

Bayesian analysis of groundwater quality in a semi-arid coastal county of south Texas

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Abstract Bayesian frameworks for comparing water quality information to a pre-specified standard or goal and comparing water quality characteristics among two different entities are presented and illustrated using chloride and total dissolved solids (TDS) measurements obtained in the shallower Chicot and the deeper Evangeline formations of the Gulf coast aquifer underlying Refugio County, TX. The Bayesian approach seeks to present evidence in favor of the competing hypotheses which are weighed equally and unlike classical statistics do not make a decision in favor of one hypothesis. When comparing water quality information to a specified goal, the Bayesian approach addresses the more practical question—given all the information, what is the probability of meeting the goal? Similarly, when comparing the water quality between two entities, the approach simply emphasizes the nature and extent of differences and as such is better suited for evaluative studies. Bayesian analysis indicated that average chloride concentrations in the Evangeline formation was 1.65 times the concentrations in the Chicot formation while the corresponding TDS concentration ratio was close to unity. The probability of identifying water with $\text{TDS} \leq 1,000 \text{ g/m}^3$ was extremely low, especially in the more prolific Evangeline formation. The probability of groundwater supplies with mean chloride concentrations $\leq 500 \text{ g/m}^3$ was relatively high in the Chicot formation but very

low in the Evangeline formation indicating the possible need for blending groundwater with other sources to meet municipal water quality goals.

Keywords Statistics · Bayes' theorem · Data mining · Refugio County · Texas · USA

Introduction

The quality of groundwater dictates the uses it can be put to and as such controls the patterns of growth and development in any region. The impacts of water quality are even more critical when the available groundwater is limited. A wide range of natural and anthropogenic factors affect the groundwater quality in any region. Groundwater quality data are not routinely collected unless there is some severe evidence of contamination. Even then, data collection tends to be intermittent and localized as cost and logistic considerations often prohibit extensive analysis and testing. Therefore, regional-scale groundwater quality assessment for water resources planning is a challenging task. Given the relatively high costs of water quality monitoring, the available data for statistical analysis often tend to be sparse. In such situations, conventional statistical tools like parametric hypothesis testing, regression and discriminant analysis tend to be of limited value. In addition, the application of these methods is somewhat complicated when the outputs are categorical in nature (Hamilton 1993).

Bayesian statistics offers a convenient set of techniques to obtain insights from existing data (Roiger and Geatz 2003). Bayesian probabilistic approaches can be used with numeric as well as categorical data.

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Additionally, in the Bayesian approach, the subjective beliefs held by decision-makers can be factored in and conditioned using collected data (Schmidtt 1969). Data mining using concepts from probability theory is extensively being used to mine medical datasets (Ouali et al. 2006). Bayesian weight of evidence approaches have also been used in mining and landslide risk evaluation applications (Bonham-Carter et al. 1989; Lee et al. 2002). Lately, there has been a renewed interest in using such probabilistic schemes in ecological and environmental applications as well (Hobbs 1997; Borsuk et al. 2001; Termansen et al. 2006).

In this study, the utility of Bayesian approaches to understand regional-scale groundwater quality was evaluated. More specifically, concepts from Bayesian inferential approaches were adapted to evaluate groundwater quality related hypothesis. It is hoped that the present study will illustrate how such techniques can be used by decision-makers for analysis and evaluation of groundwater quality within a region.

Materials and methods

Collection of groundwater quality data

A synoptic groundwater assessment study was carried out in Refugio county, TX over a 1-year period (Jan 2004–Dec 2004). A total of 22 wells were sampled in the shallower Chicot formation (0–125 m bgs) and 21 wells were sampled in the deeper Evangeline formation (125–300 m bgs). The locations of the wells are depicted in Fig. 1. In this study, the chloride and the

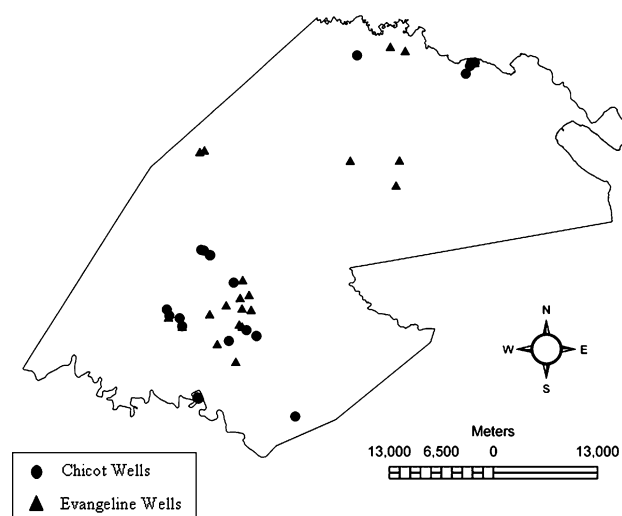


Fig. 1 Map depicting the location of monitoring wells used in this study

total dissolved solids (TDS) measurements collected in the Chicot and Evangeline formations are studied using Bayesian techniques. The TDS was measured in the field using a YSI 600 QS multi-parameter probe (YSI Inc., OH) and chloride was measured using the mercuric thiocyanate method (APHA 1995). The sample collection and analysis followed standard protocols (APHA 1995; USEPA 2002). Groundwater samples were obtained using pumps existing at the wells. The water in the appurtenances was initially purged prior to the sample collection. The stabilization of pH and conductivity values was used as an indicator to obtain representative field samples. All field and laboratory samples were measured in duplicate and an average value was used for the data analysis. The sampling procedure was repeated if the variability among the duplicates was greater than 5%. A rigorous quality control/quality assurance (QA/QC) protocol was developed to guide sampling activities and included routine calibration of the instruments and use of appropriate standards, trip and field blanks. Additional details of the field sampling program from which the TDS and chloride data used in this study were obtained can be found in Moorthy (2005).

