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Application Bootstrap to Estimate the Confidence Intervals of NO2 Levels in the Kriging Method

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ABSTRAK

Kadar NO2 perlu dipantau secara terus menerus untuk meminimalisir dampak negatif terhadap lingkungan. Pada umumnya, estimasi kadar NO2 menggunakan metode kriging menghasilkan estimasi titik. Pada penelitian ini akan dikembangkan estimasi selang untuk kadar NO2 dengan mengaplikasikan metode resampling *quasi-random* bootstrap. Data yang digunakan adalah kadar NO2 pada 14 wilayah di Kota Tangerang Selatan tahun 2021. Data tersebut stasioner sehingga metode estimasi yang digunakan adalah *ordinary kriging*. Untuk pembentukan selang kepercayaan 95% diaplikasikan 1000 resampling pada metode bootstrap. Hasil estimasi menunjukkan bahwa selang kepercayaan kadar NO2 terkecil berada pada rentang nilai 25,23123 – 27,82351 $\mu gr/m^3$ yang berlokasi di Kelurahan Pamulang Timur dan selang kepercayaan kadar NO2 terbesar berada pada rentang 45,59886 – 46,08371 $\mu gr/m^3$ yang berlokasi di Kelurahan Ciater.

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ABSTRACT

NO2 levels must be monitored continuously to minimize negative environmental impacts. In general, the estimation of NO2 levels using the Kriging method produces point estimates. In this study, we developed an interval estimate for NO2 levels by applying the quasi-random Bootstrap resampling method. We used data on NO2 levels in 14 areas in South Tangerang City in 2021. The data is stationary, so the appropriate estimation method is ordinary kriging. To develop the 95% confidence interval, we applied 1000 resamplings to the Bootstrap. The estimation results show that the lowest 95% confidence interval for NO2 levels is in the range of 25.23123 – 27.82351 $\mu gr/m^3$ in Pamulang Timur Village, and the highest 95% confidence interval for NO2 levels is in the range of 45.59886 – 46.08371 $\mu gr/m^3$ in the Ciater Village.

Keywords:
Bootstrap,
Confidence interval,
Kriging,
Quasi-random.

1. INTRODUCTION

The nitrogen dioxide (NO2) level is one of the crucial components affecting air quality. NO2 is a reddish-brown toxic gas with a sharp smell. When it exceeds the set threshold, NO2 levels can cause the air to appear brownish, leading to acid rain that can result in lung and respiratory infections. It also plays a role in forming fine particles and ground-level ozone. Apart from posing a threat to human health, air pollution also incurs significant economic losses (Zhu, et al., 2019), affecting transportation, water, and energy exchange at the land-air interface, thus influencing climate change (Zheng, et al., 2016). Elevated NO2 levels can even lead to fatalities (Öztürk & Öztürk, 2023).

Efforts to reduce NO2 pollution often involve implementing stricter emission standards for vehicles and industrial sources, promoting cleaner technologies, and encouraging sustainable transportation practices. Monitoring and controlling NO2 levels are crucial to protect human health and the environment. Therefore, some research recommends preventive measures against NO2 pollution, including consuming foods rich in vitamins C and E, using masks, enforcing smoke-free areas (Darmawan, 2018), and using activated carbon cabin air filters in vehicles to prevent exposure to NO2 pollutants for drivers and passengers (Matthaios, et al., 2022).

Reducing airborne NO2 levels can be achieved by regulating emissions through emission standards, promoting public transportation, and encouraging electric vehicles (Krecl, et al., 2021). Traffic management is also necessary to reduce congestion, especially in city centers, and the implementation of emission-free zones (Tang, et al., 2020). Other efforts are using clean and environmentally friendly industrial technologies (Ajmal, et al., 2022) and establishing air quality monitoring systems to monitor NO2 pollution levels and provide information to the public about the health impacts of NO2 pollution and how they can protect themselves from exceeding NO2 levels (Manusmare & Gajarlawar, 2023).

Several methods have been developed to estimate NO2 levels. (Wu, et al., 2021) developed a spatial-temporal kriging regression model to map NO2 concentrations in China. (Bertero, et al., 2020) Monitored NO2 concentrations in Marseille, France, focusing on using private bike fleets. (Lee & Lee, 2019) predicted annual and monthly average NO2 concentrations in the United States using land-use regression (LUR) analysis. This study also assessed environmental risks, exploring the relationship between NO2 concentrations and potentially exposed individuals in 377 metropolitan statistical areas (MSA).

