GeoThermalCloud Utah

October 16, 2021

1 GeoThermalCloud: Geothermal Machine Learning Analysis: Utah

This notebook is a part of the GeoThermalCloud.jl: Machine Learning Framework for Geothermal Exploration.

<img src="https://raw.githubusercontent.com/SmartTensors/GeoThermalCloud.jl/master/logos/geothermalCloud.jl/master/logos/

1.1 GeoThermalCloud installation

import Pkg

If **GeoThermalCloud** is not installed, first execute in the Julia REPL:

```
Pkg.add("GeoThermalCloud")
    Pkg.add("NMFk")
    Pkg.add("Mads")
    Pkg.add("DelimitedFiles")
    Pkg.add("JLD")
    Pkg.add("Gadfly")
    Pkg.add("Cairo")
    Pkg.add("Fontconfig")
    Pkg.add("Kriging")
    Pkg.add("GMT")
    Pkg.add("Images")
[1]: import GeoThermalCloud
     import NMFk
     import Mads
     import DelimitedFiles
     import JLD
     import Gadfly
     import Cairo
     import Fontconfig
     import Kriging
     import GMT
     import Images
```

1.2 Load data

```
[2]: Xdat, headers = DelimitedFiles.readdlm("utah/data/utah_geothermal_data.csv", 

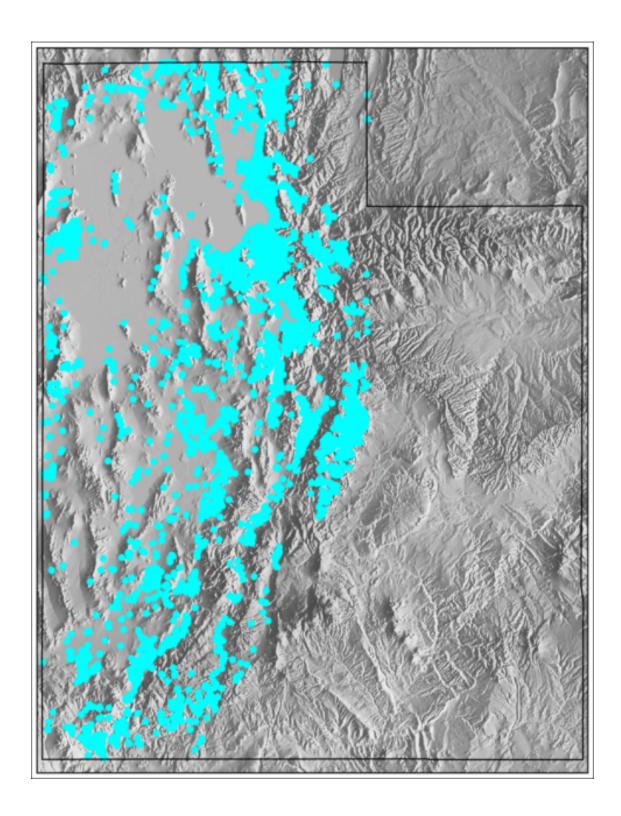
→',', header=true);
```

Set coordinates:

```
[3]: xcoord = Array{Float32}(Xdat[:, 2])
ycoord = Array{Float32}(Xdat[:, 1]);
```

1.3 Data Locations

Plot data locations on a map:



1.4 Define data attributes

We can use attribute names from the header in the input file.

However, the names are short.

For better understanding the variable names in the plots generated bellow, we are defining short and long attribute names:

```
[5]: attributes = ["Temperature", "Quartz", "Chalcedony", "pH", "TDS", "Al", "B", □ □ "Ba", "Be", "Br", "Ca", "Cl", "HCO3", "K", "Li", "Mg", "Na", "018"]

attributes_long = ["Temperature (C)", "GTM quartz (C)", "GTM chalcedony (C)", □ □ "pH ()", "TDS (ppm)", "Al (ppm)", "B (ppm)", "Ba (ppm)", "Be (ppm)", "Br □ □ (ppm)", "Ca (ppm)", "Cl (ppm)", "HCO3 (ppm)", "K (ppm)", "Li (ppm)", "Mg □ □ (ppm)", "Na (ppm)", "018 (%)"];
```

1.5 Pre-processing

Set empty data entries to NaN:

```
[6]: Xdat[Xdat .== ""] .= NaN;
```

Convert to Float32:

```
[7]: X = convert.(Float32, Xdat[:,3:end]);
```

Rescale O18 data (%):

```
[8]: X[:,18] .+= 20;
```

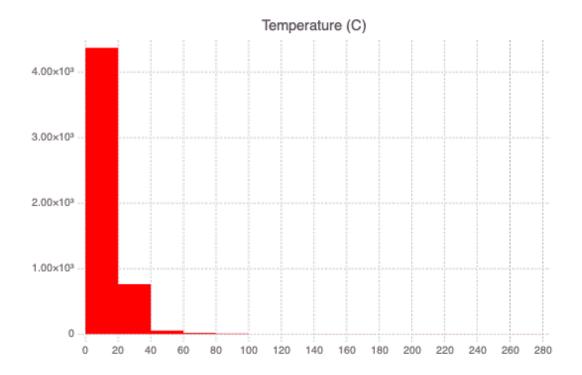
Set variables for the number of attributes and points:

```
[9]: nattributes = length(attributes_long)
npoints = size(Xdat, 1)
```

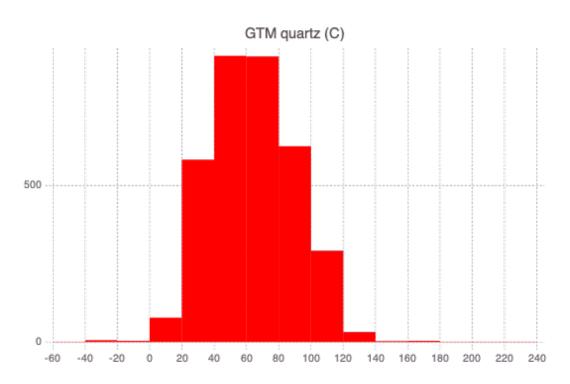
5218

Plot histograms and compute data statistics:

```
[10]: NMFk.datanalytics(X, attributes_long; dims=2);
```

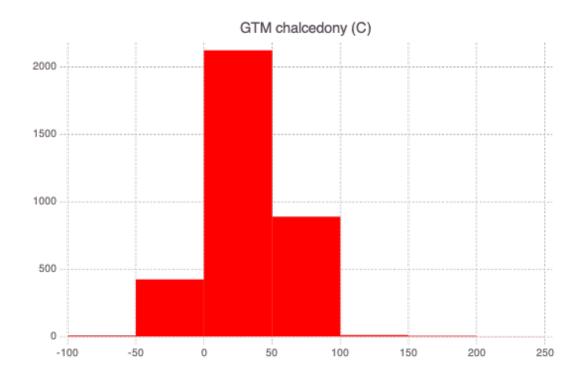


Info: Temperature (C)
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54



Temperature (C): Min 0.1 Max 261.0 StdDev 9.497179 Skewness 10.095466 Count 5214 Info: GTM quartz (C)

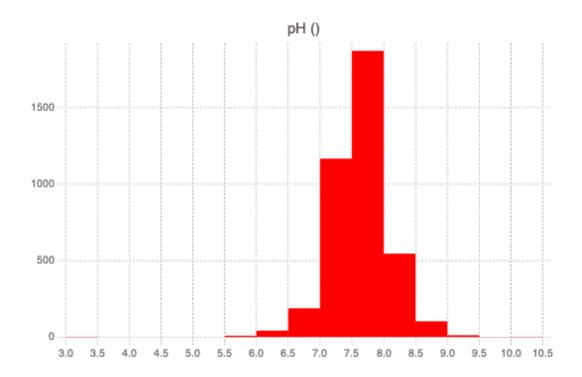
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54



GTM quartz (C): Min -50.870045 Max 222.28357 StdDev 26.329222 Skewness

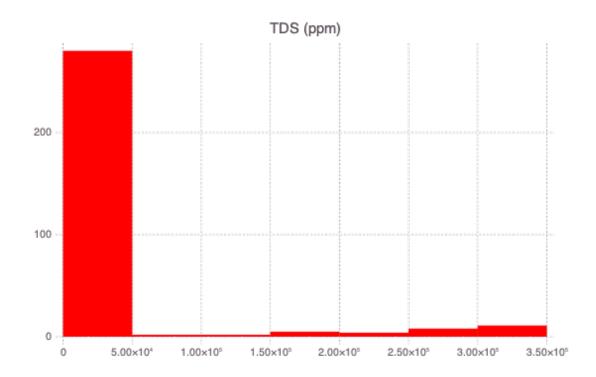
0.24256101 Count 3460

Info: GTM chalcedony (C)

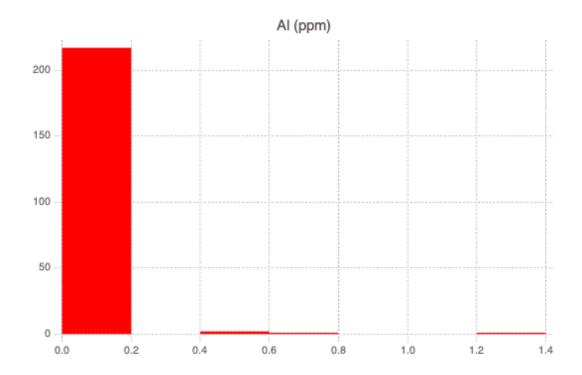


GTM chalcedony (C): Min -81.64773 Max 208.67426 StdDev 27.450817 Skewness 0.3369881 Count 3460

Info: pH ()

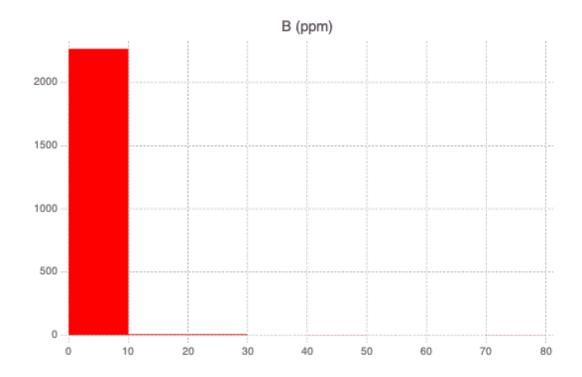


pH (): Min 3.4 Max 10.2 StdDev 0.44822767 Skewness -0.45681924 Count 3941 Info: TDS (ppm) @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54



