



Technical Basis for the EPA's Development of the Significant Impact Thresholds for PM_{2.5} and Ozone

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PM_{2.5} and Ozone

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1.0 Introduction:

In order to understand the nature of air quality, the EPA statistically estimates the distribution of pollutants contributing to ambient air quality and the variation in that air quality. The statistical methods and analysis detailed in this report focus on using the conceptual framework of *statistical significance* to calculate levels of change in air quality concentrations that have a “significant impact” or an “insignificant impact” on air quality degradation. *Statistical significance* is a well-established concept with a basis in commonly accepted scientific and mathematical theory. This analysis examines *statistical significance* for a range of values measured by air quality monitors. The statistical methods and data reflected in this analysis may be applicable for multiple regulatory applications where EPA and state agencies seek to quantify a level of impact on air quality that they consider to be either “significant” or “not significant.” Note: We have adopted the following convention throughout the document: a “significant impact” (in quotes) refers to a level of air quality change that can be used in the permit analysis of the ambient impacts from a facility to determine if it “causes, or contributes to” a violation of the applicable National Ambient Air Quality Standards (NAAQS) or Prevention of Significant Deterioration (PSD) increment, whereas we use *significant* (italicized) to refer to a mathematical assessment of probabilistic properties.

While this technical analysis may have utility in several contexts, the primary purpose of this document is to quantify the degree of air quality impacts corresponding to different confidence intervals (related to the statistical analysis presented here) that can be used in determining what is an “insignificant impact” when considering an application for a permit under the PSD program. In order to obtain a preconstruction permit under the PSD program, an applicant must demonstrate that the increased emissions from its proposed modification or construction will not “cause or contribute to” a violation of any NAAQS or PSD increment.¹ One way that this criterion can be met is by showing that the increased emissions from a proposed source will not have a significant impact on ambient air quality at any location, including locations where an exceedance of the NAAQS or PSD increment is occurring or may be projected to occur.² For the purposes of a PSD permit, the EPA has promulgated analytical methods involving air quality modeling and monitoring for conducting these compliance demonstrations.³ More generally (*e.g.*, for purposes of designating areas as attainment or nonattainment), compliance with the NAAQS is determined by comparing the measured “design value” (DV) at an air quality monitor to the level of the NAAQS for the relevant pollutant.⁴ A DV is a statistic or summary metric based on the most recent one or three years (depending on the specific standard) of

¹ 40 Code of Federal Regulations (CFR) 51.166 and 52.21.

² Memorandum from Peter Tsigotis, EPA Office of Air Quality Planning and Standards, Guidance on Significant Impact Levels for Ozone and Fine Particles in the Prevention of Significant Deterioration Permitting Program, April 17, 2018.

³ 40 CFR, part 51, Appendix W, 82 FR 5182 (January 17, 2017), Revisions to the Guideline on Air Quality Models: Enhancements to the AERMOD Dispersion Modeling System and Incorporation of Approaches to Address Ozone and Fine Particulate Matter.

⁴ A design value is a statistic that describes the air quality status of a given location relative to the level of the NAAQS. More information may be found at: <http://www3.epa.gov/airtrends/values.html>.

monitored data that describes the air quality status of a given location relative to the level of the NAAQS.

The EPA has decided that an “insignificant impact” level of change in ambient air quality can be characterized by the observed variability of ambient air quality levels. Since the cause or contribute test is applied to the NAAQS in the PSD program, this analysis has been designed to take into account the ambient data used to determine DVs and the form of the relevant NAAQS. The EPA’s technical approach, referred to as the “Air Quality Variability” approach, relies upon the fact that there is inherent variability in the observed ambient data, which is in part due to the intrinsic variability of the emissions and meteorology controlling transport and formation of pollutants, and uses statistical theory and methods to model that intrinsic variability in order to facilitate identification of a level of change in DVs that is acceptably similar to the original DV, thereby representing a change in air quality that is not significant.⁵ The DVs and background ambient concentrations that are used in the PSD compliance demonstrations are obtained through the U.S. ambient monitoring network with measured data being archived for analysis in the EPA’s Air Quality System (AQS).⁶

Based on these observed ambient data, the EPA has estimated the variability of the air quality levels of ozone and PM_{2.5} through applying a well-established statistical approach known as bootstrapping. Bootstrapping is a method that allows one to construct measures to quantify the uncertainty of sample statistics (*e.g.*, mean, percentiles) for a population of data.^{7,8} The bootstrap approach applied here uses a non-parametric, random resampling with replacement on the sample dataset (in this case, the ambient air quality concentration data underlying the DVs), resulting in many resampled datasets. This approach allows measures of uncertainty for sample statistics when the underlying distribution of the sample statistic is unknown and/or the derivation of the corresponding estimates is computationally unfeasible or intractable.⁷ Bootstrapping is also commonly utilized to overcome issues that can occur when quantifying uncertainty in samples with correlated measurements. Bootstrapping has been used across a variety of scientific disciplines and in a wide range of applications within the environmental sciences.^{9,10,11,12} For example, bootstrapping has been used to evaluate the economic value of

⁵ This approach is applied here strictly for the purpose of section 165(a)(3) and no other parts of the Clean Air Act.

⁶ The AQS contains ambient air pollution data collected by EPA, state, local, and tribal air pollution control agencies from over thousands of monitors. These data are used to assess air quality, assist in attainment/nonattainment designations, evaluate State Implementation Plans for nonattainment areas, perform modeling for permit review analysis, and other air quality management functions. More information may be found at: <http://www.epa.gov/aqs>.

⁷ Efron, B. (1979); Bootstrap methods: Another look at the jackknife. *The Annals of Statistics* 7 (1): 1–26. doi:10.1214/aos/1176344552.

⁸ Efron, B. (2003); Second Thoughts on the Bootstrap. *Stat. Sci.*, 18, 135-140.

⁹ Schuenemeyer, J., Drew, L. (2010); *Statistics for Earth and Environmental Scientists*, John Wiley & Sons, Inc. <http://dx.doi.org/10.1002/9780470650707.ch3>.

¹⁰ Park, Lek, Baehr, Jørgensen, eds. (2015); *Advanced Modelling Techniques Studying Global Changes in Environmental Sciences*, 1st Edition, Elsevier. ISBN 9780444635365.

¹¹ Chandler, R., Scott, M. (2011); *Statistical Methods for Trend Detection and Analysis in the Environmental Sciences*, John Wiley & Sons, Inc. ISBN: 978-0-470-01543-8.

¹² Mudelsee, M. & Alkio, M. (2007); Quantifying effects in two-sample environmental experiments using bootstrap confidence intervals, *Env. Mod. & Software*, 22, 84-96.

clinical health analyses¹³ and environmental policies,¹⁴ in evaluations of environmental monitoring programs,¹⁵ and in determining uncertainty in emissions inventories.¹⁶ Additionally, the EPA has used bootstrapping techniques as a key component in evaluating air quality model performance for use in our nation's air quality management system.^{17,18}

The bootstrap technique, as applied in this analysis, quantifies the degree of air quality variability at an ambient monitoring site and allows one to determine confidence intervals (CIs), *i.e.*, statistical measures of the variability associated with the monitor-based DVs, to inform the degree of air quality change that can be considered an “insignificant impact” for PSD applications. This approach is fundamentally based on the idea that an anthropogenic perturbation of air quality that is within a specified range may be considered indistinguishable from the inherent variability in the measured atmospheric concentrations and is, from a statistical standpoint, *not significant* at the given confidence level. Specifically, the analysis uses 17 years (2000-2016) of nationwide ambient ozone and PM_{2.5} measurement data from the AQS database to generate a large number of resampled datasets for ozone and PM_{2.5} DVs at each monitor from which the appropriate design values are calculated. The DVs from the resampled datasets are used to determine CIs that provide a measure of the inherent variability in air quality at the monitor location. This variability may be driven by the frequency of various types of meteorological and/or emissions conditions impacting a particular location. The analysis estimates a range of CIs for each monitor. As discussed in Section 4.1.1 of this document and in the Policy Document,² the 50% CI was chosen to quantify the bounds of a change in air quality that can be considered an “insignificant impact” for the purposes of meeting requirements under the PSD program.

This technical basis document explains the analysis design and results provide the EPA's rational basis to recommend Significant Impact Levels (SILs) values that can be applied as a tool for making the PSD compliance demonstration required by the Clean Air Act (CAA) and PSD regulations. The second section of this document provides an overview of EPA's Air Quality Variability approach, including details on the ambient monitoring network, the ambient ozone and PM_{2.5} data from AQS that are used to derive monitor-specific DVs, a general review of *statistical significance* and confidence intervals, and a description of the bootstrap technique as applied to characterize air quality variability. The third section presents the measures of air quality variability determined from applying the bootstrap technique to the AQS data for ozone and PM_{2.5}. The last section provides an analysis of confidence intervals for the ozone and PM_{2.5} DVs and the implications of the geographical analysis performed in response to peer reviewer

¹³ Campbell, M., & Torgerson, D. (1999); Bootstrapping: Estimating Confidence Intervals for Cost-effectiveness Ratios, *Q. J. of Med.*, 92, 177-182.

¹⁴ Kochi, I., Hubbell, B., & Kramer, R. (2006); An Empirical Bayes Approach to Combining and Comparing Estimates of the Value of a Statistical Life for Environmental Policy Analysis, *Env. & Resource Econ.*, 34, 385-406.

¹⁵ Levine, C., et al (2014); Evaluating the efficiency of environmental monitoring programs, *Ecol. Ind.*, 39, 94-101.

¹⁶ Tong, L., et al (2012); Quantifying uncertainty of emission estimates in National Greenhouse Gas Inventories using bootstrap confidence intervals, *Atm. Env.*, 56, 80-87.

¹⁷ Hanna, S. (1989); Confidence limits for air quality model evaluations, as estimated by bootstrap and jackknife resampling methods, *Atm. Env.*, 6, 1385-1398.

¹⁸ Cox, W. & J. Tikvart (1980); A statistical procedure for determining the best performing air quality simulation model, *Atm. Env.*, 9, 2387-2395.

comments. The resulting values chosen by the EPA can serve as SIL levels for the ozone NAAQS and the annual and 24-hour PM_{2.5} NAAQS.

2.0 Background on Air Quality Variability Approach

This section provides details on the ambient monitoring data for ozone and PM_{2.5} that were used in the EPA's Air Quality Variability approach and the statistical methods that form the technical basis for the EPA's Air Quality Variability approach.

2.1 U.S. Ambient Monitoring Data

The EPA's understanding of the nation's air quality is based on an extensive ambient monitoring network, which is used for multiple purposes, including to determine compliance with the various NAAQS. In addition, the monitoring network is used to inform the public about the status of air quality across the nation and to support air pollution research, particularly in the evaluation and development of updated NAAQS. The general requirements of the monitoring network are given in 40 CFR part 58, Appendix D (Network Design Criteria for Ambient Air Quality Monitoring). These general requirements and choices made by the state and local air agencies conducting monitoring have resulted in monitoring sites across the nation with a variety of characteristics in terms of location, monitoring equipment, and operating schedule.

NAAQS compliance is determined by comparing the measured DV derived from a monitor's data to the level of the NAAQS for the relevant pollutant. The DV is a particular statistic determined from the distribution of data from each monitor and is consistent with the averaging period and statistical form of the relevant NAAQS. The DVs from an area's monitoring network are used to determine attainment status for that area. The DVs for PM_{2.5} and ozone are determined as follows:

- For the primary ozone NAAQS, the DV is the 3-year average of the annual 4th-highest daily maximum 8-hr average (MDA8) ozone concentration.¹⁹ A monitor is in compliance if the DV is less than or equal to the level of the standard, which was recently revised to be 0.070 ppm (70 ppb.)²⁰
- For the primary annual PM_{2.5} NAAQS, the DV is the 3-year average of the PM_{2.5} annual mean mass concentrations.²¹ The annual mean is defined as the mean of the data in each of the 4 quarters of the year (*i.e.*, the mean of the quarterly means). A monitor is in compliance with the 2012 annual primary PM_{2.5} standard if the DV is less than or equal to 12.0 µg/m³.²²

¹⁹ Appendix U to Part 50 - Interpretation of the Primary and Secondary National Ambient Air Quality Standards for Ozone.

²⁰ National Ambient Air Quality Standards for Ozone, 80 FR 65292 – 65468 (Oct. 26, 2015).

²¹ Appendix N to Part 50—Interpretation of the National Ambient Air Quality Standards for PM_{2.5}.

²² There is a secondary PM_{2.5} NAAQS, with a level of 15.0 µg/m³. The work here focuses only on the primary NAAQS at 12.0 µg/m³, since compliance with the primary standard explicitly implies compliance with the secondary standard as well.

- For the 24-hr PM_{2.5} NAAQS, the DV is the 3-year average of the annual 98th percentile 24-hr average PM_{2.5} mass concentration. A monitor is in compliance with the 24-hr PM_{2.5} standard if the DV is less than or equal to 35 µg/m³.

2.1.1 Ozone Monitoring Network

The ozone monitoring network consists of only one type of monitor, Federal Equivalent Method (FEM) monitors.²³ The FEM for ozone uses ultraviolet (UV) light to determine ozone concentrations at high temporal resolutions, on the order of seconds to minutes, although only hourly averages are typically recorded. Unlike PM_{2.5} monitors, most ozone monitors are not required to operate year-round, and are instead required to operate only during the “ozone season.” The ozone season is the time of year that high ozone concentrations (which may potentially exceed the NAAQS) can be expected at a particular location. The ozone season varies widely by location, but is generally focused on the summer months, with a typical season spanning March through October. During the period of 2000 through 2016, a total of 1,708 ozone monitors reported data, with the locations of the ozone monitors shown in Figure 1 along with the average number of days sampled each year that the monitor was active.

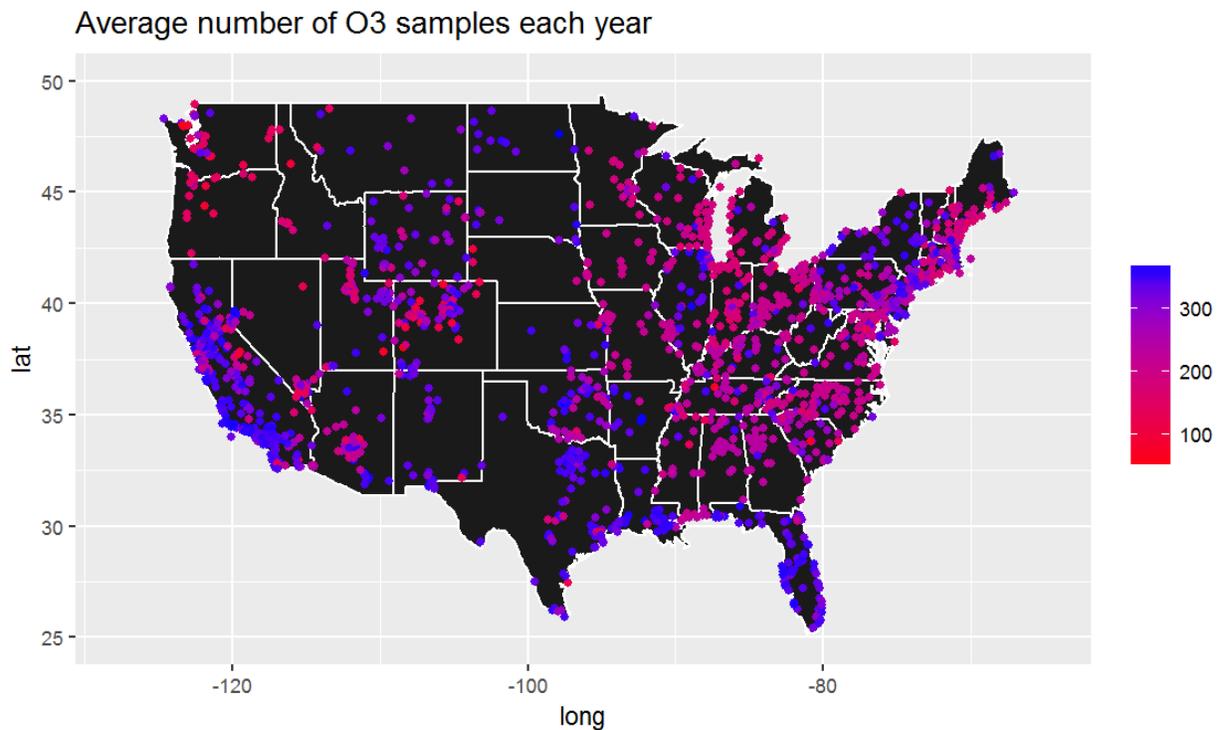


Figure 1 - Location and average number of monitored ozone days each year from the ozone sampling network for the years 2000-2016.

²³ FEM monitors are approved on an individual basis. The list of approved monitors and the accompanying CFR references can be found at <http://www3.epa.gov/ttn/amtic/criteria.html>.

