# 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++14. They rely on the Armadillo library (Sanderson & Curtin, 2016, 2018) at <a href="http://arma.sourceforge.net">http://arma.sourceforge.net</a>, the StatsLib library at <a href="https://www.kthohr.com/statslib.html">https://www.kthohr.com/statslib.html</a>, and the Boost library at <a href="https://www.boost.org">https://www.boost.org</a>. Unless otherwise noted, for the library members considered, it is assumed that users have verified that function arguments are valid. Namespaces assumed where relevant are std, arma, and boost::math. The following functions are found in the library, with files in the source code with the suffix .cpp.

- addsel
- berresp
- conjgrad
- contresp
- cumresp
- CX
- $\bullet$  eaps

- fitquad
- genfact
- $\bullet$  genprods
- genresp
- genresplik
- genrespmle
- gradascent
- gradresp
- gumbel
- hermcoeff
- hermpoly
- $\bullet$  hermpw
- intsel
- invcdf
- irtm
- irtmle
- irtms
- irtmsave
- irtmsaves
- ivecsel
- linsel
- loggamma
- logistic
- logit
- logitbeta

- $\bullet$  logitdirichlet
- loglog
- $\bullet$  logmean
- lw
- lwm
- maxberresp
- maxf2vvar
- maxlinq2
- maxquad
- maxselect
- $\bullet$  multlogit
- modit
- normal
- normalv
- normwt
- nrv
- pack
- posterior
- posteriors
- probit
- qnormpw
- $\bullet$  ranklogit
- rebound
- savmaxf2v
- sintsel

- sivecsel
- starttwoparamirt
- svecsel
- truncresp
- twoparamirt
- unpack
- vecsel
- wmc

# 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

The function lw finds the probability mass function of the sum S of mutually independent Bernoulli random variables  $X_j$ ,  $0 \le j < n$ . 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  $0 \le j < n$ , 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 reduces to the conventional algorithm. The probability mass function is provided by lw, a vector with n+1 elements. For  $0 \le k \le n$ , element k of lw is the probability that S = k.

#### lwm

The function lwm finds the probability mass function of the sum S of n mutually independent random variables  $X_j$ ,  $0 \le j <$  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 field < vec > & p).

Here p has n members. For  $0 \le j < n$ , member j of p is the vector p[j] with  $I_j$  nonnegative elements. The sum of these elements is 1, and element k,  $0 \le k < I_j$ ,

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,  $0 \le k < K$ , 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 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  $\eta$ ,  $\gamma_1$ ,  $\gamma_2$ , and  $\kappa$  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

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

 $\max f2v \max linq2(const int \& order, const params \& mparams, const vec \& v, const \max f2v \& vary0, const function < f2v(const int \&, const vec \&) > f).$ 

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{bool print; int maxit; int maxits; double eta; double gamma1; double gamma2; double kappa; double tol;}.

Here mparams.print is used for output of the iteration number and function value at the end of the iteration, mparams.maxit is the number of primary iterations, mparams.maxits is the maximum number of uses of maxquad permitted for each primary iteration, mparams.eta is  $\eta$ , mparams.gamma1 is  $\gamma_1$ , mparams.gamma2 is  $\gamma_2$ , and mparams.kappa is  $\kappa$ . 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, maxquad, modit, and rebound are all used.

# maxquad

The function *maxquad* 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

The function modit 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  $\infty$ . 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  $\eta$ , 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

The function rebound 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  $\infty$ . The function declaration is

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

The struct bounds is defined as in modit. 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

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

 $\max f2v \max f2vvar(const int \& order, const vec \& y, const f2v \& fy);$ 

The structs f2v and maxf2v are defined as in maxlinq2. The returned value maxf2vvar.locmax is y, while maxf2vvar.max is fy.value, maxf2var.grad is fy.grad, and maxf2var.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.

#### $\mathbf{nrv}$

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

maxf2v nrv(const int & order, const params & mparams, const vec & start, const function $\langle f2v(\text{const int }\&,\,\text{vec }\&)\rangle f)$ .

The structs f2v, maxf2v, and params are defined as in maxling2. The starting vector start must be in O.

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

#### savmaxf2v

The function savmaxf2v is used to save basic results of maximization. The declaration is

void savmaxf2v(const int & order , const maxf2v & vlm, const string & out, const bool & fflag, const bool & pflag).

The value of order is 1, 2, or 3. The struct maxf2v is defined as in maxlinq2. If fflag is true, then the output file is defined by out. The output file must be a binary file used by Armadillo for storage. If pflag is true, then standard output is employed. Both fflag and pflag may have the same value. If order is 1, output is vlm.max, vlm.locmax, and vlm.grad. If order exceeds2, then output also includes vlm.hess, the inverse of -1 times vlm.hess, and the square roots of the diagonal elements of this inverse.

