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REPLY COMMENT

Minmax solutions for underdetermined isotope mixing problems: Reply to Semmens et al. (2013)

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ABSTRACT: Stable isotope tracers are used to solve ecological problems, and sophisticated modelling approaches are now available to help interpret measured isotope data. However, models such as IsoSource and SIAR can go a step too far in producing mean and median values when there are too many sources and not enough tracers. The models solve these underdetermined problems by assuming that some of the many possible or feasible solutions are more likely than others. I promote the alternative idea that all feasible solutions are equally likely, and support use of minimum and maximum ('minmax') solutions as the appropriate way to view results from underdetermined systems.

KEY WORDS: Stable isotopes · Mixing models · Tracers · Food web · IsoSource · SIAR

Introduction

Ecologists are increasingly using sophisticated models for dealing with measured data. Advances in computing make it possible to create virtual data streams that are almost as complex as real-world systems, and these computational advances are being utilized increasingly by field biologists. Fry (2013) reviewed models and other approaches for dealing with complex field data on marine food webs, especially in underdetermined cases where multiple outcomes are feasible from isotope tracer measurements. For the growing number of isotopic studies on marine food webs, modelling approaches such as IsoSource (Phillips & Gregg 2003) and SIAR (Parnell et al. 2010) offer powerful ways to process and summarize the field measurements. Semmens et al. (2013) find that Fry (2013) did not discuss these Bayesian models adequately.

Minmax examples from seagrass ecosystems

The IsoSource and SIAR programs are useful to ecologists. Nonetheless, I found it hard to understand the details of model assumptions, so I developed a graph-based method to generate the same average (mean) results (Fig. 1 in Fry 2013). The analysis accompanying this example showed that the isotope information is simply not sufficient to reach a mean solution for such an underdetermined system, and, as noted previously (Benstead et al. 2006), only the conservative minmax (minimum and maximum) information gives the reliable source solutions for these underdetermined problems.

This conservative perspective stems from my graduate work in the 1970s, when I used stable isotopes to extract information about seagrass food webs that constituted underdetermined isotope systems. Because I considered minmax solutions first and foremost in those systems, I will briefly review this experience. The general isotope problem was that there were 3 food sources (–10‰ seagrass, –15‰ epiphytes + macroalgae and –20‰ phytoplankton), most consumer isotope values were near –15‰, and with only one tracer ($\delta^{13}C$), the system was underdetermined.

I thought about using some generalized model estimate of, for example, 1/3 importance for each source for the –15‰ consumers, but some senior ecologists of that era challenged such estimates. They wanted estimates that I could defend strictly from the measured

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data. This forced me to acknowledge that the system was underdetermined and that especially the middle source was poorly resolved, with a 0–100% minmax range (Fig. 1 in Fry & Sherr 1984). Then, as today, we did not have other definitive sources of information (prior knowledge or 'priors') to use in these complex marine food webs, so we were forced to narrowly rely on the isotope data. We aggregated sources (Fry & Parker 1979) and developed other information to find a way out of the 'mixing muddle', my nickname for these underdetermined problems (Sec. 5.1 in Fry 2006). Source contributions were easier to identify in food webs where isotope values of epiphytes departed strongly from seagrass values (Fry 1984, Kitting et al. 1984), but this situation was rare and occurred only in about half the systems studied (Fry et al. 1987). We realized that underdetermined systems are often just difficult, and cannot be resolved without additional information (Secs. 5.4 & 5.5 in Fry 2006). Using more tracers than just $\delta^{13}C$ alone is usually required to solve these systems (Fry 2006, 2013).

Underdetermined systems and modelling assumptions

Semmens et al. (2013) describe their procedures and terminology, but do not come to the heart of my concerns, i.e. they assume that some of the many feasible solutions are more likely than others. This assumption is implicit in their procedures and allows them to solve underdetermined mixing problems. This article elaborates on these points with a focus on mean values, but applies equally to probability distributions from which these means (and medians) are drawn.