2.1.2 PM_{2.5} Monitoring Network

The PM_{2.5} monitoring network consists of two types of monitors: Federal Reference Method (FRM)²⁴ and FEM²³ monitors. FRM monitors use a filter-based system, passing a low volume of air through a filter over a period of 24 hours (midnight to midnight) to determine 24-hr average concentrations. All monitors operate year-round, but not all monitors operate every day throughout the year. Although some FRM sites operate every day (*i.e.*, 1:1 monitors), most operate every third day (1:3 monitors), while a smaller number of monitors operate only every sixth day (1:6 monitors), according to a common schedule provided by the EPA. Newer FEM monitors are “continuous” monitors that can provide hourly (or shorter) PM_{2.5} measurements and have undergone testing to demonstrate conformance (including linear regression, slope/intercept, time series, and mean concentration ratios) with the FRM monitors.²⁵ FEM monitors operate on a 1:1 schedule and daily averages from FEM monitors are determined by averaging the 24 hourly measurements collected throughout the day. FEM monitors are slowly replacing FRM monitors, so monitoring sites with a long data record may have data derived from either an FEM, FRM, or combination of both types of monitors. Although the FRM and FEM monitors have small differences in their performance, the largest impact to the bootstrap technique of this transition from all FRM monitors to a mix of FRM and FEM monitors is the gradual increase in the frequency of PM_{2.5} measurements over time. During the period of 2000 through 2016, a total of 1,773 PM_{2.5} monitors reported data, with the locations of the PM_{2.5} monitors shown in Figure 2 along with the average number of days sampled each year that the monitor was active.

²⁴ Appendix B to Part 50—Reference Method for the Determination of Suspended Particulate Matter in the Atmosphere (High-Volume Method).

²⁵ Noble, C. A. et al (2001); Federal Reference and Equivalent Methods for Measuring Fine Particulate Matter, *Aerosol Sci. & Tech*, 34:5, 457-464.

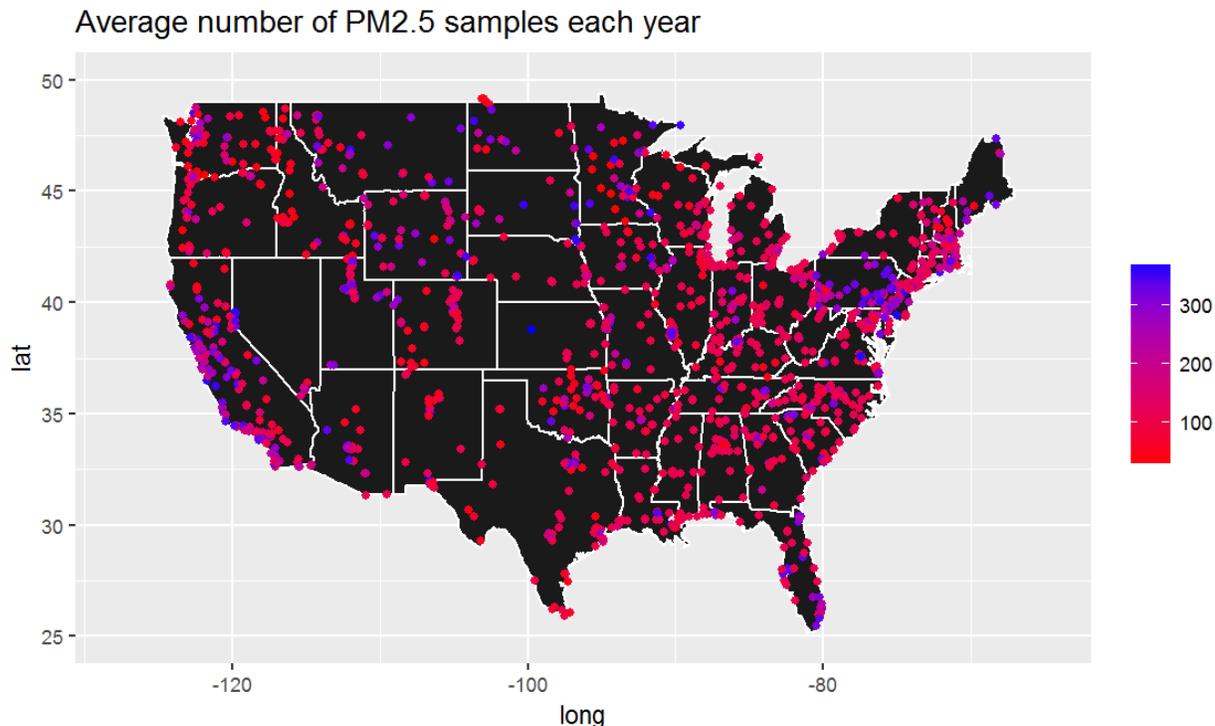


Figure 2 - Location and average number of monitored PM days each year from the PM_{2.5} sampling network for the years 2000-2016.

2.1.3 Monitoring Network Design

The ambient air monitoring network is designed to support several objectives. In consideration of the location and measurement taken, each monitor is assigned a spatial scale. Spatial scales are generally associated with the size of the area that a pollutant monitor represents. The monitor spatial scales are defined in 40 CFR part 58, Appendix D as:

1. *Microscale*—Defines the concentrations in air volumes associated with area dimensions ranging from several meters up to about 100 meters.
2. *Middle scale*—Defines the concentration typical of areas up to several city blocks in size with dimensions ranging from about 100 meters to 0.5 kilometer.
3. *Neighborhood scale*—Defines concentrations within some extended area of the city that has relatively uniform land use with dimensions in the 0.5 to 4.0 kilometers range. The neighborhood and urban scales listed below have the potential to overlap in applications that concern secondarily formed or homogeneously distributed air pollutants.
4. *Urban scale*—Defines concentrations within an area of city-like dimensions, on the order of 4 to 50 kilometers. Within a city, the geographic placement of sources may result in there being no single site that can be said to represent air quality on an urban scale.
5. *Regional scale*—Defines usually a rural area of reasonably homogeneous geography without large sources, and extends from tens to hundreds of kilometers.

6. *National and global scales*—These measurement scales represent concentrations characterizing the nation and the globe as a whole.

Depending on the distribution and types of sources in an area and the need to determine particular aspects of the air quality, there may be multiple types of monitors placed in an area. For example, a large metropolitan area, due to its size, may require several “urban scale” or “neighborhood” scale monitors to capture the range of air quality in the area. Such an area might also have “microscale” monitors placed in order to assess the impacts from a single source or small group of sources as well as a “regional scale” monitor to establish the background air quality in an area in order to differentiate the impacts from the urban area. Conversely, for a smaller urban area a single “urban scale” monitor may be considered sufficient to fully characterize the local air quality. Thus, there are wide variety of monitors in any area, covering a range of air quality monitoring needs. For ozone, the appropriate spatial scales are neighborhood, urban, and regional scale. For PM_{2.5}, in most cases the appropriate spatial scales are neighborhood, urban, or regional scales; however, in some cases it may be appropriate to monitor at smaller scales, depending on the monitoring objective.

2.1.4 Air Quality System (AQS) Database

The EPA’s AQS database contains ambient air pollution data collected by state, local, and tribal air pollution control agencies, as well as EPA and other federal agencies, from the monitoring stations described above (as well as monitoring stations for other NAAQS).⁶ AQS also contains meteorological data, descriptive information about each monitoring station, and data quality assurance/quality control information. The Office of Air Quality Planning and Standards (OAQPS), state and local air agencies, tribes, and other AQS users rely upon the system data to assess air quality, assist in attainment/nonattainment designations, evaluate state implementation plans for nonattainment areas, perform modeling for permit review analysis, and execute other air quality management functions related to the CAA.

2.2 Statistical Methods and Assessing Significance Using Confidence Intervals

This section provides a general overview of statistical methods, how air quality variability is characterized for this analysis, and the bootstrapping approach employed to estimate air quality variability.

2.2.1 General Overview of Statistical Methods

Statistics is the application of mathematical and scientific methods used to interpret, analyze and organize collections of data. Most statistical techniques are based on two concepts, a “population” and a “sample.” The *population* represents all possible measurements or instances of the entity being studied. The *sample* is a subset of the *population* that is able to be collected or measured. Since the *sample* is only a portion of the *population*, any observations or conclusions made about the *population* based on the *sample* will have uncertainty, *i.e.*, there will be some error in those observations or conclusions due to the fact that only a subset of the population was sampled or measured. Consider the following example:

As discussed above, the ambient monitoring network is designed to capture a range of ambient impacts from facilities and to characterize both background and local air quality. Suppose we want to determine the average ground-level PM_{2.5} levels in a remote state wilderness area over the course of a year. Assuming the wilderness area does not have major PM_{2.5} sources and the area is remote (*i.e.*, there are no major metropolitan areas upwind), a single, well-placed “regional scale” monitor may be sufficient to capture the nature of PM_{2.5} levels in the area (*i.e.*, the PM_{2.5} levels within the wilderness area are homogenous). Due to the remote nature of the monitor, it is only operated on a 1-in-every-6 days schedule, such that one 24-hr average PM_{2.5} measurement is made every six days. In this case, we may consider the *population* to be the 24-hr average PM_{2.5} concentrations every day (365 potential samples over the whole year) within the wilderness area. The *sample* would be the 1-in-every-6 days 24-hr average PM_{2.5} measurements (60 samples taken over the whole year). From this *sample* of the *population*, a mean 24-hr average PM_{2.5} concentration can be calculated, which can be characterized as representing the mean 24-hr average PM_{2.5} concentration from the *population*, with some amount of error between the *sample* mean and the *population* mean. By using information about the size and distribution of the *sample*, an estimate of the population variability (*i.e.*, the spread of the distribution), can be determined (*e.g.*, the standard deviation).

Significance testing, or determining the *statistical significance* of a particular value as it relates to a *sample*, is a major application of statistics. In formal hypothesis testing, a statement of non-effect or no difference – termed the null hypothesis – is established prior to taking a sample in order to test the effect of interest. A statistical test is then carried out to determine whether a *significant* effect (or difference) is present at the desired level of confidence. Note that not finding a *statistically significant* difference is not a claim of the null hypothesis being true or a claimed probability of the truth of the null hypothesis.²⁶ *Non-significance* simply shows the data to be compatible with the null hypothesis under the set of assumptions associated with the statistical test.²⁶ A CI can be used as a mathematically equivalent procedure²⁶ to a formal hypothesis test for significance. CIs are constructed based on the desired confidence level and characteristics of the *sample*, including the sample variance, to determine error bars for the statistic of interest, such as the mean. Error bars constructed in this fashion are referred to as CI because they convey the confidence in the *sample* estimate of the *population* given the size of and the variability in the sample. This can then be used to determine if the mean is *significantly* different from a particular value of interest, such as zero or some other threshold for the pollutant, by examining whether the value of interest is within the CI or outside the bounds of the CI.

The most well-known approach to deriving CIs uses the characteristics of sampling distributions and the Central Limit Theorem. The sampling distribution of the mean results from sampling all possible samples of a specified size *n* from the true population and considering the distribution of the resulting means from each sample. The Central Limit Theorem is based on the fact that the

²⁶ Gelman, A. P values and Statistical Practice, *Epidemiology*, 2013, Vol 24, Num 1, pg 70.

sampling distribution of the sample mean will center around the population mean. Regardless of the distribution of the original population, the sampling distribution of the mean will be normally distributed.²⁷ Additionally, the sampling distribution will have a spread, with a standard deviation that is inversely proportional to the square root of the sample size n (*i.e.*, the larger the sample size, the tighter the spread of the sampling distribution of the mean around the true mean of the population). This allows for the derivation of a CI by calculating the estimated mean plus/minus the standard error, which is a function of the sample size, the standard deviation, and the desired level of confidence.

To relate these statistical tests to a practical application, we continue the hypothetical example from above:

Suppose that the observed annual mean PM_{2.5} concentration for a given year is $7 \mu\text{g}/\text{m}^3$, and that based on the Central Limit Theorem utilizing the properties of the sampling distribution, the 95% CI for the annual mean is determined to be $6.4\text{-}7.6 \mu\text{g}/\text{m}^3$ ($7 \mu\text{g}/\text{m}^3 \pm 0.6 \mu\text{g}/\text{m}^3$, where $0.6 \mu\text{g}/\text{m}^3$ has been determined based on the standard error and the desired level of confidence). Since the CI contains the value $7.5 \mu\text{g}/\text{m}^3$, we may, therefore, conclude based on this specific sample that the mean of the population is *not significantly* different from $7.5 \mu\text{g}/\text{m}^3$ at the 0.95 confidence level. Conversely, if the 95% CI for the annual mean PM_{2.5} concentration is $6.7\text{-}7.3 \mu\text{g}/\text{m}^3$ ($7 \mu\text{g}/\text{m}^3 \pm 0.3 \mu\text{g}/\text{m}^3$), then the CI does not contain $7.5 \mu\text{g}/\text{m}^3$ and it could be concluded that the mean of the population is *significantly* different from $7.5 \mu\text{g}/\text{m}^3$ at the 0.95 confidence level.

The Central Limit Theorem also tells us that due to the Gaussian (Normal Distribution) properties of a sampling distribution, 68/95/99.7 percent of the values in the theoretical sampling distribution will be within 1/2/3 standard deviations of the true population mean respectively. Additionally, in any symmetric distribution such as the Gaussian obtained with the theoretical sampling distribution, the mean is equal to the median, where the median is the center value such that 50% of the values are below the median and 50% above. Thus, an alternative approach to deriving a CI directly utilizes these characteristics of the sampling distribution to consider the spread around the sampling distribution mean. For example, a 95% CI would be defined as the lowest value to the highest value of the 95% of the distribution that centers around the sampling distribution mean. This corresponds to the 0.025 and 0.975 quantiles of the sampling distribution. An example of this method of determining CIs is given in Figure 3, which shows a distribution of the mean determined from repeated *samples* from the *population*. Note that in practice the sampling distribution is approximately Normal. The average of the sample means is $6.98 \mu\text{g}/\text{m}^3$. In order to determine the 95% CI, the data are first rank-ordered from smallest to the largest concentration value, then the bounds of the 0.025 and 0.975 quantiles are the bounds of the CI (the 50% CI is also shown as an example).

²⁷ These are asymptotic properties given that the sample size n is large and that the number of samples (N) drawn from the population is large – in theory, all possible samples of size n are drawn from the population. (Moore and McCabe, 4th Ed, 2003 – p. 262.) In practice, $n \geq 30$ and N is often 1,000, 10,000, or as determined by convergence of distributional characteristics, and the resulting sampling distribution is approximately normal.

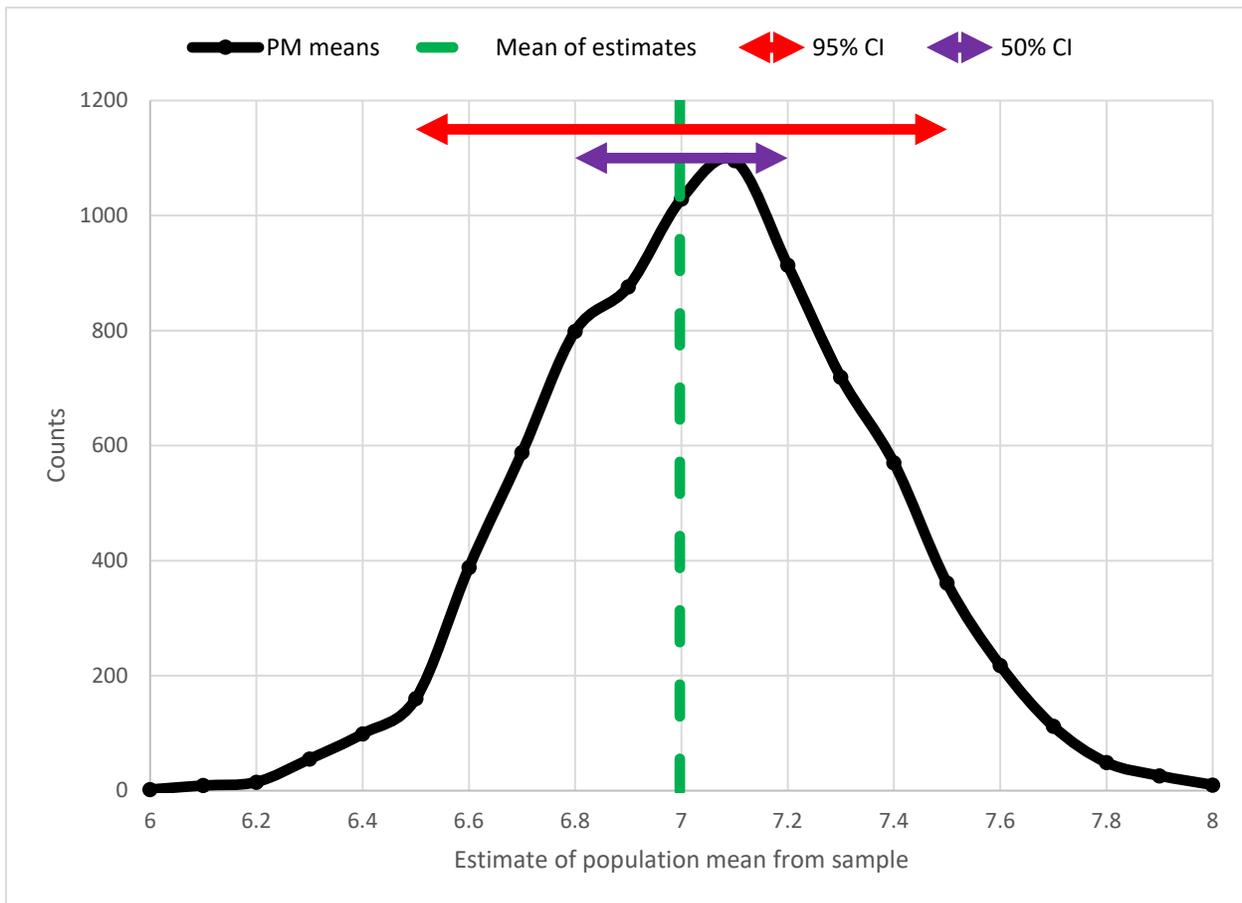


Figure 3- Example of CIs determined from a distribution of sample means.

