A machine learning approach for prioritizing groundwater testing for per-and polyfluoroalkyl substances (PFAS)

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Abstract

Regulatory agencies are beginning to recognize per-and polyfluoroalkyl substances (PFAS) as concerning and bioaccumulative compounds of which the use and environmental burden must be reduced. In the specific context of groundwater management, testing and mitigation strategies are desirable but can be time and cost-intensive processes. As a result, only a fraction of all groundwater wells has had testing performed to determine the abundance of PFAS compounds. In this study, we build machine learning models based on real-world groundwater databases from California to accurately predict PFAS levels in the absence of testing. We project that this machine learning model can predict individual PFAS compound abundances with and R^2 of 0.72. It can also predict groundwater wells likely to have concerningly high overall levels of PFAS with an accuracy of 91% and an AUC of 0.93. We propose a new regulatory paradigm in which prioritization of PFAS testing in groundwater wells can be supported by such a machine learning approach. Additionally, we believe this approach may have widespread applicability for other hazardous anthropogenic compounds in groundwater.

Introduction:

Per-and poly- fluoroalkyl substances (PFAS) are a class of water-soluble anthropogenic contaminants of increasing global concern due to their ubiquity in the global environment, persistence, and toxicity. Management of PFAS contamination in water resources requires cross-cutting approaches in multiple industries, from management of solid and liquid wastes to monitoring and regulation of industrial operations and drinking water. PFAS have been used extensively in many industrial products including textile coatings, surfactants, pesticides, food contact materials, and fire-fighting foams since the mid-20th century (Prevedouros et al., 2006; Wang et al., 2017). The primary source of PFAS to the environment is estimated to be industrial emissions (Prevedouros et al., 2006), however, PFAS are also known to be formed as the result of breakdown of "precursor" compounds such as fluorotelomer alcohols and perfluoroalkyl sulfonamido alcohols (Fasano et al., 2006; Martin et al., 2006, 2005). Many studies have shown that PFAS compounds persist in the environment, bioaccumulate, and are toxic (Conder et al., 2008; Frömel and Knepper, 2010; Parsons et al., 2008; Young and Mabury, 2010). PFAS have been detected throughout the global environment, biota, and humans (Giesy and Kannan, 2001; Rayne and Forest, 2009; Vestergren and Cousins, 2009). Studies have linked several PFAS

including perfluorooctanonate (PFOA) and perfluorooctane sulfonate (PFOS) with adverse effects on environmental and human health including decreased birth weight and increased incidence of liver, pancreas and testicular tumors (Biege et al., 2001). The primary pathways of human exposure to PFAS is include diet, indoor environments polluted with PFAS, and drinking water (Domingo and Nadal, 2019; Sjogren et al., 2016; Vestergren and Cousins, 2009). Blood serum PFAS has been shown to be positively related to drinking water PFAS concentration (Ericson et al., 2008; Kannan et al., 2004; Xu et al., 2020).

In California, which is the focus of this study, approximately 40 percent of drinking water is supplied by groundwater wells; in drought years, up to 60% of drinking water is sourced from groundwater (Carle, 2015). Between 2013-2015, six PFAS contaminants were systematically sampled in drinking water in the United States for the first time as part of the Third Unregulated Monitoring Rule, or UCMR3 Report; this study showed widespread PFAS contamination at concerning concentrations in drinking water sources (Crone et al., 2019; US EPA, n.d.). Given the region's reliance on groundwater and the known susceptibility of groundwater to PFAS contamination, the California State Water Resources Control Board began issuing investigative orders in 2019 targeting high-risk drinking water systems and known potential source sites (State Water Resources Control Board, 2020). Results of these analyses have been publicly shared on the Groundwater Ambient Monitoring and Assessment (GAMA) database, which, in addition to this new PFAS data, hosts more than 20 years of groundwater chemical monitoring data for more than 200 analytes for public supply, drinking water, and environmental monitoring groundwater wells across the State of California.

Both in the State of California, and globally, current frameworks for prioritizing drinking water testing for PFAS are poorly suited to identifying contamination in areas not directly adjacent to

known source industries and facilities; furthermore, representative sampling of the more than one million groundwater wells in California, particularly private wells, will take years. This study applies supervised machine learning to identify high-risk groundwater wells for elevated PFAS concentration using co-contaminant fingerprints, with the goal of identifying high-risk areas to be prioritized for sampling. The hypotheses driving this investigation are (1) that anthropogenic contaminants, including PFAS, follow consistent patterns in the environment both in terms of patterns of release from source areas and transport/transformation over time (Alimi et al., 2003; Barrett et al., 1999; Douglas et al., 2007; Stout et al., 1998) and (2) these consistent patterns can be leveraged to predict accurately the risk that PFAS will exceed regulatory thresholds using supervised machine learning.

Materials and Methods

Generation and curation of dataset

Data was downloaded from Geotracker Groundwater Ambient Monitoring and Assessment (GAMA) database (https://gamagroundwater.waterboards.ca.gov/gama/gamamap/public/Default.asp). The GAMA Program is California's comprehensive groundwater quality monitoring program that was created by the State Water Resources Control Board (State Water Board) in 2000. It was later expanded by Assembly Bill 599–the Groundwater Quality Monitoring Act of 2001–requiring the State Water Board to assess groundwater quality in basins that account for 95% of the state's groundwater use. This system provides access to approximately 87 million analytical results from over 290,000 wells in California for more than 200 analytes. This dataset was leniently filtered based on duplicate wells and wells with extremely high data missingness to a set of 189,208 wells across 196 analytes (approximately 5.5% of the values of this dataset are not

missing). This data was normalized using a log10(analyte in parts per trillion+1) transformation. It was then combined with geospatial data including latitude, longitude, and metadata about the well itself. The characteristics of the PFAS subcomponent of the data are summarized in **Table 1** below and in for the rest of the chemicals in **Table S1**.

