Using Ordinary Kriging to Estimate the Seasonal W126 and N100 24-h Concentrations for the Years 2004 and 2005

by

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1. Introduction

This report describes how Ordinary Kriging was used to estimate the 6-month W126 and N100 24-h ozone exposure values for the years 2004 and 2005 for the United States. A.S.L. & Associates has published previously its kriging results in peer-review papers and reports (Knudsen and Lefohn, 1988; Lefohn *et al*., 1988; Lefohn *et al*., 1992; Lefohn *et al*., 1997).

Kriging is a family of estimators used to interpolate spatial data. This family includes Ordinary Kriging, Universal Kriging, Indicator Kriging, Co-kriging, and others. The choice of which kriging to use depends on the characteristics of the data and the type of spatial model desired. The most commonly used method is Ordinary Kriging, which was selected for this study.

Ordinary Kriging was selected for this study based on how well it has performed on prior years data and because the statistical characteristics of the data in 2004 and 2005 make Ordinary Kriging the appropriate choice of estimator. Because the data display no trend at the scale of the modeling, Universal Kriging is not appropriate. The covariance models (i.e., variogram) exhibit local stationary and thus Ordinary Kriging was the appropriate method to use.

The authors have used Ordinary Kriging to make surface-level ozone models for the W126 exposure index for the years from 1982 through 2005. While the ozone values vary from year to year, the statistical character of the data remains remarkably constant from year to year. The covariance models are similar in each year and the spatial anisotropy exhibited by the co-variance models is similar in each year.

1.1 Approach

A.S.L. & Associates provided the 2004 and 2005 ozone hourly data to Mr. Douglas Shadwick for characterizing the 24-hour W126 and N100 monthly values and then summarizing the information into 6-month (April – September) values. In addition, the second highest daily maximum concentration, and the 4^{th} highest 8-hour daily maximum average concentration were calculated for the EPA-defined ozone season. The data capture was determined based on the April – September period. Following receipt of the data from Mr. Shadwick and checking of the results, A.S.L. & Associates provided Dr. Knudsen with the April – September (6 month) W126 and N100 24-h exposure indices for monitoring sites in 2004 and 2005. The computer files provided contained summarized air quality data, a monitoring site identification codes, site latitude and longitude, and site characterization code information (i.e., urban, suburban, rural, etc.).

Mr. Shadwick corrected the characterized data for missing values. The estimate of cumulative indices from hourly average data (e.g., the W126 cumulative and N100 ozone indices) will be biased low if a part of the hourly average data is missing. A correction scheme has been adopted to estimate, in particular, a cumulative index for seasonal values of the indices.

The correction scheme has two components.

1. A monthly value of each index is calculated. If at least 75% of the hourly data are available for the month, a corrected monthly cumulative index is calculated as the uncorrected monthly cumulative index divided by the data capture (as a fraction).

2. If there are any months with less that 75% data capture and the two chronologically adjacent months each have at least 75% data capture, then a corrected monthly cumulative index for the month with less than 75% data capture is calculated as the arithmetic average of the corrected monthly cumulative indices for the two adjacent months.

If all of the months contained within a season have valid estimates (in the sense described above) of the corrected monthly cumulative index, the corrected seasonal cumulative index is calculated as the sum of the corrected monthly cumulative indices. Otherwise, there is not a valid estimate of the corrected seasonal cumulative index.

In addition to the data provided to Dr. Knudsen, the second highest daily maximum 1-hour concentration and the fourth highest 8-hour average daily maximum concentration that occurred over the EPA-defined ozone season for each monitoring site that experienced sufficient data capture was provided by A.S.L. & Associates to the U.S. Forest Service project manager.

2. Scope of Work

Estimate the seasonal W126 and N100 exposure index value for each 1/2^o by 1/2^o cell in the United States excluding Alaska and Hawaii.