An overview of Bayesian statistics

Bayesian statistics is based on the notion that the probability is a measure of uncertainty (Winkler 1972). It departs from the frequentist notion of probability which is based on the idea of the chance of observing a certain value (state), given repeated experimentation. Being more generic, Bayesian statistics can deal with subjective probabilistic notions held by decision-makers as well as objective measurements obtained via observations and experimentation. Fundamental to the study of Bayesian statistics is the Bayes' theorem. Given two random variables, A and B , which describe a system of interest, Bayes' theorem can be mathematically described as follows:

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)} = \frac{L(A|B)P(A)}{P(B)} \quad (1)$$

where $P(A|B)$ is the conditional probability of A (i.e., the probability of obtaining A given B); $P(A)$ is the marginal probability of A (i.e., probability of obtaining A without considering B) and $P(B|A)$ is the conditional probability of B and $P(B)$ is the marginal probability of B . The conditional probability $P(B|A)$ is also referred to as the likelihood of A [i.e., $L(A|B)$]. The conditional probability $P(A|B)$ is referred to as the posterior probability and $P(A)$ as the prior probability and $P(B)$

is the normalizing constant. Thus, Bayes’ theorem can be described in words as

$$\text{Posterior} \propto \text{prior} \times \text{likelihood} \quad (2)$$

The prior information can represent the subjective notions about the probability of a random variable that is held by the decision-makers or can be defined based on any previous data (such as those obtained from a literature review). The likelihood on the other hand is the information gleaned from the data arising from a specific study carried out to update the insights about the system of interest. Therefore, the likelihood is always calculated from the data. The prior on the other hand represents knowledge before these data were available. Therefore, the posterior probability represents the updated understanding of the system that is obtained by conditioning prior beliefs with experimental insights.

In some instances, when there is very little prior information available, the posterior probabilities are strictly based on the likelihood function estimated from the data. In such instances, the numerical values for probabilities will be the same in Bayesian and the conventional (frequentist) approaches. Despite this numerical equivalence, it is important to remember that the interpretation of probability is different for the two approaches. The conventional approach is based on the notion of relative frequency, while the Bayesian is based on the subjective belief. The reader is referred to Schmidt (1969) and Sivia (2003) for a practical introduction to Bayesian statistics. The application of Bayesian statistics to water resources problems has been discussed by Hobbs (1997). However, Bayesian hypothesis testing has not been explored extensively in the groundwater literature and as such pertinent concepts are presented next.

Generally, in groundwater quality assessments, statistical hypothesis testing is usually carried out to (1) demonstrate that the concentration of a chemical at a location is less than (greater than) or equal to some allowable standard or goal; or (2) compare concentrations between two or more entities (e.g., up-gradient and down-gradient of a landfill) to see if they are equal. These tests are carried out by assuming the measured concentrations as random variables and using point-estimates such as the mean or the median. In the following, Bayesian approaches are presented for the above two cases and are compared to conventional statistical tests.

Bayesian hypothesis testing—comparing to a standard

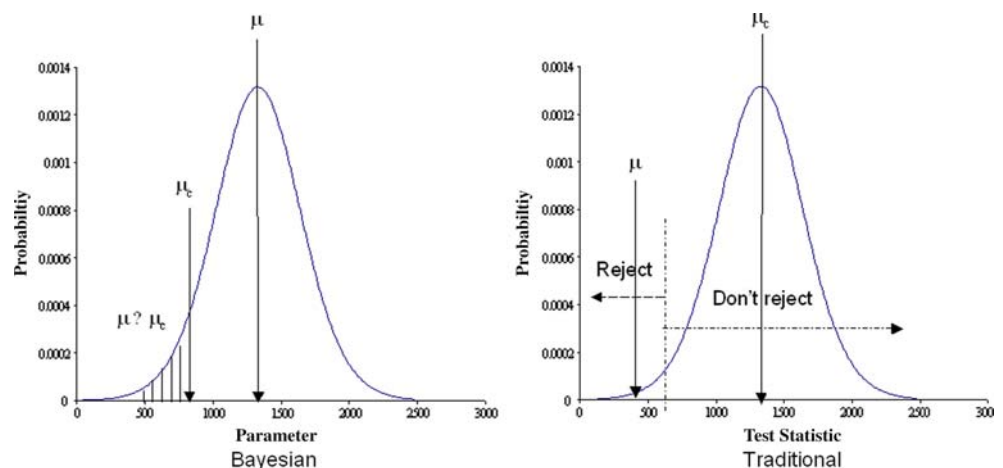
For a given random variable A , the competing hypotheses can be written as follows:

$$H_1 : \mu_A \leq \mu_c \text{ i.e., the concentration is less than or equal to the standard} \quad (3)$$

$$H_2 : \mu_A > \mu_c \text{ i.e., the concentration is greater than the standard } (\mu_c) \quad (4)$$