	number of measurements	mean	standard deviation	min	25%	50%	75%	max
PFPA	90	1.81	0.99	0.41	1.02	1.62	2.43	4.51
PFOS	502	1.19	0.6	0.01	0.72	1.15	1.51	3.78
PFHA	409	1.08	0.72	0	0.66	0.86	1.26	4.41
PFPES	50	1.52	1.05	0.45	0.68	1.34	1.86	4.66
PFNA	160	0.83	0.58	0	0.54	0.65	0.86	4.28
PFNDCA	59	0.77	0.44	0	0.52	0.62	0.86	2.3
PFHPA	308	0.93	0.67	0	0.56	0.72	1.02	4.69
PFHXSA	526	1.04	0.61	0.29	0.66	0.9	1.19	4.84
6:2FTS	33	2.16	0.99	0.3	1.51	2.24	2.73	4.08
PFOA	466	1.11	0.66	0	0.69	1.04	1.32	4.78
PFBSA	412	0.99	0.52	0.28	0.65	0.89	1.16	4.6
PFBTA	71	1.49	0.72	0.46	0.96	1.34	1.95	3.51

Table 1: Summary of PFAS measurements in dataset. Values are based on a log10(PFAS compound in part per trillion+1) scale.

Estimating correlation structure between features in GAMA dataset

In order to understand the overall correlation structure between geospatial and chemical measurements in this groundwater dataset, we computed the pairwise correlation matrix between all quantitative features present across all wells for each pair of features that had at least five wells in which both were measured. The Pearson correlation measure was used to obtain this result.

Imputation training, ML training, and testing split and cross-validation

In order to evaluate the performance of a machine learning approach to predict PFAS levels, data was split into three separate subcomponents. The first component (imputation training set) was used to train either the kNN imputer or a custom imputer we developed. The second component (machine learning training set) was used to take the imputed results and train a machine learning model. The third component (testing set) was used to evaluate the machine learning model. In both the second and third components all PFAS measurements were masked and the ability of the machine learning model to recover the known PFAS value was evaluated. Each component is performed via random sampling without replacement from the previous component.

In order to obtain estimates of the robustness of the machine learning model's performance, Monte Carlo cross-validation was performed in which the three splits of the data described above were repeatedly constructed and model performance reevaluated. We repeated the steps 20 times for each model to obtain the estimates.

kNN Imputation

kNN imputation is a method for filling in missing data by using the mean of the relevant values from a fixed number of nearest neighbors. The *sklearn.impute.KNNImputer* method in Python was used to perform kNN for this study with the number of neighbors set to 10. The Euclidean distance metric was used to evaluate nearest neighbors. After fitting the imputer on the first subcomponent of the split data, it was applied to both the second and third subcomponents with their PFAS levels masked.

Kernel based Random Forest Imputation

In our custom imputation framework, the overall similarity of a given well to other wells was determined using a pairwise correlation matrix. This similarity score alongside the original chemical measurements was used to train a Random Forest Regressor on the machine learning training set. The *sklearn.ensemble.RandomForestRegressor* method in Python was used to perform Random Forest Regressor with the number of estimators set to 1000. The performance of the Random Forest Regressor was evaluated on the testing set.

Results:

We sought to leverage the public datasets available through the California GAMA system as described in **Methods**, to build a machine learning approach that could predict groundwater wells that would be most likely to contain high PFAS levels (**Figure 1**). The machine learning model would predict known PFAS measurements given other chemical measurements (i.e. potential co-contaminants of PFAS) (**Supplementary Table 1**) and geospatial data (latitude, longitude). This machine learning model can then be applied to wells in which PFAS levels have not been measured in order to make predictions of what the expected PFAS level would be (**Figure 1E**).

