Local Predictive Influence

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0. Introduction

This paper gives a specific application of a general paradigm that was described by Cook (1986), and McCulloch (1985). Let M represent the ingredients of a statistical problem, M = (model, data) where the model consists of a set of sampling distributions and, for Bayesians, a set of prior distributions on the sampling distributions. An analysis technique T maps each M into an answer: T(M) = a where a might be a parameter estimate, a confidence interval, a probability or any other type of inference.

Let M be a function of a vector ω where ω_0 is a standard and other values of ω represent perturbations of the standard. For example, in a regression setting, ω may be an n-vector of case weights, an n-vector of perturbations in the observations, or an $n \times p$ matrix of perturbations in the covariates. For these examples, ω_0 would be the vector of all 1's, the 0 vector, and the 0 matrix.

Let D be a discrepancy function between pairs of answers, where $D(a_1, a_2) \in R$. The function D measures the influence that a perturbation scheme has on the outcome of the analysis. Cook (1986) suggests that we often want to examine the function

$$h(\omega) = D\left[T(M(\omega_0)),\ T(M(\omega))\right] \text{ for } \omega\text{'s}$$

in a neighborhood around ω_0.

Many useful choices for D will satisfy $D(a_1, a_2) \geq 0$ and $D(a, a) = 0$. Assume, from now on, that these conditions are met and therefore that h has a local minimum at $\omega = \omega_0$. The shape of h at ω_0 is an indicator of how drastically the inference changes as a function of ω, at least locally.

When h is twice differentiable the shape of h at ω_0 can be studied through the curvature, which in turn can be studied through the curvature in one direction at a time. Any vector ω can be written as $\omega = r \cdot d$ where r is a scalar and d is a unit vector. The curvature C_d in the direction d is defined to be

$$C_d = \left.\frac{\partial^2 h(\omega)}{\partial r^2}\right|_{r=0}.$$

If the maximum curvature, $\sup_d C_d$, is large then small changes in ω can make large changes in the inference. On the other hand, a small maximum curvature is evidence that the analysis is robust to small changes in M.

The remaining sections of this paper show to to compute c_d and $\sup C_d$ for one particular type of analysis, perturbation scheme and discrepancy function.

1.2 Framework

Let the data consist of independent random variables $Y_1, \ldots, Y_n$ and p-dimensional covariates $X_1, \ldots, X_n$. Assume that the normal linear model with different case weights applies, i.e.,

$$Y_i \sim N(X_i^t \beta, \sigma_i^2)$$

Let X be the matrix $(X_1, X_2, \ldots, X_n)^t$ so the model can be written

$$Y \sim N(X^t \beta, \sigma^2 S)$$

where β is the p×1 vector of regression coefficients, σ^2 is a positive scalar, and S is a positive-definite diagonal matrix. A standard assumption is that all the case weights are equal. Let $\omega = (\omega_1, \ldots, \omega_n)^t$ be a vector representing changes from identical case weights, so that the diagonal of S is $(1/(1+\omega_1), \ldots, 1/(1+\omega_n))$. The 0 vector is ω_0.

Let the prior be the usual improper, non-informative prior proportional to $\sigma^{-2} d\beta d\sigma^2$, and suppose that the goal of the analysis is to compute a predictive density for a future random variable Z at known covariate w that satisfies

$$Z \sim N(w^t \beta, \sigma^2).$$

The Kullback-Leibler directed divergence betwen two densities f and g is defined to be $I(f,g) = \int ln(f(x)/g(x))f(x)dx$. Let the discrepancy function D be the Kullback-Leibler divergence, so that $h(\omega) = I(f, f_\omega)$ where f is the predictive density computed with equal weights and f_ω is the predictive density computed with weights $(1+\omega_i)$.

