

USING BIVARIATE BÉZIER DISTRIBUTIONS TO MODEL SIMULATION INPUT PROCESSES

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ABSTRACT

We describe a graphical, interactive technique for modeling bivariate simulation input processes using a distribution family based on Bézier curves and surfaces. This family has an open-ended parameterization and is capable of accurately representing an unlimited variety of shapes for marginal distributions together with many common types of bivariate stochastic dependence. Our input-modeling technique is implemented in a Windows-based software system called PRIME—PRObabilistic Input Modeling Environment. Several examples illustrate the application of PRIME to subjective and data-driven estimation of bivariate distributions representing simulation inputs.

1 INTRODUCTION

One of the central problems in the design and construction of large-scale stochastic simulation experiments is the selection of valid input models—that is, probability distributions that accurately mimic the behavior of the random input processes driving the system. In many applications, it is critical not only to capture the shape of the marginal distribution of each major input random variable but also to represent accurately the stochastic dependencies between those variates (Lewis and Orav 1989). Although many practitioners appreciate the need for valid models of multivariate simulation inputs, they lack effective tools for building such input models. For many simulation experiments in which stochastic dependencies between input variates are explicitly modeled, ad hoc methods must be used to incorporate those features into the experiment; for example, see Veeramani, Barash, and Wilson (1991).

In this paper we extend the univariate input-modeling methodology of Wagner and Wilson (1993) to handle continuous bivariate populations, and we present a flexible, interactive, graphical technique for

modeling a broad range of input processes. We introduce Bézier surfaces as the parametric form for the representation of the bivariate input processes that arise in simulation experiments. We implemented this methodology in a Microsoft Windows-based software system called PRIME—PRObabilistic Input Modeling Environment.

The remainder of this paper is organized as follows. In Section 2 we describe our technique for the construction, manipulation, and simulation of bivariate Bézier distributions as well as the corresponding conditional univariate Bézier distributions. In Section 3 we describe the implementation of this methodology in PRIME, and in Section 4 we present some examples illustrating the diversity of bivariate distributions that can be modeled using this methodology. Finally, in Section 5 we summarize the main contributions of this work. This paper is based on Flanigan (1993).

2 FORMULATION OF BIVARIATE BÉZIER DISTRIBUTIONS

2.1 Definition of Bézier Surfaces

Starting from a set of *control points* represented by the column vectors $\{q_{i,j} \equiv (x_{i,j}, y_{i,j}, z_{i,j})^T : i = 0, 1, \dots, n_x, j = 0, 1, \dots, n_y\}$, we have the corresponding two-dimensional Bézier surface in three-dimensional space that is given parametrically as

$$Q(t_x, t_y) = \sum_{i=0}^{n_x} \sum_{j=0}^{n_y} B_{n_x,i}(t_x) B_{n_y,j}(t_y) q_{i,j} \quad (1)$$

for all $t_x, t_y \in [0, 1]$, where

$$B_{m,\ell}(t) \equiv \frac{m!}{\ell!(m-\ell)!} t^\ell (1-t)^{m-\ell} \text{ for } t \in [0, 1] \quad (2)$$

is the ℓ th Bernstein polynomial of degree m ; see Farin (1990). Wagner and Wilson (1993) provide some motivation for using weights of the form (2) to construct

a parametric representation of a curve or surface as a convex combination of a set of appropriately defined control points.

2.2 Bivariate Bézier Distribution Functions

If $(X, Y)^T$ is a continuous random vector with bounded support $[x_*, x^*] \times [y_*, y^*]$, unknown cumulative distribution function (c.d.f.) $F_{XY}(\cdot, \cdot)$, and unknown probability density function (p.d.f.) $f_{XY}(\cdot, \cdot)$, then we can approximate $F_{XY}(\cdot, \cdot)$ with an appropriate Bézier surface of the form (1), where the control points $\{q_{i,j}\}$ have been arranged so as to ensure the basic requirements of a joint distribution function: (a) $F_{XY}(x, y)$ is monotonically non-decreasing and continuous from the right in x and y ; (b) $F_{XY}(x_*, y) = 0$ for all y and $F_{XY}(x, y_*) = 0$ for all x ; (c) $F_{XY}(x^*, y^*) = 1$; and (d) $F_{XY}(x_2, y_2) - F_{XY}(x_1, y_2) - F_{XY}(x_2, y_1) + F_{XY}(x_1, y_1) \geq 0$ if $x_1 < x_2$ and $y_1 < y_2$.