Generally, the kriging estimation methods in the mentioned studies provide point estimates. Therefore, this study discusses interval estimates (in the form of confidence intervals) for NO2 levels by applying quasi-random Bootstrap resampling. The data used are NO2 levels in 14 regions of South Tangerang City in 2021. Preliminary research indicates that the data are stationary, so the appropriate estimation method is ordinary kriging. The estimated NO2 levels using this method are then resampled using quasi-random Bootstrap to develop confidence intervals.

2. METHOD

This study focuses on NO2 levels at South Tangerang City. We use data on the NO2 level at 14 regions in 2021 (Table 1). The distribution map of NO2 levels can be seen in Figure 1. According to this table, the minimum NO2 level is 24.10 $(\mu gr/m^3)$, the maximum is 51.00 $(\mu gr/m^3)$, the average is $(\mu gr/m^3)$, and the variance is 78.43 $(\mu gr/m^3)$.

Table 1. NO2 Level in 14 Regions of South Tangerang City

No	Region	Coordinate		NO_2 Level
		Lattitude	***Longitude***	$(\mu gr/m^3)$
1	Setu	-6.343361	106.7325	44.0
2	Pondok Jagung	-6.273778	106.7104	40.0
3	Paku Jaya	-6.287972	106.6759	45.0
4	Serpong	-6.316417	106.7089	51.0
5	Rawa Mekar Jaya	-6.298778	106.7616	48.0
6	Cilenggang	-6.298306	106.6552	42.0
7	Pondok Aren	-6.236122	106.6786	39.0
8	Perigi Baru	-6.327864	106.6738	30.2
9	Pamulang Barat	-6.314614	106.6614	33.9
10	Pondok Benda	-6.255775	106.6615	25.1
11	Rempoa	-6.274897	106.6923	31.2
12	Pondok Ranji	-6.344812	106.735	24.1
13	Serua	-6.288728	106.7459	26.4
14	Sawah Lama	-6.290467	106.7294	30.2

