

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> and the StatsLib library at <https://www.kthohr.com/statslib.html>. 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
- adaptpwr.cpp
- adaptv.cpp
- addsel.cpp
- berresp.cpp
- conjgrad.cpp
- contresp.cpp
- cumresp.cpp
- genfact.cpp

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- genprods.cpp
- genresp.cpp
- genresplik.cpp
- genrespmle.cpp
- gradascent.cpp
- gradresp.cpp
- gumbel.cpp
- hermcoeff.cpp
- hermpoly.cpp
- hermpw.cpp
- irtc.cpp
- irtm.cpp
- irtmle.cpp
- irtms.cpp
- ivecsel.cpp
- linsel.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
- normwt.cpp
- nrv.cpp
- pack.cpp
- probit.cpp
- qnormpw.cpp
- quadmax.cpp
- ranklogit.cpp
- rebound.cpp
- rescale.cpp
- trisym.cpp
- truncresp.cpp
- unpack.cpp
- vecsel.cpp
- wcrossprod.cpp

Distributions of Sums of Independent Multinomial Variables

The functions in this section implement a modified and generalized version of the Lord-Wingersky algorithm (Lord & Wingersky, 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-Wingersky 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 Hessian of $f.value$ at *vary0.locmax*, and *maxlinq2.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 *maxlinq2.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 $\alpha0 + \text{stepmax}$ and $\alpha0 + \eta(b.\text{upper} - \alpha0)$, while if *alpha1* is less than *alpha0*, then *modit* is truncated below so that it is at least the maximum of $\alpha0 - \text{stepmax}$ and $\alpha0 + \eta(b.\text{lower} - \alpha0)$.

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. A component has the form $\ell_c(\beta; \mathbf{Y}, A, F, q, r)$. Here the character *A* defines the type of model component involved, *F* is a distribution function with a positive and twice-continuously differentiable derivative F_1 such that $\log F_1$ has a negative second derivative. The integer $q > 0$ is the parameter dimension, and the integer $r > 0$ is the data dimension. The character *A* is in the set \mathcal{A} with elements *C* (cumulative), *D* (continuous), *G* (graded), *L* (multinomial logit), *M* (maximum of two independent Bernoulli variables), *N* (multivariate normal), *P* (log-mean Poisson case), *R* (rank logit), *S* (Bernoulli), and *T* (censored continuous). Distribution functions used in this section are in the set \mathcal{F} with three members, *G*, the standard Gumbel distribution function with value $G(y) = \exp(-\exp(-y))$ for *y* real, Ψ , the standard logistic distribution function with value $\Psi(y) = 1/[1 + \exp(-y)]$ for *y* real, and Φ , the standard normal distribution function with derivative $\Phi_1(y) = \exp(-y^2/2)/(2\pi)^{1/2}$ for real *y*. The value of *F* is only relevant in the cumulative, continuous, graded, Bernoulli, and censored continuous cases. The variables *M*, *F*, *q*, and *r* then define an open convex

subset $O(A, F, q, r)$ of q -dimensional vectors and a set $\mathcal{Y}(A, F, q, r)$ of r -dimensional vectors. The vector β is in $O(A, F, q, r)$, and \mathbf{Y} is in $\mathcal{Y}(A, F, q, r)$.

To treat both continuous and discrete log-likelihood components, the integral symbol \int is used in the following sense. Consider a real function g on a nonempty finite-dimensional set C . If C is convex and has a nonempty interior and g is integrable, then $\int(g)$ denotes the integral of g over C . If C is finite or countably infinite and g is summable, then $\int(g)$ is the sum of $g(\mathbf{c})$ over \mathbf{c} in C . More generally, let \mathcal{D} be a finite or countably infinite collection of nonempty disjoint sets D that are either convex sets with nonempty interior or finite or countably-infinite sets. Let C be the union of the sets in \mathcal{D} , and let g_D denotes the restriction of g to D in \mathcal{D} . Let $\int(g_D)$ be defined for D in \mathcal{D} , and let the $\int(g_D)$, D in \mathcal{D} , be summable. Then $\int(g)$ is the sum of $\int(g_D)$ over D in \mathcal{D} . Similar conventions apply if g is vector-valued or matrix-valued. The requirement is imposed here that, for β in $O(A, F, q, r)$, $\int(\exp(\ell_c(\beta; \cdot, A, F, q, r))) = 1$. Here $\exp(\ell_c(\beta; \cdot, A, F, q, r))$ is the function on $\mathcal{Y}(A, F, q, r)$ equal to $\exp(\ell_c(\beta; \mathbf{y}, A, F, q, r))$ if \mathbf{y} is in $\mathcal{Y}(A, F, q, r)$. The gradient function of $\ell_c(\cdot; \mathbf{y}, A, F, q, r)$ is $\nabla \ell_c(\cdot; \mathbf{y}, A, F, q, r)$ and the corresponding Hessian matrix is $\nabla^2 \ell_c(\cdot; \mathbf{y}, A, F, q, r)$.

