Statistical power of trend detection methods and sampling schedules for *Escherichia coli* concentrations

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 This is the abstract.  
  
 It consists of two paragraphs.

**Keywords** trend detection; *E. coli*, statistical power

**Abbreviations**

|  |  |
| --- | --- |
| Short Name | Descriptive Name |
| *E. coli* | *Escherichia coli* |
| GAM | generalized additive model |
| mL | milliliter |
| MPN | most probable number |
| SWQM | Surface Water Quality Monitoring |
| TCEQ | Texas Commission on Environmental Quality |

# Introduction

Fecal indicator bacteria are used to assess the sanitary quality of water for recreational and water supply purposes. Fecal indicator bacteria themselves are not dangerous but are utilized as an indicator of potential health risks associated with exposure to pathogens associated with fecal matter. *Escherichia coli* (*E. coli*) is used as a fecal indicator bacteria in Texas to assess if streams and other freshwater bodies meet numeric criteria for contact recreation. *E. coli* is a non-host specific bacteria found in the gut of warm-blooded animals, the presence of *E. coli* is used to indicate the potential for recent fecal contamination.

In-stream fecal indicator bacteria concentrations typically follow a log-normal distribution (Novotny 2004). As a result, the Texas Commission on Environmental Quality (TCEQ) biennially evaluates compliance with the in-stream criterion of 126 most probable number (MPN)/ 100 milliliters (mL) using the geometric mean over a seven-year assessment period. The geometric mean is simply a measure of central tendency calculated as the exponential of the arithmetic mean of logarithms:

Simplified, the geometric mean computes the arithmetic mean of *log(y)* and exponentiation returns the mean to the original scale. An alternative approach is to take the *n*th root of the product of *y\_i*. The current assessment approach requires a sample size of 20 over the previous 7-years with an 80% confidence interval that exceeds the 126 MPN/100 mL criterion at the lower bound in order to be determined impaired (TCEQ 2019 a). Delistings require 20 samples and the geometric mean below the 126/100 mL criterion. TCEQ (2019 a) does not specify how the confidence interval should be calculated. Traditional methods multiply a critical value (obtained from the standard normal distribution or Student’s t-distribution) by the standard error. Alternatively, the confidence intervals can be obtained by parametric bootstrap methods (Wilcox 2013). At 20 samples the method is fairly robust for estimating exceedance of the water quality criterion.

As of 2018, TCEQ identified 237 water bodies impaired due to elevated fecal indicator bacteria (TCEQ 2019 b). Total Maximum Daily Loads and Implementation Plans or Watershed Protection Plans are developed for these impaired water bodies to address potential fecal indicator bacteria sources. As part of these plans, trend analysis is typically conducted to assess if bacterial concentrations have increased or decreased over time. Two common methods for assessing statistical significance of monotonic trends are the modified Mann-Kendall test and linear regression on fecal indicator bacteria concentration values (Helsel and Hirsch 2002; Yue and Wang 2002).

Yue and Wang (2002) described the calculation of the Mann-Kendall test and the modifications for correlated data. In short, when the Mann-Kendall test statistic, *S* is negative, newer values tend to be smaller than older values and indicate a downward trend. A small absolute value of *S* indicates no trend. The *P* value of the test statistic is estimated using the normal cumulative distribution function. The null hypothesis of the Mann-Kendall test is that there is no trend.

Simple linear regression on log-transformed *E. coli* concentrations are also suitable for identifying trends. In order to assess presence of a trend, the following linear regression is used:

where *y* is *E. coli* concentration, *β0* is the intercept, *β1* is the coefficient of time variable *x*, and ε are model residuals assumed normally distributed around mean zero. If linear regressions are utilized to assess *E. coli* trends, the analyst should plot residuals to ensure model residuals meet assumptions of heterogeneity and normal distribution around mean zero.

