package: mecdf 0.6.0

Multivariate Empirical Cumulative Distribution Functions

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This vignette gives an overview of the mecdf package. The main purpose of the package, is to use multivariate empirical cumulative distribution functions (multivariate ECDFs) to model real-world data. The package also supports both step functions and continuous functions.

Introduction

We will assume the reader has a basic understanding of both multivariate CDFs and univariate ECDFs. Noting that the mvtnorm package and the standard "ecdf" function in R, are both good references. Essentially, a cumulative distribution function defines the probably that a random variable takes a value less than or equal to some other value from the random variable's sample space. So for the univariate case:

$$\mathrm{F}_X(x) = \mathbb{P}(X \le x)$$

For the bivariate case, we now have two random variables. We are interested in the probably that the first random variable takes some value less than or equal to some other value and that the second random variable also takes some value less than or equal to some other value:

$$\mathrm{F}_{X_1,X_2}(x_1, x_2) = \mathbb{P}(X_1 \le x_1, X_2 \le x_2)$$

These expressions generalise to k random variables:

$$\mathrm{F}_{X_1,X_2,\ldots,X_k}(x_1, x_2, \ldots, x_k) = \mathbb{P}(X_1 \le x_1, X_2 \le x_2, \ldots, X_k \le x_k)$$

Often we are interested in estimating the distribution from some data (most commonly the PDF, however we will focus on the CDF). The standard approach is to make some assumption about the distribution (i.e. that the actual distribution is one of a set of distributions, distinguished from each other by some parameters). The problem then simplifies to one of estimating the parameters only. An alternative approach, where we estimate the distribution directly from the data, what we will denote as $\hat{\mathrm{F}}$, without assumptions and without parameters, is to use an ECDF model. By definition a (univariate) ECDF is a step function. It's the proportion of realised (or "observed") values of a random variable, that are less than or equal to some value. We can write it as:

$$\hat{\mathrm{F}}_X(u) = \frac{\sum_{\forall i} \mathrm{I}(\mathbf{x}_{[i]} \le u)}{n}$$

In the expression above, x has been replaced with with u and $\mathbf{x}$ (here a vector) denotes the realised values of the random variable X. The function I is an indicator function, which is equal one when the enclosed expression is true, and zero otherwise.

The Multivariate ECDF

Following the above expressions, we can formulate the bivariate and k-variate ECDFs as:

$$\hat{\mathrm{F}}_{X_1,X_2}(u_1,u_2) = \frac{\sum_{\forall i} \mathrm{I}(\mathbf{x}_{[i,1]} \leq u_1, \mathbf{x}_{[i,2]} \leq u_2)}{n}$$

$$\hat{\mathrm{F}}_{X_1,X_2,\ldots,X_k}(u_1,u_2,\ldots,u_k) = \frac{\sum_{\forall i} \mathrm{I}(\mathbf{x}_{[i,1]} \leq u_1, \mathbf{x}_{[i,2]} \leq u_2, \ldots, \mathbf{x}_{[i,k]} \leq u_k)}{n}$$

Note that now $\mathbf{x}$ is a matrix. Each row of the matrix represents one multivariate realisation. Each column represents realisations of one random variable. Let us consider an example of a bivariate ECDF.

```
> #get warmed up
> library (mecdf, warn=FALSE)
```

```
> #simulated data
> x1 = runif (10)
> x2 = runif (10)
> x = cbind (x1, x2)
```