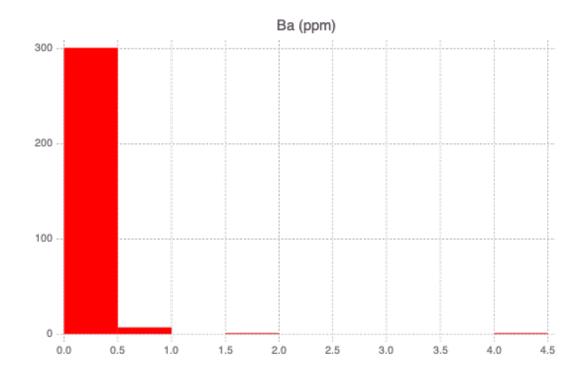
TDS (ppm): Min 122.0 Max 329000.0 StdDev 78777.95 Skewness 2.9479313 Count 312

Info: Al (ppm)

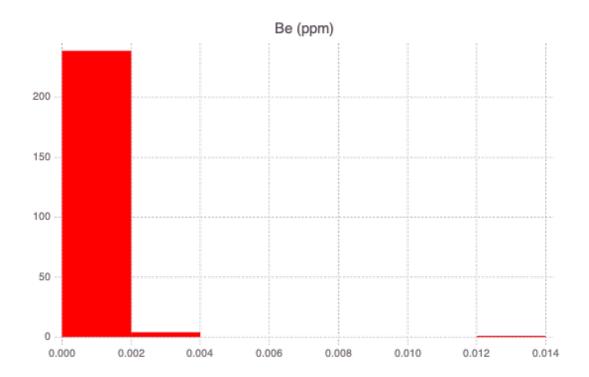


Al (ppm): Min 0.0 Max 1.251 StdDev 0.10527698 Skewness 9.031239 Count 221

Info: B (ppm)

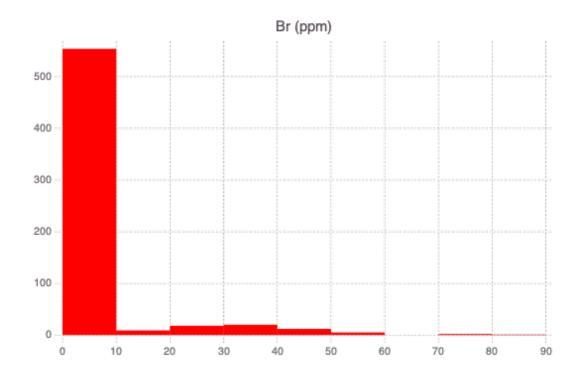


B (ppm): Min 0.0 Max 76.5 StdDev 2.6950865 Skewness 15.190172 Count 2284 Info: Ba (ppm)



Ba (ppm): Min 0.002 Max 4.5 StdDev 0.2898333 Skewness 11.825817 Count 310 $\,$

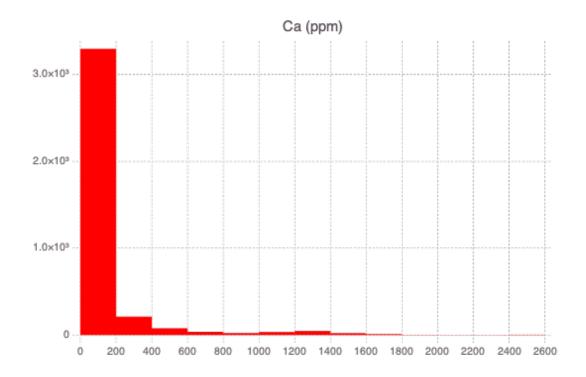
Info: Be (ppm)



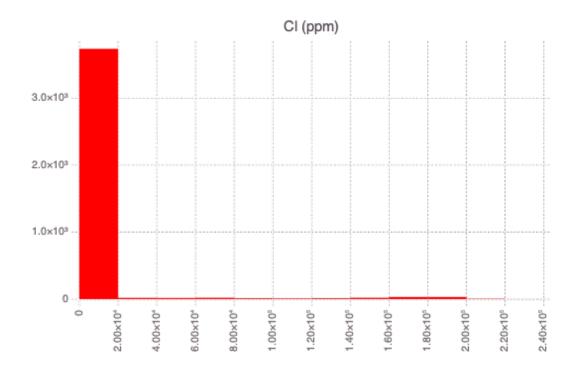
Be (ppm): Min 5.33333338-5 Max 0.013 StdDev 0.00089295243 Skewness 10.968073

Count 244

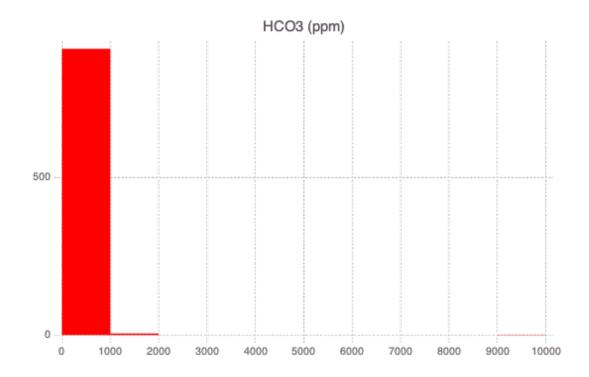
Info: Br (ppm)



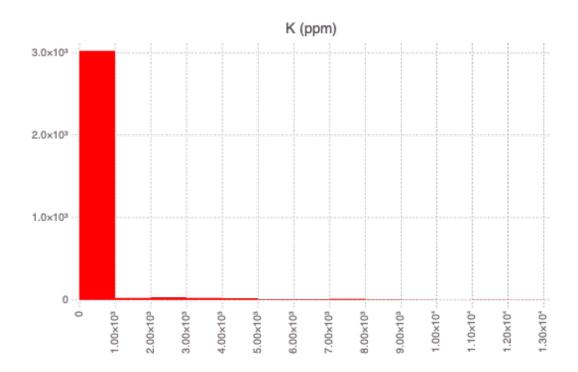
Br (ppm): Min 0.0 Max 84.0 StdDev 11.680384 Skewness 3.435088 Count 621
 Info: Ca (ppm)

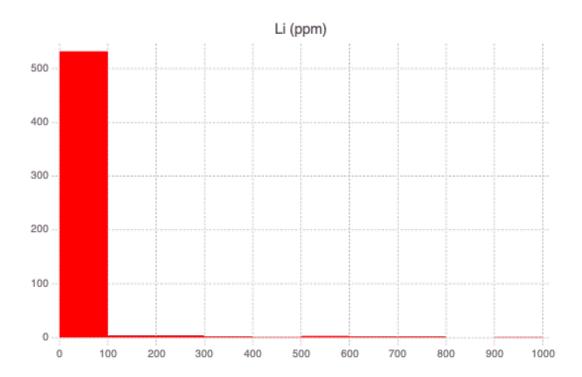


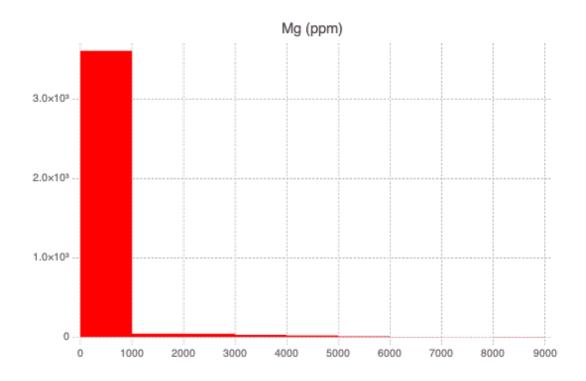
Ca (ppm): Min 0.6 Max 2566.6667 StdDev 262.82578 Skewness 4.424904 Count 3772 Info: Cl (ppm)



Cl (ppm): Min 0.6 Max 240000.0 StdDev 28681.555 Skewness 5.21565 Count 3923 Info: HCO3 (ppm)







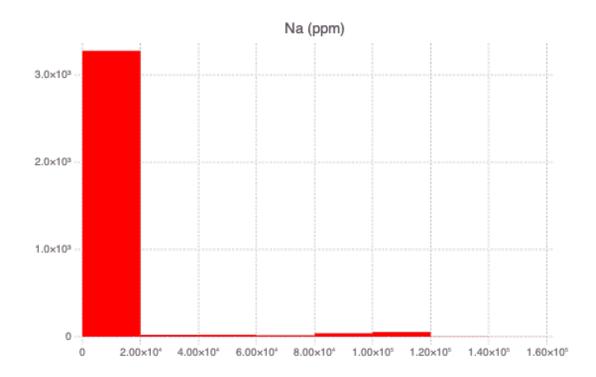
HCO3 (ppm): Min 37.0 Max 9217.0 StdDev 329.8163 Skewness 22.165213 Count 915 K (ppm): Min 0.0 Max 13000.0 StdDev 1063.7937 Skewness 6.380783 Count 3177 Li (ppm): Min 0.0 Max 970.0 StdDev 90.79041 Skewness 6.6990304 Count 551 Info: K (ppm)

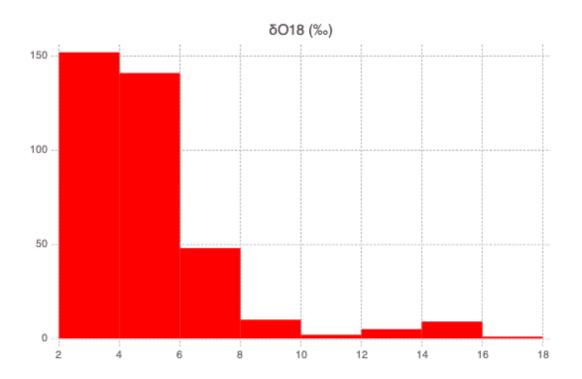
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54