Both the Mann-Kendall test and linear regression are straight forward methods for water quality analysts to apply and assess trends in *E. coli* concentrations. They are well accepted and have routines available in most statistical software. However, general guidance is not available for the number of samples required to detect given effect sizes. Current guidance for assessment of attainment of the water quality criterion (20 samples over 7-years) is adequate given the ability to estimate confidence intervals for the geometric mean calculation. As a result, many monitoring programs across the state utilize quarterly routine sampling regimes, which equate to approximately 4 samples per year or 28 samples over a 7-year assessment period. Reporting the results of trend detection test implies the test has the statistical power to detect trends of certain magnitudes. However, that information is rarely reported and unlikely that it is routinely calculated by water quality analysts. Therefore, there is considerable uncertainty if monitoring schedules (especially those designed around quarterly monitoring) used across the state are adequate for detecting trends in fecal indicator bacteria.

Statistical power refers to the probability that a statistical test rejects the null hypothesis when the alternative hypothesis is actually true. In the case of the discussed trend tests, power is the probability that the null hypothesis of no trend is rejected when there is in fact a trend in the data. Statistical power is a function of pre-assigned significance level (α), effect size, sample size, and variance within the time series (Yue et al. 2002). First, a meaningful effect size must be determined. The effect size might be biologically meaningful or informed by stakeholder input. Statistical power can be determined for a range of sample size, significance levels, effect sizes and sample variance. The purpose of this article is to provide some guidance and context in determining monitoring frequency for trend analysis of fecal indicator bacteria, specifically *E. coli*. First, we estimate the statistical power of Mann-Kendall and linear regression trend tests at sampling sites across the state using Monte Carlo simulation. Second, we provide statistical power plots at different effect sizes for a range of observed variance values. Finally, we model the likelihood of adequate statistical power for *E. coli* trend detection at sampling sites across Texas.

# Methods

## Data

TCEQ Surface Water Quality Monitoring (SWQM) site information and associated *E. coli* samples collected during the 7-year period from January 2012 through December 2019 were obtained from the Water Quality Portal (<https://www.waterqualitydata.us/>) using the dataRetrieval package in R (De Cicco et al. 2018; R Core Team 2019). Data was restricted to river or stream sampling sites, and SWQM sites with fewer than 1 sample per year were removed from analysis. In total, *E. coli* data was assessed from 984 SWQM sites.

## Statistical Power Computation

The significance level, α, is the probability of rejecting the null hypothesis when it is true (Type I error). The probability of accepting the null hypothesis when it is false is a Type II error (*β*). The statistical power of a test is the probability of rejecting the null hypothesis when the alternative hypothesis is true and is equal to 1 - *β*. A power of 0.80 is typically considered appropriate, which equates to a 20% likelihood of encountering a Type II error. If sampling from a population where the null hypothesis is false, power is calculated as:

where *N* is the total number of tests and *Nrejected* are the total number of times the test rejected the null hypothesis.

For each SWQM site, Monte Carlo simulation was used to observe the statistical power of the Mann-Kendall and linear regression test for detecting trends (Sigal and Chalmers 2016). The simulation generates 1000 independent log-normal distributed time series samples per evaluated effect size for every SWQM site using the site specific log-transformed mean and standard deviation. Effect sizes were induced by reducing the annual log-transformed mean over the 7-year sampling period by 10, 20, 40, and 80 percent. Over 3.93 million simulations were run per trend detection method. Significance level, α, was set at 0.10. The Mann-Kendall test and linear regression is applied to each simulation sample and the number of times the tests correctly reject the null hypothesis (*Nrejected*) are tabulated. Statistical power plots were also generated using Monte Carlo simulation on sample datasets generated using the quartiles (lower, median and upper) of the observed coefficient of variation (CV) of *E. coli* from SWQM sites. CV is a method of measuring the spread of a distribution relative to the size of the mean; specifically, it is ratio of the standard deviation to the mean. These power plots provide a general idea of the expected statistical power of characteristic *E. coli* datasets in the state using typical sampling intervals. They are not intended to be a replacement for conducting a statistical power test using site specific data.

