NO_2 Concentration Analysis based on Mathematical and Geospatial Approaches

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Abstract

Motivation: NO_2 is one combustion byproduct associated with multiple adverse health outcomes

Data: Air Quality System (AQS) NO_2 monitoring networks over the contiguous United States of the Environmental Protection Agency (EPA) [1] from 2000–2016

Goals:

- predict average daily NO_2 concentration for contiguous US
- find potential correlations between NO_2 concentration and socioeconomic status

Model-Driven Approach

- Mathematical model of NO_2 average daily concentration
- Exponential decay and seasonal oscillation

$$y_{\text{model}}(t; \mathbf{p}) = p_1 + p_2 e^{-p_3(t-p_4)} + p_5 \cos(2\pi p_6(t+p_7))$$

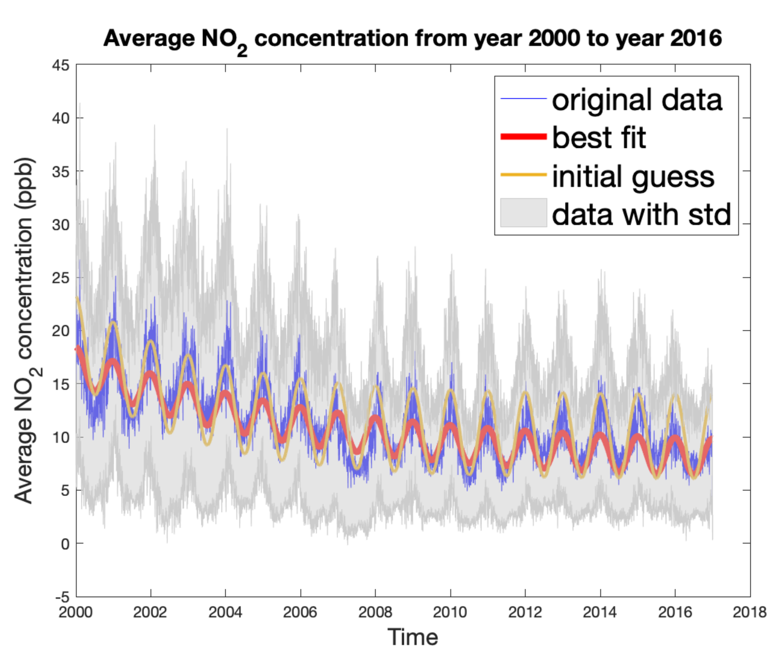
p_1: average NO_2 concentration in US before 2000	p_5: oscillation amplitude
p_2: scale factor	p_6: oscillation frequency
p_3: decay rate	p_7: shift
p_4: initial time	

Data Fitting Approach

Nonlinear least squares problem

$$\arg\min_{\mathbf{p}} \|\mathbf{W}(\mathbf{y}_{\text{model}}(\mathbf{p}) - \mathbf{y}_{\text{data}})\|_2^2$$

$\mathbf{W}$: diagonal weight matrix (standard deviation (std)$^{-1}$)	$\mathbf{y}_{\text{data}}$: original data
$\mathbf{y}_{\text{model}}$: data predicted from the model	



Optimization via Nelder-Mead method (MATLAB `fminsearch`)

Bayesian Approach

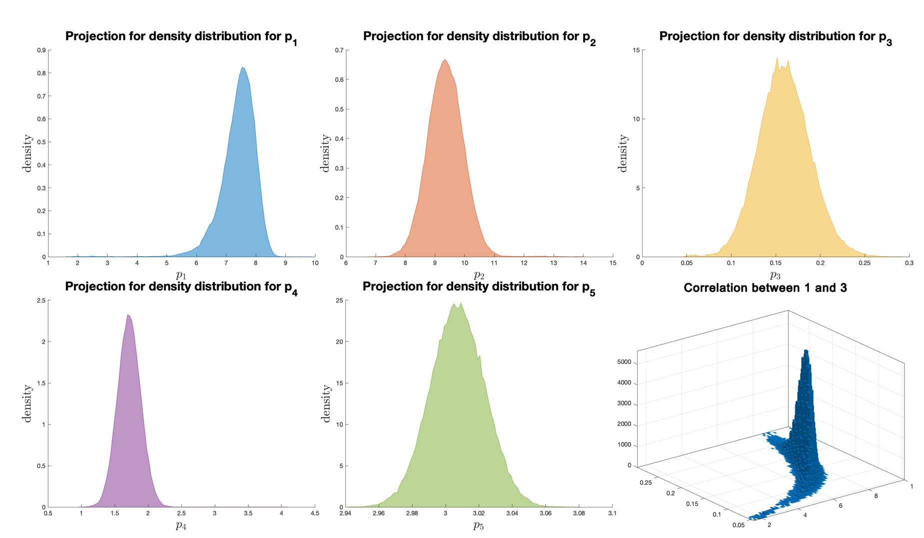
Use Bayes' Theorem [2]

