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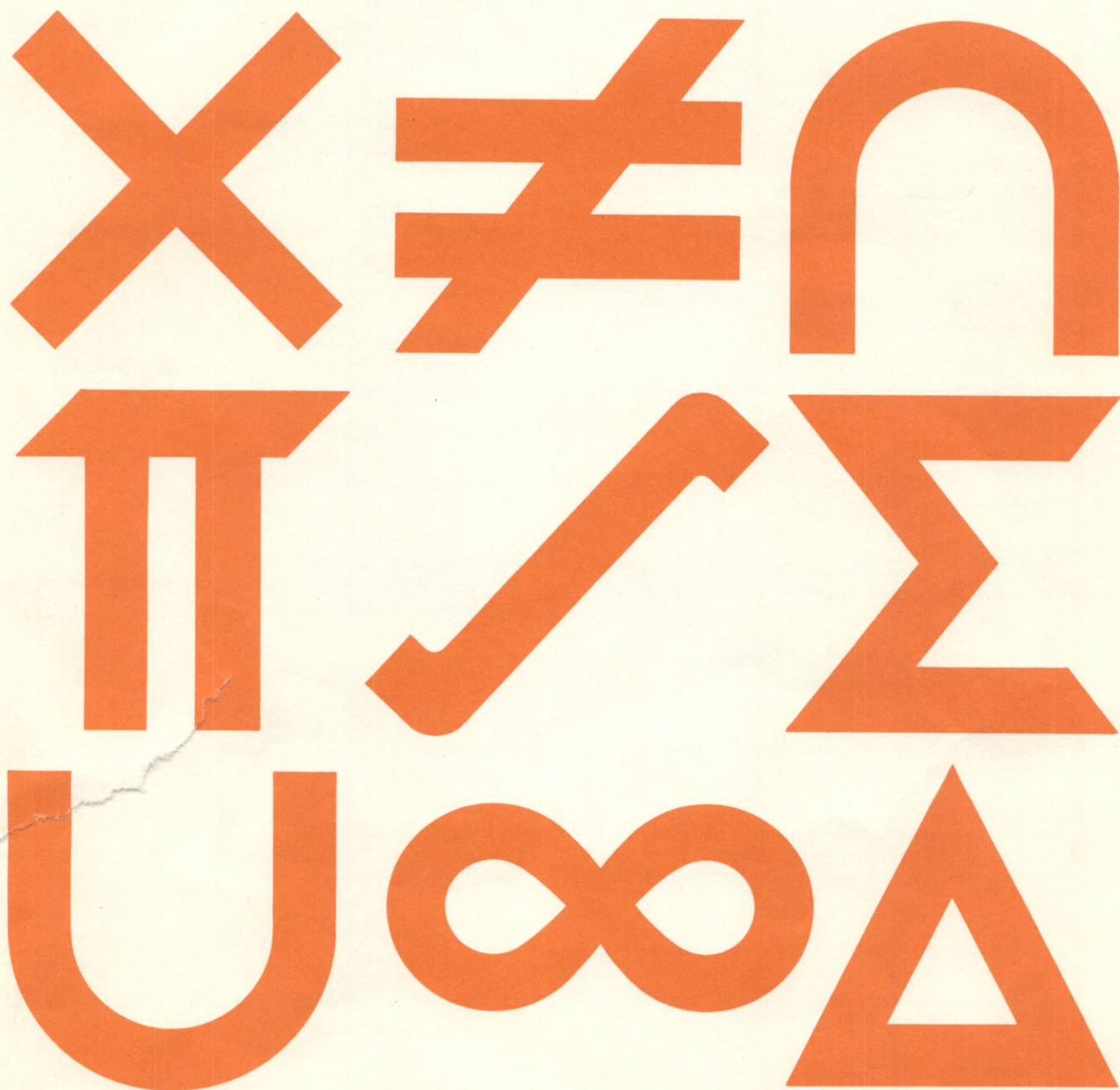
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THE KALMAN FILTERING METHOD AND ITS APPLICATION  
TO AIR POLLUTION EPISODE FORECASTING

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## Abstract

This paper presents an application of the Kalman filtering method to multi-station air pollution modeling in order to obtain a useful real-time predictor of concentration levels, especially during episode situations. Special attention has been paid to avoiding certain high dimensionality problems of the Kalman filter while still retaining some of the deterministic "physical" information of the transport and diffusion phenomena. Moreover, a method is proposed to forecast future state values using only a probabilistic knowledge of future state-transition matrices, which is the most common situation in air pollution real-time forecasting with probabilistic meteorological input. Specifically, the method is applied to SO<sub>2</sub> and meteorological data (Summer 1975) supplied by the RAMS network (Environmental Protection Agency's Regional Air Pollution Study) installed in the St. Louis Missouri area. The results of the proposed methodology are compared with those supplied by single-station predictors.