## Likelihood of adequate statistical power

We modeled the likelihood that a SWQM site would have adequate statistical power (≥ 0.80) as a function of sample size, variance, and effect size using generalized linear models (GLMs). GLMs are an extension of linear regression that allows for response variable with non-normal error distributions through the use of a link function. GLMs were setup as a logistic regression model of form:

where the probability of detecting the trends is response on the right hand side of the equation and is a function of the sum of the dependent variables with their corresponding coefficients (*β*) and random errors (*ε*). GLMs were fit using the glm function in R with the binomial family and logit link function.

# Results

## Monitoring Frequency

Out of the 984 evaluated SWQM sites, 329 were located in water bodies with a TMDL. SWQM sites located on water bodies without a TMDL were generally sampled 3 to 4 times per year (Figure ). SWQM sites with a TMDL skewed higher, with a peak at 9 times per year and smaller peaks at 4 and 6 times per year. This suggests that increased monitoring efforts are being targets towards sites where planning efforts have been implemented. Similarly, the *E. coli* geometric mean skewed higher at sites with a TMDL (Figure ).

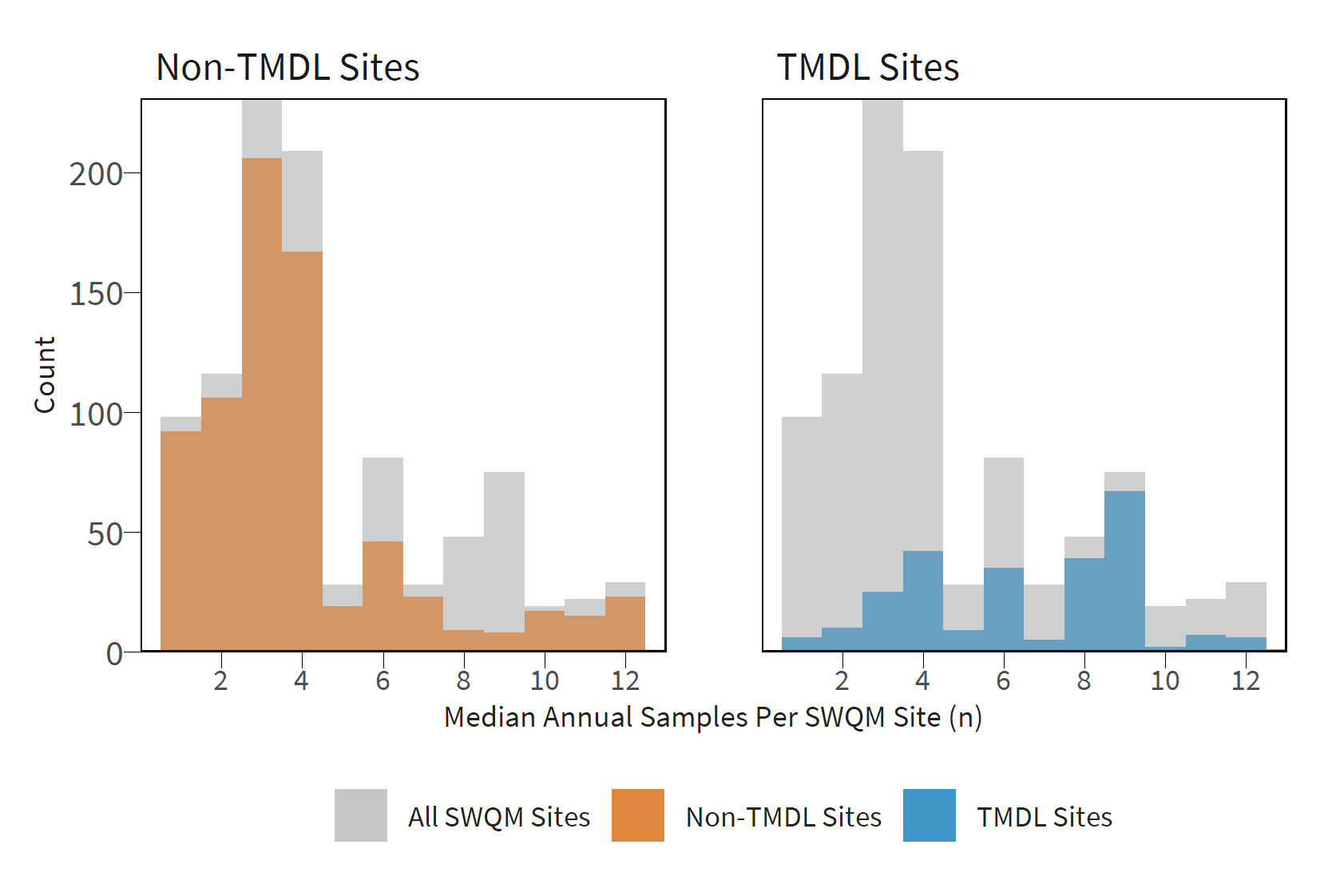


Figure : Histograms of annual *E. coli* sampling distribution for TMDL and non-TMDL SWQM sites across Texas.