The techniques utilizing the sampling distribution to make inferences about the population mean can be applied to other statistics as well, such as sample quantiles. Additionally, a statistical technique applied as resampling from one particular drawn sample, known as bootstrapping, can be used to generate estimated CIs for any desired statistic. Bootstrapping is further explained in Section 2.2.3.

The CIs for any sample comparison are generally affected by three main factors: the size of the sample, the variability within the sample, and the confidence limits desired for the comparison (*e.g.*, 0.95 level of confidence was used in the example above). Increasing the sample size (taking more measurements or samples) will increase the representativeness of the sample of the population and decrease the variance associated with the calculated measurement, resulting in narrower CIs. Samples from populations with greater inherent variability will have greater uncertainty and result in larger CIs. Finally, increasing the confidence level of the inferred conclusion will necessitate larger CIs, while lower confidence thresholds will result in narrower CIs. There are clearly many complicated aspects of significance testing, many of which require subjective selections by the analyst to insure that the results are appropriate to the application

and to reduce the influence of uncontrolled variables on the results and conclusions. These selections are usually made based on convention and standard practice, such as choosing a 95% CI. While there are many more applications of statistical techniques and nuances of the principles described above, these basic concepts of the population, sample, CIs (and their relationship to probability) are the fundamental concepts used in the development of “significant impact” thresholds presented here.

2.2.2 Characterizing Air Quality Variability

As discussed in Section 2.1, the DV from a particular monitor is the air quality statistic that is used to describe the air quality in an area (*e.g.*, the annual mean was the statistic from the example above) and is compared to the NAAQS to determine attainment status for that area. Within the conceptual framework discussed in the previous section, the ambient data from a single monitor are a *sample* of a *population* of the air quality in an area and the uncertainty in that sample stems from the inherent variability that occurs in air quality. The inherent variability is driven by a collection of factors, both natural (meteorological) and anthropogenic (emissions), which can be grouped into spatial and temporal categories.

2.2.2.1 Spatial variability

The spatial variability is the change in air quality that is present at any one moment across an area. This variability is driven by the spatial distribution of sources (causing localized increases in ambient concentrations due to their emissions), removal or sinks (causing localized decreases in ambient concentrations due to physical or chemical processes), variations in chemical production for secondarily formed PM_{2.5} and ozone (which do not have direct emissions sources), and meteorology (wind patterns may transport air from areas with higher emissions to areas that typically have lower concentrations due to fewer localized emissions). The spatial variability is directly addressed in the network design (*i.e.*, the spatial scale associated with each monitor and the potential need for multiple monitors to characterize the air quality in an area). One way to estimate the spatial variability is to compare ambient monitors that are in close proximity to one another. Such monitors would likely show similar trends in the ambient concentrations, with some variation due to changes in emissions and meteorology responsible for transporting pollutants and affecting chemical conversion, creation, and removal of atmospheric species that are specific to each individual location.

These spatial variations occur in the population of air quality levels and can be estimated from the existing sample (*i.e.*, data available from the ambient monitoring network). Depending on the intended scale of the monitor, there is some room for interpretation as to the population that sample represents (*e.g.*, a sample from an area-wide monitor theoretically represents the population of air quality across a wide area), and this interpretation has implications for the determination of the uncertainty associated with the sample (*e.g.*, a sample from an area-wide monitor is less likely to accurately represent air quality across the whole area at any moment, thus having greater uncertainty as to its ability to characterize the population of air quality it is intended to represent). Given the nature of the variability in air quality, there are three potential

populations represented by the sample and the spatial variability between the sample and the population:

1. If the population is considered to be the air quality at the location of the monitor only, then there is no spatial variability.
2. If the population is considered to be the air quality in the immediate vicinity of the monitor, then there will be some spatial variability, the degree of which will depend on nearby sources and sinks and the distance of the location of interest from these sources and sinks. For $PM_{2.5}$, if there is a nearby source of primary $PM_{2.5}$, changes in wind direction and mixing conditions will change where these nearby sources have impacts, such that there would be more spatial variability on this small scale. If there is no nearby source of primary $PM_{2.5}$, then secondary $PM_{2.5}$ would dominate and there would likely be little small-scale spatial variability on this small scale. For ozone, the same is true, in that there will likely be little spatial variability unless there are nearby sources that act as a sink (*i.e.*, major NO_x source such as a highway or point source). Without a nearby sink, then the secondary nature of ozone would generally indicate that there is little spatial variability on this small scale.
3. If the population is considered to be the air quality over a larger scale (*e.g.*, a county or Core Based Statistical Area or CBSA), then there is much more spatial variability. As with case 2, the presence and location of sources and sinks will impact how much spatial variability is present, though on such a large scale, there are likely to be many sources and sinks across the area, resulting in more spatial variability.

As discussed in Section 2.2.1, monitoring sites are assigned a spatial scale, which are associated with the size of the area for which a particular monitoring site should be representative of the air quality. For secondarily formed pollutants, Appendix D to Part 58 states that the highest concentration monitors may include urban or regional scale monitors (*i.e.*, 50 to hundreds of km spatial scale). Intuitively, it would be expected that the air quality changes across these distance scales, such that the air quality across such a large area is not identical to the air quality as determined by a single monitor. Indeed, these classifications are supportive of the idea that there are spatial variations, such that multiple monitors are generally needed to adequately characterize the air quality in an urban area. However, in rural areas with few emissions sources, a single monitor may be sufficient to characterize the air quality over hundreds of square km (as was the case in the example above).

2.2.2.2 Temporal variability

In the example introduced in Section 2.2.1, there may be uncertainty not only from the limited sampling of the population, but also based on changes in the *population* occurring with time.

Temporal variability is the variability in air quality that occurs over time, which is driven by changes in emissions and meteorology over a range of time scales. For shorter time scales, diurnal patterns in both emissions and meteorological processes can impact most atmospheric pollutants. Mobile source emissions, which can substantially contribute to atmospheric pollution, have particularly strong daily (*i.e.*, rush-hour) and weekly (no rush-hour on the weekends)

patterns. Day-to-day meteorological variability (*i.e.*, frontal passages and synoptic weather patterns) can also cause temporal variability on the timescale of days to weeks. At intermediate time scales, seasonal changes in weather can have a major impact in transport patterns and chemical reactions. There can be seasonal trends in emission patterns as well, particularly those associated with energy production and mobile source emissions. At longer time scales, there can be longer-term trends in meteorology (*e.g.*, particularly warm or wet years) and emission sources (sources being added or removed or changes in emissions due to emissions controls or economic conditions) that result in long-term air quality variability. Temporal variability is reflected in the form of the standard (*i.e.*, compliance with each ozone and PM_{2.5} standard is based on 3 years of data in order to reduce from the impact of temporal variability on NAAQS implementation programs). This variability can be addressed by requiring continuous monitoring in an area, even after air quality levels in an area are below the level of the standard. The long-term temporal variability can be characterized by examining changes in air quality over time at a particular monitor (*e.g.*, trends in DVs or other metrics from the monitor). The shorter-term temporal variability can be described by examining the hourly and daily changes in air quality or by comparing data from periods with similar meteorological conditions (*e.g.*, afternoon, weekdays versus weekends, or summertime concentrations).

Whatever the spatial scale of the monitor, temporal variability will always contribute to the air quality variability, as there will always be day-to-day changes in meteorology and emissions and variability between seasons and years, which may or may not include any trends in emissions and meteorology. The form of the standard (*e.g.*, annual average or a ranked daily value), the temporal resolution of the monitoring data (*e.g.*, hourly or 24-hr averaged samples), and the frequency of the sampling (*e.g.*, daily samples or samples taken every sixth day) may affect the ability of the monitoring data to fully capture the inherent temporal variability and thus increase the uncertainty in any statistic or DV derived from a particular sample. If a monitor has some missing data, then it is easy to conceptualize that there is some uncertainty caused by temporal variability in that there are days and hours that are not represented by the monitor. On the other hand, if a monitor has a perfect sampling record, then the uncertainty due to reduced sampling frequency is eliminated, but there remains long-term variability. Since the PM_{2.5} and ozone DVs are based on 3 years of data, there is variability between the years that affect the DVs. As noted above, the use of a 3-year DV, rather than a DV derived from 1 or 2 years of data, is intended to increase the stability (or reduce the variability) of the DVs.

The importance of temporal variability is perhaps more apparent when the application of the DVs are considered. For area designations purposes, the DVs are historical (updated DVs for a particular year are published in the following calendar year), such that the DV is an estimate of the current state of the air quality in an area. Furthermore, in the permitting process, DVs are paired with modeling of past years of meteorology and planned future emissions. Thus, the changes from year-to-year and the uncertainty in estimating future air quality levels are illustrative of important factors affecting temporal variability that impacts regulatory applications and exists regardless of the completeness of the sampling record or the spatial scale defining the population discussed above.

Continuing the example from Section 2.2.1:

Suppose that after 1 year of sampling, there is some commercial development adjacent to the wilderness area, such that new buildings and larger traffic volumes are present during the second year of the monitor's operation. One might want to assess whether or not the new activity has had a notable impact on the average $PM_{2.5}$ concentrations within the wilderness area. A comparison between the scenarios can be considered, and the idea that the difference between the two may be "notable" can be evaluated by comparing that difference to the estimated CIs created by the bootstrap procedure using the concepts in significance testing (Section 2.2.1).

2.2.2.3 Assessing air quality variability

Based on the description of the population determined above, the DV can be understood to be a statistic determined from a sample of the population. CI's for a particular DV can then be used to compare the DV with another DV or a constant value (*e.g.*, the NAAQS). If the CI for the DV contains the value of interest, then the DV and the value of interest are statistically indistinguishable from one another, given the sample data available at a particular confidence level. In the context of an air quality analysis, if a CI can be determined for a DV, then it can be concluded that a value within some given amount of variation of a DV (*i.e.*, within a CI for that DV) is statistically not significant with respect to that selected level of confidence. Note that in this context *non-significance* simply shows the data to be compatible with an assumption of no difference between the value and the DV.²⁶

2.2.3 Bootstrapping Method

For annual-average standards (*i.e.*, averages of many samples during 1 or 3 years), there are standard parametric methods (*e.g.*, the standard deviation) that might be used to estimate variability associated with DVs. When the statistic of interest has a variance that is difficult to estimate with parametric assumptions, such as a rank order statistic, some other approach must be taken to determine CIs. For non-normal populations, there are some adjustments that can be made to determine CIs of the mean if the data conform to some standard distribution (*e.g.*, log-normal). For small sample sizes, other non-parametric tests such as the Mann-Whitney²⁸ test or the Wilcoxon signed-rank test²⁹ may be used. However, for many statistics (*e.g.*, the 98th percentile), the underlying distribution of the statistic may be complicated or unknown, and thus determination of the CIs for these statistics can be difficult or impossible to determine with traditional metrics.³⁰ Of the three NAAQS considered here, the annual $PM_{2.5}$ standard is the only NAAQS that is based on a sample mean. However, the calculation of the DV statistic for the annual $PM_{2.5}$ NAAQS is more complicated than merely taking a simple arithmetic average of the 24-hr $PM_{2.5}$ values across 3 years; thus, deriving the distribution of the annual $PM_{2.5}$ DV statistic

²⁸ Mann, H. B.; Whitney, D. R. (1947). On a Test of Whether one of Two Random Variables is Stochastically Larger than the Other. *Annals of Mathematical Statistics* 18 (1): 50–60. doi:10.1214/aoms/1177730491.

²⁹ Wilcoxon, F. (Dec 1945). Individual comparisons by ranking methods. *Biometrics Bulletin* 1 (6): 80–83.

³⁰ Woodruff, R. S. (1952); Confidence intervals for medians and other position measure. *J. Amer. Stat. Assoc.*, 47, 635–646, doi:10.1080/01621459.1952.10483443.

is not straightforward. The CIs for the 24-hr PM_{2.5} and ozone NAAQS are based on rank-order statistics (98th percentile for PM_{2.5} and 4th highest daily maximum 8-hr ozone concentration, see Section 2.1), which cannot be easily described using standard statistical techniques. Thus, for the three DV statistics being analyzed here, an alternative technique to determine CIs is needed.

The bootstrapping method mentioned above is a well-established and accepted statistical method that allows one to estimate the underlying distribution of many sample statistics (*e.g.*, mean, percentiles, and correlation coefficients) when the theoretical distribution is complicated or unknown.^{7, 8, 9} The bootstrap method relies on the underpinnings and characteristics of sampling distributions discussed in Section 2.2. The estimate of the distribution is accomplished by resampling with replacement from the initial dataset many times, resulting in many resampled datasets (bootstrapped samples). The sample statistic of interest is then computed from each resampled dataset, resulting in an empirical estimate of the sampling distribution for the desired statistic. This estimate of the sampling distribution can then be used to determine CIs for the statistic of interest. Bootstrapping does not require any distributional assumptions for the population, nor does it require that there be an established formula for estimating the uncertainty in the statistic.

Meaningful information on the variability associated with the ozone and PM_{2.5} DVs can be derived by using bootstrapping to assess the variability associated with the three DV statistics (*i.e.*, the ozone DV, the annual PM_{2.5} DV, and the 24-hr PM_{2.5} DV).⁹ This analysis uses ambient PM_{2.5} and ozone measurement data taken from the EPA's AQS database to determine CIs for each monitor for 3-year DV periods (*i.e.*, the 3 years of ambient data required to compute a DV for these NAAQS). The CIs give a measure of the temporal and spatial variability in the air quality represented by each monitor. A nationwide analysis of the variability and changes in this variability over time is also conducted. Finally, the results from this analysis of air quality variability are used to calculate levels of change in pollutant concentrations that can serve as “significant impact” thresholds in the context of source-specific “cause or contribute” determinations.

The dataset used for this technical analysis comes from the AQS database described in Section 2.1 and is the same dataset that would be used for determining the DV at any particular monitor. The ambient PM_{2.5} concentration data used for this analysis consist of 24-hr averaged samples, while the ozone data consist of 8-hr averaged concentrations (*i.e.*, the MDA8's). This includes data from all of the monitoring sites in the EPA's AQS database from the years of 2000 to 2016.³¹

The bootstrapping estimates used in this analysis were calculated independently for each monitoring site, and the bootstrapping resamples at each site were taken independently within

³¹ Raw daily and hourly measurements from FRM and FEM monitors are aggregated by AQS into a single daily value for each sampling site and NAAQS (annual and 24-hr) according to the procedures described in Appendix N of Part 50. The aggregation procedures in AQS include accounting for multiple monitors at sites, handling of exceptional events (which can be different between the two PM_{2.5} NAAQS), and calculating a 24-hr value from 1-hr measurements. These results reside in the "site_daily_values" table of AQS, which were downloaded for use in the current analysis.

each calendar year. The re-sampling within each year is completed such that the re-sampled year contains the same number of days as the original data. The number of measurements varies by monitoring site and can have important implications for the inherent variability. The variation in the sampling schedule is explored further in Section 3.2.2. The re-sampling and computation of new DVs at each site are conducted to mimic the DV calculation procedures as closely as possible, which differ for each NAAQS.^{19,21}

- For the annual PM_{2.5} NAAQS, the data from each year was further subset by quarter (*i.e.*, Jan-Mar, Apr-Jun, Jul-Sep, Oct-Dec), such that the re-sampling did not allow for data from one quarter to occur in another quarter. The resulting re-sampled dataset was averaged by quarter; then the quarterly means were averaged to find the annual mean, with the DV being computed as the average of the three annual means. Design values for the annual PM_{2.5} NAAQS were rounded to the tenth $\mu\text{g}/\text{m}^3$ (*i.e.*, the one decimal), consistent with the computation of DVs for designation purposes.
- For the 24-hr PM_{2.5} NAAQS, the data from each year was subset by quarter (*i.e.*, Jan-Mar, Apr-Jun, Jul-Sep, Oct-Dec), such that the re-sampling did not allow for data from one quarter to occur in another quarter. The number of days in each quarter was kept equal to the corresponding number in the original dataset. While this isolation of quarters is not a feature of the DV calculation procedure, it was applied as a precaution to avoid changing the seasonal balance in the bootstrapped samples. The resulting re-sampled dataset was then ranked, and the 98th percentile value was selected based on the number of daily measurements in each year, as described in Table 1 of Appendix N. The DVs were then computed as the average of the three annual 98th percentile values. Design values for the 24-hr PM_{2.5} NAAQS were rounded to the nearest $\mu\text{g}/\text{m}^3$, consistent with the computation of design values for designation purposes.
- For the ozone NAAQS, all available data at each site were used. The ozone monitoring regulations require monitoring for the “ozone season,” which varies by state. Many states operate a subset of ozone monitors outside of the required monitoring season and when those data are available it is used in determining DVs for regulatory purposes. Therefore, if a monitor operated beyond the required ozone season, all valid data were included in the DV calculation. For example, if the required monitoring season was from April-October, but data from November were also available, then the MDA8 values from April-November were ranked in order to find the 4th highest value. The DVs were then computed as the average of the three annual 4th highest MDA8 values. Design values for the ozone NAAQS were truncated to the nearest ppb, consistent with the computation of design values for designation purposes. Though the regulations for processing ozone data to compute a DV do not involve segregation of the data by season, a sensitivity analysis was conducted to determine the impact of applying the same quarterly segregation used for PM_{2.5}. The results are summarized in Section A.4 of the Appendix, but the results indicated relatively little sensitivity to this choice for most sites and, thus, no quarterly segregation was applied for the final analysis.

