Application of Generalized Least Squares Regression in Bottom-Hole Temperature Corrections

Calvin A. Whealton, Jery R. Stedinger, Franklin G. Horowotiz

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Abstract

Bottom-hole temperature (BHT) corrections are a subject of great interest to those interested in using non-equilibrium temperature data from well log headers. This article develops BHT corrections for New York, Pennsylvania, and West Virginia, using generalized least squares regression (GLS). It is shown that GLS regression can give more reasonable estimates of the BHT correction than traditional least squares when spatial clustering is present. Additionally, a nonlinear function for BHT corrections is proposed that explicitly avoids negative corrections at shallow depth and avoids the instabilities of extrapolated high-order polynomials.

1 Introduction

Bottom-hole temperature (BHT) corrections have been of continued interest for several decades because researchers want to use BHT datasets, which are often large and freely available; however, BHTs are notoriously problematic because they generally represent a temperature field that was disturbed by the drilling process (Deming, 1989). As a result, BHT corrections, both from theoretical models of the heat transfer in the well and from empirical comparison of data, have been developed.

This paper derives empirical BHT corrections for portions of New York, Pennsylvania, and West Virginia. The method of deriving the temperature correction dataset required spatial clustering of points, which meant that the alternatives to ordinary least squares fitting could be explored. Additionally, in part of the region there was available information on borehole fluid so separate models should be fit based on the expected drilling technology. Lastly,

we provide a functional form that avoids problems with the correction being negative at shallow depths or unstable in deeper data.

2 Literature Review

Empirical temperature corrections have generally been polynomials of depth. For instance, Kehle (1973) presents a quartic function of depth and the correction presented by Harrison et al. (1983) is often taken as a quadratic. Other examples include Förster et al. (1997) who report a linear function and Scott (1982) who presents linear to cubic polynomials.

Polynomials are typically well-behaved over the range of the data, but extrapolation of quadratic and higher-order models beyond the dataset can cause the BHT correction to become unstable: shallow trends can reverse. Another problem with polynomials is that the fitted equation is often negative at shallow depth, which is generally considered unreasonable because drilling should not substantially increase the temperature.

Several BHT corrections have been used in the area of interest (NY, PA, and WV). Hendry et al. (1982) did not correct BHTs in their study of West Virginia, Hodge et al. (1981) presented results for western NY with and without a BHT correction. Aguirre (2014) used the Harrison correction in her study of PA and western NY based on the work of Frone and Blackwell (2010), who evaluated the correction based on it generally moving the data closer to the Spicer (1964) wells. Frone and Blackwell (2010) recommended capping Harrison correction and using the peak value for deeper BHTs and Shope (2012) noticed that Harrison correction seemed less accurate than uncorrected BHTs for wells shallower than 1,000 m in NY and PA. No studies have tried to systematically look at the region to determine where the corrections are more or less accurate.

3 Regions, Data, and Clusters

The analysis uses data from New York, Pennsylvania, and West Virginia, mainly areas within the Appalachian Basin. Figure 1 shows the area and features discussed in this section. The region was partitioned into three areas based on data divisions and geologic features or the data sources. The first region was is the Rome Trough in PA, a rift (Shope, 2012), which curves from the south-west corner of PA towards northern PA (Repetski et al., 2008). The second region is the Allegheny Plateau, which is north of the Rome Trough and extends into western NY. West Virginia is considered as a

separate region because the data came from a separate source with different characteristics.

The data used for the Rome Trough and Allegheny Plateau are based on data collected for Whealton (2015). This dataset includes much of the information listed on well log headers including bottom-hole temperature (BHT), depth, and fluid recorded as in the borehole (Whealton, 2015). Data from West Virginia are from the National Geothermal Data System (NGDS) (Saucer, 2011).

All of the datasets contained raw BHTs, so the equilibrium temperature had to be estimated from "reliable" temperature logs. The Spicer (1964) temperature profiles are considered equilibrated because they are from wells drilled with older technology that does not disturb the temperature field as much (Frone and Blackwell, 2010). These were supplemented with temperature logs identified as close to equilibrium, mainly wells explicitly noted as air-drilled with at least several hundred meters of temperature log (Whealton, 2015). The Spicer wells were the only source of equilibrium profiles in West Virginia and were the majority of equilibrium profiles for the Allegheny Plateau. The equilibrium temperature profile was estimated for each "reliable" log by a linear gradient, which was estimated after removing temperature inversions and shallow portions of the log that did not appear to follow the same trends as the deeper well log.