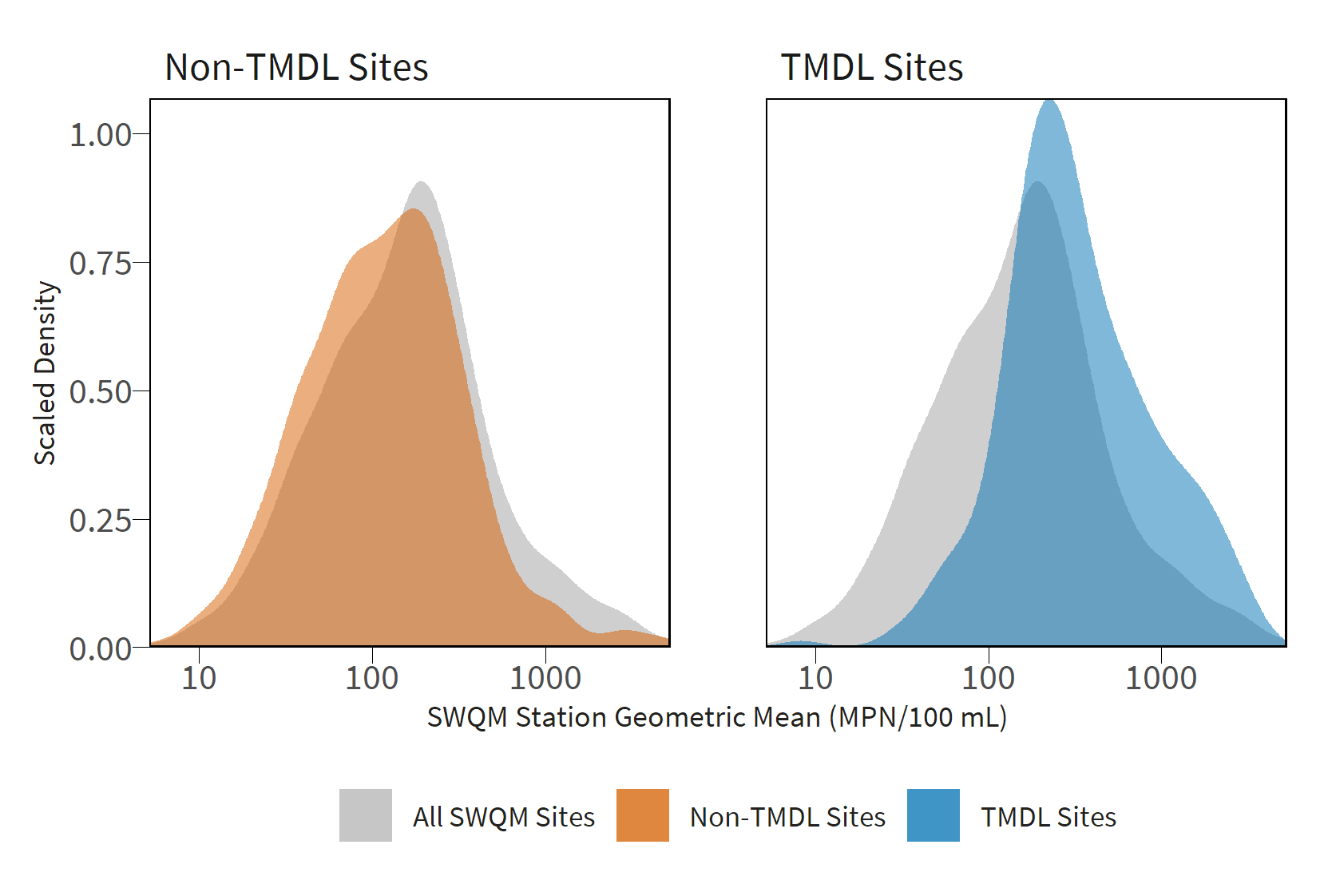


Figure : Scaled density plots of of *E. coli* geometric mean distribution for TMDL and non-TMDL SWQM sites across Texas.

## Estimated Statistical Power at SWQM Sites

At current annual sampling regimes, all SWQM sites fell below 0.80 power for detecting effect sizes of 10% (Figure . At non-TMDL sites, the vast majority of SWQM sites would fail to detect a 20% change. Since SWQM sites with a TMDL typically had a higher frequency of sampling, it is evident that a larger proportion of those sites had adequate statistical power to detect trends at the 40% effect size than non-TMDL SWQM sites. At 80% changes, the vast majority of SWQM sites displayed adequate power for trend detection.

