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. Except if otherwise stated, functions rely on the Armadillo library (Sanderson & Curtin, 2016, 2018) at http://arma.sourceforge.net. The following functions are found in the library:

- adapt.cpp
- adaptv.cpp
- cloglog.cpp
- cloglog1.cpp
- conjgrad.cpp
- cumlogit.cpp
- cumlogit1.cpp
- cumloglog.cpp
- cumloglog1.cpp

- cumprobit.cpp
- cumprobit1.cpp
- genfact.cpp
- genprods.cpp
- gradascent.cpp
- gradlogit.cpp
- gradlogit1.cpp
- gradloglog.cpp
- gradloglog1.cpp
- gradprobit.cpp
- gradprobit1.cpp
- hermcoeff.cpp
- hermpoly.cpp
- hermpw.cpp
- lw.cpp
- lwm.cpp
- maxf1vvar.cpp
- maxf2vvar.cpp
- maxlin2.cpp
- maxlin.cpp
- modit.cpp
- nrv.cpp
- rebound.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(double & c, 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(double & cc,int & n,vec p[]).

The array p of vectors 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 is provided 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.

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 double & lower, const double & upper).

Here eta is a positive multiplier less than 1, alpha0 is the previous location, alpha1 is the proposed new location, stepmax is the positive limit on step size, lower is the lower bound, and 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(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(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

void rebound(const double & y,const double & der,double & lower,double & upper).

Here y is the current location, der is the function derivative at y, lower is the lower bound, and upper is the upper bound. It is assumed that der is not 0. If der is positive, lower is changed to y. If der is negative, upper is changed to y.

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.

maxlin2.cpp

The function maxlin2.cpp performs a line seach based on the Newton-Raphson algorithm. The gradient of *f.value* is *f.grad*. The Hessian matrix of *f.value* is *f.hess*. The function declaration is

```
\max f2v \max lin2(const paramnr \& nrparams, const vec \& v, \\ \max f2v \& vary0, function < f2v(vec) > f).
```

The struct maxf2v has the definition

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

The struct paramnr has the definition

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

The struct f2v has the definition

struct f2v{double value; vec grad;};.

The gradient of f.value is f.grad. The Hessian matrix is f.hess. Parameters used are defined in nrparams. The maximum number of primary iterations used in nrv.cpp is nparams.maxit. The maximum number of secondary iterations per main iteration used in the line search is nrparams.maxits. The maximum fraction of a step toward a boundary is nrparams.eta. For secondary iterations, the improvement check is nrparams.gamma1<1. The value of nparams.gamma2 is used in nrv.cpp to ensure that the direction of v is satisfactory. The largest permitted step length is nrparams.kappa>0. The convergence criterion for primary iterations is nparams.tol.

Information concerning the starting point of the line search is in vy0, while v provides the starting direction. The initial location is vy0.locmax, the value of f.value at vy0.locmax is vy0.max, the gradient of f.value at vy0.locmax is vy0.grad, and the Hessian matrix of f.value at vy0.locmax is vy0.hess. It is assumed that the inner product of v and vy0.grad is positive. The returned value includes the approximate location maxlin2.locmax of the maximum value of f.value at a point on the ray with origin vy0.locmax that has direction v. In addition, maxlin2.max is the value of f.value at maxlin2.locmax, maxlin2.grad is the gradient of f.value at maxlin2.locmax, and maxlin2.hess is the Hessian matrix of f.value at maxlin2.locmax.

The function maxlin2.cpp uses maxf2vvar.cpp, modit.cpp, and rebound.cpp.

maxf2vvar.cpp

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

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

The structs f2v and maxf2v are defined as in maxlin2.cpp. The returned value maxf2vvar.locmax is y, while maxf2vvar.max is the value of f.value at y, maxf2var.gad is the gradient of f.value at y, and maxf2var.hess is the Hessian matrix of f.value at y.

