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AN ALGORITHM FOR NONPARAMETRIC DENSITY ESTIMATION,(U)
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AN ALGORITHM FOR NONPARAMETRIC DENSITY ESTIMATION[1]

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ABSTRACT

A numerical algorithm is given for implementing a nonparametric maximum penalized likelihood estimator similar to those proposed by Good and Gaskins and those proposed by de Montricher, Tapia and Thompson. It is shown how the resulting nonlinear constrained optimization problem may be effectively solved by using Tapia's approach to Newton's method for constrained problems.

1. Introduction. de Montricher, Tapia and Thompson demonstrated that the standard histogram was an unstable maximum likelihood density estimator and considered maximum penalized likelihood estimators similar to those previously considered by Good and Gaskins (1971). Specifically suppose we are given the random sample $x_1,\ldots,x_N \in (a,b)$. Let $H_0^1(a,b)$ consist of the functions f defined on (a,b) with the property that $f(a) = f(b) = 0$ and f' is a member of $L^2(a,b)$. Estimate the density function which gave rise to the random sample $x_1,\ldots,x_N$ by the solution of the constrained optimization problem

(1.1) $\max L(f); f \in H_0^1(a,b),\ f \geq 0$ and

$$\int_a^b f(x)dx = 1,$$

where

(1.2) $$L(f) = \prod_{i=1}^{N} f(x_i)\exp\left(-\alpha\int_a^b |f'(x)|^2 dx\right),\ (\alpha > 0).$$

The functional L in (1.2) is called the penalized likelihood and the solution of (1.1) is called the maximum penalized likelihood estimator based on the random sample $x_1,\ldots,x_N$. de Montricher, Tapia and Thompson (1975) proved that problem (1.1) has a unique solution and is a monospline of degree two, i.e., a polynomial of degree two plus a spline of degree one. We now give a numerical algorithm for approximating this monospline.

2. The Discrete Problem. For given n, consider the mesh $t_0,\ldots,t_{n+1}$ where $t_i = a + ih$, $i = 0,\ldots,n+1$ with $h = (b-a)/(n+1)$. Let $\hat{H}_0^1$ denote the vector space of all continuous piecewise linear functions which have knots at $t_1,\ldots,t_n$ and vanish at a and b. For $p \in \hat{H}_0^1$ let $y_i = p(t_i)$, $i = 0,\ldots,n+1$. Then $y_0 = y_{n+1} = 0$ and

(2.1) $p(x) \geq 0 \Leftrightarrow y_i \geq 0,\quad i = 1,\ldots,n$

(2.2) $$\int_a^b p(x)dx = h\sum_{i=0}^{n} y_i$$

(2.3) $$\int_a^b p'(x)^2 dx = \frac{1}{h}\sum_{i=0}^{n}(y_{i+1} - y_i)^2 .$$

Let

(2.4) $\nu_1 = \#\text{of } x_i \text{ in } [a, t_1 + \frac{h}{2})$

(2.5) $\nu_i = \#\text{of } x_i \text{ in } [t_{i-1} + \frac{h}{2},\ t_i + \frac{h}{2}),\quad i = 2,\ldots,n-1$

(2.6) $\nu_n = \#\text{of } x_i \text{ in } [t_{n-1} + \frac{h}{2}, b).$

We shall assume that we have enough data so that $\nu_i > 0\ \forall\ i$. Our finite dimensional

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(15)

approximation to problem (1.1) is

(2.7) max $\hat{L}(y); y_i \geq 0 \ \forall\, i$ and $\sum_{i=1}^{n} y_i = h^{-1}$

where

(2.8) $\hat{L}(y) = \prod_{i=1}^{n} y_i^{\nu_i} \exp(-\alpha h^{-1} \sum_{i=1}^{n} (y_{i+1}-y_i)^2)$.

Clearly (2.7) is a constrained optimization problem in R^n.

Proposition 2.1. The constraints $y_i \geq 0$ of problem (2.7) are not active at the solution.