$$\pi_{\text{post}}(\mathbf{p} \mid \mathbf{y}_{\text{data}}) = \frac{\pi_{\text{like}}(\mathbf{y}_{\text{data}} \mid \mathbf{p})\pi_{\text{prior}}(\mathbf{p})}{\pi_{\text{marg}}(\mathbf{y}_{\text{data}})}$$

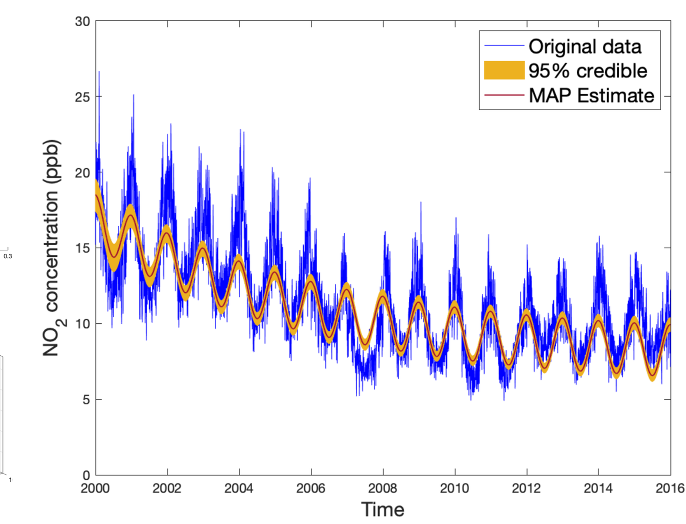
- Generate random samples from posterior distribution using Adaptive Metropolis (fixed $p_4 = 2000$ and $p_6 = 1$) with maximum a-posteriori estimate (MAP)

$$\mathbf{p}_{\text{MAP}} = \arg\max_{\mathbf{p}} \ \pi_{\text{post}}(\mathbf{p}|\mathbf{y}_{\text{data}})$$

Projections of Posterior Distribution:



Model Predictions:



Hybrid Model and Data-Driven Approach

Goal: Train a Long-Term Short-Term Memory Model (LSTM)[3] to predict the residual $\mathbf{r} = \mathbf{y}_{\text{model}} - \mathbf{y}_{\text{data}}$ of the "Model-Driven Approach"

Computational Approach:

- 60 time points used to predict the next time point
- Train on the first 5000 time points, test on the last 1000

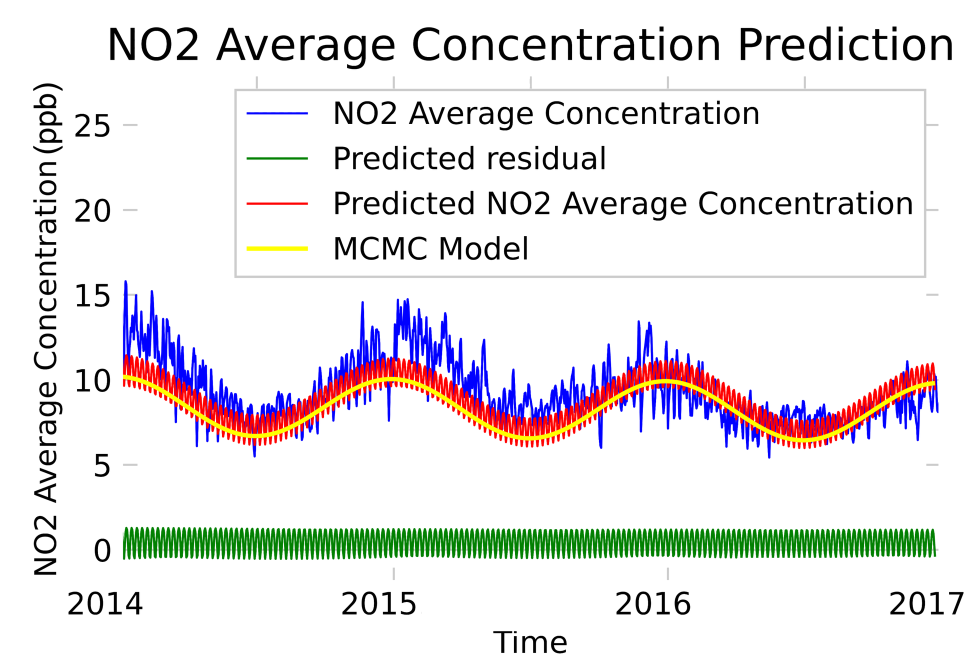
$$\min_{\boldsymbol{\theta}} \ \|\boldsymbol{\Phi}(\mathbf{r}; \boldsymbol{\theta}) - \mathbf{r}\|_2^2$$

