C++ Functions in Maxliklib Library

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Abstract

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

Keywords: Maximization procedures, quadrature procedures, maximum likelihood

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

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

- genresplik.cpp
- genrespmle.cpp
- gradascent.cpp
- gradresp.cpp
- gumbel.cpp
- hermcoeff.cpp
- hermpoly.cpp
- hermpw.cpp
- irtc.cpp
- logistic.cpp
- loglog.cpp
- logit.cpp
- logmean.cpp
- lw.cpp
- lwm.cpp
- maxberresp.cpp
- maxf2vvar.cpp
- maxlinq2.cpp
- maxquad.cpp
- multlogit.cpp
- modit.cpp
- \bullet normal.cpp
- \bullet normalv.cpp
- nrv.cpp
- pack.cpp

- probit.cpp
- ranklogit.cpp
- rebound.cpp
- truncresp.cpp
- unpack.cpp
- vecsel.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

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

Here the definition of maxf2v is

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

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

The definition of params is

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

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

The definition of f2v is

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

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

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

maxquad.cpp

The function maxquad.cpp approximates the maximum of *f.value* along a halfline 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 & v, 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.

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

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

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.

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

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

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

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

gradascent.cpp

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

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

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

Log-likelihood Components

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

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

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

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

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

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

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

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

(Haberman, 2013; Louis, 1982).

Many standard cases of $\ell_i(\cdot; \mathbf{y})$ exist, some of which are examined in the literature on survival analysis (Cox, 1972; Kalbfleisch & Prentice, 2002), generalized linear models (McCullagh & Nelder, 1989), multivariate analysis (Anderson, 2003), and discrete choice (McFadden, 1973). It should be noted that names for models are somewhat variable in different references, especially for graded and cumulative cases. In addition, graded and cumulative cases are defined to be consistent with the

Bernoulli cases. The following C++ functions are employed for common examples. The structs f2v are defined as in maxling2.cpp. If the argument beta is not in O_i , then all values returned equal NaN. It is assumed that the user of the function has verified that the input vector y is in \mathcal{Y}_i . In the cases under study in this section, unless otherwise stated, the components are strictly concave, so that ℓ is strictly concave whenever \mathbf{X}_i , $0 \leq i < n$, spans a space of dimension p. Conditions for a unique $\hat{\boldsymbol{\tau}}$ in O such that $\ell(\hat{\tau})$ 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 $\nabla \ell(\hat{\boldsymbol{\tau}})$ is the p-dimensional vector $\mathbf{0}_p$ with all elements 0 and $\nabla^2 \ell(\hat{\boldsymbol{\tau}})$ is negative definite, then O can be restricted to ensure that ℓ is strictly concave on O and $\hat{\tau}$ 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 β 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.

berresp.cpp

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

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

The function declaration is

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

If transform is G, then F = G, the standard Gumbel distribution function with value $G(y) = \exp(-\exp(-y))$ for y real. If transform is L, then $F = \Psi$, the standard logistic distribution function with value $\Psi(y) = 1/[1 + \exp(-y)]$ for y real. If transform is N, then $F = \Phi$, the standard normal distribution function with derivative $\phi(y) = \exp(-y^2/2)/(2\pi)^{1/2}$ for real y. The function berresp.value is $\ell_i(\beta; \mathbf{y})$ 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 $r_i = 1$, $q_i = 2$, \mathcal{Y}_i is the set of all one-dimensional vectors, O_i is the set of all two-dimensional vectors $\boldsymbol{\beta}$ with element $\beta(1) > 0$, and F and f are defined as in berresp.cpp. For \mathbf{y} in \mathcal{Y}_i and $\boldsymbol{\beta}$ in O_i ,

