Detecting Plumes in Mobile Air Quality Monitoring Time Series with Density-based Spatial Clustering of Applications with Noise (DBSCAN)

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Section S1. Temporal rescaling procedure for census tract comparisons.

Section S2. Anomaly type detection probability error estimation procedure.

Figures S1-S8

Tables S1-S8

**Section S1.** Temporal rescaling procedure for census tract comparisons

To remove temporal effects from census tract comparisons of anomaly type detection probability, we performed a rescaling procedure. The approach was to transform each census tract’s sampling distribution into a uniform distribution, then multiply each hour of the newly transformed uniform distribution by the fraction of detected anomalies in that hour.

Out of 35 census tracts sampled in the Houston area, we restrict our analysis to 19 to ensure that each hour between 8 AM and 4 PM CST, had at least 1,000 samples for each individual census tract. The lowest number of samples in any given hour for a census tract was 1,061, which equates to 17 minutes of sampling. For each census tract, we calculate the average number of samples per hour, determined by calculating the total number of samples and dividing by 8, the number of analyzed hours. In addition to calculating the average number of samples, we calculate for each hour in each census tract the fraction of that hour’s measurement that are of a given anomaly type (“CO2 – Rich”, “Transition”, “BC/UFP – Rich”). In the final step, we multiply the hourly fraction of each anomaly type by the average number of measurements for the census tract, and then sum the results. To determine the % probability of detection for a given anomaly type, we divide these weighted totals by the number of measurements made within the census tract.

Figures S1 and S2 display the effects of implementing the rescaling procedure on the calculated probabilities of anomaly detection for the 19 census tracts. In general, we note that implementing the rescaling procedure results in modest increases in these probabilities across the board. A notable exception is the North Rice polygon for CO2 anomaly detections. Figure S3 displays the (a) total sampling distribution and (b) anomaly sampling distribution for the North Rice polygon. We note that the 8 AM hour was oversampled relative to other hours sampled and argue that implementing the rescaling procedure decreases the effects of this hour relative to other sampling times in the census tract.

**Section S2.** Anomaly detection type probability error estimation procedure.

We provide error estimates of our calculated anomaly type detection probabilities and present them in Tables S6, S7, and S8. To do this, we implement the bootstrap for each anomaly detection type probability for each census tract to generate sampling distributions.1

We create 1000 synthetic distributions for each census tract by sampling with replacement measurements within each census tract. For each synthetic distribution, we calculate the probability of each anomaly detection type, repeating the same temporal rescaling procedure described in Section S1 1000 times for each census tract to generate 1000 probabilities of each type. From the resultant sampling distributions, we report the lower and upper bounds of the 90% confidence interval (5th to 95th percentiles), the mean, and bias. We define bias as the difference between the originally calculated probability and its mean probability estimate from its corresponding sampling distribution (in effect, taking the difference between columns in Table 2 and mean columns in Tables S6, S7, and S8).

**Graphical user interface

Description automatically generated**

**Figure S1.** Illustration of manually flagged plumes for CO2. Points in blue are labeled as plume, while points in red are labeled as anomaly. Circles represent manually flagged plumes for this portion of the CO2 time series. Note – not all blue colored points correspond to CO2 plumes, but can represent plume detections in other pollutants not shown here.

Chart, bar chart

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**Figure S2.** Effects of scaling on the probability of CO2 anomaly type detection for each census tract.

Chart, bar chart

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**Figure S3.** Effects of rescaling on probability of BC/UFP anomaly type detection for each census tract.

Chart

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**Figure S4.** Sampling distributions for (a) all measurements and (b) anomalies in the North Rice census tract.

Chart, scatter chart

Description automatically generated**Figure S5.** Visualizing cluster assignment on the first two principal component axes for DBSCAN-derived anomalies.

**Chart, bar chart, histogram

Description automatically generatedFigure S6.** Total anomaly type counts per census tract normalized by the total number of measurements within each census tract. a) CO2 b) BC/UFP

Chart, bar chart

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**Figure S7.** Probability of detecting BC/UFP anomaly type with highways in the analysis (green) and without highways in the analysis (blue).

Chart, bar chart

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**Figure S8.** Probability of detecting CO2 anomaly type with and without highways.

**Table S1.** Instruments used in the Houston mobile monitoring campaign.

|  |  |
| --- | --- |
| Measured Pollutant | Instrument |
| Black Carbon (BC) (ng/m3) | AE33 (Aethalometer) |
| Carbon Dioxide (CO2) (ppm) | LI-7000 CO2/H2O Analyzer (Spectroscopy) |
| Nitric Oxide (NO) (ppb) | Teledyne T200 (Chemiluminescence) |
| Nitrogen Dioxide (NO2) (ppb) | Teledyne T500U (CAPS) |
| Ultrafine Particle Counts (UFP) (p/cm3) | Aerosol Dynamics MAGIC 200p (CPC) |

**Table S2.** Cross validation results for 5 folds.

|  |  |  |
| --- | --- | --- |
| Fold | Trained | Testing Performance (%) |
| 1 | 0.01 | 85.05 |
| 2 | 0.03 | 85.93 |
| 3 | 0.03 | 87.39 |
| 4 | 0.03 | 84.09 |
| 5 | 0.03 | 88.57 |