The estimated equilibrium wells were used to define spatial clusters. In West Virginia, the clusters were defined by taking a 0.05°buffer around each of the Spicer wells, therefore a single BHT could be in multiple clusters. The West Virginia clusters are also almost exclusively defined in the Rome Trough portion of the state (see Figure 1). In the Rome Trough and Allegheny Plateau clusters are defined based on averaging two or more reliable temperature profiles and then taking BHTs close to the averaged wells, but without crossing the boundary of the regions. In this scheme a BHT can only belong to a single cluster.

The regression datasets are defined by taking all BHTs and correcting them to the estimated equilibrium temperature-at-depth for that cluster. This assumes that over small areal extents the equilibrium temperature at depth does not change significantly. The depth used in the Allegheny Plateau and Rome Trough was the minimum of the depth of the driller, depth of the logger, and bottom logged interval as reported on the well log header because the depth of the BHT measurement is generally not recorded. A few points were assigned a different depth because the BHT seemed consistent with much deeper data from that cluster and the unusual values could be attributed to incorrectly entered data for one of the depths. In West Virginia, the depth of the measurement was used, when possible, otherwise the true

vertical depth was used.

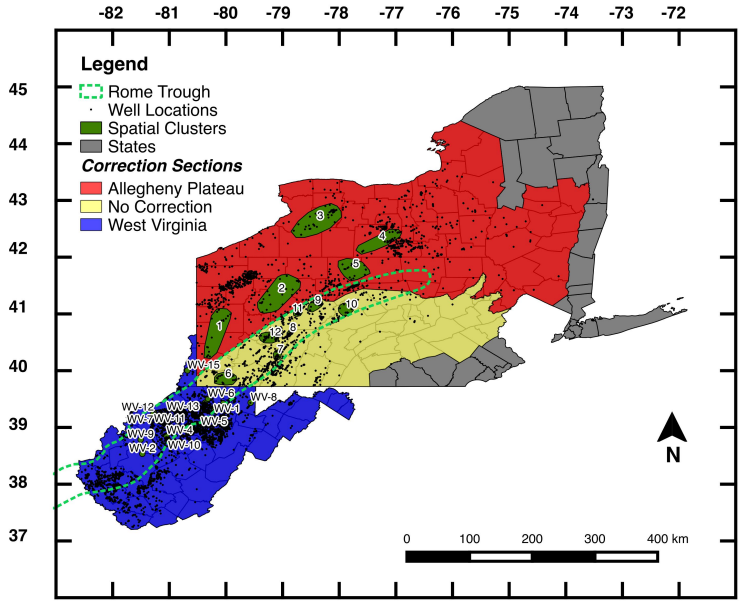

Figure 1: Map of NY, PA, and WV with the Rome Trough (Repetski et al., 2008) and spatial clusters used in analysis. Data sources:Bureau (2014),Saucer (2011); software: QGIS Development Team (2009)

4 Definition of Drilling Types

The data collected by Whealton (2015) included information on the fluid recorded in the borehole, which we used as a proxy for the well's drilling technology. The main categorization is into air-wells versus mud-wells. The classification scheme defined air-wells as those where the fluid listed on the well log header was air, gas, foam, soap, dusted, dry, or some combination of those. Mud-wells are classified as containing mud, gel, polymer, water (fresh, salt, brine), formation fluid, produced fluid, or some combination of those fluids. The categorization is defined to try and separate fluids that have mostly air in the borehole from those where water or other high heat capacity fluid is present. Additionally, some wells could not be categorized because no fluid was recorded or the fluid listed was empty or none.

The West Virginia dataset does not contain information on the type of fluid present in the borehole (Saucer, 2011).

5 Regression Statistical Models

Least squares regression assumes that the error (residual, difference in true and predicted BHT correction) are independent and identically distributed with zero mean. If the dataset contained paired data where each BHT is matched to an equilibrium temperature from the same well at the same depth, such as a drill-stem test, then this assumption might be valid. This assumption is also likely valid when all points are corrected to a region-wide estimate of the temperature-at-depth.