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

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

For all cases, the function declaration is

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

The variable transform is defined as in berresp.cpp. The function contresp.value is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ 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 $r_i = 1$, $q_i \ge 1$, \mathcal{Y}_i is the set of one-dimensional vectors \mathbf{y} such that y(0) is a nonnegative integer no greater than q_i , $q_i = n_i - 1$, O_i is the set of all vectors of dimension q_i , and F is defined as in berresp.cpp. For $\boldsymbol{\beta}$ in O_i and \mathbf{y} in \mathcal{Y}_i ,

$$\ell_{i}(\boldsymbol{\beta}; \mathbf{y}) = \begin{cases} \log(1 - F(\beta(y(0))), & y(0) = 0, \\ \log(1 - F(\beta(y(0)))) + \sum_{i=0}^{y(0)-1} \log(F(\beta(i))), & 0 < y(0) < q_{i}, \\ \sum_{i=0}^{y(0)-1} \log(F(\beta(i))), & y(0) = q_{i}. \end{cases}$$
(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 $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if y.iresp is \mathbf{y} and beta is $\boldsymbol{\beta}$. The function cumresp.cpp requires berresp.cpp, loglog.cpp, logit.cpp, and probit.cpp. If $r_i = 1$, then use of cumresp.cpp is equivalent to use of berresp.cpp. In general, $\ell_i(\cdot; \mathbf{y})$ is concave. Strict concavity holds if $q_i - y(0)$ does not exceed 1.

gradresp.cpp

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

$$\ell_{i}(\boldsymbol{\beta}; \mathbf{y}) = \begin{cases} \log(1 - F(\beta(y(0))), & y(0) = 0, \\ \log(F(\beta(y(0) - 1)) - F(\beta(y(0)))), & 0 < y(0) < q_{i}, \\ \log(F(\beta(y(0) - 1))), & y(0) = q_{i}. \end{cases}$$
(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 $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if y.iresp is \mathbf{y} and beta is $\boldsymbol{\beta}$. If $q_i = 1$, then berresp.cpp, cumresp.cpp and gradresp.cpp yield the same result. The function $\ell_i(\cdot; \mathbf{y})$ is concave. Strict concavity only holds if q_i is 1 or q_i is 2 and y(0) = 1.

gumbel.cpp

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

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

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

logistic.cpp

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

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

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

logit.cpp

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

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

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

loglog.cpp

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

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

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

logmean.cpp

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

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

The function declaration is

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

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

maxberresp.cpp

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

$$\ell_i(\boldsymbol{\beta}; \mathbf{y}) = \begin{cases} \log(F(\beta(0) + F(\beta(1) - F(\beta(0)F(\beta(1)), \quad y(0) = 1, \\ \log(1 - F(\beta(0))) + \log(1 - F(\beta(1)), \quad y(0) = 0. \end{cases}$$
(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 $\ell_i(\cdot; \mathbf{y})$ is not necessarily concave if y(0) = 1.

The function declaration is

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

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

multlogit.cpp

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

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

The function declaration is

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

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

normal.cpp

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

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

normalv.cpp

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

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

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

$$\ell_i(\boldsymbol{\beta}; \mathbf{y}) = \left[\sum_{j=0}^{r_i - 1} \log(\beta(j)) \right] + \log(\phi(\mathbf{a}(\boldsymbol{\beta}) + \mathbf{B}(\boldsymbol{\beta})\mathbf{y}; r_i)).$$
 (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_i -dimensional multivariate normal random vector with zero mean and with covariance matrix equal to the identity matrix. The function $\ell_i(\cdot; \mathbf{y})$ is always concave but is not strictly concave. The function declaration is

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

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

pack.cpp

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

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

The function declaration is

vec pack(const vecmat & u).

If u.v is a and u.m is B, then pack is the corresponding vector β .

probit.cpp

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

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

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

ranklogit.cpp

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

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

The function declaration is

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

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

truncresp.cpp

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

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

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

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

The function declaration is

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

Here yiresp has the single element y(1), and yidresp has the single element y(0).

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

unpack.cpp

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

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

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

Computation of Log Likelihood Functions

genresp.cpp

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

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

Here model has the definition

struct model{char type; char transform}.