In conventional statistics, mean value μ is computed from the data and compared to the distribution of the test statistic (μ_c) which is centered at μ_c . Hypothesis 1 is favored if the computed value of μ_A is farther to the left of the distribution and hypothesis 2 is favored when the computed value μ_A is farther to the right (Fig. 2). On the other hand, in the Bayesian approach, the posterior probability distribution of A is constructed by combining any prior information with collected data using Eq. 2. The cumulative probabilities in favor of hypothesis 1 and hypothesis 2 are then ascer-

Fig. 2 A comparison of classical and Bayesian approaches to hypothesis testing



tained from the posterior distribution, to identify which hypothesis is favored (Fig. 2). The posterior probability distribution is centered at the mean μ_A and computed as follows:

$$\frac{P''(H_1 = \text{TRUE})}{P''(H_1 = \text{TRUE})} = \frac{P''(\mu_A \leq \mu_c)}{P''(\mu_A > \mu_c)} \propto \frac{P'(\mu_A \leq \mu_c)}{P'(\mu_A > \mu_c)} \times \frac{L(\mu_A \leq \mu_c|D)}{L(\mu_A > \mu_c|D)} \quad (5)$$

where P'' represents the posterior probability, L represents the likelihood and P' represents the prior.

If the prior is considered non-informative, then the numerical value of μ_A in the Bayesian method might be the same as that used in the conventional method. However, the computed probabilities are interpreted differently. In the conventional statistics, the unusualness of the sample is measured, given the distribution of the hypothesis. In other words, the probability is an indicator of the frequency (or risk) of incorrectly rejecting the hypothesis, when in fact it is true. The significance level indicates the tolerance of the decision-maker to such a risk and is subjectively assigned. In contrast, Bayesian statistics explicitly measures the evidence in support of each hypothesis and provides a more intuitive explanation of whether the hypothesis should be rejected or not. The actual rejection or acceptance of a hypothesis, however, has to be carried out separately.

From a conservative standpoint, hypothesis H_2 (Eq. 4) is favored over hypothesis H_1 (Eq. 3). This conservatism can be incorporated into the decision-making process by multiplying the posterior probabilities by a factor of safety. Mathematically, the odds ratio (Ω'') for competing hypotheses can be written as follows (Winkler 1972):

$$\Omega'' = \frac{P''(H_1 = \text{TRUE})}{P''(H_2 = \text{TRUE})} \times \frac{1}{X} \quad \forall X \geq 1 \quad (6)$$

Clearly, X denotes the extent of conservatism on part of the decision makers.

Bayesian hypothesis testing—comparing two or more entities

The posterior probabilities can be computed at individual locations using Eq. 2 and compared to see the behavior of the random variable of interest among different entities. As the entire probability distribution is available at each of these locations, the comparison need not be restricted to point estimates like the mean and the standard deviation. For ad hoc comparisons,

the highest posterior density interval (HPDI) of the mean value can be ascertained from the posterior distribution and used for comparing different sites. HPDI is analogous to the confidence interval in conventional statistics and is also referred to as the credible level (Koop 2003). Ninety percent and 95% HPDI are commonly used and imply that the decision-maker is (90 or 95%) certain that the value of the mean lies in the HPDI.

It is interesting to note that only one-sided hypothesis (e.g., $H_1: \mu_a = \mu_b$ and $H_2: \mu_a > \mu_b$ or $\mu_a < \mu_b$) can be inferred using Bayesian hypothesis testing. The two-sided hypothesis (e.g., $H_1: \mu_a = \mu_b$ and $H_2: \mu_a \neq \mu_b$) cannot be tested as the focus of the Bayesian statistics is not point estimates, but rather the entire probability distribution of the mean or any other statistical moment being tested (Winkler 1972).

Development of prior and likelihood distributions

The specification of prior and likelihood probability distributions is an important step for carrying out Bayesian statistics. In theory, any probability distribution function can be used. As the likelihood function is based on data, it can be developed by fitting the data to any known distribution function. If there is very little information available before the sampling campaign, it is common to use a non-informative prior, which is also referred to as the Jeffreys' prior and typically represented using an uniform distribution (Borsuk and Stow 2000). From a mathematical standpoint it is convenient to specify a conjugate prior. A conjugate prior has a distribution which, when combined with the likelihood, will yield a posterior that falls in the same family of distribution (Koop 2003). The choice of the conjugate prior depends upon the distribution chosen for the likelihood function. The conjugate prior simplifies the mathematical tractability of the model and is often easy to interpret. If a non-conjugate prior is chosen, then the posterior distribution has to be computed numerically. Monte Carlo techniques are commonly used for numerical evaluations and the suitability of available algorithms has been discussed by Qian et al. (2003).

For the purposes of this study, the measured water quality parameters (or their log-transformed counterparts) are assumed to arise from a normal distribution with unknown mean (μ) but a known standard deviation (σ) (i.e., the likelihood function is normally distributed). It is useful to define the standard deviation in terms of precision R which is the inverse of the variance of the distribution (i.e., $R = 1/\sigma^2$). If the prior distribution of mean (μ) is also normal, then the

posterior distribution (μ) follows normal distribution as well (Winkler 1972).

