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

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 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 |
| GLM | generalized linear 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 2019a). Delistings require 20 samples and the geometric mean below the 126/100 mL criterion. TCEQ (2019a) 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 2019b). 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 generalized linear models (GLMs) 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.

GLMs are an semiparamteric extension of simple linear regression suitable for log-normally distributed data. GLMs incorporate a link function that transform the mean instead of relying on a transformed response variable to meet assumptions of normal distribution in a linear regression. In order to assess presence of a trend, the following GLM equation 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 GLMs are utilized to assess *E. coli* trends, a Gaussian distribution with log link function is appropriate to ensure model residuals meet assumptions of heterogeneity and normal distribution around mean zero. Lindsey and Jones (1998) discuss the advantages of utilizing the GLM family of models compared to linear models applied to transformed response variables including interpretation of the measured response, fitting skewed distributions, and allowing for non-constant variance. These advantages do require additional model diagnostics and additional model terms; however, GLMs provide relatively flexible approaches for assessing trends.

Both the Mann-Kendall test and GLMs 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 GLM trend tests at sampling sites across the state using Monte Carlo simulation. Second, we describe functional relationships between the statistical power of the two trends tests, effect size, variance, and number of samples across sampling sites in 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 5, 10, 20, 40, and 80 percent. In total, 4.92 million simulations were run per trend detection method. Significance level, α, was set at 0.10. The Mann-Kendall test and GLM is applied to each simulation sample and the number of times the tests correctly reject the null hypothesis (*Nrejected*) are tabulated.

## Describing Functional Relationships

The functional observed relationships between variance, sample size, and effect size at SWQM sites across Texas were described and visualized using generalized additive models (GAMs). GAMs are a flexible semi-parametric approach for modeling non-linear relationships between variables (Wood 2011; Wood 2017). GAM were fit with the mgcv package in R (Wood 2017). The general form of the GAM equation was:

where *s* is a spline based smoothing function applied to each covariate, *mu* is the log-transformed *E. coli* mean, *sd* is the log-transformed site standard deviation, *sample size* is the annual number of samples collected at the site, and *effect size* is the specified percent decrease to detect in the Monte Carlo simulation. The response variable *Power* is the statistical power within the interval [0,1]. GAMs were fit using the beta regression family and the logit link function. GAMs were not used to specifically test for relationships but only to describe and visualize the known functional relationships that influence statistical power of trend tests as they apply to SWQM stations.

