

# Overview of Bayesian mixing models

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# Outline

- Evolution of mixing models from IsoSource forward
- Understanding priors in Bayesian mixing models
- Challenges / future work

# Objective

- Estimate the relative proportions ('p') of 'm' sources to a mixture with  $t$  tracers (d13C, d15N, d18O)
  - Widely range of applications (hydrology, geology, chemistry, ecology)
  - Data don't have to be stable isotopes (FAs, soil samples)

## Additional complications in ecology / diet studies

- Account for isotope specific fractionation / TEFs
- Concentration dependence: different food sources may contain different amounts of C/N – omnivores may have more dN15 from animals than plants (Phillips & Koch 2002)
- Assimilation efficiency / digestibility (Martinez del Rio & Wolf 2005, Chiaradia et al. 2014)

# IsoSource (Phillips & Gregg 2003)

- Visual Basic program
- Good at examining range of potential source combinations
- User specified tolerance controls what solutions are acceptable
- Not likelihood based
- Doesn't incorporate uncertainty in sources
- As it's not Bayesian, the ranges of solutions can't be interpreted as probabilities
- Though in some cases the ranges give similar solutions to more recent mixing models

# MixSIR (Moore & Semmens 2008)

- MATLAB code / GUI
- First Bayesian mixing model
- User inputs: source & consumer signatures, isotope specific TEFs
- User can input priors from other studies
- Assumes all consumers to have the same mean diet
- Variance of mixture =  $f(\text{proportions, source variances})$

# Semmens et al. (2009)

- First hierarchical mixing model
- Includes both fixed / random effects
- Multiple layers of nested random effects
- Code published with paper, no separate software
- Also illustrates a complication in working with compositional data: need to some transformation (CLR, ILR, multivariate logit)
- \*Check out `compositions()` package in R!

# SIAR (Parnell et al. 2010)

- Menu driven interface in R
- Same basic assumptions as MixSIR
- BUT extra isotope-specific additive residual error estimated
- Also includes concentration dependence (MixSIR does not)
- Need multiple consumers to estimate residual error
- GUI also allows SIAR model to be applied to different groups (factors)

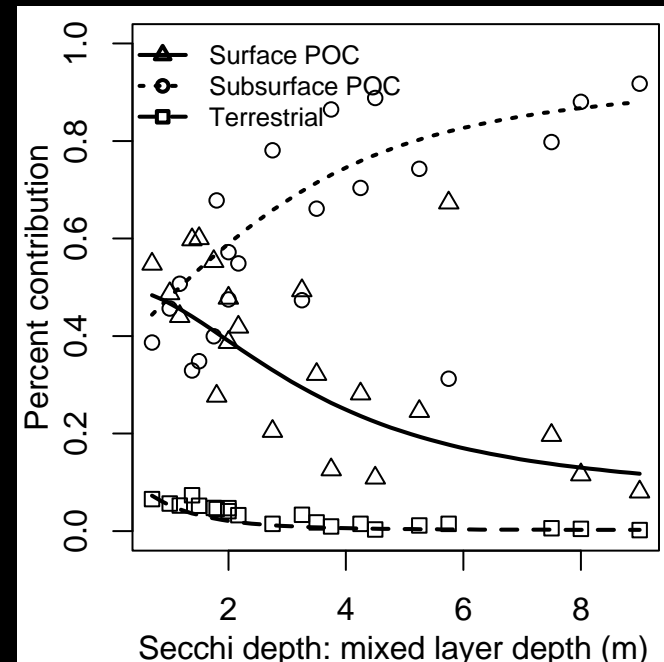
# Ward et al. (2010)

- “Fully Bayesian” versions of MixSIR / SIAR
- Flexible, incorporates uncertainty in source means / variances
- Code published with paper, no separate software
- By treating sources as parameters, informative priors can be useful



# Francis et al. 2011

- Extension of MixSIR / SIAR to include continuous covariates
- Application was on 1-D, but easily extendable to 2D
- Code provided with paper, not separate software



- There are  $(m-1)$  slope / intercepts estimated, so more parameters than basic regression!

