

Digital Spatial Data for Observed, Predicted, and Misclassification Errors for Observations in the Training Dataset for Nitrate and Arsenic Concentrations in Basin-Fill Aquifers in the Southwest Principal Aquifers Study Area

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Abstract

This product “Digital spatial data for observed, predicted, and misclassification errors for observations in the training dataset for nitrate and arsenic concentrations in basin-fill aquifers in the Southwest Principal Aquifers study area” is a 1:250,000-scale point spatial dataset developed as part of a regional Southwest Principal Aquifers (SWPA) study (Anning and others, 2012). The study examined the vulnerability of basin-fill aquifers in the southwestern United States to nitrate contamination and arsenic enrichment. Statistical models were developed by using the random forest classifier algorithm to predict concentrations of nitrate and arsenic across a model grid that represents local- and basin-scale measures of source, aquifer susceptibility, and geochemical conditions.

Background

This dataset was developed as part of a regional Southwest Principal Aquifers (SWPA) study and for the National Water-Quality Assessment (NAWQA) Program. The dataset represents observed nitrate and arsenic concentrations that were used to train the confirmatory and prediction classifiers.

Development of Classifiers

Separate classifiers were developed for nitrate and arsenic because each constituent was expected to be affected by a different set of factors, and each factor could have a different magnitude or directional influence (increase/decrease) on concentration. For each constituent, two different classifiers were developed: a prediction classifier and a confirmatory classifier. The prediction classifiers were developed specifically to predict nitrate and arsenic concentrations in basin-fill aquifers across the SWPA study area and were based on explanatory variables representing source and susceptibility conditions. These explanatory variables were available throughout the entire SWPA study area and, therefore, did not pose a limitation for using the classifiers to predict concentrations.

The confirmatory classifiers were developed to supplement the prediction classifiers in the evaluation of the conceptual model. The name, “confirmatory,” reflects the classifier’s purpose for evaluation of a-priori hypotheses and contrasts other general types of statistical models, such as those used for prediction or exploratory purposes. The confirmatory classifiers included the explanatory variables used in the prediction classifiers, as well as additional variables representing geochemical conditions and basin groundwater budget components. The inclusion of the geochemical and basin groundwater budget variables in the confirmatory classifiers allowed for further evaluation of the conceptual models, which was not possible with the prediction classifiers alone. The geochemical data, however, were only available at specific well locations, and consistent water-budget data were not available for every basin in the study area. The limited availability of the data for these variables constrained the confirmatory classifiers to observations from 16 case-study basins and precluded use of the confirmatory classifier for predicting concentrations across the SWPA study area. To contrast the scope of the two classifiers, the confirmatory classifiers were developed by using all available explanatory variables but with observations restricted to the 16 case-study basins, whereas the prediction classifiers were unrestricted with respect to spatial extent because these were developed by using a subset of the explanatory variables that were available throughout the study area.

Supplemental Information

The nitrate and arsenic observations, predictions, and misclassification error data for observations are part of a larger dataset of explanatory variables and model input data. Those data are archived in tabular form along with the model report. The explanatory data may be joined to this dataset via the site identifier. For more information on the development of the explanatory variables, see “Compilation and Processing of Explanatory Variables” in the “Approach and Methods” section of Anning and others (2012).

The digital dataset can be downloaded from the USGS at http://water.usgs.gov/lookup/getspatial?ds2012-697_SWPA_NO3_As_training

References Cited

Anning, D.W., Paul, A.P., McKinney, T.S., Huntington, J.M., Bexfield, L.M., and Thiros, S.A., 2012, Predicted nitrate and arsenic concentrations in basin-fill aquifers of the southwestern United States: U.S. Geological Survey Scientific Investigations Report 2012–5065, 78 p. Available at <http://pubs.usgs.gov/sir/2012/5065>.