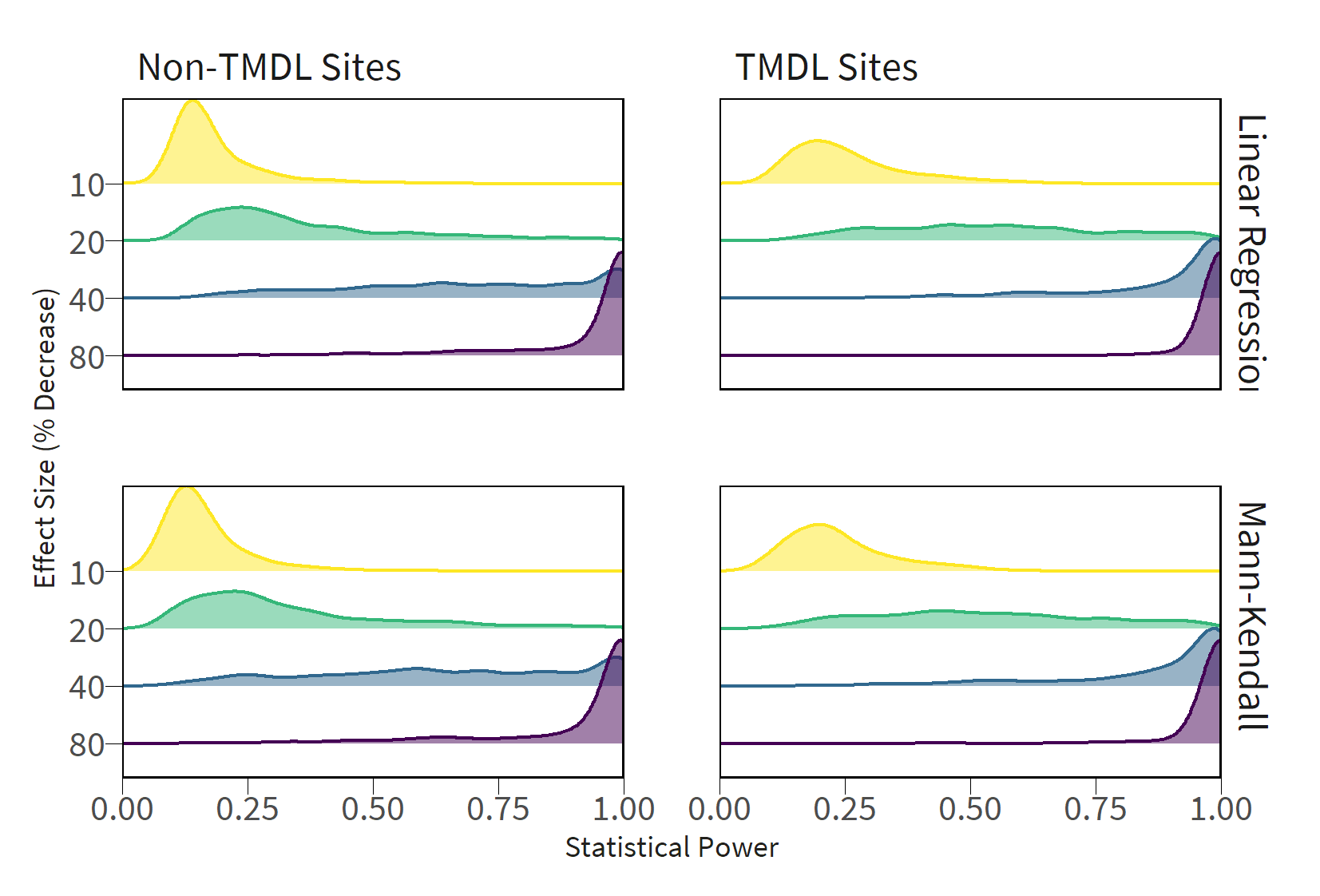


Figure : Scaled density plots of Mann-Kendall and GLM statistical power distribution for TMDL and non-TMDL SWQM sites as a function of effect size at ɑ = 0.1. Individual curves represent the scaled density estimate of statistical power values calculated for SWQM sites at a given effect size (y-axis values).

\*\* add table reporting summary of average sample size, mean (cv), statistical power \*\*

## Likliehood of Obtaining Statistical Power

Variance, sample size, and effect size are significant and substantial predictors of the probability that a SWQM site will have adequate power for detecting trends using linear regression or Mann-Kendall test methods (). Figure displays the marginal effect of sample size and effect size on probability of adequate statistical power being obtained at a SWQM site. At mean variance values and large effect sizes, it is likely that adequate power will be obtained regardless of sample size. Probability decreases substantially as effect size and sample size decrease. Even with monthly sampling, there is only 0.5 probability that a SWQM site will obtain 0.80 power with monthly sampling.

Table : GLMs for probability of adequate statistical power.

|  | Mann-Kendall | | | Linear Regression | | |
| --- | --- | --- | --- | --- | --- | --- |
| Variable | OR1 | 95% CI1 | p-value | OR1 | 95% CI1 | p-value |
| cv | 0.39 | 0.34, 0.45 | <0.001 | 0.38 | 0.33, 0.43 | <0.001 |
| Sample Size | 1.74 | 1.66, 1.83 | <0.001 | 1.72 | 1.63, 1.80 | <0.001 |
| Effect Size | 0.90 | 0.89, 0.90 | <0.001 | 0.89 | 0.89, 0.90 | <0.001 |
| 1OR = Odds Ratio, CI = Confidence Interval | | | | | | |

