

NOAA Technical Memorandum EDS CEDDA-6

DATA EDITING--SUBROUTINE EDITQ

Donald T. Acheson

Center for Experiment Design and Data Analysis Washington, D.C. June 1975

NATIONAL OCEANIC AND ATMOSPHERIC ADMINISTRATION

Environmental Data Service

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DATA EDITING - SUBROUTINE EDITQ

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Abstract. EDITQ is a FORTRAN subroutine designed to recursively edit, i.e., remove wild or suspicious points from a data sequence. Editing is done by fitting a second-order polynomial $\hat{y}_i = a_2 + a_1x_i + a_2x_i^2$, i = 1, 2, ..., N to a paired sequence $\{(y_1, x_1), (y_2, x_2), ..., (y_N, x_N)\}$, computing the residual variance

$$\sigma_{\rm R}^2 = 1/(N-3)\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$
,

and forming the dimensionless ratio $R_i^2 = (y_i - \hat{y}_i)^2 / \sigma_R^2$ for each point. If R_i^2 exceeds some specified limit, the point (y_i, x_i) is rejected, and the residual variance and polynomial coefficients are recomputed without this data point. The process continues until no further data points are rejected in subsequent passes over the entire sequence. The subroutine returns the original sequence with flagged rejected values of y, the final values of the residual variance and polynomial coefficients, and the covariance matrix of the coefficients.

1. INTRODUCTION

EDITQ is a general-purpose routine designed to edit data, i.e., to remove or flag wild or ridiculous or merely suspicious data values. Data are input as a sequence of paired independent and dependent variables. The principal outputs are the same data with edited data points flagged; the three coefficients of a second-order polynomial fitted to all accepted, but no rejected, data points; the covariance matrix of these coefficients; and the residual variance.

Editing is done as follows:

(1) The dependent variable is least-squares fitted with a second-order polynomial in the independent variable, and the residual variance is calculated.

(2) The absolute value of the deviation of each dependent datum from the fitted polynomial is compared with the square root of the residual variance. If their ratio exceeds a specified limit, the dependent datum is flagged and rejected from further consideration.

(3) When a datum is rejected, the polynomial coefficients and residual variances are recomputed without this data point, and the next dependent datum is examined in the same way. This process continues until no further points are removed, or a fixed number of passes have already been made over the entire data sequence.

The principal advantages of EDITQ are:

(1) The accept/reject criterion for editing described in step (2) above automatically accomodates both very noisy and very clean data.

(2) EDITQ is recursive. Once a data point, no matter how wild, is rejected, it no longer figures in any further computations and cannot obscure other data points with much smaller error content but still worthy of rejection.

(3) The polynomial coefficients returned provide a simple means to compute replacement values for those rejected in the process.

The principal restrictions on the use of EDITQ are:

(1) If we view the dependent data as describing an underlying physical process more or less obscured by noise, it must be possible to approximate the underlying physical process by a second-order polynomial in the independent variable over the range of the data sequence. In other words, the modeling error must be significantly less than the residual variance returned. For example, a rapidly varying dependent variable, say surface solar radiation, could only be edited effectively if the sample rate were very high to allow EDITQ to operate on a sequence with a sufficient number of points to do useful editing but sufficiently short in duration for a second-order polynomial to be a good approximation to the real physical process.

(2) The independent variable is not edited. Unpredictable results occur when this variable contains errors.

(3) There is no physics in EDITQ. It has utterly no capability for editing consistently ridiculous data, say a sequence of absolute zeroes in temperature as a function of time. EDITQ is adept at editing outliers in a statistical sense, but must be preceded by a physical credibility window.

2. USE

With reference to the listing in the appendix to this discussion, users must input the two-dimensional array DATA, its dimensions in storage LENGTH and IMAX, the index IND at the independent variable and the index I of the dependent variable, the maximum number of points MAXOUT that may be rejected and also the dimension of array NLOST, the value BOUND that must be more negative than the negative of the absolute value of any acceptable dependent datum, and the accept/reject ratio SDLIM.