If the prior mean (μ') and variance (σ') are known (or assumed) and N samples are obtained from a normally distributed process with standard deviation (σ) to yield a mean (m), then the posterior mean (μ'') and variance (σ'') can be computed as follows:

$$\frac{1}{\sigma''^2} = \frac{1}{\sigma'^2} + \frac{n}{\sigma^2} \quad \text{or} \quad R'' = R' + nR \tag{7}$$

$$m = \frac{R'\mu' + nR}{R' + nR} \tag{8}$$

Also, the probability distribution function for the normal distribution function of a random variable x with mean m and standard deviation d is given as follows:

$$f(x|m, d) = \frac{1}{\sqrt{2\pi}d} e^{-\frac{(m-x)^2}{2d^2}} \tag{9}$$

Equations 7, 8 and 9 can be used to construct the required prior, likelihood and posterior distribution. The choice of the normal–normal conjugate prior does considerably simplify the underlying mathematics, but requires the decision-maker to know the variance of the likelihood function. As a first approximation, the sample variance can be used for the population variance. The validity of this approximation increases with increasing number of samples used in the analysis (Winkler 1972). The prior mean and variance can be obtained from any previous studies carried out in similar systems or specified based on professional judgment of the analyst. If the variance of the prior distribution is not known, a large number can be specified to imply ignorance on part of the decision-maker with regard to the variability of the water quality parameter under consideration.

As stated earlier, the conjugate normal distribution approach adopted in this study considerably simplifies the mathematics but requires the decision-maker to specify the variance of the prior and the likelihood function. This assumption is commonly made in Bayesian analysis (Dilks et al. 1992). However, if both the mean and the variance of the prior are assumed to be unknown, then the variance has to be treated as a random variable. The marginal probability of the posterior mean has to be obtained by calculating the joint probability of the mean and the variance. In such instances, it is advisable to assume the mean of the random variable to be normally distributed while the reciprocal of the variance (precision) to follow gamma distribution. The normal-gamma distribution is

a conjugate distribution that can be used to estimate the posterior probability distribution of the random variable when both the mean and the variance are assumed to be unknown (Koop 2003).

Results and discussion

Specification of the prior and exploratory data analysis

The Bayesian approach is illustrated using the concentrations of TDS and chloride in Chicot and Evangeline formations of the Gulf Coast aquifer in Refugio County, TX. The prior mean values were chosen to be 500 g/m³ for chloride and 1,250 g/m³ for TDS in Chicot and Evangeline formations based on typical values found in the groundwater database put forth by the Texas Water Development Board (TWDB) and other reports (Mason 1963). The analysis of data from other locations also indicated that these water quality parameters exhibited high variability. As such, the coefficient of variation was assumed to be 1.25 and the prior standard deviation was specified as 625.00 g/m³ and 1562.50 g/m³ for chloride and TDS, respectively.

Exploratory data analysis (EDA) (Table 1) indicated that the water quality parameters exhibited considerable variability. In general, the variability was more pronounced in the shallower Chicot formation and this is to be expected as this aquifer is in direct contact with the soil and the atmosphere. The TDS exhibited greater variability than the chloride and again this result is to be expected since TDS is a bulk measure and the aquifer material is known to possess

Table 1 Exploratory data analysis of the selected water quality parameters

Statistic	Chicot		Evangeline	
	Chloride	TDS	Chloride	TDS
Mean	442.95	1339.67	739.44	1423.02
Standard error	61.73	327.54	84.66	167.66
Median	358.00	958.75	587.50	1113.00
Mode	1075.00	935.00	785.00	NA
Standard deviation	282.89	1536.31	378.61	768.31
Sample variance	80027.04	2360248.02	143343.68	590294.31
Kurtosis	1.13	19.76	-0.03	6.07
Skewness	1.33	4.35	0.99	2.24
Range	975.00	7737.00	1300.00	3292.00
Minimum	100.00	323.00	320.00	741.00
Maximum	1075.00	8060.00	1620.00	4033.00
COV	0.64	1.15	0.51	0.54
Count	21.00	22.00	20.00	21.00

NA not available

several mineral and inorganic matter that readily dissolve into the water. The summary statistics also indicate that the assumption of normality may not be entirely appropriate for this dataset. A variety of transformations were attempted to normalize the data but did not lead to significant improvements and as such, the raw data were used in the analysis. However, as the focus of this study is on relative comparisons and not on obtaining any absolute values, the assumption of normality may not be too restrictive. However, the screening nature of the results must be borne in mind during their use.

Analysis of prior, likelihood and posterior distributions

The first two moments, namely the mean and the standard deviation, of the prior, likelihood and posterior distributions for chloride and TDS in Chicot and Evangeline formations are summarized in Table 2. Note that the moments of the posterior distribution are closer to the moments of the likelihood function than the prior distribution. This result is to be expected as the prior distribution was largely rendered non-informative due to the specification of a large value for the variance.