Proof. If $y^* = (hN)^{-1}(1,\ldots,1)$, then y^* satisfies all the constraints of problem (2.7) and $\hat{L}(y) > 0$. Moreover, if $y = (y_1,\ldots,y_n)$ is such that $y_i = 0$ for some i, then $L(y) = 0$. This proves the proposition.

It follows that we can obtain the solution of problem (2.7) by solving

(2.9) $\min(-\log \hat{L}(y)); \sum_{i=1}^{n} y_i = h^{-1}$

where from (2.8) we see that

(2.10) $-\log(\hat{L}(y)) = -\sum_{i=1}^{n} \nu_i \log(y_i) + \alpha h^{-1} \sum_{i=1}^{n} (y_{i+1} - y_i)^2$.

3. The Algorithm. The Lagrangian for problem (2.9) is

(3.1) $\ell(y,\lambda) = -\sum_{i=1}^{n} \nu_i \log(y_i) + \alpha h^{-1} \sum_{i=0}^{n} (y_{i+1} - y_i)^2 + \lambda(\sum_{i=1}^{n} y_i - h^{-1})$.

The gradient of the Lagrangian is

(3.2) $\nabla\ell(y,\lambda) = (\ldots, -\nu_i y_i^{-1} + 2\alpha h^{-1}(-y_{i+1} + 2y_i - y_{i-1}) + \lambda, \ldots)^T$

and the Hessian of the Lagrangian is the diagonally dominant tridiagonal matrix

(3.3) $\nabla^2\ell(y,\lambda) = \begin{pmatrix} d_o^1 & d_1 & & & \\ d_{-1} & d_o^2 & d_1 & & \\ & \ddots & \ddots & \ddots & \\ & & d_{-1} & d_o^{n-1} & d_1 \\ & & & d_{-1} & d_o^n \end{pmatrix}$

where $d_{-1} = d_1 = -2\alpha h^{-1}$ and

$d_o^i = 4\alpha h^{-1} + \nu_i (y_i^{-1})^2$.

It therefore follows that Tapia's (1974), (1976) approach to Newton's method for constrained problems is a natural one for this problem and the operation count will be $O(n)$ per iteration instead of the usual $O(n^3)$ expected from Newton's method.

Let $g(y) = \sum_{i=1}^{n} y_i - h^{-1}$. Then $U = \nabla g(y) = (1,\ldots,1)^T$. We use $\langle , \rangle$ to denote the inner product in R^n.

The Newton-like Algorithm.

Step 1. Determine $\alpha > 0$, $\epsilon > 0$, y^o, λ^o and set $k := 0$.

Step 2. Calculate

$\lambda^{k+1} = \langle U, \nabla^2\ell(y^k,\lambda^k)^{-1}U\rangle^{-1}(g(y^k) - \langle U, \nabla^2 L(y^k,\lambda^k)^{-1}U\rangle)$

and

$y^{k+1} = y^k - \nabla^2\ell(y^k,\lambda^k)^{-1}\nabla\ell(y^k,\lambda^{k+1})$

Step 3. If $\|\nabla\ell(x^k,\lambda^k)\| \leq \epsilon$, then stop. If not, then set $k := k+1$ and go to Step 2.

Initialization values could be

$\epsilon = 10^{-4}$

$\alpha = 5.0$

$y^o = (nh)^{-1}(1,\ldots,1)$

and

$\lambda^o = -2(nh)^{-1}(y_1 + y_n) + \sum_{i=1}^{n} \nu_i (ny_i)^{-1}$.

This λ^o is given by the projection formula in Tapia (1976).

For a complete description of this algorithm and related quasi-Newton methods for constrained optimization the reader is referred to Tapia (1976).

Proposition 3.1. The above algorithm is locally quadratically convergent and requires only $O(n)$ operations per iteration.

4. Some Numerical Examples. Although for reasons of conciseness it was appropriate to develop the above discrete maximum penalized likelihood algorithm using the integral of the square of the first derivative in the penalty team, we have found by experience that the slightly more complicated second derivative approach gives less locally "rough" estimators. Namely we consider the problem

(4.1) Max $L(f); f \in H_o^2(a,b)$, $f \geq 0$ and $\int_a^b f(x)dx = 1$

where

(4.2) $L(f) = \prod_{i=1}^{n} f(x_i) \exp[-\alpha \int_a^b |f''(x)|^2 dx]$, $(\alpha > 0)$.

