *modit* is truncated below so that it is at least the maximum of *alpha0-stepmax* and *alpha0+eta(b.lower-alpha0)*.

rebound.cpp

The function *rebound.cpp* updates the lower and upper bounds for maximization of a differentiable real function on the real line with a unique critical point and a limit of $-\infty$ as the absolute value of the function argument approaches ∞ . The function declaration is

bounds rebound(const double & y, const double & der, const bounds & b).

The struct *bounds* is defined as in *modit.cpp*. Here *y* is the current location, *der* is the function derivative at *y*, *b.lower* is the current lower bound, and *b.upper* is the current upper bound. It is assumed that *der* is not 0. If *der* is positive, *modit.lower* is *y* and *modit.upper* is *b.upper*. If *der* is negative, *modit.upper* is *y* and *modit.lower* is *b.lower*.

Functions related to the Newton-Raphson algorithm

In this section, functions are discussed that are related to the Newton-Raphson algorithm. It should be noted that references to function values, gradients, and Hessian matrices do not address computational methods. In fact, the function values, gradients, and Hessian matrices employed may be approximations derived by numerical differentiation or large-sample approximations. In this section, *f.value* is assumed to be twice continuously differentiable.

maxf2vvar.cpp

The function *maxf2vvar.cpp* is used to combine information on a location and on a function's value, gradient, and Hessian matrix at the location. The function *maxf2vvar.cpp* has declaration

maxf2v maxf2vvar(const int & order, const vec & y, const f2v & fy);

The structs *f2v* and *maxf2v* are defined as in *maxlinq2.cpp*. The returned value *maxf2vvar.locmax* is *y*, while *maxf2vvar.max* is *fy.value*, *maxf2vvar.grad* is *fy.grad*, and *maxf2vvar.hess* is *fy.hess* at *y*. If *order* is less than 1, only *fy.value* is considered. If *order* is 1, *fy.value* and *fy.grad* are considered. If *order* exceeds 1, then *fy.value*, *fy.grad*, and *fy.hess* are used.

nrv.cpp

The function *nrv.cpp* applies a modified version of the Newton-Raphson algorithm to maximization of *f.value*. The function *nrv.cpp* has declaration

maxf2v nrv(const int & order, const params & mparams, const vec & start, const std::function<f2v(const int &, vec &)> f).

The structs *f2v*, *maxf2v*, and *params* are defined as in *maxlinq2.cpp*. The starting vector *start* must be in *O*.

The function *nrv.cpp* uses *maxf2vvar.cpp*, *maxlinq2.cpp*, *maxquad.cpp*, *modit.cpp*, and *rebound.cpp*. The value of *order* should be at least 2.

Functions Related to Gradient Methods

In this section, functions are considered based on gradient-based methods.

conjgrad.cpp

The function *conjgrad.cpp* implements a conjugate gradient algorithm for maximization of *f.value*. The function declaration is

maxf2v conjgrad(const int & order, const params & mparams, const vec & start, const std::function<f2v(const int &, const vec &)> f).

The starting vector is *start*. The value of *order* must be at least 1. If *order* is at least 2, Hessian matrices are computed even though not used in the algorithm.

The function *conjgrad.cpp* uses *maxf2vvar.cpp*, *maxlinq2.cpp*, *maxquad.cpp*, *modit.cpp*, and *rebound.cpp*.

gradascent.cpp

The function *gradascent.cpp* uses a gradient-ascent algorithm for maximization of *f.value*. The function declaration for *gradascent.cpp* is

maxf2v gradascent(const order &, const params & mparams, const vec & start, const std::function<f2v(const int &, const vec &)> f).

The functions `maxf2vvar.cpp`, `maxlinq2.cpp`, `maxquad.cpp`, `modit.cpp`, and `rebound.cpp` are used. Definitions are as in `conjgrad.cpp`.

Log-likelihood Components

In this section, components of log-likelihood functions are provided. For a positive integer n and an observation i , $0 \leq i < n$, positive integers r_i and q_i are given. The component of the log likelihood for observation i involves the predicted random vector \mathbf{Y}_i in a nonempty subset \mathcal{Y}_i of r_i -dimensional vectors with elements $Y_i(j)$, $0 \leq j < r_i$, the q_i by p predicting matrix \mathbf{X}_i in a nonempty set \mathcal{X}_i , the q_i -dimensional vector \mathbf{o}_i , and the positive real weight w_i . If $\boldsymbol{\tau}$ is in O , then let $\boldsymbol{\lambda}_i(\boldsymbol{\tau}) = \mathbf{o}_i + \mathbf{X}_i\boldsymbol{\tau}$ for $0 \leq i < n$, and let the log-likelihood function under study have the form

$$\ell(\boldsymbol{\tau}) = \sum_{i=0}^{n-1} w_i \ell_i(\boldsymbol{\lambda}_i(\boldsymbol{\tau}); \mathbf{Y}_i). \quad (1)$$