# 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 ).

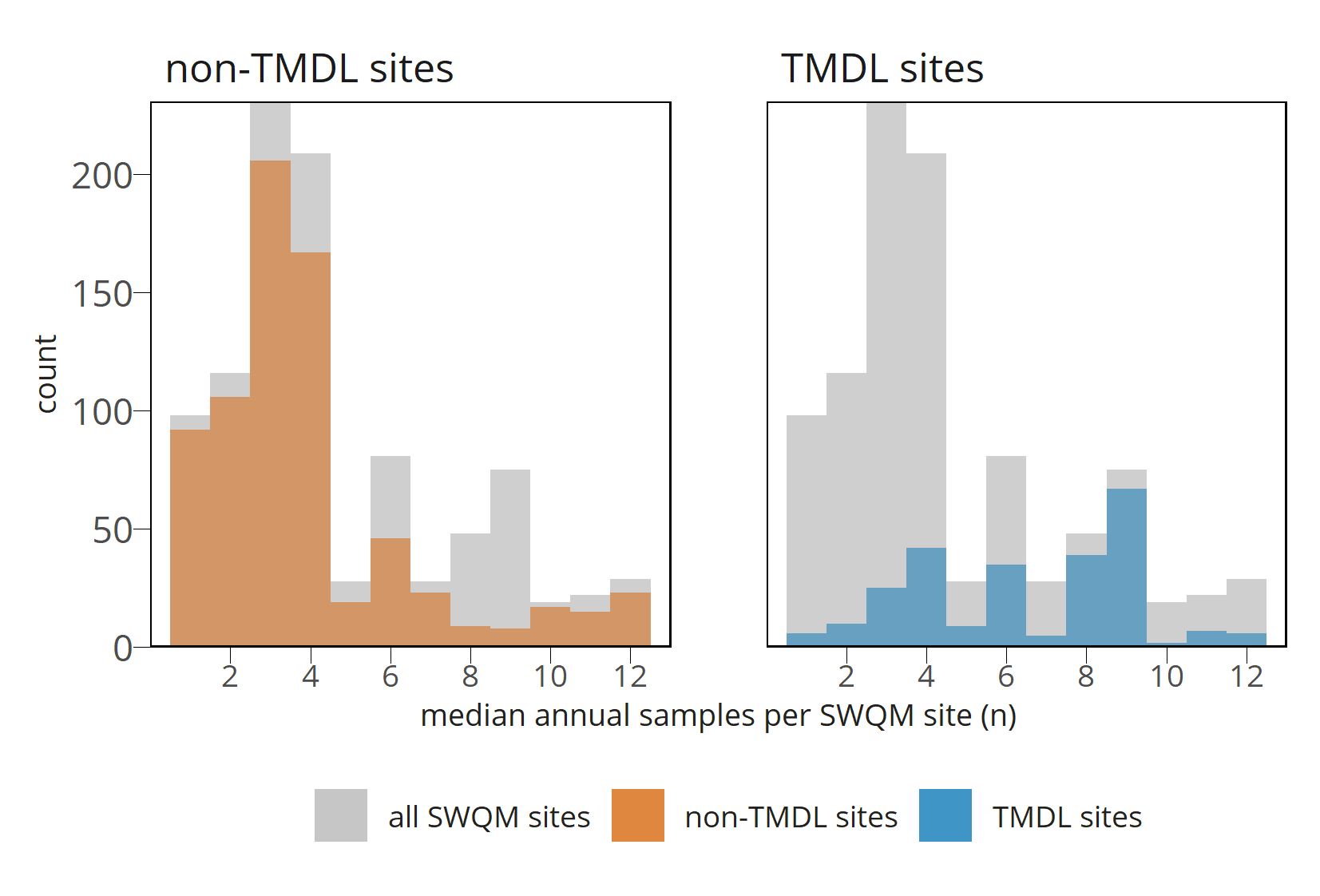


Figure : Histograms of annual *E. coli* sampling distribution for TMDL and non-TMDL SWQM sites across Texas.

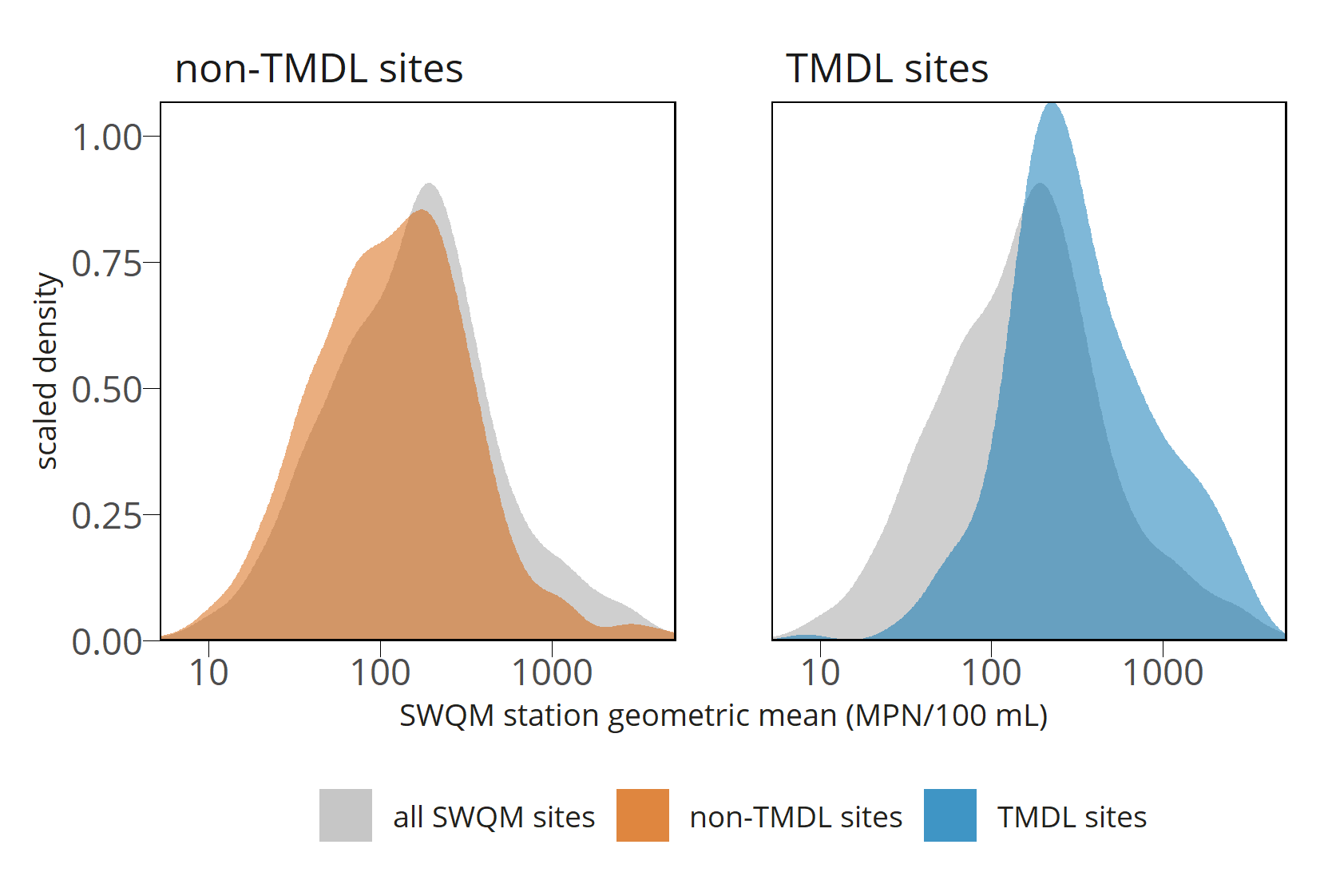


Figure : Scaled density plots of of *E. coli* geometric mean distribution for TMDL and non-TMDL SWQM sites across Texas.