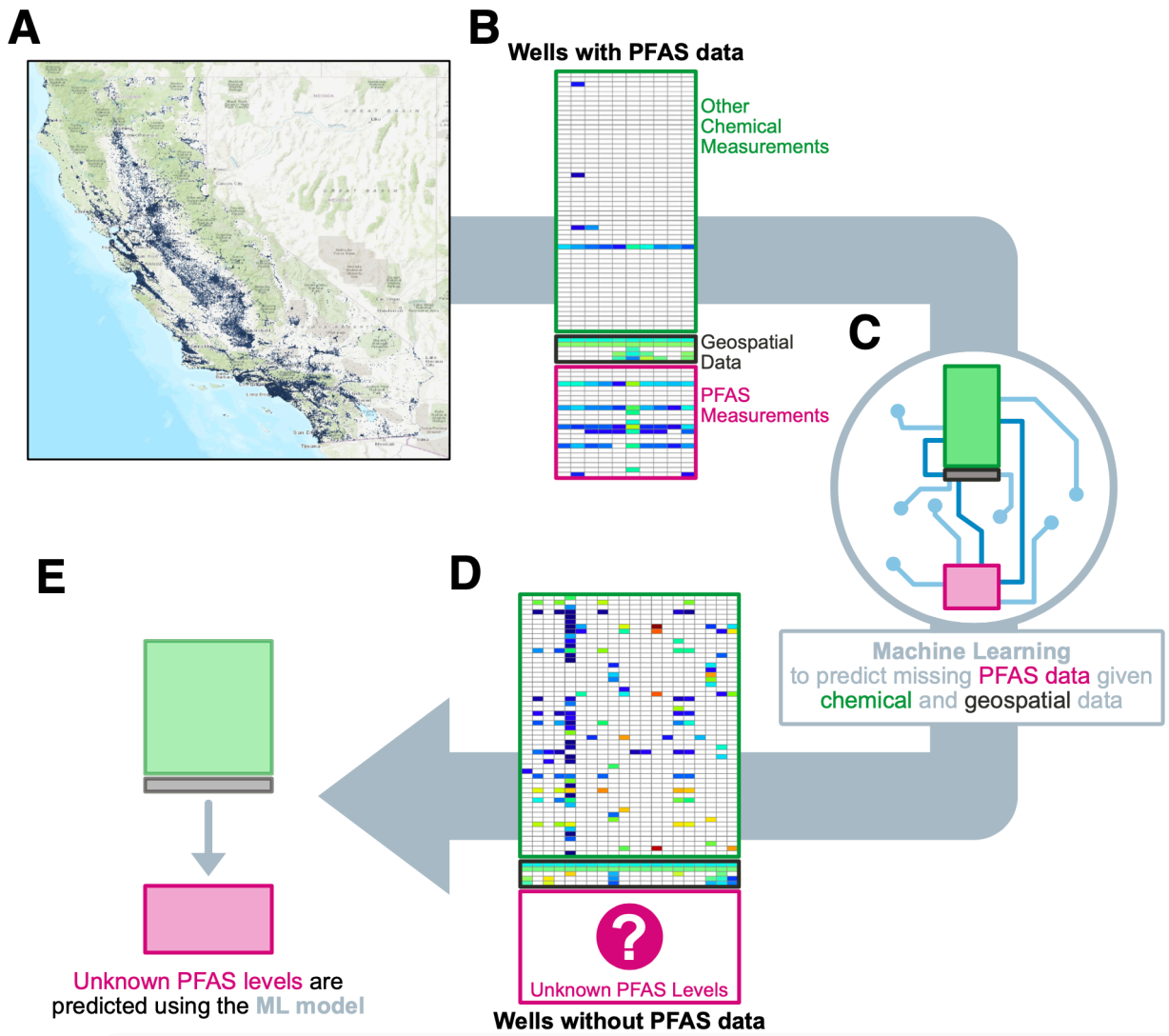

Figure 1. An overview of a machine learning approach to enable proactive water resource management for PFAS

(**a**) Visualization of the location of each of the 189,208 groundwater wells in the State of California that were used as part of this study (**b**) Visualization of the chemical (outlined in green), geospatial data (outlined in black), and PFAS measurements (outlined in pink) included in the California groundwater dataset. Columns corresponded to different wells and rows correspond to different measurements. White entries correspond to missing data. (**c**) A machine learning approach is used to predict PFAS data (pink) given other chemical (green) and geospatial data (black) (**d**) This

machine learning model can then be applied to predict unknown PFAS levels in wells with no PFAS testing performed (**e**) this results in predicted PFAS levels that can be used to prioritize testing.

PFAS measurements in our curated dataset were distributed throughout the State of California (**Figure 2A**). A particular challenge in this, and other similar datasets, is that very few wells have been tested across every possible analyte. In the entire dataset, only 5.5% of chemical measurements across all possible analytes and all possible wells have been tested. A naïve solution to handling this level of missing data would be to focus on a subset of analytes and wells in which the data is relatively complete. However, this would discard a tremendous resource associated with rich correlation structure associated with co-contaminants in this dataset (**Supplementary Figure S1**). In particular, PFAS compounds themselves have extremely strong co-contaminant profiles in this dataset supported primarily by strong positive correlations between compounds such as PFOA and PFOS. Negative correlations are rare and supported by few common data points such as the relationship between PFOA and ADONA (**Figure 2B**). PFAS values are strongly right-tailed (meaning that there a small number of values with extremely high analyte values (ex: PFOA); when the geometric mean PFAS values for a given well is taken, the distribution is closer to normally distributed (**Figure 2C**). There are many non-PFAS analytes/features with notably positive or negative correlations with the PFAS values including Latitude (negatively correlated) and antimony (positively correlated) (**Figure 2D**). Correlations such as these form the basis for which a machine learning model can learn to extrapolate PFAS measurements in the absence of their direct measurement.