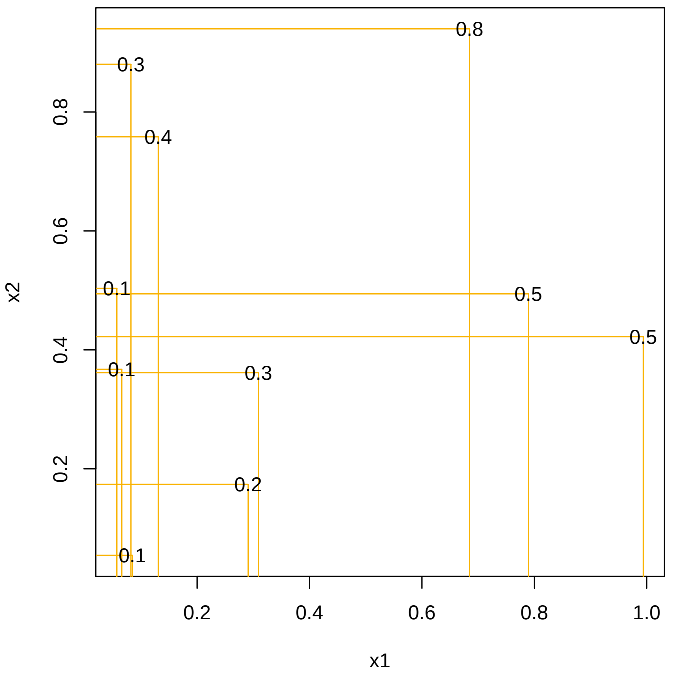
```
> #fit the model
> m = mecdf (x)
> m
mecdf_{bivariate, step}
           x1        x2
1  0.30920709 0.3616129
2  0.08229845 0.8802995
3  0.06604260 0.3673871
8  0.99384799 0.4221490
9  0.13095568 0.7582902
10 0.78943494 0.4942096
```

Our model, is also an R function and we can use it to evaluate the estimated distribution function over some point.

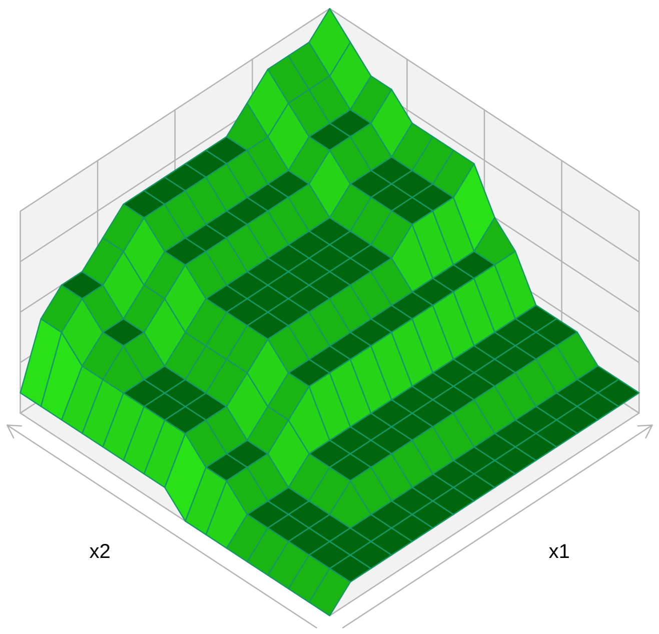
```
> m (c (0.5, 0.5) )
[1] 0.4
```

The mecdf package provides multiple ways to visualise bivariate ECDFs. That standard way, via plot, produces a plot of one variable against the other, with the values of the distribution function shown on the plot. There are also 3D plots using the function plotbcdf. By default, these produce surfaces evaluated over a regularly spaced grid. However, by including the argument regular=FALSE (not recommended for large samples), we can produce a surface over the actual realised values (which form an irregularly spaced grid). For step functions (which is what we have here), our surface is discontinuous. In the next section (with continuous functions) our surface is continuous.

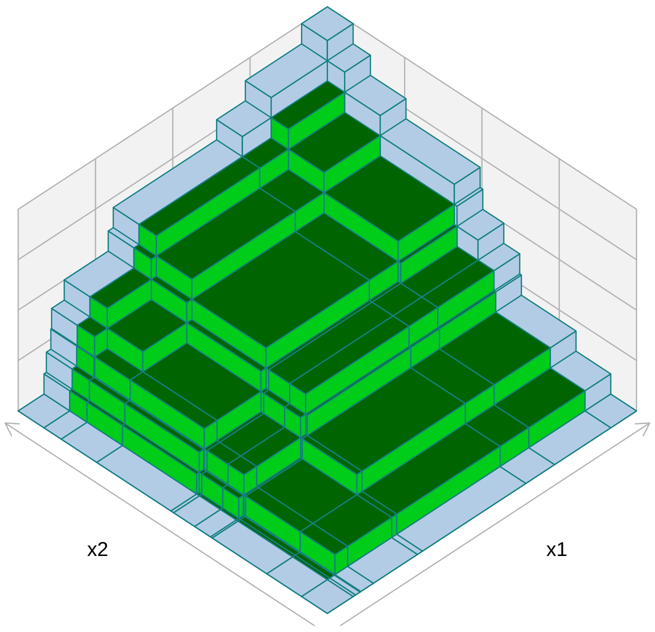
```
> plot (m)
```



```
> plotbcdf (m)
```



```
> plotbcdf (m, regular=FALSE)
```