## Mann-Kendall Power

At small effect sizes (5-10 percent decrease in *E. coli* concentration), all SWQM stations have relatively low statistical power (<0.30) for detecting effects (Figure ). Most stations have less than 0.30 power to detect trends of this magnitude using the Mann-Kendall test. With a 40 percent decrease in *E. coli* concentrations, a large proportion of TMDL sites have sufficient statistical power. Adequate power is achieved for most sites in both groups at 90 percent effect sizes.

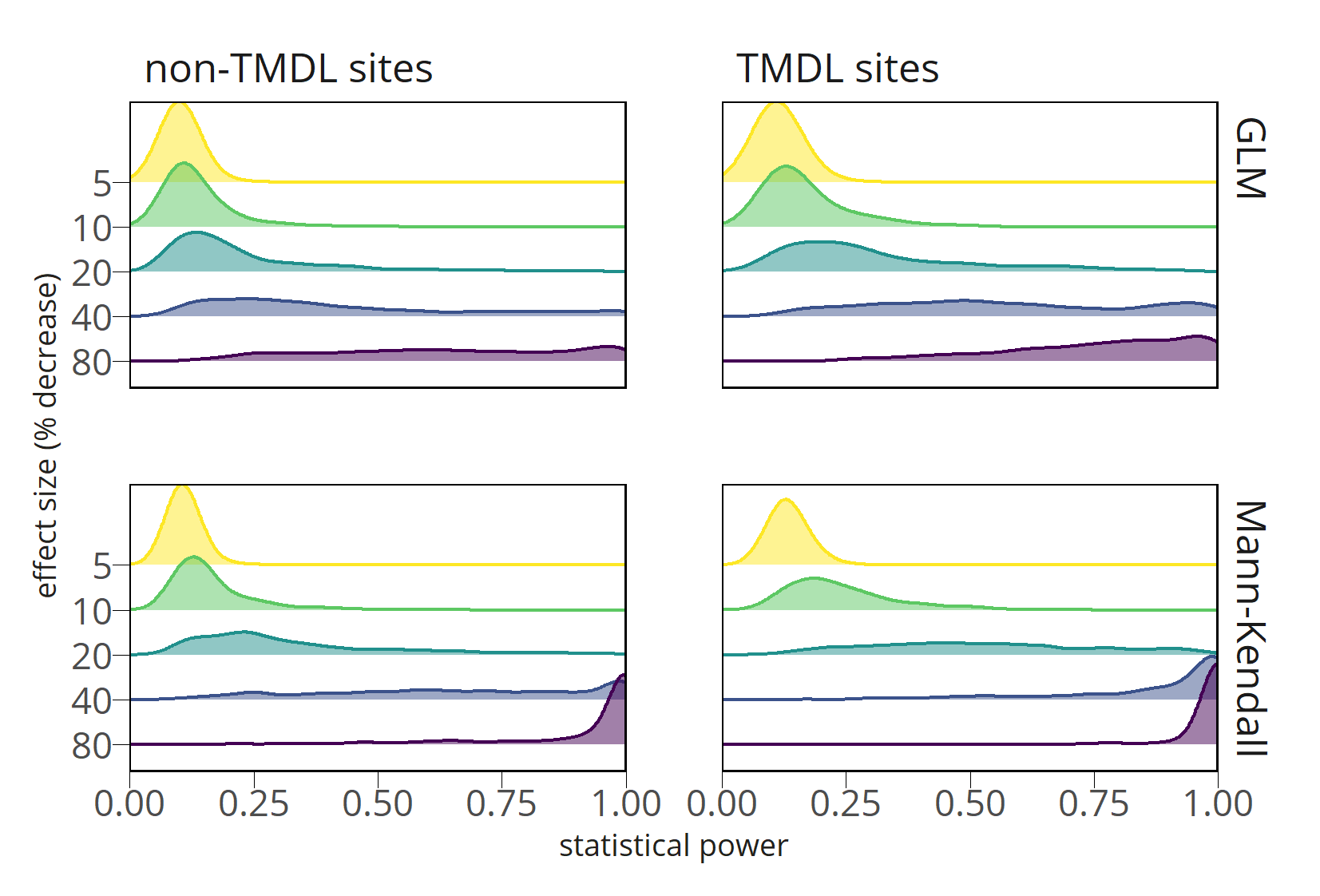


Figure : Scaled density plots of Mann-Kendall statistical power distribution for TMDL and non-TMDL SWQM stations as a function of detectable effect size at ɑ = 0.1. Individual curves represent the scaled density estimate of statistical power values calculated for SWQM stations at a given effect size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

## Generalized linear model

# Discussion

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