The details of the algorithm to approximate the solution to this problem are omitted, since they are very similar to the argument in Section 2. The operation count is still $O(n)$ per iteration.

In Figure 1, we demonstrate the solution to (4.1) using a random sample of size 20 from the standard normal distribution with mean 0 and variance 1. In Figure 2, we show the

estimator based on a sample of size 100. In Figures 3 and 4 we show the D.M.P.L.E.estimators for the 50-50 mixture of two normal distributions, both having variance 1 and with means at -1.5 and +1.5 for samples of size 25 and 100 respectively.

One comforting feature of the maximum penalized likelihood procedure is the relatively robust quality of the estimator in that changes of the optimal α with N and from distribution to distribution tend not to be traumatic, and that a rough and ready guess for α (e.g., 10) is frequently satisfactory. In Figures 5 and 6 we show an estimate for the Gaussian mexture mentioned above for a sample size of 300 and α values of 10 and .1.

If the density to be estimated is denoted by $f(\cdot)$ and the D.M.P.L.E. is denoted by $\hat{f}(\cdot)$, then we consider as one measure of estimate quality the average integrated mean square error

$$(4.3)\quad \text{IMSE} = \int (\hat{f}(x) - f(x))^2 f(x)dx \ .$$

I.M.S.E.'s for various α and N are given in Table 1 for the standard normal, the 50-50 normal mixture mentioned above, the t distribution with 5 degrees of freedom and the F distribution with (10,10) degrees of freedom.

TABLE 1

Average I.M.S.E. of the D.M.P.L.E. for α Perturbed by a Factor of Two. Divide α by 10 for the $F_{10,10}$ Samples.

	I.M.S.E. for		
Sample	$\alpha = 5$	$\alpha = 10$	$\alpha = 20$
N(0.1) N = 25	.00242	.00267	.00427
N(0.1) N = 100	.00093	.00079	.00089
N(0,1) N = 400	.00037	.00033	.00035
N(0.1) N = 800	.00028	.00022	.00019
Bimodal N = 25	.00197	.00159	.00152
Bimodal N = 100	.00070	.00054	.00171
Bimodal N = 400	.00030	.00024	.00022
t_5 N = 25	.00297	.00282	.00350
t_5 N = 100	.00092	.00084	.00101
t_5 N = 400	.00039	.00032	.00030
$F_{10,10}$ N = 25	.03208	.03865	.05519
$F_{10,10}$ N = 100	.00996	.01390	.02411
$F_{10,10}$ N = 400	.00292	.00450	.00740

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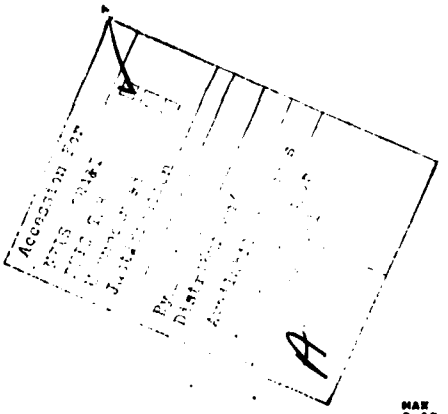

NORMAL [0,1] SAMPLE OF SIZE 20 VS.
DISCRETIZED MAXIMUM LIKELIHOOD PENALIZED ESTIMATE
WITH WEIGHING PARAMETER ALPHA 0.1000000000D+02
37 MESH POINTS FROM -3.25000 TO 3.25000
DISCRETE MESH INTERVAL 0.25000
INTEGRATED MEAN SQUARE ERROR 0.2810760180D-03
INTEGRATED SQUARE ERROR 0.9547291814D-02
MAXIMUM ABSOLUTE DIFFERENCE 0.7201856563D-01
LOG LIKELIHOOD TERM -0.2724104296D+02
LOG PENALTY TERM -0.1255486707D+01

