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 http://arma.sourceforge.net, the StatsLib library at https://www.kthohr.com/statslib.html, and the Boost library at https://www.boost.org. 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.

- adaptpwr.cpp
- addsel.cpp
- berresp.cpp
- conjgrad.cpp
- conjgradn.cpp
- contresp.cpp
- cumresp.cpp

- eaps.cpp
- genfact.cpp
- genprods.cpp
- genresp.cpp
- genresplik.cpp
- genrespmle.cpp
- gradascent.cpp
- gradascentn.cpp
- gradresp.cpp
- \bullet gumbel.cpp
- \bullet hermcoeff.cpp
- hermpoly.cpp
- hermpw.cpp
- irtc.cpp
- irtm.cpp
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- \bullet irtms.cpp
- ivecsel.cpp
- linsel.cpp
- loggamma.cpp
- logistic.cpp
- logit.cpp
- logitbeta.cpp
- logitdirichlet.cpp
- loglog.cpp

- logmean.cpp
- lw.cpp
- lwm.cpp
- maxberresp.cpp
- maxf2vvar.cpp
- maxlinq2.cpp
- maxquad.cpp
- multlogit.cpp
- modit.cpp
- ngh.cpp
- \bullet normal.cpp
- normalv.cpp
- normwt.cpp
- nrv.cpp
- nrvn.cpp
- pack.cpp
- posterior.cpp
- posteriors.cpp
- probit.cpp
- qnormpw.cpp
- quadmax.cpp
- ranklogit.cpp
- rebound.cpp
- rescale.cpp
- trisym.cpp

- truncresp.cpp
- unpack.cpp
- vecsel.cpp
- wmc.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 , $0 \le j < n$. 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.cpp 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.cpp

The function lwm.cpp 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 vector < 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.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

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

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.cpp permitted for each primary iteration, mparams.eta is η , mparams.gamma1 is γ_1 , mparams.gamma2 is γ_2 , and mparams.kappa is κ . Iterations cease if the function value changes less than mparams.tol after a primary iteration.

The definition of f2v is

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

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

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

maxquad.cpp

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

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

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

modit.cpp

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

double modit(const double & eta, const double & alpha0, const double & alpha1, const double & stepmax, const bounds & b),

and the struct bounds is defined as

struct bounds {double lower; double upper;}.

Here eta corresponds to η , alpha0 is the previous location, alpha1 is the proposed new location, stepmax is the positive limit on step size, b.lower is the lower

bound, and b.upper is the upper bound. It is assumed that alpha0 and alpha1 are different. The function returns a value modit that is normally alpha1; however, if alpha1 exceeds alpha0, then modit is truncated above so that it does not exceed the minimum of alpha0+stepmax and alpha0+eta(b.upper-alpha0), while if alpha1 is less than alpha0, then modit is truncated below so that it is at least the maximum of alpha0-stepmax and alpha0+eta(b.lower-alpha0).

rebound.cpp

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

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

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

Functions related to the Newton-Raphson algorithm

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

maxf2vvar.cpp

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

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

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

ngh.cpp

The function ngh.cpp finds gradients and Hessian matrices via numerical differentiation. The function declaration is

f2v ngh(const int & order, const double & delta, const vec & x, const function $\langle f2v(const \text{ int } \& , const \text{ vec } \&)\rangle f)$.

If the variable order is 0, only the function value f.value at x at is reported. If order is 1, then f.grad at x is also reported by a numerical approximation with step size delta. If order is at least 2, then both f.grad and f.hess at x are reported by use of numerical approximations with step size delta. Values of f.grad are found by evaluation of f.value at vectors that differ from x in only one element. When an element of these vectors differ from those of x, the difference has absolute value delta. Values of f.hess are found by evaluation of f.value at vectors that differ from x in no more than two elements. When an element of these vectors differ from those of x, the difference has absolute value delta.

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

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

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.

nrvn.cpp

The function nrvn.cpp uses numerical differentiation for a modified version of the Newton-Raphson algorithm to maximization of f.value. The function nrvn.cpp has declaration

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

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.

conjgradn.cpp

The function conjgradn.cpp uses numerical differentiation to implement a conjugate gradient algorithm for maximization of f.value. The function declaration is

maxf2v conjgradn(const int & order, const params & mparams, const vec & start, const double & step, 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 positive step size for differentiation is *step*.

The function conjgradn.cpp uses conjgrad.cpp, ngh.cpp, 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

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

The functions $\max f2vvar.cpp$, $\max f2vpar.cpp$, $\max f2vpar.cpp$, $\max f2vpar.cpp$, $\max f2vpar.cpp$, and rebound.cpp are used. Definitions are as in conjgrad.cpp.

gradascentn.cpp

The function gradascent.ncpp uses numerical differentiation to implement a gradient-ascent algorithm for maximization of f.value. The function declaration for gradascent.ncpp is

maxf2v gradascentn(const order & , const params & mparams, const vec & start, const double & step, const function<f2v(const int & , const vec &)> f).

