Can soil geochemistry predict the mercury concentration in fish?

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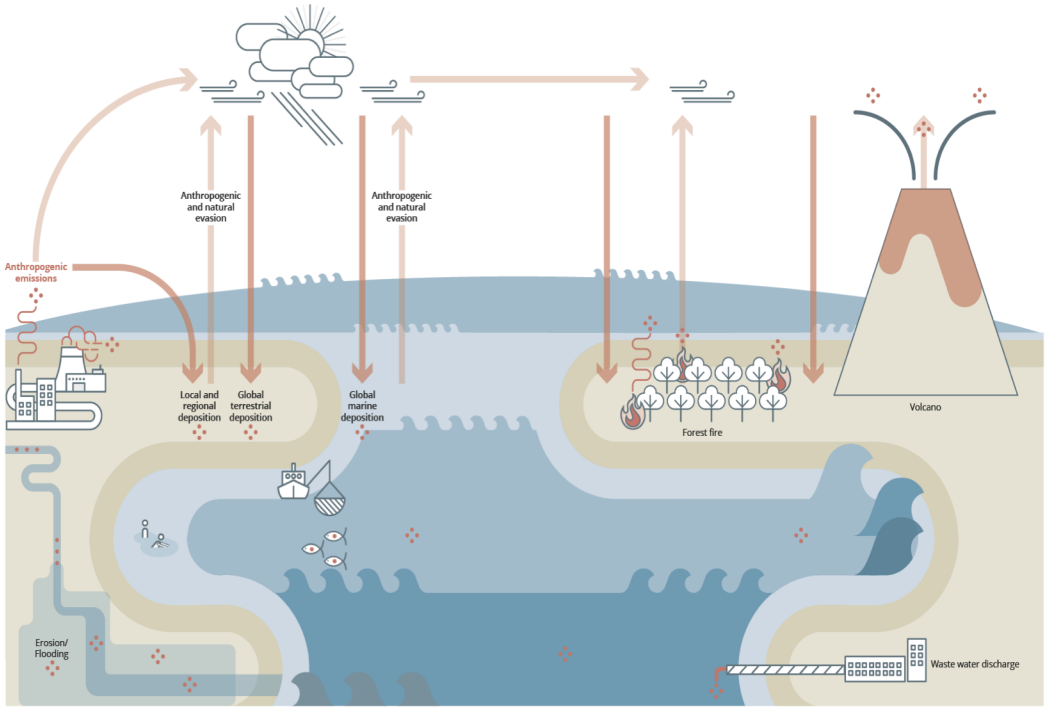
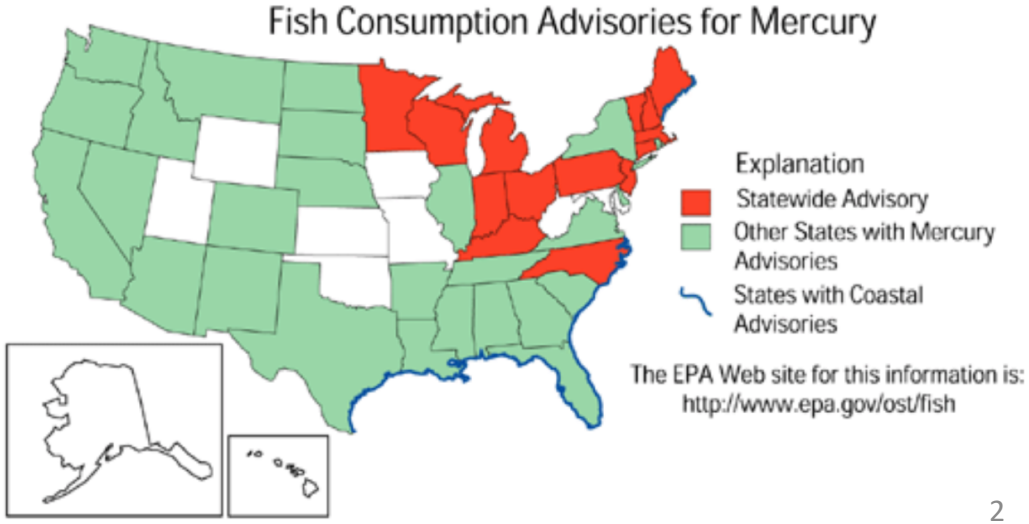
Background/ Context