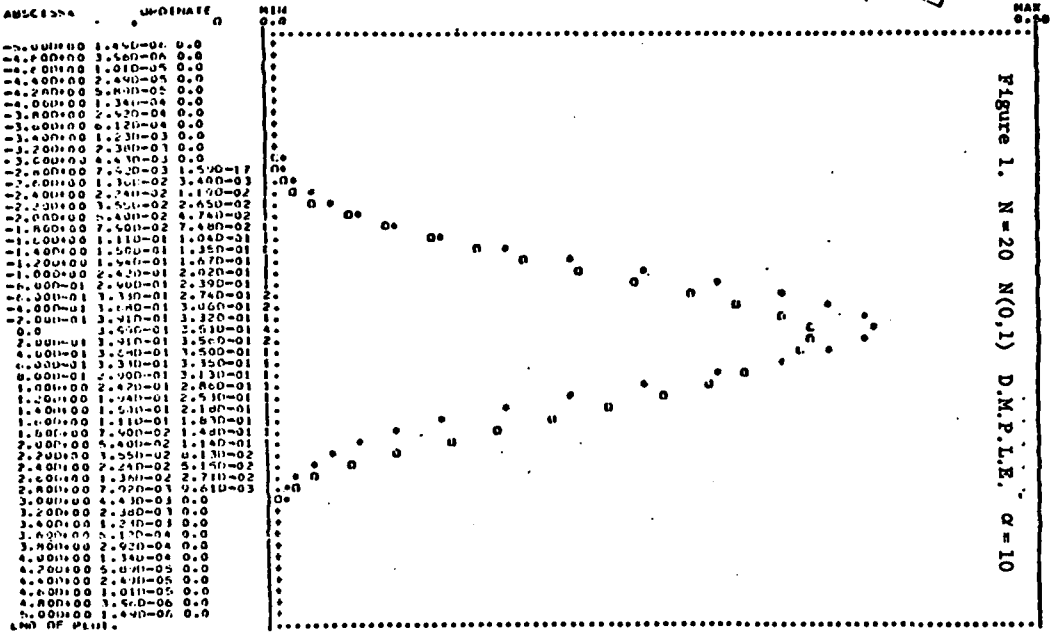

Figure 1. N = 20 N(0,1) D.M.P.L.E. $\alpha = 10$

NORMAL [0,1] SAMPLE OF SIZE 100 VS.
DISCRETIZED MAXIMUM LIKELIHOOD PENALIZED ESTIMATE
WITH WEIGHING PARAMETER ALPHA 0.1000000000D+02
37 MESH POINTS FROM -3.25000 TO 3.25000
DISCRETE MESH INTERVAL 0.25000
INTEGRATED MEAN SQUARE ERROR 0.3462435498D-02
INTEGRATED SQUARE ERROR 0.4731637930D-01
MAXIMUM ABSOLUTE DIFFERENCE 0.4116194257D+03
LOG LIKELIHOOD TERM -0.1401337549D+01
LOG PENALTY TERM