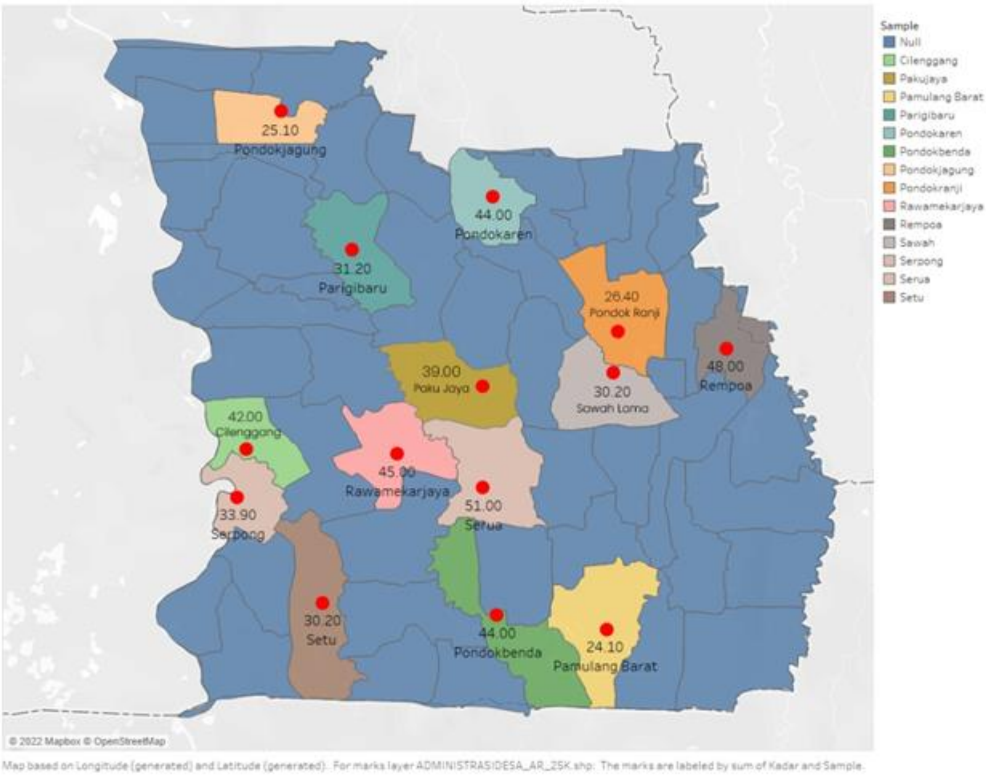


Figure 1. Distribution maps of NO_2 levels in South Tangerang City

This study uses the simple kriging interpolation method to estimate the NO2 levels. These estimations will be resampled using Bootstrap to determine the confidence interval. The first step is checking the data stationarity to decide the appropriate type of kriging method. If the data is stationary (does not have a trend), then the appropriate method is simple or ordinary kriging. Conversely, the appropriate method is universal kriging.

Next, we form a matrix of distances between sample points using the equation:

$$|h| = |s_i - s_j| = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}, \tag{1}$$

where (x) and y are the coordinates of the sample's location. Subsequently, these data pairs are divided into several classes, which are calculated using the Sturges equation (Scott, 2010):

$$k = 1 + 3.3\log(n), \tag{2}$$

where k is the number of class intervals, and n is the sample size. Next, calculate the experimental semivariogram using the equation (Beers & Kleijinen, 2003):

$$\gamma(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} [Z(s_i + h) - Z(s_i)]^2, \tag{3}$$

where $\gamma(h)$ is the semivariogram value between s_i and $s_i + h$, $Z(s_i)$ is an observation on point s_i, $Z(s_i + h)$ is an observation on point $s_i + h$, and $N(h)$ is the number of point pairs at a distance h. We will compare the experimental and the theoretical semivariogram values. Theoretical semivariogram values are calculated using three models, i.e., Spherical, Exponential, and Gaussian, as follows (Sari, et al., 2015):

a. *Spherical*

$$\gamma(h) = \begin{cases} C\left[\left(\frac{3h}{2a}\right) + \left(\frac{h}{2a}\right)^3\right], for\ h \le a, \\ C, for\ h > a. \end{cases} \tag{4}$$

b. *Exponential*

$$\gamma(h) = C\left[1 - exp\left(-\frac{h}{a}\right)\right], \tag{5}$$

c. *Gaussian*

$$\gamma(h) = C\left[1 - exp\left(-\frac{h^2}{a^2}\right)\right], \tag{6}$$

where h is the location distance between the sample, and C is the sill (variogram value for distance when the magnitude is constant). The sill value is the same as the data variance. The value of a represents the range (the distance when the semivariogram value reaches the sill). After getting the experimental semivariogram, sill, and range values from the three theoretical semivariogram models, complete the structural analysis, matching the experimental semivariogram with the theoretical semivariogram. This analysis was carried out by calculating the Root Mean Square Error (RMSE) of the two semivariograms using the equation:

$$RMSE = \sqrt{\tfrac{1}{k}\textstyle\sum_{i=1}^{k}(\gamma(h) - \hat{\gamma}(h))^2}, \tag{7}$$

where $\gamma(h)$ is the experimental value of the semivariogram, and $\hat{\gamma}(h)$ is the theoretical semivariogram value. A model with the smallest RSME will be the best model.

The NO2 levels are estimated using the ordinary kriging method at unsampled areas using the equation:

$$\hat{Z}(s_0) = \sum_{i=1}^{n} w_i Z(s_i), \tag{8}$$

where $\hat{Z}(s_0)$ estimates unsampled locations, and w_i is weighted for $Z(s_i)$ with $\sum_{i=1}^{n} w_i = 1$.

This research contributes to developing the confidence intervals based on the point estimation resulting from equation (8). We resampled the point estimation using the Bootstrap method. The detailed steps used are as follows.