Consider observation i for $0 \leq i < n$. For a nonempty open convex set O_i of q_i -dimensional vectors, $\ell_i(\cdot; \mathbf{y})$ is a twice continuously differentiable real function on O_i for all \mathbf{y} in \mathcal{Y}_i . For any $\boldsymbol{\tau}$ in O and \mathbf{X} in \mathcal{X}_i , $\boldsymbol{\lambda}_i(\boldsymbol{\tau})$ is in O_i . If \mathcal{Y}_i is finite or countably infinite and $\boldsymbol{\beta}$ is in O_i , then 1 is the sum of the $\exp(\ell_i(\boldsymbol{\beta}; \mathbf{y}))$ over \mathbf{y} in \mathcal{Y}_i and some random vector \mathbf{Y} equals \mathbf{y} with probability $\exp(\ell_i(\boldsymbol{\beta}; \mathbf{y}))$ for each \mathbf{y} in \mathcal{Y}_i . If \mathcal{Y}_i is a convex set with a nonempty interior and $\boldsymbol{\beta}$ is in O_i , then the integral of $\exp(\ell_i(\boldsymbol{\tau}; \mathbf{y}))$ over \mathbf{y} in \mathcal{Y}_i is 1 and a continuous random vector \mathbf{Y}_i has density $\exp(\ell_i(\boldsymbol{\beta}; \mathbf{y}))$ at \mathbf{y} in \mathcal{Y}_i . In some cases involving censorship, more complex structures arise. The gradient function of $\ell_i(\cdot; \mathbf{y})$ is $\nabla \ell_i(\cdot; \mathbf{y})$ and the corresponding Hessian matrix is $\nabla^2 \ell_i(\cdot; \mathbf{y})$. It follows that the gradient of ℓ at $\boldsymbol{\tau}$ in O is

$$\nabla \ell(\boldsymbol{\tau}) = \sum_{i=0}^{n-1} w_i \mathbf{X}_i^T \nabla \ell_i(\boldsymbol{\lambda}_i(\boldsymbol{\tau}); \mathbf{Y}_i), \quad (2)$$

and the Hessian matrix of ℓ at $\boldsymbol{\tau}$ is

$$\nabla^2 \ell(\boldsymbol{\tau}) = \sum_{i=0}^{n-1} w_i \mathbf{X}_i^T \nabla^2 \ell_i(\boldsymbol{\lambda}_i(\boldsymbol{\tau}); \mathbf{Y}_i) \mathbf{X}_i. \quad (3)$$

The Hessian matrix $\nabla^2 \ell(\boldsymbol{\tau})$ has an approximation

$$\tilde{\nabla}^2 \ell(\boldsymbol{\tau}) = - \sum_{i=0}^{n-1} w_i \mathbf{X}_i^T \nabla \ell_i(\boldsymbol{\lambda}_i(\boldsymbol{\tau}); \mathbf{Y}_i) [\nabla \ell_i(\boldsymbol{\lambda}_i(\boldsymbol{\tau}); \mathbf{Y}_i)]^T \mathbf{X}_i \quad (4)$$

(Haberman, 2013; Louis, 1982) .

Many standard cases of $\ell_i(\cdot; \mathbf{y})$ exist, some of which are examined in the literature on survival analysis (Cox, 1972; Kalbfleisch & Prentice, 2002), generalized linear models (McCullagh & Nelder, 1989), multivariate analysis (Anderson, 2003),

and discrete choice (McFadden, 1973). It should be noted that names for models are somewhat variable in different references, especially for graded and cumulative cases. In addition, graded and cumulative cases are defined to be consistent with the Bernoulli cases. The following C++ functions are employed for common examples. The structs *f2v* are defined as in *maxliq2.cpp*. If the argument *beta* is not in O_i , then all values returned equal *NaN*. It is assumed that the user of the function has verified that the input vector *y* is in \mathcal{Y}_i . In the cases under study in this section, unless otherwise stated, the components are strictly concave, so that ℓ is strictly concave whenever \mathbf{X}_i , $0 \leq i < n$, spans a space of dimension p . Conditions for a unique $\hat{\boldsymbol{\tau}}$ in O such that $\ell(\hat{\boldsymbol{\tau}})$ equals the supremum of ℓ over O are relatively complex (Haber-
man, 1974, 1977, 1980). It is worth noting that in cases in which $\hat{\boldsymbol{\tau}}$ in O satisfies the conditions that $\nabla \ell(\hat{\boldsymbol{\tau}})$ is the p -dimensional vector $\mathbf{0}_p$ with all elements 0 and $\nabla^2 \ell(\hat{\boldsymbol{\tau}})$ is negative definite, then O can be restricted to ensure that ℓ is strictly concave on O and $\hat{\boldsymbol{\tau}}$ is the only member of O such that $\ell(\hat{\boldsymbol{\tau}})$ equals the supremum of ℓ on O and, for $\boldsymbol{\tau}$ in O , $\nabla \ell(\boldsymbol{\tau})$ is only the vector with all elements 0 if $\boldsymbol{\beta}$ equals $\hat{\boldsymbol{\beta}}$. In all component functions, *order* is less than 1 if only the component value is computed, 1 if the component value and gradient are found, and greater than 1 if the component value, gradient, and Hessian are found.