The routine returns the array DATA in which all values of the independent data and all accepted dependent data values are as input, while those rejected have the value DATA ($J_{rejected}$, I) + 2 x BOUND; the number of points rejected NCORR; the indices of rejected points NLOST (k), k = 1, 2, ..., NCORR; the final polynomial coefficients AØ, Al, and A2; the covariance matrix COVAR of these three coefficients; the square root of the residual variance STD, and the maximum deviation DEVMAX of any data point from the polynomial current at the time DEVMAX was found.

Appropriate choices of some of these parameters lend considerable flexibility to the use of EDITQ, e.g.,

(1) SDLIM - If SDLIM is greater than $[LENGTH-3]^{1/2}$, no editing will take place, and the routine serves simply to least-squares fit the data and return the residual variance, polynomial coefficients, and their covariance matrix.

(2) BOUND - If attention is paid to the number of significant digits that can be represented in the computer being used, original data values of rejected points can be recovered by addressing the array NLOST for the indices $J_{rejected} = NLOST$ (k), k = 1, 2, ..., NCORR and subtracting 2 x BOUND from the returned values in DATA. If preliminary editing has been done, say simple checking for physically impossible values, and points failing this test are assigned values less than BOUND, EDITQ will not consider them further.

3. POLYNOMIAL FITTING AS A FILTER

Since a least-squares fitted second-order polynomial is, in general, a smooth estimator of noisy data, it is suitable to compare this estimate with simple arithmetic averaging.

Define time-centered simple arithmetic averaging as

$$\overline{y}_{N}(o) = 1/(2N+1) \sum_{j=-N}^{N} y_{j}, y_{j} = y(t_{j}),$$
 (1)

where t_j is time centered (without loss of generality) at $t_0 = 0$. The analogous second-order least-squares fitted estimate is

$$\hat{y}_{N}(o) = a_{0} + a_{1}t_{0} + a_{2}t_{0}^{2} = a_{0} , \qquad (2)$$

$$a_{0} = (\Sigma t_{j}^{4} \Sigma y_{j} - \Sigma t_{j}^{2} \Sigma t_{j}^{2} y_{j}) / [(2N + 1) \Sigma t_{j}^{4} - (\Sigma t_{j}^{2})^{2}] ,$$

all sums being j = -N, ..., N.

The transfer function of a filter is defined as the ratio of the Fourier transform F of output to that of the input,

$$\begin{split} \overline{Y}_{N}(\omega) &= F(\overline{y}_{N})/F(y) , \\ \hat{Y}_{N}(\omega) &= F(\hat{y}_{N})/F(y) . \end{split}$$

3.

Since both smoothing operations defined in (1) and (2) are linear, their transfer functions are easily written down for the time-centered, equispaced sampling case $(t_i = j\Delta t)$,

$$\overline{\overline{Y}}_{N}(\omega) = (1/2N + 1)(1 + 2 \Sigma \cos \omega j \Delta t)$$

$$j=1$$

(4)

=
$$(1/2N + 1) \sin [(2N + 1) \omega \Delta t/2]/\sin (\omega \Delta t/2)$$

$$\hat{Y}_{N}(\omega) = \left(\left[(3N^{2} + 3N - 1)/S \right] (1 + 2 \sum_{j=1}^{N} \cos \omega_{j} \Delta t) \right]_{j=1}^{N}$$

$$- 2 \sum_{j=1}^{N} j^{2} \cos \omega_{j} \Delta t \right) / \left[(2N + 1) (3N^{2} + 3N - 1)/S - N(N + 1) (2N + 1)/3 \right].$$
(5)

Eqs. (4) and (5) are plotted in figure 1 for N = 6, 12, and 24.

It is evident from figure 1 that the shape of the transfer functions for either simple averaging or least-squares polynomial fitting do not change appreciably as N is increased. As N is decreased, this is no longer true. In fact, for N = 1, the polynomial transfer function $\hat{Y}_{N}(\omega)$ equals 1, as can be seen from (5). This is not surprising since a second-order polynomial exactly fits three data points.

