# CoDaPack Tutorial

Data Science for the Geosciences, 2022

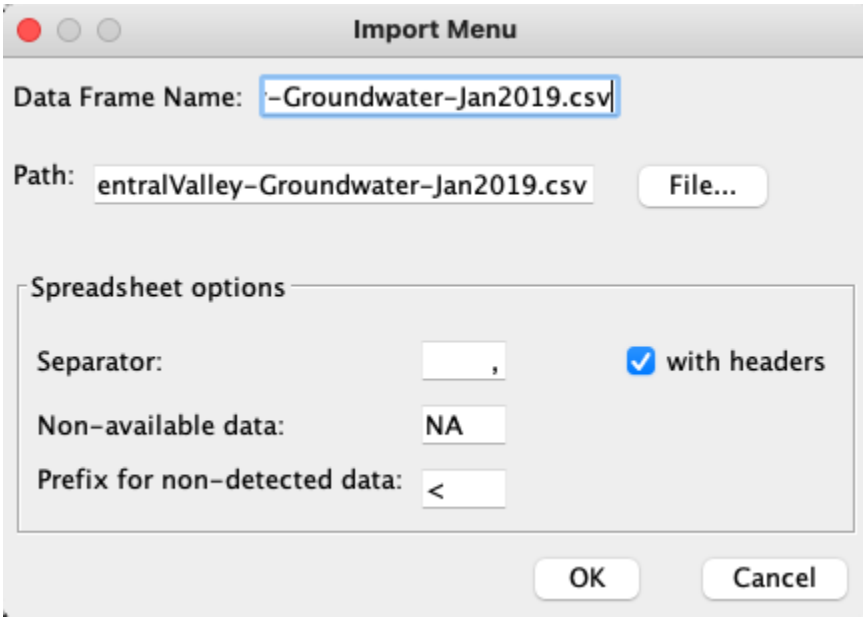
Author: Lijing Wang, David Yin, Jef Caers

## Download CoDaPack

- Download CoDAPACK from this link: http://ima.udg.edu/codapack/.
- Then click on the windows, Mac or Java icon depending on where to install it.

## Load data to CoDaPack

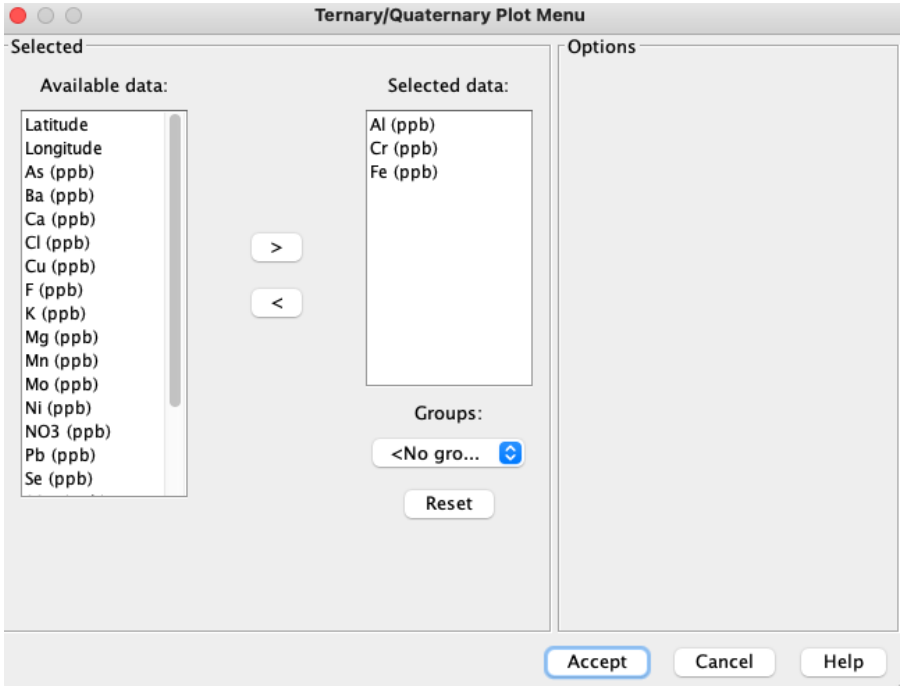
- Download the groundwater quality dataset, using right click and save as….
- Open CoDaPack
- Click File -> Import -> Import CSV/Text Data… to import our dataset. Please change the separator to comma ‘,’.