berresp.cpp

The function *berresp.cpp* is used to handle standard models for Bernoulli random variables. If this choice applies to observation i , \mathcal{Y}_i is the set of one-dimensional vectors \mathbf{y} with $y(0)$ equal 0 or 1, $r_i = 1$, $q_i = 1$, O_i is the set of all one-dimensional vectors, and F is a three-times continuously differentiable cumulative distribution function with a positive derivative f such that $\log(f)$ has a negative second derivative. For y in \mathcal{Y}_i and $\boldsymbol{\beta}$ in O_i ,

$$\ell_i(\boldsymbol{\beta}; \mathbf{y}) = \begin{cases} \log(F(\beta(0))), & y(0) = 1, \\ \log(1 - F(\beta(0))), & y(0) = 0. \end{cases} \quad (5)$$

The function declaration is

```
f2v berresp(const int & order, const char & transform, const resp & y,  
const vec & beta).
```

If *transform* is G , then $F = G$, the standard Gumbel distribution function with value $G(y) = \exp(-\exp(-y))$ for y real. If *transform* is L , then $F = \Psi$, the standard logistic distribution function with value $\Psi(y) = 1/[1 + \exp(-y)]$ for y real. If *transform* is N , then $F = \Phi$, the standard normal distribution function with derivative $\phi(y) = \exp(-y^2/2)/(2\pi)^{1/2}$ for real y . The function *berresp.value* is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if *y.iresp* is \mathbf{y} and *beta* is $\boldsymbol{\beta}$.

The function *berresp.cpp* requires *loglog.cpp*, *logit.cpp*, and *probit.cpp*.

contresp.cpp

The function `contresp.cpp` computes the function value, gradient, and Hessian matrix associated with the distribution of a location and scale model for a continuous random vector. Here $r_i = 1$, $q_i = 2$, \mathcal{Y}_i is the set of all one-dimensional vectors, O_i is the set of all two-dimensional vectors β with element $\beta(1) > 0$, and F and f are defined as in `berresp.cpp`. For \mathbf{y} in \mathcal{Y}_i and β in O_i ,

$$\ell_i(\beta; \mathbf{y}) = \log(\beta(1)) + \log(f(\beta(0) + \beta(1)y(0))). \quad (6)$$

These cases correspond to a model that a random variable has a distribution $\beta(0) + \beta(1)Z$, where Z has a distribution function F . Here $\ell_i(\cdot; \mathbf{y})$ is concave, and the function is strictly concave if $y(0)$ is not 0.

For all cases, the function declaration is

*f2v contresp(const int & order, const char & transform, const resp & y,
const vec & beta).*

The variable *transform* is defined as in `berresp.cpp`. The function *contresp.value* is $\ell_i(\beta; \mathbf{y})$ if *y.dresp* is \mathbf{y} and *beta* is β . The function `contresp.cpp` requires `gumbel.cpp`, `logistic.cpp`, and `normal.cpp`.

cumresp.cpp

The function `cumresp.cpp` computes the function value, gradient, and Hessian matrix associated with a cumulative response transformation. Here $r_i = 1$, $q_i \geq 1$, \mathcal{Y}_i is the set of one-dimensional vectors \mathbf{y} such that $y(0)$ is a nonnegative integer no greater than q_i , $q_i = n_i - 1$, O_i is the set of all vectors of dimension q_i , and F is defined as in `berresp.cpp`. For β in O_i and \mathbf{y} in \mathcal{Y}_i ,

$$\ell_i(\beta; \mathbf{y}) = \begin{cases} \log(1 - F(\beta(y(0)))), & y(0) = 0, \\ \log(1 - F(\beta(y(0)))) + \sum_{i=0}^{y(0)-1} \log(F(\beta(i))), & 0 < y(0) < q_i, \\ \sum_{i=0}^{y(0)-1} \log(F(\beta(i))), & y(0) = q_i. \end{cases} \quad (7)$$

The function declaration is

*f2v cumresp(const int & order, const char & transform, const resp & y,
const vec & beta).*

Here *transform* is defined as in `berresp.cpp`. The function *cumresp.value* is $\ell_i(\beta; \mathbf{y})$ if *y.iresp* is \mathbf{y} and *beta* is β . The function `cumresp.cpp` requires `berresp.cpp`, `loglog.cpp`, `logit.cpp`, and `probit.cpp`. If $r_i = 1$, then use of `cumresp.cpp` is equivalent to use of `berresp.cpp`. In general, $\ell_i(\cdot; \mathbf{y})$ is concave. Strict concavity holds if $q_i - y(0)$ does not exceed 1.

gradresp.cpp

The function `gradresp.cpp` computes the function value, gradient, and Hessian matrix associated with a graded response transformation. Define F as in `berresp.cpp`. Then $r_i = 1$, $q_i \geq 1$, O_i is the set of all vectors of dimension q_i with strictly decreasing elements, \mathcal{Y}_i is the set of one-dimensional vectors \mathbf{y} with $y(0)$ a nonnegative integer no greater than q_i , and, for β in O_i and \mathbf{y} in \mathcal{Y}_i ,

$$\ell_i(\beta; \mathbf{y}) = \begin{cases} \log(1 - F(\beta(y(0)))), & y(0) = 0, \\ \log(F(\beta(y(0) - 1)) - F(\beta(y(0)))), & 0 < y(0) < q_i, \\ \log(F(\beta(y(0) - 1))), & y(0) = q_i. \end{cases} \quad (8)$$