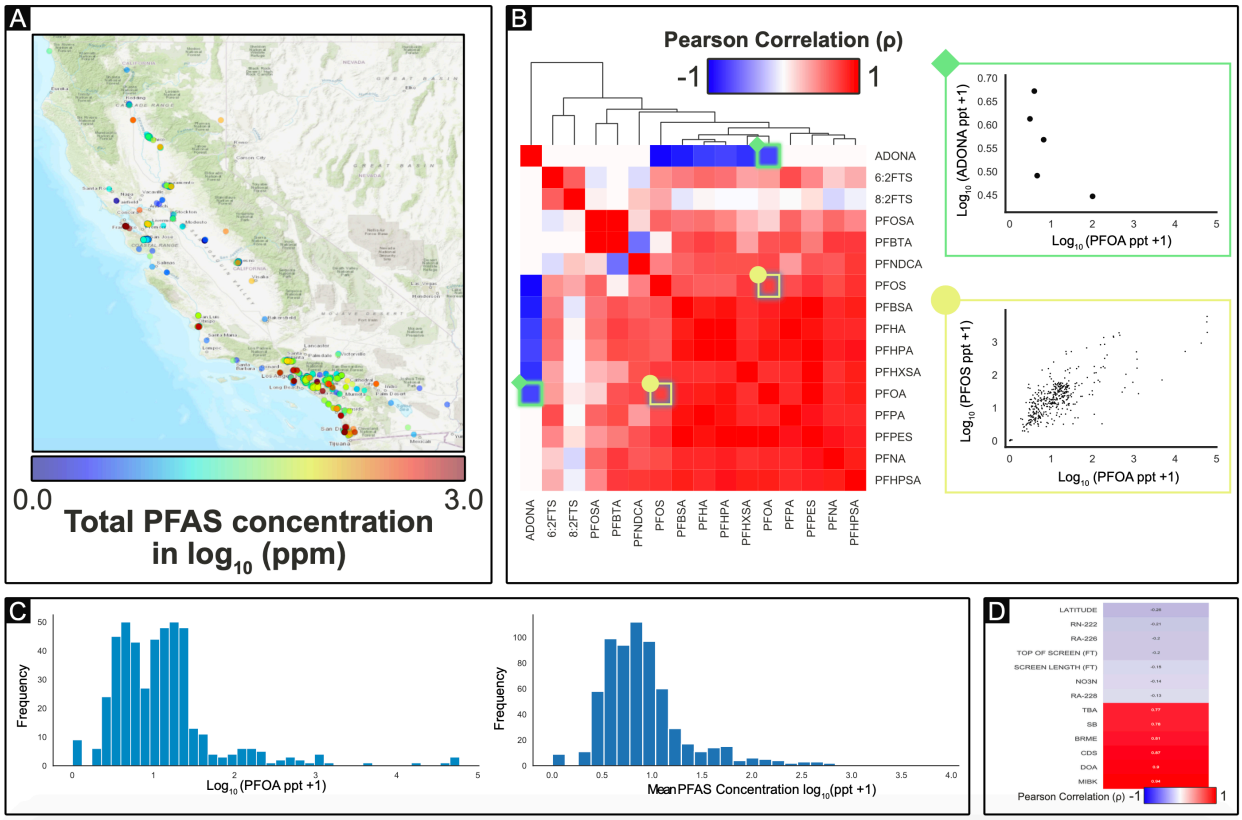

Figure 2. PFAS levels vary over a 1,000x scale have significant correlations within themselves and between different chemicals/geospatial data.

(**a**) Visualization of the location of each of the 663 groundwater wells (dots) in the State of California that had associated PFAS measurements. Each well is colored by total PFAS concentration on a log10 scale. (**b**) A correlation matrix visualization of pairwise correlations between PFAS compounds. Each cell represents the Pearson correlation between the respective elements as shown in the yellow and purple scatter plots. The more red the cell the closer the correlation is to 1.0, the more blue the value the closer the correlation is to -1.0. (**c**) Histogram of the log10(PFOA in ppt +1) abundances across groundwater wells in the dataset for which it was measured (top). Histogram of the Total PFAS concentration [sum of individual log10(PFAS compound in ppt +1)] abundances across groundwater wells in the dataset for which there are

measurements (bottom). (**d**) Visualization of non-PFAS features in the dataset that most strongly correlate positively (red) and most strongly correlated negatively (blue) with overall PFAS levels.

Next, we sought to apply these correlations to predicting PFAS values. We split the data into distinct groups on which we could separately train and evaluate our predictions. In general, we built models which could predict PFAS levels given all other information that was present for a given well. We tried two different methods to estimate PFAS levels. The first involved, kNN imputation (see **Methods**), in which missing data was filled in based on an average of a certain number of most similar wells. The second involved a kernel-based machine learning (ML) approach (see **Methods**) in which the overall similarity score of a well to other related wells was used in combination with the observed measurements themselves. These were integrated into a random forest regressor to predict individual PFAS levels. To compare these methods, we created a reference scatter plots of what the result of predicting the average PFAS level would be if applied to wells a model had not previously seen, which would result in an overall R^2 of 0.0. This result is contrasted with the results from the kNN and kernel (R^2 of 0.50) based ML approach (R^2 of 0.72). (**Figure 3A, B**). We then applied the results of our ML approach to all wells in the GAMA dataset that have not yet been tested. This resulted in a nearly 50-fold increase in the number of wells with PFAS estimates as well as the identification of a sizable number of wells with concerningly high predicted PFAS levels (**Figure 3C**).