## 1. Introduction

Kalman filters are a class of linear minimum-error-variance sequential state estimation algorithms. They have been used in many applied fields and, in particular, in navigation space guidance and orbit determination<sup>1</sup> and in hydrology<sup>2</sup>. The linear discrete version of this methodology can be used for forecasting problems where the transition mechanism of a discrete system is described by the discrete "message model"

$$\tilde{x}(t+1) = \tilde{\Phi}(t+1,t)\tilde{x}(t) + \tilde{\Gamma}(t)\tilde{w}(t+1) \quad (1)$$

In this equation,  $\tilde{\Phi}(t+1,t)$  is the state-transition matrix from  $t$  to  $t+1$ ,  $\tilde{x}(t)$  is the state vector at time  $t$ ,  $\tilde{w}(t+1)$  is a zero-mean white noise stochastic process with covariance matrix  $\tilde{V}_w(t+1)$ , and  $\tilde{\Gamma}(t)$  is the noise transition matrix. The dimension of  $\tilde{w}$  is not necessarily equal to that of  $\tilde{x}$ .

In the general theory, the state  $\tilde{x}(t)$  is not observed directly. Instead, observations have the form of an "observation model"

$$\tilde{z}(t) = \tilde{H}(t)\tilde{x}(t) + \tilde{v}(t) \quad (2)$$

included in the system noise process  $\tilde{w}(t)$ .

A very important problem arises in the application of the Kalman filter to air pollution problems. In fact, it is necessary to avoid the high dimensionality of the resulting Kalman filter equations. For example, when  $\tilde{\Phi}$  is the time-evolution transition matrix of the K-model, a simple spatial grid of  $20 \times 20 \times 10$  points produces Kalman filter matrices of dimension  $4000 \times 4000$ . Many proposals have been made for the simplification of this problem. In particular, either the Green function can be used<sup>5</sup> to reduce the equation of the K-model to a difference equation of relatively small dimension, or a discrete form of Chandrasekar-type equations can be applied<sup>6</sup> for the same goal. Alternatively, the region can be partitioned into subregions<sup>3</sup> and, if the subvectors of the subregions are not coupled (or weakly coupled), the filter algorithm can be applied separately to each of the subvectors, so reducing the size of the matrices which must be manipulated. Finally, a multiple linear regression model can be used<sup>4</sup> for  $\tilde{\Phi}$ , so reducing the dimension of the filter to the number of monitoring stations in the area, losing however the "physical" information of the diffusion phenomenon.

Our proposed method uses for the dimension of the filter the number of monitoring stations, but it incorpo-

ithm (Kalman filter) for the estimation of the state of a linear time-varying dynamic system, driven by white noise of zero mean and known variance. Under the further assumptions that  $\tilde{v}$ ,  $\tilde{w}$  and  $\tilde{x}$  are mutually uncorrelated, the relevant formulas are  $[\tilde{x}(t_2|t_1)]$  is the estimate at time  $t_1$  of  $\tilde{x}(t_2)$ :

$$\text{predicted state } \tilde{x}(t+1|t) = \tilde{\Phi}(t+1, t)\tilde{x}(t|t); \quad (3)$$

predicted error covariance matrix

$$\tilde{V}_{\tilde{x}}(t+1|t) = \tilde{\Phi}(t+1, t)\tilde{V}_{\tilde{x}}(t|t)\tilde{\Phi}^T(t+1, t) + \tilde{\Gamma}(t)\tilde{V}_{\tilde{w}}(t+1)\tilde{\Gamma}^T(t); \quad (4)$$