Info: Li (ppm)

 ${\tt @ NMFk / Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.j1:54}\\$

Info: Mg (ppm)





```
Mg (ppm): Min 0.0 Max 8500.0 StdDev 663.7361 Skewness 6.581147 Count 3760
Na (ppm): Min 0.5 Max 160000.0 StdDev 17983.25 Skewness 4.946034 Count 3437
018 (%): Min 2.1499996 Max 16.36 StdDev 2.4535506 Skewness 2.5710073 Count 368
Name Min Max StdDev Count (non-NaN's)
Temperature (C) 0.1 261.0 9.497179 10.095466 5214
GTM quartz (C) -50.870045 222.28357 26.329222 0.24256101 3460
GTM chalcedony (C) -81.64773 208.67426 27.450817 0.3369881 3460
pH () 3.4 10.2 0.44822767 -0.45681924 3941
TDS (ppm) 122.0 329000.0 78777.95 2.9479313 312
Al (ppm) 0.0 1.251 0.10527698 9.031239 221
B (ppm) 0.0 76.5 2.6950865 15.190172 2284
Ba (ppm) 0.002 4.5 0.2898333 11.825817 310
Be (ppm) 5.3333333e-5 0.013 0.00089295243 10.968073 244
Br (ppm) 0.0 84.0 11.680384 3.435088 621
Ca (ppm) 0.6 2566.6667 262.82578 4.424904 3772
Cl (ppm) 0.6 240000.0 28681.555 5.21565 3923
HCO3 (ppm) 37.0 9217.0 329.8163 22.165213 915
K (ppm) 0.0 13000.0 1063.7937 6.380783 3177
Li (ppm) 0.0 970.0 90.79041 6.6990304 551
Mg (ppm) 0.0 8500.0 663.7361 6.581147 3760
Na (ppm) 0.5 160000.0 17983.25 4.946034 3437
018 (%) 2.1499996 16.36 2.4535506 2.5710073 368
 Info: Na (ppm)
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
 Info: 018 (%)
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54
 Info: Attributes
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:70
```

Note that the data entries for TDS, A1, and O18 are heavily missing.

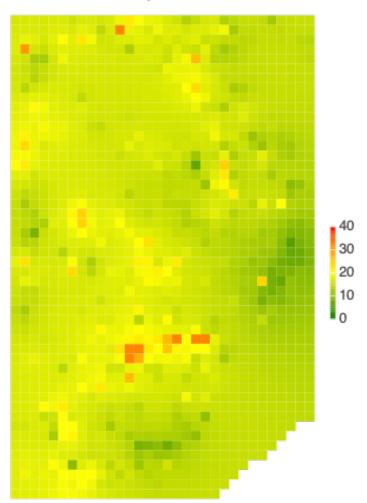
Even though the dataset is very sparse, our ML methods can analyze the inputs.

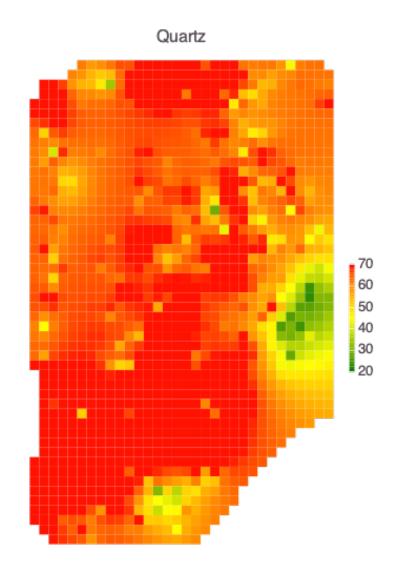
Most of the commonly used ML methods cannot process datasets that are sparse.

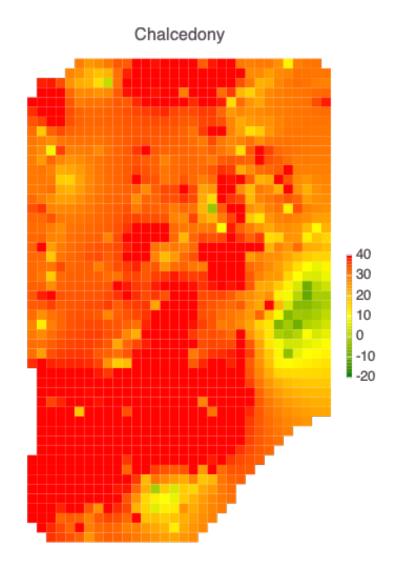
Furthermore, different attributes in the Great Basin dataset cover different areas.

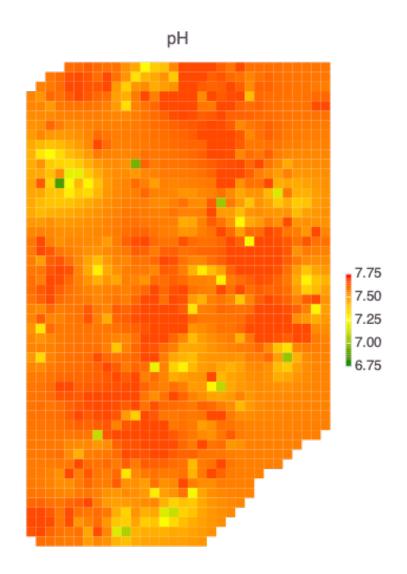
This is demonstrated in the maps generated below.