# Functions Related to Gradient Methods

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

# conjgrad

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

## gradascent

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

 $\max f2v \text{ gradascent}(\text{const order } \& \text{, const params } \& \text{ mparams,}$  $\operatorname{const vec } \& \operatorname{start, const function} < f2v(\operatorname{const int } \& \text{, const vec } \& \text{)} > f).$ 

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

#### maxselect

The function maxselect uses either the conjugate-gradient, gradient-ascent, or modified Newton-Raphson algorithm for maximization of f.value. The function declaration for maxselect is

 $\max f2v$  maxselect(const order & , const params & mparams, const char & algorithm const vec & start, const function< f2v(const int & , const vec & )> f).

The functions conjgrad, gradascent, maxf2vvar, maxlinq2, maxquad, modit, nrv, and rebound are used. Definitions are as in conjgrad, except that algorithm is C for conjugate gradient, G for gradient ascent, and N for Newton-Raphson.

# 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 differential 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 A with elements  $B(\log t beta)$ , C (cumulative), D (continuous), E (logit Dirichlet), G (graded), H (log gamma), E (multinomial logit), E (log-mean Poisson case), E (rank logit), E (Bernoulli), and E (censored continuous). Distribution functions used in this section are in the set E with three members, E0, the standard Gumbel distribution function with value

 $G(y) = 1 - \exp(-\exp(-y))$  for y real,  $\Psi$ , the standard logistic distribution function with value  $\Psi(y) = 1/[1 + \exp(-y)]$  for y real, and  $\Phi$ , 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  $\boldsymbol{\beta}$  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 f 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 f(g) denotes the integral of g over G. If G is finite or countably infinite and G is summable, then f(g) is the sum of f(g) over f(g)

For a positive integer n and an observation i,  $0 \le i < n$ , positive integers  $q_i$  and  $r_i$  and character variables  $A_i$  in  $\mathcal{A}$  and  $F_i$  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  $\boldsymbol{\tau}$  is in O, then let  $\boldsymbol{\lambda}_i(\boldsymbol{\tau}) = \mathbf{o}_i + \mathbf{X}_i \boldsymbol{\tau}$  be in  $O(A_i, F_i, q_i, r_i)$  for  $0 \le i < n$ , and let the log-likelihood function under study have the form

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

It follows that the gradient of  $\ell$  at  $\tau$  in O is

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

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

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

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

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

(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 maxling2. 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  $\ell$ is strictly concave whenever  $X_i$ ,  $0 \le i < n$ , spans a space of dimension p. Conditions for a unique  $\hat{\tau}$  in O such that  $\ell(\hat{\tau})$  equals the supremum of  $\ell$  over O are relatively complex (Haberman, 1974, 1977, 1980). It is worth noting that in cases in which  $\hat{\tau}$  in O satisfies the conditions that  $\nabla \ell(\hat{\tau})$  is the p-dimensional vector  $\mathbf{0}_p$  with all elements 0 and  $\nabla^2 \ell(\hat{\tau})$  is negative definite, then O can be restricted to ensure that  $\ell$  is strictly concave on O and  $\hat{\tau}$  is the only member of O such that  $\ell(\hat{\tau})$  equals the supremum of  $\ell$ on O and, for  $\tau$  in O,  $\nabla \ell(\tau)$  is only the vector with all elements 0 if  $\beta$  equals  $\hat{\beta}$ . 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. In typical cases, resp. dresp or resp. iresp has no elements; however, exceptions do exist.

#### berresp

The function *berresp* 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  $\mathbf{y}$  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  $\mathbf{y}$  in  $\mathcal{Y}(A, F, q, r)$  and  $\boldsymbol{\beta}$  in O(A, F, q, r),

$$\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r) = \begin{cases} \log(F(\beta(0)), & y(0) = 1, \\ \log(1 - F(\beta(0))), & y(0) = 0. \end{cases}$$
 (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  $\ell_c(\beta; \mathbf{y}, A, F, q, r)$  if y iresp is  $\mathbf{y}$  and beta is  $\beta$ . The function berresp requires loglog, logit, and probit.

### contresp

The function contresp 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  $\boldsymbol{\beta}$  with element  $\beta(1) > 0$ , and F is in  $\mathcal{F}$ . For  $\mathbf{y}$  in  $\mathcal{Y}(A, F, q, r)$  and  $\boldsymbol{\beta}$  in O(A, F, q, r),

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

These cases correspond to a model that a random variable Y has a distribution function  $F(\beta(0) + \beta(1)y)$ , where F is the distribution function of a random variable Z. 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. The function contresp.value is  $\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r)$  if y.dresp is  $\mathbf{y}$  and beta is  $\boldsymbol{\beta}$ . The function contresp requires gumbel, logistic, and normal.