Because of spatial clustering, it is likely that all observations from a given cluster will be too high or too low relative to the region-wide average. Hence, observations in a cluster are "biased" on average. One possible reason for the differences is that drilling practices vary enough in the clusters so that there are systematic differences. Another potential cause is that the estimated equilibrium temperature for the clusters was imperfect, so errors in the estimation and extrapolation of equilibrium temperature could cause systematic tendencies for a cluster. Many of the well logs used to estimate equilibrium temperature were offset from each other but showed roughly the same gradient.

With clustering, the error between an observation and the region-wide model has two components: a cluster-specific "bias" and a random noise term. The cluster-specific "bias" represents how the points in a cluster are systematically different from the region-wide model. Several statistical models could be used to address the cluster-specific "biases" including using least-squares coefficient estimates with cluster-robust standard errors, least squares estimation of a model with cluster-specific constants and use of an average constant, and feasible generalized least squares. More details on these approaches can be found in an Econometrics text, such as Greene (2012, Ch. 11) or Kmenta (1986, Ch. 12), under methods used for panel data. The method used here is generalized least squares (GLS) which should increase efficiency for small datasets.

In GLS the goal is not to minimize the simple sum of squares errors, as in least squares regression, but to weight observations in a way that accounts for shared "bias" and their inherent noise. More details are provided in Appendix A. If the cluster "biases" are fairly small compared to the noise in the data, then the result will look very similar to a least squares fit and the fitting procedure will tend to treat the points as fairly independent; however, when the "biases" are large compared to the noise, each cluster is nearly treated as a separate point because additional points in a single cluster are highly discounted when fitting the model.

6 Regression Results

The regression results are reported for each of the three separate regions defined above. The fitted models for each region are summarized in Table 1. All depths are in meters and all BHT corrections are in °C.

6.1 West Virginia

West Virginia dataset included 187 points and did not have information on drilling fluid, so the comparison is between fitting a linear model (first-order function of depth) with least squares versus generalized least squares. Figure 2 shows the data and fitted lines and Table 1 shows the fitted coefficients. The models differ by minor amounts over the range of the data. Because the GLS model should be more efficient, it is recommended as the base model (Equation 1) but the temperature correction should be capped at 15°C (2,606 m). Although the regression dataset does not contain data to this depth, some alternative datasets that contained deeper observations did indicate corrections of about 15 °C. Generally, data used in studies is deeper than the depth at which the temperature correction becomes positive (305 m), so practically it is positive over the range of interest.

$$\Delta T_{West\ VA} = -1.99 + 0.00652z, \qquad 305\text{m} < z < 2606\text{m} \tag{1}$$

6.2 Rome Trough of PA

The Pennsylvania Rome Trough dataset had 181 points. Regressions are plotted in Figure 3. The results do not conform to the expected model of BHT corrections, which is positive and increasing with depth. This behavior was regardless of the fitting procedure or whether the data was split based on fluid. Because of the lack of a credible model for this region the conservative approach is to apply no temperature correction. This recognizes that our knowledge of this region is not sufficient to justify any correction.

$$\Delta T_{Rome\ Tr.} = 0, \qquad z > 0\text{m} \tag{2}$$

6.3 Allegheny Plateau

The Allegheny Plateau dataset of 121 points has some of the largest signal in all of the data analyzed, as can be seen in Figure 4. When a linear depth model was fit to the data the correction was negative until about 1,100 m.