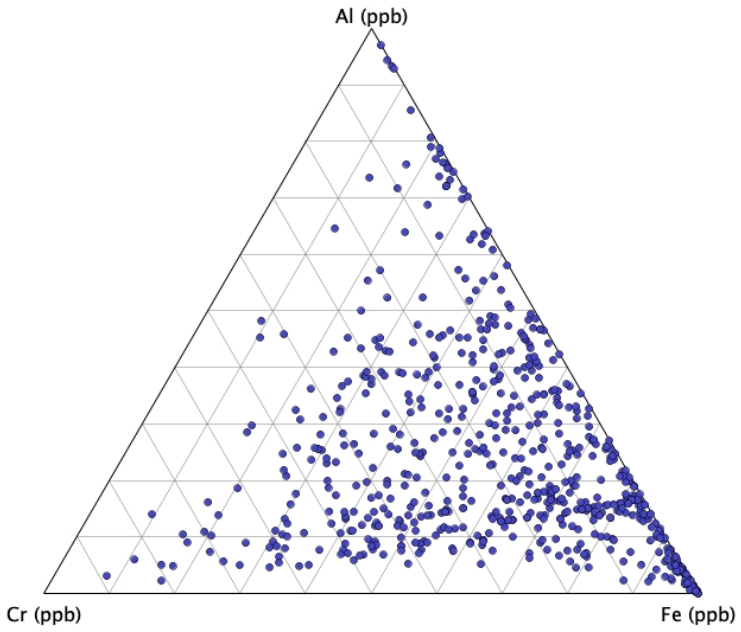



## Ternary Diagram

- Click Graph -> Ternary/Quaternary plot

- Select the data you would like to plot in a ternary diagram

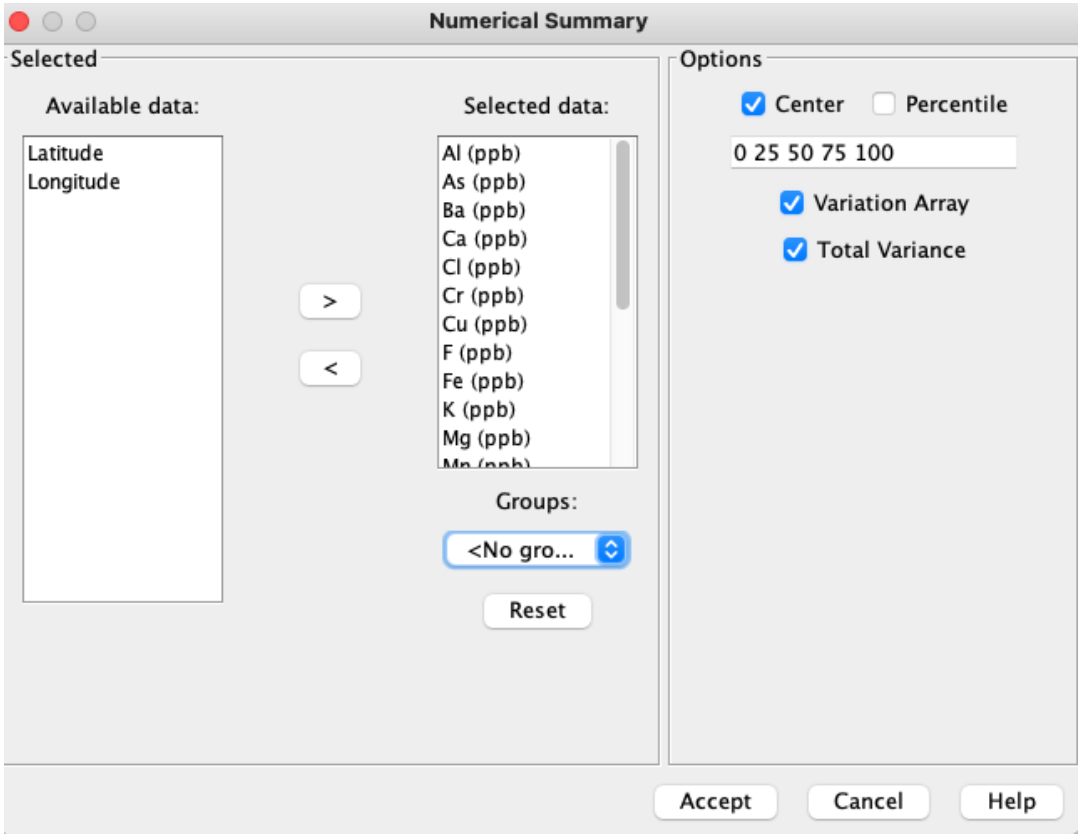