filter gain matrix

$$\tilde{K}(t+1) = \tilde{V}_{\tilde{x}}(t+1|t)\tilde{H}^T(t+1)[\tilde{H}(t+1)\tilde{V}_{\tilde{x}}(t+1|t)\tilde{H}^T(t+1) + \tilde{V}_{\tilde{v}}(t+1)]^{-1}; \quad (5)$$

after processing the observation  $\tilde{z}(t+1)$

$$\tilde{x}(t+1|t+1) = \tilde{x}(t+1|t) + \tilde{K}(t+1)[\tilde{z}(t+1) - \tilde{H}(t+1)\tilde{x}(t+1|t)]; \quad (6)$$

new error covariance matrix

$$\tilde{V}_{\tilde{x}}(t+1|t+1) = [\tilde{I} - \tilde{K}(t+1)\tilde{H}(t+1)]\tilde{V}_{\tilde{x}}(t+1|t); \quad (7)$$

where  $\tilde{V}_{\tilde{x}}(t_2|t_1)$  is the covariance matrix of the error  $\tilde{x}(t_2) - \tilde{x}(t_2|t_1)$ .

In the Appendix a computer oriented scheme of equations (1-7) is developed. This method uses equation (3) recursively in order to obtain the forecast up to  $p$  time-steps ahead. This forecast requires, at each time  $t$ , the estimates  $\tilde{\Phi}(t+k, t+k-1|t)$ ,  $k=1, 2, \dots, p$  of future state-transition matrices which may be highly time dependent. In air pollution, for example, the state-transition matrix



### 3. An application of the Kalman filter to SO<sub>2</sub> forecasting

The methodology of the previous section has been applied to hourly meteorological and SO<sub>2</sub> data. The period of analysis is Summer 1975 (2208 hourly time periods) and the data was supplied by three monitoring stations of the RAMS network (Environmental Protection Agency's Regional Air Pollution Study) installed in St. Louis, Missouri (Figure 1). The following time series have been used: three SO<sub>2</sub> time series, (Station 3, industrial area; Station 5, commercial area; Station 13, suburban area) wind speed (Station 3), wind direction (Station 3), temperature vertical gradient (Station 5), and hour of the day. All these, except SO<sub>2</sub>, have been categorized as follows:

- wind speed, 3 classes ( $\leq 2\text{m/s}$ ,  $> 2\text{m/s}$  and  $\leq 6\text{m/s}$ ,  $> 6\text{m/s}$ );
- wind direction, 8 classes

(N-NE, NE-E, E-SE, SE-S, S-SW, SW-W, W-NW, NW-N);

- temperature vertical gradient, 3 classes based on the variable

$$s = \frac{\Delta T}{\Delta z} + \frac{1^\circ\text{C}}{100\text{m}} \quad (s < -0.005 \text{ unstable, } s \geq -0.005 \text{ and } s \leq 0.005 \text{ neutral, } s > 0.005 \text{ stable}); \text{ and}$$

- hour of the day, 5 classes (night, transition, low

$$q_{\alpha\alpha'}^{h+1} = \sum_{\alpha''=1}^{57} q_{\alpha\alpha''}^h q_{\alpha''\alpha'}^1, \quad h=1, \dots, k-1 \quad (9)$$

The transition matrix estimates, given the system state  $\alpha(t)$  at time  $t$ , are then ( $p=8$ )

$$\Phi_{\alpha'}(t+k, t+k-1 | t) = \sum_{\alpha=1}^{57} \Phi_{\alpha} q_{\alpha\alpha'}^k, \quad k=1, \dots, 8 \quad (10)$$

The general program scheme, described in the Appendix, has been applied to our data in the following way. The state vector  $\tilde{x}(t)$  has four components given by the three  $SO_2$  hourly concentrations measured for the time  $t$  in ppm at the three selected stations, and a fourth component which is identically 1 as required for the easier application of multiple regression methods. For each of the 57 meteorological-time-of-day categories  $\alpha$ , we have in Table V a  $4 \times 4$  state-transition matrix  $\Phi_{\alpha}$  which is estimated by multiple regression methods. A simplified version of the general methodology (1-7) has been used in which, for computational purposes, the covariance  $\hat{\tilde{V}}_{\tilde{\Gamma}\tilde{w}}$  of  $\tilde{\Gamma}\tilde{w}$ , expressed in  $\text{ppm}^2$  and estimated from the data, has been completely ascribed to  $\tilde{w}$  by setting

$$\hat{\tilde{V}}_{\tilde{w}} = \hat{\tilde{V}}_{\tilde{\Gamma}\tilde{w}} = \begin{pmatrix} 2.436 & 10^{-5} & 6.495 & 10^{-6} & 2.656 & 10^{-6} \\ 6.495 & 10^{-6} & 5.160 & 10^{-5} & -2.626 & 10^{-6} \\ 2.656 & 10^{-6} & -2.626 & 10^{-6} & 2.561 & 10^{-4} \end{pmatrix}, \quad \tilde{\Gamma} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \quad (11)$$