In view of the computational and statistical advantages of univariate Bézier distributions detailed in Wagner and Wilson (1993), we seek to formulate the bivariate Bézier c.d.f. $F_{XY}(\cdot, \cdot)$ so that the marginal distribution of X is a univariate Bézier distribution whose c.d.f. $F_X(\cdot)$ is represented parametrically by

$$P(t_x) \equiv [P_x(t_x), P_z(t_x)]^T \equiv \sum_{i=0}^{n_x} B_{n_x,i}(t_x) p_i \quad (3)$$

for all $t_x \in [0, 1]$, where the i th control point in (3) is $p_i \equiv [x_i^{(X)}, z_i^{(X)}]^T$. Similarly, we seek a setup in which the marginal distribution of Y is a univariate Bézier distribution whose c.d.f. $F_Y(\cdot)$ is represented parametrically by

$$L(t_y) \equiv [L_y(t_y), L_z(t_y)]^T \equiv \sum_{j=0}^{n_y} B_{n_y,j}(t_y) l_j \quad (4)$$

for all $t_y \in [0, 1]$, where the j th control point in (4) is $l_j \equiv [y_j^{(Y)}, z_j^{(Y)}]^T$. As explained in Flanigan (1993), the coordinates of the control points used in displays (1), (3), and (4) must related as follows:

$$\left. \begin{matrix} x_{i,j} = x_i^{(X)} \\ y_{i,j} = y_j^{(Y)} \end{matrix} \right\} \text{ for } i = 0, 1, \dots, n_x \text{ \& } j = 0, 1, \dots, n_y; \quad (5)$$

and

$$z_{i,j} = \begin{cases} 0 & [= z_0^{(X)} = z_0^{(Y)}] \text{ if } i = 0 \text{ or } j = 0 \\ z_j^{(Y)} & \text{ for } i = n_x \text{ and } j = 1, 2, \dots, n_y - 1 \\ z_i^{(X)} & \text{ for } j = n_y \text{ and } i = 1, 2, \dots, n_x - 1 \\ 1 & [= z_{n_x}^{(X)} = z_{n_y}^{(Y)}] \text{ for } i = n_x, j = n_y \end{cases} \quad (6)$$

In terms of the setup specified by displays (3)–(6), we see that the joint c.d.f. $F_{XY}(\cdot, \cdot)$ of the Bézier random vector $(X, Y)^T$ is given parametrically by

$$\begin{aligned} Q(t_x, t_y) & \quad (7) \\ & \equiv [Q_x(t_x, t_y), Q_y(t_x, t_y), Q_z(t_x, t_y)]^T \\ & = [P_x(t_x), L_y(t_y), Q_z(t_x, t_y)]^T \end{aligned}$$

for all $t_x, t_y \in [0, 1]$; and it is straightforward to verify that a bivariate Bézier distribution for $(X, Y)^T$ whose c.d.f. $F_{XY}(\cdot, \cdot)$ is defined by equations (5)–(7) will have marginal c.d.f.'s $F_X(\cdot)$ and $F_Y(\cdot)$ for X and Y that are given parametrically by (3) and (4), respectively. Notice that the stochastic dependency between X and Y is represented by the $\{z_{i,j} : i = 1, \dots, n_x - 1; j = 1, \dots, n_y - 1\}$ —that is, by the z -coordinates that are *not* specified in (6).

If X and Y are independent, then we take $z_{i,j} = z_i^{(X)} \cdot z_j^{(Y)}$ for $i = 1, \dots, n_x - 1$ and $j = 1, \dots, n_y - 1$ so that the joint distribution function factors into the product of the two marginal distribution functions:

$$Q_z(t_x, t_y) = P_z(t_x) \cdot L_z(t_y) \text{ for all } t_x, t_y \in [0, 1]; \quad (8)$$

and (8) is equivalent to the more familiar factorization $F_{XY}(x, y) = F_X(x) \cdot F_Y(y)$ for all x, y .