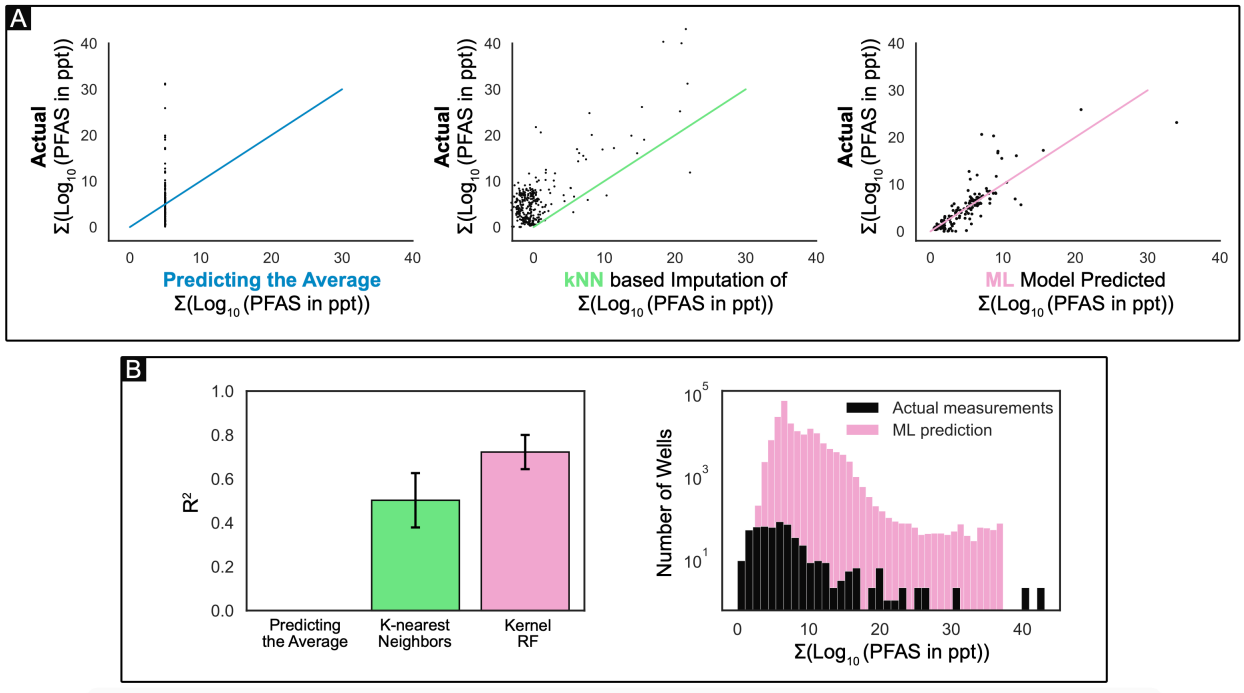

Figure 3. Machine learning model accurately predicts individual PFAS compounds and overall PFAS abundances

(**a**) Comparison of three approaches to predict PFAS levels. Predicting the average overall PFAS level for each well (left), predicting PFAS levels using a k-nearest neighbors approach in which the average PFAS level of wells with similar chemical and geospatial profiles levels is used to create an informed predictions (center), predicting PFAS levels using a Random Forest regressor built on top of a custom imputation framework (right). (**b**) The R^2 or variance explained for each of the three models described in (**a**). Black error bars represent standard deviation for the R^2 across 20 independent train/test splits of the dataset. (**c**) Histogram of the distribution of predicted PFAS values (in blue) compared to wells where PFAS was actually measured (in orange). PFAS values are summed on a log 10 scale. Y-axis is on a log10 scale.

Lastly, we sought to quantify the model's performance when applied to a specific regulatory threshold. Specifically, we quantified its performance for identifying wells whose PFOA + PFOS levels are greater than 70 parts per trillion, equivalent to the current United States EPA Health Advisory Level. At a 5% false positive rate, the model was able to recover 70% of the true positives results in an overall area under the curve of 0.93 (**Figure 4A**). To demonstrate how this model would be used in a real world context, we simulated how quickly all wells with PFOA + PFOS levels greater than 70 parts per trillion would be discovered using a random sampling strategy or a strategy in which the wells with the highest machine learning predicted PFOA+PFOS levels were tested first (**Figure 4B**). The ML informed strategy significantly outperformed a random sampling approach ($p<0.00001$).

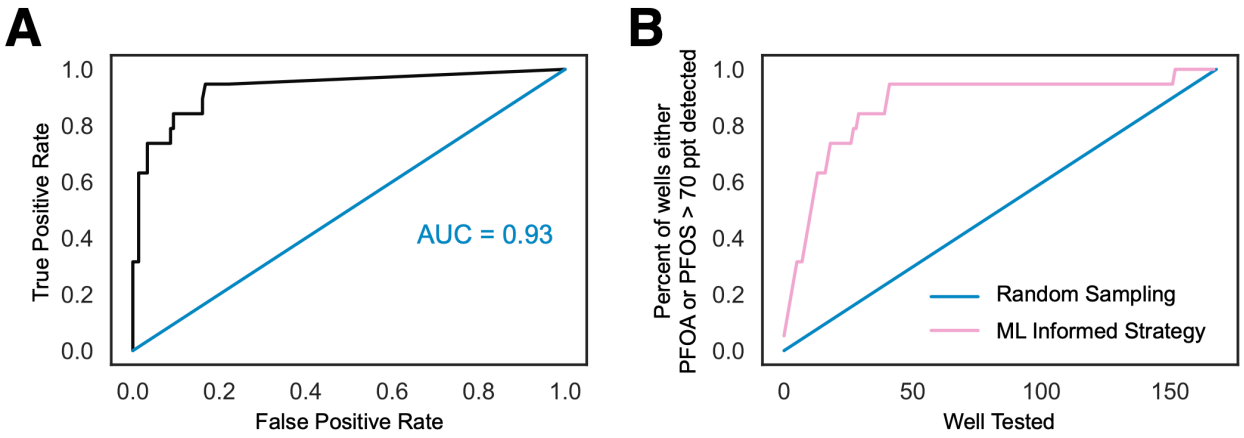

Figure 4. Practical advantage of a risk adjusted testing strategy based on a machine learning model.

(**a**) Receiver operating characteristic curve demonstrating model performance for predicting wells where the sum of PFOA and PFOS exceeds 70 ppt. Red diagonal line represents the expected model performance for a model which guess randomly based on the average likelihood of a well exceeding the threshold. (**b**) Results of a machine learning informed testing strategy in which the

wells are tested in order of which ones have the highest predicted probabilities of exceeding the combined PFOS and PFOA threshold (orange line). This result is compared to a strategy in which wells are tested randomly (blue line).

Discussion:

Co-occurrence of geospatial and chemical analytes in drinking water can be used for accurate machine learning approaches for PFAS

Other studies have applied machine learning to gridded spatial predictors such as topography, groundwater flow direction, land use, and soil conditions; for example, a previous study achieved an R^2 of 0.54 using machine learning on spatial data for groundwater nitrate concentrations (Knoll et al., 2019). For predicting groundwater PFAS concentrations, our model reaches an R^2 of 0.72, demonstrating the power of including full co-contaminant and geochemical data even without additional spatial predictors like topography and groundwater flow direction. Our kernel-based machine learning framework includes information on the total concentration of salts in local groundwater, which acts as a proxy for water management practices like water recycling and wastewater injection, as well as for land use practices because various industries tend to test groundwater for different contaminants (e.g. pesticides in agricultural areas and chlorinated solvents in industrial areas).