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

 $\max f2v \operatorname{nrv}(\operatorname{const} \operatorname{paramnr} \& \operatorname{nrparams}, \operatorname{const} \operatorname{vec} \& \operatorname{start}, \operatorname{function} < f2v(\operatorname{vec}) > f).$

The structs f2v, maxf2v, and paramnr are defined as in maxlin2.cpp and maxf2vvar.cpp. In convergence.pdf, γ_1 corresponds to nparams.gamma1, γ_2 corresponds to nrparams.gamma2, and κ corresponds to nrparams.kappa. The starting vector start must be in O. Iterations cease once the value of f.value increases by less than nrparams.tol after a primary iteration.

The function nrv.cpp uses maxf2vvar.cpp, maxlin2.cpp, modit.cpp, and rebound.cpp.

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

```
maxf1v conjgrad(const paramga & gaparams,
const vec & start, const function<f1v(vec)>f).
```

The definition of maxf1v is

struct maxf1v{vec locmax; double max; vec grad;};.

The definition of paramga is

struct paramga{int maxit; int maxits; function < double (vec) > c; double eta; double gamma1; double gamma2; double kappa; double tol;}.

The definition of f1v is

struct f1v{double value; vec grad;};.

The starting vector is start. The maximum number of main iterations is gaparams.maxit. The maximum number of secondary iterations per main iteration is gaparams.maxits. The function gaparams.c specifies the step size for numerical differentiation of the gradient f.grad of f.value. It must be the case that, for any vector y in the domain of f.value, y+c(y) is also in that domain. The maximum fraction of a step toward a boundary is gaparams.eta. In convergence.pdf, γ_1 corresponds to gaparams.gamma1, γ_2 corresponds to gaparams.gamma2, and κ corresponds to gaparams.kappa. Iterations cease once the value of f.value increases by less than gaparams.tol after a primary iteration.

The function conjgrad.cpp uses $\max f1vvar.cpp$, $\max lin.cpp$, 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 gradient.cpp is

```
maxf1v \ gradascent(const \ paramga \ \& \ gaparams, const vec \ \& \ start, \ const \ function < f1v(vec) > f).
```

The definitions of gaparams, paramga, f1v, and f are the same as in conjgrad.cpp, and maxf1vvar.cpp, maxlin.cpp, modit.cpp, and rebound.cpp are used.

maxf1vvar.cpp

The function maxf1vvar.cpp is used to combine information on a location and on a functions value and gradient at the location. The function maxf1vvar.cpp has declaration

maxf1v maxf1vvar(const vec & y,const f1v & fy).

The structs f1v and maxf1v are defined as in conjgrad.cpp. The returned value maxf1vvar.locmax is y, while maxf1vvar.max is the value of f.value at y and maxf1var.gad is the gradient of f.value at y.

maxlin.cpp

The function *maxlin.cpp* uses numerical differentiation to provide an approximate Newton-Raphson procedure for a line search. The function declaration is

maxf1v maxlin(const paramga & gaparams, const vec & v, maxf1v & vary0, function<f1v(vec)>f).

The structs maxf1v, paramga, and f1v are defined as in conjgrad.cpp. The functions maxf1vvar.cpp, modit.cpp, and rebound.cpp are all used.

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 r_i and q_i are given. The component of the log likelihood for observation i involves the predicted random vector \mathbf{Y}_i in a nonempty subset \mathcal{Y}_i of r_i -dimensional vectors and the q_i by p predicting matrix \mathbf{X}_i in a nonempty set \mathcal{X}_i . The log-likelihood function under study has the form

$$\ell(\gamma) = \sum_{i=0}^{n-1} w_i \ell_i(\mathbf{X}_i \boldsymbol{\gamma}; \mathbf{Y}_i)$$
 (1)

for γ in O. 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 γ in O and \mathbf{X} in \mathcal{X}_i , $\mathbf{X}\gamma$ 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 $\exp(\ell_i(\boldsymbol{\beta}; \mathbf{y}))$ over \mathbf{y} in \mathcal{Y}_i is 1 and a continuous random vector \mathbf{Y} has density $\exp(\ell_i(\boldsymbol{\beta}; \mathbf{y}))$ at \mathbf{y} in \mathcal{Y}_i . The gradient function of $\ell_i(\cdot; \mathbf{y})$ is $\nabla \ell_i(\cdot; \mathbf{y})$ and corresponding Hessian matrix is $\nabla^2 \ell_i(\cdot; \mathbf{y})$. It follows that the gradient of ℓ at γ is

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

and the Hessian matrix of ℓ at γ is

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

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.