# Variation array

- Click Statistics -> Compositional statistics summary

- Select the data you would like to perform summary statistics

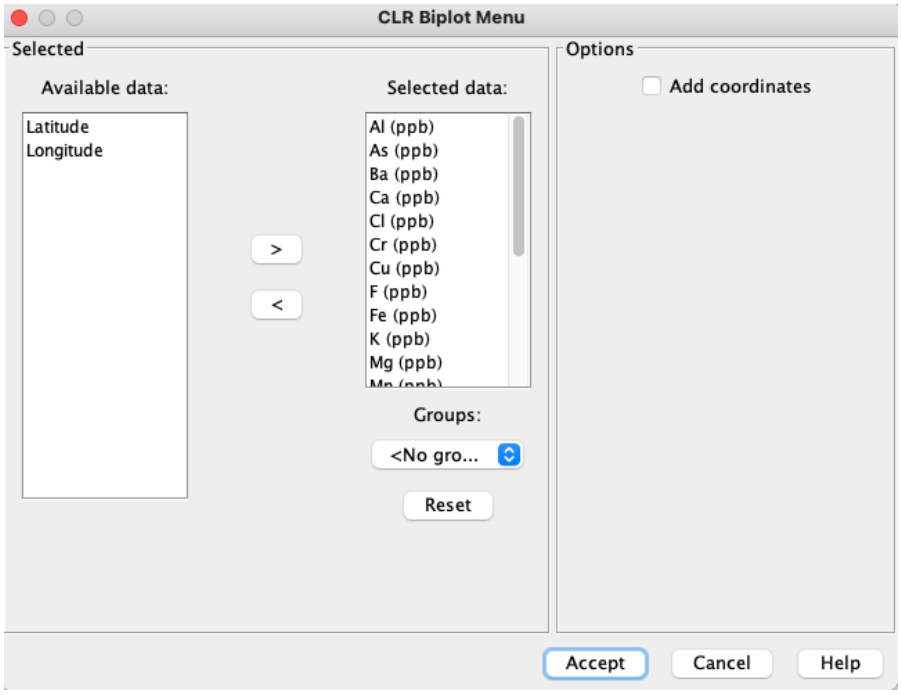


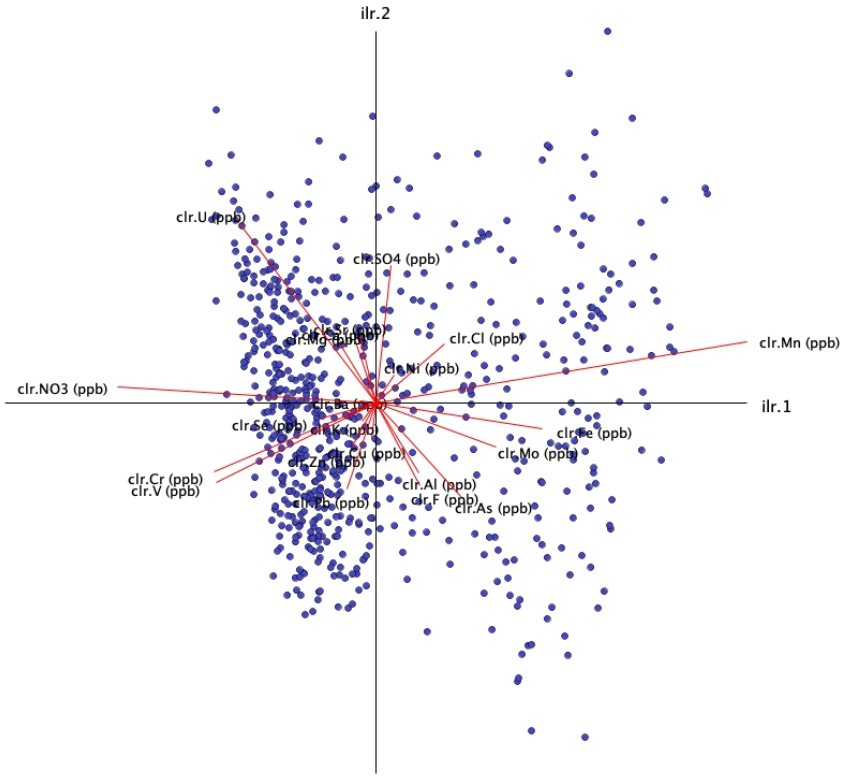

Variation array:

| Xi\Xj | Al (ppb) | As (ppb) | Ba (ppb) | Ca (ppb) | Cl (ppb) | Cr (ppb) | Cu (ppb) | F (ppb) | Fe (ppb) | K (ppb) | Mg (ppb) | Mn (ppb) | Mo (ppb) | Ni (ppb) | NO3 (ppb) | Pb (ppb) | Se (ppb) | SO4 (ppb) | Sr (ppb) | U (ppb) | V (ppb) | Zn (ppb) | clr variances | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Al (ppb) | | 1.8187 | 2.6682 | 1.9893 | 2.1355 | 3.5242 | 1.1581 | 1.0255 | 2.3620 | 1.8338 | 4.1912 | 6.6286 | 1.7172 | 1.9756 | 5.4229 | 2.1832 | 2.6592 | 3.1857 | 2.1296 | 5.2488 | 3.7094 | 2.5702 | 1.0462 | |
| As (ppb) | -0.0966 | | 2.5670 | 2.7044 | 2.8402 | 4.5382 | 2.1868 | 1.4208 | 2.5411 | 2.0357 | 4.5807 | 5.7295 | 1.6976 | 2.5908 | 7.1786 | 3.1766 | 3.3522 | 4.4754 | 2.9287 | 6.0916 | 3.7045 | 3.8042 | 1.5852 | |
| Ba (ppb) | 3.0667 | 3.1633 | | 0.3068 | 2.2382 | 2.8771 | 1.6654 | 2.0214 | 2.7381 | 1.0430 | 1.6823 | 7.2436 | 3.3026 | 1.6875 | 4.1130 | 2.4539 | 2.6873 | 3.8088 | 0.3422 | 4.4961 | 2.8349 | 2.5804 | 0.8841 | |
| Ca (ppb) | 9.2750 | 9.3716 | 6.2083 | | 1.3796 | 2.4694 | 1.0475 | 1.7167 | 2.5409 | 0.8455 | 1.1961 | 6.9099 | 2.6064 | 1.0655 | 3.5544 | 2.1517 | 1.8480 | 1.7179 | 0.1461 | 3.1504 | 2.7995 | 2.2050 | 0.3574 | |
| Cl (ppb) | 9.0297 | 9.1263 | 5.9630 | -0.2453 | | 4.2549 | 1.8750 | 2.1040 | 2.5367 | 2.0206 | 3.1572 | 5.5405 | 2.2614 | 1.9252 | 6.0837 | 3.1944 | 2.5372 | 2.0810 | 1.3246 | 5.0272 | 5.2024 | 3.1880 | 1.1735 | |
| Cr (ppb) | -0.8984 | -0.8018 | -3.9651 | -10.1734 | -9.9281 | | 2.5871 | 3.0743 | 5.7430 | 2.3790 | 3.1370 | 13.1485 | 5.3106 | 3.3445 | 3.0060 | 3.1409 | 2.3335 | 4.7090 | 2.4849 | 5.3227 | 2.2625 | 3.6873 | 2.1111 | |
| Cu (ppb) | -1.0244 | -0.9278 | -4.0911 | -10.2994 | -10.0541 | -0.1259 | | 1.0796 | 2.5512 | 1.1314 | 2.5072 | 7.0683 | 2.1379 | 1.3784 | 4.1586 | 1.3014 | 2.0256 | 2.5722 | 1.1905 | 4.3186 | 2.7016 | 1.6756 | 0.5099 | |