# Solomon et al. 2011

- 3 source model (C, N, H)
- Extended mixing model to include extra source ( $H^2O$ ) for H
- Software included with paper, not separate package
- Extra tracer improves ability to discriminate
- Makes Dirichlet prior slightly more complex, because the number of sources varies by isotope / tracer

# IsotopeR (Hopkins & Ferguson 2012)

- R package incorporating models through 2010
- Also includes measurement error (mass spec)
- Also includes correlation between sources
  - e.g. C/N sometimes positively correlated
  - Incorporating this correlation may yield better predictions / estimation

# MixSIAR

- Fusion of previous tools
- New features:
- User friendly GUI
- Grouping variables may be fixed / random
- Hierarchical models
- Inclusion of covariates
- New options for modeling residual errors (soon!)
- Data can be input in a number of formats
- Source means / variances
- Very active SIAR / MixSIAR Facebook group (led by A. Jackson)
  - Lots of users helping each other

FB group: <https://www.facebook.com/pages/SIAR-Stable-Isotope-Analysis-in-R/148501811896914>

MixSIAR: <https://github.com/brianstock/MixSIAR>

# Field is evolving rapidly

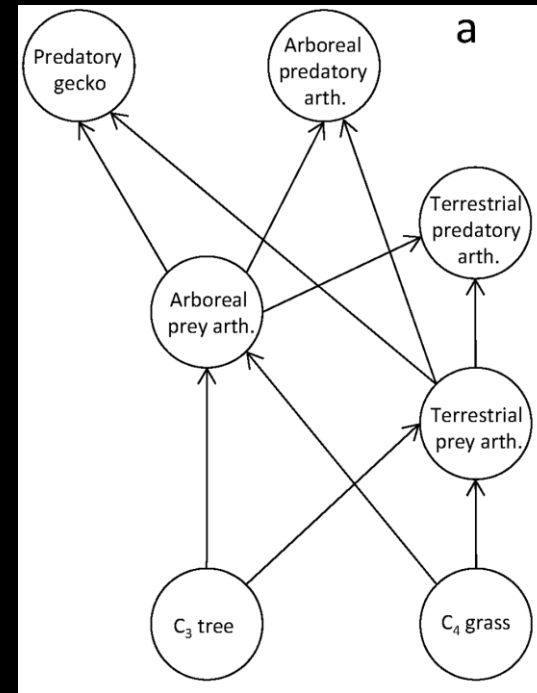
- Improvements in theory (Parnell et al. 2013)
  - “kitchen sink” mixing model
  - Lots of potential parameters that can be estimated with other types of data, informed by priors, etc
- Many tangential applications

# Yeakel et al. 2011

- One potential flaw with all previous approaches is that the available biomass of all sources is assumed equal
- Demonstrated post-hoc resampling with MixSIR – but is broadly applicable to all other models
- Moose v mice
- Script provided with paper, not separate software

# IsoWeb (Kadoya et al. 2012)

- User inputs food web structure & SI values
- Incorporates uncertainty in TEFs
- Can compare likelihood of different food web topologies
- Script available with paper, not separate software



# SISUS (Erhardt et al. 2014)

- Update / improvement on IsoSource
- Estimates ranges of feasible proportions
  - Like isosource, not to be confused with Bayesian mixing models
- Used to be available as an R package, but defunct as of 08-2014



# FRUITS (Fernandes et al. 2014)

- Mixing model that incorporates dietary routing
  - Incorporates differential weight of sources
- More mechanistic mixing model
- Need additional priors from feeding studies, experiments, etc.
- Software as R package on sourceforge