For both PM_{2.5} and ozone, each year of data from each site was re-sampled 20,000 times. During initial development of the method, the distributions derived from the bootstrap analysis did not appear to change after 3,000-4,000 re-samples for several single calendar years. Therefore, 20,000 re-samples were chosen to conservatively ensure that stable results were obtained for all cases. For each 1-year re-sample for each pollutant, the relevant annual statistic was computed (annual mean for PM_{2.5}, 98th percentile for PM_{2.5}, and 4th highest MDA8), giving 20,000 estimates of the annual statistic for each year. In order to replicate the way in which the standard is calculated, the data from each year are resampled separately from the other years. In order to calculate the bootstrap samples in a manner consistent with the DV calculations (*i.e.*, calculating averages and 98th percentile values in each year independently), then averaging the three annual values, each of the 20,000 estimates for year 1 were averaged with the corresponding 20,000 estimates for year 2 and year 3, giving 20,000 estimates of the DV. From the 20,000 estimates, the mean, median, standard deviation, maximum, minimum, 25%, 50%, 68%, 75% and 95% CIs for the mean,³² were computed and retained for further analysis. For symmetric distribution such as the Normal Distribution obtained with the sampling distribution, the mean is equal to the median, where the median is the center value such that 50% of the values are below the median and 50% above. Thus, a bootstrapped CI for the mean is analogous to a bootstrapped CI for the median and the CIs can be calculated by rank-ordering the bootstrap results and selecting the bounds that contain the corresponding percentage of data. Since data from 2000-2014 were processed, all possible 3-year DVs from 2002-2014 were computed, for a total of 13 DV-years, including five 3-year periods that had non-overlapping years (*i.e.*, 2000-2002, 2003-2005, 2006-2008, 2009-2011, and 2012-2016).³³ As we are defining the CIs as the bounds of the uncertainty and a measure of the air quality variability, we frequently refer to each CI as the uncertainty associated with the actual DV.

The following gives an example of how the CIs are determined utilizing the percentile method³⁴ for the 24-hr PM_{2.5} DVs from a monitor:

- Consider the dataset X_0 , which contains 150 measurements of 24-hr averaged PM_{2.5} monitoring values from year 1. Datasets Y_0 and Z_0 contain data from the same site, but for years 2 and 3 respectively, and contain 250 and 350 days of data respectively.
- From X_0 , we calculate the 98th percentile as the 3rd highest value in the dataset. From Y_0 , we calculate the 98th percentile as the 5th highest value in the dataset. From Z_0 , we calculate the 98th percentile as the 7th highest value in the dataset. The DV for this site is the average of the 98th percentiles from X_0 , Y_0 , and Z_0 .

³² Here, and elsewhere in this document, a CI for the median is the interval spanning the data that contains ½ of the CI of the data above the median and ½ of the CI of the data below the median of the re-sampled DV estimates. For example, the 50% CI consists of the 25% of the data above the median and the 25% of the data below the median.

³³ Later in this document, whenever a single year is used to identify a DV, it refers to the last year of the 3-year period.

³⁴ Efron, B.; Tibshirani, R. (1993); An Introduction to the Bootstrap. Boca Raton, FL: Chapman & Hall/CRC. ISBN 0-412-04231-2.

- From X_0 , 20,000 new sample datasets, $X_1, X_2, \dots, X_{20,000}$, each with 150 measurements of $PM_{2.5}$ are sampled with replacement from the original dataset X_0 . Likewise, 20,000 new sample datasets are sampled with replacement from Y_0 , and Z_0 .
- For each X_i , the 98th percentile value is the 3rd highest value, for each Y_i , the 98th percentile is the 5th highest value, and for each Z_i , the 98th percentile is the 7th highest value. Thus, the DV for each subset, DV_i , is the average of the 3rd high value from X_i , the 5th highest value from Y_i , and the 7th highest value from Z_i . This calculation yields 20,000 different DVs.
- To determine the CIs from these 20,000 DVs, the DVs are ranked from low to high. Then the lower bound for the 50% CI is the 5,000th ranked DV, and the upper bound for the 50% CI is the 15,000th ranked DV. That is, the CIs are determined simply by ranking the resulting distribution of DVs and the $(1-q)\%$ CI for the mean is the bounds of the center of the data that contains q percentage of the results (*i.e.*, the lower bound is the $(q/2)$ th percentile and the upper bound is the $(1-q/2)$ th percentile).

Section A.1 provides several illustrative examples of the bootstrapping analysis for both the annual and 24-hr $PM_{2.5}$ NAAQS with actual data from six different sites.

3.0 Results of the Air Quality Variability Approach

This section provides results on characterizing the variability of air quality for ozone and $PM_{2.5}$ based on EPA's Air Quality Variability approach.

3.1 Ozone results

The results from the bootstrap analysis for the 2014-2016 ozone DVs are shown in Figure 4, which shows the mean, median, minimum, and maximum bootstrap DVs for each monitor, as well as the upper and lower bounds of the 25%, 50%, 68%, 75%, and 95% CIs for the median DV calculated from the 20,000 bootstrap samples as a function of the DV determined from the original dataset (top panel), the relative differences between the CI DVs and the actual DVs (middle panel), and box-and-whisker plots of the distribution of the relative difference at each CI (bottom plot). The mean and median of the bootstrap DVs for the ozone NAAQS replicate the actual DV from the original site data fairly well, with some very small deviations (maximum deviation is less than 5%). Even though the ozone NAAQS is based on peak values (similar to the 24-hr $PM_{2.5}$ NAAQS), the magnitude of the relative variability in the ozone bootstrap DVs ranges from 1-5%, with maximums around 25-30%. This is likely due to the nature of ozone formation (*i.e.*, ozone is almost exclusively a secondarily formed pollutant, with precursors typically originating from multiple sources, rather than a single source). There is a component of reaction/formation time, both of which are likely to reduce the spatial variability and temporal variability of the ambient ozone. There is an increase in the absolute variability with an increase in the baseline DVs, but there is not an apparent trend in the relative variability. This indicates that the baseline air quality does not systematically affect the relative amount of variability at a site. This is especially important because it indicates that a central tendency value for the relative

variability in the DV for the ozone NAAQS is stable across levels of ozone concentrations. Therefore, a representative value can be multiplied by the level of that NAAQS to obtain a value in concentration units (ppb for ozone) that is appropriately used to characterize variability for sites with air quality that “just complies” with the NAAQS.

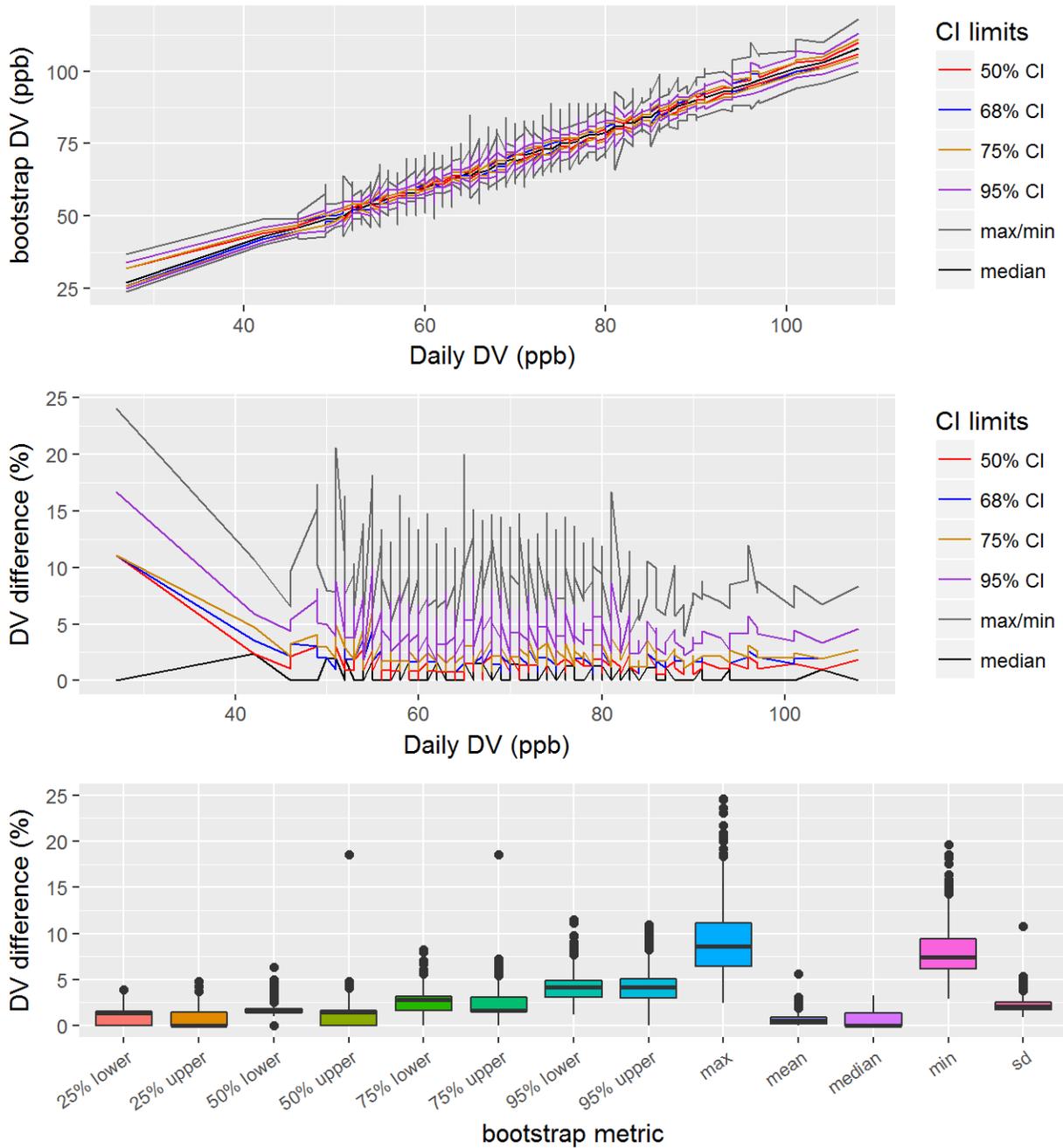


Figure 4 - Bootstrap results for the ozone 2014-2016 DVs (25%, 50%, 68%, 75%, and 95% CIs, along with the mean and median bootstrap DVs) Top panel shows the values for the DVs at the various CIs, the middle panel shows the average of the relative difference between the upper and lower bounds of the CI and the actual DV, and the bottom panel shows the distribution of the relative differences between the CI and the actual DV.

3.2 PM_{2.5} Results (Annual and 24-hr)

The results from the bootstrap analysis for the 2014-2016 DVs are shown in Figures 5 and 6. The top two panels of Figure 5 show the upper and lower limits of the 25%, 50%, 68%, 75%, and 95% CIs for the median as well as the mean, median, minimum and maximum DVs calculated from the 20,000 bootstrap samples as a function of the DV determined from the original dataset. Variability is greater for the 24-hr PM_{2.5} NAAQS than the annual PM_{2.5} NAAQS. This is not surprising since the mean is expected to be a more stable statistic than the 98th percentile. Since the PM_{2.5} data distributions tend to be skewed to the right (see examples in the Appendix), the presence of a few very high concentration values, or “outliers,” in the original dataset for a year would tend to increase the variability associated with any metric based on the highest concentrations (*e.g.*, if the 50th percentile value were determined, it would likely have much less variability than the 98th percentile). The mean and median of the bootstrap DVs for the annual NAAQS almost perfectly replicate the actual DV from the original site data. While some deviations of the mean and median bootstrap DVs from the actual 24-hr NAAQS DV are evident, there are only a few sites where the mean and median bootstrap DVs deviate substantially from the actual DV.

The relative variability (*i.e.*, the difference between the bounds of the bootstrapped CI and the actual design value for a single monitoring site, divided by the actual design value for the site) is also shown in Figure 5, with distributions of the relative differences for each CI across monitoring sites shown in Figure 6. Viewing the results on a relative scale allows the display of finer details of the deviations between the bootstrap results and the actual DVs. The relative variability shows that for the annual NAAQS there are relatively small differences in the values corresponding to the 25%, 50%, 68%, and 75% CIs compared to the difference between these and the 95% CI. Similarly, for the 24-hr NAAQS, the values corresponding to the 50%, 68% and 75% CIs are fairly close to each other, with greater differences between these and the 25% CI on the low end and the 95% CI on the high end. The relative variability shows an important feature: that from a relative sense, the air quality variability is fairly stable as the baseline air quality worsens. That is, there is no notable increase in the relative variability of the bootstrap DV as the actual DV increases. This is important because it indicates that the magnitude of the actual DV does not systematically affect the relative variability in the bootstrap DV at a site and because it indicates that a central tendency value for the relative variability in the DV. Therefore, a representative value can be multiplied by the level of that NAAQS to obtain a value in concentration units ($\mu\text{g}/\text{m}^3$ for PM_{2.5}) that is appropriately used to characterize variability for sites with air quality that “just complies” with that NAAQS.

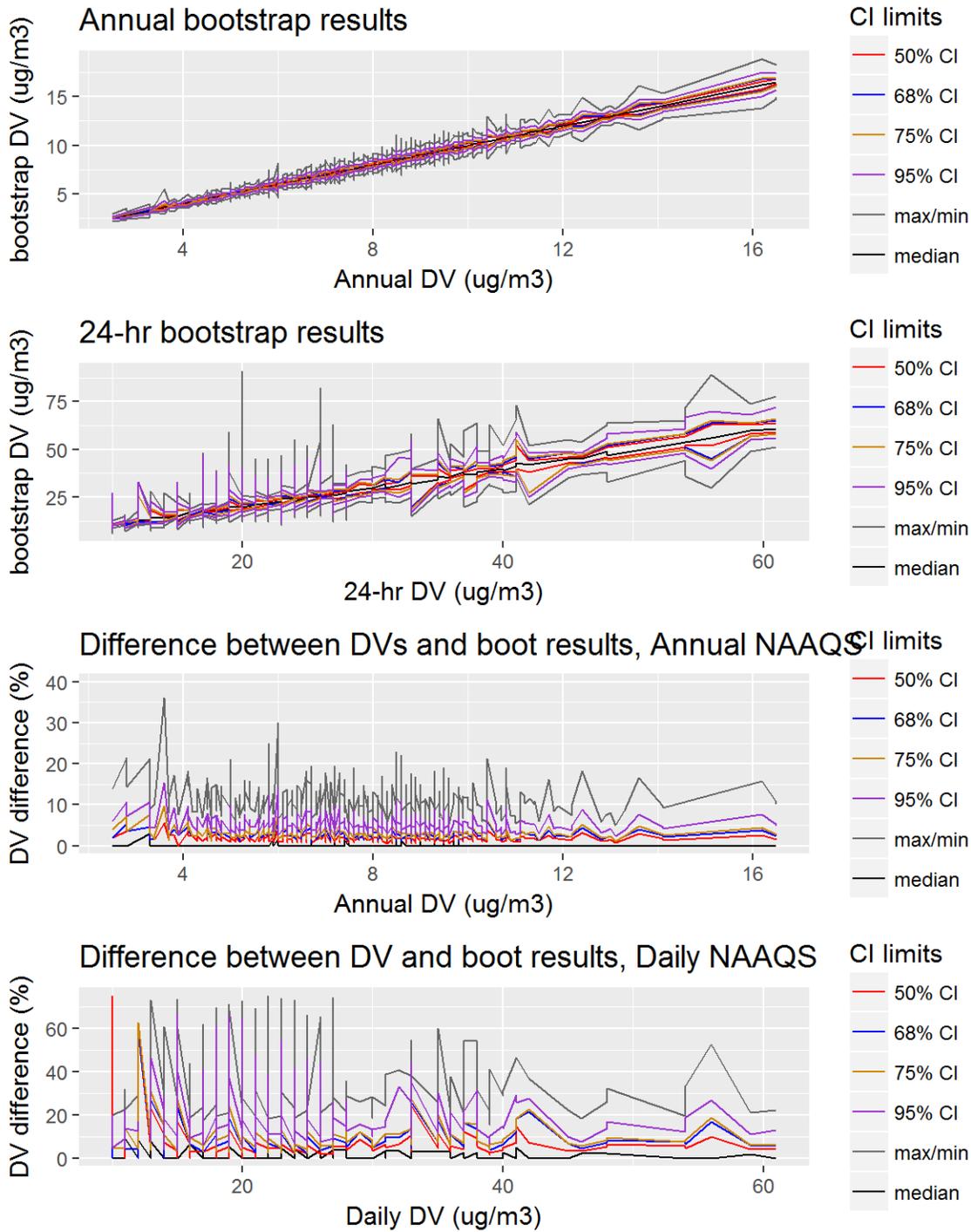


Figure 5 - Bootstrap results for the PM_{2.5} 2014-2016 DVs (25%, 50%, 68%, 75%, and 95% CIs, along with the mean and median bootstrap DVs). The top two panels show the values for the DVs at the various CIs, while the bottom two panels show the average of the percent difference between the upper and lower bounds of the CI and the actual DV.