Recommendations to stakeholders

In the United States, many State governments are beginning to make historical groundwater (and other environmental) monitoring data available to the public, but these resources have thus far been underutilized. Application of computational techniques on existing monitoring datasets is a

promising method for improving detection of groundwater wells which pose a threat to human health. It may even reveal previously unknown areas of concern for well-characterized contaminants in addition to investigating emerging contaminants like the PFAS. As more regional and Federal governments make these data available, it will become possible to create massive datasets of high-resolution historical groundwater data for many contaminants, which may aid in scientific understanding of the patterns of release and transport. Better understanding of release and transport of contaminants that pose a threat to public health may enable proactive management and protection of groundwater resources, both by regulating facilities and industries known to discharge contaminants of concern, and by optimizing pumping and blending of extracted groundwater to protect human health.

With the application of any computational method which makes predictions on historical data, inherent biases in the data are a significant concern when evaluating and applying predictions, particularly when predictions can affect public health. In particular, we emphasize the potential environmental justice pitfalls of relying naively on machine learning predictions to make regulatory decisions. In the United States, heavy-polluting industries and facilities have historically been built in or adjacent to socioeconomically and racially segregated neighborhoods due to a combined history of exclusionary residential real estate practices and zoning laws (Maantay, 2002; Mohai et al., 2009; Mohai and Saha, 2015). It is possible that these areas are under-monitored relative to their contamination risk, and as a result of this sparse monitoring, the model results may underestimate the level of contamination in historically disadvantaged communities. This invisible socioeconomic overprint on the groundwater monitoring data is not unique to the United States and will need to be investigated further as a central aspect of

integrating machine learning and other big-data approaches into water management and regulation.

While under-sampling of disadvantaged communities is a concern, machine learning tools such as this one also may aid in better characterizing the relative groundwater contamination burden in different communities by providing robust aggregate predictions of overall exposure to related compounds classes such as PFAS built upon a small number of existing measurements.

A future scientific challenge remains to tie individual chemical dose-effects to multi-chemical integrated hazard indices for human and environmental health; key to this is understanding how multiple chemical exposures interact to produce cumulative health effects. Such efforts should drive the determination of regulatory limits that machine learning models such as the one described here can be optimized towards.

Generalization across other contaminants and geographies

We have demonstrated that approaches similar to the ones outlines above can perform extremely well for chemicals such as TCE and PCATE (results not shown). Indeed, for these chemicals the total number of available measurements exceeds that available for the PFAS chemicals by >10-fold. Generally, the performance of machine learning methods such as those we have outlined in this paper improve with the amount of data available. We have demonstrated the potential of aggregating groundwater contaminant measurements despite a significant level of sparsity with a high degree of missing data elements (in this case excess of >94% missing). We believe that this result highlights the need for collaborations between regulatory bodies across state and national

boundaries to bring together contamination datasets in an open data framework. In such a framework, machine learning methods such as these could be used to rapidly identify and mitigate the most dangerous sources of anthropogenic groundwater contamination.

Conclusions:

In this study, we were able to demonstrate the utility of collating diverse geospatial and chemical measurements to a single database for the purpose of prioritizing groundwater wells for testing. Despite the high levels of missing data (in which only a small portion of the total possible measurements are available for a given well), we demonstrate that the correlations between chemicals and geospatial features provide sufficient structure to create accurate predictive models. Specifically, our model for predicting PFAS has the potential to significantly accelerate the ability to identify groundwater sources with concerningly high PFAS concentrations. In general, we believe our approach could have broad utility in aiding regulatory agencies in overseeing the management of anthropogenic contaminants in groundwater using predictive analytics to guide testing strategies.

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Declaration of competing interest

A.D. is a founder of and equity holder in Coral Genomics. The authors alone are responsible for the views expressed in this publication and they do not necessarily represent the views, decisions or policies of the institutions with which they are affiliated.

Author Contributions

SB and AD worked on all aspects of the paper together including data curation, analysis, figure generation, and writing of the manuscript.