The function declaration is

```
f2v gradresp(const int & order, const char & transform, const resp & y,
const vec & beta).
```

Here *transform* is defined as in `berresp.cpp`. The function *gradresp.value* is $\ell_i(\beta; \mathbf{y})$ if *y.iresp* is \mathbf{y} and *beta* is β . If $q_i = 1$, then `berresp.cpp`, `cumresp.cpp` and `gradresp.cpp` yield the same result. The function $\ell_i(\cdot; \mathbf{y})$ is concave. Strict concavity only holds if q_i is 1 or q_i is 2 and $y(0) = 1$.

gumbel.cpp

The function `gumbel.cpp` provides the computations required in `contresp.cpp` for $\ell_i(\cdot; \mathbf{y})$ for the Gumbel case of $F = G$. The function declaration is

```
f2v gumbel(const int & order, const resp & y, const vec & beta).
```

The function *gumbel.value* is then $\ell_i(\beta; \mathbf{y})$ if *y.dresp* is \mathbf{y} and *beta* is β .

logistic.cpp

The function `logistic.cpp` provides the computations required in `contresp.cpp` for $\ell_i(\cdot; \mathbf{y})$ for the logistic case $F = \Psi$ in `contresp.cpp`. The function declaration is

```
f2v logistic(const int & order, const resp & y, const vec & beta).
```

The function *logistic.value* is $\ell_i(\beta; \mathbf{y})$ if *y.dresp* is \mathbf{y} and *beta* is β .

logit.cpp

The function `logit.cpp` computes the function value, gradient, and Hessian matrix associated with the logit case in `berresp.cpp` with $F = \Psi$. The function declaration is

f2v logit(const int & order, const resp & y, const vec & beta).

The function *logit.value* is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if *y.iresp* is \mathbf{y} and *beta* is $\boldsymbol{\beta}$.

loglog.cpp

The function *loglog.cpp* computes the function value, gradient, and Hessian matrix associated with the log-log case of *berresp.cpp* with $F = G$. The function declaration is

f2v loglog(const int & order, const resp & y, const vec & beta).

The function *loglog.value* is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if *y.iresp* is \mathbf{y} and *beta* is $\boldsymbol{\beta}$.

logmean.cpp

The function *logmean.cpp* computes the function value, gradient, and Hessian matrix associated with a log-mean transformation for a Poisson random variable. In this case, $r_i = 1$, \mathcal{Y}_i is the set of one-dimensional vectors \mathbf{y} such that $y(0)$ is a nonnegative integer, $q_i = 1$, and O_i is the set of all one-dimensional vectors. For $\boldsymbol{\beta}$ in O_i and \mathbf{y} in \mathcal{Y}_i ,

$$\ell_i(\boldsymbol{\beta}; \mathbf{y}) = y(0)\beta(0) - \exp(\beta(0)) - \log([y(0)]!). \quad (9)$$

The function declaration is

f2v logmean(const int & order, const resp & y, const vec & beta).

The function *logmean.value* is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if *y.iresp* is \mathbf{y} and *beta* is $\boldsymbol{\beta}$.

maxberresp.cpp

The function *maxberresp.cpp* finds the log likelihood component, gradient, and Hessian matrix for the maximum of two unobserved Bernoulli random variables. The function F is defined as in *berresp.cpp*, \mathcal{Y}_i is the set of one-dimensional vectors \mathbf{y} with $y(0)$ equal 0 or 1, $r_i = 1$, $q_i = 2$, and O_i is the set of all two-dimensional vectors. For y in \mathcal{Y}_i and $\boldsymbol{\beta}$ in O_i ,

$$\ell_i(\boldsymbol{\beta}; \mathbf{y}) = \begin{cases} \log(F(\beta(0) + F(\beta(1) - F(\beta(0)F(\beta(1))), & y(0) = 1, \\ \log(1 - F(\beta(0))) + \log(1 - F(\beta(1))), & y(0) = 0. \end{cases} \quad (10)$$

It should be noted that

$$F(\beta(0) + F(\beta(1) - F(\beta(0)F(\beta(1))) = 1 - [1 - F(\beta(0))][1 - F(\beta(1))] \quad (11)$$

and

$$\log(1 - F(\beta(0))) + \log(1 - F(\beta(1))) = \log([1 - F(\beta(0))][1 - F(\beta(1))]). \quad (12)$$

The function $\ell_i(\cdot; \mathbf{y})$ is not necessarily concave if $y(0) = 1$.

The function declaration is

f2v maxberresp(const int & order, const char & transform, const resp & y, const vec & beta).

The variables *transform*, *y*, and *beta* are defined as in *berresp.cpp*. The functions *berresp.cpp*, *logit.cpp*, *loglog.cpp*, and *probit.cpp* are required.

multlogit.cpp

The function *multlogit.cpp* computes the function value, gradient, and Hessian matrix associated with a multinomial logit transformation. In this case, $r_i = 1$, \mathcal{Y}_i is the set of one-dimensional vectors \mathbf{y} such that $y(0)$ is a nonnegative integer no greater than $q_i \geq 1$, and O_i is the set of all q_i -dimensional vectors. For β in O_i and \mathbf{y} in \mathcal{Y}_i ,

$$\ell_i(\beta; \mathbf{y}) = \begin{cases} -\log \left(1 + \sum_{k=0}^{q_i-1} \exp(\beta(k)) \right), & y(0) = 0, \\ \beta(y(0) - 1) + \ell_i(\beta; \mathbf{0}_1), & y(0) > 0. \end{cases} \quad (13)$$

The function declaration is

f2v multlogit(const int & order, const resp & y, const vec & beta).