The Continuous ECDF

Not only can be generalise ECDFs to the multivariate case, we can also generalise them to the continuous case. In principle, continuous distribution functions should be better estimates than step distribution functions (for continuous random variables). However, estimating the continuous ECDF requires a high computational cost (often with only a small improvement in the estimate). There is another problem with continuous ECDFs. The method presented here has the potential to produce negative values for the distribution function. The solution is discussed later (in the section on model correction).

We can treat our realised values, as forming an irregularly spaced grid. This allows us to produce a continuous distribution function by linear interpolation over vertices of that grid. This is simple in the univariate case (where a one dimension grid, is quite trivial). For any vertex (here simply any realised value, $u \in \mathbf{x}$), we can compute the value of a distribution function $\mathrm{F}^*_X(u)$ over that vertex. We make a slight modification to our standard expression so that the values of our distribution function are between 0 and 1.

$$\mathrm{F}^*_X(u) = \frac{\sum_{\forall i} \mathrm{I}(\mathbf{x}_{[i]} \leq u) - 1}{n - 1}$$

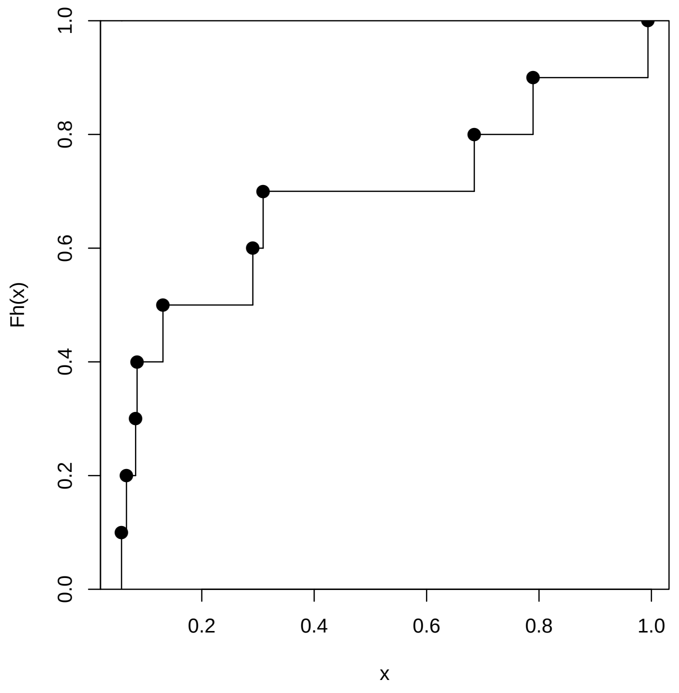
We have four possible cases:

1. If $u \leq \min(\mathbf{x})$, then $\hat{\mathrm{F}}_X = 0$.
2. Else if $u \geq \max(\mathbf{x})$, then $\hat{\mathrm{F}}_X = 1$.
3. Else if $u \in \mathbf{x}$, then $\hat{\mathrm{F}}_X(u) = \mathrm{F}^*_X(u)$
4. Otherwise we interpolate...

$$\hat{\mathrm{F}}_X(u) = q\mathrm{F}^*_X(a) + p\mathrm{F}^*_X(b)$$

Where: a, the greatest realised value less than u; b, the smallest realised value greater than u; p, the distance from a to u as a proportion of the distance between a and b; and q, which equals $1 - p$. Noting that $a < u < b$. Using the vector x1 created earlier:

```
> m = mecdf (x1)
> plot (m)
> points (x1, m (x1), pch=16, cex=1.5)
```



To move from the univariate case to the bivariate case, we define a function $\mathrm{F}^*_{X_1,X_2}$, however our grid is no longer trivial. We have vertex whenever $u_1 \in \mathbf{x}_{[,1]}$ and $u_2 \in \mathbf{x}_{[,2]}$.