1. Prepare vector $\vec{Z} = \begin{pmatrix} Z(s_1) \\ Z(s_2) \\ \cdot \\ \cdot \\ Z(s_n) \end{pmatrix}$,
2. Forms a matrix C with the size of $n \times n$. C contains the value of the chosen theoretical semivariogram,
3. Decompose matrix C using Cholesky. The result is the Cholesky factor matrix (L) and its inverse (L^{-1}) so that $C = LL^{-1}$,
4. Transform correlated data $Z(s_i), i = 1,2,\ldots,n$, into uncorrelated using:
$$\vec{U} = L^{-1}\vec{Z}, \tag{9}$$
where $\vec{U} = \begin{pmatrix} U_1 \\ U_2 \\ \vdots \\ U_{n-1} \\ U_n \end{pmatrix}$,
5. Resampling $\vec{U}$ using the Bootstrap b times. In this study, we use $b = 1000$ to obtain samples $\vec{U}^{*(b)}$, $b = 1,2, \ldots,1000$,
6. Transform the Bootstrap sample in Stage 5 back into a correlated form using equations:
$$Z_i^{*(b)} = LU_i^{*(b)}, i = 1, \ldots, n. \tag{10}$$
This stage is called quasi-random Bootstrap.
7. Use $Z_i^{*(b)}$ to find $\hat{Z}(s_0)_i^{*(b)}$ in equation (8).

The next step is to calculate the standard error at each estimation point in step 7 using:

$$s\hat{e} = \sqrt{\frac{\sum_{b=1}^{1000}\left(\hat{Z}(s_0)^{*(b)} - \hat{Z}(s_0)^{*(.)}\right)^2}{1000-1}}, \tag{11}$$

where $\hat{Z}(s_0)^{*(.)} = \frac{\sum_{b=1}^{1000} \hat{Z}(s_0)^{*(b)}}{1000}$. Use the following equation to calculate a $(1-\alpha)$ confidence interval for NO2 levels in unsampled points:

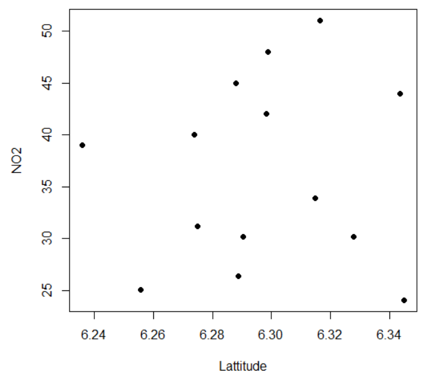
$$\hat{\theta}_{lower} = \hat{Z}(s_0) - z_{\alpha/2} \times s\hat{e}, \tag{12}$$

$$\hat{\theta}_{upper} = \hat{Z}(s_0) + z_{\alpha/2} \times s\hat{e}, \tag{13}$$

Where $\hat{\theta}_{lower}$ dan $\hat{\theta}_{upper}$ are the lower and upper bound of the confidence interval, and $z_{\alpha/2}$ is a normal distribution table value with significance level α.

3. RESULTS AND DISCUSSION

Figure 2 shows the scatter plot between the NO2 level on the X-axis (left) and the Y-axis (right). Based on this figure, it can be seen that the plot of NO2 levels spreads randomly (have no trend) both on the X and Y axes. So, the NO2 level data is stationary. Therefore, the appropriate estimation method is ordinary kriging.



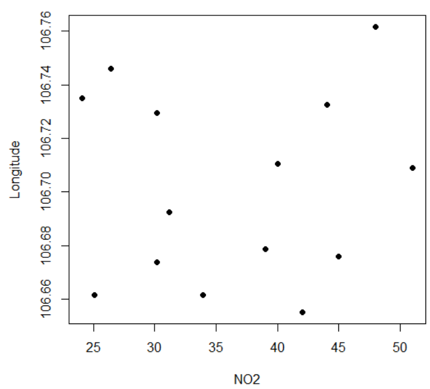


Figure 2. Scatterplot of NO2 levels on the X-Axis (left) and (b) Y-Axis (right).

The next step is grouping the samples into several classes. Based on equation (2), the samples are grouped into five classes, with the class interval calculated by the maximum distance divided by the number of classes. Then, the experimental semivariogram values will be calculated, and the results are presented in Table 2. The plot of the distance between data pairs and the experimental semivariogram is presented in Figure 3. From Figure 3, it can be seen that the experimental semivariogram values look stable.