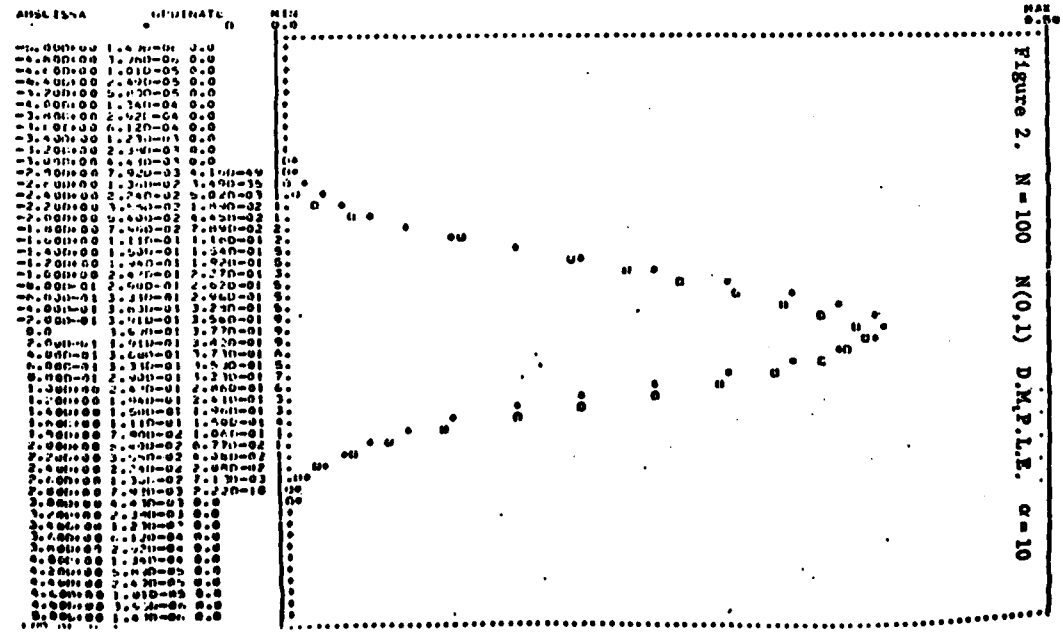

Figure 2. N = 100 N(0,1) D.M.P.L.E. $\alpha = 10$

BIMODAL NORMAL WITH MEANS = +- 1.50 VARIANCE OF LEFT = 1 WITH WEIGHT AND VARIANCE OF RIGHT = 0.5000 1.0000
SAMPLE SIZE = 25 WITH 13 SAMPLES ON RIGHT VS.
DISCRETIZED MAXIMUM LIKELIHOOD PENALIZED ESTIMATE
WITH WEIGHTING PARAMETER ALPHA 0.1000000000D+02
41 MESH POINTS FROM -5.00000 TO 5.00000
DISCRETE MESH INTERVAL 0.25000
INTEGRATED MEAN SQUARE ERROR 0.7011074430D-03
INTEGRATED SQUARE ERROR 0.6220122060D-02
MAXIMUM ABSOLUTE DIFFERENCE 0.6347762952D-01
LOG LIKELIHOOD TERM -0.4521376387D+02
LOG PENALTY TERM -0.2351619451D+01

ABSCISSA	ORDINATE *	ORDINATE O
-5.000D+00	4.36D-04	0.0
-4.800D+00	8.61D-04	0.0
-4.600D+00	1.63D-03	3.79D-03
-4.400D+00	2.94D-03	1.09D-02
-4.200D+00	5.21D-03	2.00D-02
-4.000D+00	8.76D-03	2.91D-02
-3.800D+00	1.42D-02	3.08D-02
-3.600D+00	2.20D-02	3.07D-02
-3.400D+00	3.28D-02	3.22D-02
-3.200D+00	4.70D-02	3.65D-02
-3.000D+00	6.49D-02	5.11D-02
-2.800D+00	8.57D-02	7.46D-02
-2.600D+00	1.09D-01	1.04D-01
-2.400D+00	1.33D-01	1.37D-01
-2.200D+00	1.56D-01	1.69D-01
-2.000D+00	1.76D-01	1.98D-01
-1.800D+00	1.92D-01	2.18D-01
-1.600D+00	2.00D-01	2.28D-01
-1.400D+00	2.01D-01	2.28D-01
-1.200D+00	1.96D-01	2.20D-01
-1.000D+00	1.85D-01	2.05D-01
-8.000D-01	1.70D-01	1.89D-01
-6.000D-01	1.55D-01	1.73D-01
-4.000D-01	1.42D-01	1.60D-01
-2.000D-01	1.33D-01	1.52D-01
0.0	1.30D-01	1.49D-01
2.000D-01	1.33D-01	1.55D-01
4.000D-01	1.42D-01	1.65D-01
6.000D-01	1.55D-01	1.77D-01
8.000D-01	1.70D-01	1.90D-01
1.000D+00	1.85D-01	2.02D-01
1.200D+00	1.96D-01	2.10D-01
1.400D+00	2.01D-01	2.03D-01
1.600D+00	2.00D-01	1.95D-01
1.800D+00	1.92D-01	1.72D-01
2.000D+00	1.76D-01	1.47D-01
2.200D+00	1.56D-01	1.11D-01
2.400D+00	1.33D-01	7.62D-02
2.600D+00	1.09D-01	4.61D-02
2.800D+00	8.57D-02	2.28D-02
3.000D+00	6.49D-02	7.24D-03
3.200D+00	4.70D-02	1.45D-03
3.400D+00	3.28D-02	5.03D-16
3.600D+00	2.20D-02	1.82D-32
3.800D+00	1.42D-02	3.12D-03
4.000D+00	8.76D-03	1.56D-02
4.200D+00	5.21D-03	1.69D-02
4.400D+00	2.94D-03	1.18D-02
4.600D+00	1.63D-03	4.92D-03
4.800D+00	8.61D-04	0.0
5.000D+00	4.36D-04	0.0