The function *multlogit.value* is $\ell_i(\beta; \mathbf{y})$ if *y.iresp* is \mathbf{y} and *beta* is β . If $q_i = 1$, use of *multlogit.cpp* gives the same result as use of *logit.cpp* and as use of *berresp.cpp*, *cumresp.cpp*, or *gradresp.cpp* with *transform* equal *L*.

normal.cpp

The function *normal.cpp* computes the function value, gradient, and Hessian matrix associated with the normal case in *contresp.cpp* if \mathcal{Y}_i is the space of one-dimensional vectors and $F = \Phi$. The function declaration is

f2v normal(const int & order, const vec & y, const vec & beta).

normalv.cpp

The function *normalv.cpp* computes the function value, gradient, and Hessian matrix associated with the log-likelihood component associated with a multivariate normal model with r_i positive, $q_i = r_i(r_i + 3)/2$, \mathcal{Y}_i the set of all r_i -dimensional real vectors, and O_i the set of q_i -dimensional vectors β with elements β_h , $0 \leq h < q_i$ such

that $\beta_h > 0$ if $h = r_i + j(j+3)/2$ and $0 \leq j < r_i$. For such β , let $\mathbf{a}(\beta)$ be the r_i -dimensional vector with elements $a_j(\beta) = \beta_j$ for $0 \leq j < r_i$, and let $\mathbf{B}(\beta)$ be the lower-triangular r_i by r_i matrix with row j and column k equal to β_h if $0 \leq k \leq j < r_i$ and $h = r_i + k + (j(j+1)/2)$. For an r_i -dimensional vector \mathbf{z} with elements z_j , $0 \leq j < r_i$, let $\phi(\mathbf{z}; r_i)$ be the product of the $\phi(z_j)$, $0 \leq j < r_i$.

For \mathbf{y} in \mathcal{Y}_i ,

$$\ell_i(\beta; \mathbf{y}) = \left[\sum_{j=0}^{r_i-1} \log(\beta(j)) \right] + \log(\phi(\mathbf{a}(\beta) + \mathbf{B}(\beta)\mathbf{y}; r_i)). \quad (14)$$

This case corresponds to a model that a random vector has a distribution $\mathbf{a}(\beta) + \mathbf{B}(\beta)\mathbf{Z}$, where \mathbf{Z} is an r_i -dimensional multivariate normal random vector with zero mean and with covariance matrix equal to the identity matrix. The function $\ell_i(\cdot; \mathbf{y})$ is always concave but is not strictly concave. The function declaration is

f2v normalv(const int & order, const resp & y, const vec & beta).

The function *normalv.value* is $\ell_i(\beta; \mathbf{y})$ if *y.dresp* is \mathbf{y} and *beta* is β . If r_i is 1, then *normalv.cpp* reduces to *normal.cpp*. The function *normalv.cpp* requires *pack.cpp* and *unpack.cpp*.

pack.cpp

The function *pack.cpp* is used in *normalv.cpp* to take an r_i -dimensional vector \mathbf{a} and an r_i by r_i lower-triangular matrix \mathbf{B} and convert the combination to the β in *normalv.cpp* such that $\mathbf{a}(\beta) = \mathbf{a}$ and $\mathbf{B}(\beta) = \mathbf{B}$. The vector \mathbf{a} and the matrix \mathbf{B} appear in the struct *vecmat* defined by

struct vecmat{vec v; mat m;};

The function declaration is

vec pack(const vecmat & u).

If *u.v* is \mathbf{a} and *u.m* is \mathbf{B} , then *pack* is the corresponding vector β .

probit.cpp

The function *probit.cpp* computes the function value, gradient, and Hessian matrix associated with a probit transformation in *berresp.cpp* with $F = \Phi$. The function declaration is

f2v probit(const int & order, const resp & y, const vec & beta).

The function *probit.value* is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if *y.iresp* is \mathbf{y} , *beta* is $\boldsymbol{\beta}$, and $F = \Phi$.