This estimate,  $\hat{\tilde{V}}_{\tilde{\Gamma}\tilde{w}}$ , has been calculated using the error series  $\tilde{x}(t+1) - \Phi_{\alpha(t+1)} \tilde{x}(t)$  during the analyzed period



single-station fitting predictor defined in another paper<sup>9</sup>.

This latter predictor has been defined in the following way. For any given combined class  $\alpha$  ( $\alpha=1,2,\dots,57$ ) let  $T_{\alpha}^0 = \{t_1, t_2, \dots\}$  be the collection of hourly periods during which that condition  $\alpha$  obtained. Define  $\mu_{\alpha}^0$  and  $\sigma_{\alpha}^0$  to be the mean and the standard deviation of the observed  $SO_2$  hourly concentrations at time  $T_{\alpha}^0$ . Similarly define  $T_{\alpha}^k = \{t_1+k, t_2+k, \dots\}$  and let  $\mu_{\alpha}^k$ ,  $\sigma_{\alpha}^k$  be the mean and standard deviation of the observed  $SO_2$  hourly concentrations at times  $T_{\alpha}^k$ . Finally, define  $\rho_{\alpha}^k$  to be the lag  $k$  autocorrelation between the  $SO_2$  concentrations at times  $T_{\alpha}^0$  and those at times  $T_{\alpha}^k$ . With these  $5 \times n$  parameters (in our case 285) for each  $k$ , we apply the following  $k$ -hours-ahead predictor:

$$\frac{c(t+k|t) - \mu_{\alpha}^k(t)}{\sigma_{\alpha}^k(t)} = \rho_{\alpha}^k \frac{c(t) - \mu_{\alpha}^0(t)}{\sigma_{\alpha}^0(t)} \quad (12)$$

that allows the concentration estimation  $c(t+k|t)$  on the basis of the observed combined class  $\alpha(t)$  and  $SO_2$  concentration  $c(t)$  at time  $t$ . In the case where  $c(t)$  and  $c(t+k)$  are modeled to have a joint normal distribution in each condition class, then this predictor is equivalent to the conditional mean of  $c(t+k)$  given the data at time  $t$ . The predictor may also be regarded as an AR(1) model conditioned on the meteorological-time-of-day class.

improvement may be expected by better taking into account, in the definition of matrices  $\Phi$ , the physics of the diffusion phenomena.

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F. Saving

Forcing of the symmetry of VX for numerical stability,  
And saving of its main diagonal

G. Filter gain matrix

$$K = VX \cdot H_1^T \cdot [H_1 \cdot VX \cdot H_1^T + VV]^{-1}$$

H. Process the observation  $Z = \tilde{z}(T+1)$

$$X = X_1 + K \cdot [Z - H_1 \cdot X_1]$$

I. A-posteriori error covariance matrix with a formula  
numerically more stable<sup>1</sup> than (7)

$$VX = [I - K \cdot H_1] \cdot VX \cdot [I - K \cdot H_1]^T + K \cdot VV \cdot K^T$$

J. Saving

Forcing of the symmetry of VX for numerical stability,  
and saving of its main diagonal

K. Loop

$T = T + 1$ , then end if  $T > T_{MAX}$ , otherwise go to step B.

For a more complete documentation on this subject, the APL version of the main program of the algorithm is included in this Appendix. This main program calls other APL functions whose role is easily understandable by their names.

		day-hour																							
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
m	June 75	1	1	1	1	1	2	2	3	4	5	5	5	5	5	5	4	3	3	2	2	2	1	1	1
n	July 75	1	1	1	1	1	2	2	3	4	4	5	5	5	5	4	4	3	3	2	2	1	1	1	1
t	August 75	1	1	1	1	1	2	2	3	4	4	5	5	5	4	4	4	3	3	2	2	1	1	1	1
h																									

Table I. Determination of the hour-of-day classes (insolation) based on the month and the hour of the day.