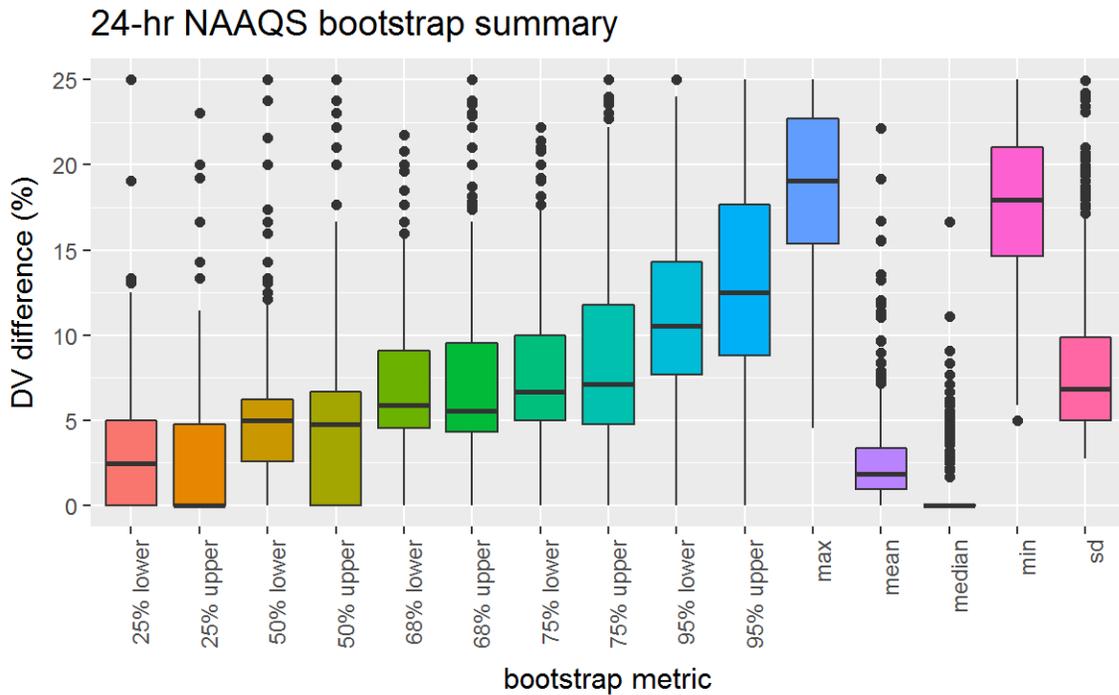
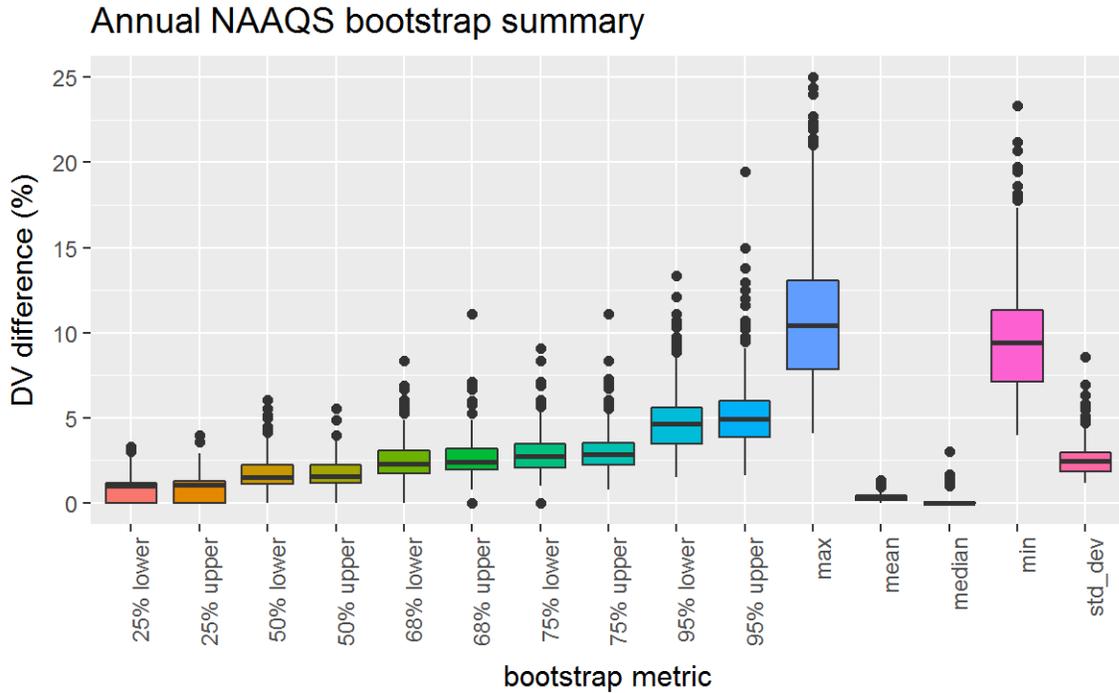


Figure 6 - Bootstrap results for the PM_{2.5} 2014-2016 DVs, showing distribution of the relative differences between the upper and lower bounds of the bootstrap DVs and the actual DV at the 25%, 50%, 68%, 75%, and 95% CIs, along with the mean, median, maximum, minimum, standard deviations of the relative differences.

3.2.1 Analysis of PM_{2.5} Spatial Variability

Section 2.1.3 discusses the design of the monitoring network and the spatial scales associated with each monitor. While there may be changes to the area around a monitor after the scale was determined when the monitor was sited, the monitor scale should be somewhat reflective of air quality within the area indicated. This basic need for multiple monitor scales and multiple monitors in an area to assess an area's air quality is due to the fact that there is an inherent spatial variability of air quality. For example, due to the inherent variability in the location of emission sources and changes in meteorological patterns, two “urban scale” monitors located a few blocks from each other would likely record different daily values, resulting in different DVs. The analysis conducted here seeks to quantify that spatial variability by identifying pairs of monitors that are located in proximity to one another to determine the relative difference between the two monitors, as indicated by the DVs. The differences between the DVs are interpreted as a measure of the spatial variability in the area and provide a benchmark to evaluate the variability determined from the Bootstrap analysis.

The analysis was conducted using the 2012-2016 annual and 24-hr PM_{2.5} DVs and focused on pairs of monitors which collected PM_{2.5} samples every day (1:1 monitors) in order to reduce the impact of temporal variability (see Section 4.3.1 for an analysis of the temporal variability). A total of 70 1:1 monitors were identified that were separated by a distance of less than 50 km, with 13 less than 10 km apart. We did not investigate whether -- based on emission sources, winds, and terrain -- any of these sites could reasonably be considered representative for particular locations at which a new source could seek a permit in the future.

The results from the analysis are summarized in Table 1 (monitor pairs within 10 km) and in Figures 7, 8 and 9 (monitor pairs within 50 km). There is a fairly strong correlation between the DVs in the site pairs (top panels in Figure 7), with a slope of 0.8 (r^2 of 0.51) between monitor pairs less than 50 km apart for the annual NAAQS and a slope of 0.87 (r^2 of 0.59) for the 24-hr NAAQS. There are no obvious trends in the differences between the monitors, either the absolute differences or the relative differences (defined as the absolute difference between the DVs from the two monitors divided by the average DV). The relative differences range from 0% to 66%, with a median relative difference of 9% for the annual DVs. For the 24-hr DVs, the relative differences range from 0% to 67%, with a median relative difference of 6%. When the subset of monitors within 10 km are considered, the slope between paired monitors is similar for the annual NAAQS, though the r^2 increases to 0.82, while the slope for the 24-hr NAAQS increases to 0.97 and the r^2 increases to 0.94. For this subset, the maximum relative differences drop to 23% and 16% for the annual and 24-hr DVs, respectively, and the median relative differences drop to 5% and 4%, respectively.

These results are interesting and seem to somewhat contrast the results from the bootstrap analysis, which suggest less variability in the annual NAAQS than in the 24-hr NAAQS. This comparison suggests that there is more spatial variability associated with the annual NAAQS, while the bootstrap results show that there is less variability in the annual NAAQS. Conversely, this comparison suggests that there is less spatial variability associated with the 24-hr NAAQS, while the bootstrap results show that there is more variability in the 24-hr NAAQS. Despite this

apparent contradiction, these results make sense in the context of secondary pollutants, particularly $PM_{2.5}$. In general, the highest concentrations associated with pollutants that have a substantial portion due to secondary formation occur in widespread “events”. These events are an important aspect of the air quality in an area and are associated with unique meteorological conditions, which can either transport air from polluted upwind regions, increasing the background concentrations, or trap local pollutants and facilitate in-situ production. Events are also associated with unique emissions episodes, such as dust storms or biomass burning events that emit large quantities of primary and precursor pollutants. Because of the nature of $PM_{2.5}$ events, there would tend to be a stronger correlation of the higher concentrations across larger spatial scales. The average air quality (annual NAAQS), on the other hand, would not be as heavily impacted by the unique (and wide-spread events) and instead would be more heavily affected by local emissions and production. As such, the prevailing meteorological conditions and the prevalent local emission sources would have the most impact on the annual DVs. In this case, localized differences in emissions could cause monitors to have greater differences in the annual DVs than is seen at a number of site pairs.

The result from the spatial variability analysis of $PM_{2.5}$ also suggests an important link to temporal variability of $PM_{2.5}$. The occurrence of these transport and emissions events is infrequent with varying intensity, such that they may not occur in every year and their frequency and duration would vary. Even when these events do occur, the intensity and impact on regional and local air quality would vary and also be difficult to predict. Since the bootstrap results show that 24-hr NAAQS has the most variability, this seems to imply that temporal variability is the most important component of the 24-hr NAAQS variability, while the spatial variability may be the most important component of the annual NAAQS variability, based on the results from the spatial analysis.

Table 1 - Summary of results from PM_{2.5} spatial variability analysis for monitor pairs within 10 km of one another.

State	City	Dist (km)	Monitor 1 ID	Annual DV 1	Monitor 2 ID	Annual DV 2	Delta (%) ³⁵
Minnesota	Washington	1.0	271630447	8.1 µg/m ³	271630448	8.8 µg/m ³	8%
Hawaii	Honolulu	1.7	150031001	4.9 µg/m ³	150031004	5.6 µg/m ³	14%
Pennsylvania	Philadelphia	2.6	421010047	10.3 µg/m ³	421010057	10.9 µg/m ³	5%
Pennsylvania	Philadelphia	3.1	421010055	11.6 µg/m ³	421010047	10.3 µg/m ³	12%
Louisiana	East Baton Rouge	5.4	220330009	9.0 µg/m ³	221210001	9.2 µg/m ³	3%
Nevada	Washoe	5.5	320310016	7.9 µg/m ³	320311005	10.0 µg/m ³	23%
Pennsylvania	Northampton	5.7	420950025	10.5 µg/m ³	420950027	10.1 µg/m ³	4%
Rhode Island	Providence	5.9	440070022	7.1 µg/m ³	440071010	7.4 µg/m ³	3%
Iowa	Clinton	6.4	190450019	10.6 µg/m ³	190450021	9.4 µg/m ³	11%
Utah	Salt Lake	7.3	490353006	9.2 µg/m ³	490353010	9.7 µg/m ³	5%
New Mexico	Bernalillo	7.9	350010023	6.5 µg/m ³	350010024	6.3 µg/m ³	3%
Indiana	Marion	8.9	180970078	11.1 µg/m ³	180970081	11.8 µg/m ³	6%
Indiana	Clark	9.3	180190006	11.8 µg/m ³	211110067	11.3 µg/m ³	4%
State	City	Dist (km)	Monitor 1 ID	24-hr DV 1	Monitor 2 ID	24-hr DV 2	Delta (%) ³⁵
Minnesota	Washington	1.0	271630447	20.6 µg/m ³	271630448	21.1 µg/m ³	3%
Hawaii	Honolulu	1.7	150031001	10.9 µg/m ³	150031004	11.4 µg/m ³	5%
Pennsylvania	Philadelphia	2.6	421010047	24.3 µg/m ³	421010057	25.2 µg/m ³	4%
Pennsylvania	Philadelphia	3.1	421010055	26.4 µg/m ³	421010047	24.3 µg/m ³	8%
Louisiana	East Baton Rouge	5.4	220330009	19.7 µg/m ³	221210001	19.4 µg/m ³	2%
Nevada	Washoe	5.5	320310016	26.8 µg/m ³	320311005	31.5 µg/m ³	16%
Pennsylvania	Northampton	5.7	420950025	27.2 µg/m ³	420950027	28.3 µg/m ³	4%
Rhode Island	Providence	5.9	440070022	18.3 µg/m ³	440071010	18.6 µg/m ³	2%
Iowa	Clinton	6.4	190450019	24.7 µg/m ³	190450021	22.8 µg/m ³	8%
Utah	Salt Lake	7.3	490353006	42.3 µg/m ³	490353010	41.0 µg/m ³	3%
New Mexico	Bernalillo	7.9	350010023	15.4 µg/m ³	350010024	15.1 µg/m ³	2%
Indiana	Marion	8.9	180970078	25.0 µg/m ³	180970081	26.4 µg/m ³	5%
Indiana	Clark	9.3	180190006	24.2 µg/m ³	211110067	22.8 µg/m ³	6%

³⁵ Defined as the difference between the two monitored DVs divided by the mean DV of the two monitors.

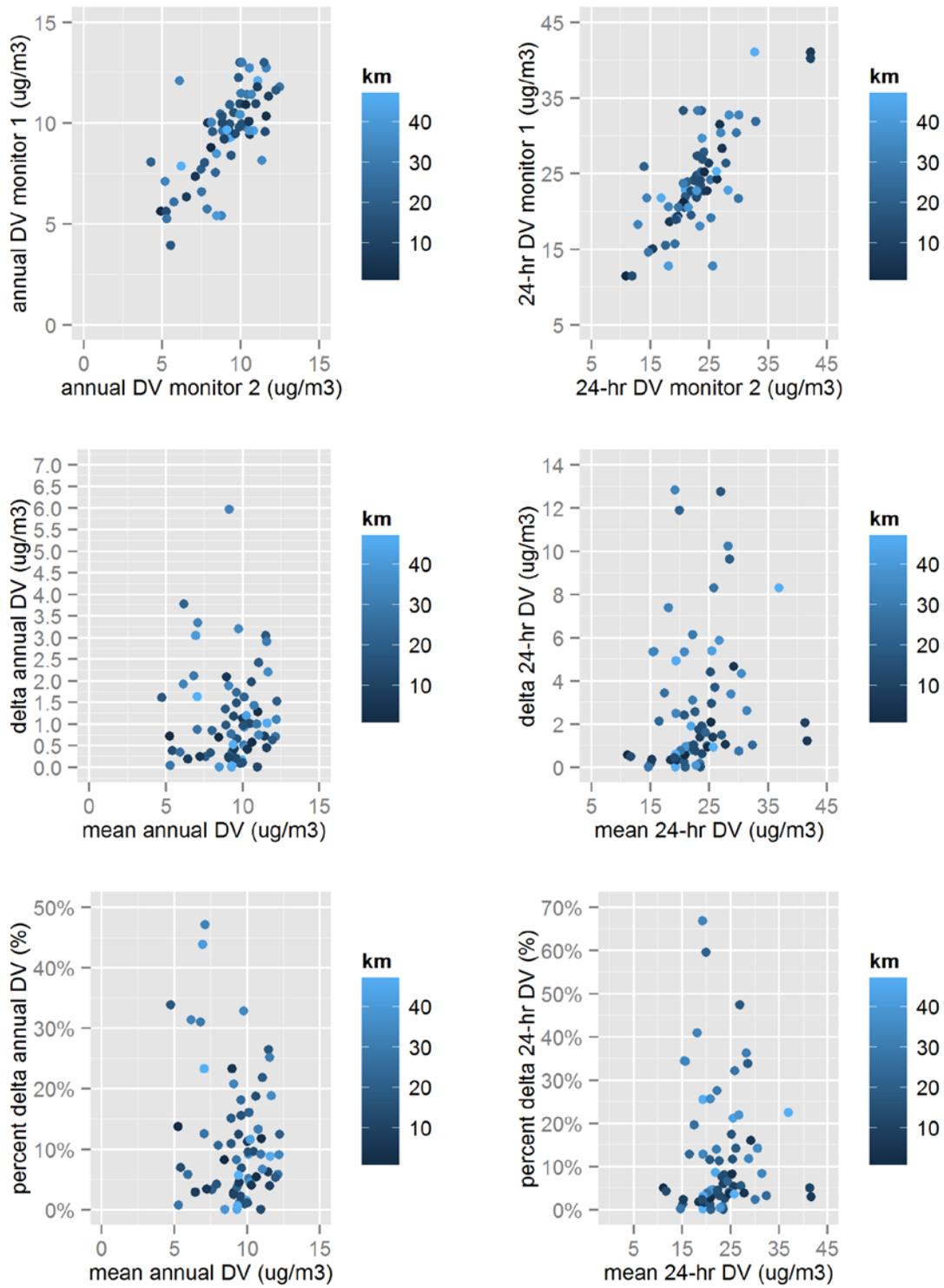


Figure 7 - Results from the analysis of spatial variability. Left column shows results for annual PM_{2.5} NAAQS and the right column shows the results for the 24-hr PM_{2.5} NAAQS.