2.3 Bivariate Bézier Density Functions

For the bivariate random vector $(X, Y)^T$ whose joint c.d.f. $F_{XY}(\cdot, \cdot)$ is specified by equation (1), the corresponding joint p.d.f. $f_{XY}(\cdot, \cdot)$ is given parametrically by

$$\begin{aligned} Q^*(t_x, t_y) & \quad (9) \\ & \equiv [Q_x^*(t_x, t_y), Q_y^*(t_x, t_y), Q_z^*(t_x, t_y)]^T \\ & = [P_x(t_x), L_y(t_y), Q_z^*(t_x, t_y)]^T \end{aligned}$$

for all $t_x, t_y \in [0, 1]$, where

$$Q_z^*(t_x, t_y) = \frac{\sum_{i=0}^{n_x-1} \sum_{j=0}^{n_y-1} B_{n_x-1,i}(t_x) B_{n_y-1,j}(t_y) \Delta_i \Delta_j z_{i,j}}{\left[\sum_{i=0}^{n_x-1} B_{n_x-1,i}(t_x) \Delta x_i \right] \left[\sum_{j=0}^{n_y-1} B_{n_y-1,j}(t_y) \Delta y_j \right]}, \quad (10)$$

with $\Delta x_i \equiv x_{i+1} - x_i$ (for $i = 0, 1, \dots, n_x - 1$) and $\Delta y_j \equiv y_{j+1} - y_j$ (for $j = 0, 1, \dots, n_y - 1$) respectively representing the corresponding first differences of the x - and y -coordinates of the control points $\{q_{i,j}\}$ in the formulation (1) of the joint c.d.f., and

$$\Delta_i \Delta_j z_{i,j} \equiv z_{i+1,j+1} - z_{i,j+1} - z_{i+1,j} + z_{i,j} \quad (11)$$

(for $i = 0, 1, \dots, n_x - 1$ and $j = 0, 1, \dots, n_y - 1$) representing the corresponding second partial differences of the z -coordinates of those control points. A detailed justification of (9)–(11) is given in Flanigan (1993).

2.4 Conditional Bézier Distributions

Given $Y = y(t_y) \equiv L_y(t_y)$, the conditional c.d.f. of X at the point $x(t_x) \equiv P_x(t_x)$ is univariate Bézier with

$$F_{X|Y}[x(t_x)|y(t_y)] = \frac{\sum_{i=1}^{n_x} B_{n_x,i}(t_x) \left\{ \sum_{j=0}^{n_y-1} B_{n_y-1,j}(t_y) [z_{i,j+1} - z_{i,j}] \right\}}{\sum_{j=0}^{n_y-1} B_{n_y-1,j}(t_y) \Delta z_j^{(Y)}} \quad (12)$$

provided $f_Y[y(t_y)] > 0$. It follows from (12) that the control points $\{[x_i, z_i^{(X|Y)}]^T : i = 0, 1, \dots, n_x\}$ for the Bézier curve representing the conditional distribution of X given $Y = y(t_y)$ have the same x -coordinates as in (3); and the corresponding z -coordinates are given by

$$z_i^{(X|Y)} = \frac{\sum_{j=0}^{n_y-1} B_{n_y-1,j}(t_y) [z_{i,j+1} - z_{i,j}]}{\sum_{j=0}^{n_y-1} B_{n_y-1,j}(t_y) \Delta z_j^{(Y)}} \quad (13)$$

for $i = 0, 1, \dots, n_x$. An analogous formulation yields $F_{Y|X}(\cdot)$, the conditional distribution of Y given X .