Generally, underdetermined systems do not have enough equations to allow unique solutions. A simple example of an underdetermined system is the equation $x^2 = 1$, where 2 equally likely solutions are $x = -1$ and $x = +1$. We really cannot decide between these 2 alternatives without further information. But if, for example, we assume that only values >0 will occur in the system, then the -1 solution is eliminated and we can solve the problem, i.e. $x = 1$. This example illustrates that underdetermined systems cannot be solved without extra information, but are rather easily solved with assumption. That is, assumptions can convert underdetermined systems into determined systems. Other underdetermined systems such as $a + b = 7$ share these same characteristics of multiple, equally likely solutions (e.g. $a + b = 7$ has solutions $2 + 5$, $1 + 6$, etc.).

The assumptions of the Bayesian approaches used by Semmens et al. (2013) are tied to the use of the Monte Carlo sampling schemes for accumulating feasible solutions. This Monte Carlo approach was first used for underdetermined systems by Minagawa (1992), then adopted in IsoSource (Phillips & Gregg 2003) and SIAR (Parnell et al. 2010, Semmens et al. 2013). To see how this works, let us reconsider the case of a sample in the middle of the 4-source square (Fig. 1 in Fry 2013), which is also discussed by Semmens et al. (2013). The point in the middle is the least determined point of the mixing polygon, and so represents the place where solutions are least constrained by data and where assumption is strongest. Monte Carlo procedures (in IsoSource) produce a mean ± SD for the feasible solutions for each source, with values of 25 ± 14% applying for each source. The minmax solutions for each source are also identical: 0% minimum and 50% maximum. A 25 ± 14% mean estimate looks like a real solution, and it has a strong generalist bias because on average, all sources are used equally. But we can sense a problem with this answer. Specifically, our logic tells us that although this generalist solution is possible, so are the other specialist solutions, for instance those along diagonal lines connecting sources in this square (Fig. 1 in Fry 2013). Is the Monte Carlo mean really more likely or not? There seem to be 2 views on this issue:

(1) Semmens et al. (2013) consider it useful to produce these Monte Carlo means in a standardized manner and to embrace them as preliminary estimates, keeping in mind that the variability estimates are important along with the mean and median values. Especially, the variability estimates include the possibility (though unlikely) of the specialist solutions at the end of the probability distributions. These means and associated variability are useful in many further modelling steps where various uncertainties can be incorporated, and this is a strong feature of SIAR. Also, where any priors or other information are available, they can be applied to narrow the variability range towards a more certain or determined value. However, some or all of the original Monte Carlo estimates of the mean and variability are likely to survive in the final solutions, especially when priors are weak or absent.

(2) By contrast I consider all feasible solutions to be equally likely, i.e. the generalist solution is no more likely than the specialist one. The Monte Carlo method just produces a range of solutions, and the minimum and maximum ends of this range are the useful results from the models, not means, medians, etc. and their associated errors. Presentation of the

frequency distribution of the Monte Carlo results, advocated as the appropriate way to summarize results analysed with IsoSource (Phillips & Gregg 2003) or SIAR (Semmens et al. 2013), is unnecessary from this minmax viewpoint. I recognize that each feasible solution could have associated probability distributions or errors, such as standard deviations. But because the location of the real mean in the spectrum of feasible solutions is unknown, one refrains from adopting any particular feasible solution to represent that unknown mean. In this view, the fact that there will be variability in the real-world answer is not a strong guide for determining a mean (or median) within the range of feasible solutions.

I prefer the equal likelihood, minmax approach, because: (1) it is the conservative, data-supported way to view the results with minimal assumption; (2) underdetermined systems such as the example $x^2 = 1$ generally have solutions that are equally likely; and (3) other modellers working with complex marine systems also state that feasible solutions are equally likely for underdetermined systems (e.g. see the Fig. 4 caption in Soetaert & van Oevelen 2009). The Monte Carlo method can be very useful for determined systems, but its usefulness is much more limited for underdetermined systems where especially Monte Carlo solutions for points near the middle of mixing diagrams contain large amounts of assumption (Fry 2013). The Monte Carlo approaches can produce widely divergent estimates of source contributions when different feasible solutions are assumed for the same data, but using the minmax solutions will produce consistent, reliable source estimates that represent the whole solution range.