ranklogit.cpp

The function *ranklogit.cpp* computes the function value, gradient, and Hessian matrix associated with a model for discrete choice in which $q_i + 1$ objects are ranked for some positive integer q_i and the r_i most preferred objects are recorded for some positive integer $r_i \leq q_i$. The set \mathcal{Y}_i consists of the vectors \mathbf{y} of dimension r_i with distinct nonnegative integer elements that are no greater than q_i , and O_i is the set of all q_i -dimensional vectors. Let $\mathbf{0}_1$ be the one-dimensional vector with the single element 0. To describe the model, consider the standard Gumbel distribution function G defined in *contresp.cpp*. Consider $\boldsymbol{\beta}$ in O_i . Let U_j , $0 \leq j \leq q_i$, be independent random variables such that U_0 and $U_j - \beta_j$, $1 \leq j \leq q_i$, have the common distribution function G . Let \mathbf{Y} be a random vector with values in \mathcal{Y}_i such that \mathbf{Y} is the member \mathbf{y} of \mathcal{Y}_i with elements y_j , $0 \leq j < r_i$, if U_{y_j} is nonincreasing in j and $U_{y_j} \geq U_k$ if k is a nonnegative integer no greater than q_i that does not equal y_h for any nonnegative integer element $h < r_i$. For $\boldsymbol{\beta}$ in O_i and \mathbf{y} in \mathcal{Y}_i , let $\boldsymbol{\alpha}(\boldsymbol{\beta})$ be the vector of dimension $q_i + 1$ such that element j , $0 \leq j \leq q_i$, is $\alpha_j(\boldsymbol{\beta}) = 0$ if $j = 0$ and $\alpha_j(\boldsymbol{\beta}) = \beta_{j-1}$ if $j > 0$. For \mathbf{y} in \mathcal{Y}_i and $0 \leq j < r_i$, let $K_j(\mathbf{y})$ be the set of nonnegative integers no greater than q_i not equal to y_h for any nonnegative integer $h < j$. Thus $K_0(\mathbf{y})$ is the set of nonnegative integers no greater than q_i . Then the log-likelihood component is

$$\ell_i(\boldsymbol{\beta}; \mathbf{y}) = \sum_{j=0}^{r_i-1} \left[\alpha_{y_j}(\boldsymbol{\beta}) - \log \left(\sum_{h \in K_j(\mathbf{y})} \exp(\alpha_h(\boldsymbol{\beta})) \right) \right]. \quad (15)$$

The function declaration is

f2v ranklogit(const int & order, const resp & y, const vec & beta).

The function *ranklogit.value* is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if *y.iresp* is \mathbf{y} and *beta* is $\boldsymbol{\beta}$. If $r_i = 1$, use of *ranklogit.cpp* gives the same result as use of *multlogit.cpp*.

truncresp.cpp

The function *truncresp.cpp* computes the function value, gradient, and Hessian matrix associated with a right-censored continuous random variable with the distribution of $\beta(0) + \beta(1)Z$ for some real $\beta(0)$ and positive real $\beta(1)$, where, as in *contresp.cpp*, Z has distribution function F equal to G , Ψ , or Φ . In this case, $r_i = 2$, \mathcal{Y}_i consists of two-dimensional vectors \mathbf{y} such that $y(0)$ is a real number and $y(1)$ is 0 or 1, $q_i = 2$, and O_i is the set of all two-dimensional vectors $\boldsymbol{\beta}$ with element $\beta(1) > 0$. As in *berresp.cpp*, let f be the derivative of F . For $\boldsymbol{\beta}$ in O_i and \mathbf{y} in \mathcal{Y}_i , if $y(1) = 0$, then the observation is not censored and the corresponding log-likelihood component is

$$\ell_i(\boldsymbol{\beta}; \mathbf{y}) = \log(\beta(1)) + \log(f(\beta(0) + \beta(1)y(0))), \quad (16)$$

while in the case of $y(1) = 1$, the the observation is censored at $y(0)$ and the log-likelihood component is

$$\ell_i(\boldsymbol{\beta}; \mathbf{y}) = \log(1 - F(\beta(0) + \beta(1)y(0))). \quad (17)$$

The function declaration is

f2v truncresp(const int & order, const char & transform, const resp & y, const vec & beta).

Here *y.iresp* has the single element $y(1)$, and *y.dresp* has the single element $y(0)$.

In the function declaration, *beta* is $\boldsymbol{\beta}$, *transform* is defined as in *berresp.cpp*, and *truncresp.value* is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$. Functions required are *berresp.cpp*, *contresp.cpp*, and their respective required functions.

unpack.cpp

The function *unpack.cpp* is used in *normalv.cpp* to convert a vector $\boldsymbol{\beta}$ of dimension $q_i = r_i(r_i + 3)/2$ to the *vecmat* format described in *pack.cpp*. The function declaration is

vecmat unpack(const int & d, const vec & beta).

Here *d* is r_i , *beta* is $\boldsymbol{\beta}$, *unpack.v* is $\mathbf{a}(\boldsymbol{\beta})$, and *unpack.m* is $\mathbf{B}(\boldsymbol{\beta})$.

Computation of Log Likelihood Functions

genresp.cpp

The function *genresp.cpp* provides a general tool for computation of a a component of a log-likelihood function, its gradient, and its Hessian matrix. The function declaration is

f2v genresp(const int & order, const model & choice, const resp & y, const vec & beta).

Here *model* has the definition

struct model{char type; char transform}.

In *choice*, *choice.type* has value *C* for a cumulative case, *D* for a continuous case, *G* for a graded response, *L* for the multinomial logit case, *M* for the maximum of two independent Bernoulli variables, *P* for the log-mean Poisson case, *R* for the rank-logit case, *S* for the Bernoulli case, and *T* for the censored continuous case. For discrete

cases, *choice.transform* has possible values *G* for log-log cases, *L* for logit cases, and *N* for probit cases. For continuous cases, *G* is for the Gumbel distribution, *L* is for the logistic case, and *N* is for the normal case. For example, *choice.type* is *C* and *choice.transform* is *G* for the cumulative log-log case, while *choice.type* is *S* and *choice.type* is *N* in the probit case. The variable *choice.transform* is only relevant if *choice.type* is *C*, *D*, *G*, *M*, *S*, or *T*.