While the prior is developed using subjective judgments and data from previous experiments, it can be interpreted to arise from a set of hypothetical equivalent observations obtained prior to the development of the likelihood function. The variance of the prior and the likelihood functions can be used to estimate the

number of hypothetical observations that led to the prior as follows (Winkler 1972):

$$N' = \frac{\sigma^2}{\sigma'^2} = \frac{R'}{R} \quad (10)$$

where N' is the number of hypothetical equivalent observations that generated the prior information; R' and σ' are the precision and standard deviation of the prior and R and σ are the precision and standard deviation of the likelihood, respectively. Also, as the posterior synthesizes prior and likelihood information, it can be interpreted to arise from a set of N'' ($N'' = N + N'$) observations, where N is the number of observations used to define the likelihood function. As can be seen from Table 2, the specified priors were highly non-informative and conceptualized to stem from no more than one observation. Clearly, the information in the posterior is weighted more heavily by the likelihood function.

The prior, likelihood and posterior probability distribution functions for chloride concentrations in the Chicot aquifer are schematically depicted in Fig. 3. The distributions for water quality parameters also exhibited similar behavior and as such are not presented here for brevity. However, they can be readily constructed using information contained in Table 2 in Eq. 9. The non-informative nature of the prior is readily evidenced by the relatively flat line in Fig. 3. While the likelihood function is not as flat, it also exhibits a fair amount of variance. As evidenced in Fig. 3, a distinguishing feature of the Bayesian approach is that the posterior distribution exhibits less variability than the prior and the likelihood functions. Therefore, good quality field data when combined with limited prior information will result in posterior distributions that are based primarily on field data but improved by whatever prior information was available (Dilks and others 1992). The extent of improvement in this case depends upon the variability in the prior. Again, as can be seen from Fig. 3, even a fairly non-informative prior can lead to substantial improvements.

Testing water quality parameters against specified goals

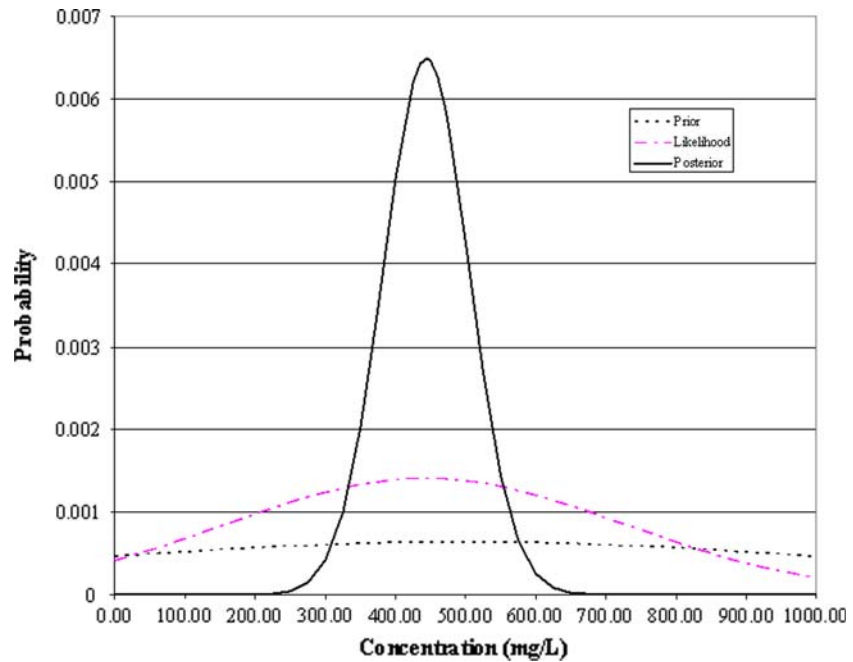
The USEPA recommended secondary drinking water standards for chloride and TDS are 250 and 500 g/m³, respectively (USEPA 2006). Groundwater concentrations of these parameters typically tend to be higher in the county, given the geochemical makeup of the aquifers and the proximity to the coast. For water

Table 2 Prior, likelihood and posterior distributions for the water quality parameters

	Chicot formation		Evangeline formation	
	Chloride	TDS	Chloride	TDS
Prior				
Mean	500.00	1250.00	500.00	1250.00
SD	625.00	1562.50	625.00	1562.50
Precision	2.56E-06	4.10E-07	2.56E-06	4.10E-07
Observations	NA	1	NA	NA
Likelihood				
Mean	442.95	1339.67	739.44	1423.02
SD	282.89	1536.31	378.61	768.31
Precision	1.25E-05	4.24E-07	6.98E-06	1.69E-06
Observations	21	22	20	21
Posterior				
Mean	443.51	1335.90	735.12	1421.05
SD	61.43	320.57	83.89	166.70
Precision	2.65E-04	9.73E-06	1.42E-04	3.60E-05
N	21	23	20	21

NA not available

Fig. 3 Prior, likelihood and posterior distributions for chloride concentrations in the Chicot aquifer formation



supply projects, groundwater with TDS less than 1,000 g/m³ and chloride less than 500 g/m³ (i.e., two times the recommended limits) are usually sought to keep treatment costs to a minimum. The probability of finding, on average, groundwater with these characteristics (i.e., TDS ≤ 1,000 g/m³ and chloride ≤ 500 g/m³) would be of interest to municipalities and regional development groups.