| F (ppb) | 3.9325 | 4.0291 | 0.8658 | -5.3425 | -5.0972 | 4.8309 | 4.9569 | | 2.0675 | 1.4894 | 3.1684 | 6.2731 | 1.2303 | 1.8045 | 5.3947 | 1.9459 | 2.2395 | 2.9779 | 1.7929 | 5.6410 | 3.0204 | 2.5623 | 0.7709 | |
| Fe (ppb) | 1.3216 | 1.4182 | -1.7451 | -7.9534 | -7.7081 | 2.2200 | 2.3460 | -2.6109 | | 2.4695 | 3.9974 | 3.3353 | 2.3659 | 2.5155 | 8.5683 | 3.7891 | 4.2673 | 4.1205 | 2.6756 | 7.6642 | 6.1828 | 3.8637 | 1.9003 | |
| K (ppb) | 6.4901 | 6.5867 | 3.4234 | -2.7849 | -2.5396 | 7.3885 | 7.5145 | 2.5576 | 5.1685 | | 1.7956 | 7.1053 | 2.3328 | 1.4111 | 3.9573 | 2.0800 | 2.2077 | 3.0126 | 1.0361 | 4.1834 | 2.2581 | 2.2948 | 0.5379 | |
| Mg (ppb) | 8.1303 | 8.2269 | 5.0636 | -1.1447 | -0.8995 | 9.0287 | 9.1546 | 4.1978 | 6.8086 | 1.6401 | | 8.4092 | 4.5855 | 2.4941 | 4.8319 | 3.4626 | 3.1330 | 3.5508 | 1.1643 | 5.2725 | 3.6823 | 3.6446 | 1.6616 | |
| Mn (ppb) | -0.3370 | -0.2403 | -3.4037 | -9.6120 | -9.3667 | 0.5615 | 0.6874 | -4.2695 | -1.6586 | -6.8271 | -8.4672 | | 4.9701 | 6.3523 | 16.8681 | 6.9577 | 9.1711 | 7.5425 | 6.8397 | 12.6992 | 12.8144 | 8.8038 | 6.1630 | |
| Mo (ppb) | -0.5877 | -0.4910 | -3.6543 | -9.8626 | -9.6174 | 0.3108 | 0.4367 | -4.5202 | -1.9093 | -7.0778 | -8.7179 | -0.2507 | | 2.5989 | 7.6506 | 3.4035 | 3.3647 | 3.0836 | 2.7453 | 6.3469 | 4.9932 | 3.7352 | 1.6068 | |
| Ni (ppb) | -1.8410 | -1.7443 | -4.9077 | -11.1160 | -10.8707 | -0.9425 | -0.8166 | -5.7735 | -3.1626 | -8.3311 | -9.9712 | -1.5040 | -1.2533 | | 4.7209 | 2.5908 | 2.4320 | 2.5995 | 1.1994 | 4.2121 | 3.4366 | 2.7337 | 0.8172 | |
| NO3 (ppb) | 5.8463 | 5.9429 | 2.7796 | -3.4287 | -3.1834 | 6.7447 | 6.8706 | 1.9138 | 4.5246 | -0.6439 | -2.2840 | 6.1832 | 6.4339 | 7.6872 | | 5.0086 | 4.0750 | 5.7725 | 3.8228 | 4.3911 | 2.7573 | 5.1202 | 3.6073 | |
| Pb (ppb) | -2.7303 | -2.6337 | -5.7970 | -12.0053 | -11.7600 | -1.8319 | -1.7060 | -6.6628 | -4.0520 | -9.2205 | -10.8606 | -2.3934 | -2.1427 | -0.8894 | -8.5766 | | 2.7125 | 4.1529 | 2.2235 | 5.5691 | 3.2901 | 2.5293 | 1.4649 | |