The major change in either transfer function with varying N occurs when Δt , the data sampling interval, is kept constant. If we define the simple averaging filter "bandwidth" as $\omega' = \pi$ in figure 1, then the "bandwidth" = $2\pi/(2N + 1)\Delta t$ decreases rapidly with increasing N as one expects for any averaging or smoothing filter. From figure 1 it is also easy to compare the effects of simple averaging and second-order polynomial fitting. Since the side-lobe structure of both filters is essentially the same, we need only be concerned with the bandwidths. The polynomial filter bandwidth is about 1.75 times that of simple averaging for the same number of points, so comparability is obtained when $(2N + 1)_{polynomial} \tilde{=} 1.75 (2N + 1)_{simple}$ averaging.

4. OPERATION AND FLOW

EDITQ is shown in figure 2. The basic equations are given below.

The least-squares coefficients of a second-order polynomial $y = a_0 + a_1x + a_2x^2$ are

$$a_{0} = [s_{y}(s_{x2}s_{x4} - s_{x3}^{2}) + s_{xy}(s_{x3}s_{x2} - s_{x}s_{x4}) + s_{x2y}(s_{x}s_{x3} - s_{x2}^{2})]/D, \quad (6)$$

$$a_{1} = [L(S_{xy}S_{x4} - S_{x2y}S_{x3}) + S_{x}(S_{x2y}S_{x2} - S_{y}S_{x4}) + S_{x2}(S_{y}S_{x3} - S_{xy}S_{x2})]/D, \quad (7)$$

$$a_{2} = [L(S_{x2}S_{x2y} - S_{x3}S_{xy}) + S_{x}(S_{x3}S_{y} - S_{x}S_{x2y}) + S_{x2}(S_{x}S_{xy} - S_{x2}S_{y})]/D , (8)$$

$$D = [L(S_{x2}S_{x4} - S_{x3}^{2}) + S_{x}(S_{x3}S_{x2} - S_{x}S_{x4}) + S_{x2}(S_{x}S_{x3} - S_{x2}^{2})] , (9)$$

where

$$S_{x} = \sum_{j=1}^{L} x_{j},$$

$$S_{x2} = \sum_{j=1}^{L} x_{j}^{2},$$

$$S_{x2y} = \sum_{j=1}^{L} x_{j}^{2}y_{j}, \text{ etc.}$$

The residual variance σ^2 is given by

$$\sigma^{2} = 1/(L - 3)\sum_{j=1}^{L} (y_{j} - a_{0} - a_{1}x_{j} - a_{2}x_{j}^{2})^{2}$$

but can be expanded and summed and more efficiently written as

$$\sigma^{2} = (S_{y2} - 2a_{0}S_{y} - 2a_{1}S_{xy} - 2a_{2}S_{x2y} + La_{0}^{2} + 2a_{0}a_{1}S_{x} + 2a_{0}a_{1}S_{x2} + a_{1}^{2}S_{x2} + 2a_{1}a_{2}S_{x3} + a_{2}^{2}S_{x4})/(L - 3)$$
(10)

The covariance matrix C_{ov} of a_0 , a_1 , and a_2 , is given by (Jenkins and Watts, 1968)

$$C_{ov} = \begin{pmatrix} L & S_{x} & S_{x2} \\ S_{x} & S_{x2} & S_{x3} \\ S_{x2} & S_{x3} & S_{x4} \end{pmatrix}^{-1} \sigma^{2} .$$
(11)

In (11), the element C_{ov} (1, 1) is the estimated error variance in the coefficient a_0 , C_{ov} (1, 2) is the estimated error covariance between a_0 and a_1 , and so forth.

REFERENCE

Jenkins, A.M., and D.G. Watts, <u>Spectral Analysis and Its Applications</u>, Holden-Day, San Francisco, 1968, 525 pp.





Figure 1.--Plot of $\overline{Y}_N(\omega')$ and $\hat{Y}_N(\omega')$ for N = 6, 12, and 24. Note that the differences between N = 6, 12, and 24 are too small to show clearly on this plot. As N increases, there is a slight suppression of the side lobes.



Figure 2.--Flow chart.





Figure 2.--Flow chart (continued).