The competing hypotheses can be stated as follows:

$$H_1 : \mu \leq \mu_c \tag{11}$$

$$H_2 : \mu > \mu_c \tag{12}$$

where μ is the mean concentration of the water quality constituent (chloride or TDS) and μ_c is the concentration goal for the water quality constituent (i.e., 500 and 1,000 g/m³ for chloride and TDS, respectively). If the observations are assumed to stem from a normal distribution with a known variance, then the posterior probabilities supporting hypothesis H_1 and H_2 can be written as follows:

$$P''(H_1) = P''(\mu \leq \mu_c) = P\left(\frac{\mu - \mu''}{\sigma''} \leq \frac{\mu_c - \mu''}{\sigma''}\right) \Rightarrow P\left(z \leq \frac{\mu_c - \mu''}{\sigma''}\right) \tag{13}$$

$$P''(H_2) = 1 - P''(\mu \leq \mu_c) = 1 - P\left(\frac{\mu - \mu''}{\sigma''} \leq \frac{\mu_c - \mu''}{\sigma''}\right) \Rightarrow P\left(z > \frac{\mu_c - \mu''}{\sigma''}\right) \tag{14}$$

The prior evidence in support of the hypothesis and the likelihood of observing each of the hypotheses can also be computed using Eqs. 13 and 14 but substituting the posterior mean and standard deviations with respective parameters for prior and likelihood function.

The evidence supporting each hypothesis is presented in Table 3. From prior values, it can be seen that the evidence (prior probabilities) in support of either hypothesis is roughly the same. These probabilities highlight general ignorance on the part of the decision-maker with regard to the water quality characteristics in the county due to lack of sufficient data prior to this study. However, the posterior probabilities present more conclusive evidence as they incorporate the information obtained from the sampling campaign.

Table 3 Prior, likelihood and posterior probabilities supporting the competing claims of finding water with specified water quality goals

	Chicot		Evangeline	
	Chloride	TDS	Chloride	TDS
Prior				
$P(\mu \leq \mu_c)$	0.500	0.436	0.500	0.436
$P(\mu > \mu_c)$	0.500	0.564	0.500	0.564
Likelihood				
$P(\mu \leq \mu_c)$	0.580	0.413	0.264	0.291
$P(\mu > \mu_c)$	0.420	0.587	0.736	0.709
Posterior				
$P(\mu \leq \mu_c)$	0.821	0.147	0.003	0.006
$P(\mu > \mu_c)$	0.179	0.853	0.997	0.994

As can be seen, there is a little over 80% probability of finding groundwater with chloride concentration less than or equal to 500 g/m³ in the shallower Chicot formation, indicating that the groundwater interactions with marine aerosols and other surficial salt deposits are probably low. However, the evidence in favor of finding groundwater with TDS less than or equal to 1,000 g/m³ is rather low indicating the importance of geochemical reactions that contribute to the TDS in the Chicot formation.

The probability of finding groundwater with specified quality (as measured using chloride and TDS) is very low in the Evangeline formation in comparison to the Chicot formation. The groundwater flow in the Evangeline formation is significantly slower than that in the Chicot formation (Chowdhury et al. 2004) indicating longer residence times in the deeper Evangeline aquifer. In addition, the water in the Evangeline formation has had to traverse a considerable distance (~100 km) from the outcrops to the sampling wells. As such, the groundwater in this deeper aquifer formation is considerably older than that in the surficial Chicot formation. These factors increase the potential for mineral precipitation, dissolution and other geochemical reactions that deteriorate the groundwater quality.

Groundwater quality sampling in the northwestern sections of the county was rather spotty, due to lack of access to wells and probably affected the computed posterior probabilities. The groundwater quality in the Evangeline formation is probably better in this area, as outcrops of the formation can be found in relatively pristine northwestern sections. The data from the current study could serve as useful prior to update the water quality characteristics of the Evangeline formation as more data are collected in the northwestern sections of the county.

While Chicot formation has slightly better water quality than the deeper Evangeline formation, the deeper aquifer formation is known to have considerable sand thicknesses and is more prolific than the shallower Chicot formation (Mason 1963). Hence, blending of groundwater obtained from shallow and deep formations with other sources is probably necessary to satisfy the quantity and quality needs for municipal water supply purposes.

Comparing water quality in different aquifer formations

The Bayesian posterior estimates can be directly used to informally compare water quality characteristics among the two aquifer formations. For informal

comparisons, the posterior ratio for the mean values can be written as follows:

$$M'' = \frac{\mu''|_{\text{Evangaline}}}{\mu''|_{\text{Chicot}}} \quad (15)$$

Similar ratios for prior and likelihood means can also be developed for informal comparison. If the posterior mean ratio is close to unity, then, on average, there is no difference in the water quality parameter in the two formations. If the means ratio as written is much greater than one, then the average concentration in the Evangeline formation is greater than that in the Chicot formation. Alternatively, if the means ratio as written is much less than unity, then the average concentration of the water quality parameter is higher in the Chicot formation. Similar comparison can also be carried out using standard deviations to assess the differences in variability of the water quality parameters in the two formations. As stated previously, the HPDI provides a useful estimate for the range of variability of the mean at a specified level of confidence. HPDI is analogous to the confidence interval in conventional statistics and is also referred to as the credible level (Koop 2003) and combines the mean and variance into a composite metric. For the assumed normal-normal conjugate pair, and given posterior distribution with mean μ'' and standard deviation σ'' , the 95% HPDI can be computed as follows (Winkler 1972):

$$\text{HPDI} = \mu'' \pm 1.96\sigma'' \quad (16)$$

Highest posterior density interval can be used to make more formal comparisons of the mean values observed in the two entities. In addition to comparing expected values, the entire posterior probability distribution function can also be used to visually compare groundwater quality parameters in two formations of interest. If the overlap between the two distributions is significant, then the water quality parameters are said to exhibit similar behavior. Alternatively, if the water quality parameters behave differently then they will only minimally overlap, if any.