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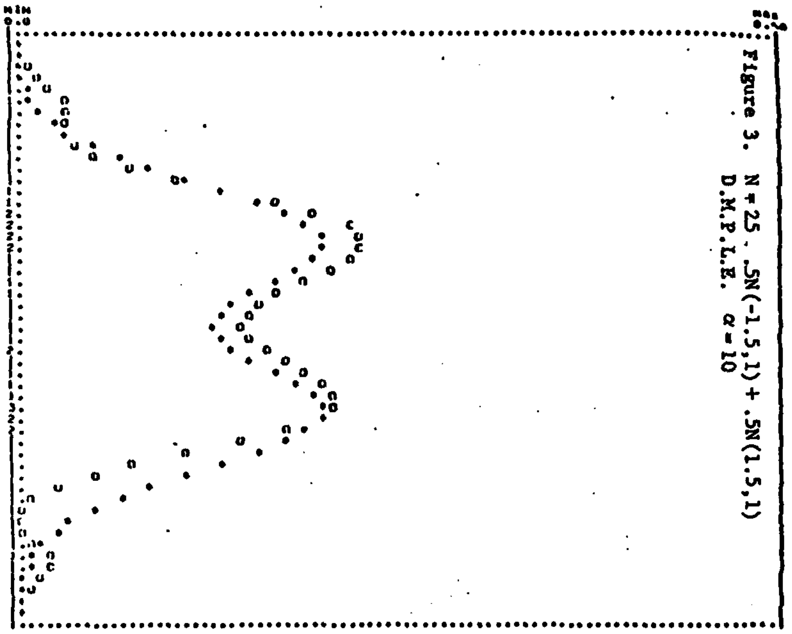

Figure 3. N = 25 .5N(-1.5,1) + .5N(1.5,1) D.M.P.L.E. α = 10

BIMODAL NORMAL WITH MEANS = +- 1.50 VARIANCE OF LEFT = 1 WITH WEIGHT AND VARIANCE OF RIGHT = 0.5000 1.0000
SAMPLE SIZE = 100 WITH 50 SAMPLES ON RIGHT VS.
DISCRETIZED MAXIMUM LIKELIHOOD PENALIZED ESTIMATE
WITH WEIGHTING PARAMETER ALPHA 0.1000000000D+02
41 MESH POINTS FROM -5.00000 TO 5.00000
DISCRETE MESH INTERVAL 0.25000
INTEGRATED MEAN SQUARE ERROR 0.1126789964D-01
INTEGRATED SQUARE ERROR 0.5476640062D-01
MAXIMUM ABSOLUTE DIFFERENCE 0.2323925084D-01
LOG LIKELIHOOD TERM -0.1867027496D+03
LOG PENALTY TERM -0.1713146243D+01