Assumptions about generalist solutions

Consider a consumer whose isotope values lie in the middle of a 4-source square mixing model (Fig. 1 in Fry 2013). Is it really a good assumption that this consumer is a generalist? The assumption may not be valid in real-world situations. Consumer use of any single source reflects the interaction of many factors, e.g. source availability, quantity, digestibility, nutritional quality, and predation risk associated with feeding on that source. Consumption of even a single source is thus complex and subject to change, so the generalist solution that assumes equal use of 4 sources is unlikely. Generalist behaviour is reflected in most solutions generated by IsoSource and SIAR, and stems from assumptions that some feasible solutions are more likely than others (Fry 2013, this article). Generalist behaviour is not very likely in many real-world situations, and for this reason, minmax estimates may be the simpler solutions that ecologists should adopt.

Problems with Monte Carlo solutions for underdetermined systems

Problems can occur when questionable food sources are included as potentially important in isotope mixing diagrams. For example, in the first study to use the Monte Carlo accumulation of feasible solutions, Minagawa (1992) included C_4 plants as a potentially important food source in the diets of Japanese people. The Monte Carlo simulations for underdetermined solutions based on isotope data indicated a 10 to 20% contribution of protein from C_4 plants, but this was not supported when further information was incorporated in mass balance equations.

In a more recent study, Kon et al. (2009) considered shrimp farm effluent as a food source for crabs in 2 mangrove creeks. The effluent contributed means of at least 5 to 15% to crab diets at all sampling stations (summarized in Fig. 5A in Fry 2013), a result that could have been interpreted as effluent spreading throughout the entire mangrove system. It is instructive that Kon et al. (2009) did not use these Monte Carlo model means in their final evaluation, highlighting instead the much stronger contributions of shrimp effluent at just the 2 stations closest to the shrimp farm. If the IsoSource mean results had been emphasized, quite a different scientific message of broad-scale pollution would have resulted from the study.

Both studies (Minagawa 1992, Kon et al. 2009) observed that mean contributions of some sources were too high and not zero in underdetermined mixing models. These high values occur because the Monte Carlo procedures give the result that all sources are used and important for points near the middle of underdetermined mixing diagrams. Stated another way, an unfortunate artefact associated with Monte Carlo approaches is that just including a source in an underdetermined mixing diagram assures that the source will have a non-zero contribution in final mean solutions for points near the middle of these diagrams. Also, the Monte Carlo means and medians for underdetermined systems usually contain substantial amounts of questionable assumption (Fry 2013, this article). Overall, these examples show that problems have emerged for Monte Carlo approaches when they are used for estimating means (and medians) in underdetermined systems. The strength of these Monte Carlo approaches advocated by Semmens et al. (2013) lies in the treatment of variability issues and error propagation.

Concluding remarks

Hopefully, a robust mixing model approach will be developed over time that uses an optimal mix of Bayesian and minmax approaches. Elements of such an approach might include: (1) a graph of the data and sources, presented so that underdetermined aspects of solutions can be identified visually towards the center of the source mixing polygons, with the central danger zone of Fry (2013) added as appropriate; (2) where informative priors are used to strongly narrow the range of feasible solutions, these priors are discussed in a stepwise manner to make sure that their use is logical and appropriate; (3) conservative minmax source values are clearly presented to identify the range of feasible solutions, with values for Σ_{MIN} and % resolved (Fry 2013) calculated from the min and max values. The minmax information can be calculated conveniently with IsoSource where priors are not easily incorporated, or the minmax information can be approximated after consideration of priors and variability issues using the error bar ranges generated in SIAR output.

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