The function `genresp.cpp` uses `berresp.cpp`, `contresp.cpp`, `cumresp.cpp`, `gradresp.cpp`, `logmean.cpp`, `maxberresp.cpp`, `multlogit.cpp`, `ranklogit.cpp`, and `truncresp.cpp`, together with the functions they in turn require.

genrespplik.cpp

The function `genrespplik.cpp` computes the log-likelihood function and its gradient and Hessian matrix. The function declaration is

f2v genrespplik(const std::vector<dat> & data, const vec & beta).

The struct *dat* is defined by

struct dat{model choice; double weight; resp dep; vec offset; mat indep; xsel xselect;}.

Here *model* is defined as in `genresp.cpp`, *resp* is defined as in `truncresp.cpp`, and the struct *xsel* is defined by

struct xsel{bool all; ivec list}.

For $0 \leq i < n$, *data[i]* corresponds to observation *i*. Thus *data[i].choice* defines the model, *data[i].weight* is the observation weight, w_i , *data[i].resp* defines the dependent vector, \mathbf{Y}_i , *data[i].offset* is the offset vector \mathbf{o}_i , *data[i].indep* provides the matrix \mathbf{X}_i of independent variables, and *data[i].xselect* are defined so that $x[i]$ is \mathbf{X}_i if *data[i].xselect[i].all* is *true*. Otherwise, two cases exist for $0 \leq j < p$. If *xselect[i].list* has K_i elements and *j* is *xselect[i].list(k)* for a nonnegative integer $k < K_i$, then column *j* of \mathbf{X}_i is column *k* of *data[i].indep*. If *j* is not equal to any element of *x[i].list*, then column *j* of \mathbf{X}_i is the q_i -dimensional vector with all elements 0.

The function `genrespplik.cpp` uses `genresp.cpp` plus all C++ functions it in turn requires.

genrespplikl.cpp

The function `genrespplikl.cpp` computes the log-likelihood function, its gradient, and its approximate Hessian matrix from Equation 4 when all components involve only discrete variables. The function declaration is

f2v genrespplik(const std::vector<dat> & data, const vec & beta).

Definitions of arguments of the function are the same as in `genrespplik.cpp`. The function `genrespplik.cpp` uses `genresp.cpp` plus all C++ functions it in turn requires.

genrespmle.cpp

The function `genrespmle.cpp` applies the Newton-Raphson algorithm in `nrv.cpp` to the log-likelihood function, gradient, and Hessian matrix of `genrespplik.cpp`. The function declaration is

maxf2v genrespmle(const params & mparams, const std::vector<dat> & data, const vec & start).

Here the structs *maxf2v* and *mparams* are defined as in `maxlinq2.cpp` and `maxf2vvar.cpp`. The vector *start* is the starting vector. The global variables of `genrespplik.cpp` are required. The functions `nrv.cpp` and `genrespplik.cpp` are required, together with all C++ functions they in turn require.

genrespmle1.cpp

The function `genrespmle1.cpp` applies the conjugate gradient algorithm in `conjgrad.cpp` to the log-likelihood function and gradient of `genrespplik.cpp`. The function declaration is

maxf2v genrespmle1(const params & mparams, const std::vector<dat> & data, const vec & start).

Here the structs *maxf2v* and *params* are defined as in `maxlinq2.cpp`. The vector *start* is the starting vector. The global variables of `genrespplik.cpp` are required. The functions `conjgrad.cpp` and `genrespplik.cpp` are required, together with all functions they in turn require.

genrespmleg.cpp

The function `genrespmleg.cpp` applies the gradient ascent algorithm in `gradascent.cpp` to the log-likelihood function and gradient of `genrespplik.cpp`. The function declaration is

maxf1v genrespmle1(const params & mparams, const std::vector<dat> & data, const vec & start).

Here the structs *maxf2v* and *params* are defined as in `maxlinq2.cpp`. The vector *start* is the starting vector. The global variables used in `genrespplik.cpp` are

required. The functions `conjgrad.cpp` and `genresplik.cpp` are required, together with all functions they in turn require.

genresplml.cpp

The function `genresplml.cpp` applies the Newton-Raphson algorithm in `nrv.cpp` to the log-likelihood function, gradient, and approximate Hessian matrix of `genresplikl.cpp`. The function declaration is

```
maxf2v genresplml(const params & mparams, const std::vector<dat> & data, const
vec & start).
```

Here the structs *maxf2v* and *params* are defined as in `maxlinq2.cpp` and `maxf2vvar.cpp`. The vector *start* is the starting vector. The global variables of `genresplik.cpp` are required. The functions `nrv.cpp` and `genresplikl.cpp` are required, together with all functions they in turn require.