**Table S3.** Error estimates for CO2 anomaly detection type probabilities (in %) by census tract determined from a sampling distribution composed of 1000 bootstrap replicates. “Mean” is the mean of the sampling distribution, “Lower” is the 5th percentile of the sampling distribution, “Upper” is the 95th percentile of the sampling distribution, “Bias” is the originally calculated value – “Mean”.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Census Tract | CO2 Mean | CO­2 Lower | CO2 Upper | Bias |
| Bayland Park | 1.7 | 1.6 | 1.8 | 0 |
| Washington Corridor | 2.8 | 2.7 | 2.9 | 0 |
| Manchester | 0.8 | 0.8 | 0.9 | 0 |
| East Galena Park | 0.7 | 0.7 | 0.8 | 0 |
| Milby Park | 1.2 | 1.2 | 1.3 | 0 |
| Sharpstown | 4.6 | 4.5 | 4.8 | 0 |
| Sharpstown South | 2.2 | 2.1 | 2.3 | 0 |
| West Galena Park | 1.5 | 1.4 | 1.6 | 0 |
| North Spring Branch | 2.1 | 1.9 | 2.2 | 0 |
| North Rice | 5.8 | 5.7 | 5.8 | 0 |
| Clinton | 1.1 | 1.1 | 1.2 | 0.1 |
| West Eastex | 1.1 | 1.0 | 1.1 | 0 |
| North Heights | 1.4 | 1.4 | 1.5 | 0 |
| South Rice | 5.0 | 4.9 | 5.1 | 0 |
| Harrisburg | 1.0 | 1.0 | 1.1 | 0 |
| Sharpstown North | 3.6 | 3.4 | 3.7 | 0 |
| Westchase | 3.4 | 3.2 | 3.5 | 0 |
| South Spring Branch | 2.3 | 2.2 | 2.4 | 0 |
| South Beltway Central | 0.9 | 0.9 | 0.9 | 0 |

**Table S4.** Error estimates for BC/UFP anomaly detection type probabilities (in %) by census tract determined from a sampling distribution composed of 1000 bootstrap replicates. “Mean” is the mean of the sampling distribution, “Lower” is the 5th percentile of the sampling distribution, “Upper” is the 95th percentile of the sampling distribution, “Bias” is the originally calculated value – “Mean”.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Census Tract | BC/UFP Mean | BC/UFP Lower | BC/UFP Upper | Bias |
| Bayland Park | 0.8 | 0.8 | 0.9 | 0 |
| Washington Corridor | 1.9 | 1.8 | 2.0 | 0 |
| Manchester | 5.6 | 5.5 | 5.8 | 0 |
| East Galena Park | 0.7 | 0.6 | 0.7 | 0 |
| Milby Park | 10.6 | 10.3 | 11.0 | 0 |
| Sharpstown | 2.8 | 2.6 | 2.9 | 0 |
| Sharpstown South | 1.3 | 1.2 | 1.4 | 0 |
| West Galena Park | 6.0 | 5.8 | 6.1 | 0 |
| North Spring Branch | 1.0 | 0.9 | 1.0 | 0 |
| North Rice | 0.6 | 0.5 | 0.6 | 0 |
| Clinton | 4.4 | 4.3 | 4.5 | 0 |
| West Eastex | 2.6 | 2.5 | 2.6 | -0.1 |
| North Heights | 1.4 | 1.4 | 1.5 | 0 |
| South Rice | 0.6 | 0.6 | 0.7 | 0 |
| Harrisburg | 4.2 | 4.0 | 4.3 | 0 |
| Sharpstown North | 1.2 | 1.1 | 1.2 | 0 |
| Westchase | 1.3 | 1.2 | 1.4 | 0 |
| South Spring Branch | 2.4 | 2.3 | 2.5 | 0 |
| South Beltway Central | 2.2 | 2.1 | 2.2 | 0 |

**Table S5.** Error estimates for Transition anomaly detection type probabilities (in %) by census tract determined from a sampling distribution composed of 1000 bootstrap replicates. “Mean” is the mean of the sampling distribution, “Lower” is the 5th percentile of the sampling distribution, “Upper” is the 95th percentile of the sampling distribution, “Bias” is the originally calculated value – “Mean”.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Census Tract | Transition Mean | Transition Lower | Transition Upper | Bias |
| Bayland Park | 8.6 | 8.4 | 8.7 | 0 |
| Washington Corridor | 13.3 | 13.2 | 13.4 | 0 |
| Manchester | 19.6 | 19.4 | 19.8 | 0 |
| East Galena Park | 8.6 | 8.5 | 8.8 | 0 |
| Milby Park | 16.7 | 16.4 | 17.1 | 0.1 |
| Sharpstown | 17.8 | 17.6 | 18.1 | 0 |
| Sharpstown South | 9.5 | 9.3 | 9.7 | 0 |
| West Galena Park | 16.5 | 16.3 | 16.7 | 0 |
| North Spring Branch | 12.0 | 11.7 | 12.2 | 0 |
| North Rice | 14.4 | 14.3 | 14.5 | 0 |
| Clinton | 20.1 | 19.9 | 20.3 | 0 |
| West Eastex | 12.7 | 12.6 | 12.9 | 0.1 |
| North Heights | 10.4 | 10.3 | 10.5 | 0 |
| South Rice | 13.4 | 13.2 | 13.5 | 0 |
| Harrisburg | 16.9 | 16.7 | 17.1 | 0 |
| Sharpstown North | 18.7 | 18.4 | 19.0 | 0 |
| Westchase | 12.7 | 12.5 | 13.0 | 0 |
| South Spring Branch | 13.3 | 13.1 | 13.6 | 0 |
| South Beltway Central | 16.3 | 16.2 | 16.4 | 0 |