For a positive integer n and an observation i , $0 \leq i < n$, positive integers q_i and r_i and character variables A_i in \mathcal{A} and F in \mathcal{F} are given. The component of the log likelihood for observation i involves the predicted random vector \mathbf{Y}_i in $\mathcal{Y}(A_i, F_i, q_i, r_i)$, 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 τ is in O , then let $\lambda_i(\tau) = \mathbf{o}_i + \mathbf{X}_i \tau$ be in $O(A_i, F_i, q_i, r_i)$ for $0 \leq i < n$, and let the log-likelihood function under study have the form

$$\ell(\tau) = \sum_{i=0}^{n-1} w_i \ell_c(\lambda_i(\tau); \mathbf{Y}_i, A_i, F_i, q_i, r_i). \quad (1)$$

It follows that the gradient of ℓ at τ in O is

$$\nabla \ell(\tau) = \sum_{i=0}^{n-1} w_i \mathbf{X}_i^T \nabla \ell_c(\lambda_i(\tau); \mathbf{Y}_i, A_i, F_i, q_i, r_i), \quad (2)$$

and the Hessian matrix of ℓ at τ is

$$\nabla^2 \ell(\tau) = \sum_{i=0}^{n-1} w_i \mathbf{X}_i^T \nabla^2 \ell_c(\lambda_i(\tau); \mathbf{Y}_i, A_i, F_i, q_i, r_i) \mathbf{X}_i. \quad (3)$$

The Hessian matrix $\nabla^2 \ell(\tau)$ has the approximation

$$\tilde{\nabla}^2 \ell(\tau) = - \sum_{i=0}^{n-1} w_i \mathbf{X}_i^T \nabla \ell_c(\lambda_i(\tau); \mathbf{Y}_i, A_i, F_i, q_i, r_i) [\nabla \ell_i(\lambda_i(\tau); \mathbf{Y}_i, A_i, F_i, q_i)]^T \mathbf{X}_i \quad (4)$$

(Haberman, 2013; Louis, 1982) .

The functions $\ell_c(\cdot; \mathbf{y}, A, F, q, r)$ used are considered in this section. Some 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 (Haberman, 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. If *order* exceeds 2, the approximation of the Hessian by Equation 4 is employed. Repeated use is made of the struct *resp* with *vec* component *dresp* and *ivec* component *iresp*.

berresp.cpp

The function *berresp.cpp* is used to handle standard models for Bernoulli random variables. Here $q = r = 1$, A is S , $\mathcal{Y}(A, F, q, r)$ is the set of one-dimensional vectors *y* with $y(0)$ equal 0 or 1, and $O(A, F, q, r)$ is the set of all one-dimensional vectors, and F is in \mathcal{F} . For *y* in $\mathcal{Y}(A, F, q, r)$ and $\boldsymbol{\beta}$ in $O(A, F, q, r)$,

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

The function declaration is

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

If *transform* is G , then $F = G$, If *transform* is L , then $F = \Psi$. If *transform* is N , then $F = \Phi$. The function *berresp.value* is $\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r)$ if *y.iresp* is *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 $r = 1$, $q = 2$, A is D , $\mathcal{Y}(A, F, q, r)$ is the set of all one-dimensional vectors, $O(A, F, q, r)$ is the set of all two-dimensional vectors β with element $\beta(1) > 0$, and F is in \mathcal{F} . For \mathbf{y} in $\mathcal{Y}(A, F, q, r)$ and β in $O(A, F, q, r)$,

$$\ell_c(\beta; \mathbf{y}, A, F, q, r) = \log(\beta(1)) + \log(F_1(\beta(0) + \beta(1)y(0))). \quad (6)$$

These cases correspond to a model that a random variable has a distribution $\beta(0) + \beta(1)Z$, where Z has distribution function F . Here $\ell_c(\cdot; \mathbf{y}, A, F, q, r)$ 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 $\ell_c(\beta; \mathbf{y}, A, F, q, r)$ 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 $r = 1$, $q \geq 1$, A is C , F is in \mathcal{F} , $\mathcal{Y}(A, F, q, r)$ is the set of one-dimensional vectors \mathbf{y} such that $y(0)$ is a nonnegative integer no greater than q , $O(A, F, q, r)$ is the set of all vectors of dimension q , and F is defined as in `berresp.cpp`. For β in $O(A, F, q, r)$ and \mathbf{y} in $\mathcal{Y}(A, F, q, r)$,

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

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 $\ell_c(\beta; \mathbf{y}, A, F, q, r)$ 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 $r = 1$, then use of `cumresp.cpp` is equivalent to use of `berresp.cpp`. In general, $\ell_c(\cdot; \mathbf{y}, A, F, q, r)$ is concave. Strict concavity holds if $q - y(0)$ does not exceed 1.

gradresp.cpp

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

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

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 $\ell_c(\beta; \mathbf{y}, A, F, q, r)$ if *y.iresp* is \mathbf{y} and *beta* is β . If $q = 1$, then `berresp.cpp`, `cumresp.cpp` and `gradresp.cpp` yield the same result. The function $\ell_c(\cdot; \mathbf{y}, A, F, q, r)$ is concave. Strict concavity only holds if q is 1 or q is 2 and $y(0) = 1$.

gumbel.cpp

The function `gumbel.cpp` provides the computations required in `contresp.cpp` for $\ell_c(\cdot; \mathbf{y}, A, F, q, r)$ for the simple Gumbel case of $F = G$, A with value D , $q = 2$, $r = 1$, $\mathcal{Y}(A, F, q, r)$ the set of real numbers, and $O(A, F, q, r)$ the set of two-dimensional vectors β with $\beta(1) > 0$. The function declaration is