# cumresp

The function cumresp computes the function value, gradient, and Hessian matrix associated with a cumulative response transformation. Here r = 1,  $q \ge 1$ , 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. For  $\boldsymbol{\beta}$  in O(A, F, q, r) and  $\mathbf{y}$  in  $\mathcal{Y}(A, F, q, r)$ ,

$$\ell_{i}(\boldsymbol{\beta}; \mathbf{y}) = \begin{cases} \log(1 - F(\beta(y(0))), & y(0) = 0, \\ \log(1 - F(\beta(y(0)))) + \sum_{i=0}^{y(0)-1} \log(F(\beta(i))), & 0 < y(0) < q, \\ \sum_{i=0}^{y(0)-1} \log(F(\beta(i))), & y(0) = q. \end{cases}$$
(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. The function cumresp.value is  $\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r)$  if y.iresp is  $\mathbf{y}$  and beta is  $\boldsymbol{\beta}$ . The function cumresp requires berresp, loglog, logit, and probit. If r = 1, then use of cumresp is equivalent to use of berresp. 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

The function gradresp computes the function value, gradient, and Hessian matrix associated with a graded response transformation. Then r = 1,  $q \ge 1$ , 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  $\boldsymbol{\beta}$  in O(A, F, q, r) and  $\mathbf{y}$  in  $\mathcal{Y}(A, F, q, r)$ ,

$$\ell_{i}(\boldsymbol{\beta}; \mathbf{y}) = \begin{cases} \log(1 - F(\beta(y(0))), & y(0) = 0, \\ \log(F(\beta(y(0) - 1)) - F(\beta(y(0)))), & 0 < y(0) < q, \\ \log(F(\beta(y(0) - 1))), & y(0) = q. \end{cases}$$
(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. The function gradresp.value is  $\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r)$  if y.iresp is  $\mathbf{y}$  and beta is  $\boldsymbol{\beta}$ . If q = 1, then berresp, cumresp and gradresp 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

The function gumbel provides the computations required in contresp 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  $\boldsymbol{\beta}$  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  $\boldsymbol{\beta}$ .

# loggamma

The function loggamma provides the computations required for  $\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r)$  for the log-gamma distribution with A with value  $H, q = 2, r = 1, \mathcal{Y}(A, F, q, r)$  the set of real numbers, and O(A, F, q, r) the set of two-dimensional vectors  $\boldsymbol{\beta}$  with positive elements. The function declaration is

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

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

# logistic

The function logistic provides the computations required in contresp for  $\ell_c(\cdot; \mathbf{y}, A, F, q, r)$  for the logistic case  $F = \Psi$  in contresp 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  $\boldsymbol{\beta}$  with  $\beta(1) > 0$ . The function declaration is

f2v logistic(const int & order, const resp & v, 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  $\boldsymbol{\beta}$ .

# logit

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

 $f2v \log it(const int \& order, const resp \& y, const vec \& beta).$ 

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

# logitbeta

The function logitbeta computes the function value, gradient, and Hessian matrix associated with the logit of a beta distribution with a two-dimensional parameter vector  $\boldsymbol{\beta}$  with positive elements. Here  $\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r)$  has A with value  $H, q = 2, r = 1, \mathcal{Y}(A, F, q, r)$  the set of real numbers, and O(A, F, q, r) the set of two-dimensional vectors  $\boldsymbol{\beta}$  with positive elements. The function declaration is

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

The function logitbeta value is  $\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r)$  if q = 2, r = 1, y iresp is  $\mathbf{y}$ , A is B, and beta is  $\boldsymbol{\beta}$ .

# logitdirichlet

The function logitdirichlet computes the function value, gradient, and Hessian matrix associated with the logits of a Dirichlet distribution with a q = r + 1dimensional parameter vector  $\boldsymbol{\beta}$  with positive elements. Here  $\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r)$  has A with value E,  $\mathcal{Y}(A, F, q, r)$  the set of r-dimensional vectors, and O(A, F, q, r) the set of q-dimensional vectors  $\boldsymbol{\beta}$  with positive elements. The function declaration is

f2v logitdirichlet(const int & order, const resp & v, const vec & beta).

The function logitdirichlet.value is  $\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r)$  if y.iresp is  $\mathbf{y}$ , beta is  $\boldsymbol{\beta}$ , and A is E. The q-dimensional random variable  $\mathbf{u}$  has a Dirichlet distribution with parameter vector  $\boldsymbol{\beta}$  if 1 is the sum of the elements of  $\mathbf{u}$  and  $y_i = \log(u_i/u_q)$  for integers i from 1 to r. If r = 1, then the logit Dirichlet case reduces to the case of a logit beta.

## loglog

The function loglog computes the function value, gradient, and Hessian matrix associated with the log-log case of berresp 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  $\ell_c(\beta; \mathbf{y}, A, F, q, r)$  if y iresp is  $\mathbf{y}$  and beta is  $\beta$ .

## logmean

The function logmean 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  $\mathcal{Y}(A, F, q, r)$ ,

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

The function declaration is

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

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

### maxberresp

The function maxberresp 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 y in  $\mathcal{Y}(A, F, q, r)$  and  $\boldsymbol{\beta}$  in O(A, F, q, r),

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

It should be noted that

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

and

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

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. The function maxberesp.value is  $\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r)$  if y.iresp is  $\mathbf{y}$  and beta is  $\boldsymbol{\beta}$ . The functions berresp, logit, loglog, and probit are required.