The following C++ functions are employed for common examples. The structs f1v and f2v are defined as in maxlin2.cpp and maxlin.cpp.

cloglog.cpp

The function cloglog.cpp computes the function value, gradient, and Hessian matrix associated with a complementary log-log transformation. Let G be the cumulative distribution function with $G(y) = 1 - \exp(-\exp(y))$ for real y. Thus G is the cumulative distribution function of a version of the Gumbel distribution. The inverse function G^{-1} of G is the complementary log-log transformation with $G^{-1}(x) = \log(-\log(1-x))$ for real x such that 0 < x < 1. In this case, $r_i = 1$, \mathcal{Y}_i is the set of one-dimensional vectors \mathbf{y} such that y(0) is 0 or 1, $q_i = 1$, O_i is the set of all one-dimensional vectors. For $\mathbf{\beta}$ in O_i and \mathbf{y} in \mathcal{Y}_i , $\ell_i(\mathbf{\beta}; \mathbf{y}) = \log(1 - G(\mathbf{\beta}(0)))$ if y(0) = 0, and $\ell_i(\mathbf{\beta}; \mathbf{y}) = \log(G(\mathbf{\beta}(0)))$ if y(0) = 1. The function declaration is

f2v cloglog(ivec & y, vec & beta).

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

cloglog1.cpp

The function cloglog1.cpp computes the function value and gradient associated with a complementary log-log transformation. The definitions of r_i , q_i , O_i , \mathcal{Y}_i , and $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ are the same as in cloglog.cpp. The function declaration is

 $f1v \ cloglog1(ivec \& y, vec \& beta).$

The function cloglog1.value is $\ell_i(\beta; \mathbf{y})$ if y is \mathbf{y} and beta is $\boldsymbol{\beta}$.

cumlogit.cpp

The function cumlogit.cpp computes the function value, gradient, and Hessian matrix associated with a cumulative logit transformation. Let L be the distribution function of a standard logistic random variable, so that $L(y) = 1/[1 + \exp(-y)]$ for real y and the inverse function L^{-1} of L is the logit transformation with $L^{-1}(x) = \log(x/(1-x))$ for real x such that 0 < x < 1. In this case, $r_i = 1$, n_i is an integer greater than 1, \mathcal{Y}_i is the set of one-dimensional vectors \mathbf{y} such that y(0) is a nonnegative integer less than n_i , $q_i = n_i - 1$, and O_i is the set of all vectors of dimension $n_i - 1$. For $\boldsymbol{\beta}$ in O_i and \mathbf{y} in \mathcal{Y}_i ,

$$\ell_{i}(\boldsymbol{\beta}; \mathbf{y}) = \begin{cases} \log(1 - L(\beta(y(0))), & y(0) = 0, \\ \log(1 - L(\beta(y(0)))) + \sum_{i=0}^{y(0)-1} \log(L(\beta(i))), & 0 < y(0) < n_{i} - 1, \\ \sum_{i=0}^{y(0)-1} \log(L(\beta(i))), & y(0) = n_{i} - 1. \end{cases}$$
(4)

The function declaration is

 $f2v \ cumlogit(ivec \& y, vec \& beta).$

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

cumlogit1.cpp

The function cumlogit1.cpp computes the function value and gradient associated with a cumulative logit transformation. As in cumlogit.cpp, r_i , n_i , q_i , O_i , and \mathcal{Y}_i are defined as in cumlogit.cpp, and Equation 4 holds for $\boldsymbol{\beta}$ in O_i and \mathbf{y} in \mathcal{Y}_i . The function declaration is

f1v cumlogit1(ivec & y, vec & beta).