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

The function *gumbel.value* is then $\ell_c(\beta; \mathbf{y}, A, F, q, r)$ if *y.dresp* is \mathbf{y} and *beta* is β .

logistic.cpp

The function `logistic.cpp` provides the computations required in `contresp.cpp` for $\ell_c(\cdot; \mathbf{y}, A, F, q, r)$ for the logistic case $F = \Psi$ in `contresp.cpp` with A with value D , $q = 2$, $r = 1$, $\mathcal{Y}(A, F, q, r)$ the set of real numbers, and $O(A, F, q, r)$ the set of two-dimensional vectors β with $\beta(1) > 0$. The function declaration is

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

The function *logistic.value* is $\ell_c(\beta; \mathbf{y}, A, F, q, r)$ 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 A equal to S , $F = \Psi$, and $q = r = 1$. The function declaration is

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

The function `logit.value` is $\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r)$ 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 A equal to S , $F = G$, and $q = r = 1$. The function declaration is

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

The function `loglog.value` is $\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r)$ 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, $q = r = 1$, A is P , the value of F in \mathcal{F} is irrelevant, $\mathcal{Y}(A, F, q, r)$ is the set of one-dimensional vectors \mathbf{y} such that $y(0)$ is a nonnegative integer, and $O(A, F, Q, R)$ is the set of all one-dimensional vectors. For $\boldsymbol{\beta}$ in $O(A, F, q, r)$ and \mathbf{y} in $\mathcal{Y}(A, F, q, r)$,

$$\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r) = y(0)\beta(0) - \exp(\beta(0)) - \log([y(0)]!). \quad (9)$$

The function declaration is

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

The function `logmean.value` is $\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r)$ 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. Here $q = 2$, $r = 1$, A is M , F is in \mathcal{F} , $O(A, F, q, r)$ is the set of two-dimensional vectors, and $\mathcal{Y}(A, F, q, r)$ is the set of one-dimensional vectors \mathbf{y} with $y(0)$ equal 0 or 1. For \mathbf{y} in $\mathcal{Y}(A, F, q, r)$ and $\boldsymbol{\beta}$ in $O(A, F, q, r)$,

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

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 $\ell_c(\cdot; \mathbf{y}, A, F, q, r)$ 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 variable *transform* is defined as in *berresp.cpp*. The function *maxberresp.value* is $\ell_c(\beta; \mathbf{y}, A, F, q, r)$ if *y.iresp* is \mathbf{y} and *beta* is β . 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, $r = 1$, $q \geq 1$, F is irrelevant, A is L , $\mathcal{Y}(A, F, q, r)$ is the set of one-dimensional vectors \mathbf{y} such that $y(0)$ is a nonnegative integer no greater than q , and $O(A, F, q, r)$ is the set of all q -dimensional vectors. For β in $O(A, F, q, r)$ and \mathbf{y} in $\mathcal{Y}(A, F, q, r)$,

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

The function declaration is

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

The function *multlogit.value* is $\ell_c(\beta; \mathbf{y}, A, F, q, r)$ if *y.iresp* is \mathbf{y} and *beta* is β . If $q = 1$, 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*. Thus A is D , $F = \Phi$, $q = 2$, $r = 1$, $\mathcal{Y}(A, F, q, r)$ is the space of one-dimensional vectors, and $O(A, F, q, r)$ is the set of two-dimensional vectors β with $\beta(1) > 0$. The function declaration is

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

The function *normal.value* is $\ell_c(\beta; \mathbf{y}, A, F, q, r)$ if *y.dresp* is \mathbf{y} and *beta* is β .

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 positive, $q = r(r + 3)/2$, A equal to N , F is irrelevant, $\mathcal{Y}(A, F, q, r)$ the set of all r -dimensional real vectors, and $O(A, F, q, r)$ the set of q -dimensional vectors $\boldsymbol{\beta}$ with elements β_h , $0 \leq h < q$ such that $\beta_h > 0$ if $h = r + j(j + 3)/2$ and $0 \leq j < r$. For such $\boldsymbol{\beta}$, let $\mathbf{a}(\boldsymbol{\beta})$ be the r -dimensional vector with elements $a_j(\boldsymbol{\beta}) = \beta_j$ for $0 \leq j < r$, and let $\mathbf{B}(\boldsymbol{\beta})$ be the lower-triangular r by r matrix with row j and column k equal to β_h if $0 \leq k \leq j < r$ and $h = r + k + (j(j + 1))/2$. For an r -dimensional vector \mathbf{z} with elements z_j , $0 \leq j < r$, let $\phi(\mathbf{z}; r)$ be the product of the $\Phi_1(z_j)$, $0 \leq j < r$.