The functions gradascent.cpp, ngh.cpp, maxf2vvar.cpp, maxlinq2.cpp, maxquad.cpp, modit.cpp, and rebound.cpp are used. Definitions are as in conjgradn.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 twicecontinuously 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 \mathcal{A} with elements B(logit beta), C (cumulative), D (continuous), E (logit Dirichlet), G (graded), H (log gamma), 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 $\boldsymbol{\beta}$ is in O(A, F, q, r), and **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 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 D, and let g_D denotes the restriction of g to D in D. Let $\int(g_D)$ be defined for D in D, and let the $\int(g_D)$, D in 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 $\boldsymbol{\beta}$ in O(A, F, q, r), $\int (\exp(\ell_c(\boldsymbol{\beta}; \cdot, A, F, q, r))) = 1$. Here $\exp(\ell_c(\boldsymbol{\beta}; \cdot, A, F, q, r))$ is the function on $\mathcal{Y}(A, F, q, r)$ equal to $\exp(\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r))$ 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_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 $0 \leq i < n$, and let the log-likelihood function under study have the form

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

It follows that the gradient of ℓ at τ 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 ℓ 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 maxlinq2.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 , $0 \le i < n$, spans a space of dimension p. Conditions for a unique $\hat{\tau}$ in O such that $\ell(\hat{\tau})$ equals the supremum of ℓ 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 ℓ is strictly concave on O and $\hat{\tau}$ is the only member of O such that $\ell(\hat{\tau})$ equals the supremum of ℓ on O and, for τ in O, $\nabla \ell(\tau)$ 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. In typical cases, resp.dresp or resp.iresp has no elements; however, exceptions do exist.

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 \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 β . 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 $\boldsymbol{\beta}$ 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.cpp. 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.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 $\boldsymbol{\beta}$ 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.cpp. 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.cpp requires berresp.cpp, logiog.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, $q \ge 1$, 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.cpp. 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.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 $\boldsymbol{\beta}$ 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.cpp

The function loggamma.cpp 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 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 $\boldsymbol{\beta}$ 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 $\boldsymbol{\beta}$.

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

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

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

logitbeta.cpp

The function logitbeta.cpp 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 & v, 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.cpp

The function logit dirichlet.cpp computes the function value, gradient, and Hessian matrix associated with the logits of a Dirichlet distribution with a q = r + 1-dimensional 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 & y, 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.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

 $f2v \log\log(\text{const int } \& \text{ order, const resp } \& v, \text{ const vec } \& \text{ beta}).$

The function loglog value is $\ell_c(\beta; \mathbf{y}, A, F, q, r)$ 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 $\mathcal{Y}(A, F, q, r)$,

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

The function declaration is

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

The function logmean value is $\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r)$ 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 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.cpp. 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.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, $q \ge 1$, 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 $\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r)$ if y.iresp is \mathbf{y} and beta is $\boldsymbol{\beta}$. 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 $\boldsymbol{\beta}$ 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 β .

normalv.cpp

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 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 , $0 \le h < q$ 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 β_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.cpp reduces to normal.cpp. The function normalv.cpp requires pack.cpp and unpack.cpp.

pack.cpp

For the struct vecmat defined by

struct vecmax{vec v; mat m;};,

the function pack.cpp 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.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 $\ell_c(\boldsymbol{\beta}; \mathbf{y}, A, F, q, r)$ if y iresp is \mathbf{y} and beta is $\boldsymbol{\beta}$. $F = \Phi$. 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 $\boldsymbol{\beta}$.

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), $0 \le j \le q$, 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 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 $y(j), 0 \leq j < r$, 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 y in $\mathcal{Y}(A, F, q, r)$, let $\alpha(\beta)$ be the vector of dimension q+1 such that element $j, 0 \le j \le q$, 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 $\boldsymbol{\beta}$. 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 β 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 β , transform is defined as in berresp.cpp, and truncresp.value is $\ell_c(\beta; \mathbf{y}, A, F, q, r)$. Functions required are berresp.cpp, contresp.cpp, and their respective required functions.

unpack.cpp

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

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

genresplik.cpp

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

f2v genresplik(const int & order, const vector<dat> & data, const xsel & obssel, 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 x select[i] list has K_i elements and j is x select[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. If obssel.all is

true, then all observations data[i] are used. Otherwise, data[i] is only used for i in obssel.list.