## multlogit

The function multlogit computes the function value, gradient, and Hessian matrix associated with a multinomial logit transformation. In this case, r = 1,  $q \ge 1$ , 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  $\boldsymbol{\beta}$  in O(A, F, q, r) and  $\mathbf{y}$  in  $\mathcal{Y}(A, F, q, r)$ ,

$$\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r) = \begin{cases} -\log\left(1 + \sum_{k=0}^{q-1} \exp(\beta(k)), & y(0) = 0, \\ \beta(y(0) - 1) + \ell_c(\boldsymbol{\beta}; \mathbf{0}_1, A, F, q, r), & y(0) > 0. \end{cases}$$
(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  $\beta$ . If q = 1, use of multlogit gives the same result as use of logit and as use of berresp, cumresp, or gradresp with transform equal L.

#### normal

The function normal computes the function value, gradient, and Hessian matrix associated with the normal case in contresp. 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  $\boldsymbol{\beta}$  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  $\boldsymbol{\beta}$ .

#### normalv

The function normaly 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 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  $\beta_h$ ,  $0 \le h < q$  such that  $\beta_h > 0$  if h = r + j(j+3)/2 and  $0 \le j < r$ . For such  $\boldsymbol{\beta}$ , let  $\mathbf{a}(\boldsymbol{\beta})$  be the r-dimensional vector with elements  $a_j(\boldsymbol{\beta}) = \beta_j$  for  $0 \le j < r$ , and let  $\mathbf{B}(\boldsymbol{\beta})$  be the symmetric positive-definite r by r matrix with row j and column k equal to  $\beta_h$  if  $0 \le k \le j < r$  and h = r + k + (j(j+1)/2. For an r-dimensional vector  $\mathbf{z}$  with elements  $z_j$ ,  $0 \le j < q$ , let  $\phi(\mathbf{z}; r)$  be the product of the  $\Phi_1(z_j)$ ,  $0 \le j < r$ .

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

$$\ell_c(\boldsymbol{\beta}; \mathbf{y}) = \left[ \sum_{j=0}^{r-1} \log(\beta(r+j(j+3)/2)) \right] + \log(\phi(\mathbf{a}(\boldsymbol{\beta}) + \mathbf{B}(\boldsymbol{\beta})\mathbf{y}; r)).$$
 (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 reduces to normal. The function normalv requires pack and unpack.

### pack

For the struct vecmat defined by

struct vecmax{vec v; mat m;};

the function pack converts a d-dimensional vector pack.v and a d by d symmetric matrix pack.m to a vector with dimension d(d+3)/2 with d initial elements the vector pack.v and element h = d + k + (j(j+1)/2) equal to row j and column k of pack.m for nonnegative k no greater than j < d. The function declaration is

vec pack(const vecmat & u).

Diagonal elements of the matrix equal the corresponding elements of u, and off-diagonal elements are twice the corresponding elements of the vector.

# probit

The function probit computes the function value, gradient, and Hessian matrix associated with a probit transformation in berresp 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  $\boldsymbol{\beta}$ .

## ranklogit

The function ranklogit 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 < 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  $\beta$  in O(A, F, q, r). Let U(j),  $0 \le j \le q$ , be independent random variables such that U(0) and  $U(j) - \beta(j)$ ,  $1 \le j \le q$ , have the common distribution function G. Let Y be a random vector with values in  $\mathcal{Y}(A, F, q, r)$  such that Y is the member y of  $\mathcal{Y}(A, F, q, r)$  with elements y(j), 0 < 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  $\beta$  in O(A, F, q, r) and 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 y in  $\mathcal{Y}(A,F,q,r)$  and  $0 \le i \le r$ , let  $K(i, \mathbf{y})$  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

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

The function declaration is

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

The function ranklogit value is  $\ell_c(\beta; \mathbf{y}, A, F, q, r)$  if y iresp is  $\mathbf{y}$  and beta is  $\beta$ . If r = 1, use of ranklogit gives the same result as use of multlogit.

#### truncresp

The function truncresp computes the function value, gradient, and Hessian matrix associated with a right-censored continuous random variable with the distri-

bution of  $\beta(0) + \beta(1)Z$  for some real  $\beta(0)$  and positive real  $\beta(1)$ , where, as in contresp, 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

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

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

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

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  $\beta$ , transform is defined as in berresp, and truncresp.value is  $\ell_c(\beta; \mathbf{y}, A, F, q, r)$ . Functions required are berresp, contresp, and their respective required functions.

# unpack

The function unpack converts a vector of dimension d(d+3)/2 to the vecmat format described in pack. The function declaration is

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

The vector unpack.v contains the first d elements of beta and row j and column k of unpack.m is element d+k+j(j+3)/2 of beta for nonnegative integers k < j < d.

# Computation of Log Likelihood Functions

#### genresp

The function genresp 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}.