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

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

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

The struct dat is defined by

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

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

struct xsel{bool all; ivec list}.

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

The function genresplik.cpp uses genresp.cpp plus all C++ functions it in turn 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 std::vector<dat> & data, const vec & start).

Here the structs maxf2v and mparams are defined as in maxlinq2.cpp and maxf2vvar.cpp. The vector start is the starting vector. The variable algorithm determines the algorithm, with N for Newton-Raphson, L for Newton-Raphson with the Hessian approximation of Equation 4, C for conjugate gradient, and G for gradient ascent. The functions nrv.cpp, conjgrad.cpp, gradascent.cpp, and genresplik.cpp are required, together with all C++ functions that these four functions need.

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. Data involve multiple responses for each individual observation. For a positive integer m, m observations are present. For observation h, $0 \le h < m$, n_h responses are observed and one latent . For response i, $0 \le i < n_h$, positive integers q_{hi} and r_{hi} are given. The component of the log likelihood for response i involves the predicted random vector \mathbf{Y}_{hi} in a nonempty subset \mathcal{Y}_{hi} of r_{hi} -dimensional vectors with elements $Y_{hi}(j)$, $0 \le j < r_{hi}$, 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} , and the positive real weight w_{hi} . In addition, for some positive integers Q and R and some nonempty subset Θ of R-dimensional vectors, a latent vector $\boldsymbol{\theta}_h$ in Θ and an R by p predicting matrix \mathbf{Z}_h is associated with observation h. If $\boldsymbol{\tau}$ is in O, then let $\boldsymbol{\lambda}_i(\boldsymbol{\tau}|\boldsymbol{\theta}) = \mathbf{o}_i + \mathbf{X}_i\boldsymbol{\tau}$ for $0 \le i < n$, and let the log-likelihood function under study have the form

$$\ell(\boldsymbol{\tau}) = \sum_{i=0}^{n-1} w_i \ell_i(\boldsymbol{\lambda}_i(\boldsymbol{\tau}); \mathbf{Y}_i). \tag{18}$$

irtc.cpp

The function irtc.cpp finds the conditional log likelihood and associated gradient and Hessian matrix for a latent structure model. The function declaration is

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

In this declaration, *order* is less than 1 if only the function value is returned, at least 1 if the gradient is required, 2 if the Hessian is produced, and more than 2 if the approximate Hessian matrix is found.

The struct thetamap is defined by

struct thetamap{bool dep; int respno; ivec indcols; ivec thetas;}.

The function genresplik.cpp and its associated functions are required by irtc.cpp.

Integration Tools

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

adapt.cpp

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

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

The struct pw has the definition

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

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

adaptv.cpp

The function adaptv.cpp provides a linear transformation of a set of D-dimensional quadrature points and adjusts the corresponding weights for each point, where D is a positive integer. The linear transformation has the form $L(\mathbf{x}) = \mathbf{a} + \mathbf{B}\mathbf{x}$ for the D-dimensional vector \mathbf{x} , where \mathbf{a} is a D-dimensional vector and \mathbf{B} is a D-dimensional vector \mathbf{x} .

by D lower triangular matrix. The linear transformation is applied to each quadrature point and the weights are multiplied by the determinant of \mathbf{B} . The function declaration is

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

The struct pwv has the definition

struct pwv{mat points; vec weights;};.

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

genfact.cpp

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

imat genfact(const ivec & sizes).

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

genprods.cpp

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

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

The struct pw is defined as in adapt.cpp, and the struct pw is defined as in adaptv.cpp. Consider the case of Q quadrature points for a multidimensional integral on the space of D-dimensional vectors, where Q and D are positive integers.

Then genprods.points has Q columns and genprods.weights has Q elements. The matrix genprods.points has D rows. The array pws has D members. For $0 \le d < D$, 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.points is pws[d].points(indices(d,k)). Element k of genprods.weights is the product of pws[d].weights(indices(d,k)) for $0 \le d < D$.

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.

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