The function genresplik.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 genresplik.cpp. The function declaration is

maxf2v genrespmle(const int & order, const params & mparams, const char & algorithm, const vector<dat> & data, const xsel & obssel, 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 genresplik.cpp are required, together with all C++ functions that these four functions need.

Tools for Computation of Log Likelihood Functions

addsel.cpp

The function add sel.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, $0 \le h < m$, 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_* , r_* , and r_* , and r_* , r_* in rackleta, and r_* , r_* in rackleta, and r_* in the nonempty set rackleta, and the fixed rackleta, dimensional vector rackleta, is in rackleta, is in rackleta, and rackleta, is in rackleta, and rackleta, and rackleta, and rackleta, and rackleta, is in rackleta, and rackleta, and rackleta, is in rackleta, and rackleta, in the nonempty set rackleta, is in rackleta, and rackleta, in the nonempty set rackleta, in the nonempty set

 \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 τ in O, the log-likelihood has the form

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

where $\ell_h(\tau)$ is the component of the log-likelihood for observation h. Thus the gradient function of ℓ at τ 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 ℓ_h at τ . The Hessian function of ℓ at τ 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 ℓ_h at τ . 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, $\ell_h(\tau)$ 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

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

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 $\mathcal{Y}(A_*, F_*, q_*, r_*)$.

irtc.cpp

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

f2v irtc (const int & order, const vector<dat> & data, const vector<thetamap> & thetamaps, const resp & theta, const xsel & datasel, 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 genresplik.cpp, the latent vector value is provided by theta, and beta is defined as usual as the parameter vector. Use of datasel is the same as use of obssel in genresplik.cpp.

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].drespcols, and other 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 ivecsel.cpp and genresplik.cpp, together with their associated functions, are required by irtc.cpp.

irtm.cpp

The function irtm.cpp finds the log likelihood component $\ell_h(\tau)$ 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 vector<dat> & data, const vector<thetamap> & thetamaps, const adq & scale, const params & mparamsn, rescale & newscale, const vector<pwr> & thetas, const xsel & datasel, 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 definition of *datasel* is as in irtc.cpp.

The struct pwr is defined by

```
struct pwr{double weight; resp theta;},
the struct adq is
struct adq{bool adapt; xsel xselect; double step;},
and the struct rescale
struct rescale{double mult; vecmat tran},
```

The structs scale and newscale are important in adaptive quadrature (Naylor & Smith, 1982) and are used in irtmle.cpp to improve efficiency and accuracy of computations involving continuous latent vectors. Let thetas have Q elements thetas [k]such that thetas[k].theta corresponds to the q_* -dimensional vector $\boldsymbol{\theta}_k$. If scale.adapt is false, scale.xselect.all is false and scale.xselect.list has no elements, or scale.xselect.all is true and thetas[0].theta.dresp has no elements, then u_{hk} is thetas[k].weight and $\boldsymbol{\theta}_{hk}$ is θ_k . Consider the case of scale.adapt equal true, thetas[0].theta.dresp has a positive number of elements, and either scale.xselect.all is true or scale.xselect.list has a positive number of distinct nonnegative integer elements less than q_* such that each element of scale.xselect.list corresponds to an element of thetas[0].theta.dresp. Then $\theta_{hk} = \mathbf{v}_h + \mathbf{M}_h \theta_k$ for a q_* -dimensional vector \mathbf{v}_h and a symmetric q_* by q_* matrix \mathbf{M}_h . An element of \mathbf{v}_h is forced to be 0 if the corresponding element of $\boldsymbol{\theta}_0$ does not correspond to an element of thetas[0].theta.dresp and, in the case of scale.xselect.all equal false, does not correspond to an element of thetas[0].theta.dresp specified by scale.xselect.list. All members of a row of \mathbf{M}_h are forced to be 0 if the corresponding element of \mathbf{v}_h is forced to be 0. The elements of \mathbf{v}_h not forced to be 0 are given in rescale.tran.v, and elements of \mathbf{M}_h not forced to be 0 are given by rescale.tran.m. The matrix rescale.tran.m is positive-definite and rescale.mult is its determinant. If rescale.tran.v is used, then \mathbf{v}_h is selected to maximize $\ell_h(\boldsymbol{\tau}|\boldsymbol{\theta})$ subject to the constraint that an element of θ must equal the corresponding element of θ_0 when that element of \mathbf{v}_h must be 0. Let this location of the maximum be $\boldsymbol{\theta}_{h0}$. This maximization is normally accomplished with nrvn.cpp with step size scale.mult. The starting value is a previously specified rescale.tran.v. The matrix rescale.tran.m is normally the symmetric matrix square root of the inverse of the matrix formed from the rows and columns of the negative Hessian matrix of $\ell_h(\tau|\cdot)$ at $\hat{\theta}_{h0}$ that correspond to elements of \mathbf{v}_h not restricted to be 0, and rescale.mult is the corresponding determinant. If the desired symmetric square root does not exist, then rescale is unchanged from its previous value. The function irtm.cpp uses the functions irtc.cpp, adaptpwr.cpp, and nrvn.cpp, together with their required functions. The parameters in mparamsn are defined as in maxlinq2.cpp. They are used with nrvn.cpp to find rescale.tran.v.