For \mathbf{y} in $\mathcal{Y}(A, F, q, r)$,

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

This case corresponds to a model that a random vector has a distribution $\mathbf{a}(\boldsymbol{\beta}) + \mathbf{B}(\boldsymbol{\beta})\mathbf{Z}$, where \mathbf{Z} is an r -dimensional multivariate normal random vector with zero mean and with covariance matrix equal to the identity matrix. The function $\ell_c(\cdot; \mathbf{y}, A, F, q, r)$ 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 $\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r)$ if $y.dresp$ is \mathbf{y} and $beta$ is $\boldsymbol{\beta}$. If r 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 -dimensional vector \mathbf{a} and an r by r lower-triangular matrix \mathbf{B} and convert the combination to the $\boldsymbol{\beta}$ in `normalv.cpp` such that $\mathbf{a}(\boldsymbol{\beta}) = \mathbf{a}$ and $\mathbf{B}(\boldsymbol{\beta}) = \mathbf{B}$. 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 $\boldsymbol{\beta}$.

probit.cpp

The function `probit.cpp` computes the function value, gradient, and Hessian matrix associated with a probit transformation in `berresp.cpp` with A equal to S , $F = \Psi$, and $q = r = 1$. The function declaration is

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

The function `probit.value` is $\ell_c(\beta; \mathbf{y}, A, F, q, r)$ if `y.iresp` is \mathbf{y} and `beta` is β . $F = \Phi$. The function declaration is

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

The function `probit.value` is $\ell_c(\beta; \mathbf{y}, A, F, q, r)$ if `y.iresp` is \mathbf{y} and `beta` is β .

ranklogit.cpp

The function `ranklogit.cpp` computes the function value, gradient, and Hessian matrix associated with a model for discrete choice in which $q + 1$ objects are ranked for some positive integer q and the r most-preferred objects are recorded for some positive integer $r \leq q$. Here A has value R , F is irrelevant, the set $\mathcal{Y}(A, F, q, r)$ consists of the vectors \mathbf{y} of dimension r with distinct nonnegative integer elements that are no greater than q , and $O(A, F, q, r)$ is the set of all q -dimensional vectors. To describe the model, consider the standard Gumbel distribution function G . Consider β in $O(A, F, q, r)$. Let $U(j)$, $0 \leq j \leq q$, be independent random variables such that $U(0)$ and $U(j) - \beta(j)$, $1 \leq j \leq q$, have the common distribution function G . Let \mathbf{Y} be a random vector with values in $\mathcal{Y}(A, F, q, r)$ such that \mathbf{Y} is the member \mathbf{y} of $\mathcal{Y}(A, F, q, r)$ with elements $y(j)$, $0 \leq j < r$, 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 that does not equal $y(h)$ for any nonnegative integer element $h < r$. For β in $O(A, F, q, r)$ and \mathbf{y} in $\mathcal{Y}(A, F, q, r)$, let $\alpha(\beta)$ be the vector of dimension $q + 1$ such that element j , $0 \leq j \leq q$, is $\alpha(j; \beta) = 0$ if $j = 0$ and $\alpha(j; \beta) = \beta(j - 1)$ if $j > 0$. For \mathbf{y} in $\mathcal{Y}(A, F, q, r)$ and $0 \leq j < r$, let $K(j; \mathbf{y})$ be the set of nonnegative integers no greater than q 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 . Then the log-likelihood component is

$$\ell_c(\beta; \mathbf{y}, A, F, q, r) = \sum_{j=0}^{r-1} \left[\alpha(y_j; \beta) - \log \left(\sum_{h \in K(j; \mathbf{y})} \exp(\alpha(h; \beta)) \right) \right]. \quad (15)$$

The function declaration is

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

The function *ranklogit.value* is $\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r)$ if *y.iresp* is \mathbf{y} and *beta* is $\boldsymbol{\beta}$. If $r = 1$, 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 in \mathcal{F} . In this case, $q = r = 2$, A is T . $\mathcal{Y}(A, F, q, r)$ consists of two-dimensional vectors \mathbf{y} such that $y(0)$ is a real number and $y(1)$ is 0 or 1, and $O(A, F, q, r)$ is the set of all two-dimensional vectors $\boldsymbol{\beta}$ with element $\beta(1) > 0$. For $\boldsymbol{\beta}$ in $O(A, F, q, r)$ and \mathbf{y} in $\mathcal{Y}(A, F, q, r)$, if $y(1) = 0$, then the observation is not censored and the corresponding log-likelihood component is

$$\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r) = \log(\beta(1)) + \log(F_1(\beta(0) + \beta(1)y(0))), \quad (16)$$

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

$$\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r) = \log(1 - F(\beta(0) + \beta(1)y(0))). \quad (17)$$

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 $y(1)$, *y.dresp* has the single element $y(0)$, *beta* is $\boldsymbol{\beta}$, *transform* is defined as in *berresp.cpp*, and *truncresp.value* is $\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r)$. 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 $q = r(r + 3)/2$ to the *vecmat* format described in *pack.cpp*. The function declaration is

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

Here d is r , *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 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 int & order, 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; uvec 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* is 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 *addsel.cpp*, *linsel.cpp*, *vecsel.cpp*, *genresp.cpp*, and all C++ functions *genresp.cpp* requires.

genrespmle.cpp

The function *genrespmle.cpp* applies maximizes the log-likelihood function, gradient, and Hessian matrix of *genrespplik.cpp*. The function declaration is

maxf2v genrespmle(const int & order, const params & mparams,
const char & algorithm, 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 variable *algorithm* determines the algorithm, with *N* for Newton-Raphson, *L* for Newton-Raphson with the Hessian approximation of Equation 4, *C* for conjugate gradient, and *G* for gradient ascent. The functions *nrv.cpp*, *conjgrad.cpp*, *gradascent.cpp*, and *genrespplik.cpp* are required, together with all C++ functions that these four functions need.