By the linear transformation $X^*=S^{1/2}X$ and $Y^*=S^{1/2}Y$ we get the new model $Y^* \sim N(X^{*t}\beta, \sigma^2 I)$ that has the same weight for every case.

he distribution of Z given w, X and Y is the Student distribution $St(n-p, w^t\hat{\beta}, (1+v)s^2)$ where p is the dimension of β, $\hat{\beta}=(X^{*t}X^*)^{-1}X^{*t}Y^*$, $v=w^t(X^{*t}X^*)^{-1}w$, $s^2=Y^{*t}QY^*/(n-p)$, $Q=I-X^*(X^{*t}X^*)^{-1}X^{*t}$ is the orthogonal projection operator parallel to the column space of X^* and the distribution St(a,b,c) has density proportional to $dz[1+(z-b)^2/ac]^{-(b+1)/2}$ (Geisser (1965), Johnson and Geisser (1982)).

By interchanging integration and differentiation and after some tedious calculus we see that

$$C_d \text{ is } d^t(M1 + M2 + M3 + M4)d$$

where M1, M2, M3, and M4 are each rank one matrices. They are defined in terms of $z^t=(z_1,\ldots,z_n)=w^t(X^tX)^{-1}X^t$ and the vector of residuals $QY=r=(r_1,\ldots,r_n)^t$. The four matrices are

$M1 = (n-p)/(2(n-p+3)(1+v)^2) \cdot [z^\circ z]\ [z^\circ z]^t$

$M2 = -(n-p)/((n-p+3)(1+v)Y^tQY) \cdot [z^\circ z]\ [r^\circ r]^t$

$M3 = (n-p)/(2(n-p+3)(Y^tQY)^2) \cdot [r^\circ r]\ [r^\circ r]^t$

$M4 = (n-p)(n-p+1)/((n-p+3)(1+v)(Y^tQY)) \cdot [r^\circ z]\ [r^\circ z]^t$

where ° denotes elementwise multiplication. Section 3 sketches a proof of this result.

The direction that maximizes the second derivative is the eigenvector corresponding to the largest eigenvalue of M1 + M2 + M3 + M4. Since each summand has rank 1 the sum has at most rank 4. Thus there is only a four dimensional space of weight changes that effect the Kullback-Leibler divergence of the predictive density, at least locally.

2. Example

For a numerical example consider, as does Cook (1986), the Snow Geese data for observer 1 from Weisberg (1985). The data are X=flock size estimated by the observer and Y=flock size determined from a photograph. We believe Y to be the true flock size. We are interested in true flock size Z for flocks which have not been photographed but whose sizes have been estimated as w by the same observer. Figure 1 is a scatterplot of the data.

This is a calibration problem. Aitchison and Dunsmore (1975) show that if

1) the conditional distribution of X_i given Y_i, β and σ^2 is $N(\beta_0+\beta_1 Y_i, \sigma^2)$,
2) the conditional distribution of w given Z, β and σ^2 is $N(\beta_0+\beta_1 Z, \sigma^2)$,
3) the conditional distribution of Z given Y is $St(n-3, \bar{Y}, (1+1/n)\Sigma(Y_i-\bar{Y})^2/(n-3))$ and
4) the prior for β and σ^2 is proportional to $\sigma^{-2}d\beta d\sigma^2$

then the predictive distribution for Z given X, Y and w is St(n-2,a,b) where

$$a = \frac{\bar{Y} + (Z-\bar{X})\cdot\Sigma(X_i-\bar{X})(Y_i-\bar{Y})}{\Sigma(X_i-\bar{X})^2} \quad \text{and}$$

$$b = \frac{RSS\cdot\Sigma(X_i-\bar{X})^2}{(n-2)\cdot\Sigma(Y_i-\bar{Y})^2}\left(1 + \frac{1}{n} + \frac{(Z-\bar{Y})^2}{\Sigma(X_i-\bar{X})^2} \right) \quad \text{and}$$

RSS is the residual sum of squares from the regression of Y on X. Geisser (1985) points out that the Aitchison and Dunsmore result is identical to the predictive distribution for Z given X, Y and w if

1′) the conditional distribution of Y_i given X_i, β and σ^2 is $N(\beta_0+\beta_1X_i,\sigma^2)$,

2′) the conditional distribution of Z given w, β and σ^2 is $N(\beta_0+\beta_1w,\sigma^2)$ and

4′) (=4) the prior for β and σ^2 is proportional to $\sigma^{-2}d\beta d\sigma^2$.