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

# genresplik

The function genresplik computes the log-likelihood function and its gradient and Hessian matrix. The function declaration is

```
f2v genresplik(const int & order, const field<pattern> & patterns, const xsel & patternnumber, const field<resp> & data, const resp & theta, const field<xsel> & selectbeta, const xsel & selectbetano, const field<xsel> & selectbetac, const xsel & selectbetacno, const field<xsel> & selectthetai, const xsel & selectthetaino, const field<xsel> & selectthetad, const xsel & selectthetadno, const field<xsel> & selectthetac, const xsel & selectthetacno, const field<xsel> & selectthetac, const xsel & selectthetacno, const vec & w, const xsel & obssel, const vec & beta).
```

The definitions of arguments and structs rely the the definition of *model* in genresp and the definition of *resp* in truncresp. The variable *theta* is a supplemental variable often used with item-response models.

In the case of xsel, the struct is defined as

struct xsel{bool all; uvec list}.

The struct is applied to a finite and nonempty collection collection of k objects numbered from 0 to k-1. If all is true, all members of the collection are considered. Otherwise, only members in *list* are used. Thus in the case of *obssel*, the observation

numbers i to be used are specified. The function intsel is used for selections based on xsel. If xsel.bool is true, then an integer i is mapped by intsel to i, whereis if bool is false, then i is mapped to element i of xsel.list.

If patternnumber maps the integer i to j(1), then patterns(j(1)) defines the function  $\lambda_i$  and the model used for the response  $\mathbf{Y}_i$ . In addition, the weight  $w_i$  assigned to  $\mathbf{Y}_i$  is element i of w, and selectbeta(j(2)) specifies the elements of beta used to define  $\lambda_i$  if selectbetano maps i to j(2).

The struct pattern is defined as

struct pattern{model choice; vec o; mat x; cube c;}.

Thus patterns(j(1)).choice defines the model for  $\mathbf{Y}_i$ . The vector patterns(j(1)).o is then  $\mathbf{o}_i$ , while patterns(j(1)).x and patterns(j(1)).c are used to find  $\mathbf{X}_i$ . Definition of  $\mathbf{X}_i$  is somewhat complex. Let selectbetacno map i to j(2), and let selectthetacno map i to j(3). If k is not selected by selectbeta(j(2)), then column k of  $\mathbf{X}_i$  is the zero vector. Otherwise, let k(2) be element m(2) selected by selectbeta(j(2)). If m(2) is not selected by selectbetac(j(2)), then column k(2) of  $\mathbf{X}_i$  is column m(2) of m(2) of m(3) of m(3) of the sums of the products of m(3) of m(3) of the sums of the products of m(3) is integer m(4) of m(3) of m(3).

In the case of  $\mathbf{Y}_i$ , let thetaino(i) select j(5) and thetadno(i) select j(6). If thetai(j(5)) does not select anything, data(i).iresp is the int component of  $\mathbf{Y}_i$ . Otherwise, the int component of  $\mathbf{Y}_i$  consists of the elements of theta.iresp selected in thetai(j(5)). If thetad(j(6)) does not select anything, data(i).dresp is the double component of  $\mathbf{Y}_i$ . Otherwise, the double component of  $\mathbf{Y}_i$  consists of the elements of theta.dresp selected in thetad(j(6)). The function genresplik uses addsel, cx, intsel, linsel, sintsel, sivesel, svecsel, vecsel, genresp, and all C++ functions genresp requires.

### genrespmle

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

```
maxf2v genrespmle(const int & order, const params & mparams, const char & algorithm, const field<pattern> & patterns, const xsel & patternnumber, const field<resp> & data, const resp & theta, const field<xsel> & selectbeta, const xsel & selectbetano, const field<xsel> & selectbetac, const xsel & selectbetacno, const field<xsel> & selectthetai, const xsel & selectthetaino, const field<xsel> & selectthetad, const xsel & selectthetadno, const field<xsel> & selectthetac, const xsel & selectthetacno,
```

const vec & w, const xsel & obssel, const vec & start).

Definitions are as in maxlinq2, maxf2vvar, maxselect, and genresplik. The functions maxselect and genresplik are required, together with all C++ functions that these two functions need.

## Tools for Computation of Log Likelihood Functions

### addsel

The function addsel 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.

#### $\mathbf{c}\mathbf{x}$

The function cx is used to multiply a cube by a vector to yield a matrix. The function declaration is

mat cx(const cube & c, const vec & x).

The result is that cx(i,j) is the sum over k of c(i,j,k)x(k).

### intsel

The function *ivecsel* selects a nonnegative integer from a struct *xsel* defined as in genresplik. The function declaration is

int intsel(const xsel & xselect, const int & i).

The value of *intsel* is the *i*th integer from xselect.

#### ivecsel

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

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

Here the struct xsel is defined as in genresplik. 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

The function linsel 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.

#### sintsel

The function sintsel counts the number of integers selected from the first n nonnegative integers. The function declaration is

int sintsel(const xsel & xselect, const int & n).

The integers from 0 to n are selected according to xselect, where xsel is defined as in genresplik.