Tools for Computation of Log Likelihood Functions

addsel.cpp

The function *addsel.cpp* is used to add *f2v* structures. The function declaration is

void addsel(const int & order, const xsel & xselect,
const f2v & x, f2v & y, const double & a).

Here *order* and *xselect* are defined as in Log-likelihood Components. The struct *y* is modified by use of the struct *x* and the multiplier *a*. In all cases, *ax.value* is added to *y.value*. If *xselect.all* is *true*, then *x* and *y* have compatible dimensions, *ax.grad* is added to *y.grad* if *order* is at least 1, and *ax.hess* is added to *y.hess* if *order* is at least 2. If *xselect.all* is *false*, then *ax.grad* is added to *y.grad.elem(xselect.list)*

if *order* is at least 1 and *ax.hess* is added to *y.hess.submat(xselect.list,xselect.list)* if *order* is at least 2.

ivecsel.cpp

The function *ivecsel.cpp* is employed to create a new integer vector from an old vector by extracting of elements of the old integer vector. The function declaration is

ivec ivecsel(const xsel & xselect, const ivec & y).

Here the struct *xsel* is defined as in *genresplik.cpp*. If *xselect.all* is *true*, then *ivecsel* is *y*. Otherwise, *ivecsel* is a vector with the number of elements in *xselect.list*, and element *i* of *ivecsel* is element *xselect.list(i)* of *y*.

linsel.cpp

The function *linsel.cpp* is used to apply a linear transformation to an *f2v* struct. The function declaration is

f2v linsel(const int & order, const f2v & x, const mat & a).

Here *order* is defined as in Log-likelihood Components. It is always the case that *linsel.value* is *x.value*. If *order* is positive, then *linsel.grad* is the product of the transpose of *a* and the gradient *x.grad*. If *order* exceeds 1, then *linsel.hess* is the product of the transpose of *a*, the Hessian *x.hess*, and the matrix *a*.

vecsel.cpp

The function *vecsel.cpp* is employed to create a new vector from an old vector by extracting of elements of the old vector. The function declaration is

vec vecsel(const xsel & xselect, const vec & y).

Here the struct *xsel* is defined as in *genresplik.cpp*. If *xselect.all* is *true*, then *vecsel* is *y*. Otherwise, *vecsel* is a vector with the number of elements in *xselect.list*, and element *i* of *vecsel* is element *xselect.list(i)* of *y*.

Latent Structures

In this section, functions useful for analysis of latent structures are considered. The log-likelihood function in this section is defined based on the definitions in Log-likelihood Components; however, use of latent variables is involved. In typical cases, data involve multiple responses for each individual observation. For a positive integer *m*, *m* observations are present. For observation *h*, $0 \leq h < m$, the observation

has weight $w_{h*} > 0$, and n_h responses are observed. In addition, a latent vector appears in the model. Associated with the latent vector are positive integers q_* and r_* , A_* in \mathcal{A} , and F_* in \mathcal{F} . The latent vector $\boldsymbol{\theta}_h$ is in $\mathcal{Y}(A_*, F_*, q_*, r_*)$. The latent variable is predicted by the q_* by p predicting matrix \mathbf{X}_{h*} in the nonempty set \mathcal{X}_* and the fixed q_* -dimensional vector \mathbf{o}_* . It is assumed that $\boldsymbol{\lambda}_*(\boldsymbol{\tau}) = \mathbf{o}_* + \mathbf{X}_*\boldsymbol{\tau}$ is in $O(A_*, F_*, q_*, r_*)$ as long as \mathbf{X}_* is in \mathcal{X}_* and $\boldsymbol{\tau}$ is in O . For response i , $0 \leq i < n_h$, positive integers q_{hi} and r_{hi} are given. The variable A_{hi} is in \mathcal{A} and F_{hi} is in \mathcal{F} . The component of the log likelihood for response i involves the predicted random vector \mathbf{Y}_{hi} in $\mathcal{Y}(A_{hi}, F_{hi}, q_{hi}, r_{hi})$, the latent vector $\boldsymbol{\theta}_h$, the q_{hi} by p predicting matrix \mathbf{X}_{hi} in a nonempty set \mathcal{X}_{hi} , the q_{hi} -dimensional vector \mathbf{o}_{hi} , the q_{hi} by q_* matrix \mathbf{D}_{hi} , the positive real weight w_{hi} , the q_{hi} by p matrix \mathbf{D}_{hik} , $0 \leq k < q_*$, and the function $\ell_c(\cdot; \mathbf{y}, A_{hi}, F_{hi}, q_{hi}, r_{hi})$ on $O(A_{hi}, F_{hi}, q_{hi}, r_{hi})$ defined for \mathbf{y} in $\mathcal{Y}(A_{hi}, F_{hi}, q_{hi}, r_{hi})$. For any $\boldsymbol{\tau}$ in O , \mathbf{X} in \mathcal{X}_{hi} , and $\boldsymbol{\theta}$ in $\mathcal{Y}(A_*, F_*, q_*, r_*)$,

$$\boldsymbol{\lambda}_{hi}(\boldsymbol{\tau}|\boldsymbol{\theta}) = \mathbf{o}_{hi} + \mathbf{X}_{hi}\boldsymbol{\tau} + \mathbf{D}_{hi}\boldsymbol{\theta} + \sum_{k=0}^{p-1} \theta_k \mathbf{D}_{hik}\boldsymbol{\tau} \quad (18)$$

is in $O(A_{hi}, F_{hi}, q_{hi}, r_{hi})$.