ABSCISSA	ORDINATE *	ORDINATE O
-5.000D+00	4.36D-04	0.0
-4.800D+00	8.61D-04	0.0
-4.600D+00	1.63D-03	2.03D-60
-4.400D+00	2.94D-03	1.51D-56
-4.200D+00	5.21D-03	3.01D-56
-4.000D+00	8.76D-03	3.31D-64
-3.800D+00	1.42D-02	1.96D-47
-3.600D+00	2.20D-02	2.25D-03
-3.400D+00	3.28D-02	1.27D-02
-3.200D+00	4.70D-02	3.15D-02
-3.000D+00	6.49D-02	4.80D-02
-2.800D+00	8.57D-02	8.14D-02
-2.600D+00	1.09D-01	1.05D-01
-2.400D+00	1.33D-01	1.29D-01
-2.200D+00	1.56D-01	1.52D-01
-2.000D+00	1.76D-01	1.75D-01
-1.800D+00	1.92D-01	1.83D-01
-1.600D+00	2.00D-01	1.95D-01
-1.400D+00	2.01D-01	1.96D-01
-1.200D+00	1.96D-01	1.92D-01
-1.000D+00	1.85D-01	1.82D-01
-8.000D-01	1.70D-01	1.67D-01
-6.000D-01	1.55D-01	1.54D-01
-4.000D-01	1.42D-01	1.44D-01
-2.000D-01	1.33D-01	1.35D-01
0.0	1.30D-01	1.30D-01
2.000D-01	1.33D-01	1.24D-01
4.000D-01	1.42D-01	1.31D-01
6.000D-01	1.55D-01	1.42D-01
8.000D-01	1.70D-01	1.61D-01
1.000D+00	1.85D-01	1.86D-01
1.200D+00	1.96D-01	2.07D-01
1.400D+00	2.01D-01	2.19D-01
1.600D+00	2.00D-01	2.20D-01
1.800D+00	1.92D-01	2.10D-01
2.000D+00	1.76D-01	1.93D-01
2.200D+00	1.56D-01	1.72D-01
2.400D+00	1.33D-01	1.50D-01
2.600D+00	1.09D-01	1.26D-01
2.800D+00	8.57D-02	1.00D-01
3.000D+00	6.49D-02	7.41D-02
3.200D+00	4.70D-02	5.11D-02
3.400D+00	3.28D-02	3.60D-02
3.600D+00	2.20D-02	2.80D-02
3.800D+00	1.42D-02	2.00D-02
4.000D+00	8.76D-03	1.02D-02
4.200D+00	5.21D-03	2.03D-03
4.400D+00	2.94D-03	5.44D-18
4.600D+00	1.63D-03	8.46D-32
4.800D+00	8.61D-04	0.0
5.000D+00	4.36D-04	0.0

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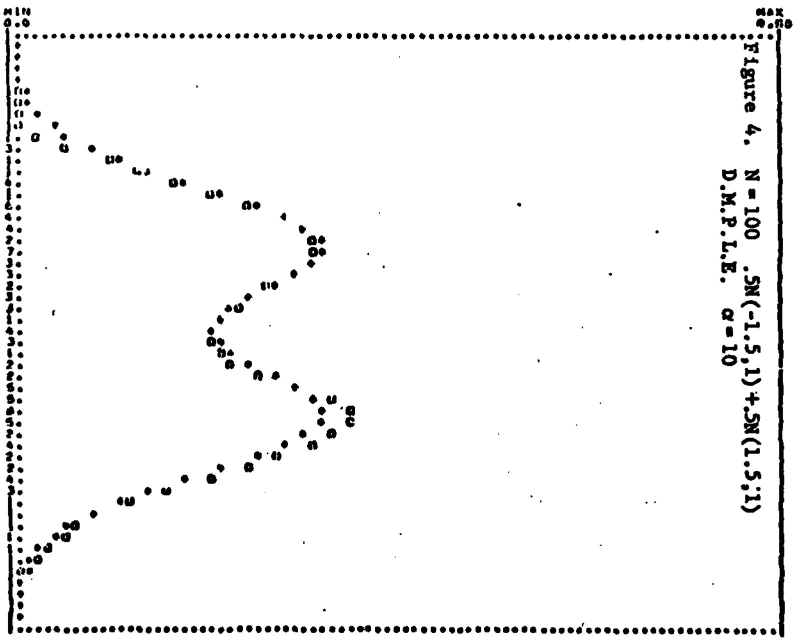