Table 2. Experimental Semivariogram Values

Class k^{th}	Class Interval	Number of Distance Pairs $N(h)$	Distance Total	Experimental Semivariogram $\gamma(h)$
1	0 – 0.02560	9	0.01791	73.99303
2	0.025602 – 0.05120	24	0.03953	107.60041
3	0.05120 – 0.07680	32	0.06282	54.52787
4	0.07680 – 0.10241	19	0.08616	81.38977
5	0.10241 – 0.12801	7	0.11284	78.69214

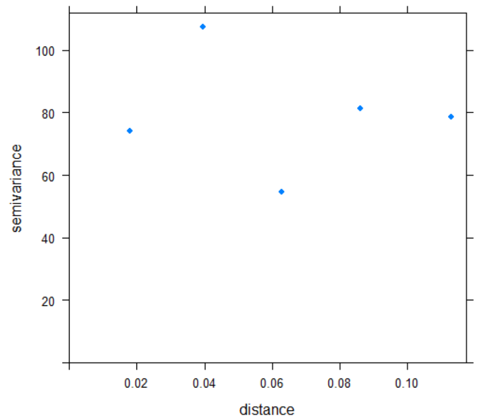


Figure 3. The plot of distance between data pairs vs experimental semivariogram values

The sill value (c) is obtained from the data variance value, i.e., 78.43 µgr/m^3. Meanwhile, range (a) is obtained from the middle value of the interval in the class, which has a semivariogram value close to the sill value. Because the sill value is close to the 5th class experimental semivariogram value in Table 2 (78.6921), the class interval chosen to determine the range is 0.10241140 – 0.12801425. So, $a = 0.1152$. Based on the sill and range values, the nugget effect parameter value for the three theoretical semivariogram models (equations (4) – (6)) is zero when $h = 0$. The theoretical semivariogram values for the Spherical, Exponential, and Gaussian models are listed in Table 3. Based on the smallest RSME value in Table 3, it can be concluded that the best model to estimate NO2 levels is the Exponential. This estimate was calculated using equation (8) at 40 South Tangerang City area points, as shown in table 4. Meanwhile, the map of the estimation results is shown in Figure 2. Based on Table 4, the largest estimated value of NO2 levels is in the Ciater area at 45.84128 ($\mu gr/m^3$), and the smallest estimated value is in the East Pamulang area with an estimated value of 26.52737 ($\mu gr/m^3$).

Table 3. Experimental and Theoretical Semivariogam Values

Class k^{th}	Distance Total	Experimental Semivariaogram	Theoretical Semivariaogram		
			Spherical	**Exponential**	**Gaussian**
1	0.01791	73.99303	18.14843	29.24224	5.48883
2	0.03953	107.60041	38.78539	50.41574	23.33985
3	0.06282	54.52787	57.79388	63.15588	46.28756
4	0.08616	81.38977	71.58676	70.11603	63.78945
5	0.11284	78.69214	78.38559	74.28181	74.02372
		RMSE	39.90233	33.14727	49.38041

Table 4. Point estimates of NO2 levels at 40 areas of South Tangerang City using the Exponential Model.

No.	Region	Estimation of NO_2 level ($\mu gr/m^3$)
1	Pamulang Timur	26.52737
2	Pakulonan	30.35174
3	Pondok Cabe Udik	30.43661
4	Pondok Jagung Timur	30.48084

5	Kademangan	30.79205
6	Keranggan	30.79205
7	Muncul	31.13489
8	Jelupang	32.24183
9	Pondok Karya	32.47729
10	Rengas	32.81675
11	Parigi	33.34769
12	Paku Alam	33.87592
13	Pondok Betung	33.90319
14	Pondok Kacang Barat	34.05360
15	Sawah Baru	34.05370
16	Jurangmangu Timur	34.10586
17	Pondok Kacang Timur	34.25171
18	Jurang Mangu Barat	35.25273
19	Bakti Jaya	35.63790
20	Pondok Cabe Ilir	35.78812
21	Pondok Jaya	37.06014
22	Rawabuntu	37.36694
23	Buaran	37.55341
24	Babakan	37.74739
25	Lengkong Karya	37.97086
26	Lengkong Wetan	37.97615
27	Pondok Pucung	38.38206
28	Ciputat	39.13030
29	Cempaka Putih	39.33554
30	Cipayung	39.61343
31	Kedaung	40.22329
32	Jombang	40.75590
33	Pisangan	41.34482
34	Serua Indah	41.78560
35	Lengkong Gudang Timur	42.14297
36	Cireundeu	42.35209
37	Bambu Apus	42.72107
38	Lengkong Gudang	42.96277
39	Benda Baru	44.95925
40	Ciater	45.84128