For $\boldsymbol{\tau}$ in O , the log-likelihood has the form

$$\ell(\boldsymbol{\tau}) = \sum_{h=0}^{m-1} w_{h*} \ell_h(\boldsymbol{\tau}), \quad (19)$$

where $\ell_h(\boldsymbol{\tau})$ is the component of the log-likelihood for observation h . Thus the gradient function of ℓ at $\boldsymbol{\tau}$ satisfies

$$\nabla \ell(\boldsymbol{\tau}) = \sum_{h=0}^{m-1} w_{h*} \nabla \ell_h(\boldsymbol{\tau}), \quad (20)$$

where $\nabla \ell_h(\boldsymbol{\tau})$ is the gradient function of ℓ_h at $\boldsymbol{\tau}$. The Hessian function of ℓ at $\boldsymbol{\tau}$ satisfies

$$\nabla^2 \ell(\boldsymbol{\tau}) = \sum_{h=0}^{m-1} w_{h*} \nabla^2 \ell_h(\boldsymbol{\tau}), \quad (21)$$

where $\nabla^2 \ell_h(\boldsymbol{\tau})$ is the Hessian function of ℓ_h at $\boldsymbol{\tau}$. The approximation

$$\tilde{\nabla}^2 \ell(\boldsymbol{\tau}) = - \sum_{h=0}^{m-1} w_{h*} \nabla \ell_h(\boldsymbol{\tau}) [\nabla \ell_h(\boldsymbol{\tau})]^T, \quad (22)$$

may also be considered.

In turn, $\ell_h(\boldsymbol{\tau})$ involves the product

$$\ell_h(\boldsymbol{\tau}|\boldsymbol{\theta}) = \ell_c(\boldsymbol{\lambda}_*(\boldsymbol{\tau}); \boldsymbol{\theta}, A_*, F_*, q_*, r_*) \sum_{i=0}^{n_h-1} w_{hi} \ell_c(\boldsymbol{\lambda}_{hi}(\boldsymbol{\tau}|\boldsymbol{\theta}); \mathbf{Y}_{hi}, A_{hi}, F_{hi}, q_{hi}, r_{hi}) \quad (23)$$

for $\boldsymbol{\theta}$ in $\mathcal{Y}(A_*, F_*, q_*, r_*)$. The component

$$\ell_h(\boldsymbol{\tau}) = \log \int (\exp(\ell_h(\boldsymbol{\tau}|\cdot))), \quad (24)$$

where $\exp(\ell_h(\boldsymbol{\tau}|\cdot))$ is the function with value $\exp(\ell_h(\boldsymbol{\tau}|\boldsymbol{\theta}))$ for $\boldsymbol{\theta}$ in $\mathcal{Y}(A_*, F_*, q_*, r_*)$. In practice, $\ell_h(\boldsymbol{\tau})$ is evaluated by

$$\tilde{\ell}_h(\boldsymbol{\tau}) = \log \left[\sum_{k=1}^{Q_h} u_{hk} \exp(\ell_h(\boldsymbol{\tau}|\boldsymbol{\theta}_{hk})) \right], \quad (25)$$

for some positive weights u_{hk} and elements $\boldsymbol{\theta}_{hk}$ in $\mathcal{Y}(A_*, F_*, q_*, r_*)$.

irtc.cpp

The function `irtc.cpp` finds the conditional log likelihood component $\ell_h(\boldsymbol{\tau}|\boldsymbol{\theta})$ and associated gradient and Hessian matrix for a latent structure model. The function declaration is

```
f2v irtc (const int & order, const std::vector<dat> & data,
const std::vector<thetamap> & thetamaps, const resp & theta,
const vec & beta).
```

In this declaration, *order* is less than 1 if only the function value is returned, at least 1 if the gradient is required, 2 if the Hessian is produced, and more than 2 if the approximate Hessian matrix is found. The use of *dat* is as in `genrespplik.cpp`, the latent vector value is provided by *theta*, and *beta* is defined as usual as the parameter vector.

The struct *thetamap* is defined by

```
struct thetamap{bool dep; xsel drespcols; xsel irespcols; mat offsets; cube indeps;}.
```

Here *dep* is true if the response is derived from *theta*, *drespcols* gives the elements of *theta.dresp* used in the response, and *irespcols* gives the elements of *theta.iresp* in the response. For item *h* and observation *i*, the matrix *thetamaps[i].offsets* contains each column *k* of \mathbf{D}_{hi} such that *k* is specified in *thetamaps[i].drespcols*, and other columns of \mathbf{D}_{hi} are zero vectors. In the cube *thetamaps[i].indeps*, each \mathbf{D}_{hik} is given for *k* specified in *thetamaps[i].drespcols*, and column *j* of \mathbf{D}_{hik} is provided if *j* is in the elements specified in *theta[i].drespcols* for item *h* and observation *i*. Other columns of \mathbf{D}_{hik} are vectors of zeros. Element *i* of *data* corresponds to \mathbf{Y}_{hi} .