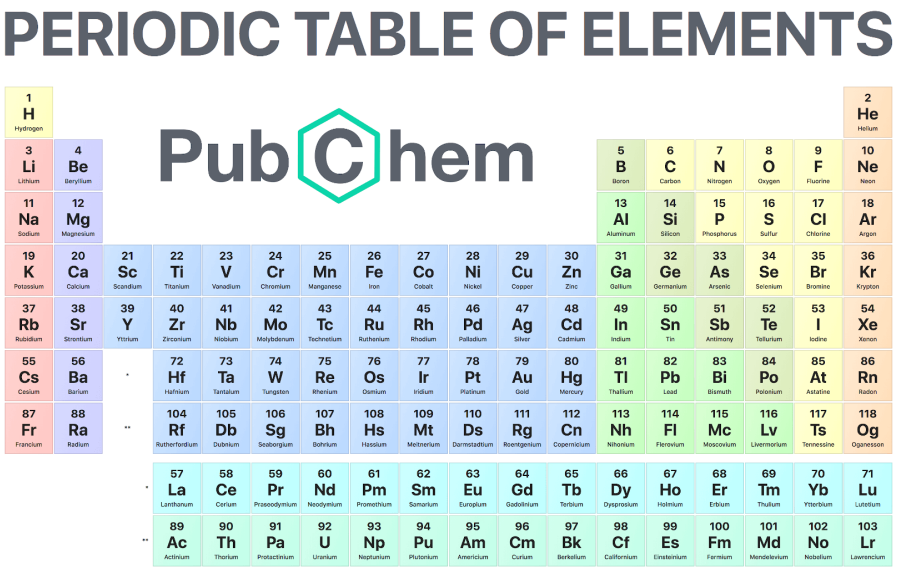
- Mercury is considered by WHO as one of the top ten chemicals or groups of chemicals of major public health concern
- Toxic effects:
  - Nervous system
  - Endocrine system
  - Immune system
  - Cardiovascular system
  - Gastrointestinal tract
- Top predators have the highest risk of exposure do to bioaccumulation and biomagnification
- Humans are primarily exposure though a fish diet





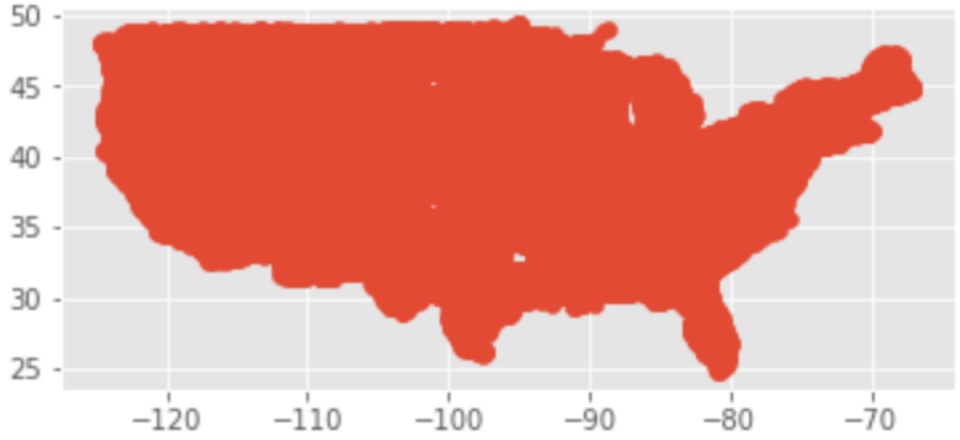
Research Question:

Since mercury biomagnification and accumulation is controlled by environmental factors can we use soil geochemistry to predict fish tissue Hg in the United States?