The function cumlogit1.value is $\ell_i(\beta; y)$ if y is y and beta is β .

cumloglog.cpp

The function cumloglog.cpp computes the function value, gradient, and Hessian matrix associated with a cumulative complementary log-log transformation. Define G as in cloglog.cpp. Then r_i , n_i , q_i , O_i , and \mathcal{Y}_i are defined as in cumlogit.cpp, and, for β in O_i and \mathbf{y} in \mathcal{Y}_i ,

$$\ell_{i}(\boldsymbol{\beta}; \mathbf{y}) = \begin{cases} \log(1 - G(\beta(y(0))), & y(0) = 0, \\ \log[1 - G(\beta(y(0))) + \sum_{i=0}^{y(0)-1} \log(G(\beta(i))), & 0 < y(0) < n_{i} - 1, \\ \sum_{i=0}^{y(0)-1} \log(1 - G(\beta(i))), & y(0) = n_{i} - 1. \end{cases}$$
(5)

The function declaration is

f2v cumloglog(ivec & y, vec & beta).

The function cumloglog.value is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if y is \mathbf{y} and beta is $\boldsymbol{\beta}$. If n = 2, then cumloglog.cpp and cloglog.cpp yield the same result.

cumloglog1.cpp

The function cumloglog1.cpp computes the function value and gradient associated with a cumulative log-log transformation. Here r_i , n_i , q_i , O_i , and \mathcal{Y}_i are defined as in cumlogit.cpp. As in cloglog.cpp, Equation 5 holds for $\boldsymbol{\beta}$ in O_i and \mathbf{y} in \mathcal{Y}_i . The function declaration is

f1v cumloglog1(ivec & y, vec & beta).

The function cumloglog1.value is $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ if y is \mathbf{y} and beta is $\boldsymbol{\beta}$. If $n_i = 2$, then cumloglog1.cpp and cloglog1.cpp yield the same result.

cumprobit.cpp

The function cumprobit.cpp computes the function value, gradient, and Hessian matrix associated with a cumulative probit transformation. Let Φ be the cumulative distribution function of the standard normal distribution with expectation 0 and variance 1, so that the inverse function Φ^{-1} defined on the interval (0,1) is the probit transformation. In this case, r_i , n_i , q_i , O_i , and \mathcal{Y}_i are defined as in cumlogit.cpp, and, for β in O_i and \mathbf{y} in \mathcal{Y}_i ,

$$\ell_{i}(\boldsymbol{\beta}; \mathbf{y}) = \begin{cases} \log[1 - \Phi(\beta(y(0))), & y(0) = 0, \\ \log(1 - \Phi(\beta(y(0)))) + \sum_{i=0}^{y(0)-1} \log(\Phi(\beta(i))), & 0 < y(0) < n_{i} - 1, \\ \sum_{i=0}^{y(0)-1} \log(\Phi(\beta(i))), & y(0) = n_{i} - 1. \end{cases}$$
(6)

The function declaration is

f2v cumprobit(ivec & y, vec & beta).

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

cumprobit1.cpp

The function cumprobit1.cpp computes the function value and gradient associated with a cumulative probit transformation. Definitions of r_i , n_i , q_i , \mathcal{Y}_i , and $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ are the same as in cumprobit.cpp. The function declaration is

f1v cumprobit1(ivec & y, vec & beta).

The function *cumprobit1.value* is $\ell_i(\beta; \mathbf{y})$ if y if y and beta is β .

gradlogit.cpp

The function gradlogit.cpp computes the function value, gradient, and Hessian matrix associated with a graded logit transformation. Define L as in cumlogit.cpp. Then $r_i = 1$, n_i is an integer greater than 1, $q_i = n_i - 1$, O_i is the set of all vectors of dimension $n_i - 1$ with strictly increasing elements, \mathcal{Y}_i is the set of one-dimensional vectors \mathbf{y} with y(0) a nonnegative integer less than n_i , and, for $\boldsymbol{\beta}$ in O_i and \mathbf{y} in \mathcal{Y}_i ,

$$\ell_{i}(\boldsymbol{\beta}; \mathbf{y}) = \begin{cases} \log(L(\beta(y(0)))) & y(0) = 0, \\ \log(L(\beta(y(0))) - L(\beta(y(0) - 1))), & 0 < y(0) < n_{i} - 1, \\ \log[1 - L(\beta(y(0) - 1))), & y(0) = n_{i} - 1. \end{cases}$$
(7)

The function declaration is

f2v gradlogit(ivec & y, vec & beta).