Table 5 shows the Bootstrap quasi-random samples that contain vector $\vec{U}$ and several Bootstrap resampling from vector $\vec{U}$ at 14 points. Vector $\vec{U}$ is the result of transforming observational data to become uncorrelated based on equation (9). It then transformed $\vec{U}$ into quasi Bootstrap samples $\vec{Z}^{*(b)}$ using equation (10) for $b = 1, \ldots, 1000$. Table 6 contains $\vec{Z}^{*(b)}$. These $\vec{Z}^{*(1)}$ to $\vec{Z}^{*(1000)}$ will be used as new samples to estimate NO2 levels at 40 unsampled regions using the ordinary kriging method using equation (8).

Table 5. Bootstrap Resampling from Vector $\vec{U}$

No	$\vec{U}$	$\vec{U}^{*(1)}$	$\vec{U}^{*(2)}$	...	$\vec{U}^{*(1000)}$
1	1.12832	0.92553	1.10663	...	0.52503
2	0.99524	0.84481	0.41621	...	1.08935
3	1.08935	0.84481	0.52503	...	1.10663
4	1.19690	0.41127	1.10663	...	0.56599
5	1.10663	1.12832	0.37055	...	0.92553
6	0.92553	0.41621	1.19690	...	0.47487
7	0.84481	1.19690	0.41127	...	1.19690
8	0.56599	0.41127	1.08935	...	0.47487
9	0.63835	1.08935	0.63835	...	1.19690
10	0.41621	0.47487	0.84481	...	1.08935
11	0.52503	0.84481	1.10663	...	0.37055
12	0.37055	0.37055	0.84481	...	0.37055
13	0.41127	0.41621	0.84481	...	0.56599
14	0.47487	0.63835	0.63835	...	1.08935

Table 6. Resampling using Quasi-random Bootstrap

No	$\vec{Z}^{*(1)}$	$\vec{Z}^{*(2)}$	...	$\vec{Z}^{*(1000)}$
1	36.09207	43.15444	...	20.47443
2	33.91967	17.40573	...	43.02472
3	35.05370	22.16735	...	45.19772
4	19.60295	45.94474	...	25.70293
5	47.30906	18.03049	...	39.60156
6	20.57868	50.38309	...	23.22514
7	50.91461	20.35088	...	51.31152
8	21.99952	48.47781	...	24.75157
9	49.00643	32.61194	...	53.66487
10	26.16110	39.79306	...	50.65106
11	42.01500	51.90078	...	24.99932
12	22.59479	41.53944	...	22.42821
13	25.38694	42.09116	...	31.32140
14	35.19577	36.14696	...	53.17094

Table 7 contains the standard error for $\hat{Z}(s_0)^{*(1)}$ to $\hat{Z}(s_0)^{*(1000)}$, which is calculated using equation (11), the lower and upper bound of the 95% confidence interval for NO2 levels at 40 unsampled regions. From this table, it can be seen that the smallest 95% confidence interval is in the value range 25.23123 – 27.82351 at East Pamulang, and the largest 95% confidence interval is in the value range 45.59886 - 46.08371 at Ciater. From the lower and upper bounds of the estimation of NO2 levels at 40 unsampled regions, they are still in the good category following the Decree of the Minister of the Environment Number: KEP 45/MENLH/1997 concerning air pollutant standard indices.

Table 7. Standard error and 95% Confidence Interval for NO_2 level at 40 unsampled areas.