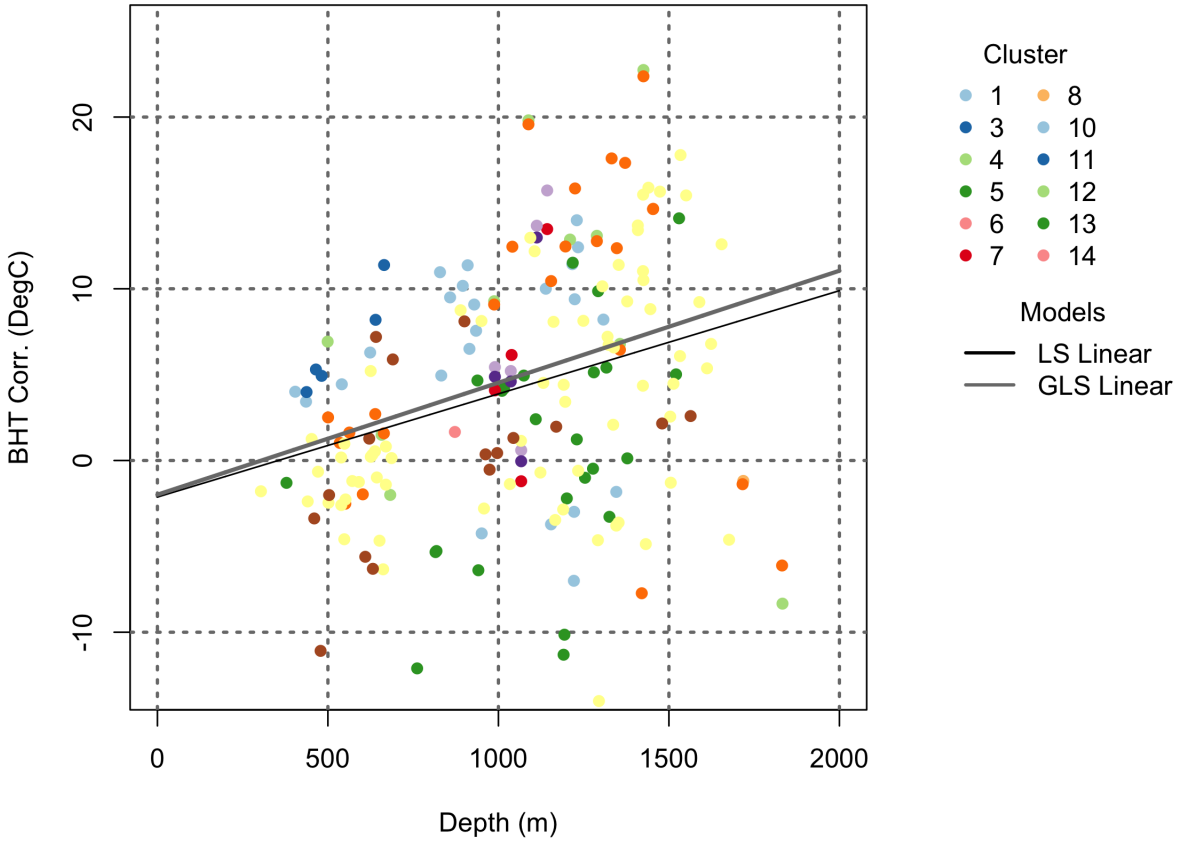

Figure 2: Plot of West Virginia data with ordinary least squares (OLS) and generalized least squares (GLS) fits for a linear model. Points are color-coded based on the cluster definition, which is based on spatial buffering of the Spicer wells. The Spicer well number is used as the identification of the cluster.