Comb. Class	Meteo Class	hour-type Class	Comb. Class	Meteo Class	hour-type Class	Comb. Class	Meteo Class	hour-type Class
1	1	All	20	7	5	39	13	4
2	2	1	21	8	1	40	13	5
3	2	2	22	8	2-3-4-5	41	14	1
4	2	3	23	9	1	42	14	2
5	2	4	24	9	2	43	14	3
6	2	5	25	9	3	44	14	4
7	3	All	26	9	4	45	14	5
8	4	All	27	9	5	46	15	1
9	5	1	28	10	All	47	15	2
10	5	2	29	11	1	48	15	3
11	5	3	30	11	2-3-4-5	49	15	4
12	5	4	31	12	1	50	15	5
13	5	5	32	12	2	51	16	All
14	6	1	33	12	3	52	17	1
15	6	2-3-4-5	34	12	4	53	17	2
16	7	1	35	12	5	54	17	3
17	7	2	36	13	1	55	17	4
18	7	3	37	13	2	56	17	5
19	7	4	38	13	3	57	18	All

Table III

Definition of the 57 combined classes on the basis of the 18 different meteorological classes and the 5 hour-of day classes.



Comb. Cl. $\alpha$	$\Phi_{\alpha}$ Elements											
	(1,1)	(1,2)	(1,3)	(1,4)	(2,1)	(2,2)	(2,3)	(2,4)	(3,1)	(3,2)	(3,3)	(3,4)
1	.902	.018	-.005	.001	.650	.515	-.081	.008	.063	-.015	1.167	-.001
2	1.433	-.118	-.049	.003	.560	.713	-.075	.005	-.019	-.092	.762	.004
3	.795	.131	-.018	.001	1.272	.648	.068	-.002	.087	-.182	.677	.005
4	1.211	.301	-.040	-.003	.144	1.155	-.008	-.003	.835	-.314	.673	.025
5	.846	-.038	-.055	.004	-.401	1.037	.014	.004	.145	.136	.927	.011
6	.787	.007	.031	.002	.170	.807	-.072	.004	-.604	.293	.577	.006
7	.441	-.000	-.002	.001	-1.159	.946	-.054	.006	-.136	.142	.877	-.001
8	1.111	.027	.034	-.000	.830	.501	.605	-.001	-.349	.229	.584	.003
9	.601	.001	.001	.001	.111	.833	.015	.004	2.196	-.082	.733	-.002
10	1.169	-.009	-.014	-.000	-1.928	.978	.052	.011	2.175	-.013	.596	-.005
11	.878	-.039	-.032	.001	-.028	.511	-.022	.004	3.169	.216	.794	-.006
12	.657	-.010	.012	.001	.250	.612	.033	.005	1.341	-.113	.886	-.001
13	.761	-.056	.010	.002	.050	.291	.027	.015	.969	-.039	.910	-.006
14	.769	.001	.004	.001	.241	.603	-.033	.003	-.269	-.010	.798	.002
15	.594	.036	.006	.001	-.399	1.136	-.061	.001	-.111	-.089	.623	.006
16	.166	.000	.164	.001	-.170	.658	.106	.005	.195	.003	2.008	-.005
17	.361	-.006	.056	.001	.124	.804	-.562	.018	-1.043	.038	1.474	-.000
18	.285	.002	.090	.002	1.493	.714	-.047	-.002	-.369	.072	.931	.002
19	.896	-.042	-.045	.002	.015	.627	-.069	.004	.633	-.306	.683	.008
20	.879	.066	.070	-.002	.511	.748	-.013	.000	.547	.061	.774	-.002
21	.493	.052	-.002	.002	-.036	.316	-.002	.002	2.433	-.224	.793	-.003
22	.687	.083	.001	.001	.013	.278	-.009	.002	.987	-.029	.908	-.002
23	.339	.057	.019	.002	-.002	.382	.005	.001	-.139	.228	1.138	.002