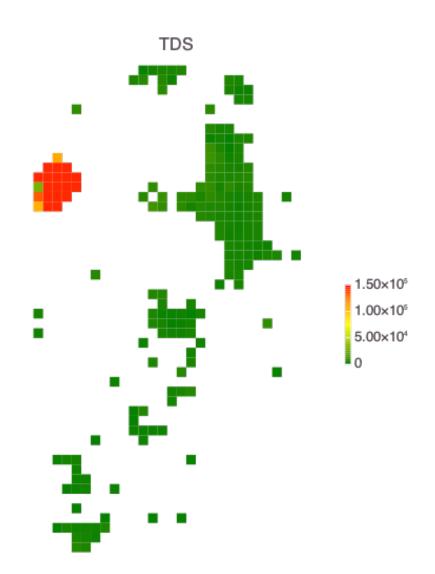
Temperature

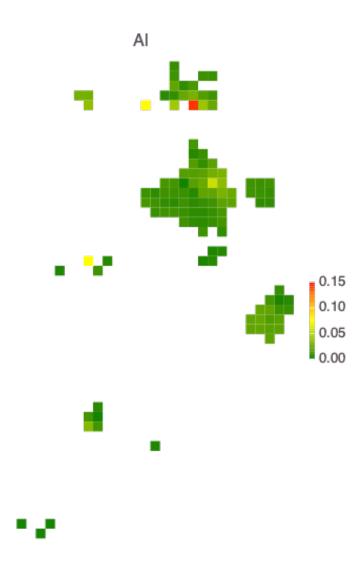


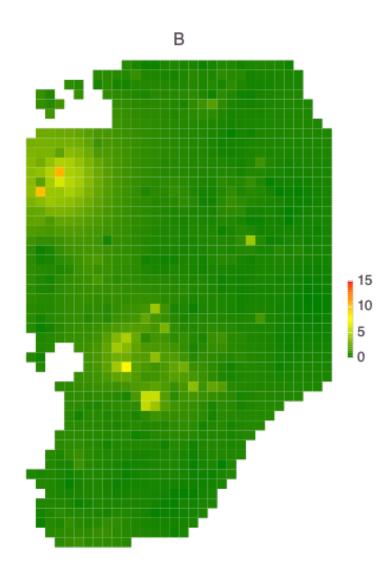


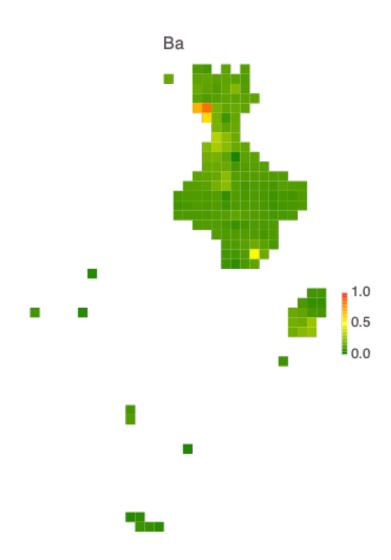


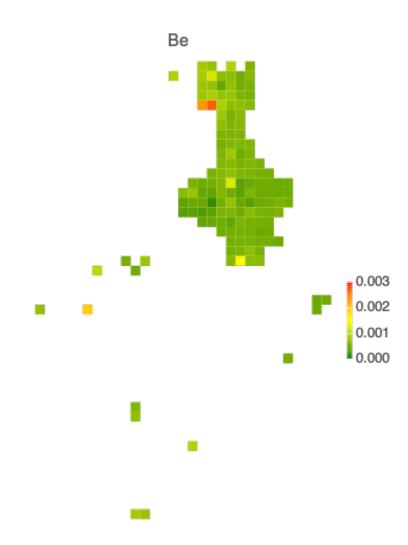


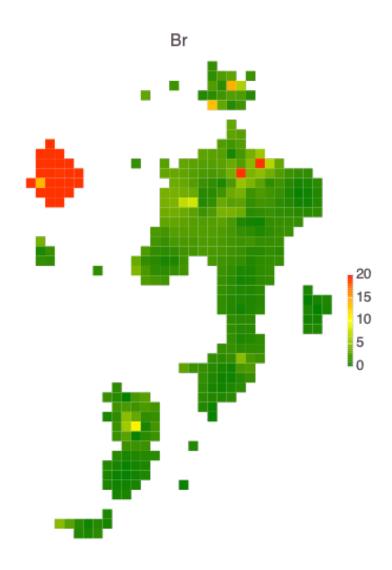


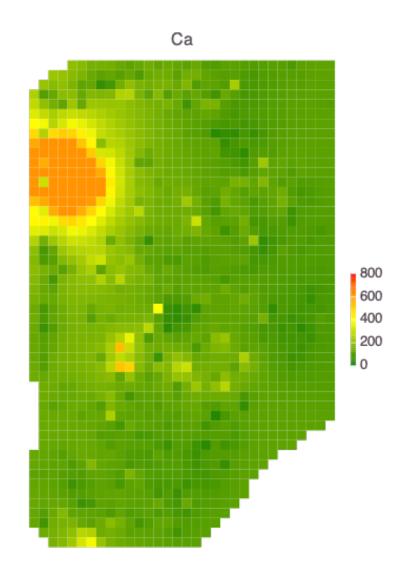


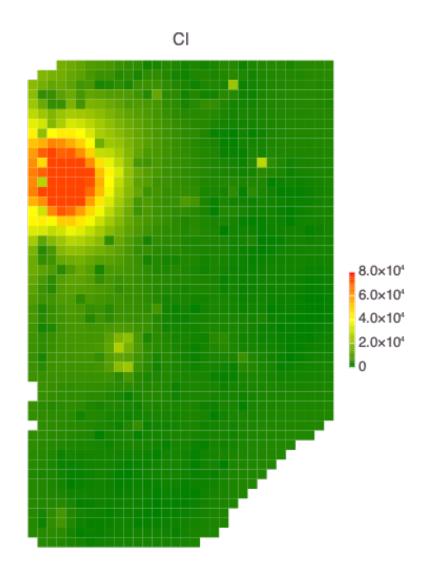


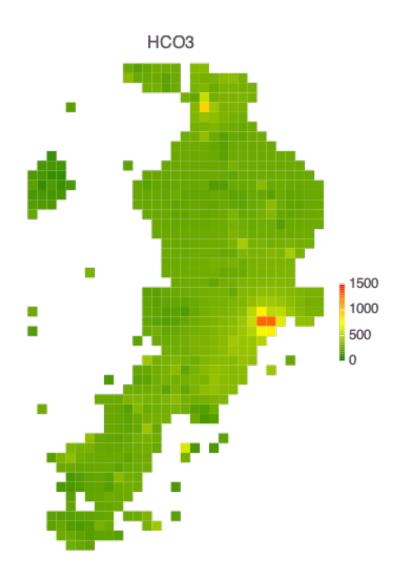


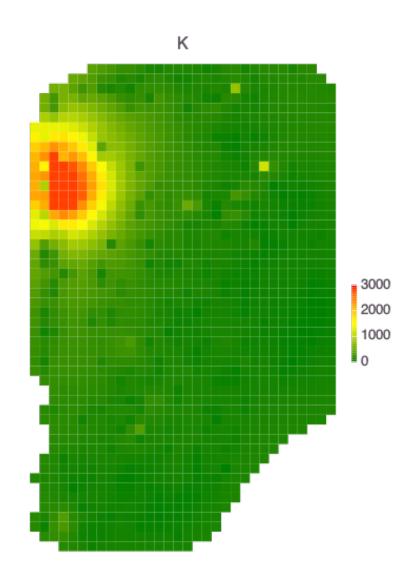


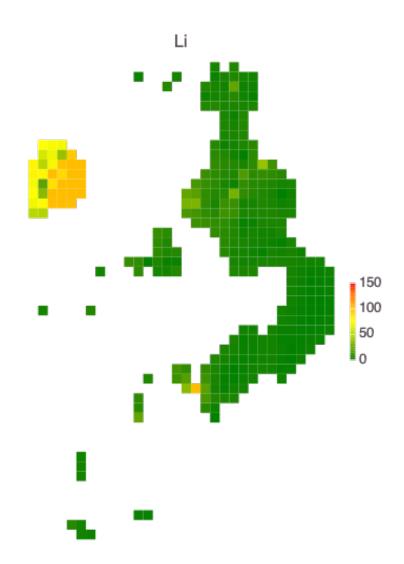


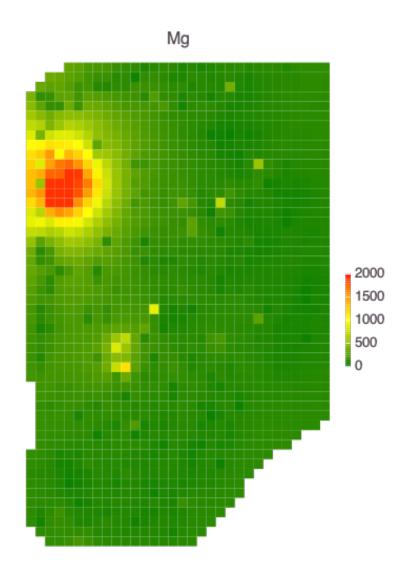


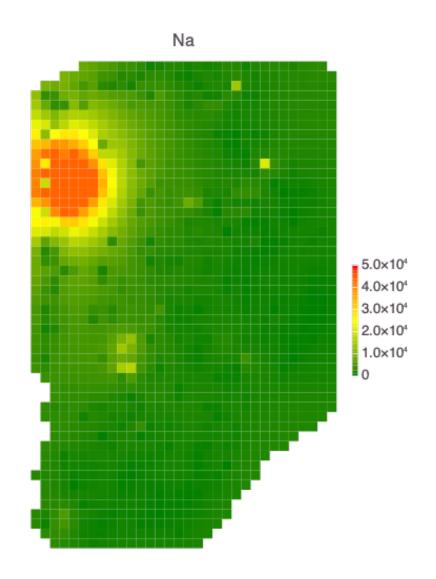


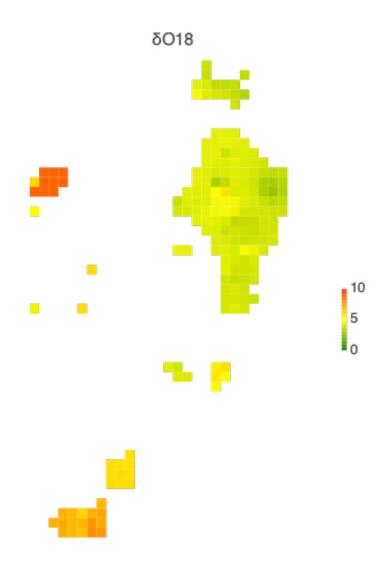












1.6 Log-transformation

Attribute values are log-transformed to better capture the order of magnitude variability.

All attributes except for Quartz, Chalcedony and pH are log-transformed (Quartz and Chalcedony have negative values).

```
[12]: logv = [true, false, false, false, true, true]

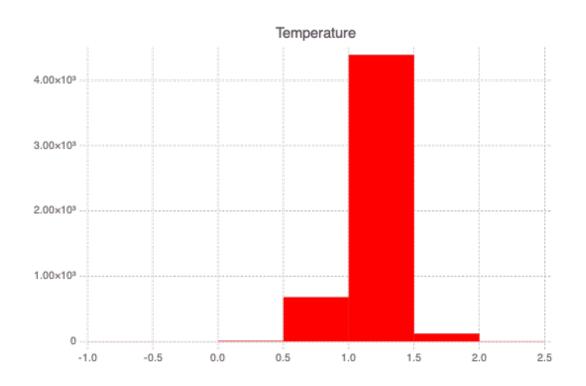
[attributes logv]
```

18×2 Matrix{Any}:

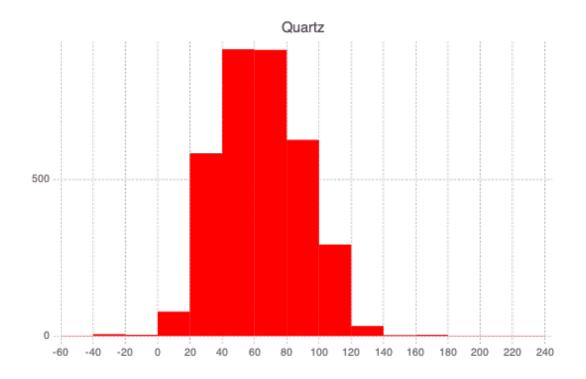
"Temperature" true

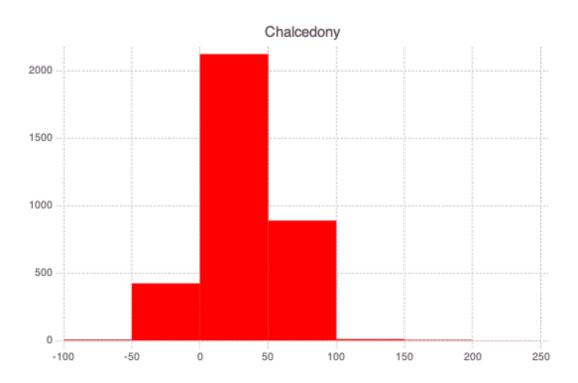
"Quartz"	false
"Chalcedony"	false
"рН"	false
"TDS"	true
"Al"	true
"B"	true
"Ba"	true
"Be"	true
"Br"	true
"Ca"	true
"Cl"	true
"HCO3"	true
"K"	true
"Li"	true
"Mg"	true
"Na"	true
" 018"	true

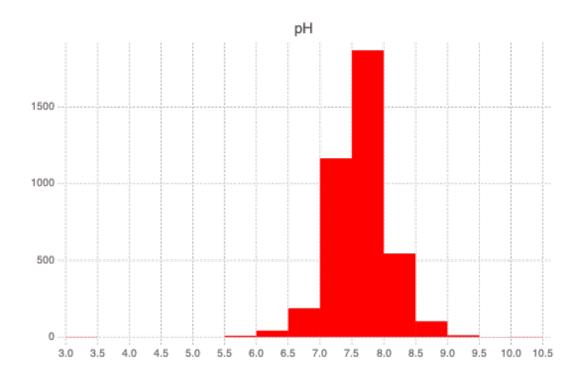
[13]: NMFk.datanalytics(X, attributes; dims=2, logv=logv);



Info: Temperature: log10-transformed
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51