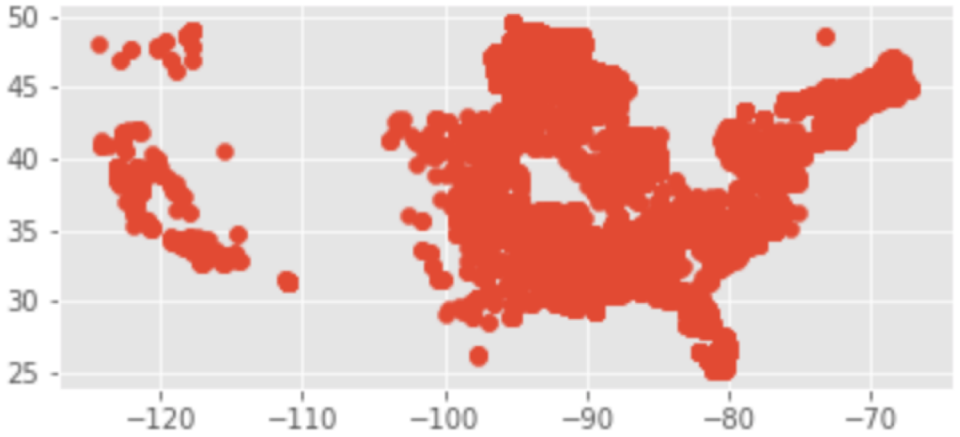


Data

- Soil Geochemistry: National Geochemical Survey
  - n= 64,756

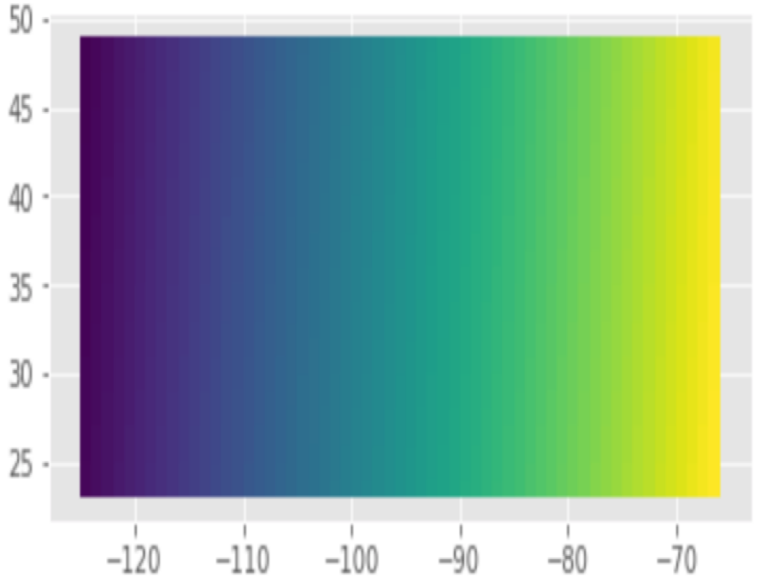


- Fish Tissue Hg: EPA Fish Hg database
  - n= 19,705

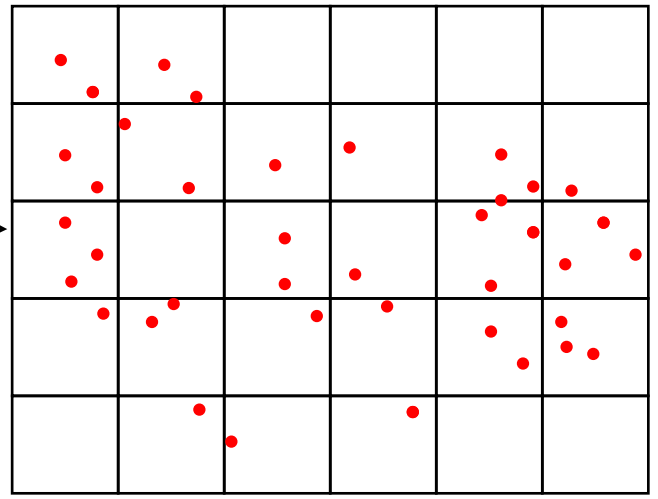


Data Processing

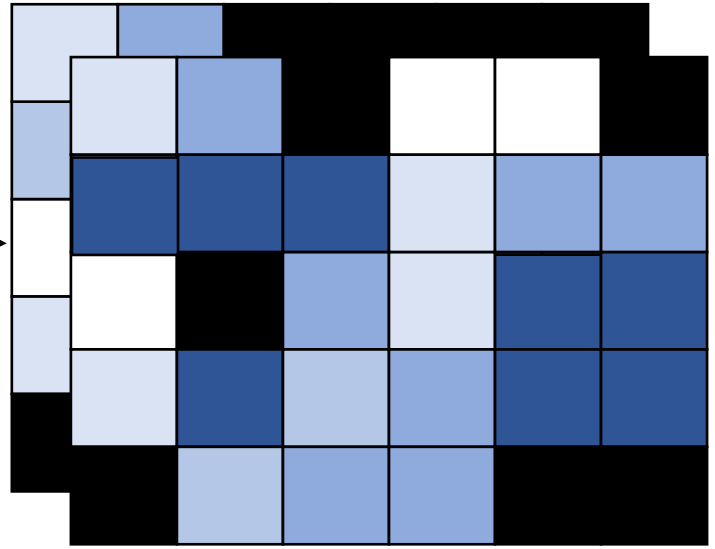
- Generate a grid
  - n= 1534



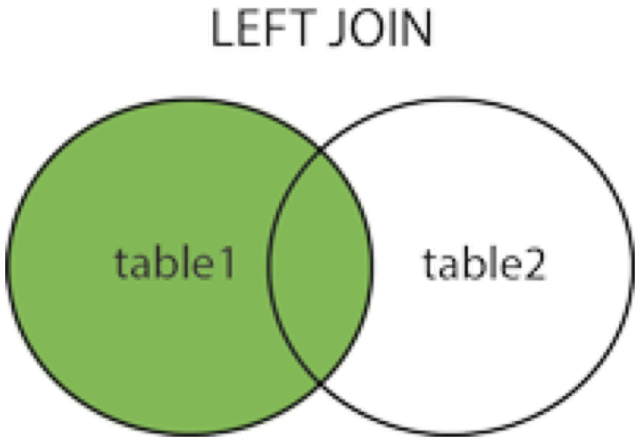
Aggregate Point → Polygon



Average NGS
Average Hg



- Merge Data frames



Grid ID

←

ID	Fish Hg

←

ID	NGS

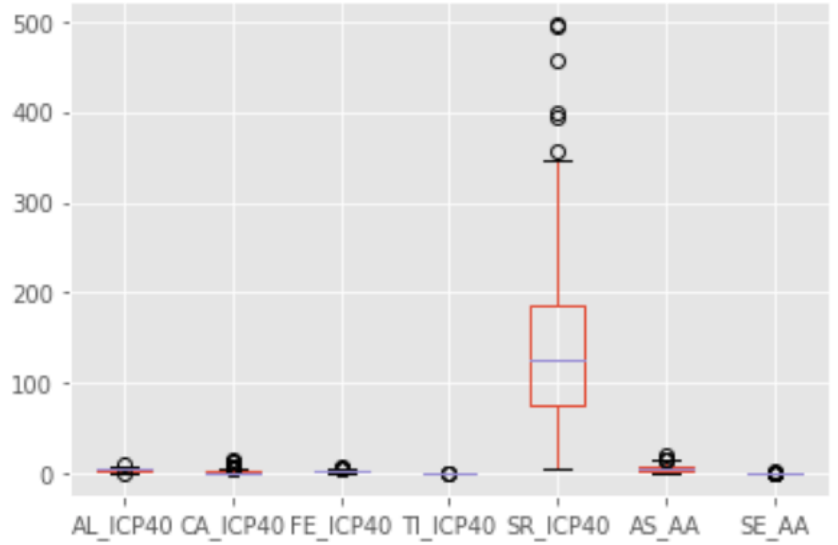
=

ID	Fish Hg	NGS