APPENDIX

SURROUTINE	EDITQ	TRACE		CDC	6600 F	TN V3.0-	-324	OPT=0	04
	SUBRO	UTINE EDIT	Q(DATA+LENGTH+IN STD+NCORR+A0+	A1,42,CC	(+MAXQU)VAR+DE	T.BOUND	SNLI	MANLOST	♥,
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с	NLO	ST(M), M=1 OR -Tu	MAXOUT IS THE A DER) OF FLAGGED E RESIDUAL STANK	ARRAY OF DATA.	INDICE	S J (IN	INCR	EASING With th	F
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40 C C C	SUBRO	UTINES CAL	LED - NONE						
C C	REFER	ENCE - JEN	KINS AND WATTS						
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	A0=	BOUND										
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	DO	3 J=1	+MAXOL	T								
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85	5 CON	TINUE										
	DAT	A(J,I)=DATA	(J+I)-	-X0							
	RJ≃l	DATA(J+IND)									
	SUM	X=SUM	X+RJ									
	SUM	XSQ=5	UMXSQ+	RJ#RJ								
90	SUM)	X3=SU	MX3+RJ	*RJ*R	J							
	SUM	X4=5U	MX4+RJ	*RJ*R	J*RJ							
			18(J+1 V-0474	<u>,</u>								
	SUM	1=50M	TTURIA UNVCO-									
95	SUM	1302-3 XY=SII	UMIS⊌+ MXY≠R.		TUATA	J						
	SUM	X2Y=S	UMX2Y+	R.I#R I	U BOATA							
	81 =1	RI +1.	0	10 10	DATA	•						
	10 CON	TINUE	•									
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	DENO	OM≈RL	# (SUMX	SQ#SU	MX4-S	UMX3*	SUM	(3)				
	1	+SU	MX#(SU	MX3*S	UMXSQ	-SUMX	#SUI	1X4)			
	2	+SU	MXSQ# (SUMX*	SUMX3	-SUMX	SQ#S	5UM	XSQ)			
AT	A0=	SUMY	+ (SUHX	SQ#SU	MX4-S	UMX3*	SUM	(3)				
05	1 1	+SUMX	1 = (SUM	X3#SU	MXSQ-	SUMX*	SUM	(4)	.		_	
	2 41-	+5UMX	21=(50		MX3-S	UMXSQ	#SUN	łXŚ	a))/	DENON	4	
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.... FTN V3.0-324 OPT=0 04 . ---