where $\boldsymbol{\Phi}$ is an LSTM network with network parameters $\boldsymbol{\theta}$

- 50 epochs for the training via 'Adam' optimizer

Observations:

- Hybrid approach captures oscillation trend
- Large deviations still exist
- Data-driven approaches require larger datasets



References/Acknowledgement

[1] Qian Di et al. "Assessing NO2 concentration and model uncertainty with high spatiotemporal resolution across the contiguous United States using ensemble model averaging". In: *Environmental science & technology* 54.3 (2019), pp. 1372–1384.

[2] Arianna Krinos and Aimee Maurais. "Parameter and Uncertainty Estimation for a Model of Atmospheric CO2 Observations". In: *SIAM Undergraduate Research Online* (2019).

[3] Palash Sharma. *Keras LSTM Layer Explained for Beginners with Example.* MLK - Machine Learning Knowledge. Feb. 1, 2021. URL: https://machinelearningknowledge.ai/keras-lstm-layer-explained-for-beginners-with-example/ (visited on 06/29/2023).

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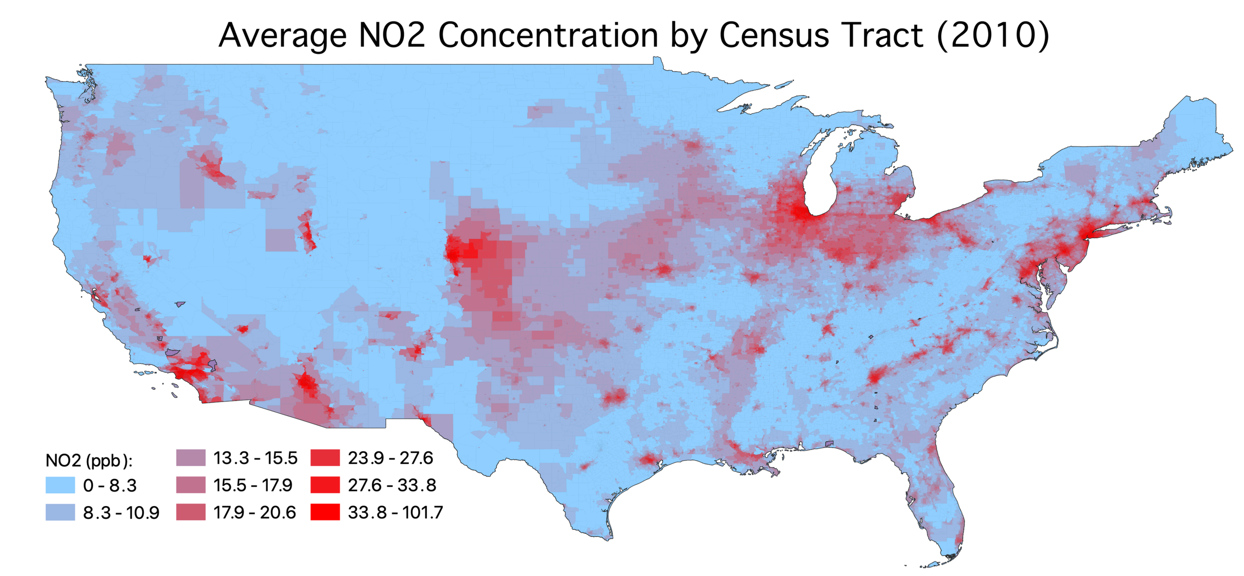