2.5 Covariance between Bézier Variates

The covariance between X and Y is given by

$$\text{Cov}(X, Y) = \sum_{i=0}^{n_x-1} \sum_{j=0}^{n_y-1} \vartheta_i^{(X)} \vartheta_j^{(Y)} \Delta_i \Delta_j z_{i,j}, \quad (14)$$

where

$$\vartheta_i^{(X)} \equiv \left[\frac{1}{2} \sum_{\ell=0}^{n_x} \frac{\binom{n_x}{\ell} \binom{n_x-1}{i} x_\ell}{\binom{2n_x-1}{i+\ell}} \right] - E[X] \quad (15)$$

for $i = 0, 1, \dots, n_x$,

$$\vartheta_j^{(Y)} \equiv \left[\frac{1}{2} \sum_{k=0}^{n_y} \frac{\binom{n_y}{k} \binom{n_y-1}{j} y_k}{\binom{2n_y-1}{j+k}} \right] - E[Y] \quad (16)$$

for $j = 0, 1, \dots, n_y$, and $\Delta_i \Delta_j z_{i,j}$ is defined by (11). For the random variable X (respectively, Y), the expected value $E[X]$ (respectively, $E[Y]$) and the variance $\text{Var}[X]$ (respectively, $\text{Var}[Y]$) are readily evaluated using computational formulas given in Wagner

and Wilson (1993) and derived in Flanigan (1993). Thus $\text{Corr}(X, Y)$, the correlation between X and Y is readily evaluated as $\text{Cov}(X, Y)/[\text{Var}(X)\text{Var}(Y)]^{1/2}$.

2.6 Generation of Bézier Vectors

The random vector $(X, Y)^T$ can be generated using the method of conditional distributions as follows. Given a pair of independent random numbers U_1 and U_2 , we compute Y from U_1 by inversion of the marginal c.d.f. $F_X(\cdot)$; then given Y , we compute X from U_2 by inversion of the conditional c.d.f. $F_{X|Y}(\cdot|Y)$. Specifically, this involves the following steps:

1. Generate $U_1, U_2 \sim \text{Uniform}[0, 1]$ independently.
2. Find $\tilde{t}_y \in [0, 1]$ such that

$$\sum_{j=0}^{n_y} B_{n_y,j}(\tilde{t}_y) z_j^{(Y)} = U_1; \quad (17)$$

3. Find $\tilde{t}_x \in [0, 1]$ such that

$$\sum_{i=0}^{n_x} B_{n_x,i}(\tilde{t}_x) z_i^{(X|Y)} = U_2; \quad (18)$$

4. Deliver the vector

$$(X, Y)^T = \left[\sum_{i=0}^{n_x} B_{n_x,i}(\tilde{t}_x) x_i, \sum_{j=0}^{n_y} B_{n_y,j}(\tilde{t}_y) y_j \right]^T \quad (19)$$

Notice that a root-finding procedure is required to compute the solutions to equations (17) and (18).

3 MODELING BIVARIATE BÉZIER DISTRIBUTIONS USING PRIME

PRIME, PRobabilistic Input Modeling Environment, is a graphical Microsoft Windows-based software system that incorporates the methodology developed in Section 2 to help an analyst estimate the bivariate input processes that arise in large-scale simulation studies. PRIME is designed for IBM-compatible microcomputers equipped with a math coprocessor and a pointing device such as a mouse. It is written entirely in the C programming language, and it has been developed to run under version 3.1 of Microsoft Windows (Microsoft Corporation 1992). PRIME is designed to be easy and intuitive to use. The construction of a bivariate distribution is performed through