### sivecsel

The function *sivecsel* counts the number of integer vector elements selected. The function declaration is

int sivecsel(const xsel & xselect, const ivec & y).

The integers in y are selected according to xselect, where xsel is defined as in genresplik.

#### svecsel

The function svecsel counts the number of integer vector elements selected. The function declaration is

int svecsel(const xsel & xselect, const vec & y).

The integers in y are selected according to xselect, where xsel is defined as in genresplik.

#### vecsel

The function vecsel 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. 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 Loglikelihood 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  $\lambda_*(\tau) = \mathbf{o}_* + \mathbf{X}_*\tau$  is in  $O(A_*, F_*, q_*, r_*)$  as long as  $X_*$  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  $\mathcal{Y}(A_*, F_*, q_*, r_*)$ ,

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

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

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

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

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

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

where  $\nabla \ell_h(\tau)$  is the gradient function of  $\ell_h$  at  $\tau$ . The Hessian function of  $\ell$  at  $\tau$  satisfies

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

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

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

may also be considered.

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

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

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

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

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

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

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

For computations for latent-structure models, the following functions are employed.

### invcdf

The function *invcdf* finds the inverse of the cumulative distribution function and its derivative at *prob* for either the standard Gumbel (cdf equals G), logistic (cdf equals L), or normal (cdf equals N). The function declaration is

f1 invcdf(const char & cdf, const double & prob).

The struct f1 is

struct f1{double value; double der}.

At prob, the value of the inverse is invcdf.value, and the derivative is invcdf.der.

#### irtm

The function *irtm* finds the log likelihood component  $\ell_h(\beta)$  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 field<pattern> & patterns,
const xsel & patternnumber, const field<resp> & data, const field <pwr> & thetas,
const adq & scale, dovecmat & obsscale,
const field<xsel> & selectbeta, const xsel & selectbetano,
const field<xsel> & selectbetac, const xsel & selectbetacno,
const field<xsel> & selectthetai, const xsel & selectthetaino,
const field<xsel> & selectthetad, const xsel & selectthetadno,
const field<xsel> & selectthetac, const xsel & selectthetacno,
const vec & w, const xsel & obssel, const vec & beta).
```

In this declaration, almost all arguments are defined as in genresplik. The exceptions are thetas, scale, and obsscale. These arguments rely on the structs pwr, adq, and dovecmat with the following definitions:

```
struct pwr{double weight; double kernel; resp theta;},
struct adq{bool adapt; xsel linselect;xselv quadselect;},
and
struct dovecmat{double s; vec v; mat m;}.
```

The structs thetas and obsscale define the  $u_{hk}$  and  $\boldsymbol{\theta}_{hk}$  of Equation 25, while scale is used in irtmle for computation of maximum-likelihood estimates of  $\boldsymbol{\beta}$ . For element k of thetas,  $u_{hk}$  is obtained by multiplying thetas(h).weight by obsscale.s and dividing by thetas(h).kernel, the integer elements of  $\boldsymbol{\theta}_{hk}$  are the same as in thetas(h).theta.iresp, and the remaining elements of  $\boldsymbol{\theta}_{hk}$  are found by adding obsscale.v to the product of the matrix obsscale.m and the vector thetas(h).theta.dresp. Use of scale is discussed in the description of irtmle. In addition to functions needed by genresplik, fitquad and its required functions are needed.

### irtmle

The function *irtmle* finds the maximum likelihood estimate for a latent structure model. As in irtm, 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 field<patterns> & patterns,
const field < xsel & patternnumber, const xsel & patno,
const field<field<resp>> & data, const field<field <pwr>> > & thetas,
const xsel & thetano.
const field\langle adq \rangle \& scale, const xsel & scaleno, field\langle dovecmat \rangle \& obsscale,
const field<xsel> & selectbeta, const field<xsel> & selectbetano,
const xsel & selbetano,
const field < xsel > & selectbetac, const field < xsel > & selectbetacno,
const xsel & selbetacno,
const field<xsel> & selectthetai, const field<xsel> & selectthetaino,
const xsel & selthetaino,
const field < xsel > & select the tad, const field < xsel > & select the tadno,
const xsel & selthetadno,
const field < xsel > & select the tac, const field < xsel > & select the tacno,
const xsel & selthetacno,
const field < vec > & w, const xsel & wno,
const field<xsel> & obssel, const xsel & obsselno,
const vec & obsweight, const xsel & datasel,
const field < xsel & betasel, const xsel & betaselno, const vec & start).
```

In this declaration, maxf2v and mparams are defined as in maxlinq2 and maxf2vvar, while order is defined as in genresplik. whereas mparams is used for the basic iterations used for determination of the maximum-likelihood estimate, The variables algorithm and start are defined as in genrespmle. The vector obsweight provides the weights  $w_{h*}$  for  $0 \le h \le m-1$ . The variables patterns, selectbeta, selectbetac, selectthetai, selecthetad, and selectthetac are defined as in genresplik. For each observation h and each nonnegative integer  $i < n_h$ , if m(h, 1) is patno(h),

then patternno(m(h,1)) assigns i to the member of patterns that corresponds to  $\lambda_{hi}$ . Similar arguments apply to triples such as selectbeta, selectbetano, and selbeta. In the case of w and wno, for each observation h, wno assigns a vector in w of length  $n_h$  that corresponds to the  $w_{hi}$  for  $0 \le i < n_h$ . A similar relationship exists between obssel and obselno. Selection of observations h is determined by datasel, and betasel and betaselno determine which subvector of the parameter vector  $\beta$  applies to h.