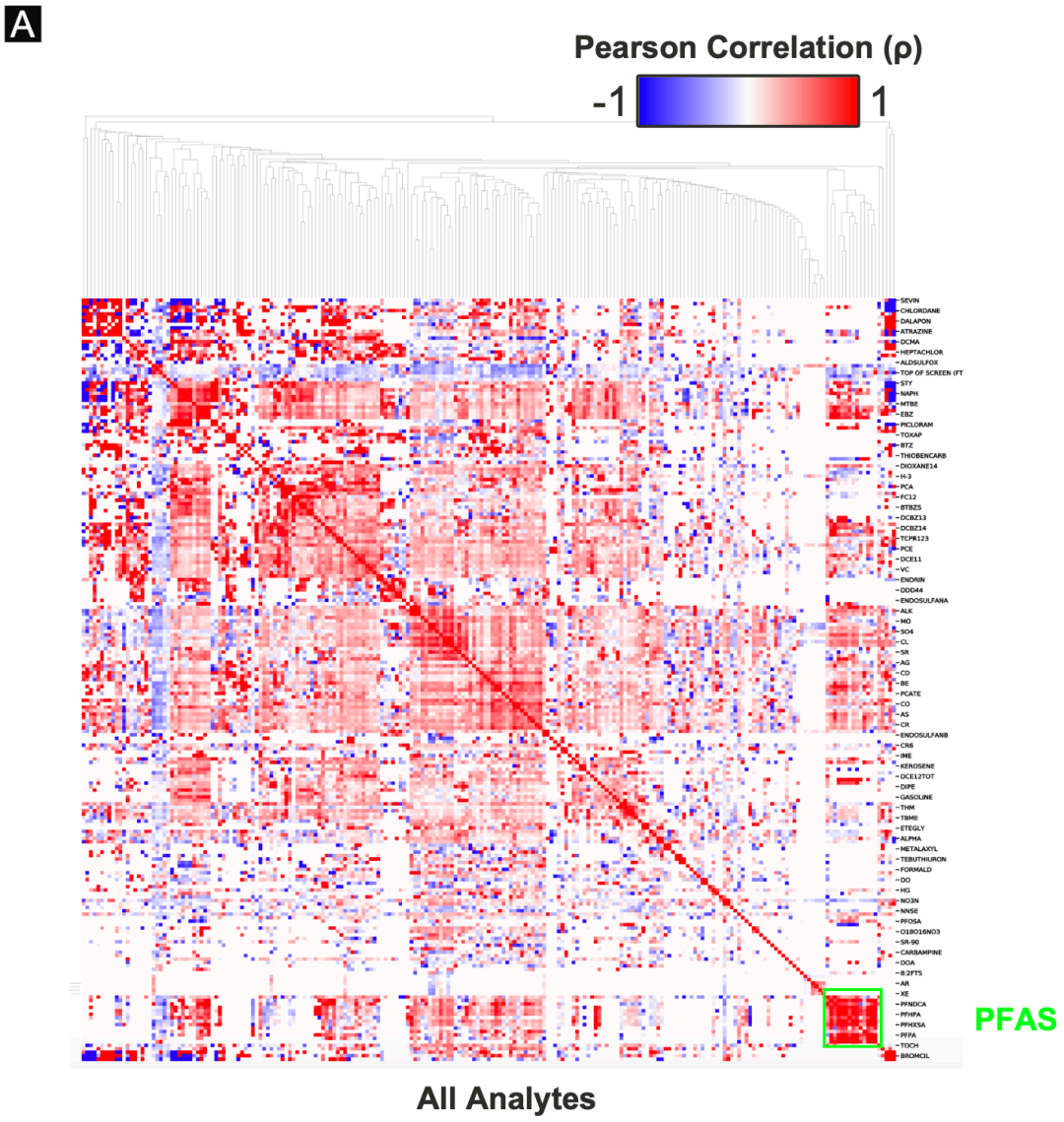

Figure S1. An overview of pairwise correlations between chemical and geospatial features in the GAMA dataset.

A correlation matrix visualization of pairwise correlations between chemical and geospatial features. Each cell represents the Pearson correlation between the respective elements as shown in the yellow and purple scatter plots. The more red the cell the closer the correlation is to 1.0, the

more blue the value the closer the correlation is to -1.0. The PFAS set of compounds is highlighted in green.

References:

Alimi, H., Ertel, T., Schug, B., 2003. Fingerprinting of hydrocarbon fuel contaminants: Literature review. Environ. Forensics. https://doi.org/10.1080/15275920303489

Barrett, M.H., Hiscock, K.M., Pedley, S., Lerner, D.N., Tellam, J.H., French, M.J., 1999. Marker species for identifying urban groundwater recharge sources: A review and case study in Nottingham, UK. Water Res. https://doi.org/10.1016/S0043-1354(99)00021-4

Biege, L.B., Hurtt, M.E., Frame, S.R., O'Connor, J.C., Cook, J.C., 2001. Mechanisms of extrahepatic tumor induction by peroxisome proliferators in male CD rats. Toxicol. Sci. 60, 44–55. https://doi.org/10.1093/toxsci/60.1.44

Carle, D., 2015. Introduction to Water in California. University of California Press.

Conder, J.M., Hoke, R.A., De Wolf, W., Russell, M.H., Buck, R.C., 2008. Are PFCAs bioaccumulative? A critical review and comparison with regulatory criteria and persistent lipophilic compounds. Environ. Sci. Technol. https://doi.org/10.1021/es070895g

Crone, B.C., Speth, T.F., Wahman, D.G., Smith, S.J., Abulikemu, G., Kleiner, E.J., Pressman, J.G., 2019. Occurrence of per- and polyfluoroalkyl substances (PFAS) in source water and their treatment in drinking water. Crit. Rev. Environ. Sci. Technol. 49, 2359–2396. https://doi.org/10.1080/10643389.2019.1614848

Domingo, J.L., Nadal, M., 2019. Human exposure to per- and polyfluoroalkyl substances (PFAS) through drinking water: A review of the recent scientific literature. Environ. Res. https://doi.org/10.1016/j.envres.2019.108648

Douglas, G.S., Emsbo-Mattingly, S.D., Stout, S.A., Uhler, A.D., McCarthy, K.J., 2007. Chemical fingerprinting methods, in: Introduction to Environmental Forensics. Elsevier Inc., pp. 311–454. https://doi.org/10.1016/B978-012369522-2/50010-5

Ericson, I., Nadal, M., Van Bavel, B., Lindström, G., Domingo, J.L., 2008. Levels of perfluorochemicals in water samples from Catalonia, Spain: Is drinking water a significant contribution to human exposure?, in: Environmental Science and Pollution Research. Springer, pp. 614–619. https://doi.org/10.1007/s11356-008-0040-1

Fasano, W.J., Carpenter, S.C., Gannon, S.A., Snow, T.A., Stadler, J.C., Kennedy, G.L., Buck, R.C., Korzeniowski, S.H., Hinderliter, P.M., Kemper, R.A., 2006. Absorption, distribution, metabolism, and elimination of 8-2 fluorotelomer alcohol in the rat. Toxicol. Sci. 91, 341–355. https://doi.org/10.1093/toxsci/kfj160