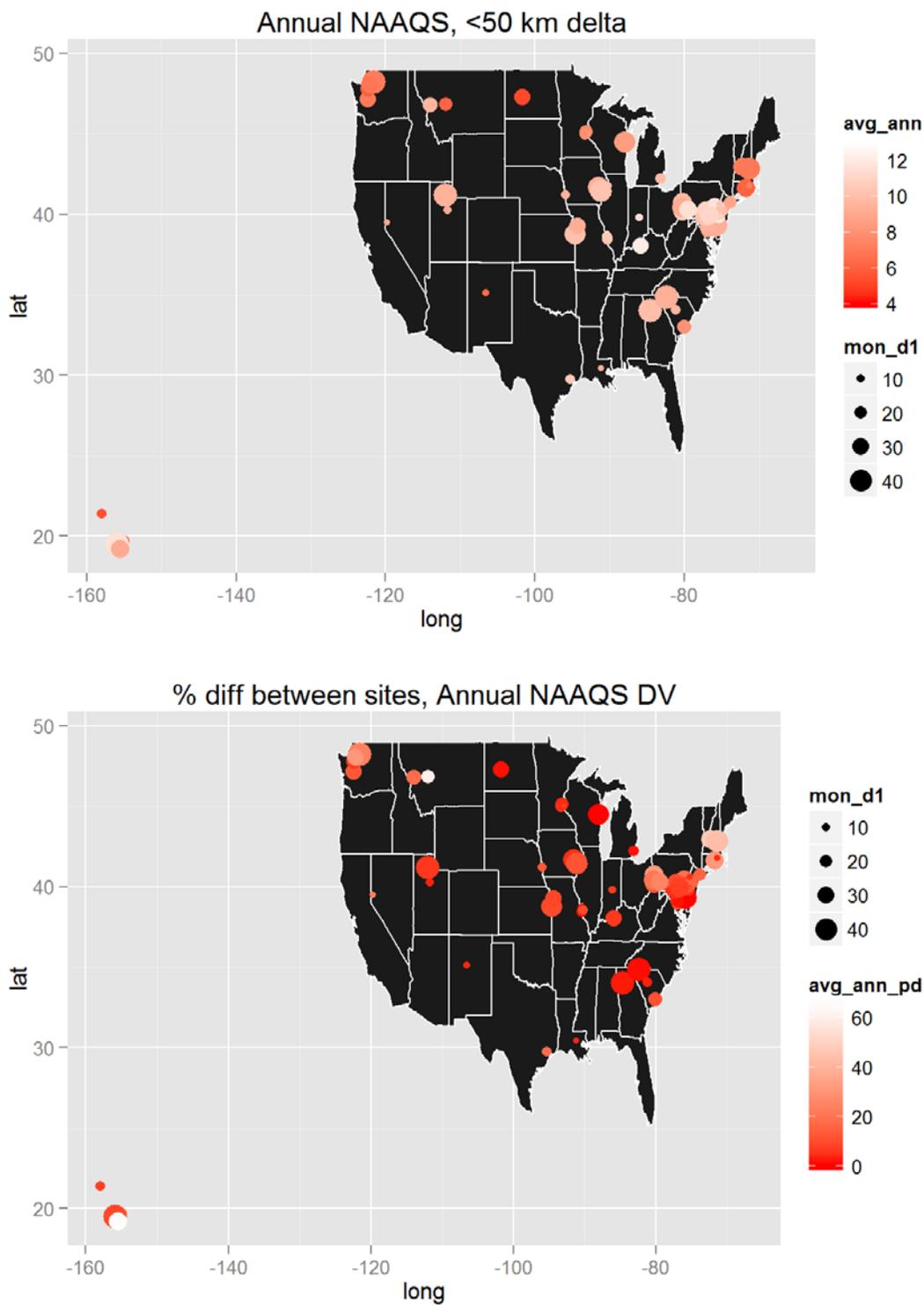


Figure 8 - Spatial distribution of the difference between the DVs from spatial analysis of the 2012-2016 PM_{2.5} annual DVs. Top panel shows the absolute value of the difference between the two monitors while the bottom panel shows the percent difference between monitors.

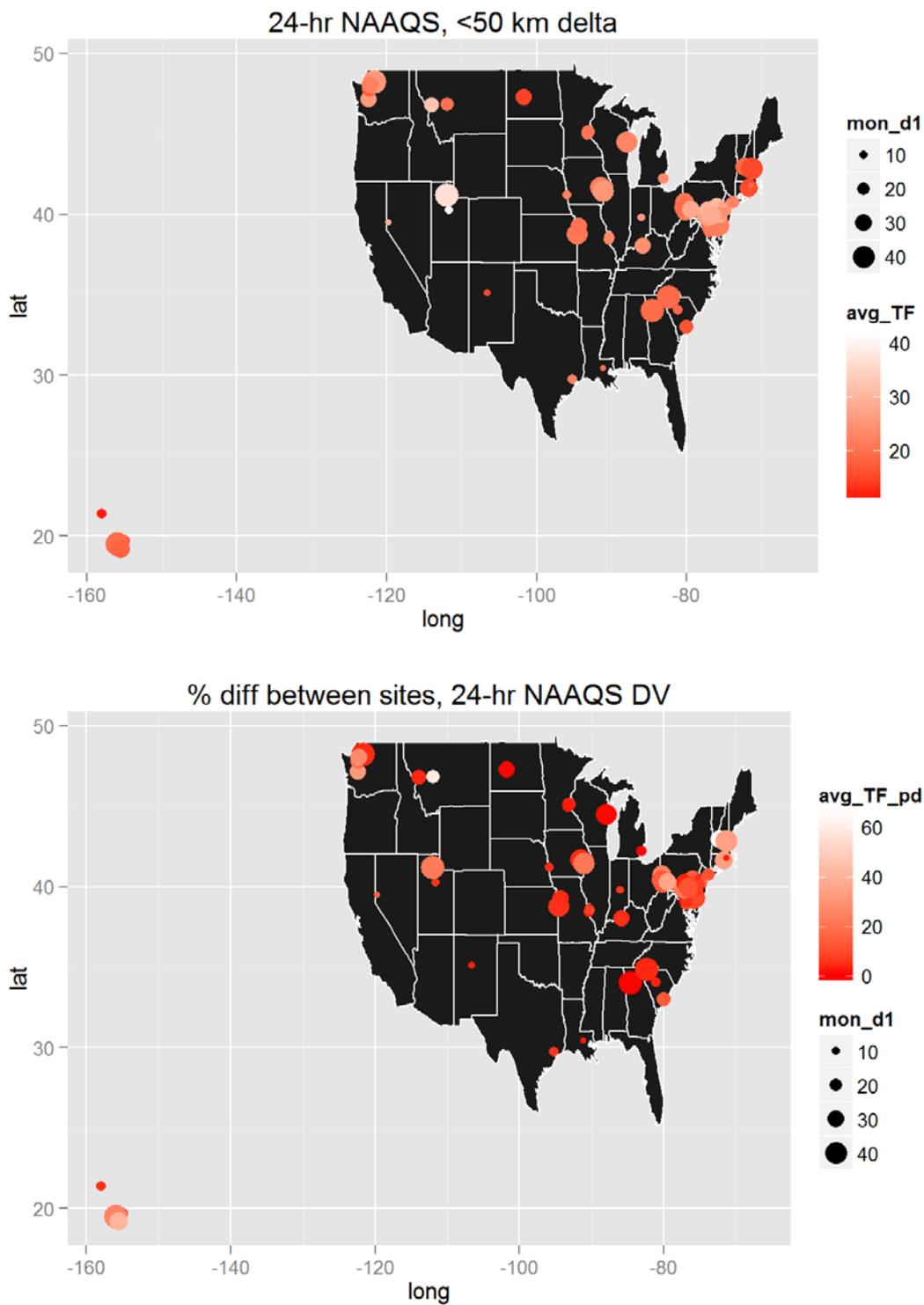


Figure 9 - Spatial distribution of the difference between the DVs from spatial analysis of the 2012-2016 PM_{2.5} 24-hr DVs. Top panel shows the absolute value of the difference between the two monitors while the bottom panel shows the percent difference between the two monitors.

3.2.2 Analysis of the Influence of PM_{2.5} Monitor Sampling Frequency

The PM monitoring network was been designed to operate continuously. When initially designed and deployed, the monitoring requirements for PM indicated that many sites only needed to sample on every third or sixth day, with a smaller number required to sample every day. This was partly due to the technology available at the time, which required a person to collect the filter sample and reload the filter cartridge for each sample taken. The filters were then transported to a laboratory for weighting analysis. While much of the PM_{2.5} network still relies on filter-based sampling, systems that can load multiple filters and automatically swap out filters after each 24-hr monitoring period have reduced the labor requirements. Non-filter based measurement techniques have also been developed that allow for continuous operation (as well as 1-hr sampling) so that concentration values are provided for every 24-hr period. Additionally, the requirements for sampling frequency have tightened, requiring more frequent sampling, particularly in areas with DVs close to the NAAQS. The result of the technological and regulatory changes is a sampling network with varied sampling frequency, with notable changes in the sampling frequency over time (see Figure 10). The total number of sites in the network has decreased, but the number of 1:1 sites has increased. Many 1:6 and 1:3 sites have been replaced by 1:1 sites, a trend most obviously starting around 2008. (The site classification was based solely on the number of daily samples during the course of the year, *i.e.*, sites with 60 or less samples were 1:6, sites with 121 samples or less but more than 60 were classified as 1:3, and sites with 122 or more samples were classified as 1:1.)

Due to the nature of temporal variability, it would generally be expected that data from datasets from sites with less frequent sampling would in general have a higher sample variance and therefore wider confidence intervals. Sensitivity tests conducted with the 2010-2013 DVs indeed showed that statistics from the subset of sites with daily monitoring (1:1) have tighter confidence intervals than the subset of sites with 1:3 monitoring and all data (which includes 1:6 monitors) (see Table 2). However, since the 1:1 monitors are not sampling the same air as the 1:3 monitors, it is difficult to directly compare the results from these subsets as a definitive indicator of the inherent increase in variability due to less frequent sampling. However, the results do support what is generally expected from reduced sampling frequency (*i.e.*, while 1:1 monitoring might capture a wider range of air quality, less frequent sampling would likely result in increased sample variance and wider confidence intervals for statistics from the air quality measurement data).

Since the monitor sampling frequency can have a notable impact on the calculated air quality variability, an important question arises regarding which monitors should be used to characterize air quality variability. Using only the 1:1 monitors would likely produce smaller estimates of the sample variance due to the increased sample size while possibly capturing a wider range of air quality across a more widely sampled spectrum. However, the 1:3 and 1:6 monitors are part of the monitoring network and will continue to be present for the foreseeable future. Additionally, despite an increase in the number of 1:1 monitors, the overall air quality variability indicated by the network has been fairly stable for the annual and 24-hr PM_{2.5} NAAQS (see Section 4.3.1). This suggests that the inherent variability in the air quality is more influential than the increased

variability induced by the presence of 1:3 and 1:6 monitors. In addition, the much greater number of monitoring sites available when sites with all schedules are considered (see Table 2) provides more confidence that the results are representative of the U.S. as a whole.

Table 2 - Summary of comparison of the air quality variability determined by the bootstrap analysis for PM for three design periods for monitors with different sampling frequencies.

Monitor class	all	1 in 1	1 in 3	all	1 in 1	1 in 3	all	1 in 1	1 in 3
Year/NAAQS	2014 annual			2015 annual			2016 annual		
Difference, median bootstrap vs actual	0.04%	0.02%	0.04%	0.03%	0.03%	0.06%	0.04%	0.03%	0.03%
Avg. 25% CI span	0.67%	0.57%	0.94%	0.70%	0.58%	0.91%	0.71%	0.62%	0.88%
Avg. 50% CI span	1.63%	1.14%	1.81%	1.65%	1.24%	1.85%	1.69%	1.22%	1.85%
Avg. 68% CI span	2.44%	1.72%	2.67%	2.46%	1.77%	2.74%	2.45%	1.79%	2.76%
Avg. 75% CI span	2.80%	1.92%	3.11%	2.83%	2.00%	3.09%	2.82%	2.08%	3.18%
Avg. 95% CI span	4.72%	3.33%	5.26%	4.86%	3.43%	5.38%	4.79%	3.47%	5.48%
Year/NAAQS	2014 24-hr			2015 24-hr			2016 24-hr		
Difference, median bootstrap vs actual	1.14%	0.67%	1.54%	1.36%	0.84%	1.78%	1.23%	1.01%	1.40%
Avg. 25% CI span	2.27%	1.89%	2.38%	2.27%	1.92%	2.50%	2.50%	2.17%	2.63%
Avg. 50% CI span	4.29%	2.94%	4.76%	4.17%	3.45%	4.65%	4.35%	3.13%	5.13%
Avg. 68% CI span	6.00%	4.76%	7.02%	6.25%	5.09%	7.14%	6.52%	5.00%	7.89%
Avg. 75% CI span	6.82%	5.36%	8.33%	7.50%	5.56%	8.33%	7.69%	5.77%	8.88%
Avg. 95% CI span	12.50%	9.40%	14.14%	12.50%	10.00%	14.81%	13.16%	9.62%	16.67%
Number of sites	507	182	274	531	210	270	535	237	240

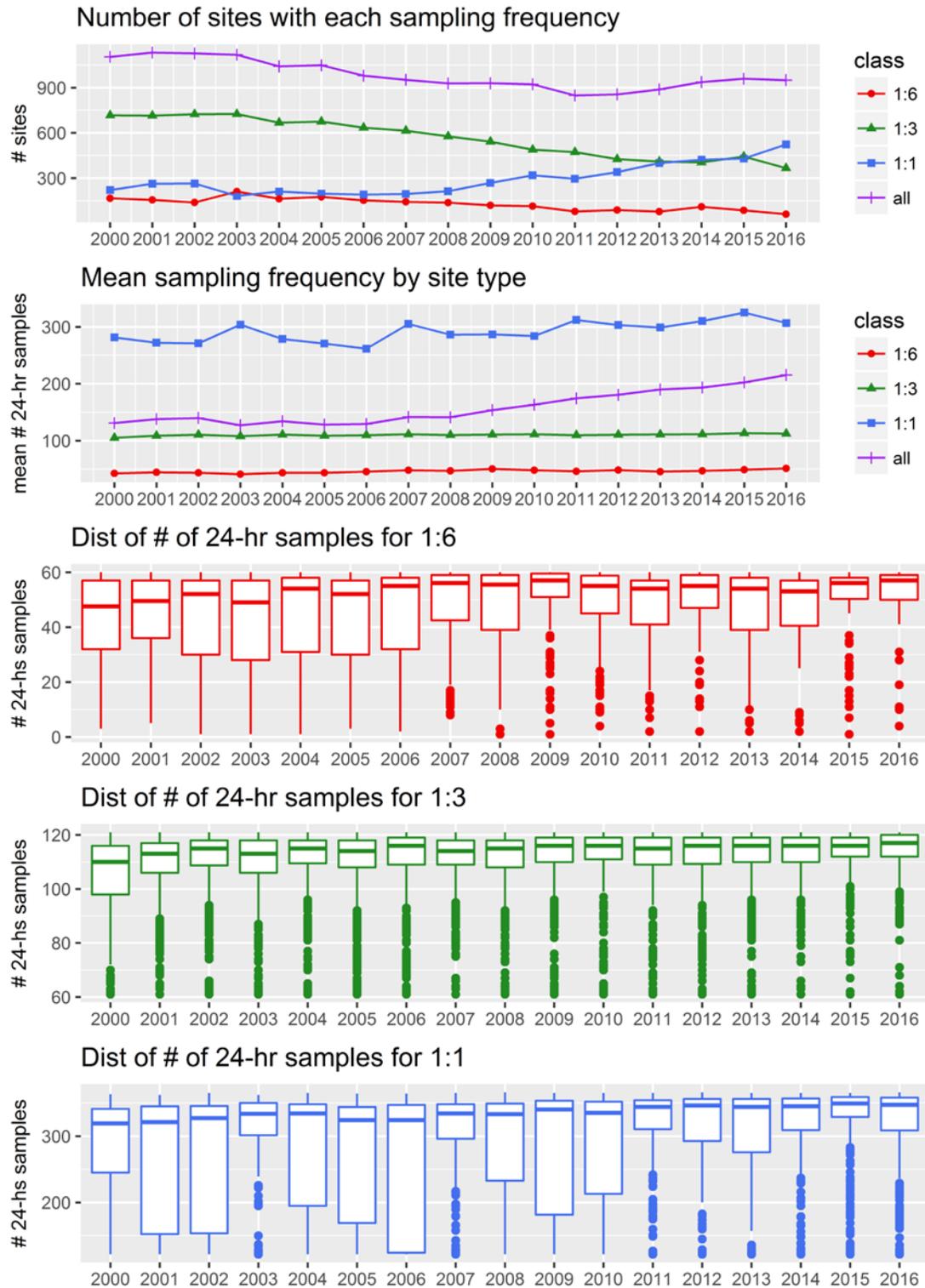


Figure 10 - PM_{2.5} monitor network statistics. Top row shows the number of sites with each sampling frequency by year. Second row shows the average number of samples at each site type. Third, fourth and fifth rows show the distribution of the number of samples for each site type.

4.0 Application of Air Quality Variability to Calculate SILs for the PSD Program

For a specific change in air quality concentrations to be used to show that a proposed source does not cause or contribute to a violation of the NAAQS, the concentration change must represent a level of impact on ambient air quality that is “insignificant” or not meaningful. The EPA has taken into account the necessary policy considerations in conjunction with the statistical analysis presented here to provide a rational basis to select values derived from the statistical analysis that can be applied to represent “insignificant impacts.”

Section 3 presented the results from the bootstrap analysis, which produced variability estimates at the 25%, 50%, 68%, 75%, and the 95% CIs for all the AQS data across the U.S. from 2000-2016. This section presents the technical considerations related to the policy² considerations guiding the application of the above results to identify an appropriate SIL for each context, and the final values the EPA has selected from the study results.³⁶

4.1 PSD Air Quality Analyses and Statistical Significance

The following four factors are important for EPA’s choice of a SIL: determining a CI to represent the inherent variability for purposes of the NAAQS compliance demonstration, an approach for scaling local variability to the level of the NAAQS, the geographic extent of each summary value, and the DV year or years from which to use the variability results. The EPA has balanced the necessary policy considerations in conjunction with technical information discussed here and in the Policy Document² to develop SIL values that represents, in the Agency’s judgment, an appropriate measure of “insignificant impact” that can be used by PSD permitting authorities to determine if emissions from proposed construction will “cause or contribute” to a violation of the corresponding NAAQS.