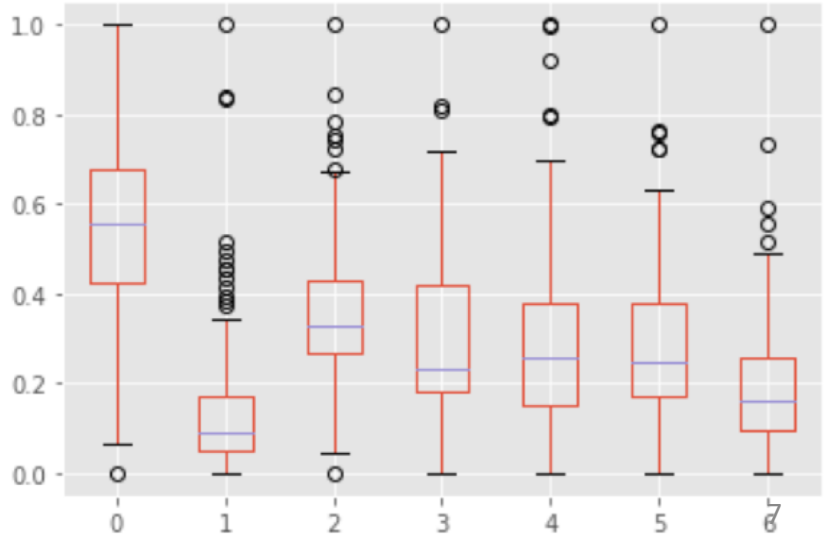
Scrub the Data

- Clean the dataset
  - Remove missing values (n=214)
- (Automated) Variable selection
  - Remove highly correlated variables (r > ± 0.80)
  - Remove variables where the p-value of the correlation with the dependent variable is more than 0.20
  - Normalize the data (this method is more appropriate for ecotoxicology data)

Before Normalization



After Normalization



Model

- Ridge regression Results
  - The root mean square error = 0.18
  - The mean absolute error = 0.15
  - R2 = 0.11