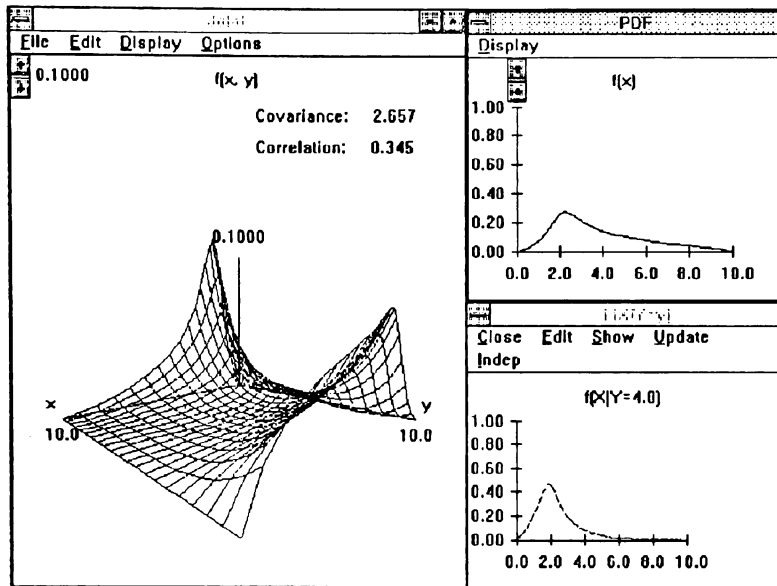


Figure 1: A Typical Bivariate PRIME Session

the actions of the mouse, and several options are conveniently available through menu selections.

In PRIME, the user manipulates the marginal distributions independently of each other; then to complete the construction of a bivariate input model, the user manipulates the joint p.d.f. (9) or selected conditional c.d.f.'s like (12). For example, to edit (subjectively estimate) the marginal c.d.f. (4) of Y , the user may add, delete, or move the control points $\{l_j : j = 0, 1, \dots, n_y\}$ by moving the mouse within a window depicting $F_Y(\cdot)$. Control points are represented as small black squares, and each control point is given a unique label corresponding to its index j in equation (4). Each control point acts like a “magnet” pulling the curve in the direction of the control point, where the Bernstein polynomials (2) govern the strength of the “magnetic attraction” of each control point. The movement of a control point causes the displayed curve to be updated (nearly) instantaneously. Figure 1 displays a typical PRIME session depicting a bivariate joint density $f_{XY}(\cdot, \cdot)$ with $\text{Cov}(X, Y) = 2.657$ and $\text{Corr}(X, Y) = 0.345$, the marginal density $f_X(\cdot)$, and the conditional density $f_{X|Y}(\cdot|Y = 4.0)$.

In addition to subjective estimation of bivariate Bézier distributions by interactive manipulation of the control points, PRIME allows data-driven estimation of the control points that yield the “best” fit to the sample data according to a variety of statistical-estimation principles. In the next section we illustrate both modes of operation for PRIME.

4 EXAMPLES

4.1 Fitting Bivariate Distributions Subjectively

In the absence of data, PRIME can be used to construct a bivariate input process conceptualized from subjective information and expertise. The representation of the conceptualized distribution is achieved by: (a) constructing the two marginal distributions by manipulating the control points associated with each marginal distribution; and (b) representing the dependencies between the two marginal distributions by either moving the control points associated with the joint density, or by moving the control points associated with the conditional distributions.

For example, suppose it is known that the processing times for two successive manufacturing operations are negatively correlated, with correlation coefficient of -0.37 . The distribution of the first processing time is denoted by X , where X is known to have a minimum value of 2 minutes, a maximum value of 6 minutes, and a most likely (modal) value of 3 minutes. The distribution of the second processing time is denoted by Y , where Y is known to have a minimum value of 3 minutes, a maximum value of 9 minutes, and a most likely (modal) value of 6 minutes. To construct the joint distribution of (X, Y) , we must first define the two marginal distributions. Figure 2 shows the two marginal distributions that were defined by placing the control points corresponding to the respective marginal distributions. After the marginal