| Se (ppb) | -2.4512 | -2.3546 | -5.5179 | -11.7262 | -11.4809 | -1.5528 | -1.4268 | -6.3837 | -3.7728 | -8.9413 | -10.5815 | -2.1143 | -1.8636 | -0.6103 | -8.2975 | 0.2791 | | 2.9739 | 1.7566 | 4.9268 | 3.1592 | 3.0273 | 1.3546 | |
| SO4 (ppb) | 8.7926 | 8.8892 | 5.7259 | -0.4824 | -0.2371 | 9.6910 | 9.8170 | 4.8601 | 7.4710 | 2.3025 | 0.6624 | 9.1296 | 9.3803 | 10.6336 | 2.9464 | 11.5230 | 11.2438 | | 1.7749 | 3.9455 | 5.2820 | 3.9269 | 1.8262 | |
| Sr (ppb) | 4.6772 | 4.7738 | 1.6105 | -4.5978 | -4.3526 | 5.5756 | 5.7015 | 0.7447 | 3.3555 | -1.8130 | -3.4531 | 5.0141 | 5.2648 | 6.5181 | -1.1691 | 7.4075 | 7.1284 | -4.1155 | | 3.4057 | 3.1406 | 2.3827 | 0.4554 | |
| U (ppb) | -0.9354 | -0.8388 | -4.0021 | -10.2104 | -9.9651 | -0.0369 | 0.0890 | -4.8679 | -2.2570 | -7.4255 | -9.0656 | -0.5984 | -0.3477 | 0.9056 | -6.7816 | 1.7950 | 1.5159 | -9.7280 | -5.6125 | | 4.4033 | 5.4980 | 3.3966 | |
| V (ppb) | 0.9079 | 1.0045 | -2.1588 | -8.3671 | -8.1218 | 1.8063 | 1.9323 | -3.0246 | -0.4137 | -5.5822 | -7.2223 | 1.2449 | 1.4956 | 2.7489 | -4.9384 | 3.6382 | 3.3591 | -7.8847 | -3.7693 | 1.8433 | | 3.7759 | 2.1965 | |
| Zn (ppb) | 0.4162 | 0.5128 | -2.6505 | -8.8588 | -8.6135 | 1.3146 | 1.4406 | -3.5163 | -0.9054 | -6.0739 | -7.7141 | 0.7532 | 1.0039 | 2.2572 | -5.4301 | 3.1465 | 2.8674 | -8.3764 | -4.2610 | 1.3516 | -0.4917 | | 1.6631 | |
| | Mean ln(Xi/Xj) | | | | | | | | | | | | | | | | | | | | | | 37.0897 | Total Variance |

# Biplot

- Click Graph -> CLR biplot
- Select the data you would like to visualize on a biplot


CLR Biplot Menu
Selected
Available data:
Latitude
Longitude
>
<
Selected data:
Al (ppb)
As (ppb)
Ba (ppb)
Ca (ppb)
Cl (ppb)
Cr (ppb)
Cu (ppb)
F (ppb)
Fe (ppb)
K (ppb)
Mg (ppb)
Groups:
<No gro...
Reset
Options
Add coordinates
Accept
Cancel
Help


ilr.2
ilr.1
clr.U (ppb)
clr.SO4 (ppb)
clr.Cl (ppb)
clr.Mn (ppb)
clr.NO3 (ppb)
clr.Fe (ppb)
clr.Mo (ppb)
clr.Cr (ppb)
clr.V (ppb)
clr.Al (ppb)
clr.F (ppb)
clr.As (ppb)