4.1.1 Confidence Interval

The bootstrap analysis produced estimates for the 25%, 50%, 68%, 75%, and 95% CIs in order to characterize the range of the inherent variability and to provide options for selecting an appropriate “insignificant impact” level that will be applied to determine each SIL. The statistical framework that forms the basis for the bootstrap CIs can be related to more traditional assessments of statistical significance and statistical significance testing. In contrast to the usage here, the traditional application of statistical significance testing seeks to determine if a deviation from the base value is *significant* (rather than *not significant*, which is the usage here). In order to make this determination, larger CIs are typically selected (*e.g.*, 90-99%, which results in a

³⁶ The methods, analysis, and application to the PSD program was subject to a peer-review. The results of that peer-review and the subsequent changes to the analysis and the document are detailed in a companion report, U.S. EPA, 2018, Peer review report for the technical basis for the EPA’s development of significant impact thresholds for PM_{2.5} and ozone, RTP, NC, EPA 454/S-18-001, available from the U.S. EPA RTP library.

high level of confidence that a deviation from the base value is indeed *significant*). In practice, the smallest CI that might be considered for a similar *significance* determination would be the 68% CI, which corresponds to one standard deviation of the mean for a normally distributed sample. Thus, any deviation larger than the bounds of the 68% CI could traditionally be identified as a *significant* deviation from the mean. In this application for the PSD program, however, we are seeking for each NAAQS a value below which we can conclude that the change in air quality is “not statistically significant” (*i.e.*, that there will not be a notable difference in air quality after the new source begins operation). Thus, a CI that could potentially be considered to represent a *significant* value would not simultaneously be appropriate for identifying a value that is *statistically not significant*. As such, CIs used for identifying a value that is *not statistically significant* value should be below 68%. For the reasons described in the Policy Document, the 50% CI was chosen as the benchmark statistic from the bootstrap analysis to represent the recommended SILs in PSD permitting for ozone and PM_{2.5} NAAQS.

4.1.2 Adjustment to the Level of the NAAQS

Since air quality variability may have different characteristics at different baseline air quality levels (e.g., areas with smaller DVs may have less variability than areas with higher DVs), it is reasonable to characterize the variation in the air quality across a range of air quality levels. Sections 4.2 and 4.3 present the 50% CI value on both an absolute scale (ug/m³ and ppb) and a relative scale (percentage), where the relative variability is defined as the percent change from the base DV at each site. The figures in these sections indicate that there is less of a trend in the relative variability compared to the absolute variability, and no trend in the relative variability for the ozone DV at any of the CIs (*i.e.*, the relative variability is not particularly higher or lower at higher or lower baseline DVs: see Figures 11 and 14). However, the relative variability was fairly consistent across the range of design values, suggesting a commonality in the relative variability across a wide range of geographic regions, chemical regimes, and baseline air quality levels. These results suggest that there is an inherent aspect to the variability, regardless of the baseline air quality. Thus, for reasons explained in the policy memorandum, the relative variability values are used for the SILs development.

4.1.3 Selection of a Geographic Scale

A fundamental question raised in using air quality variability to inform the selection of a value for a SIL is whether the variability-based SIL value should be based on an analysis of air quality variability at the particular site of the new source or modification, or whether the SIL value should reflect the central tendency of all monitored sites in the U.S., regardless of the new source’s or modification’s planned location.

The EPA recognizes that the air quality data and the nature of the emissions and chemical formation of ozone and PM_{2.5} can impact areas differently and, thus, should be considered as part of this evaluation. The analysis presented in Sections 4.2 and 4.3 (Figures 11 and 14) examine the relative variability represented by the 50% CI to explore any spatial trends in the data. The analysis indicates that while there is evidence of local spatial correlation (*i.e.*, most areas have fairly similar levels of relative variability and that sites with higher variability are isolated), there

are no large scale (*i.e.*, region-to-region) trends in ambient air variability. While there is a fairly consistent range of variability across the U.S., the magnitude of the variability differs from site-to-site within a state or region with few instances of regional patterns and no strong instances of east/west or north/south trends.

The analysis shows that a small number of sites with particularly high variability have an effect on the average network-wide variability. A median network-wide variability is not overly influenced by a few outliers. Thus, for the reasons explained in the Policy Document, the median variability from the 50% CI from the entire U.S. ambient monitoring network is used to calculate SIL values.

4.1.4 Selection of the Three Most Recent Design Value Years

Sections 4.2.1 and 4.3.1 present trends in the median nation-wide variability at the 50% CI from 2000-2016 (equivalent to DV years of 2002-2016). For all three NAAQS considered here, there are general downward trends in the computed variability across these years. Since the SILs should reflect the most representative state of the atmosphere, the analysis uses for each NAAQS the lower variability observed in the more recent periods, rather than all the data since 2000. However, it may be advantageous to avoid relying on a single 3-year period that may have been influenced by unusual circumstances, particularly in light of the slightly different trends in the last several years across pollutants (*i.e.*, most recently the 24-hr PM_{2.5} NAAQS median 50% CI has increased, while the annual PM_{2.5} and ozone NAAQS median 50% CIs have continued to decrease). Faced with a similar selection of DV periods for use in attainment demonstrations for nonattainment areas,³⁷ the EPA also recommended using the average of three DV periods to be used along with a modeling analyses. Thus, for the reasons explained in the Policy Document, the three most recent DV periods (*i.e.*, 2012-2014, 2013-2015, 2014-2016) were used for determining SILs for PM_{2.5} and ozone.

4.2 Analysis for Ozone

Figure 11 shows, for each monitoring site, the half-width of the 50% CI divided by the actual design value, from the 2014-2016 data for the ozone NAAQS.³⁸ The scatter plot for the relative variability values shows that the data are fairly well concentrated around 1-2%, with a small number of sites exceeding 3% and a maximum around 4.5% (with one exception). The variability is fairly consistent across the range of baseline air quality levels, indicating that there is no particular trend with actual design value in the site level variability. The median and mean variability values are fairly similar

The spatial distribution of the relative variability from the 50% CI is also shown in Figure 11, with 2014-2016 DV period site data colored according to their relative variability and sites with insufficient data during this period in gray. There appears to be no notable large-scale spatial

³⁷ Draft Modeling Guidance for Demonstrating Attainment of Air Quality Goals for Ozone, PM_{2.5}, and Regional Haze. R. Wayland, AQAD, Dec. 3, 2014.

³⁸ The plots for ozone show a distinct banding in the results. This is a feature of the truncation conventions that were applied to the AQS data prior to the air quality variability analysis.

trends in highest relative variability. The lack of any large-scale spatial trend indicates that there is indeed a fundamental characteristic to the relative ambient air quality variability (see Section 4.1.3).

4.2.1 Ozone Temporal Trends

The median air quality variability from the 15 DV periods for ozone is shown in Figure 12 (each period is 3 years). This analysis shows how the combination of changes in the network design (e.g., the change in the monitoring season) and the changes in emissions and meteorology over this period have impacted the variability in the DVs from the network. There has been a small decrease in the variability for ozone (0.03 percentage points per year), though most of that decrease occurred in the form of a large drop in the variability between the 2003-2005 and 2004-2006 DV periods. There were increases in the variability for the 2008 and 2012 DV periods, indicating that there is some variability between years. The median air quality variability values at the 50% CI for the three most recent DV periods (i.e., 2012-2014, 2013-2015, 2014-2016) as shown in Table 3, when averaged result in a SIL value for the ozone 8-hour NAAQS of 1.47%. This corresponds to 1.0 ppb at the level of the 2015 ozone NAAQS (70 ppb).

Table 3 - Summary of ozone bootstrap results for three design periods, 2012-2014, 2013-2015, and 2014-2016

Year/NAAQS	2014 annual	2015 annual	2016 annual
Difference, mean of median bootstrap vs actual DV	0.44%	0.48%	0.43%
Avg. 25% CI span	0.74%	0.76%	0.75%
Avg. 50% CI span	1.47%	1.47%	1.47%
Avg. 68% CI span	2.14%	2.05%	2.11%
Avg. 75% CI span	2.38%	2.34%	2.31%
Avg. 95% CI span	4.31%	3.97%	3.97%
Number of sites	1148	1131	1131

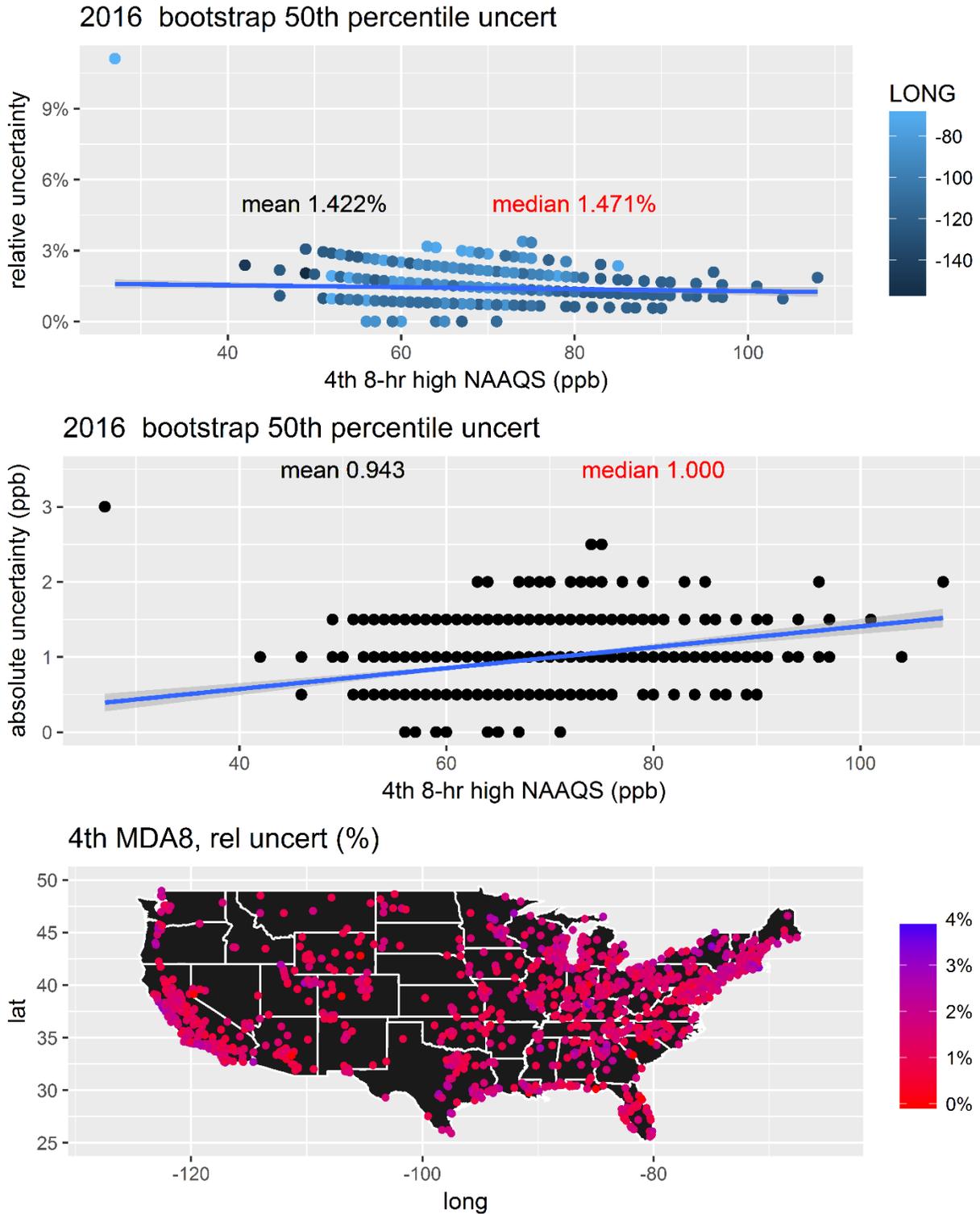


Figure 11 - Bootstrap results from the 50% CIs for the 2016 ozone DVs. The top panel shows the relative difference between the span of the CI and the actual DV across the range of actual DVs, the middle panel shows the absolute difference between the values across the same range, and

the bottom panel shows the spatial distribution of the relative difference between the values at each site.

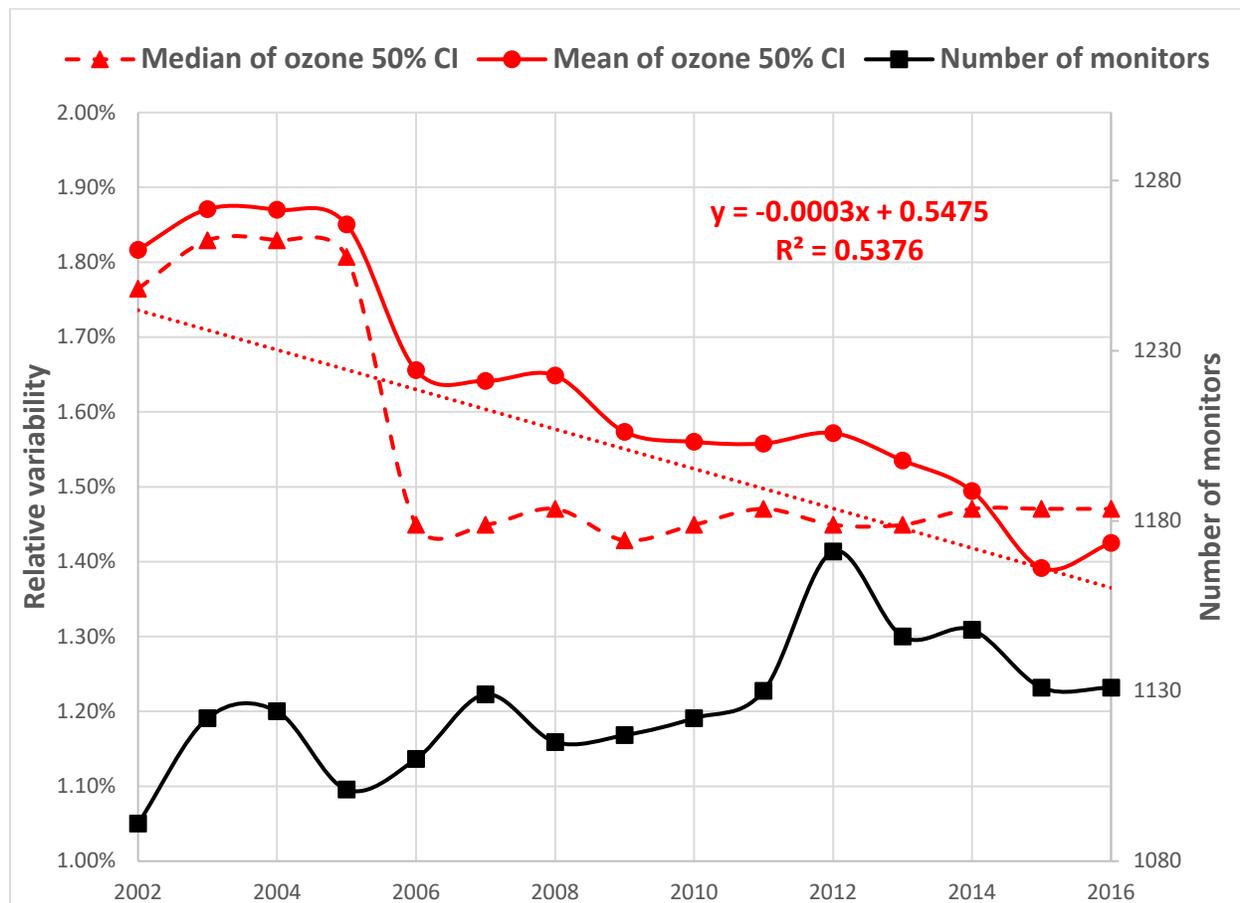


Figure 12 - Median and mean variability in the network determined from the bootstrap analysis for the 15 DV periods from 2002-2016 for ozone (each DV period represents 3 years of data and the data are plotted on the ending year, *i.e.*, the 2016 DV period is from 2014-2016 and plotted at 2016).