24	1.187	-.191	.101	-.000	.416	.657	.008	-.001	-.298	-.520	1.078	.007
25	1.012	-.155	-.055	.004	-.009	.691	.013	.002	1.120	-.289	.510	.005
26	.873	.067	-.007	.001	-.025	.986	-.023	.001	-.146	-.019	.680	.013
27	.940	.002	-.059	.002	-.022	.749	-.070	.006	.046	.082	.838	.003
28	.283	.084	-.000	.001	-.057	.936	.044	-.001	.060	.021	.274	.004
29	.698	.106	.010	.002	.065	.682	.003	.001	.167	-.796	.831	.005
30	1.002	.260	-.010	-.001	.090	.640	-.004	.001	-.054	-.080	.466	.003
31	1.209	.242	.002	-.001	.019	.760	-.008	.001	-.773	.035	.669	.010
32	.828	-.018	-.006	.003	.161	.483	-.003	.002	.106	-.377	1.104	.001
33	1.322	-.499	.051	.002	.915	-.056	.042	-.001	.925	-.598	.842	.000
34	.949	-.070	.039	.002	.135	.603	-.008	.002	-.081	-.025	.757	.011
35	.701	-.049	-.042	.006	.061	.617	.015	.001	-.151	.382	.865	.004
36	.744	-.135	-.018	.003	-.007	.749	-.037	.002	-.817	-1.033	.364	.020
37	1.002	-.543	.065	.003	.005	.214	.027	.002	-.178	-.190	.274	.007
38	.585	.022	.142	.001	.158	.355	-.037	.002	.247	-.010	.923	-.001
39	.630	.011	.043	.001	.110	.487	.053	.001	-.655	-.109	.361	.009
40	.632	-.012	-.041	.003	-.242	1.024	-.062	.003	.024	-.094	.417	.004
41	.628	.261	.088	.000	-.043	1.114	.194	-.001	.023	.096	1.088	-.001
42	.617	.162	.060	.001	-.022	.478	.006	.002	-.139	.174	.366	.004
43	.446	.604	.329	-.002	.144	.232	.008	.001	-.017	.014	.889	.000
44	.307	.062	.252	.003	.036	1.009	.202	-.001	-.046	.148	.307	.006
45	.844	.203	-.151	.002	-.074	.792	-.088	.003	.039	.576	1.087	-.002
46	1.016	-.381	.133	.000	.039	.653	.063	.001	.027	.051	.366	.002
47	.336	-.165	.004	.005	-.002	.026	-.005	.003	-.029	-.034	.133	.003
48	.840	.657	.216	-.002	.001	.790	.567	-.000	-.042	-.008	.569	.002
49	1.945	.575	.019	-.005	.038	.643	.007	.000	.184	.403	.116	.000
50	.701	-.139	.039	.003	.011	.869	-.017	.000	.130	.028	.179	.002
51	.744	.198	-.012	-.001	-.251	.939	-.004	.002	-.013	.002	1.319	-.001
52	.402	-.002	.006	.002	-.715	1.343	-.008	.003	.093	-.040	.175	.003
53	.420	-.014	-.013	.003	-.405	.758	-.052	.006	-.079	.149	.387	.002
54	1.170	.572	-.143	-.003	.357	1.032	-.091	-.001	-.507	.393	.856	.003
55	.503	.180	-.037	.003	.156	.550	.090	.002	.056	.122	.899	.001
56	.772	.041	-.011	.001	-.111	.670	.122	.002	.167	.447	.861	-.002
57	.315	-.040	-.007	.003	-.002	.811	-.011	.001	.029	-.826	.264	.009

Table V.  $\Phi_{\alpha}$  transition matrices for each combined class  $\alpha$ .  
The fourth row of each matrix is identically 0 0 0 1.