 $\label{temperature: Min -1.0 Max 2.4166405 StdDev 0.19028741 Skewness -0.5570712 Count} Temperature: Min -1.0 Max 2.4166405 StdDev 0.19028741 Skewness -0.5570712 Count} Temperature: Min -1.0 Max 2.4166405 StdDev 0.19028741 Skewness -0.5570712 Count} Temperature: Min -1.0 Max 2.4166405 StdDev 0.19028741 Skewness -0.5570712 Count} Temperature: Min -1.0 Max 2.4166405 StdDev 0.19028741 Skewness -0.5570712 Count} Temperature: Min -1.0 Max 2.4166405 StdDev 0.19028741 Skewness -0.5570712 Count} Temperature: Min -1.0 Max 2.4166405 StdDev 0.19028741 Skewness -0.5570712 Count} Temperature: Min -1.0 Max 2.4166405 StdDev 0.19028741 Skewness -0.5570712 Count} Temperature: Min -1.0 Max 2.4166405 StdDev 0.19028741 Skewness -0.5570712 Count} Temperature: Min -1.0 Max 2.4166405 StdDev 0.19028741 Skewness -0.5570712 Count} Temperature: Min -1.0 Max 2.4166405 StdDev 0.19028741 Skewness -0.5570712 Count} Temperature: Min -1.0 Max 2.4166405 StdDev 0.19028741 Skewness -0.5570712 Count} Temperature: Min -1.0 Max 2.4166405 StdDev 0.19028741 Skewness -0.5570712 Count} Temperature: Min -1.0 Max 2.4166405 StdDev 0.19028741 Skewness -0.5570712 Skewness -$

5214

Quartz: Min -50.870045 Max 222.28357 StdDev 26.329222 Skewness 0.24256101 Count

3460

Chalcedony: Min -81.64773 Max 208.67426 StdDev 27.450817 Skewness 0.3369881

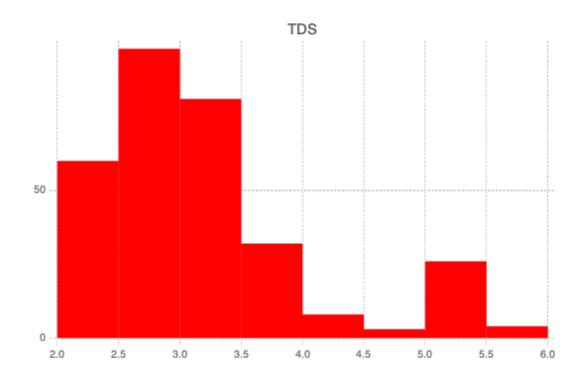
Count 3460 Info: Quartz

@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54

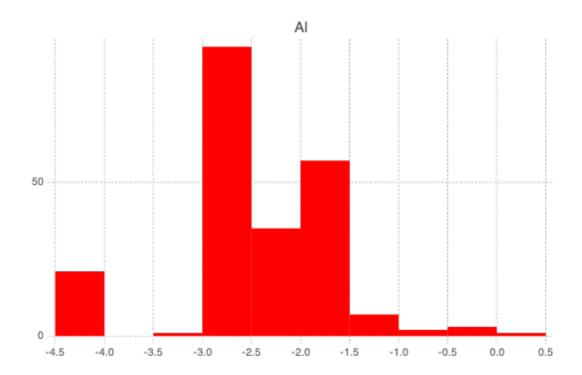
Info: Chalcedony

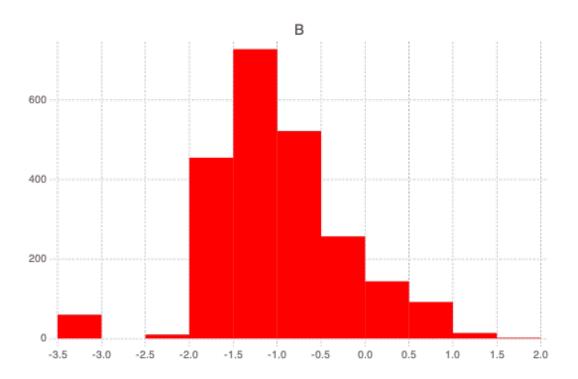
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:54

Info: pH



pH: Min 3.4 Max 10.2 StdDev 0.44822767 Skewness -0.45681924 Count 3941 Info: TDS: log10-transformed





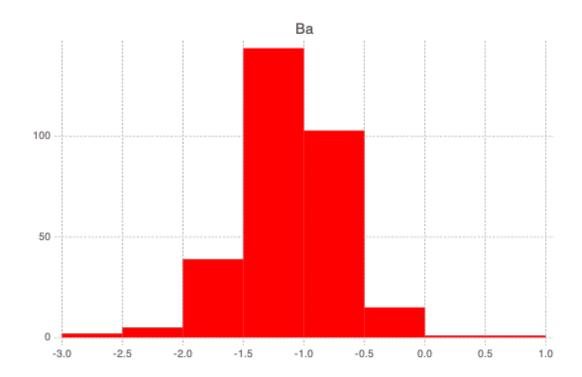
TDS: Min 2.0863597 Max 5.5171957 StdDev 0.8672777 Skewness 1.4807001 Count 312 Al: Min -4.3979397 Max 0.09725732 StdDev 0.8454361 Skewness -0.37494856 Count 221

Info: Al: log10-transformed

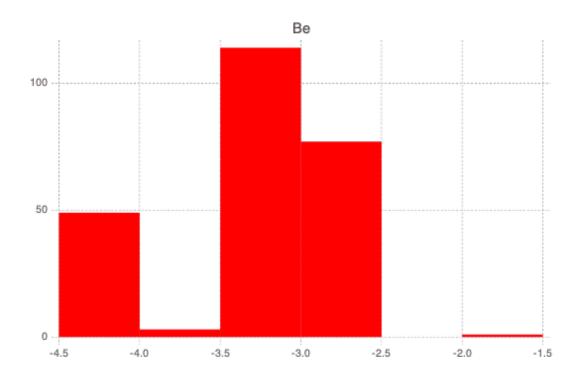
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51

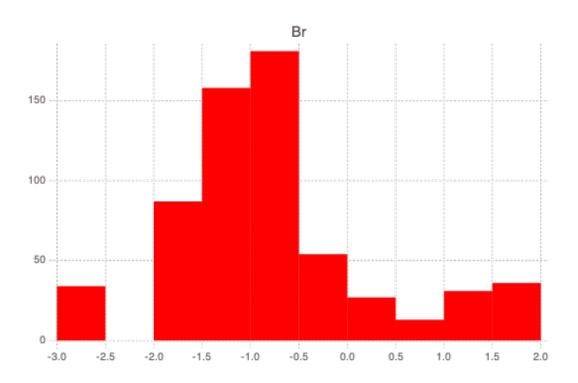
Info: B: log10-transformed

@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51



B: Min -3.30103 Max 1.8836614 StdDev 0.77384454 Skewness 0.08153698 Count 2284 Info: Ba: log10-transformed





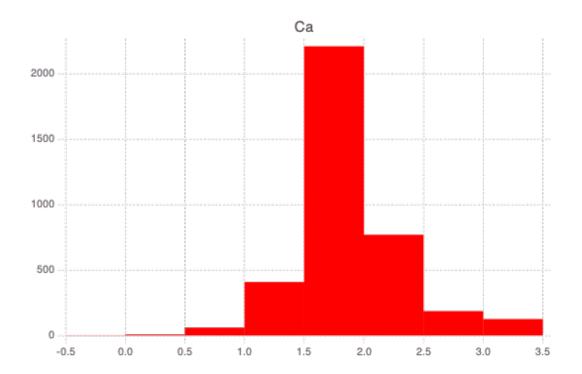
Ba: Min -2.69897 Max 0.6532125 StdDev 0.40884706 Skewness -0.013896148 Count 310 Be: Min -4.273001 Max -1.8860567 StdDev 0.46150032 Skewness -0.83869493 Count 244

Info: Be: log10-transformed

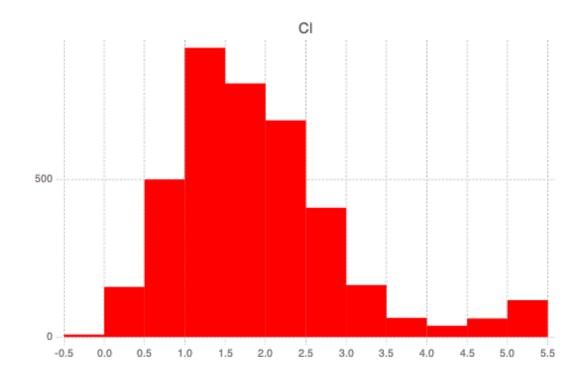
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51

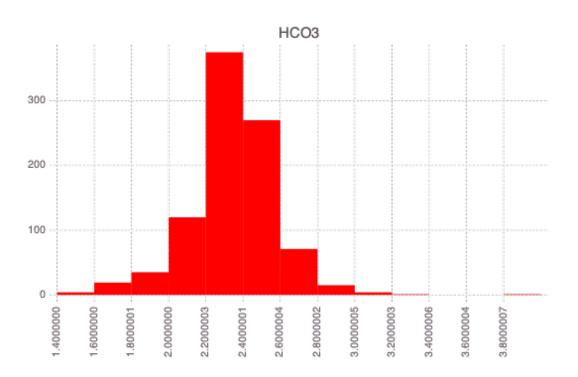
Info: Br: log10-transformed

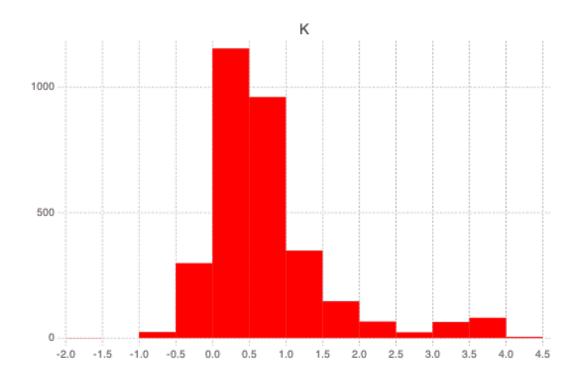
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51



Br: Min -3.0 Max 1.9242793 StdDev 1.0616237 Skewness 0.5956521 Count 621 Info: Ca: log10-transformed







Ca: Min -0.22184873 Max 3.4093695 StdDev 0.43120933 Skewness 0.5738154 Count 3772

