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Defining and evaluating the effect of redundant isotopic tracers in Bayesian unmixing models

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The prevention of the negative consequences induced by accelerated soil erosion depends on well thought out and economically viable mitigation policies that are founded on the accurate source apportionment of erosion hotspots. Typically, quantification of sediment source apportionment is difficult and requires the impractical and economically unfeasible solution of in-situ sampling at all possible erosion hotspots. An alternative and commonly applied technique is source and sediment fingerprinting with complimentary unmixing of the sediment fingerprint by mass balance equations, with a recent surge of Bayesian inference to incorporate uncertainty in sediment apportionment.

The compound-specific isotope analysis of fatty acids are commonly used for land-use specific fingerprints. However, fingerprinting using isotopic tracers has shown limitations in multiple catchments in which $\delta^{13}\text{C}$ of fatty acids plot in a 1-dimensional mixing line, resulting in the contribution of the central source being mis-classified as source contribution from either source located at the mixing line endpoints. In this study, we used $\delta^{15}\text{N}$ as an additional land-use specific tracer to expand the fatty acid linear mixing line into a more suitable N-dimensional mixing polygon. We use an initial "brute force method" with virtual mixtures to explore all combinations and permutations of tracers and their model performance.

Results show that increasing the number of fatty acid tracers had a detrimental effect on unmixing performance, suggesting that increasing the number of conservative tracers does not always produce an improved unmixing result as previously understood when using a Bayesian framework.

Expanding on this, we hypothesised that if the relative source-source values are constant between different length fatty acids, the mixing space will also be constant, resulting in the application of additional $\delta^{13}\text{C}$ of fatty acid tracers being comparable to applying repetitions of an identical tracer making additional fatty acid tracers potentially redundant. The performance of the unmixing models using $\delta^{13}\text{C}$ fatty acid tracers can then be understood to depend on the model's capacity to handle redundant tracers. The effect of tracer redundancy was quantified by adding identical duplicate tracers (repetitions of the same tracer, $\delta^{13}\text{C}$ FA C26) or different fatty acid tracers ($\delta^{13}\text{C}$ FA C24, C28, C30) to the $\delta^{15}\text{N}$ and $\delta^{13}\text{C}$ FA C26 tracer set in a three, four and five tracer set and unmixed using the Bayesian framework MixSIAR.

Increasing the number of identical tracers in a tracer set decreased model performance resulting from the propagation of the source-based uncertainty outweighing any discrimination power gained. The latter contradicts the previous idea that MixSIAR handles non-informative tracers. The addition of fatty acids (C24, C28, C30) to C26 showed a lower but proportional decrease in model performance compared to additional identical tracers. This suggests that using multiple tracers which have the same relative mixing space are practically equivalent to applying identical tracer multiple times. We conclude that when using a Bayesian framework for unmixing models, it is beneficial to remove redundant tracers which display the same relative mixing space to improve model performance.