The prior, likelihood and posterior mean ratios for chloride and TDS is presented in Table 4. As can be seen, the prior ratios were set equal to one, indicating that there is not much of a difference in the mean values in both aquifer formations. However, for chloride the likelihood and posterior ratios are close to 1.65 indicating considerable differences between the two formations. On the other hand, the posterior ratio is close to unity for TDS indicating that the mean TDS

Table 4 Prior, likelihood and posterior mean ratios for chloride and TDS (the ratios are computed as Evangeline/Chicot)

	Mean ratio		Standard deviation ratio	
	Chloride	TDS	Chloride	TDS
Prior	1.00	1.00	1.00	1.00
Likelihood	1.67	1.06	1.34	0.50
Posterior	1.66	1.06	1.37	0.52

Table 5 Ninety-five percent highest posterior density intervals (HPDI) for chloride and TDS in Chicot and Evangeline formations

95% HPDI	Chicot formation		Evangeline formation	
	Chloride	TDS	Chloride	TDS
Upper limit	563.91	1964.22	899.55	1747.78
Lower limit	323.10	707.57	570.69	1094.32

values are not very different between the two formations. Again as seen from Table 4, the variability around the mean values is about 35% higher in the Evangeline formation. On the other hand, the variability in the TDS is lower in the Evangeline formation by about 50%. The 95% HPDI are summarized in Table 5. As can be seen the 95% HPDI for TDS mean in the Evangeline formation is completely enveloped by the 95% HPDI for mean TDS concentration for the Chicot formation. Thus, the differences between the mean concentrations of TDS can be concluded to be

negligible. However, the 95% HPDI for the mean chloride concentrations have very minimal overlap indicating differences between the chloride concentrations in the two formations. The posterior probability distribution plots presented in Figs. 4 and 5 visually depict the differences in mean and variability for chloride and TDS, respectively.

The above results highlight the limitations of bulk measures like TDS in differentiating the water quality characteristics between different aquifer formations. The differences in the mean values noted in chloride and not TDS indicates that constituents other than chloride contribute significantly to the TDS in the aquifer. The lower variability of chloride in the Chicot formation indicates the stabilization of variance due to direct atmospheric exchange. On the other hand, lower variability of TDS in the deeper Evangeline formation is consistent with the longer residence times and point toward the importance of geochemical reactions in controlling the TDS in the aquifer pore water.

Contrasting classical and Bayesian approaches

In the conventional statistical approach, hypothesis testing is viewed as a decision-making problem where one hypothesis is selected over the other. The easier of the two hypotheses, namely the null hypothesis, is given the benefit of doubt and the alternative hypothesis is only selected when there is considerable evidence against the null hypothesis (i.e., the probability of incorrectly rejecting the null hypothesis is small). On

Fig. 4 A comparison of posterior distributions for chloride in Chicot and Evangeline aquifer formations

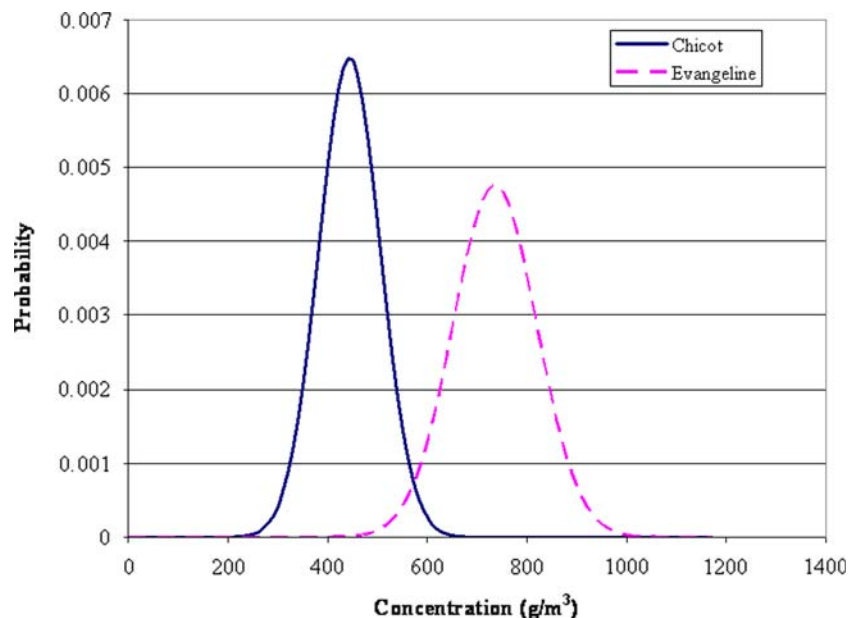
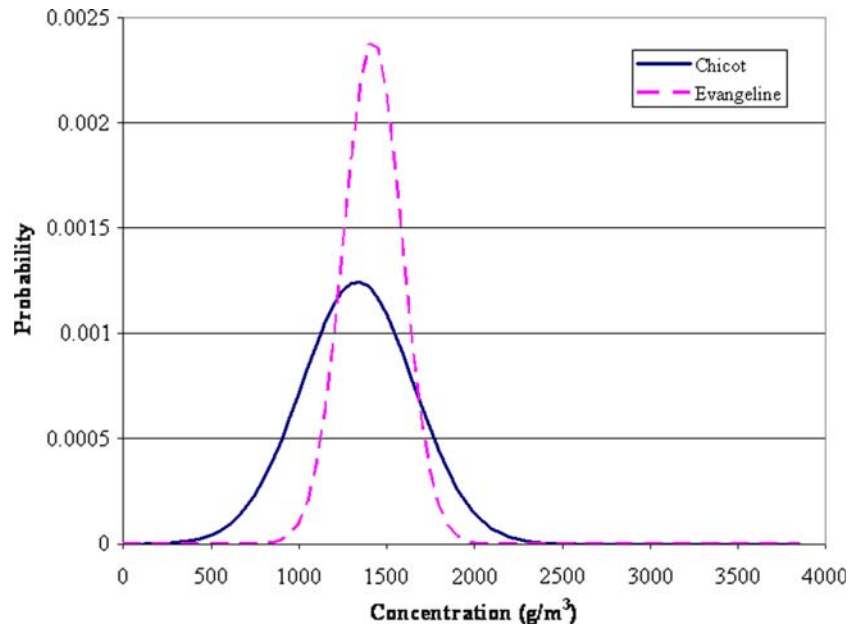