No.	Estimated Area	Standard Error	Estimation of NO_2 ($\mu gr/m^3$) level		Category
			Lower Bound	Upper Bound	
1	Pamulang Timur	0.66131	25.23123	27.82351	Good
2	Pakulonan	0.24915	29.86342	30.84005	Good
3	Pondok Cabe Udik	0.65541	29.15202	31.72119	Good
4	Pondok Jagung Timur	0.23878	30.01283	30.94884	Good
5	Kademangan	0.49627	29.81939	31.76472	Good
6	Keranggan	0.49627	29.81939	31.76472	Good
7	Muncul	0.36534	30.41883	31.85094	Good
8	Jelupang	0.29153	31.67044	32.81320	Good
9	Pondok Karya	0.08026	32.31999	32.63459	Good
10	Rengas	0.15971	32.50372	33.12978	Good
11	Parigi	0.12074	33.11104	33.58432	Good
12	Paku Alam	0.00825	33.85974	33.89209	Good
13	Pondok Betung	0.14801	33.61309	34.19329	Good
14	Pondok Kacang Barat	0.03181	33.99126	34.11593	Good
15	Sawah Baru	0.34076	33.38583	34.72157	Good
16	Jurangmangu Timur	0.13870	33.83401	34.37770	Good
17	Pondok Kacang Timur	0.06184	34.13051	34.37291	Good
18	Jurang Mangu Barat	0.17490	34.90993	35.59553	Good
19	Bakti Jaya	0.51907	34.62054	36.65526	Good
20	Pondok Cabe Ilir	0.62835	34.55658	37.01966	Good
21	Pondok Jaya	0.34551	36.38295	37.73732	Good
22	Rawabuntu	0.28002	36.81811	37.91576	Good
23	Buaran	0.48517	36.60250	38.50432	Good
24	Babakan	0.49751	36.77229	38.72249	Good
25	Lengkong Karya	0.14815	37.68049	38.26123	Good
26	Lengkong Wetan	0.14811	37.68587	38.26643	Good
27	Pondok Pucung	0.31333	37.76794	38.99617	Good
28	Ciputat	0.23924	38.66141	39.59920	Good
29	Cempaka Putih	0.31627	38.71566	39.95542	Good
30	Cipayung	0.34767	38.93201	40.29484	Good
31	Kedaung	0.35957	39.51854	40.92804	Good
32	Jombang	0.03656	40.68423	40.82756	Good
33	Pisangan	0.47717	40.40959	42.28004	Good
34	Serua Indah	0.07738	41.63394	41.93725	Good
35	Lengkong Gudang Timur	0.08487	41.97663	42.30931	Good
36	Cireundeu	0.62764	41.12193	43.58225	Good
37	Bambu Apus	0.22685	42.27646	43.16569	Good
38	Lengkong Gudang	0.01163	42.93997	42.98556	Good
39	Benda Baru	0.34242	44.28812	45.63038	Good
40	Ciater	0.12369	45.59886	46.08370	Good

According to Table 7, NO2 levels in South Tangerang City are in the good category. The results of this study can be used as a reference by local governments in establishing regional policies or regulations that focus on controlling air quality: maintaining appropriate policies and improving/adding policies needed to reduce pollution from NO2. Apart from motorized vehicles, previous research shows that higher NO2 levels can come from cooking fuels and biomass burning (Quackenboss, Spengler, Kanarek, Letz, & Duffy, 1986) (Ryan, Spengler, & Halfpenny, 1988) (Park & Ko, 2018). NO2 levels can be reduced by implementing a motor vehicle restriction policy. In DKI Jakarta, NO2 levels have decreased during the 2019-2020 COVID-19 pandemic by the Large-Scale Social Restrictions (PSBB) policy (Prasetyo, Bashit, Yusuf, & Rassarandi, 2023). (Widya, et al., 2020) suggests that local governments prioritize maintaining a greater percentage of greening when implementing urban planning and design.

The results of NO2 level estimates can provide insight into NO2 distribution patterns in various regions, helping governments and environmental organizations identify potential pollution sources and design more effective policies to reduce their negative impacts. Additionally, understanding NO2 levels can be used to monitor interim developments and measure the effectiveness of government mitigation measures. By understanding NO2 levels, we can work on better strategies to maintain global air quality and environmental and public health.

4. SUMMARY

This article successfully developed a 95% confidence interval to estimate NO2 levels in South Tangerang City. These confidence intervals developed from point estimation using the ordinary Kriging method. The point estimate and 95% confidence interval for the smallest NO2 levels are in East Pamulang, while the largest NO2 is in Ciater. In general, NO2 levels in South Tangerang City are a good category following the Decree of the Minister of Environment Number: KEP 45/MENLH/1997 concerning air pollutant standard indices.

5. REFERENCES

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