$$\mathrm{F}^*_{X_1,X_2}(u_1,u_2) = \frac{\sum_{\forall i} \mathrm{I}(\mathbf{x}_{[i,1]} \leq u_1, \mathbf{x}_{[i,2]} \leq u_2) - 1}{n-1}$$

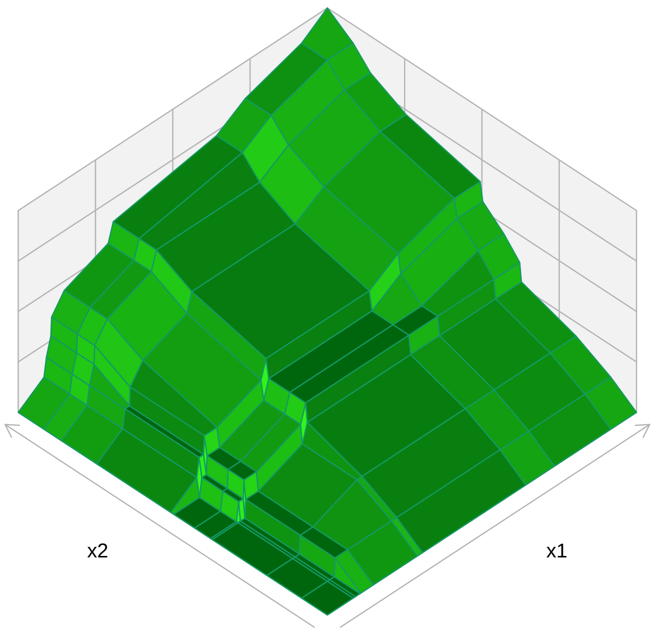
Now we have several cases:

1. If either $u_1 \leq \min(\mathbf{x}[,1])$ or $u_2 \leq \min(\mathbf{x}[,2])$, then $\hat{\mathrm{F}}_{X_1,X_2}(u_1,u_2) = 0$
2. Else if both $u_1 \geq \max(\mathbf{x}[,1])$ and $u_2 \geq \max(\mathbf{x}[,2])$, then $\hat{\mathrm{F}}_{X_1,X_2}(u_1,u_2) = 1$
3. Else if either $u_1 > \max(\mathbf{x}[,1])$ or $u_2 > \max(\mathbf{x}[,2])$, we substitute the corresponding u value with the corresponding maximum value, then start this if-else sequence again...
4. Else if both $u_1 \in \mathbf{x}_{[,1]}$ and $u_2 \in \mathbf{x}_{[,2]}$, then $\hat{\mathrm{F}}_{X_1,X_2}(u_1,u_2) = \mathrm{F}^*_{X_1,X_2}(u_1,u_2)$.
5. Else if one value is (an element) and the other isn't, we interpolate between two vertices (similar to the univariate case, except using two variables).
   e.g. $\hat{\mathrm{F}}_{X_1,X_2}(u_1,u_2) = q\mathrm{F}^*_{X_1,X_2}(u_1,a) + p\mathrm{F}^*_{X_1,X_2}(u_1,b)$.
6. Else (both values between pairs of realisations), then we compute values of a, b, p and q for each variable, and interpolate between four vertices:

$$\hat{\mathrm{F}}_{X_1,X_2}(u_1,u_2) = q_1q_2\mathrm{F}^*_{X_1,X_2}(a_1,a_2) + q_1p_2\mathrm{F}^*_{X_1,X_2}(a_1,b_2) + p_1q_2\mathrm{F}^*_{X_1,X_2}(b_1,a_2) + p_1p_2\mathrm{F}^*_{X_1,X_2}(b_1,b_2)$$

We can generalise this to k variables. For a grid with k variables, there will be up to 2^k vertices, hence the large computational cost. In many cases, some (or even all) of the vertices will have the same value, so a further simplication may be possible. Using the matrix x, created earlier:

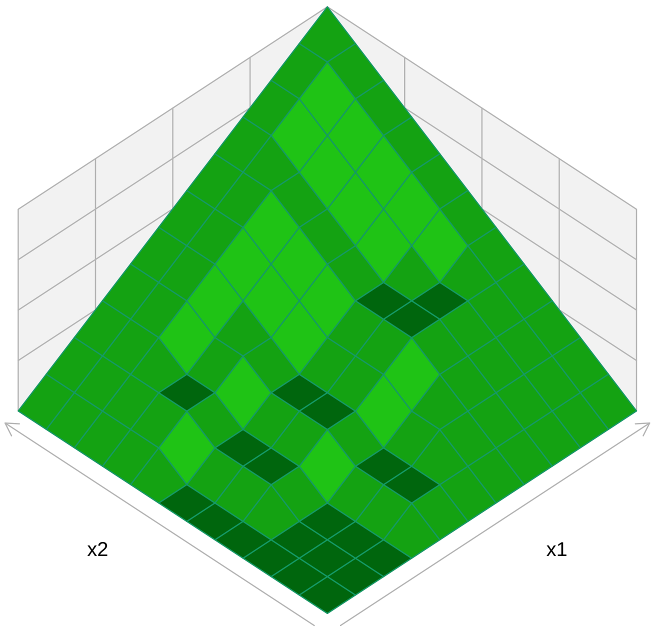
```
> m = mecdf (x, continuous=TRUE)
> plotbcdf (m, regular=FALSE)
```



Projecting ECDFs onto Unit Cubes

It is possible to project an ECDF model onto a unit (potentially hyper) cube, with uniform marginals. I have no idea if this is useful or not. However, we can do it very easily (by replacing realised values with their index, if we were to sort them, one variable at a time), it's kind of interesting, and it does have a vague resemblance to a certain other multivariate approach, so why not...

```
> m = mecdf (x, continuous=TRUE, project=TRUE)
> plotbcdf (m, regular=FALSE)
```



Model Correction

The mecdf function contains the arguments expand and expandf. The first indicates whether or not a correction should be done (by expanding the data). If a correction is done, the second indicates the expansion factor. For step functions, expand defaults to false. For continuous functions, expand defaults to true.

When expand is true, two fake observations are added to our sample. One represents the (new) minimum, over all variables. The other, the (new) maximum over all variables. They are computed as follows, for each variable, the range (difference between actual minimum and maximum value) is computed, multiplied by the expansion factor, to give an offset, then one value is computed for the minimum actual value less the offset and another value for the maximum value plus the offset.

The main reason for doing this is that the interpolation method described earlier (for two or more variables), can produce invalid models unless there's some form of correction first.

Intuitively, a continuous multivariate CDF model should be monotonically non-decreasing in the direction of each variable and only have values between 0 and 1. Not so intuitively, the empirical (continuous) case, requires that the function is zero-valued for domain values less than or equal to minimum observed values, for every variable.

This requirement isn't satisfied unless their is one single realisation, that represents the minimum observed values for every variable.

A vaguely similar argument can be constructed for domain values greater than or equal to maximum values, requiring a single realisation representing the maximum for every variable.

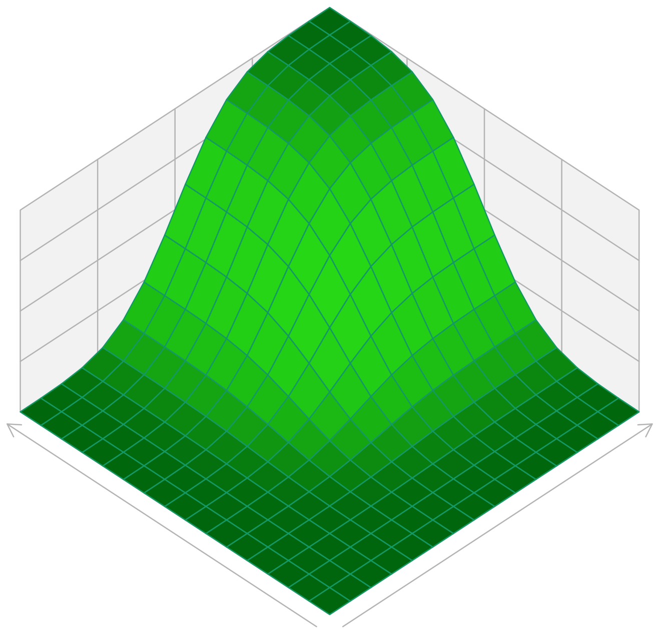
The Bivariate Normal vs The Bivariate ECDF

First let us consider a bivariate normal distribution. We will create three examples with no correlation, perfect positive correlation and perfect negative correlation. We are going to use the mvtnorm package to help us.