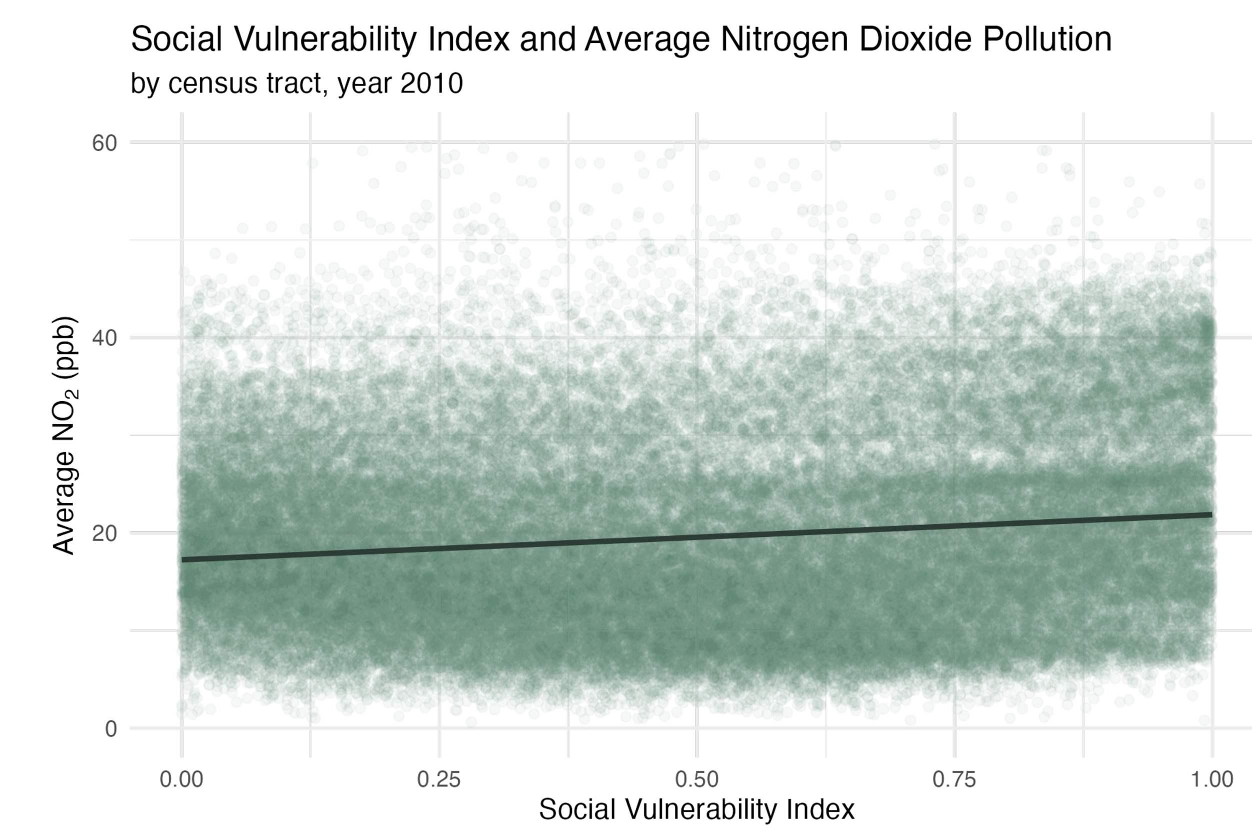
2D NO_2 Maps Analysis

- Averaged NO_2 values over each census tract for years 2000, 2010, 2014, and 2016



- Combined geographical data of census tracts with their Social Vulnerability Indexes (SVI)



Regression Table: Average NO_2 explained by SVI

	estimate	std	p val	lower CI	upper CI
intercept	17.387	0.073	0	17.245	17.530
slope	4.507	0.126	0	4.260	4.754

Conclusions

- A model-driven approach with appropriately selected parameters can provide good predictions of average daily NO_2 concentrations. Including a weight matrix in the objective function resulted in a better data fit.
- Posterior MCMC samples suggest high levels of agreement and demonstrate little uncertainty in their predictions.
- The LSTM model was not ideal for our small data set. A future step is to analyze the frequency of oscillations in the residuals.
- Although weak for some years, we observe correlations between the SVI and NO_2 concentration, most noticeable in 2010.