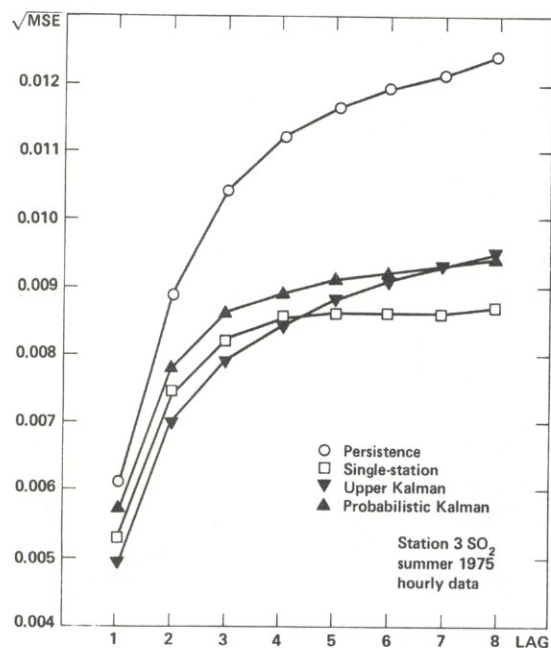


Fig. 2a

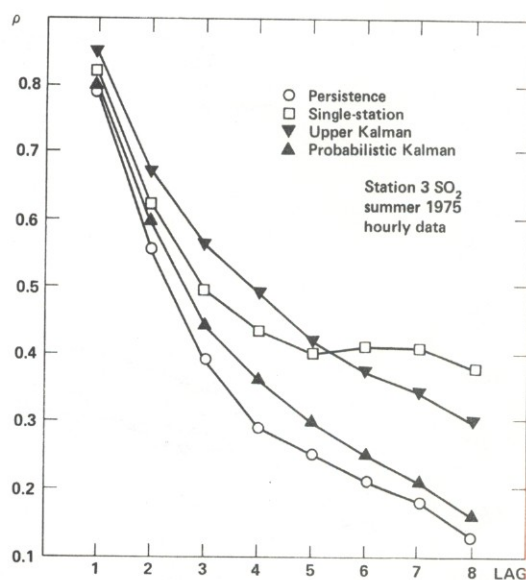


Fig. 2b

Figure 2 Root mean square error (a) and correlation coefficient (b) between measured and forecasted data, for different forecasting lags, of the following models: concentration persistence (○), single-station predictor (□), Kalman filter upper bound (▼) and probabilistic bound (▲). Data of Station 3.

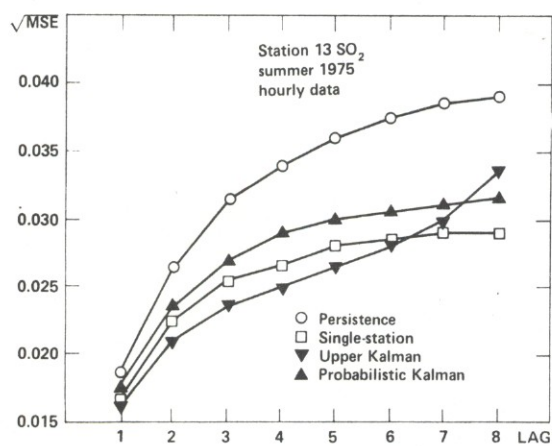


Fig. 4a

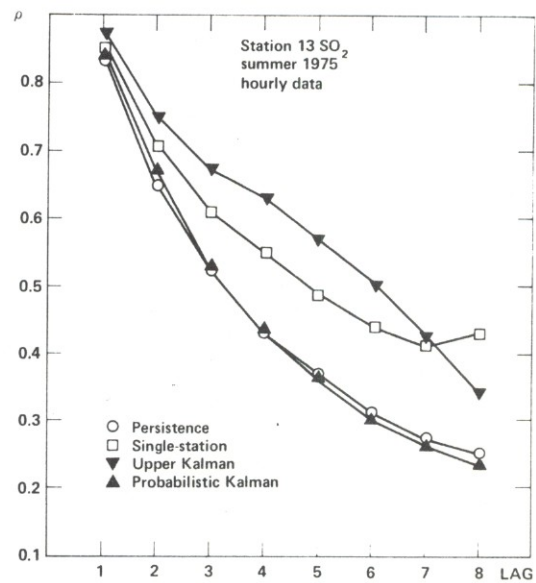


Fig. 4a

Figure 4 Same as Figure 2 for Station 13.



# SCIENTIFIC CENTER REPORT INDEXING INFORMATION

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#### 1977 PALO ALTO SCIENTIFIC CENTER OUTSIDE PUBLICATIONS

J. CANOSA & J. GAZDAG (320-3321), The Korteweg-de Vries-Burgers Equation, *Journal of Computational Physics*, Vol. 23, No. 4, April 1977, 393-403.

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