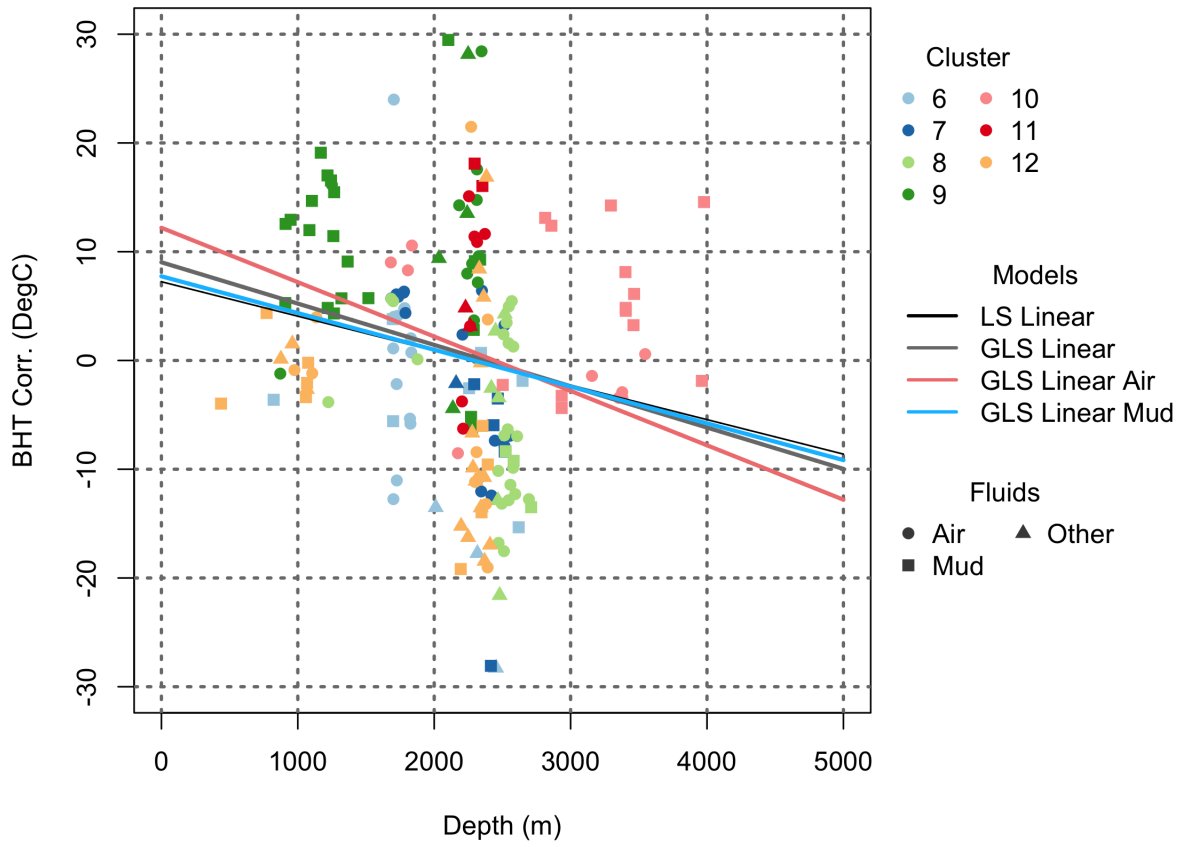

Figure 3: Plot of Rome Trough data with ordinary least squares (OLS) and generalized least squares (GLS) fits for a linear model and GLS fits for the air and mud wells. Points are color-coded based on the cluster definition in Figure 1.

There is little reason to believe in negative BHT corrections and it was more an artifact of the model, so a model of the form shown in Equation 3 was fit since it is always positive (if the initial coefficient is positive) and it behaves linearly for large depths. The curved transition zone is controlled by the exponent in the model. An exponent of 3 was used because it sufficiently matched the curvature of the data and it was conservative on the very shallow temperature corrections.

There are alternative models that could have been fit to the data. For example, the exponent parameter could be be set to a different value. This was experimented with a little when fitting the mud model and the impact

was minor. The weighted sum of squares changes from 64.1 to 66.5 when changing the exponent from 2 to 5, and the predicted correction at 4000 m changes from 38.9 to 36.8 °C. Another possibility is to include an additive constant so that the correction will not cross at the origin. When this was included it was about 5 °C and this would likely cause arbitrary signals to appear in shallow counties, so it was not included. Lastly, a limiting case of the model is for the exponential parameter being infinite, which will be a model that is zero until it reaches a threshold depth and increases linearly after that. This form has a kink in the middle which causes problems with local minima when fitting the parameters and seems less physically plausible.

The nonlinear model showed that it was sensitive to the locations of points for the air-model. Inclusion or exclusion of points, especially in the curved portion of the function, could cause the fitted model to changed from that shown in Figure 4 to one where the correction is nearly linear starting at a few hundred meters. We chose the dataset that had more points to help define the transition region because this was a larger sample and the results were more consistent with the physical intuition of the the relationship between air and mud BHT corrections.

The models for different drilling fluids showed that there was no statistically significant difference (test statistic of 0.49 on χ^2 with two degrees of freedom, p-value of $0.78 \gg 0.05$). One explanation for the lack if difference is that the air-model is not well controlled in the upper linear portion of the curve; the standard error of the slope parameter is over twice as large for the air model as it is for the mud-model. The air model is only supported for depth shallower than approximately 2,500 m whereas the mud model has data much deeper. Note: the highest air data (around 2700 m, 38 °C) was removed from fitting in all air-models because it was a rogue observation.