Integration Tools

The functions in this section aid in cases in which integration is required.

adapt.cpp

The function `adapt.cpp` provides a linear transformation of a set of real quadrature points and adjusts the corresponding weights for each point. The linear transformation has the form $L(x) = a + bx$ for x real, where a is a real number and b is a positive real number. The linear transformation is applied to each quadrature point and the weights are multiplied by b . The function declaration is

```
pw adapt(const double & loc, const double & scale, const pw & pws).
```

The struct *pw* has the definition

```
struct pw{vec points; vec weights;};
```

The variable *loc* is a and the variable *scale* is b . The original points are provided by *pws.points*, and the original positive weights are given by *pws.weights*. The transformed points are *adapt.points*, and the transformed weights are *adapt.weights*. If *scale* is not positive, then *adapt* is set equal to *pws*. The number of elements in *pws.points*, *pws.weights*, *adapt.points*, and *adapt.weights* is the same.

adaptv.cpp

The function `adaptv.cpp` provides a linear transformation of a set of D -dimensional quadrature points and adjusts the corresponding weights for each point,

where D is a positive integer. The linear transformation has the form $L(\mathbf{x}) = \mathbf{a} + \mathbf{B}\mathbf{x}$ for the D -dimensional vector \mathbf{x} , where \mathbf{a} is a D -dimensional vector and \mathbf{B} is a D by D lower triangular matrix. The linear transformation is applied to each quadrature point and the weights are multiplied by the determinant of \mathbf{B} . The function declaration is

pwv adaptv(const vec & loc, const mat & lt, const pwv & pws).

The struct *pwv* has the definition

struct pwv{mat points; vec weights;};

The variable *loc* is \mathbf{a} and the variable *lt* is \mathbf{B} . The original points are provided by *pws.points*, and the original positive weights are in *pws.weights*. The transformed points are in *adaptv.points*, and the transformed weights are in *adaptv.weights*. If any diagonal element of *lt* is not positive, then *adaptv* is set equal to *pws*. The number of elements in *pws.weights* and *adaptv.weights* is the same and is the same as both the number of columns in *adaptv.points* and the number of columns in *pws.points*. The number of rows in *adaptv.points* is equal to the number of rows in *pws.points*.

genfact.cpp

For a vector *sizes* of positive integers, the function *genfact.cpp* generates all vectors *i* of nonnegative integers with the same number of elements as *sizes* such that each element of *i* is less than the corresponding element of *sizes*. The function declaration is

imat genfact(const ivec & sizes).

The columns of *genfact* are the possible vectors *i*. For example, if the elements of *sizes* are 2 and 3, then Column 0 of *genfact* has elements 0 and 0, and Column 1 has elements 1 and 0. In all, *sizes* has 6 columns, and Column 5 has elements 1 and 2.

genprods.cpp

The function *genprods.cpp* generates a collection of quadrature points and quadrature weights for a multivariate integral from quadrature weights and quadrature points for a univariate integral. The function declaration is

pwv genprods(const imat & indices, const vector<pw> & pws).

The struct *pw* is defined as in *adapt.cpp*, and the struct *pwv* is defined as in *adaptv.cpp*. Consider the case of Q quadrature points for a multidimensional

integral on the space of D -dimensional vectors, where Q and D are positive integers. Then *genprods.points* has Q columns and *genprods.weights* has Q elements. The matrix *genprods.points* has D rows. The array *pws* has D members. For $0 \leq d < D$, *pws[d].points* and *pws[d].weights* have $m(d) > 1$ members, and the members of *pws[d].weights* are positive. The matrix *indices* specifies the quadrature vectors and quadrature weights to construct from *pws*. If *indices* has p columns, $0 \leq k < p$, and $0 \leq d < D$, then row d and column k of *indices* is nonnegative and less than $m(d)$ and the corresponding row and column of *genprods.points* is *pws[d].points(indices(d,k))*. Element k of *genprods.weights* is the product of *pws[d].weights(indices(d,k))* for $0 \leq d < D$.

hermcoeff.cpp

The function *hermcoeff.cpp* finds the coefficients of a Hermite polynomial of a given order. The function declaration is

vec hermcoeff(const int & n).

The integer variable n is the nonnegative order. The vector *hermcoeff* has $n+1$ elements. The polynomial is $H_n(x) = \sum_{i=0}^n \alpha_i x^{n-i}$ for real x , and element i of *hermcoeff* is α_i . For example, if n is 2, then the elements of *hermcoeff* are 1, 0, and -1 .

hermpoly.cpp

The function *hermpoly.cpp* evaluates the Hermite polynomials up to a given order at a specified real value. The function declaration is

vec hermpoly(const int & n, const double & x).

The order is the nonnegative integer variable n , and the real value is x . The vector *hermpoly* has $n+1$ elements. For $0 \leq k \leq n$, element k of *hermpoly* is the value of H_k at x .

hermpw.cpp

The function *hermpw.cpp* uses the algorithm of Golub and Welsch (1969) to find the quadrature points and quadrature weights for Gauss-Hermite quadrature. The function declaration is

pw hermpw(const int & n).

The struct *hermpw* has vector elements *hermpw.points* and *hermpw.weights*. The number of quadrature points is n . The ordered quadrature points are in

hermpw.points. The corresponding weights are in *hermpw.weights*.

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