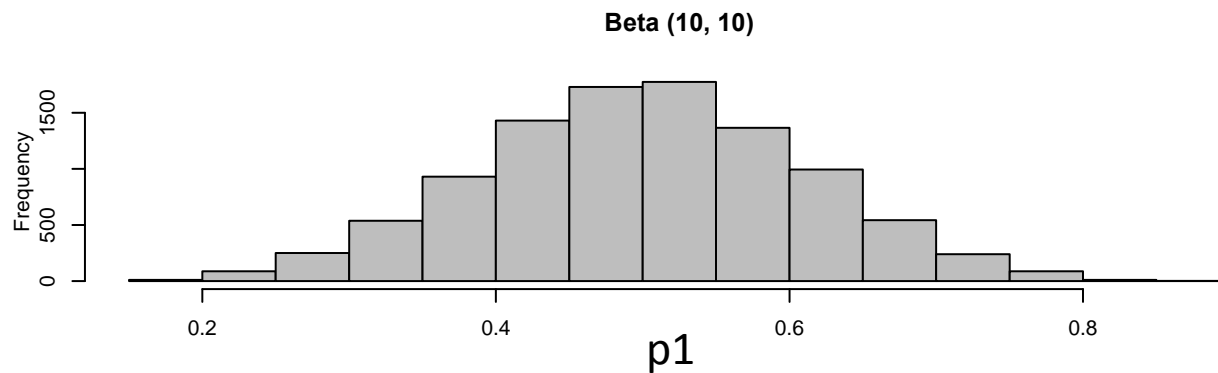
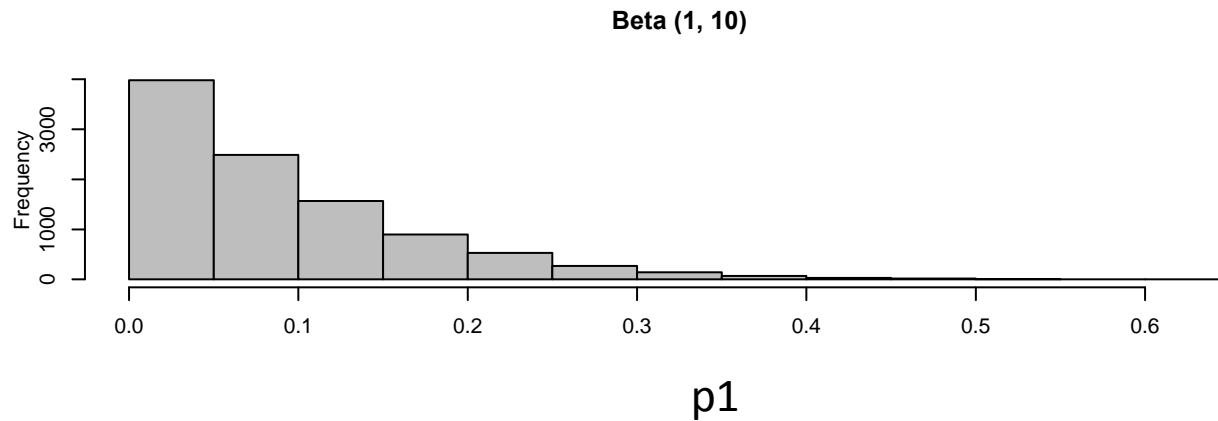
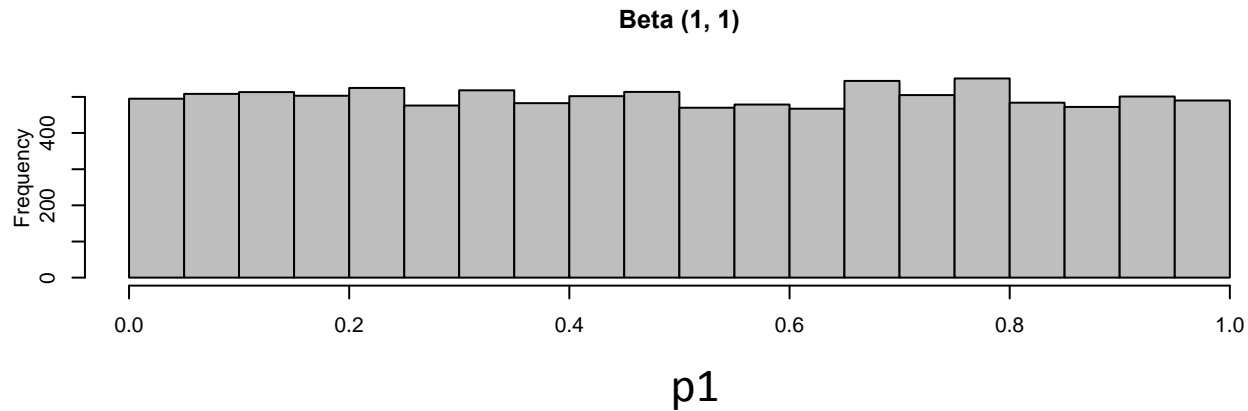
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# Priors on proportions

- All mixing models treat proportions ( $p$ ) as estimated parameters
- We assign a Dirichlet distribution as the prior
  - Constrained to sum to 1
    - For ' $m$ ' sources, there are ' $m-1$ ' parameters
  - Widely used in compositional data analysis
  - Very flexible, multivariate version of beta distribution
  - Hyperparameters =  $\alpha = c(1, 1, 1)$  whose length is the same as the number of sources