The function gradlogit value is $\ell_i(\beta; y)$ if y is y and beta is β .

gradlogit1.cpp

The function gradlogit1.cpp computes the function value and gradient associated with a graded logit transformation. Here r_i , n_i , q_i , O_i , \mathcal{Y}_i , and $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ are defined as in gradlogit.cpp. The function declaration is

f1v gradlogit1(ivec & y, vec & beta).

The function gradlogit1.value is $\ell_i(\beta; \mathbf{y})$ if y is y and beta is β .

gradloglog.cpp

The function gradlogit.cpp computes the function value, gradient, and Hessian matrix associated with a graded complementary log-log transformation. Define G as in cloglog.cpp. Then $r_i = 1$, n_i is an integer greater than 1, $q_i = n_i - 1$, O_i is the set of all vectors of dimension $n_i - 1$ with strictly increasing elements, \mathcal{Y}_i is the set of one-dimensional vectors \mathbf{y} with y(0) a nonnegative integer less than n_i , and, for $\boldsymbol{\beta}$ in O_i and \mathbf{y} in \mathcal{Y}_i ,

$$\ell_{i}(\boldsymbol{\beta}; \mathbf{y}) = \begin{cases} \log(G(\beta(y(0)))) & y(0) = 0, \\ \log(G(\beta(y(0))) - G(\beta(y(0) - 1))), & 0 < y(0) < n_{i} - 1, \\ \log[1 - G(\beta(y(0) - 1))), & y(0) = n_{i} - 1. \end{cases}$$
(8)

The function declaration is

 $f2v \operatorname{gradloglog}(ivec \& v, vec \& beta).$

The function gradloglog value is $\ell_i(\beta; y)$ if y if y and beta is β .

gradloglog1.cpp

The function gradloglog1.cpp computes the function value and gradient associated with a graded complementary log-log transformation. Here r_i , n_i , q_i , O_i , \mathcal{Y}_i , and $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ are defined as in gradloglog.cpp. The function declaration is

f1v gradloglog1(ivec & y, vec & beta).

The function gradloglog1.value is $\ell_i(\beta; \mathbf{y})$ if y is y and beta is β .

gradprobit.cpp

The function gradprobit.cpp computes the function value, gradient, and Hessian matrix associated with a graded probit transformation. Define Φ as in cumprobit.cpp. Then $r_i = 1$, n_i is an integer greater than 1, $q_i = n_i - 1$, O_i is the set of all vectors of dimension $n_i - 1$ with strictly increasing elements, \mathcal{Y}_i is the set of

one-dimensional vectors \mathbf{y} with y(0) a nonnegative integer less than n_i , and, for $\boldsymbol{\beta}$ in O_i and \mathbf{y} in \mathcal{Y}_i ,

$$\ell_{i}(\boldsymbol{\beta}; \mathbf{y}) = \begin{cases} \log(\Phi(\beta(y(0)))) & y(0) = 0, \\ \log(\Phi(\beta(y(0))) - \Phi(\beta(y(0) - 1))), & 0 < y(0) < n_{i} - 1, \\ \log[1 - \Phi(\beta(y(0) - 1))), & y(0) = n_{i} - 1. \end{cases}$$
(9)

The function declaration is

f2v gradprobit(ivec & y, vec & beta).

The function gradprobit value is $\ell_i(\beta; y)$ if y if y and beta is β .

gradprobit1.cpp

The function gradprobit1.cpp computes the function value and gradient associated with a graded probit transformation. Here r_i , n_i , q_i , O_i , \mathcal{Y}_i , and $\ell_i(\boldsymbol{\beta}; \mathbf{y})$ are defined as in gradprobit.cpp. The function declaration is

flv gradprobit1(ivec & y, vec & beta).

The function gradprobit 1. value is $\ell_i(\beta; \mathbf{y})$ if y is y and beta is β .

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

The struct pw has the definition

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

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

adaptv.cpp

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

pwv adapt(vec & loc, mat & lt, 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

 $imat\ genfact(ivec\ \&\ sizes).$

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(imat & indices,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 pw 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 order. The function declaration is

vec hermcoeff(int & n).

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

hermpoly.cpp

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

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

The order is the nonnegative integer variable n, and the real value is x. The vector hermpoly has n+1 elements. For $0 \le k \le n$, 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(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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