Cl: Min -0.22184873 Max 5.3802114 StdDev 1.0519629 Skewness 1.1927316 Count 3923 HCO3: Min 1.5682018 Max 3.9645896 StdDev 0.22752158 Skewness 0.051133487 Count 915

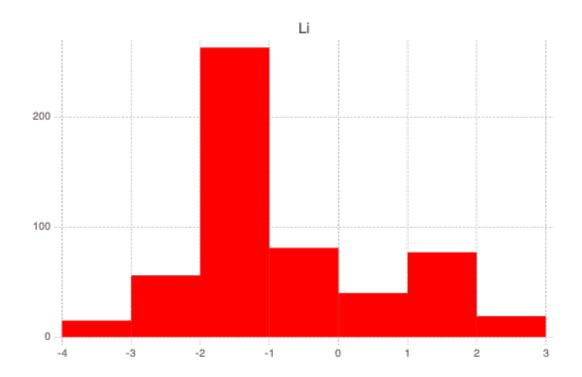
Info: Cl: log10-transformed

@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51

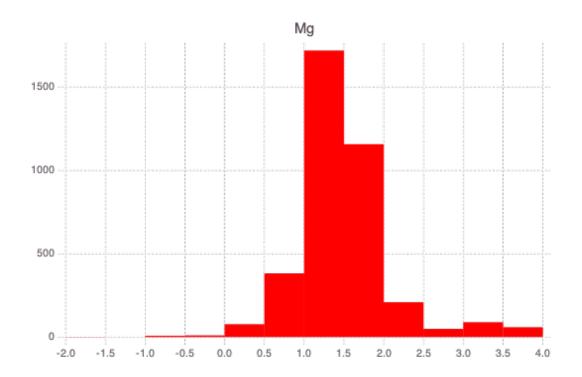
Info: HCO3: log10-transformed

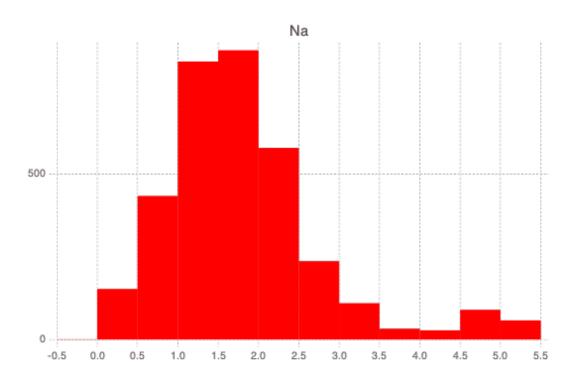
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51

Info: K: log10-transformed



K: Min -2.0 Max 4.1139436 StdDev 0.8480291 Skewness 1.8444492 Count 3177
Info: Li: log10-transformed
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51





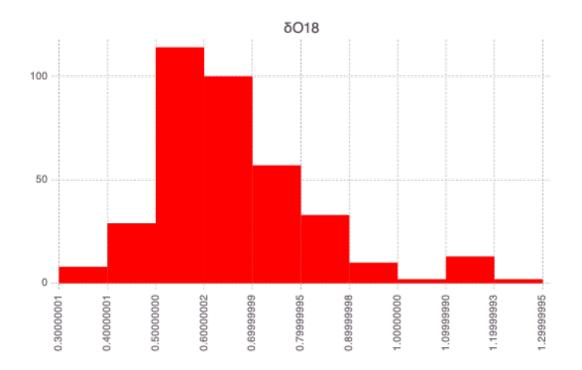
Li: Min -3.9586072 Max 2.9867718 StdDev 1.4681796 Skewness 0.6889145 Count 551 Mg: Min -2.0 Max 3.929419 StdDev 0.5826601 Skewness 1.142913 Count 3760

Info: Mg: log10-transformed

@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51

Info: Na: log10-transformed

@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51



Na: Min -0.30103 Max 5.20412 StdDev 0.985548 Skewness 1.3556563 Count 3437 018: Min 0.33243838 Max 1.2137833 StdDev 0.16311567 Skewness 1.1355046 Count 368

Name Min Max StdDev Count (non-NaN's)
Temperature -1.0 2.4166405 0.19028741 -0.5570712 5214
Quartz -50.870045 222.28357 26.329222 0.24256101 3460
Chalcedony -81.64773 208.67426 27.450817 0.3369881 3460
pH 3.4 10.2 0.44822767 -0.45681924 3941
TDS 2.0863597 5.5171957 0.8672777 1.4807001 312
Al -4.3979397 0.09725732 0.8454361 -0.37494856 221
B -3.30103 1.8836614 0.77384454 0.08153698 2284
Ba -2.69897 0.6532125 0.40884706 -0.013896148 310
Be -4.273001 -1.8860567 0.46150032 -0.83869493 244
Br -3.0 1.9242793 1.0616237 0.5956521 621
Ca -0.22184873 3.4093695 0.43120933 0.5738154 3772

Cl -0.22184873 5.3802114 1.0519629 1.1927316 3923 HCO3 1.5682018 3.9645896 0.22752158 0.051133487 915

```
K -2.0 4.1139436 0.8480291 1.8444492 3177
Li -3.9586072 2.9867718 1.4681796 0.6889145 551
Mg -2.0 3.929419 0.5826601 1.142913 3760
Na -0.30103 5.20412 0.985548 1.3556563 3437
018 0.33243838 1.2137833 0.16311567 1.1355046 368
Info: 018: log10-transformed
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:51
Info: Attributes
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPreprocess.jl:70
```

1.7 Normalize the data

```
[14]: Xnl, xlmin, xlmax, zflag = NMFk.normalizematrix_col(X; logv=logv);
```

1.8 Define the number of signatures to be explored

```
[15]: nkrange = 2:10
```

2:10

1.9 Define a directory where outputs should be stored

```
[16]: resultdir = "utah/results";
```

1.10 Define the number of NMF iterations (NMF random initial guess runs):

```
[17]: nruns = 100;
```

1.11 Run NMFk on normalized data

```
[18]: #W, H, fitquality, robustness, aic = NMFk.execute(Xnl, nkrange, nruns; cutoff=0.

→3, resultdir=resultdir, casefilename="nmfk-nl", load=true)

W, H, fitquality, robustness, aic = NMFk.load(nkrange, nruns; cutoff=0.3, □

→resultdir=resultdir, casefilename="nmfk-nl");
```

```
186.979 Silhouette:
                                            0.5600511 AIC:
                                                              -193490.6 Signal
Signals: 2 Fit:
order: [1, 2]
Signals: 3 Fit:
                    116.1197 Silhouette:
                                            0.3400365 AIC:
                                                              -202059.3 Signal
order: [1, 2, 3]
                    81.67226 Silhouette: -0.004722083 AIC:
Signals: 4 Fit:
                                                                -205653 Signal
order: [1, 2, 3, 4]
Signals: 5 Fit:
                    55.85581 Silhouette: 0.03561851 AIC:
                                                              -210367.2 Signal
order: [1, 2, 3, 4, 5]
Signals: 6 Fit:
                    37.37445 Silhouette:
                                           0.08498218 AIC:
                                                             -215954.6 Signal
order: [1, 2, 3, 4, 5, 6]
                    22.77074 Silhouette: -0.06623857 AIC:
Signals: 7 Fit:
                                                              -225288.2 Signal
order: [1, 2, 3, 4, 5, 6, 7]
                   14.94362 Silhouette:
Signals: 8 Fit:
                                            0.0637157 AIC:
                                                              -231651.2 Signal
```

```
order: [1, 2, 3, 4, 5, 6, 7, 8]
Signals: 9 Fit: 9.241436 Silhouette: -0.1125796 AIC: -240388.3 Signal order: [1, 2, 3, 4, 5, 6, 7, 8, 9]
Signals: 10 Fit: 6.104004 Silhouette: -0.01305462 AIC: -246494 Signal order: [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]
Info: Optimal solution: 3 signals
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkIO.jl:30
```

1.12 Get the acceptable solutions within the present range of number of signatures:

```
[19]: NMFk.getks(nkrange, robustness[nkrange], 0.3)
2-element Vector{Int64}:
2
3
```

1.13 Get the optimal number of signatures:

```
[20]: NMFk.getk(nkrange, robustness[nkrange], 0.3)
```

3

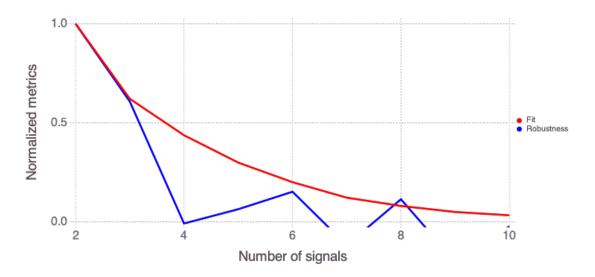
1.14 Plot the fit and robustness of the solution

```
[21]: resultdirpost = "utah/results-postprocessing-nl-$(nruns)"
figuredirpost = "utah/figures-postprocessing-nl-$(nruns)"
NMFk.plot_feature_selecton(nkrange, fitquality, robustness;

in the processing-nl-$(nruns)"

NMFk.plot_feature_selecton(nkrange, fitquality, robustness;

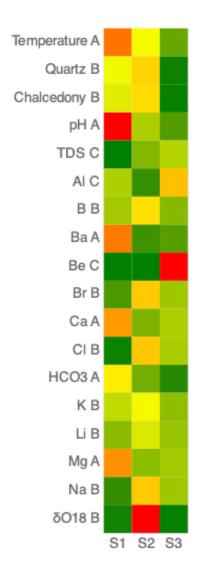
in the processing-nl-$(nruns)"
```