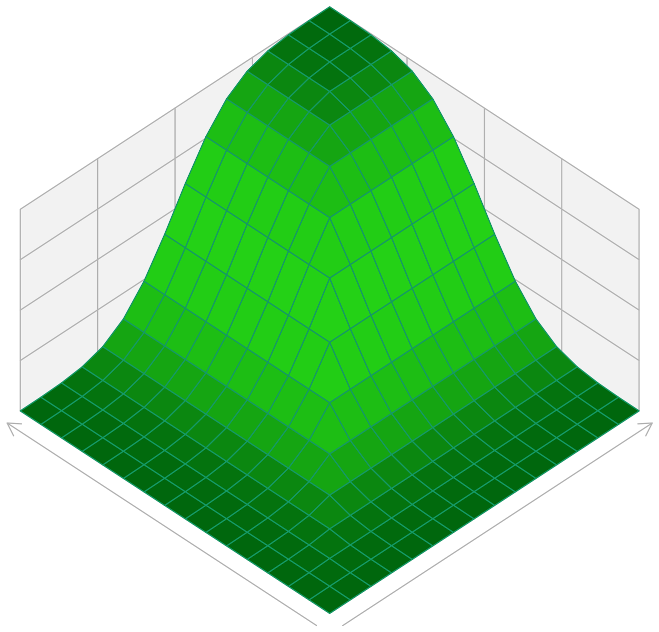
```
> #get warmed up...
> library (mvtnorm, warn=FALSE)
```

```
> #create a function, to plot the distributions
> normal.plot = function (cor=0, res=16, rng=c (-3.5, 3.5) )
 {        x1 = x2 = seq (rng [1], rng [2], length=res)
        m = matrix (numeric (), nr=res, nc=res)
        for (i in 1:res) for (j in 1:res)
                m [i, j] = pmvnorm (c (-Inf, -Inf), c (x1 [i], x2 [j]),
                        sigma=matrix (c (1, cor, cor, 1), nr=2) )
        plotbcdf (m)
 }
```

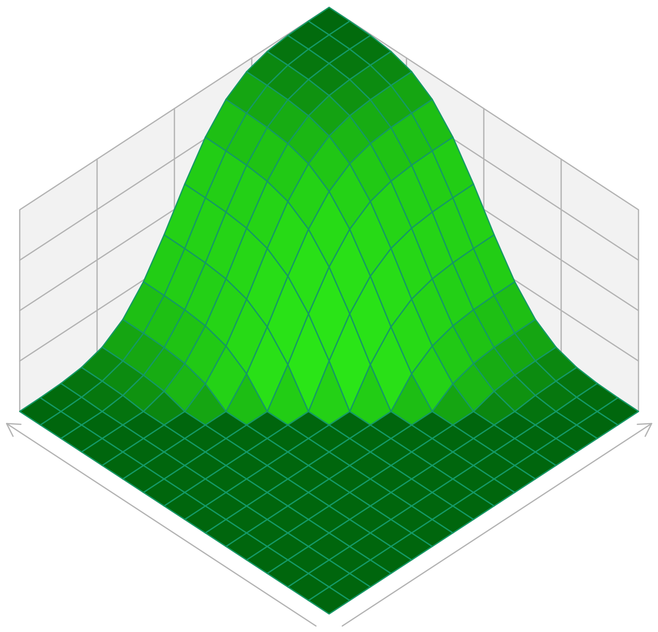
```
> normal.plot(0)
```



```
> normal.plot (1)
```



```
> normal.plot (-1)
```