Therefore we can solve the calibration problem as a straightforward linear regression prediction problem by reversing the roles of X and Y.

Let's consider predicting true flock size for three values of estimated flock size, say $w\in\{30,100,300\}$. For each value of w we can find d_{max}, the direction that maximizes C_d. Figure 8.2 is a plot of the coordinates of d_{max} for each value of w as a function of observer count. Each coordinate of d_{max} corresponds to one data case. A large coordinate indicates a case that would cause a large change in the predictive distribution if its weight were changed slightly.

These plots are similar to a plot by Cook of the coordinates of d_{max}

as a function of observer count. Cook treated σ^2 as known and used a discrepancy function that depends only on point estimates of β. The main difference between his plot and our plots is in the value for the point where X=500. In Cook's analysis that point corresponded to the largest coordinate of d_{max} and would have been the most influential under a set of small weight changes. In our analysis the influence of that point depends on the value of the covariate.

Another interesting feature is that for w=30 the biggest change in the discrepancy function comes when the points at X=500 and X=250 get weight changes of the same sign. For w=300 the biggest change comes when those points get weight changes of opposite signs. This effect may arise because for w=300 changing the weights with opposite signs will make a large change in the location of the predictive distribution. For w=30 changing the weights with the same signs will make a large change in the variance of the predictive distribution.

APPENDIX B

3. Computation of Curvature

This appendix gives a rough outline and a few intermediate calculations for proving the result in Section 1. Let r be a scalar and $d=(d_1,\ldots,d_n)^t$ be a unit vector. Define

$$S = \begin{pmatrix} 1 + r\cdot d_1 & & & 0 \\ & \cdot & & \\ & & \cdot & \\ 0 & & & 1 + r\cdot d_n \end{pmatrix}.$$

Under the linear model $Y \sim N(X^t\beta, \sigma^2(S^{-1}))$ with prior $\sigma^{-2} d\beta d\sigma^2$ the predictive distribution for a future observable Z with known covariate w is $St(n-p,\ w^t\hat{\beta},\ (1+v)s^2)$ where

X is $n \times p$

$X^* = S^{1/2}X$

$Y^* = S^{1/2}Y$

$\hat{\beta} = (X^{*t}X^*)^{-1}X^{*t}Y^*$

$v = w^t(X^{*t}X^*)^{-1}w$

$s^2 = Y^{*t}QY^*/(n-p)$

and $Q = I - X^*(X^{*t}X^*)^{-1}X^{*t}$

Let f_w be the predictive distribution of Z given above. We want to compute

$$C_d = \left.\frac{\partial\, I^2(f_0, f_w)}{\partial r^2}\right|_{r=0}$$

where I is defined in Section 1.

Let $A = (1+v)s^2, \quad A_0 = A|_{r=0}$

$B = (z-w^t\hat{\beta})^2, \quad B_0 = B|_{r=0}.$

The first step in computing C_d is to differentiate and evaluate at r=0 inside the integral. The derivatives of terms involving only A_0 and B_0 are 0 because A_0 and B_0 do not depend on r. Terms involving only A can come outside of the integral. Letting ′ denote differentiation with respect to r we get

$$C_d = -\frac{n-p}{2}\frac{AA'' - (A')^2}{A^2}\bigg|_{r=0} + \frac{n-p+1}{2}\int \frac{((n-p)A+B)\,((n-p)A''+B) - ((n-p)A'+B)^2}{((n-p)A+B)^2}\bigg|_{r=0} f_0(z)dz$$