The recommended models for this area is the the air- or mud-model (Equations 3 and 4), as applicable when the drilling fluid is known, or a weighted sum of the air- and mud-models when the fluid is unknown. The air and mud corrections should be capped at 15.4 and 37.8 °C, respectively. For unknown wells, the weighting should represent the probability that the well is air or mud.

$$\Delta T_{Alle.\ Pt.\ Air} = 0.0104((1090^3 + z^3)^{1/3} - 1090), \qquad z < 2500\text{m} \qquad (3)$$

$$\Delta T_{Alle.\ Pt.\ Mud} = 0.0155((1660^3 + z^3)^{1/3} - 1660), \qquad z < 4000\text{m} \qquad (4)$$

Although the coefficients seem very similar, the standard errors using GLS are quite different. For instance, in the Allegheny Plateau fit using least

squares the standard error of the slope and shift parameter are 0.00412 and 340, respectively. The GLS estimates of the standard errors for the two parameters are 0.00324 and 1710. Generally, the least squares estimated of the coefficient standard errors are much smaller because the estimates are based on the data being independent and it does not discount observations from the same cluster.

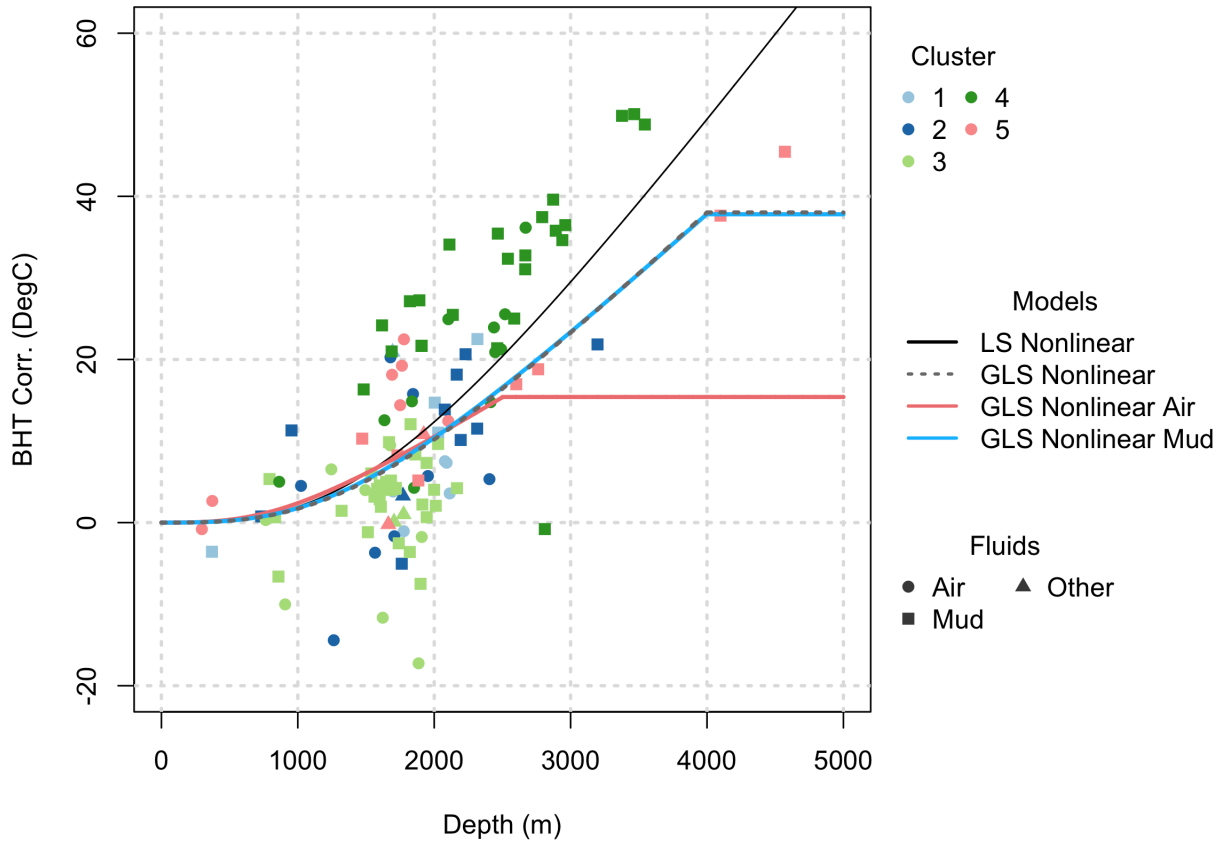

Figure 4: Plot of Allegheny Plateau data (121 points) with least squares (OLS) and generalized least squares (GLS) fits for a nonlinear model and GLS fits for the nonlinear air and mud wells. Points are color-coded based on the cluster definition in Figure 1. The GLS model is nearly hidden by the GLS mud model because their parameters are very close (see Table 1).

Table 1: Summary of fitted models. Selected models for each region are denoted with '*'. Statistically significant coefficients at the 5%-level based on two-sided tests are in bold. GLS, OLS, and LS stand for generalized least squares, ordinary least squares, and least squares respectively. The measure of fit, $\widehat{\mathrm{R}^2}$ is defined in Equation 12. All depths, z, are in meters and all temperature corrections are in °C.

Model	ΔT Equation	$\widehat{\mathrm{R}^2}$
West Virginia		