1.15 Analysis of the optimal solution

```
[22]: Sorder, Wclusters, Hclusters = NMFk.clusterresults(NMFk.getk(nkrange,
       →robustness[nkrange], 0.3), W, H, string.(collect(1:npoints)), attributes;
       →lon=xcoord, lat=ycoord, resultdir=resultdirpost, figuredir=figuredirpost,
       →ordersignal=:Wcount, Hcasefilename="attributes", Wcasefilename="locations", U
       →biplotcolor=:WH, sortmag=false, biplotlabel=:H, point_size_nolabel=2Gadfly.
       →pt, point_size_label=4Gadfly.pt)
       Info: Number of signals: 3
       @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:205
       Info: Attributes (signals=3)
       @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:209
      Warning: type
     Clustering.KmeansResult{Core.Array{Core.Float32,2},Core.Float32,Core.Int64} not
     present in workspace; reconstructing
       @ JLD /Users/vvv/.julia/packages/JLD/JHrZe/src/jld_types.jl:697
       Info: Robust k-means analysis results are loaded from file utah/results-
     postprocessing-nl-100/Hmatrix-3-3_18-1000.jld!
       @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkCluster.jl:67
      Warning: Procedure to find unique signals could not identify a solution ...
       @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkCluster.jl:158
      Warning: Procedure to find unique signals could not identify a solution ...
       @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkCluster.jl:158
      Warning: Procedure to find unique signals could not identify a solution ...
       @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkCluster.jl:158
      Warning: type
     Clustering.KmeansResult{Core.Array{Core.Float32,2},Core.Float32,Core.Int64} not
     present in workspace; reconstructing
       @ JLD /Users/vvv/.julia/packages/JLD/JHrZe/src/jld_types.jl:697
       Info: Robust k-means analysis results are loaded from file utah/results-
     postprocessing-nl-100/Wmatrix-3-3_5218-1000.jld!
       @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkCluster.jl:67
      Warning: Procedure to find unique signals could not identify a solution ...
       @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkCluster.jl:158
      Warning: Procedure to find unique signals could not identify a solution ...
       @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkCluster.jl:158
      Warning: Procedure to find unique signals could not identify a solution ...
       @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkCluster.jl:158
     6×2 Matrix{Any}:
      "Ha"
                     1.0
      "Temperature"
                     0.858848
      "Ba"
                     0.84477
      "Mg"
                     0.788068
      "Ca"
                     0.76783
```

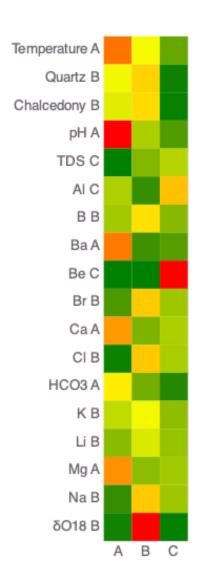
```
"HC03"
                0.549396
 Info: Signal B -> A Count: 6
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:316
 Info: Signal A -> B Count: 9
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:316
 Info: Signal C -> C Count: 3
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:316
 Info: Signal A (S1) (k-means clustering)
 @ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:333
9×2 Matrix{Any}:
 " 018"
              1.0
 "Cl"
               0.651079
 "Na"
               0.643991
 "Br"
               0.642053
 "Quartz"
               0.620207
 "Chalcedony"
               0.596872
 "B"
               0.586983
 "K"
               0.475275
"Li"
               0.414782
3×2 Matrix{Any}:
 "Be"
       1.0
 "Al"
        0.672723
 "TDS" 0.332944
```

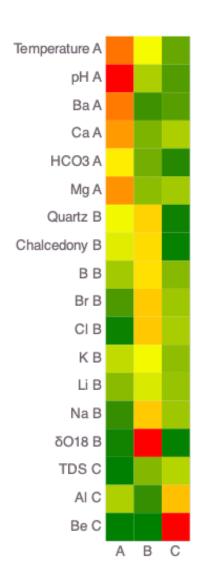


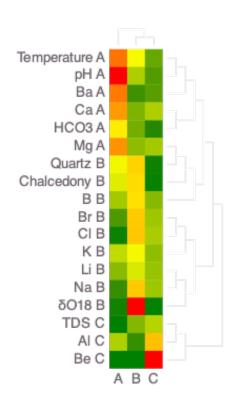
Info: Signal B (S2) (k-means clustering)

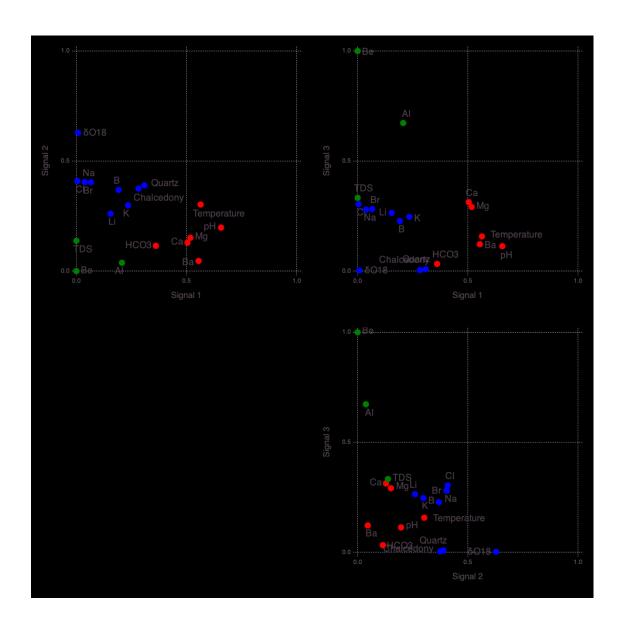
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:333

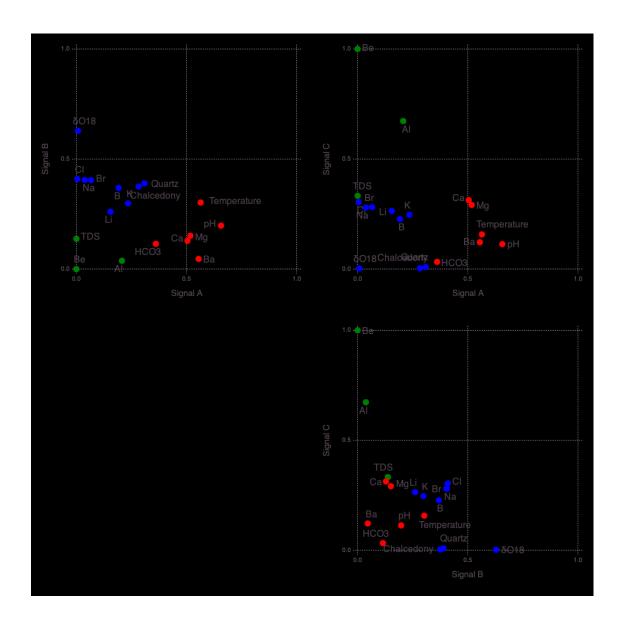
Info: Signal C (S3) (k-means clustering)











2131×2 Matrix{Any}:

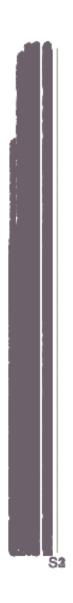
- "4816" 1.0
- "4655" 0.970208
- "4826" 0.958804
- "2260" 0.955817
- "4015" 0.938536
- "3257" 0.93743
- "4889" 0.929527
- "1797" 0.924136
- "3405"
- 0.924069 "2566" 0.905143

```
"350"
         0.492666
"341"
         0.491852
"2730"
         0.487104
"3987"
         0.47064
"483"
         0.466211
"2909"
         0.464978
"476"
         0.46367
"2931"
         0.435235
"452"
         0.359449
1966×2 Matrix{Any}:
"4430"
         1.0
         0.972819
"2992"
"2309"
         0.920633
"4913"
         0.90427
"4056"
         0.88218
"564"
         0.868838
"4978"
         0.866204
"4319"
         0.857647
"4788"
         0.855117
"2468"
         0.831267
"375"
         0.203084
         0.202853
"159"
"3798"
         0.198906
"5112"
         0.1978
"738"
         0.19415
"3317"
         0.193811
"747"
         0.189873
"10"
         0.181605
"4954"
         0.163099
1121×2 Matrix{Any}:
"5013"
         1.0
"5118"
         0.985958
"5064"
         0.978501
"5068"
         0.974911
"5126"
         0.969774
"2554"
         0.952582
"5049"
         0.948387
"5048"
         0.914722
"5006"
         0.910949
"5095"
         0.910366
"4154"
         0.174466
"4710"
         0.174457
"3376"
         0.172963
"1412"
         0.170218
```

"3662"

0.161509

```
"4300" 0.160252
"2742" 0.148677
"4289" 0.144853
"2028" 0.129906
```



Info: Locations (signals=3)
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:391
Info: Signal A (S1) Count: 2131
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:404
Info: Signal B (S2) Count: 1966
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:404
Info: Signal C (S3) Count: 1121
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:404
Info: Signal A -> A Count: 2131

@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:414
Info: Signal B -> B Count: 1966

@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:414
Info: Signal C -> C Count: 1121

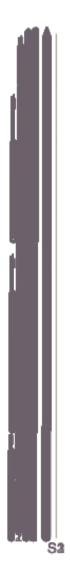
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:414 Info: Signal A (remapped k-means clustering)

@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:429

Info: Signal B (remapped k-means clustering)

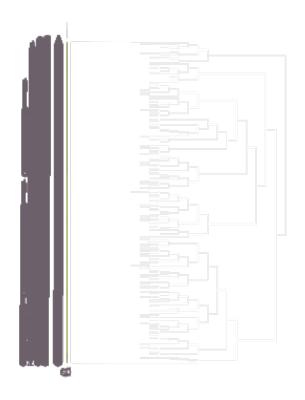
@ NMFk /Users/vvv/.julia/dev/NMFk/src/NMFkPostprocess.jl:429