- Model coefficients are:
  - X1: AL_ICP40 -0.018
  - X2: CA_ICP40 -0.034
  - X3: FE_ICP40 -0.23
  - X4: TI_ICP40 0.032
  - X5: SR_ICP40 -0.16
  - X6: AS_AA -0.12
  - **X7: SE_AA -0.36**

OLS Regression Results

Dep. Variable:	hg_mean	R-squared (uncentered):	0.327
Model:	OLS	Adj. R-squared (uncentered):	0.291
Method:	Least Squares	F-statistic:	9.092
Date:	Tue, 03 Dec 2019	Prob (F-statistic):	4.02e-09
Time:	16:32:10	Log-Likelihood:	-49.698
No. Observations:	138	AIC:	113.4
Df Residuals:	131	BIC:	133.9
Df Model:	7		
Covariance Type:	nonrobust		

	coef	std err	t	P>|t|	[0.025	0.975]
x1	0.8173	0.300	2.726	0.007	0.224	1.410
x2	0.3742	0.221	1.695	0.093	-0.063	0.811
x3	-1.0023	0.388	-2.582	0.011	-1.770	-0.234
x4	0.7521	0.193	3.904	0.000	0.371	1.133
x5	-0.5005	0.271	-1.850	0.067	-1.036	0.035
x6	0.1678	0.251	0.670	0.504	-0.328	0.663
x7	-0.2506	0.227	-1.103	0.272	-0.700	0.199

Omnibus:	157.709	Durbin-Watson:	2.143
Prob(Omnibus):	0.000	Jarque-Bera (JB):	4002.281
Skew:	4.216	Prob(JB):	0.00
Kurtosis:	27.999	Cond. No.	14.4

Untransformed data (but may violate OLS regression assumptions)

	AL_ICP40	CA_ICP40	FE_ICP40	TI_ICP40	SR_ICP40	AS_AA	SE_AA
AL_ICP40	1.000000	0.105773	0.742391	0.115026	0.736606	0.236462	0.079761
CA_ICP40	0.105773	1.000000	0.064647	-0.259561	0.379239	0.211274	0.227949
FE_ICP40	0.742391	0.064647	1.000000	0.431655	0.421571	0.247446	0.010555
TI_ICP40	0.115026	-0.259561	0.431655	1.000000	0.018363	-0.345852	-0.262499
SR_ICP40	0.736606	0.379239	0.421571	0.018363	1.000000	0.035092	0.080518
AS_AA	0.236462	0.211274	0.247446	-0.345852	0.035092	1.000000	0.464423
SE_AA	0.079761	0.227949	0.010555	-0.262499	0.080518	0.464423	1.000000

OLS Regression Results

Dep. Variable:	hg_mean	R-squared (uncentered):	0.408
Model:	OLS	Adj. R-squared (uncentered):	0.388
Method:	Least Squares	F-statistic:	20.66
Date:	Tue, 03 Dec 2019	Prob (F-statistic):	4.96e-21
Time:	16:27:58	Log-Likelihood:	-35.355
No. Observations:	217	AIC:	84.71
Df Residuals:	210	BIC:	108.4
Df Model:	7		
Covariance Type:	nonrobust		

	coef	std err	t	P>|t|	[0.025	0.975]
AL_ICP40	0.0802	0.024	3.285	0.001	0.032	0.128
CA_ICP40	0.0205	0.011	1.813	0.071	-0.002	0.043
FE_ICP40	-0.1394	0.035	-3.995	0.000	-0.208	-0.071
TI_ICP40	0.6279	0.113	5.533	0.000	0.404	0.852
SR_ICP40	-0.0009	0.000	-2.299	0.022	-0.002	-0.000
AS_AA	0.0169	0.008	2.131	0.034	0.001	0.033
SE_AA	-0.2576	0.105	-2.461	0.015	-0.464	-0.051

Omnibus:	262.458	Durbin-Watson:	1.430
Prob(Omnibus):	0.000	Jarque-Bera (JB):	13980.961
Skew:	5.031	Prob(JB):	0.00
Kurtosis:	41.013	Cond. No.	1.04e+03

Conclusions

- **As this scale** we were able to model the relationship between environmental soil geochemistry and fish tissue Hg
  - Overall good predictive power but still unexplained variance
- Issues: the order of operations matters
  - Difference between fields
- Future questions:
  - How does the grid location change the results?
  - How does the type of grid chosen affect these results? Would a honeycomb grid have been better?
  - How does the size of the grid change the results?