OLS Linear	$-2.13 + \mathbf{0.00601}z$	0.09
GLS Linear*	$-1.99 + \mathbf{0.00652}z$	0.08
Rome Trough		
OLS Linear	$\mathbf{7.24} - \mathbf{0.00317}z$	0.04
GLS Linear	$\mathbf{9.03} - \mathbf{0.00380}z$	0.03
GLS Linear Air	$\mathbf{12.2} - \mathbf{0.00500}z$	0.05
GLS Linear Mud	$\mathbf{7.74} - \mathbf{0.00338}z$	0.0
Used*	0	
Allegheny Plateau		
LS Nonlinear	$\mathbf{0.0221}\left(\left(\mathbf{1900}^3 + z^3\right)^{1/3} - \mathbf{1900}\right)$	0.55
GLS Nonlinear	$\mathbf{0.0159}\left(\left(\mathbf{1710}^3 + z^3\right)^{1/3} - \mathbf{1710}\right)$	0.50
GLS Nonlinear Air*	$0.0104\left((1090^3 + z^3)^{1/3} - 1090\right)$	0.25
GLS Nonlinear Mud*	$\mathbf{0.0155}\left(\left(\mathbf{1660}^3 + z^3\right)^{1/3} - \mathbf{1660}\right)$	0.52

7 Conclusions

This paper derived BHT corrections for NY, PA, and WV using alternative methods to traditional least squares regression. The benefits of using GLS methods with spatial clusters are present were clearly shown in the Allegheny Plateau, where a traditional fitting technique would cause the estimated BHT corrections to be much higher because it did not recognize that the data were drawn from a few clusters and instead treated all observations equally. In the Rome Trough of PA there is not sufficient understanding of the system generate a BHT correction. In neither the Rome Trough of PA nor the Allegheny Plateau were the differences in drilling fluid statistically significant, but because the air data was over a much more limited interval in the Allegheny Plateau the air-model could not be extrapolated to the depth of the mud wells. In WV, the impact of clusters did not change the fitted model much and the data looks consistent with a linear model.

8 Acknowledgments

Cornell University's Energy Institute and Southern Methodist University's Geothermal Laboratory for providing data. Code used to estimate the models is available at https://github.com/calvinwhealton/Bottom-HoleTemps. Data used in the analysis is available from the corresponding author upon request.