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

#### irtms

The function *irtms* finds the log likelihood component  $\ell(\beta)$  and associated gradient and Hessian matrix for a latent-structure model. As in irtm, 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 field<pattern> & patterns,
const field<xsel> & patternnumber, const xsel & patno,
const field<field<resp>> & data, const field<field<pwr>> > & thetas,
const xsel & thetano,
const field <adq> & scale, const xsel & scaleno, field <dovecmat> & obsscale.
const field<xsel> & selectbeta, const field<xsel> & selectbetano.
const xsel & selbetano.
const field<xsel> & selectbetac, const field<xsel> & selectbetacno,
const xsel & selbetacno,
const field<xsel> & selectthetai, const field<xsel> & selectthetaino,
const xsel & selthetaino,
const field<xsel> & selectthetad, const field<xsel> & selectthetadno,
const xsel & selthetadno,
const field<xsel> & selectthetac, const field<xsel> & selectthetacno,
const xsel & selthetacno,
const field < vec > & w, const xsel & wno, const field < xsel > & obssel,
const xsel & obsselno,
const vec & obsweight, const xsel & datasel,
const field<xsel> & betasel, const xsel & betaselno, const vec & beta).
```

Definitions are as in *irtmle*, except that *beta* is the general function argument of the log likelihood rather than a starting vector. The function irtm and its required functions are used by irtms.

#### irtmsave

The function *irtms* are finds the log likelihood components of  $\ell_h(\beta)$  and associated gradient and Hessian matrix for a latent structure model. The function declaration is

```
field<pwrf2v> irtmsave (const int & order, const field<pattern> & patterns, const xsel & patternnumber, const field<resp> & data, const field <pwr> & thetas, dovecmat & obsscale, const field<xsel> & selectbeta, const xsel & selectbetano, const field<xsel> & selectbetac, const xsel & selectbetacno, const field<xsel> & selectthetai, const xsel & selectthetaino, const field<xsel> & selectthetad, const xsel & selectthetadno, const field<xsel> & selectthetac, const xsel & selectthetacno, const field<xsel> & selectthetac, const xsel & selectthetacno, const vec & w, const xsel & obssel, const vec & beta).
```

In this declaration, almost all arguments are defined as in irtm. The struct pwr is defined as follows:

struct pwrf2v{double weight; double kernel; resp theta; double value; vec grad; mat hess;}.

For element i of thetas, element i of irtmsave has theta equal to thetas(i).theta, weight equal to thetas(i).weight, kernel equal to thetas(i).kernel, value equal to  $\ell_h(\beta|\theta)$  for  $\theta$  equal to point and  $\beta$  equal to beta, grad equal to the corresponding gradient at  $\beta$  (if order is positive), and hess equal to the corresponding Hessian at  $\beta$  (if order exceeds 1). Functions needed by genresplik are also needed in irtmsave.

### irtmsaves

The function *irtms*aves finds the log likelihood components of all the  $\ell_h(\beta)$  and associated gradient and Hessian matrix for a latent structure model. The function declaration is

```
field<pwrf2v> irtmsave s(const int & order, const field<pattern> & patterns, const xsel & patternnumber, const xsel & patno, const field<field<pre>cresp> > & data, const field<field <pwr> > & thetas, const xsel & thetano, field<dovecmat> & obsscale, const field<xsel> & selectbeta, const field<xsel> & selectbetano, const xsel & selectbetano, const xsel & selectbetaco, const field<xsel> & selectbetaco, const field<xsel> & selectbetacno, const xsel & selectbetacno, const xsel & selectbetacno.
```