Fig. 5 A comparison of posterior distributions for the total dissolved solids (TDS) in Chicot and Evangeline aquifer formations



the other hand, the Bayesian approach to hypothesis testing is more inferential in nature and a decision to accept or reject a particular hypothesis is not rigorously pursued. The two competing hypotheses are given equal preference and the evidence in favor of each hypothesis is compared only informally.

When comparing the water quality observations to a known standard or goal, the classical test indicates whether it can be inferred with certainty (at a specified significance level) that the observations are not the same as the specified standard. However, if the conclusion is that the difference is not substantial (i.e., cannot reject the null hypothesis that there is no difference between the observations and the standard), it cannot be inferred that there is no difference with the same level of certainty. It is also important to note that the specified significance level is an arbitrary specification that enters the classical analysis. The Bayesian approach on the other hand addresses the more practical question—given the data and any prior information, what is the probability of meeting the standard? The Bayesian approach does not require an arbitrary specification of the significance level for comparison. Thus, the classical approach is more useful in decision-making applications such as using water quality data to terminate remedial activities at a contaminated site, while the Bayesian approach is more useful in evaluative studies such as assessing the availability of suitable water supply sources.

Similarly, when comparing water quality between two entities (aquifer formations in this study), the classical approach emphasizes whether noted differ-

ences can be conclusively justified at an accepted significance level. The null hypothesis is stated as follows: “on average there is no difference between the two entities”—the classical statistics helps conclude if the differences are indeed significant (again at an arbitrarily specified significance level). If the null hypothesis cannot be rejected, it cannot be concluded with certainty that there is no difference between the two entities. The classical testing is only concerned with whether there is a significant difference between the two entities and typically does not quantify the nature of the differences that exist. The Bayesian approach on the other hand concerns itself with the nature of differences that exist. The decision whether the differences are significant or not is not part of the analysis and left to the interpretation of the decision-maker. From this standpoint, the Bayesian analysis can be argued to be less subjective than the classical approach. Again, the Bayesian interpretation of the probabilities and its emphasis on the nature of the differences makes it better suited for evaluative studies.

Summary and conclusions

The primary goal of this study was to demonstrate the applicability of Bayesian analysis techniques to assess water quality characteristics in a region. The Bayesian analysis based on the notion that probability is a measure of uncertainty is in contrast with the classical statistical theories that interpret probability as a mea-

sure of randomness which can be characterized by repeated measurements. Two types of water quality assessments were considered as part of this study: (1) comparing observed water quality characteristics against a water quality standard or a goal and (2) comparing observed water quality characteristics in two different entities of interest. The concepts of Bayesian analysis were illustrated to study two chemical constituents (chloride and TDS) measured in two different aquifer formations (Chicot and Evangeline) in the Gulf coast aquifer underlying Refugio County, TX.

The Bayesian interpretation of probability is based on the notion of making the best possible inference given a few measurements of these water quality parameters (Sivia 2003). Unlike conventional statistics, the Bayesian approach quantifies the probability of finding groundwater that exhibits concentration less than or equal to the prescribed goal. For the illustrative case study, the results indicated that the probability of finding groundwater with chloride concentrations less than or equal to 500 g/m³ or TDS concentrations less than or equal to 1,000 g/m³ was rather low in the more prolific Evangeline formation indicating the possible need for blending it with the groundwater from Chicot formation or other sources to obtain necessary water quality for municipal applications. The water quality characteristics between the Chicot and Evangeline formations were also assessed using Bayesian approaches. The results indicated that while the difference between the mean values of chloride was relatively high, there was very little difference between the observed mean values of TDS in the Evangeline formation. In the Bayesian approach, the competing hypotheses are given equal weights and focus is not making a decision in favor of one or the other. Rather, the evidence supporting each hypothesis is computed using any available prior information and collected data. Therefore, the Bayesian approach is better suited for evaluative water quality studies that aim to understand the differences between competing hypotheses.

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