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Hydrology and Earth System Sciences
Discussions

Interactive comment on "Machine Learning Deciphers CO_2 Sequestration and Subsurface Flowpaths from Stream Chemistry" *by* Andrew R. Shaughnessy et al.

Anonymous Referee #1

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General comments

The paper applies NMF (Non-negative Matrix Factorization), which is a machine learning technique, to EMMA (End-Member Mixing Analysis). They use this to calculate CO2 sequestration in three watersheds. The novelty is the application of NMF to EMMA. In general, the paper is well written. I suggest publication if the comments below are addressed.

Specific comments

1. Line 19-20, 44-45 and 412. You talk about a "new machine learning technique". Actually, it is not a new technique. What you do is applying an old technique (machine

learning or, more specifically, NMF) to EMMA, which is new.

2. Line 132-134. You say that NMF is unique in that it does not rely on assumptions of endmembers a priori. This is repeated throughout the whole paper (figure 2, line 172, 412 and 428). I think this is not entirely true. For instance, Carrera et al. (2004) calculate endmembers without NMF. Carrera, J., E. Vázquez-Suñé, O. Castillo, and X. Sánchez-Vila (2004), A methodology to compute mixing ratios with uncertain endmembers, Water Resour. Res., 40, W12101, doi: 10.1029/2003WR002263.

3. Line 138: You use SO4 as a reference for solute concentrations. To me it would make more sense to use Cl-, instead, because it is not likely involved in chemical reactions. Is there a particular reason for using SO4?

4. Line 145: You define end members for shallow, moderately shallow, and deep flowpaths. Of course, they may vary in time as you say in line 149. Could this create some bias? For example, end members of deep flowpaths are generally older with water that fell as rainfall earlier than end members of shallow flowpaths. As acid rain varies with time, differences in chemical signature can be affected by the age of the water.

5. Line 265: Equation 3 and kstream are not clear to me. Where does the -1 come from? I suggest adding an explanation in the SM like you have done for krock.

6. SM, section 2.2. I find this section very hard to follow. Actually, you describe mathematical equations by using text. I think you can make it more readable, if you put the equations as well.

7. SM, line 55-57. If I understand correctly, here you attribute all Ca and Mg to carbonate dissolution. However, it can also come from silicates. In fact, in figure 1 you represent silicates by CaSiO2. Do you simply neglect Ca from silicate weathering?

Technical corrections

1. SM, line 28. Change "in in" to "in".

2. SM, line 133-134. I think this equation is equation 3 from the main text, not 2.

3. SM, line 148. You refer to Fig. 3C. However, this figure contains nothing related to lag times. I think you mean Fig. 4C.

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