```
const field<xsel> & selectthetain, const field<xsel> & selectthetaino, const xsel & selthetaino, const field<xsel> & selectthetad, const field<xsel> & selectthetadno, const xsel & selthetadno, const field<xsel> & selectthetac, const field<xsel> & selectthetacno, const xsel & selthetacno, const xsel & selthetacno, const field<vec> & w, const xsel & wno, const field<xsel> & obssel, const xsel & obsselno, const vec & obsweight, const xsel & datasel, const field<xsel> & betasel, const xsel & betaselno, const vec & beta).
```

Definitions are as in irtms and irtmsave. Element i of irtmsaves(h) corresponds to  $\ell_h(\boldsymbol{\beta}|\boldsymbol{\theta}_i)$ . Functions required are irtmsave and the functions used in irtmsave.

# posterior

For an observation, the function *posterior* finds the posterior distribution of the latent vector given the observed responses. The function declaration is

field<pwr>> posterior (const field<pwrf2v> & irtcomps

The definition of pwr is in irtm, and the definition of pwrf2v is in irtmsave. The posterior is presented as q quadrature weights and points, where irtcomps has q members.

### posteriors

For a latent-structure model, the function *posteriors* finds the posterior distributions of the latent vectors given the observed responses for each observation. The function declaration is

field<field<pwr>> > posteriors (const field<field<pwrf2v>> & irtcompsm

The definition of pwr is in irtm, and the definition of pwrf2v is in irtmsave. The posterior for each observation h is presented as q(h) quadrature weights and points, where irtcompsm(h) has q(h) members.

### starttwoparamirt

The function starttwoparamirt finds a starting vector for use in two paramirt. The function declaration is

vec starttwoparamirt(const char & cdf, const imat & responses).

As in invcdf, the cumulative distribution function is specified by  $\operatorname{\mathsf{cdf}}$ . The starting vector  $\operatorname{starttwoparamirt}$  is based on the input matrix  $\operatorname{responses}$  with m rows and n columns. Each row represents n binary items.

# twoparamirt

The program twoparamirt provides a basic analysis of a two-parameter itemresponse model for binary responses with a univariate standard normal latent variable. It uses a control file controlfile read from standard input. The file is a text file with any line consisting of a pair of entries separated by a space, The entries contain no blank characters. The following cases exist.

The variable data has string value infile that specifies the input file for the data. The default is infile.csv.

The variable sf is associated with the string startvalue that specifies a file containing the vector of starting values. The default is to apply starttwoparamirt.

The variable *outfile* has string value that specifies the name of the output file for results. The default is *outfile*.

The bool variable *fflag* indicates whether an output file is used. The default is *true*.

The bool variable pflag indicates whether anything is printed in ascii form in standard output. The default is true.

The character variable dist specifies the cumulative distribution associated with the binary responses. The possibilities are N for normal, L for logistic, and G for Gumbel. The default is L.

The character variable method specifies the algorithm applied. The possibilities are G for gradient ascent, C for conjugate gradient ascent, N for modified Newton-Raphson, and L for Louis approximation. The default is N.

The positive double variable tol specifies the convergence criterion mparams.tol. The default is 0.001.

The bool variable adapt indicates whether adaptive quadrature is used. The default is true.

The character variable quadrature indicates the quadrature procedure used, with G for Gauss-Hermite and Q for normal quantiles. The default is G.

The positive integer variable *points* that exceeds 1 gives the number of quadrature points, with the default 9.

# **Integration Tools**

#### eaps

For each observation i, the function eaps generates a posterior weighted mean eaps(i).v and covariance matrix eaps(i).m that correspond to a discrete posterior distribution with points posts(i).m.col(j) with probabilities posts(i).v(j) for j from 1 to  $posts(i).m.n\_cols$ . The function declaration is

field < vecmat > eaps(const field < vecmat > & posts).

The definition of *vecmat* is as in pack. The function wmc is used.

# fitquad

The function fitquad fits a quadratic function to function values and quadrature points and finds the linear transformation that maps the origin onto the location of the maximum of the quadratic function and has a symmetric Jacobian matrix equal to the positive-definite and symmetric square root of the inverse of the Hessian matrix of the fitted quadratic function. The function declaration is

dovecmat fitquad(const field<f2v> & cresults, const field<pwr> & newthetas, const adq & scale, dovecmat & obsscale).

The structs are defined as in irtm. The linear components of the fitted quadratic not set to 0 are specified by *scale.linselect*, and the quadratic components not set to 0 are specified by *scale.quadselect*. If the fitted quadratic function is not strictly concave, then *fitquad* is *obsscale*.

## genfact

For a vector sizes of positive integers, the function genfact 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

The function genprods 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

vecmat genprods(const imat & indices, const field < pw > & pws).

The struct vecmat is defined as in pack, and the struct pw has vec elements points and weights. 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.m has Q columns and genprods.v has Q elements. The matrix genprods.m has D rows. The array pws has D members. For  $0 \le d < D$ , 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,  $0 \le k < p$ , and  $0 \le d < D$ , then row d and column k of indices is nonnegative and less than m(d) and the corresponding row and column of genprods.m is pws(d).points(indices(d,k)). Element k of genprods.v is the product of pws(d).weights(indices(d,k)) for  $0 \le d < D$ .

### hermcoeff

The function hermcoeff 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  $\alpha_i$ . For example, if n is 2, then the elements of hermcoeff are 1, 0, and -1.

# hermpoly

The function hermpoly 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  $0 \le k \le n$ , element k of hermpoly is the value of  $H_k$  at x.

# hermpw

The function hermpw 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

The function normwt 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.points. 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

The function qnormpw 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*.

#### wmc

The function wmc computes a weighted mean vector and covariance matrix. The function declaration is

vecmat wmc(const vecmat & wx).

The elements of wx.v are probabilities corresponding to the rows of wx.m.

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