4.3 Analysis for PM_{2.5}

Figure 13 shows, for each monitoring site, the half-width of the 50% CI divided by the DVs, for both the annual and 24-hr PM_{2.5} NAAQS. This figure shows that the relative variability using these assumptions is indeed stable across the range of baseline air quality levels, while the absolute variability increases as the baseline air quality levels increase.³⁹ The values for relative variability are fairly well concentrated around 1-2% for the annual NAAQS, with a small number of sites exceeding 3% and a maximum slightly less than 5%. For the 24-hr NAAQS, the data are

³⁹ The rounding conventions for PM_{2.5} result in striations in the data, which are clearly visible in Figure 13. While these striations appear to represent trends in the data, this is a function of the display and not actual trends in the data. Linear regression lines have been added to each panel, which clearly show an increase in the absolute variability with increasing DVs, while the relative variability is relatively unaffected by changes in the DVs.

concentrated around 4-5%, with a small number of sites exceeding 10%. The outliers occur across the range of baseline air quality levels, indicating that there is no particular trend with actual DV in the occurrence of sites with especially high variability. When assessed as a whole, despite their relatively infrequent occurrence, these outliers do tend to increase the average variability. As with ozone, the median variability is less influenced by these outliers and appears to be more representative of the central tendency of the distribution of relative variability values than the average. Unlike the ozone results, the median is smaller than the mean

The spatial distribution of the relative variability from Figure 13 is shown in Figure 14, with sites having data during the 2014-2016 DV period colored according to their relative variability (sites with insufficient data during the 2014-2016 DV period are not shown, data from other years are presented in the Appendix). Based solely a visual inspection, there appears to be no notable large-scale spatial trends in highest relative variability in either the annual or 24-hr PM_{2.5} NAAQS. The sites with larger variability tend to occur in the western half of the U.S., though the sites are isolated and generally not grouped into any specific geographic region. The exceptions to this appears in Western U.S. and along the Ohio River Valley, where there are a collection of sites with higher variability (generally above 7.5%) in the 24-hr NAAQS (though the annual NAAQS does not display this apparently higher variability). This result may be related to the nature of high PM events in the western half of the U.S. (*e.g.*, the typical PM_{2.5} levels may be lower in the western states, but the events that do occur produce much higher concentrations than the typical background, which would result in greater skew and thus greater variability in DVs computed from these data, particularly in the 24-hr PM_{2.5} DVs). These sites also tend to have a lower sampling frequency (see Figure 2), which we have shown to artificially increase the apparent variability. There are also trends in missing data that are important to consider when exploring regional trends in variability. In particular, for the period 2008 through 2013, the data were invalidated for several states. Late in 2014, a problem was found with the PM_{2.5} data from these states and, as a result, the data were invalidated for a number of years.⁴⁰

In response to comments received during the peer-review of the initial public draft of this document, several more detailed spatial analyses are presented for the annual and 24-hr PM_{2.5} data in Section 7 of the Appendix to this document. The analysis attempts to identify natural groupings of sites based on location and the level of air quality variability using cluster analysis. The analysis applied both an iterative (K-means) and a hierarchical clustering algorithm using various combination of the site-level variability, latitude, and longitude, resulting in 12 different sets of clusters. The analysis also considered comparing sites by grouping them using the National Oceanic and Atmospheric Administration (NOAA) “climate regions,” which are groupings of states known by NOAA to have similar climatic conditions. While some of the analysis did identify some unique clusters, these groups were often not spatially grouped. Many

⁴⁰ The dates and specific monitors affected in each state vary. For DC, data were invalidated in Q4 of 2016. For FL, data were invalidated from 2011-2014. For GA, data were invalidated in Q1 of 2011. For ME, data were invalidated from 1998-2015. For ID, data were invalidated from 2011-2014. For IL, data were invalidated from 2011-2013 and Q1-Q2 of 2014. For Louisville, KY, data were invalidated from 2009-2013. For the South Coast Air Basin, CA, data were invalidated in 2014. For MS, data were invalidated in 2014. For TN, data were invalidated from 2011-2014. For WA, data were invalidated from 2011-2015. The invalidation may not have affected every monitor in each state, but these dates cover the time spans for which the data invalidation occurred.

of the analyses did not identify any unique clusters. When the results from the special cluster analysis are considered as a whole, they do not indicate any consistent large-scale trends. The lack of any consistent regional trend indicates that there is indeed a fundamental characteristic to the relative ambient air quality variability (see Section 4.1.2).

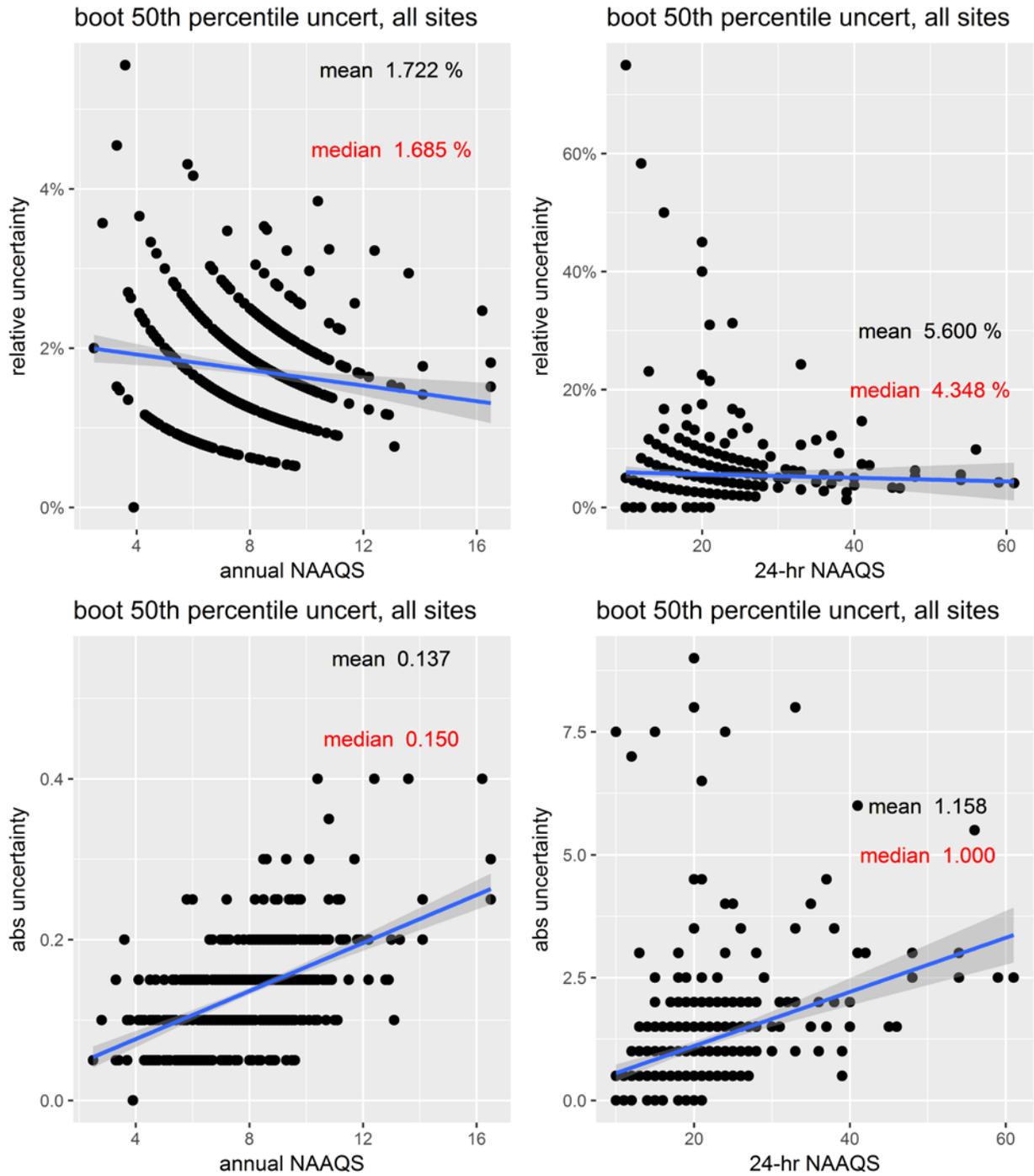


Figure 13 - Bootstrap results from the 50% CIs for the 2016 PM_{2.5} DVs. The top two panels show the relative difference between the span of the CI and the actual DV across the range of actual DV, and the bottom two panels show the absolute difference between the values across the same range.

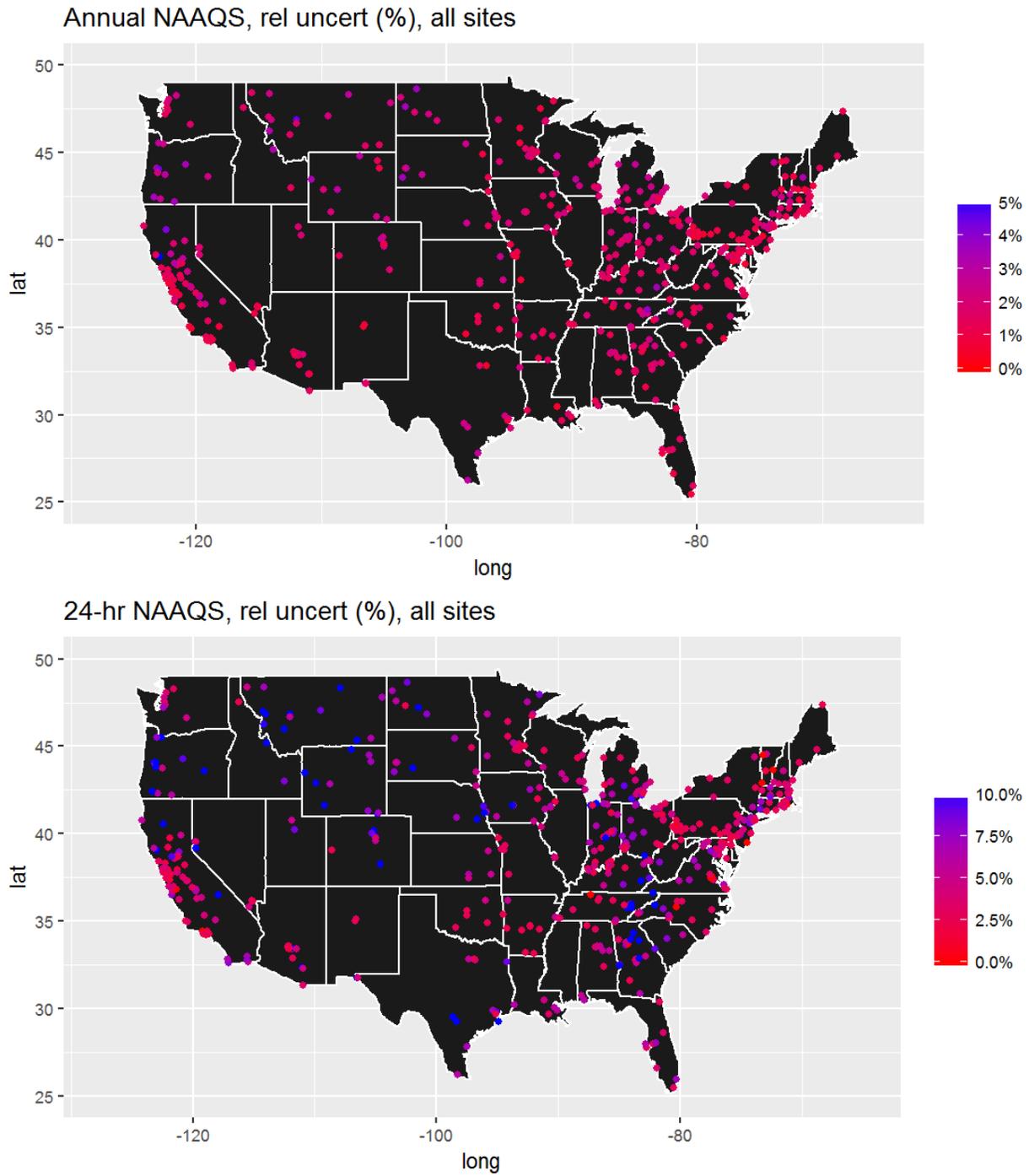


Figure 14 - Spatial distribution of the relative difference between the span of the 50% CI and the actual DV for the 2014-2016 PM_{2.5} DVs.

4.3.1 PM_{2.5} Temporal Trends

The median air quality variability from the 13 DV periods for both the annual and 24-hr PM_{2.5} NAAQS are shown in Figure 15. This analysis shows how the combination of the changes in the network design (*e.g.*, the change in the monitoring frequency) and the changes in emissions and meteorology have impacted the network variability. There has been a greater decrease in the variability in the 24-hr PM_{2.5} NAAQS than in the variability for the annual PM_{2.5} NAAQS (0.03 percentage points per year versus 0.02 percentage points per year). The analysis in Section 3.2.2 showed that the 24-hr NAAQS is more affected by the monitoring frequency than the annual NAAQS, so it is likely that the change in monitoring frequency played some role in the larger decrease in the variability for the 24-hr PM_{2.5} NAAQS. The median air quality variability at the 50% CI for the three most recent DV periods (*i.e.*, 2012-2014, 2013-2015, 2014-2016) is shown in Table 4, and when averaged result in a SIL value of 1.66% for the annual PM_{2.5} NAAQS (12 µg/m³) and 4.27% for the PM_{2.5} 24-hr NAAQS (35 µg/m³). These values correspond to 0.2 µg/m³ at the level of 12 µg/m³ for the annual NAAQS, and 1.5 µg/m³ at the level of 35 µg/m³ for the NAAQS.

Table 4 - Summary of comparison of the air quality variability determined by the bootstrap analysis for three design periods.

Year/NAAQS	2014 annual	2015 annual	2016 annual
Difference, median bootstrap vs actual	0.04%	0.03%	0.04%
Avg. 25% CI span	0.67%	0.70%	0.71%
Avg. 50% CI span	1.63%	1.65%	1.69%
Avg. 68% CI span	2.44%	2.46%	2.45%
Avg. 75% CI span	2.80%	2.83%	2.82%
Avg. 95% CI span	4.72%	4.86%	4.79%
Year/NAAQS	2014 24-hr	2015 24-hr	2016 24-hr
Difference, median bootstrap vs actual	1.14%	1.36%	1.23%
Avg. 25% CI span	2.27%	2.27%	2.50%
Avg. 50% CI span	4.29%	4.17%	4.35%
Avg. 68% CI span	6.00%	6.25%	6.52%
Avg. 75% CI span	6.82%	7.50%	7.69%
Avg. 95% CI span	12.50%	12.50%	13.16%
Number of sites	507	531	535

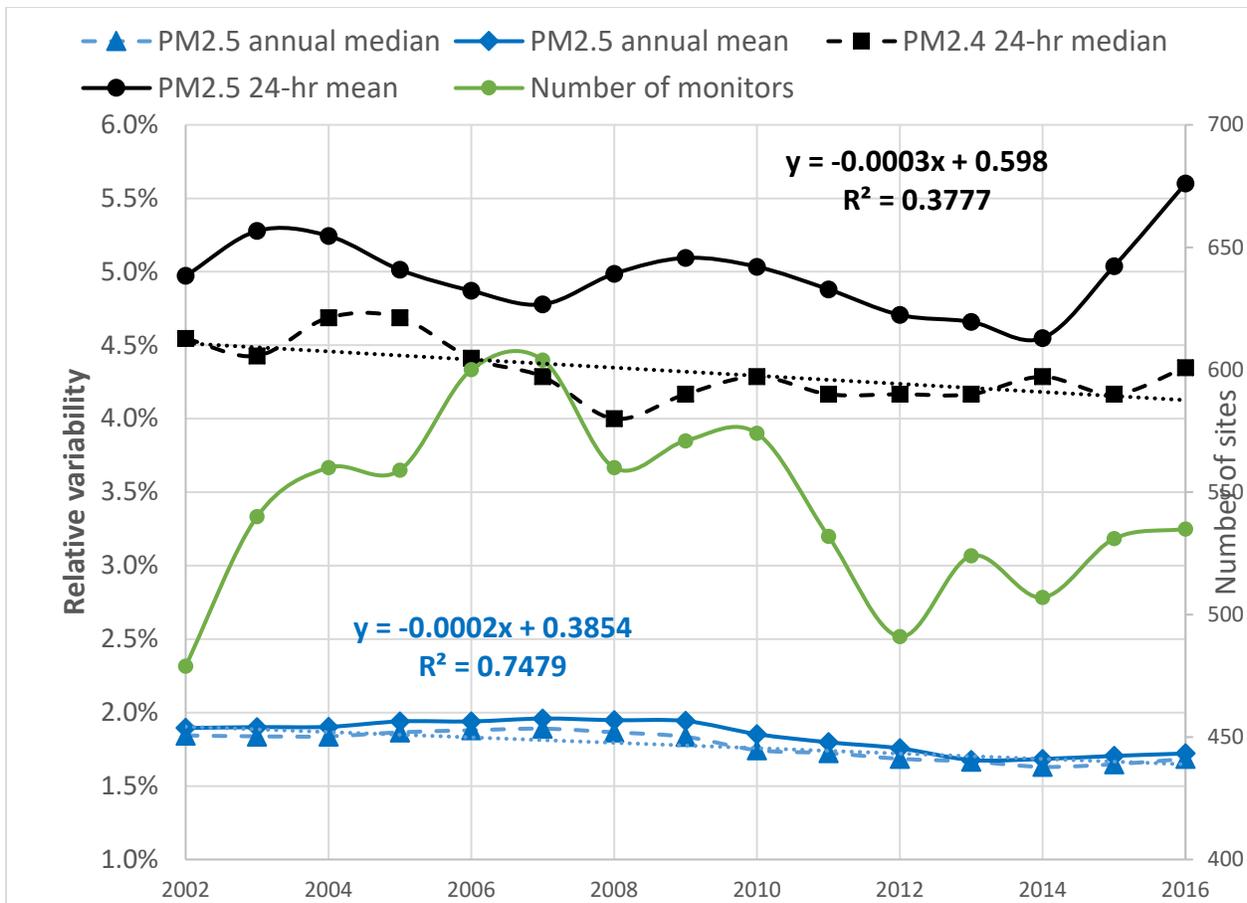


Figure 15 - Median and mean variability in the network determined from the bootstrap analysis (50% CI) for the 15 DV periods from 2002-2016 for PM_{2.5} (each DV period represents 3 years of data and the data is plotted on the ending year: *i.e.*, the 2016 DV period is from 2014-2016 and plotted at 2016).

5. Additional Information

Data for the analyses presented in this document can be obtained by contacting:

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