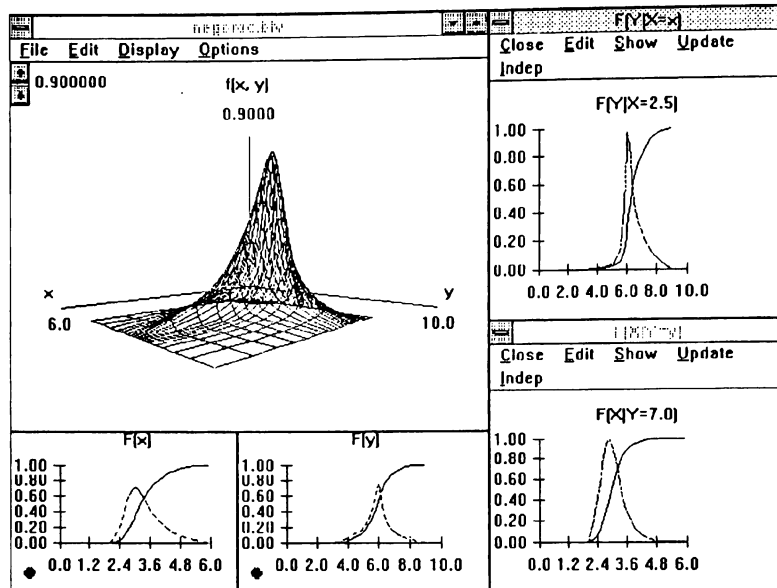


Figure 2: A Bivariate Distribution of Processing Times $(X, Y)^T$ with $\text{Corr}(X, Y) = -0.369$

distributions were satisfactorily constructed, the dependencies between X and Y were modeled. In this case, the dependencies were modeled by moving the control points associated with the conditional distributions until the correlation of the fitted joint distribution was approximately equal to -0.37 . In Figure 2, the displayed joint distribution has a correlation of -0.369 .

4.1.1 Uniform Marginal Distributions

Figure 3 depicts a PRIME session where each marginal distribution is uniform; that is, $X \sim \text{Uniform}[0, 10]$ and $Y \sim \text{Uniform}[0, 10]$. Figure 3 displays a bivariate distribution for $(X, Y)^T$ with $\text{Cov}(X, Y) = -5.322$ and $\text{Corr}(X, Y) = -0.645$. Beneath the window containing the joint p.d.f., there are two windows displaying the marginal c.d.f.'s, $F_X(\cdot)$ and $F_Y(\cdot)$; and these latter windows also display as dashed curves the corresponding marginal p.d.f.'s, $f_X(\cdot)$ and $f_Y(\cdot)$. To the right of the joint p.d.f. window are two windows depicting the conditional c.d.f.'s $F_{Y|X}(\cdot|X = 9.0)$ and $F_{X|Y}(\cdot|Y = 2.0)$; and these c.d.f. windows also display as dashed curves the corresponding conditional p.d.f.'s. As shown in the joint p.d.f. window, most of the probability mass is concentrated along the line $y = -x + 10$.

4.1.2 Nonuniform Marginal Distributions

Figure 4 depicts the joint c.d.f. and p.d.f. of the

nonuniform random vector $(X, Y)^T$. Notice that for this case, $\text{Cov}(X, Y) = 2.133$ and $\text{Corr}(X, Y) = 0.539$. Figure 4 also shows the conditional c.d.f.'s $F_{Y|X}(Y|X = 3.0)$ and $F_{X|Y}(X|Y = 8.0)$.

4.2 Fitting Bivariate Distributions to Data

Suppose that a random sample $\{(X_k, Y_k)^T : k = 1, 2, \dots, m\}$ has been taken from an unknown continuous bivariate distribution, and we seek to approximate this distribution with a bivariate Bézier c.d.f. $F_{XY}(\cdot, \cdot)$. Let

$$F_m(x, y) \equiv \#\{(X_k, Y_k) : X_k \leq x, Y_k \leq y\}/m$$

denote the corresponding empirical c.d.f., and let $F_m(x)$ and $G_m(y)$ denote the corresponding marginal empirical c.d.f.'s for X and Y , respectively.

After fitting a marginal distribution separately to each component of the random sample $\{(X_k, Y_k)^T\}$, the user can model the dependencies between these components. The dependencies are modeled by moving the control points associated with either the joint Bézier p.d.f. $f_{XY}(\cdot, \cdot)$ or the conditional Bézier c.d.f.'s or p.d.f.'s until the desired stochastic dependence is achieved. Figure 5 displays the fitted joint p.d.f., a superimposed bivariate histogram, and the fitted marginal distributions that were estimated by the method of moments from a random sample $\{(X_k, Y_k)^T : k = 1, 2, \dots, m\}$ of size $m = 44$ with sample statistics $\widehat{\text{Cov}}(X, Y) = -1.979$ and