Figure 4. N = 100 .5N(-1.5,1)+.5N(1.5,1) D.M.P.L.E. α = 10

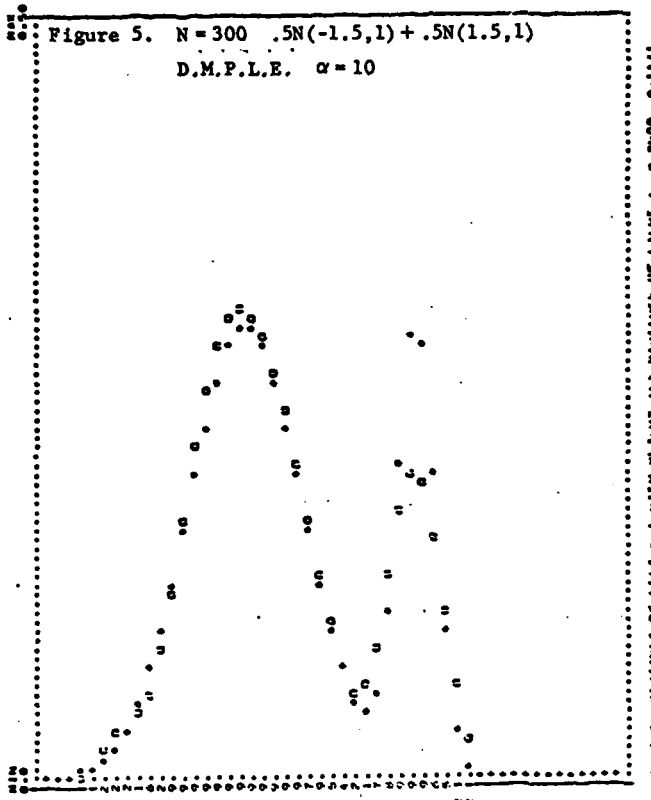

Figure 5. N = 300 .5N(-1.5,1) + .5N(1.5,1)
D.M.P.L.E. $\alpha = 10$

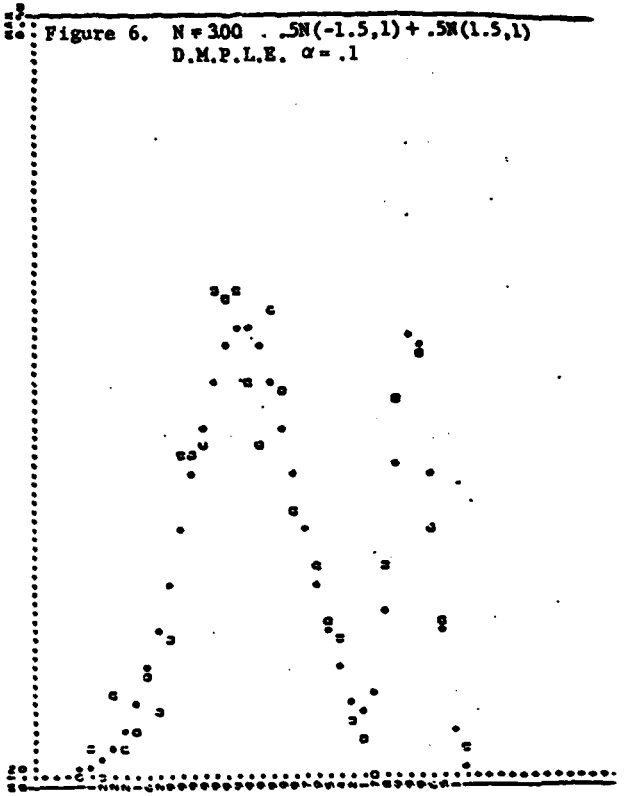

Figure 6. N = 300 .5N(-1.5,1) + .5N(1.5,1)
D.M.P.L.E. $\alpha = .1$

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