**Table S6.** Counts of when QOR or DBSCAN outperform the other under different circumstances.

|  |  |  |  |
| --- | --- | --- | --- |
| QOR Label | DBSCAN Label | Correct Label | Counts |
| “Anomaly” | “Normal” | “Normal” | 19456 |
| “Normal” | “Anomaly” | “Normal” | 6739 |
| “Normal” | “Anomaly” | “Anomaly” | 8183 |
| “Anomaly” | “Normal” | “Anomaly” | 12174 |

**Table S7.** Loadings post varimax rotation from Figure 5. Varimax rotated loadings from Larson et al. are also presented for reference.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | CO2-rich (This work) | CO-rich2 | BC-rich(This work) | BC-rich2 |
| BC | -0.02 | 0.09 | 0.76 | 0.88 |
| CO2 | 0.97 | 0.76 | 0.07 | 0.19 |
| NOx | 0.42 | 0.69 | 0.70 | 0.62 |
| UFP | 0.08 | 0.26 | 0.75 | 0.87 |

**Table S8.** Census tract characteristics reprinted from Actkinson et al.3 Data taken from U.S. Census (2010)4 and Environmental Defense Fund.5

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Census Tracts | Population  Total | # Metal Recyclers | # Concrete Batch Plants | # Petrochemical Facilities |
| Northwest Domain | **34873** | **7** | **2** | **0** |
| North Spring Branch | 5126 | 0 | 0 | 0 |
| South Spring Branch | 3604 | 0 | 0 | 0 |
| Memorial Park | 6908 | 0 | 0 | 0 |
| Washington Corridor | 5432 | 2 | 0 | 0 |
| North River Oaks | 1803 | 0 | 0 | 0 |
| South River Oaks | 2775 | 0 | 0 | 0 |
| West Eastex | 2753 | 5 | 2 | 0 |
| North Heights | 6472 | 1 | 0 | 0 |
| Southwest Domain | **24927** | **0** | **1** | **0** |
| Westchase | 5548 | 0 | 0 | 0 |
| Sharpstown | 5616 | 0 | 0 | 0 |
| Sharpstown North | 3484 | 0 | 1 | 0 |
| Sharpstown South | 5196 | 0 | 0 | 0 |
| Bayland Park | 5083 | 0 | 0 | 0 |
| South Beltway Central Domain | **2530** | **3** | **8** | **0** |
| South Beltway Central | 2530 | 3 | 8 | 0 |
| Rice Domain | **8247** | **0** | **0** | **0** |
| North Rice | 2892 | 0 | 0 | 0 |
| South Rice | 5355 | 0 | 0 | 0 |
| Ship Channel Domain | **20177** | **4** | **1** | **4** |
| Clinton | 2127 | 2 | 1 | 1 |
| West Galena Park | 5245 | 0 | 0 | 0 |
| East Galena Park | 3000 | 0 | 0 | 0 |
| Manchester | 1647 | 0 | 0 | 1 |
| Harrisburg | 1496 | 2 | 0 | 2 |
| Milby Park | 6662 | 0 | 0 | 0 |

(1) Efron, B.; Tibshirani, R. J. *An Introduction to the Bootstrap*; Chapman and Hall/CRC: New York, 1994. https://doi.org/10.1201/9780429246593.

(2) Larson, T.; Gould, T.; Riley, E. A.; Austin, E.; Fintzi, J.; Sheppard, L.; Yost, M.; Simpson, C. Ambient Air Quality Measurements from a Continuously Moving Mobile Platform: Estimation of Area-Wide, Fuel-Based, Mobile Source Emission Factors Using Absolute Principal Component Scores. *Atmos. Environ.* **2017**, *152*, 201–211. https://doi.org/10.1016/j.atmosenv.2016.12.037.

(3) Actkinson, B.; Ensor, K.; Griffin, R. J. SIBaR: A New Method for Background Quantification and Removal from Mobile Air Pollution Measurements. *Atmospheric Meas. Tech.* **2021**, *14* (8), 5809–5821. https://doi.org/10.5194/amt-14-5809-2021.

(4) Census 2010 Tracts https://cohgis-mycity.opendata.arcgis.com/datasets/census-2010-tracts (accessed 2020 -11 -23).

(5) Finding pollution—and who it impacts most—in Houston https://www.edf.org/maps/airqualitymaps/houston/pollution-map/ (accessed 2020 -11 -23).