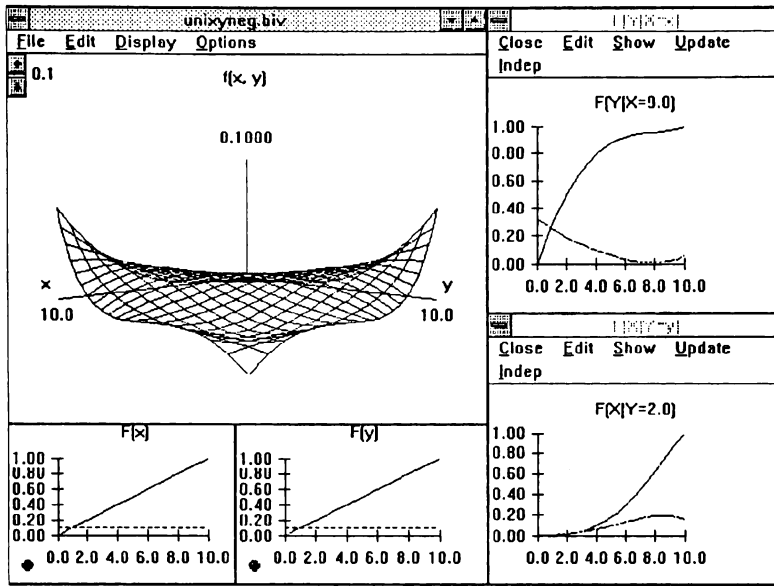


Figure 3: A Negatively Correlated Distribution with Uniform Marginals

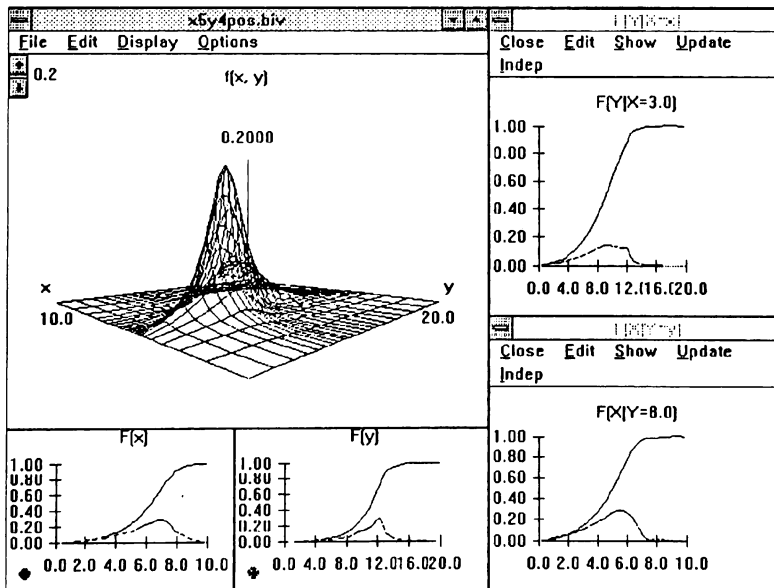


Figure 4: A Positively Correlated Distribution with Nonuniform Marginals

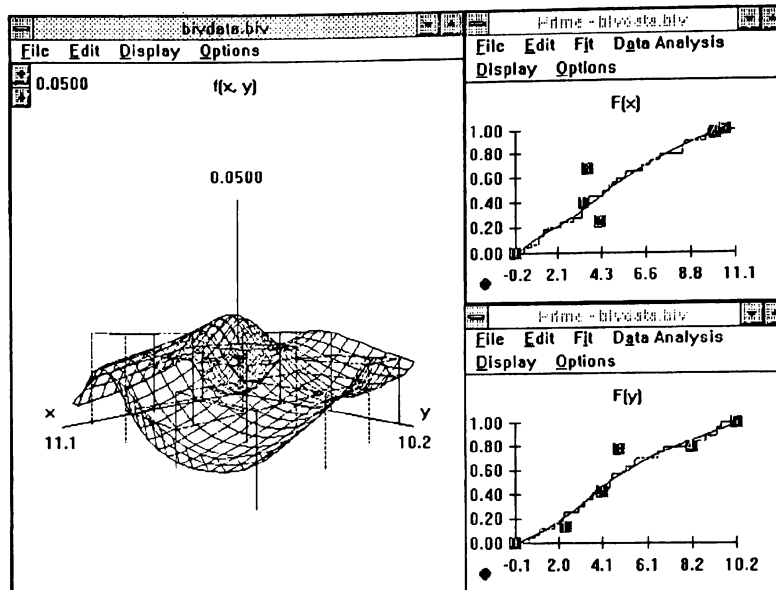


Figure 5: A Bivariate Distribution Fit to Data

$\widehat{\text{Corr}}(X, Y) = -0.255$. After each marginal distribution was satisfactorily fitted to its corresponding component of the sample $\{(X_k, Y_k)\}$, the dependencies between X and Y were modeled. The control points for the joint p.d.f. were manipulated until the theoretical covariance $\text{Cov}(X, Y)$ for the fitted distribution matched the sample covariance $\widehat{\text{Cov}}(X, Y) = -1.979$.

4.3 Manipulating Conditional Distributions

The conditional p.d.f.'s and c.d.f.'s are edited in the same manner as the marginal distributions, except that the control points for the conditional p.d.f.'s and c.d.f.'s are only allowed to move in the vertical direction.

5 SUMMARY, CONCLUSIONS, AND RECOMMENDATIONS

5.1 Bivariate Bézier Distribution Families

If $(X, Y)^T$ is a continuous random vector having a bivariate Bézier distribution function $F_{XY}(\cdot, \cdot)$ as defined in Section 2.2, then the distribution of $(X, Y)^T$ has the following properties:

- The joint c.d.f., represented parametrically by (1) as a Bézier surface, is similar in form to a Bézier curve. The Bernstein polynomials (2) are the same basis functions used for both Bézier curves and Bézier surfaces.

- The joint p.d.f., $f_{XY}(\cdot, \cdot)$, has a closed-form parametric representation as a ratio of Bézier functions, as given by (10).
- The conditional c.d.f.'s, $F_{X|Y}(\cdot|\cdot)$ and $F_{Y|X}(\cdot|\cdot)$, have the same parametric form as the univariate marginal c.d.f.'s; and the control points that define the conditional c.d.f.'s are easily related to the control points that define the joint c.d.f.