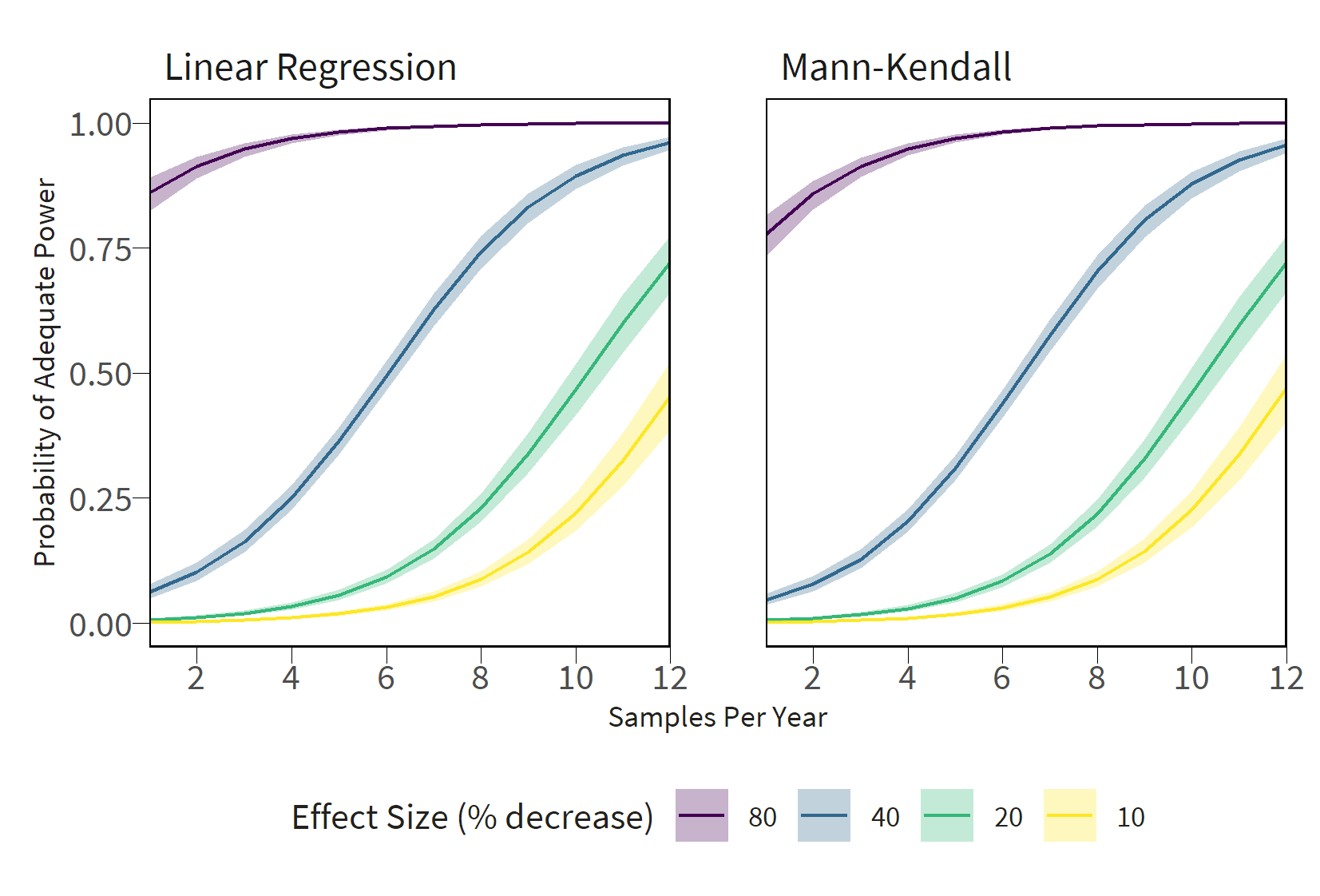


Figure : GLM marginal effects plots show the likelihood that a SWQM site has adequate statistical power for detecting trends as a function of the number of samples and desired detected effect size. CV is held constant at the mean.

# Discussion

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