Specific tasks performed included:

1. Check and verify the latitude, longitude and elevation of each site.
2. Calculate and model variograms for each exposure index values for each year.
3. Krig the seasonal W126 and N100 values for each year.
4. Prepare files that contain information describing the kriged values, the coordinates, variance, and the 95% error bound for each 1/2 ^{o} by 1/2^o cell.

The traditional kriging variance and the 95% Error bound were reported as in similar years. In addition, as mentioned above, another estimate of the error variance, which is referred to as the Ordinary Kriging interpolation variance (NKVAR), was determined (Yamamoto, 2005). The 95% error bound based on the new variance was reported also.

3. Steps in Modeling

In its 1982 Kriging study, NCLAN investigators were concerned about the selection of stations to be included in the air quality analysis (Heck *et al*., 1984). In urban settings, the ozone concentrations were thought to be lower at city-center than at rural locations because of nitric oxide titration in the city. Therefore, NCLAN investigators hypothesized that by using city-center monitoring stations to predict rural ozone levels, the resultant estimations might be biased low. Because of this concern, specific monitoring stations located in large metropolitan areas were not included in the 1982 NCLAN analysis.

Because significant changes have occurred to all metropolitan areas in the last 20 years, the method of filtering city-center sites used in the 1982 NCLAN study was re-examined. Using 2004 data, Table 1 shows statistics for several of the large metropolitan areas of the US. In Table 1, the first line in each case is the mean variance of the N100 values for the city-center sites included in the 1982 study. The second line is a summary of all the sites within the metropolitan area.

With the exception of Los Angeles, the 2004 set of sites had essentially the same N100 values as the entire metropolitan area. In Los Angeles the filtered city center sites are higher than the complete set of sites. Table 2, illustrates the same information for the W126 index.

Based on this test, it was decided to not use the filtering protocol developed in the 1982 NCLAN study and to instead use all the monitoring data.

Table 1. City-Center Site Comparison for N100.

N100 City-Center Analysis

	N	Mean	Variance
Cincinnati			
City Center	8	9.1	61.1
City plus surrounding area	19	9.4	65.5
St. Louis			
City Center	14	12.5	15.4
City plus surrounding area	20	10.3	27.3
Chicago			
City Center	15	6.3	53.7
City plus surrounding area	19	9.4	65.5
Los Angeles			
City Center	24	61.7	6591.4
City plus surrounding area	42	84.2	11289.3

Table 2 City-Center Site Comparison for W126.

W126 City-Center Analysis

	N	Mean	Variance
Cincinnati			
City Center	8	24.4	21.3
City plus surrounding area	19	23.9	45.7
St. Louis			
City Center	14	24.6	44.7
City plus surrounding area	20	24.7	34.8
Chicago			
City Center	15	17.6	36/5
City plus surrounding area	39	18.0	30.6
Los Angeles			
City Center	24	40.6	681.2
City plus surrounding area	42	50.2	1114.7

Ozone exposure indices for California are known to be significantly different (i.e., higher) from other areas of the United States. Therefore California was analyzed separately in this study.

The following steps were performed for each exposure index.

1. Data Checking

   a. The latitude, longitude of all the monitoring sites from the AIRS database were compared and updated to coordinates supplied by ASL & Associates. In addition, many of the AIRS sites have incorrect elevations, missing elevations, or elevations listed in feet rather than meters. The elevations of all monitoring sites were checked and update with elevations supplied by Bill Jackson, U.S. Forest Service using a 90-meter digital elevation model.

   b. Maps showing monitoring sites and data values were plotted.

2. Calculation of data statistics.

   a. Basic statistics histograms were calculated independently for California and for the rest of the U.S.

b. Histograms were prepared.

3. Variograms for each exposure index were calculated. Experience gained in prior studies of ozone indices was used in determining the parameters for calculating and modeling the variograms of the N100 values. Particular care was used to determine the presence and likely directions of anisotropy. After calculation of the variograms, a theoretical model was fitted to them.