Note that

$$\frac{f_0(z)dz}{((n-p)A+B)^2} = \frac{(n-p+2)(n-p)\ g(z)dz}{(n-p+3)(n-p+1)(1+v_0)^2(Y^tQ_0Y)}$$

where g is the Student $(n-p+4,\ w^t\hat{\beta}_0,\ (n-p)A_0/(n-p+4))$ density and a subscript 0 indicates evaluation at r=0. Multiplying out the numerator of the integrand gives

$$C_d = -\frac{n-p}{2}\frac{AA''-(A')^2}{A^2}\bigg|_{r=0}$$

$$+ \frac{(n-p+2)(n-p)}{2(n-p+3)(1+v_0)^2(Y^tQ_0Y)}\Big[(n-p)^2AA'' + (n-p)\int B''g(z)dz$$

$$+ (n-p)A''\int Bg(z)dz + \int BB''g(z)dz$$

$$- (n-p)^2(A')^2 - 2(n-p)A'\int B'g(z)dz$$

$$- \int (B')^2g(z)dz \Big]\Big|_{r=0}.$$

Next evaluate B and its derivatives.

$\int Bg(z)dz|_{r=0} = \text{var}(g) = (1+v_0)Y^tQ_0Y/(n-p+2)$.

$\int B'g(z)dz = 0$ because the integral is an odd central moment of a symmetric density.

B'' does not involve z and comes outside of the integral. Using $((X^tSX)^{-1})' = -(X^tSX)^{-1}(X^tSX)'(X^tSX)^{-1}$ (Rogers (1980)) and $(X^tSX)' = X^tDX$ where $D = \text{diag}(d_1,\dots,d_n)$ yields

$B''|_{r=0} = 2(w^t(X^tX)^{-1}X^tDQ_0Y)^2$.

$$\int (B')^2g(z)dz|_{r=0} = 4(w^t\hat{\beta}')^2|_{r=0} \cdot \text{var}(g)$$

$$= 4(w^t(X^tX)^{-1}X^tDQ_0Y)^2\ (1+v_0)Y^tQ_0Y/(n-p+2)$$

and hence

$$C_d = (A')^2|_{r=0} \cdot (n-p)^3/(2(n-p+3)(1+v_0)^2(Y^tQ_0Y)^2)$$

$$+ (w^t(X^tX)^{-1}X^tDQ_0Y)^2 \cdot (n-p+1)(n-p)/((n-p+3)(1+v_0)(Y^tQ_0Y)).$$

Evaluating A' at r=0 and substituting back into C_d yields C_d as the sum of four terms.

$$C_d = \frac{n-p}{2(n-p+3)(1+v_0)^2} \cdot (w^t(X^tX)^{-1}X^tDX(X^tX)^{-1}w)^2$$
$$- \frac{n-p}{(n-p+3)(1+v_0)Y^tQ_0Y} \cdot (w^t(X^tX)^{-1}X^tDX(X^tX)^{-1}w)\ (Y^tQ_0DQ_0Y)$$
$$+ \frac{n-p}{2(n-p+3)(Y^tQ_0Y)^2} \cdot (Y^tQ_0DQ_0Y)^2$$
$$+ \frac{(n-p+1)\ (n-p)}{(n-p+3)(1+v_0)(Y^tQ_0Y)} \cdot (w^t(X^tX)^{-1}X^tDQ_0Y)^2$$

Let $e = Q_0Y$, the vector of residuals.

Let $m = X(X^tX)^{-1}w$.

Let $\circ$ denote elementwise multiplication. Then

$$C_d = d^t\ (\ M1 + M2 + M3 + M4\ )\ d \text{ where}$$

$$M1 = \frac{n-p}{2(n-p+3)(1+v_0)^2} \cdot (\ m \circ m\ )(\ m \circ m\ )^t$$

$$M2 = \frac{-(\ n-p\ )}{(n-p+3)(1+v_0)Y^tQ_0Y} \cdot (\ m \circ m\ )(\ e \circ e\ )^t$$

$$M3 = \frac{n-p}{2(n-p+3)(Y^tQ_0Y)^2} \cdot (\ e \circ e\ )(\ e \circ e\ )^t$$

$$M4 = \frac{(n-p+1)\ (n-p)}{(n-p+3)(1+v_0)(Y^tQ_0Y)} \cdot (\ e \circ m\ )(\ e \circ m\ )^t$$