The functions `ivcsel.cpp` and `genrespplik.cpp`, together with their associated functions, are required by `irtc.cpp`.

irtm.cpp

The function `irtm.cpp` finds the log likelihood component $\ell_h(\boldsymbol{\tau})$ and associated gradient and Hessian matrix for a latent structure model. The function uses numerical integration if $\mathcal{Y}(A_*, F_*, q_*, r_*)$ is not finite or countably infinite. The function declaration is

```
f2v irtm (const int & order, const std::vector<dat> & data,
const std::vector<thetamap> & thetamaps, adq & scale,
const std::vector<pwr> & thetas, const vec & beta).
```

In this declaration, only the function value is returned if *order* is 0, the function value and gradient are returned if *order* is 1, and the function value, gradient, and Hessian matrix are returned if *order* is 2. The function value, gradient, and Louis approximation for the Hessian matrix are returned if *order* is 3. The use of *dat* is as in `genresplik.cpp`, and *beta* is defined as usual as the parameter vector. The struct *thetamap* is defined as in `irtc.cpp`.

The struct *pwr* is defined by

```
struct pwr{double weight; resp theta;},
```

and the struct *adq* is

```
struct adq{bool adapt; xsel xselect; vecmat tran;}.
```

The struct *scale* is important in adaptive quadrature (Naylor & Smith, 1982) and is used in `irtmle.cpp` to improve efficiency and accuracy of computations involving continuous latent vectors. Let *thetas* have Q_h elements *thetas*[*k*], and let *thetas*[*k*].*theta* correspond to the q_* -dimensional vector $\boldsymbol{\theta}_{hk0}$. In Equation 25, u_{hk} is *thetas*[*k*].*weight*, and $\boldsymbol{\theta}_{hk} = \mathbf{v}_h + \mathbf{M}_h \boldsymbol{\theta}_{hk0}$, where \mathbf{v}_h is a q_* -dimensional vector and \mathbf{M}_h is a lower-triangular q_* by q_* matrix determined by *scale*. If *scale.adapt* is *false*, then all elements of \mathbf{v}_h are 0 and \mathbf{M}_h is the identity matrix. To consider the case of *scale.adapt* equal to *true*, let Υ_h be the subset of the nonnegative integer less than q_* such that *thetas*[*k*].*theta.dresp* corresponds to the elements of $\boldsymbol{\theta}_{hk0}$ in Υ_h . If *scale.xselect.all*, let Υ_{h1} equal Υ_h . If *scale.xselect.all* is *false*, let Υ_{h1} be the elements of Υ_h that correspond to elements of *scale.xselect.list*. Then 0 is the value of any element of \mathbf{v}_h that does not correspond to an element of Υ_{h1} and *scale.tran.v* provides the values of the elements of \mathbf{v}_h that do correspond to elements of Υ_{h1} . In the case of \mathbf{M}_h , *scale.tran.m* provides the values of all elements of \mathbf{M}_h for rows and columns that both correspond to elements of Υ_h , all other off-diagonal elements of \mathbf{M}_h are 0 and all other diagonal elements of \mathbf{M}_h are 1. Thus *scale.tran.v* is \mathbf{v}_h and *scale.tran.m* is \mathbf{M}_h if *scale.adapt* and *scale.xselect.all* are *true* and *thetas*[*k*].*theta.iresp* has no elements. After computation of *irtm*, *scale* is updated if *scale.adapt* is *true* and Υ_{h1}

is nonempty. The updating fits a quadratic function to the values of $\ell_h(\beta|\theta_{hk})$. The predicting variables are the elements of θ_{hk} in Υ_{h1} .

The function `irtm.cpp` uses the functions `irtc.cpp`, `adaptpwr.cpp`, `quadmax.cpp`, and `rescale.cpp`, together with their required functions.

irtmle.cpp

The function `irtmle.cpp` finds the maximum likelihood estimate for a latent structure model. The function uses numerical integration if $\mathcal{Y}(A_*, F_*, q_*, r_*)$ is not finite or countably infinite. The function declaration is

```
maxf2v irtmle (const int & order, const params & mparams,
const char & algorithm, const vec & obsweight,
const std::vector<obs> & obsdata,
const std::vector<obsthetamap> & obsthetamaps,
const std::vector<obsttheta> & obsthetas,
std::vector<adq> & obscales,
const std::vector<xsel> betasel, const vec & start).
```

In this declaration, *maxf2v* and *mparams* are defined as in `maxlinq2.cpp` and `maxf2vvar.cpp`, while *order* is defined as in `irtc.cpp`. The variable *algorithm* is defined as in `genrespmle.cpp`. The vector *obsweight* provides the weights w_{h*} for $0 \leq h \leq m - 1$. The struct *obs* is defined as

```
struct obs{std::vector<dat> data;},
```

where *dat* is defined as in `genresplik.cpp` and *obsdata.data[h]* is the data specification for observation *h*, the struct *obsthetamap* is defined as

```
struct obsthetamap{std::vector<thetamap> thetamaps;},
```

where the struct *thetamap* is defined as in `irtc.cpp` and *obsthetamap.thetamaps[h]* provides the mapping of the latent vector for observation *h*, and the struct

```
struct obsthetas{std::vector<pwr> thetas;},
```

where the struct *pwr* is defined as in `irtm.cpp` and *thetas[h].thetas* provides the quadrature weights and points for observation *h*. The scale adjustment for observation *h* is defined by *obsscale[h]*, where the struct *adq* is defined as in `irtm.cpp`. The vector *beta* is defined as usual as the parameter vector. The value of *betasel[h].all* is *true* if all elements of *beta* are used for the log likelihood for observation *h*, and the elements of *beta* corresponding to *betasel[h].list* are used for this log likelihood if *betasel[h].all* is *false*.