irtmle.cpp

The function irrmle.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 vector<vector<dat>> & obsdata, const vector<vector<thetamap>> & obsthetamaps, const vector<xsel> & datasel, const xsel & obssel, const adq & scale, const params & mparamsn, vector <rescale> & obsscale, const vectoryet obstatel, const vector
& obsscale, const vector
& betasel, const vec & start).
```

In this declaration, maxf2v, mparams, and mparamsn are defined as in maxling2.cpp and maxf2vvar.cpp, while order is defined as in irtc.cpp. The parameters in mparamsn are used when adaptive quadrature is specified, whereas mparams is used for the basic iterations used for determination of the maximum-likelihood estimate, The variable algorithm is defined as in genrespmle.cpp. The vector obsweight provides the weights w_{h*} for $0 \le h \le m-1$. The struct dat is defined as in genresplik.cpp, obsdata[h] is the data specification for observation h, the struct thetamap is defined as in irtc.cpp, obsthetamap[h] provides the mapping of the latent vector for observation h, the struct pwr is defined as in irtm.cpp, thetas is defined as in irtm.cpp, the struct adq is defined as in irtm.cpp, the scale adjustment for observation h is defined by obsscale[h], the elements of data[h] to be used are defined as in datasel[h], and the observations h used are defined by obssel. If obssel.all is true, then all observations are used. Otherwise, observation h only is used if in obssel. list. 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 $\ell(\tau)$ 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 vector<vector<dat>> & obsdata, const vector<vector<thetamap>> & obsthetamaps, const vector<xsel> & datasel, const xsel & obssel, const adq & obsscale, const params & mparamsn, vector<rescale>obsscales, const vector<pwr>> & thetas, const 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 obsweight, obsdata, obsthetamaps, datasel, obssel, scale, mparamsn, obsscales, thetas, 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 used by irtms.cpp.

posterior.cpp

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

```
vecmat posterior (const vector<dat> & data, const vector<thetamap> & thetamaps, const adq & scale, const rescale & newscale, const vector<pwr> & thetas, const xsel & datasel, const vec & beta).
```

Definitions are consistent with those in irtm.cpp. The posterior is presented as q points, each of which has r elements. Output is based on thetas. The number q of points is the number of elements of thetas, and r is the number of elements of thetas [0]. theta.dresp. The output consists of the vector posterior.v with q elements corresponding to the probabilities assigned to each point and the q by r matrix posterior.v with each row corresponding to a point of dimension v. All functions required by adaptpwr.cpp and irtc.cpp are required by posterior.cpp.

posteriors.cpp

For each observation used in irtms.cpp, the function posteriors.cpp finds the posterior distribution of the latent vector given the observed responses. The function declaration is

vector<vecmat> posteriors (const vector<vector<dat> > & obsdata, const vector<vector<thetamap> >& obsthetamaps, const vector<xsel> & datasel, const xsel obssel, const adq & scale, const vector<rescale> & obsscale, const vector<pwr>> & thetas, const vector<xsel> & betasel, const vec & beta).

Definitions are consistent with those in irtms.cpp. The posteriors for each observation are presented as in posterior.cpp. All functions required by posterior.cpp are required by posteriors.cpp.

Integration Tools

adaptpwr.cpp

The function adapt pwr.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, const rescale & newscale).

The structs pwr, adq, and rescale are defined as in irtm.cpp. If scale.adapt is false, oldtheta.theta.dresp has no elements, or scale.xselect.all is false and scale.xselect.list has no elements, then adaptpwr is oldtheta. In other cases, adapt-pwr.weight is the product of oldtheta.weight and newscale.mult, adaptpwr.theta.iresp is adaptpwr.theta.iresp, elements of adaptpwr.theta.dresp that do not correspond to elements of scale.tran.v are the same as corresponding elements of oldthat.theta.dresp, and the remaining elements of adaptpwr.theta.dresp correspond to rescale.tran.v . plus the product of rescale.tran.m and elements of oldtheta.theta.dresp that correspond to elements of rescale.tran.v.

eaps.cpp

For each observation i, the function eaps.cpp 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 $vector < vecmat > eaps(const \ vector < vecmat > & posts)$.

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

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

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

The struct vecmat is defined as in pack.cpp, 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.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 $0 \le k \le n$, 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.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.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.

wmc.cpp

The function wmc.cpp 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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