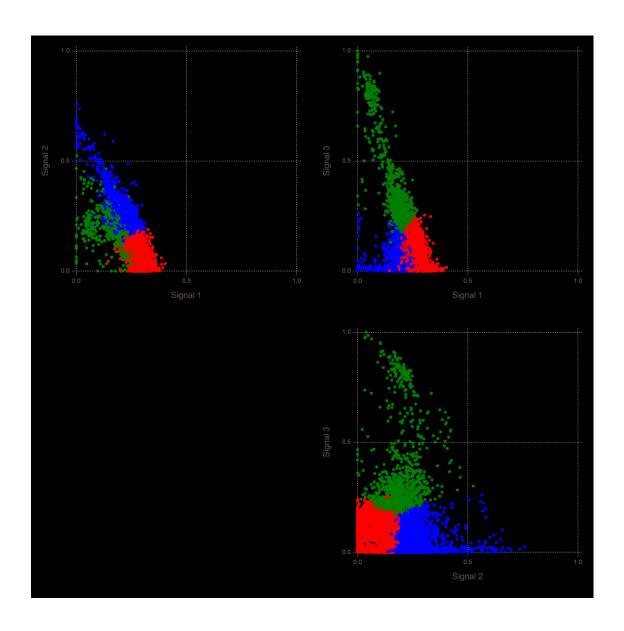
Info: Signal C (remapped k-means clustering)

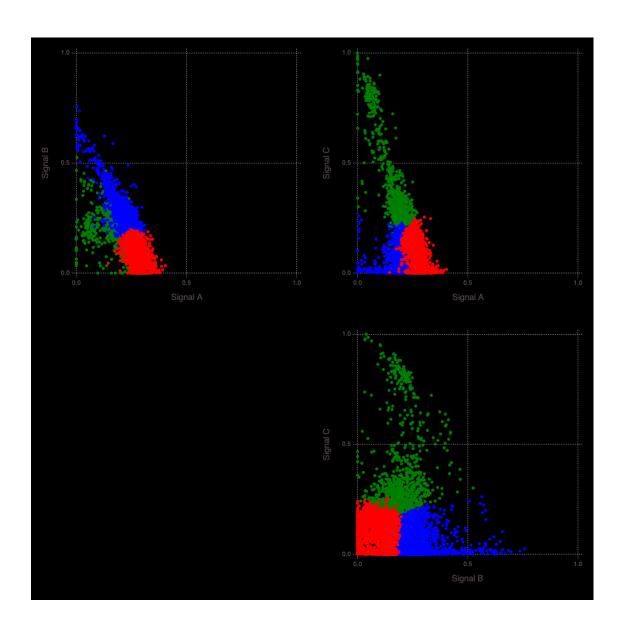


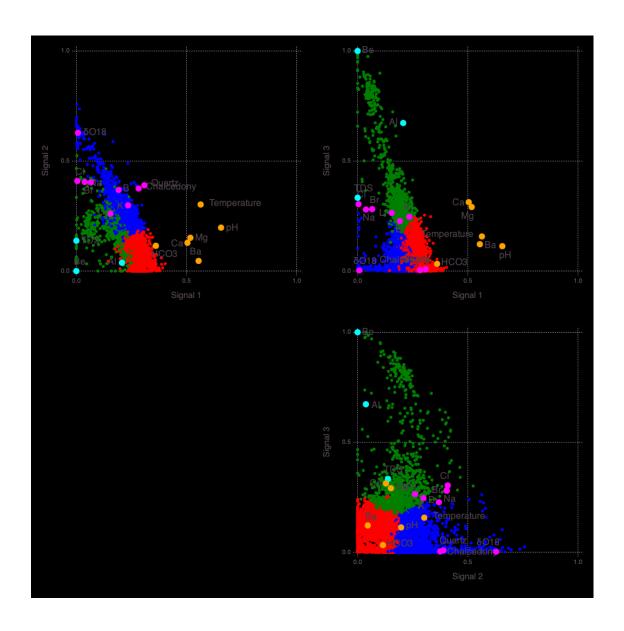


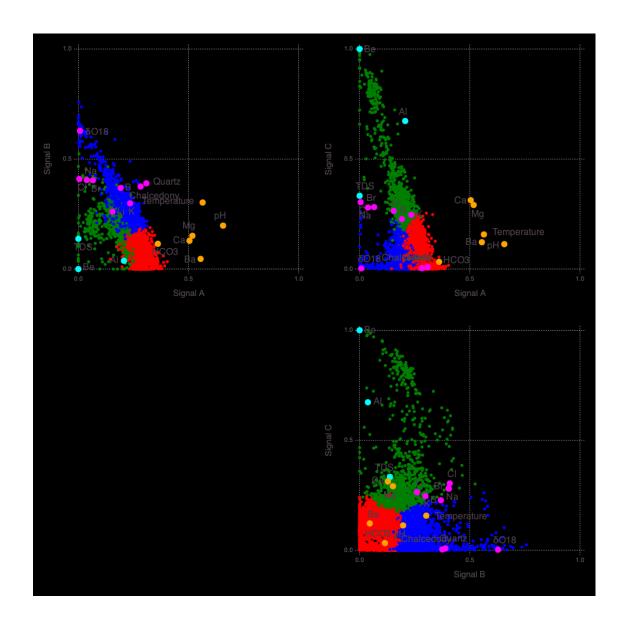












1.16 Associations of the data attributes with the extracted signatures

[23]: Mads.display("utah/results-postprocessing-nl-100/attributes-3-groups.txt")

Signal A (S1)
pH 1.0
Temperature 0.859
Ba 0.845

```
0.788
Mg
                 0.768
Ca
HCO3
                 0.549
Signal B (S2)
018
                 1.0
Cl
                 0.651
Na
                 0.644
Br
                 0.642
Quartz
                 0.62
Chalcedony
                 0.597
В
                 0.587
K
                 0.475
Li
                 0.415
Signal C (S3)
Ве
                 1.0
Al
                 0.673
TDS
                 0.333
```

1.17 Associations of the data locations with the extracted signatures

```
[24]: locations, lhs = DelimitedFiles.readdlm("utah/results-postprocessing-nl-100/
      →locations-3.csv", ',', header=true)
     clusters = sort(unique(locations[:,end]))
     for i=1:size(clusters,1)
             locations[locations .== clusters[i]] .= Integer(i)
     end
     locations = convert.(Float32, locations)
     5218×7 Matrix{Float32}:
         1.0 -111.06
                        39.4341
                               0.6627
                                          0.0234368
                                                      0.124347
                                                                  1.0
         2.0 -111.066 39.4233
                                0.670377
                                          0.0287214
                                                      0.14722
                                                                  1.0
         3.0 -111.053 39.4658 0.615474 8.88704f-7
                                                      0.203825
                                                                  1.0
         4.0 -111.07
                       39.4286 0.669782 0.0108548
                                                      0.0435491
                                                                  1.0
         5.0 -111.112
                       39.3211 0.640001 0.152409
                                                                  1.0
                                                      0.00993296
         6.0 -111.056
                       39.4947
                                0.763099 5.00038f-5
                                                      0.0934381
                                                                  1.0
         7.0 -111.056
                       39.4947
                                0.760624 0.0
                                                      0.0882335
                                                                  1.0
         8.0 -111.057
                       39.4947
                                0.69465
                                          0.0
                                                      0.175217
                                                                  1.0
         9.0 -111.116
                       39.328
                                0.855406
                                          0.0417626
                                                      0.00724127
                                                                  1.0
        10.0 -111.113
                       39.3455
                                0.528689 0.181605
                                                      0.00429201
                                                                  2.0
      5210.0 -113.908
                       41.6355
                                0.575887 0.313012
                                                      0.12041
                                                                  2.0
      5211.0 -113.908
                       41.6369
                                0.497084 0.331514
                                                                  2.0
                                                      0.00821709
      5212.0 -113.909
                       41.6333
                                0.569316
                                         0.312737
                                                      0.110429
                                                                  2.0
      5213.0 -113.935
                       41.5866
                                0.785556 0.214434
                                                      0.00475439
                                                                  1.0
```

0.103709

2.0

5214.0 -113.919 41.6333 0.607505 0.337506

```
5215.0 -113.955 41.563
                                 0.626563 0.314026
                                                       0.00605548 2.0
      5216.0 -113.936 41.6496 0.723449 0.206588
                                                       0.00947504 1.0
      5217.0 -113.926 41.7227 0.644214 0.224996
                                                       0.0861631
                                                                   1.0
      5218.0 -113.984 41.6888 0.70402 0.208866
                                                       0.0225921
                                                                   1.0
[25]: GMT.grdimage("utah/maps/utah.nc", shade=(azimuth=100, norm="e0.8"), proj=:
      →Mercator.
          color=GMT.makecpt(color=:grayC, transparency=10, range=(0,5000,500),
      ⇔continuous=true),
         figsize=8, conf=(MAP_FRAME_TYPE="plain",__
       →MAP_GRID_PEN_PRIMARY="thinnest,gray,.", MAP_GRID_CROSS_SIZE_SECONDARY=0.1, U
       →MAP_FRAME_PEN=0.5, MAP_TICK_PEN_PRIMARY=0.1, MAP_TICK_LENGTH_PRIMARY=0.01,
      →FORMAT GEO MAP="ddd", FONT ANNOT PRIMARY=0.1, FONT ANNOT SECONDARY=0.1),

→frame=(axis="lrtb"))
      GMT.legend!(box=(pen=false, fill=:white),
                  pos=(inside=true, anchor=:T, width=1.30, justify=:CM, offset=(-0.7, __
      \rightarrow-0.6)),
                  GMT.text record([
                      "S 0.10i c 0.10i red 0.25p 0.2i A"
                      "S 0.10i c 0.10i gold 0.25p 0.2i B"
                      "S 0.10i c 0.10i blue 0.25p 0.2i C"]),
                  par=(:FONT_ANNOT_PRIMARY, "8p,Arial"))
      GMT.scatter!(locations[:,2], locations[:,3], marker=:c, markersize=:0.15,
          color=(:red, :gold, :blue), zcolor=locations[:,end], alpha=10,
          coast=(proj=:Mercator,
         DCW=(country="US.UT", pen=(0.5,:black))),
         fmt=:png, savefig="utah/maps/signatures-3")
      Images.load("utah/maps/signatures-3.png")
```

**** WARNING: .setopacityalpha is deprecated (as of 9.53.0) and will be removed in a future release

**** See .setfillconstantalpha/.setalphaisshape for the improved solution **** WARNING: .setopacityalpha is deprecated (as of 9.53.0) and will be removed in a future release

**** See .setfillconstantalpha/.setalphaisshape for the improved solution pslegend [WARNING]: Representation of font type not recognized. Using default.