The functions `irtms.cpp` and its required functions and the functions that are prerequisites for `genrespmle.cpp` are required by `irtmle.cpp`.

irtms.cpp

The function `irtms.cpp` finds the log likelihood component $\ell(\boldsymbol{\tau})$ and associated gradient and Hessian matrix for a latent structure model. The function uses numerical integration if $\mathcal{Y}(A_*, F_*, q_*, r_*)$ is not finite or countably infinite. The function declaration is

```
f2v irtms (const int & order, const vec & obsweight,
const std::vector<obs> & obsdata,
const std::vector<obsthetamap> & obsthetamaps,
const std::vector<obsttheta> & obsthetas,
const std::vector<xsel> & betasel, const vec & beta).
```

In this declaration, *order* is less than 1 if only the function value is returned, at least 1 if the gradient is required, 2 if the Hessian is produced, and more than 2 if the approximate Hessian matrix is found. The use of *obs*, *obsthetamaps*, *obsthetas*, *obsscale*, and *betasel* are as in `irtmle.cpp`, and *beta* is defined as usual as the parameter vector. The function `irtm.cpp` and its required functions are required by `irtms.cpp`.

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.

adaptpwr.cpp

The function `adaptpwr.cpp` provides a linear transformation of a quadrature point. 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

pwr adaptpwr(const pwr & oldtheta, const adq & scale).

The structs *pwr* and *adq* are defined as in `irtm.cpp`. If *scale.adapt* is *false*, then *adaptpwr* is *oldtheta*. It is always the case that *adaptpwr.weight* is *oldtheta.weight* and *adaptpwr.theta.iresp* is *adaptpwr.theta.iresp*. If *scale.adapt* is *true* and *scale.xselect.all* is *true*, then *adaptpwr.theta.dresp* is *scale.tran.v* plus the product of *scale.tran.m* and *oldtheta.theta.dresp*.

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 degree. 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 degree at a specified real value. The function declaration is

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

The degree 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*. The weights are relative to the standard normal density.

normwt.cpp

The function *normwt.cpp* divides quadrature weights by the standard normal density to facilitate use with latent-structure models with latent variables that are normally distributed. The function declaration is

pw normwt(const pw & pwi).

The struct *normwt* has vector elements *normwt.points* and *normwt.weights*. The input *pwi* has elements *pwi.points* and *pwi.weights*. The ordered quadrature points are in *normwt.points*. The corresponding weights are in *normwt.weights*. The result *normwt.points* is the same as *pwi.points*, but the weights *normwt.weights* are obtained

from *pwi.weights* by dividing by the standard normal density at the corresponding points *pwi.points*.

qnormpw.cpp

The function *qnormpw.cpp* provides normal-scores quadrature of a given order. The function declaration is

```
pw qnormpw(const int & n).
```

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

quadmax.cpp

The function *quadmax.cpp* finds the maximum and its location and associated Hessian matrix for a quadratic function that best approximates a function in terms of least squares. The function declaration is

```
maxf2v quadmax(const std::vector<maxf2v> & functdat).
```

The function under study has value *functdat[i].max* at *functdat[i].locmax* for integers *i* from 0 to 1 less than the number of elements of *functdat*. If the fitted quadratic function is not strictly concave, then *quadmax.max* is NaN.

rescale.cpp

The function *rescale.cpp* is employed to update quadrature weights and points used in adaptive quadrature. The function declaration is

```
adq rescale(const adq & scale, const std::vector<maxf2v> & functdat).
```

The struct *adq* is defined as in *irtm.cpp*, and *functdat* is defined as in *quadmax.cpp*. The result *rescale.adjust* is the same as *scale.adjust*, *rescale.tran.v* have the same size as *scale.tran.v* and *rescale.tran.m* has the same dimensions as *scale.tran.m*.

trisym.cpp

The function *trisym.cpp* is used in *quadmax.cpp* to convert a vector β of dimension $q = (d + 1)(d + 2)/2$ to the *fvecmat* format defined by

```
struct fvecmat{double value;vec v;mat m;};
```

The function declaration is

fvecmat trisym(const int & d, const vec & beta).

Here d is d , β is β , $trisym.value$ is the quadratic function value $\beta(0)$ at the zero vector, $trisym.v$, the gradient of the quadratic function at the zero vector, has elements $\beta(j)$ for $1 \leq j \leq d$, and $trisym.m$, twice the Hessian of the quadratic function, is the d by d matrix with row i and column j for nonnegative integers less than d equal to $\beta(d+1+u+v(v+1)/2)/2$ if $u = \min(i, j) < v = \max(i, j)$ and equal to $\beta(d+(v+1)(v+2)/2)$ if $i = j$.

wcrossprod.cpp

The function `wcrossprod.cpp` computes a weighted cross-product matrix. The function declaration is

mat wcrossproduct(const mat & x, const vec & w).

In terms of Armadillo functions, `wcrossprod` is equal to the matrix product $x.t*\text{diagmat}(w)*x$.

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