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SURROUTINE	EDITQ	TRACE			CDC	6600	FTN	V3.0-324	0PT=0	04
	1	+SUMX#(SUM	IX3#SUMY-	SUMX+SUMX2Y)					
	2 VDV	+SUMXSQ#(S =(SUMYSQ+2		Y-SUMXSQ#SU	MY))/DE UMXY-2,	ENOM	+S(IM)	(2Y+RI #401	An+2.#A	.n#
	1	A1#SUMX+	2.0*A0*A	2*SUMXSQ+A1	*A1*SU	MXSQ+2	2.0+/	1#42#SUM	(3+A2#	V
15	2	A2+SUMX4)/(RL-3.	0)	_					
	. VDV	=ABS(VDV)								
	STU	=SORT(VDV)		105						
	16 (SID+EQ+0+0 30 NPASS#1	-10 TO	125						
20	NOU	T=0	710							
	DO	20 J=1+LEN	IGTH							
	IF(DATA(J+I).	LT. (BOUN	D+0.1)) GO '	TO 20					
	RJ=	DATA(J,IND	1) 							
25		=ABS((DATA DEV.GT.DEV	(J)I)-AU Maxi devi	≠AI⇒RJ→A2*R. MAX=nFV	J*RJ}/S	SID)				
23	IFO	DEV.LE.SDL	IM) GO T	0 20						
	NOU	T=NOUT+1								
	NCO	RR=NCORR+1								
~~	NLO	ST (NCORR) =	:J							
30	RL= SUM	RL-I.U X=SUMX-R.I								
	SUM	XSQ=SUMXSC	I − RJ#RJ							
	SUM	X3=SUMX3-R	J#RJ#RJ							
ar	SUM	X4=SUMX4-R	(J#RJ#RJ#I	RJ						
35		AJ=DAIA(J) A/ 1. T)=DAT	1] (A (1. T)	4+2 A#DOUND						
	SUM	Y=SUMY-DAT	AUJ III	0+2+0+800ND	i	i				
	SUM	YSQ=SUMYSG	-DATAJ#D	ATAJ						
	SUM	XY=SUMXY-R	J#DATAJ							
40	SUM		-RJ+RJ+D	ATAJ						
				4-5114Y3#5114	¥ 3 1					
	1	+SUMX*(S	UMX3#5UM		MX4)					
	2	+SUMXSQ#	(SUMX+SU	MX3-SUMXSQ#!	SUMXSQ)				
45	, AO=	(SUMY*(SUM	IXSQ#SUMX	4-SUMX3*SUM	X3)					
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50	2	+SUMXSQ# (S	UMY#SUMX	3-SUMXY#SUM	XSQ))/(DENOM				
	, A2=	(RL#(SUMXS		-50423+5042	Y)					
	2	+SUMX50*(5	UMX#SUMX	Y-SUMXSQ#SU	, MY11708	FNOM				
	VDV	= (SUMYSQ-2	.0*A0*SU	MY-2.0+A1+S	UMXY-2	.0*42	SUM	2Y+RL#404	A0+2.*A	0+
55	1	A1#SUMX+	2.0*A0*A	2*SUMXSQ+A1	*A1*SU	MXSQ+2	2.0+/	1*A2*SUM)	3+A2*	•
	2	A2*SUMX4)/(RL-3.	0)						
	510	=SQRT(ABS(VDV)) A), LE SD			.1300	`	•		
	IF(VDV.LE.0.0) GO TO	100	TO PERMIT		•			
60	IF(NCORR GE M	AXOUT) G	0 TO 40						
	IF (RL.LE.4.1)	GO TO 1	00						
	20 CON	HINUE	CO TO .							
	30 CON	TINUF	60 10 I	00						
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SUPROUTINE	EDITQ	TRACE		CDC 6600 F	'TN V3.0-324	OPT=0	04
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75	KSP≂N	CORR					
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	JSP=K	SP-1					
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90		4 K=KST*KSD 1					
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	NLOST	(J)=NHOLD					
85	120 CONTI						
	125 CONTI	NUE					
	A0=X0	+A0-A1*T0+A2*T0*T0					
	A1=A1	-2.0*A2*T0					
90	A2=A2		1734CI 117314	UNI ADENION			
	COADA	1=(500003005000004-500	4845114863#1				
	COAOA	2= (SUNX+SUMX3-SUMXS	SQ#SUMXSQ)#	VDV/DENOM			
	COALA	1=(RL#SUMX4-SUMXSQ	SUMXSQ) *VD	V/DENOM			
95	COALA	2=(SUMX*SUMXSQ-RL*S	5UMX3) #VDV/	DENOM			
	COA2A	2= (RL+SUMX SQ-SUMX+)	SUMX) #VDV/DI	LNUM		3.8.1	
,	1+2.#T	(191)=CUAUAU=2.************************************	-CUAUAI+2 [0+T04T0#C0.	A242	12+10+10-004	141	
	COVAR	(1,2)=COA0A1-2.*TO	*COA0A2-T0*	COA1A1+3.#1	T0*T0*C0A1A2	2	
00	1-2.*T	0#T0#T0#C0A2A2					
	COVAR	(1,3)=COA0A2-T0+CO	A1A2+T0+T0*	COA2A2			
	COVAN	(2,2) = COAIAI - 4 = 10	*UDAIA2+4•*	10*10*CUA2/	42		
	COVAR	(2+3)=COA1A2=2+*10	TUAZAC				
05	COVAR	(2,1) = COVAR(1,2)					
	COVAR	(3,1)=COVAR(1,3)					
	COVAR	(3,2)=COVAR(2,3)					
	127 CONTI			-			
10		U JEIALENGIH	• T A				
10	IF (DA	TA(J+I) LE BOUND)	GO TO 130				
	DATA	J,I)=DATA(J,I)+X0					
	130 CONTI	NUE					
15	RETUR	(N					
12	ENU						