- The conditional p.d.f.'s, $f_{X|Y}(\cdot|\cdot)$ and $f_{Y|X}(\cdot|\cdot)$, have the same parametric form as the univariate marginal p.d.f.'s; and the control points that define the conditional p.d.f.'s are easily related to the control points that define the joint c.d.f.
- The covariance between X and Y , $\text{Cov}(X, Y)$, for a joint distribution function represented parametrically as a Bézier surface, has a closed-form expression given by (14).
- The parameterization of the bivariate Bézier distribution family is both natural and open-ended. The coordinates of the control points define the distribution parameters; and if additional flexibility is required, it is easily achieved by adding more control points.

5.2 Modeling Simulation Inputs with PRIME

From the user's point of view, PRIME is an easy-to-use, intuitive, graphical software system. PRIME

provides immediate, visual feedback on the currently configured distribution. The user can easily alter an inappropriately configured distribution by adding, deleting, or relocating one or more of the relevant control points for the joint p.d.f., the marginal p.d.f.'s or c.d.f.'s, or the conditional c.d.f.'s or p.d.f.'s. PRIME also provides a framework for viewing and manipulating bivariate distributions.

5.3 Recommendations for Future Work

Several aspects of this work require further development. Of particular interest is the extension of the methodology to handle trivariate and higher-dimensional distributions. For subjective estimation of continuous multivariate distributions, we also require more comprehensive techniques for visually representing and manipulating general types of stochastic dependence. For data-driven estimation of continuous multivariate distributions, we require fully automated fitting schemes to estimate not only the marginal distributions of the target random vector but also the stochastic dependency structure between components of that random vector.

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