4. Kriged values of W126 for each 1/2^o by 1/2^o degree cell were determined. The N100 exposure for each 1/2^o by 1/2^o cell in California and the rest of US were estimated using Ordinary Kriging. The main input to a kriging program is the variogram parameters and the search parameters. The variogram parameters are listed in Tables, 5, 7, 9, and 11. The search parameters are shown below.

Search Radius		California	US
Maximum search radius	=	500 km	1100 km
Max. number of sites used to estimate a cell	=	12	12
Min. number of sites used to estimate a cell	=	1	1

5. A file with kriged values was prepared. An example is shown in Table 3.

Table 3. Example Output from Ordinary Kriging Program.

Latitude	Longitude	N100	Ordinary Kriging Var.	95%EB	OK Interpolation Variance	OKIV 95%EB	No. of Samples
44.5	-66.5	8.23	33.04	11.5	12.76	7.14	15
45	-66.5	7.53	28.34	10.65	11.68	6.83	15
44	-67	9.46	34.39	11.73	12.26	7	15
44.5	-67	8.31	28.61	10.7	13.18	7.26	15
45	-67	7.22	19.93	8.93	10.96	6.62	15

4. 2004 year data

N100 Exposure Index

Table 4 shows summary statistics for the N100 index. Table 5 shows the variogram parameters for N100.

Table 4. Year 2004 N100 Statistics.

AREA	MEAN	VARIANCE	STD.DEV.	MIN	MAX	NUMBER
California	20.2	2305.2	48.0	0.0	318.9	150
Rest of US	1.9	31.5	5.6	0.0	62.6	975

Table 5. Year 2004 N100 Variogram Parameters.

AREA	Co	C1	Range1	C2	Range2	Angle	AF ratio
CAL	200	1100	100	1100	400	135	2.5
US	5	23	180	7	1350	0	1.5

W126 Exposure Index – Basic Statistics

Table 6 shows summary statistics for the W126 index. Table 7 shows the variogram parameters for W126

Table 6. Year 2004 W126 Statistics

AREA	MEAN	VARIANCE	STD.DEV.	MIN	MAX	NUMBER
California	34.6	1043.1	32.3	0.0	148.2	150
Rest of US	17.3	71.1	8.4	0.0	69.9	975

Table 7. Year 2004 W126 Variogram Parameters.

AREA	Co	C1	Range1	C2	Range2	Angle	AF ratio
CAL	100	300	60	600	450	-45	2.0
US	20	28	180	22	800	0	1.0

5. 2005 year data

N100 Exposure Index

Table 8 shows summary statistics for the N100 index. Table 9 shows the variogram parameters for N100

Table 8. Year 2005 N100 Statistics

AREA	MEAN	VARIANCE	STD.DEV.	MIN	MAX	NUMBER
California	22.9	2086.0	45.7	0.0	299.2	141
Rest of US	4.4	54.7	7.4	0.0	41.4	966

Table 9. Year 2005 N100 Variogram Parameters.

AREA	Co	C1	Range1	C2	Range2	Angle	AF ratio
CAL	200	1100	150	900	450	135	2.5
US	10	33	150	15	500	0	1.0

W126 Exposure Index

Table 10 shows summary statistics for the W126 index. Table 11 shows the variogram parameters for W126

Table 10. Year 2005 W126 Statistics

AREA	MEAN	VARIANCE	STD.DEV.	MIN	MAX	NUMBER
California	32.5	903.9	30.1	0.4	131.3	141
Rest of US	25.9	111.3	10.5	1.2	81.1	966

Table 11. Year 2005 W126 Variogram Parameters.

AREA	Co	C1	Range1	C2	Range2	Angle	AF ratio
CAL	100	200	80	600	500	135	2.0
US	50	25	120	35	1000	0	1.3

The kriged results were prepared in 4 digital files with the following information: latitude, longitude, estimated kriged value (e.g., W126 or N100), kriged variance, 95% error bound, NKVAR, N95% error bound, and number of samples used to determine the kriged estimate.

6. References

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