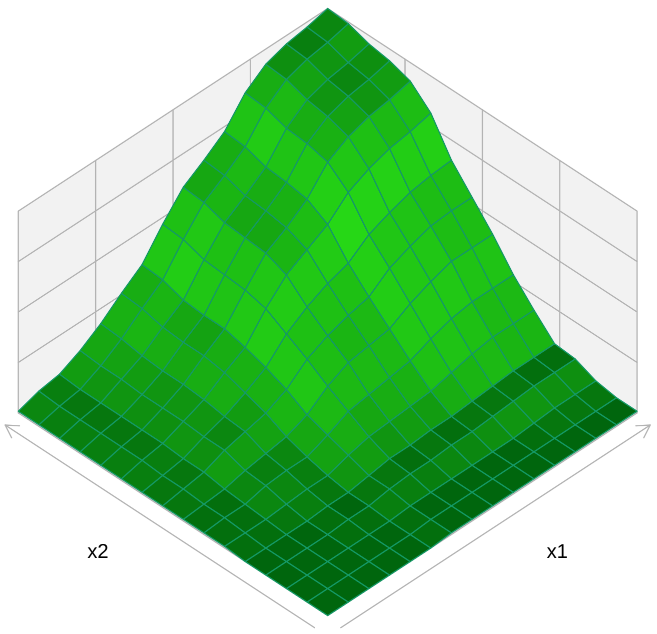


Now let's create three simulated datasets, from each of the distributions above (also using the mvtnorm package), and model the simulated data using bivariate ECDFs (from the mecdf package). We will use a sample size of 120. We could be pedantic and ensure the same ranges of the plots, however it makes little difference, so we will simply plot over the observed range.

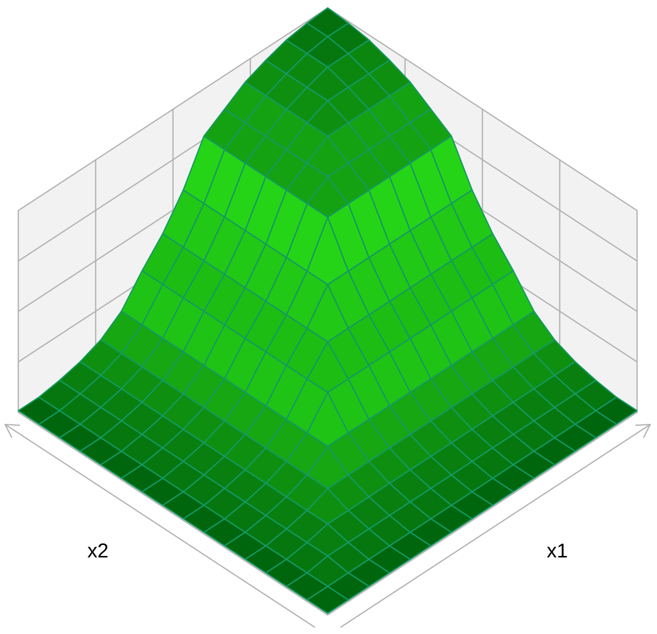
```
> #another convenience function
> normal.sim = function (n=1, cor=0)
```

```
         rmvnorm (n, c (0, 0), matrix (c (1, cor, cor, 1), nr=2) )
> m0 = mecdf (normal.sim (120, 0) )
> mpos = mecdf (normal.sim (120, 1) )
> mneg = mecdf (normal.sim (120, -1) )
```

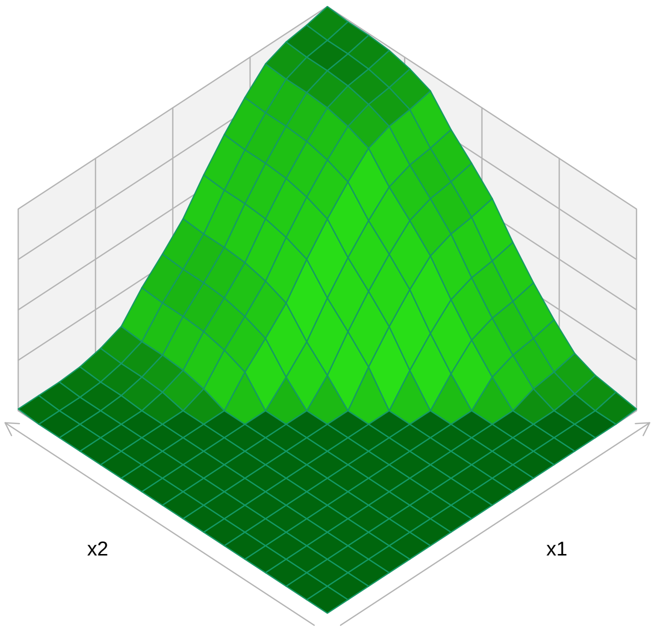
```
> plotbcdf (m0)
```



```
> plotbcdf (mpos)
```



```
> plotbcdf (mneg)
```



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