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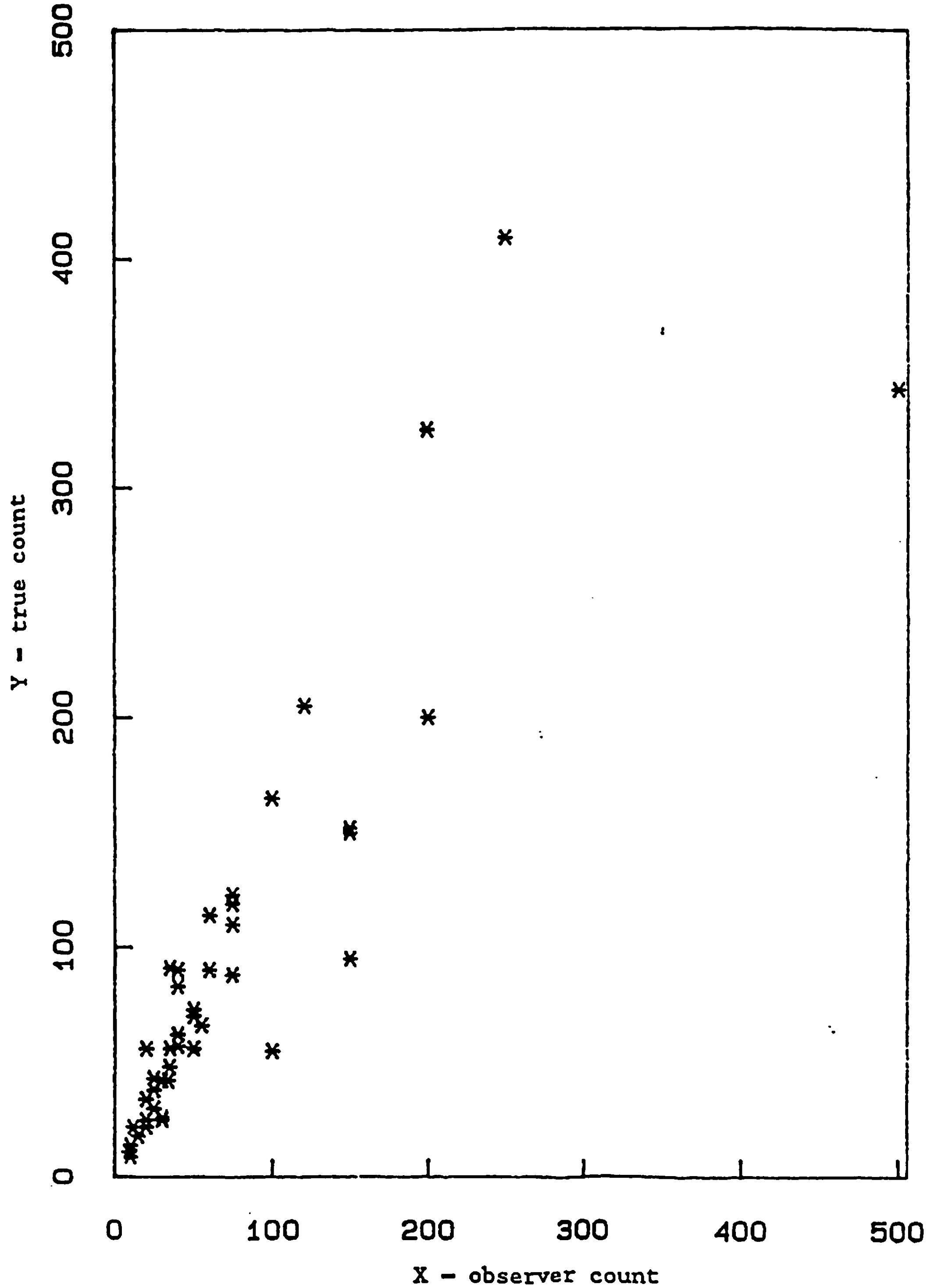
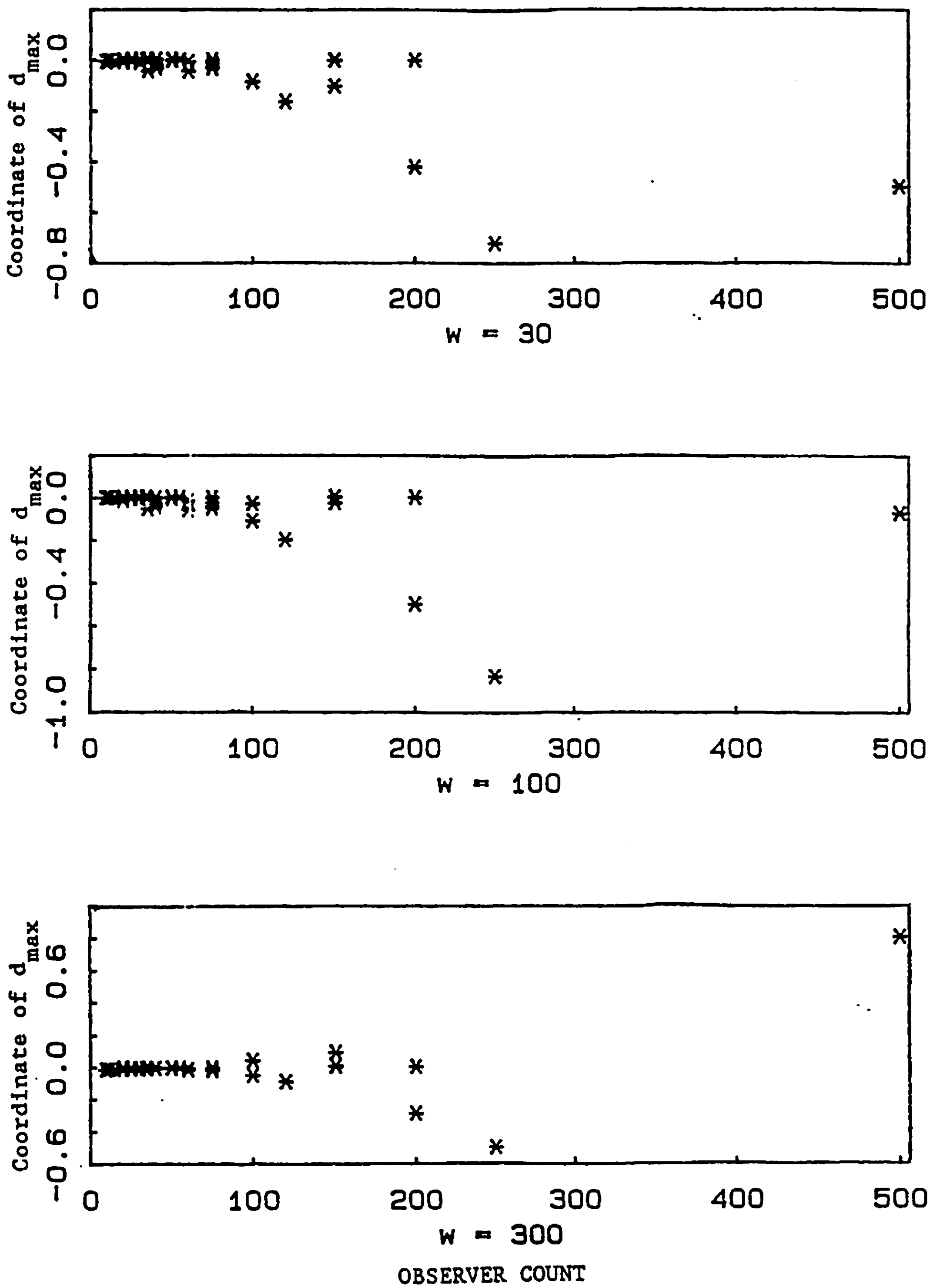


Snow Geese Data

FIGURE 1



Coordinate of d_{max}
-0.8
-0.4
0.0
0
100
200
300
400
500
W = 30
Coordinate of d_{max}
-1.0
-0.4
0.0
0
100
200
300
400
500
W = 100
Coordinate of d_{max}
-0.6
0.0
0.6
0
100
200
300
400
500
W = 300
OBSERVER COUNT

FIGURE 2