A GLS Estimation and Definition of Statistics

The first step in generalized least squares is estimation of the data covariance matrix. This is done with a model where there was a constant for each cluster c, as shown in Equation 5, where ΔT is the temperature correction, $f(.,.)$ is a function of dependent variables $\underline{x}$ and parameters $\underline{\beta}$, υ_c is cluster-specific constant, ε is the error term, and subscript i is for the observation.

$$\Delta T_i = f\left(\underline{x}_i, \underline{\beta}\right) + \upsilon_c + \varepsilon_i \tag{5}$$

From this model the variance of the cluster-specific "bias" and the variance of the noise term must both be estimated, as shown in Equations 6 and 7, respectively. In these equations, the true parameters υ and ε from Equation 5 were substituted with u and e, respectively, to show that the fitted model only gave estimates of the true parameters. These equations assume at all of the clusters will be equally noisy (homoscedastic) (Greene, 2012, Sec. 11.6.2). Although this assumption could be changed so that a separate value of s_e is estimated for each cluster, many clusters have 10 to 20 points and estimates of variances on such small samples are themselves quite variable.

$$s_u^2 = \frac{1}{C}\sum_{c=1}^{C}\left(u_c - \bar{u}\right)^2 \tag{6}$$

$$s_e^2 = \frac{1}{n}\sum_{i=1}^{n} e_i^2 \tag{7}$$

Next, the data covariance matrix for an individual cluster c can be constructed as shown in Equation 8, which will have off-diagonal elements of s_u^2 and on-diagonal elements $s_e^2 + s_u^2$ (Greene, 2012, Sec. 11.5, Eq. 11-31).

$$\mathbf{S}_c = s_e^2\mathbf{I} + s_u^2\underline{1}\ \underline{1}' \tag{8}$$

Lastly, the data covariance matrix of the entire dataset can be constructed as shown in Equation 9 (Greene, 2012, Sec. 11.5, Eq. 11-32). This is essentially a matrix of matrices with the on-diagonal matrices being the estimated data covariance structure of a given cluster. The off-diagonal matrices are zero because these observations are from separate clusters and should be uncorrelated on average, hence there is no covariance structure to this portion of the dataset.

$$\mathbf{S} = \begin{bmatrix} \mathbf{S}_1 & \mathbf{0} & \cdots \\ \mathbf{0} & \mathbf{S}_2 & \\ \vdots & & \ddots \end{bmatrix} \tag{9}$$

Now that the covariance structure of the data is estimated, the model can be fit by minimizing the "weighted" sum of squared errors. Weighted is used loosely because it employs a diagonal data covariance matrix whereas this problem has a matrix with on- and off-diagonal elements that are non-zero. Therefore, this procedure is called generalized least squares to differentiate it from weighted least squares. The problem formulation is shown in Equation 10, where the estimated model parameters are $\underline{b}$ and $\underline{e}$ is an n-by-1 vector of estimated residuals. The result is a single value, which was minimized using an optimization software (R Core Team, 2012, 'optim').

$$\underline{b} = \min_{\underline{\beta}} \underline{e}' \mathbf{S}^{-1} \underline{e} \tag{10}$$

When separate drilling fluids were considered, Equation 5 included separate predictors for each fluid but the cluster constants were the same for both fluids. The assumption is that the "bias" in a cluster is for the individual cluster and it should not depend on the type of fluid present. In the fitting of the final model the data covariance matrix was partitioned based on the drilling fluid and the model was fit to each fluid one at a time.

The model parameter covariance matrix is estimated using Equation 11. This is based on the second-order terms of a Taylor Series expansion of the objective function about the solution. The square root of the diagonal elements of this matrix represent the standard error of parameters.

$$\text{Var}\left(\underline{b}\right) = \left[\left(\frac{\partial f(\mathbf{X})}{\partial \underline{b}} \right)' \mathbf{S}^{-1} \left(\frac{\partial f(\mathbf{X})}{\partial \underline{b}} \right) \right]^{-1} \tag{11}$$

The measure of fit used in this analysis is a pseudo R^2, referred to as $\widehat{R^2}$ and defined in Equation 12, where SSE and SST are the sum of squares error (sum of squared residuals from regression) and sum of squares total in the real, un-weighted space. The regression procedure will not maximize this

metric because least squares estimates minimize SSE, and for generalized least squares this value is not bounded on [0,1] unlike traditional R^2.

$$\widehat{R^2} = 1 - \frac{SSE}{SST} \tag{12}$$

Throughout the analysis normal and χ^2 approximations, which are technically accurate only for large (asymptotic) samples, will be used when testing hypotheses and reporting p-values. The reason is that the simple degrees of freedom adjustments in linear ordinary least squares regression problem are not easily defined and the parameter covariance structure of the nonlinear models are only approximate.

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