Frömel, T., Knepper, T.P., 2010. Biodegradation of fluorinated alkyl substances. Rev. Environ. Contam. Toxicol. 208, 161–177. https://doi.org/10.1007/978-1-4419-6880-7_3

Giesy, J.P., Kannan, K., 2001. Global distribution of perfluorooctane sulfonate in wildlife. Environ. Sci. Technol. 35, 1339–1342. https://doi.org/10.1021/es001834k

Kannan, K., Corsolini, S., Falandysz, J., Fillmann, G., Kumar, K.S., Loganathan, B.G., Mohd, M.A., Olivero, J., Van Wouwe, N., Yang, J.H., Aldous, K.M., 2004. Perfluorooctanesulfonate and related fluorochemicals in human blood from several

countries. Environ. Sci. Technol. 38, 4489–4495. https://doi.org/10.1021/es0493446

Knoll, L., Breuer, L., Bach, M., 2019. Large scale prediction of groundwater nitrate concentrations from spatial data using machine learning. Sci. Total Environ. 668, 1317–1327. https://doi.org/10.1016/j.scitotenv.2019.03.045

Maantay, J., 2002. Zoning law, health, and environmental justice: What's the connection?, in: Journal of Law, Medicine and Ethics. Blackwell Publishing Inc., pp. 572–593. https://doi.org/10.1111/j.1748-720X.2002.tb00427.x

Martin, J.W., Ellis, D.A., Mabury, S.A., Hurley, M.D., Wallington, T.J., 2006. Atmospheric Chemistry of Perfluoroalkanesulfonamides: Kinetic and Product Studies of the OH Radical and Cl Atom Initiated Oxidation of *N* -Ethyl Perfluorobutanesulfonamide. Environ. Sci. Technol. 40, 864–872. https://doi.org/10.1021/es051362f

Martin, J.W., Mabury, S.A., O'Brien, P.J., 2005. Metabolic products and pathways of fluorotelomer alcohols in isolated rat hepatocytes. Chem. Biol. Interact. 155, 165–180. https://doi.org/10.1016/j.cbi.2005.06.007

Mohai, P., Pellow, D., Roberts, J.T., 2009. Environmental Justice. Annu. Rev. Environ. Resour. 34, 405–430. https://doi.org/10.1146/annurev-environ-082508-094348

Mohai, P., Saha, R., 2015. Which came first, people or pollution? A review of theory and evidence from longitudinal environmental justice studies. Environ. Res. Lett. 10, 125011. https://doi.org/10.1088/1748-9326/10/12/125011

Parsons, J.R., Sáez, M., Dolfing, J., de Voogt, P., 2008. Biodegradation of perfluorinated

compounds. Rev. Environ. Contam. Toxicol. 196, 53–71. https://doi.org/10.1007/978-0-387-78444-1_2

Prevedouros, K., Cousins, I.T., Buck, R.C., Korzeniowski, S.H., 2006. Sources, fate and transport of perfluorocarboxylates. Environ. Sci. Technol. https://doi.org/10.1021/es0512475

Rayne, S., Forest, K., 2009. Perfluoroalkyl sulfonic and carboxylic acids: A critical review of physicochemical properties, levels and patterns in waters and wastewaters, and treatment methods. J. Environ. Sci. Heal. - Part A Toxic/Hazardous Subst. Environ. Eng. https://doi.org/10.1080/10934520903139811

Sjogren, P., Montse, R., Lampa, E., Salihovic, S., van Bavel, B., Lind, L., Lind, P.M., 2016. Circulating levels of perfluoroalkyl substances are associated with dietary patterns - A cross sectional study in elderly Swedish men and women. Environ. Res. 150, 59–65. https://doi.org/10.1016/j.envres.2016.05.016

State Water Resources Control Board, 2020. California State Water Resources Control Board.

Stout, S.A., Uhler, A.D., Naymik, T.G., McCarthy, K.J., 1998. Peer Reviewed: Environmental Forensics Unraveling Site Liability. Environ. Sci. Technol. 32, 260A-264A. https://doi.org/10.1021/es983570w

US EPA, O., n.d. Data Summary of The Third Unregulated Contaminant Monitoring Rule.

Vestergren, R., Cousins, I.T., 2009. Tracking the pathways of human exposure to perfluorocarboxylates. Environ. Sci. Technol. https://doi.org/10.1021/es900228k

Wang, Z., Boucher, J.M., Scheringer, M., Cousins, I.T., Hungerbühler, K., 2017. Toward a Comprehensive Global Emission Inventory of C4-C10 Perfluoroalkanesulfonic Acids (PFSAs) and Related Precursors: Focus on the Life Cycle of C8-Based Products and Ongoing Industrial Transition. Environ. Sci. Technol. 51, 4482–4493. https://doi.org/10.1021/acs.est.6b06191

Xu, Y., Jurkovic-Mlakar, S., Li, Y., Wahlberg, K., Scott, K., Pineda, D., Lindh, C.H., Jakobsson, K., Engström, K., 2020. Association between serum concentrations of perfluoroalkyl substances (PFAS) and expression of serum microRNAs in a cohort highly exposed to PFAS from drinking water. Environ. Int. 136, 105446. https://doi.org/10.1016/j.envint.2019.105446

Young, C.J., Mabury, S.A., 2010. Atmospheric perfluorinated acid precursors: Chemistry, occurrence, and impacts. Rev. Environ. Contam. Toxicol. 208, 1–109. https://doi.org/10.1007/978-1-4419-6880-7_1