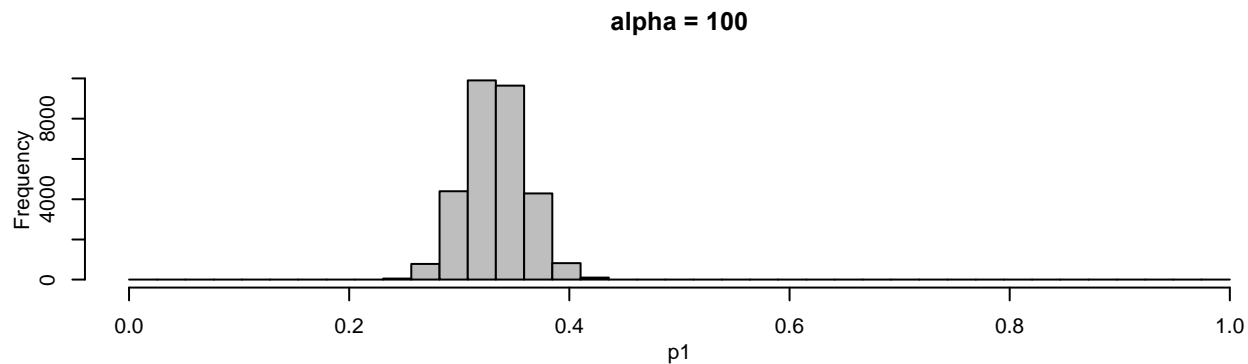
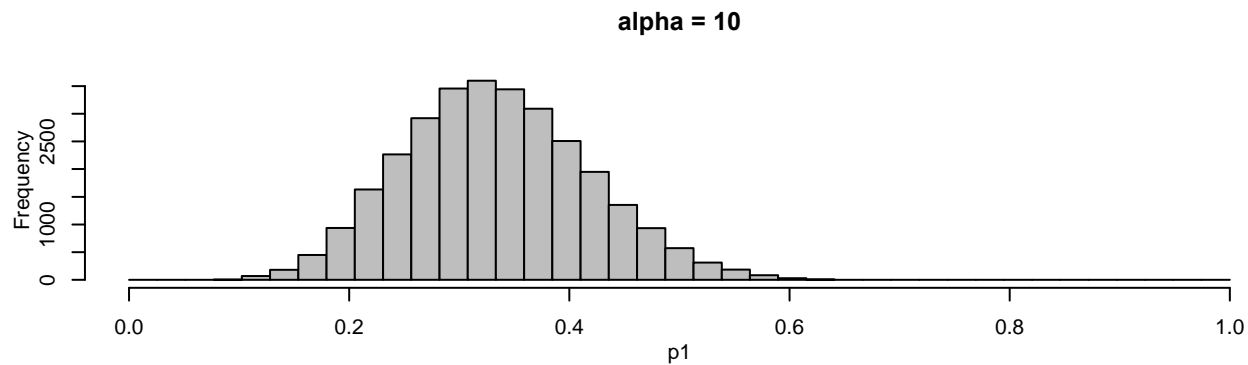
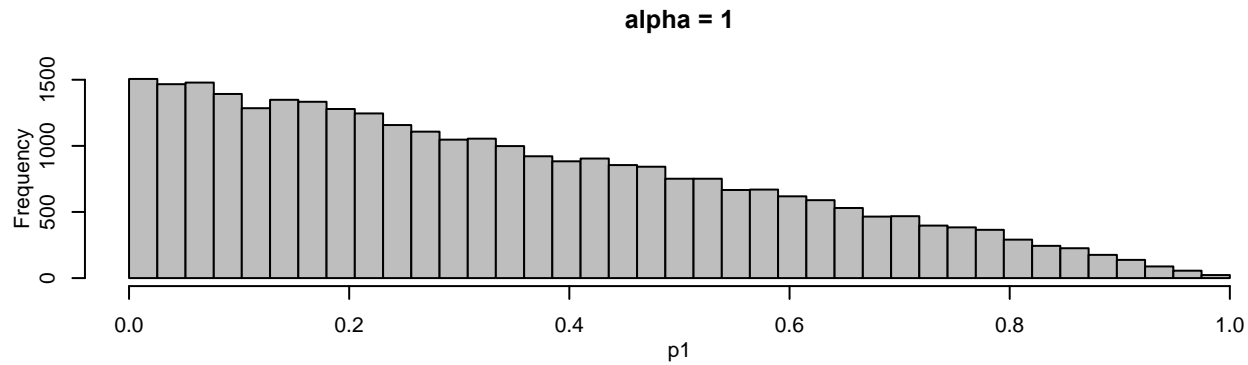
# Beta distribution



# Dirichlet: sample size

- Expected value of proportion  $i$  is just  $= \alpha_i / \text{sum}(\alpha)$
- This means  $\alpha = (1, 1, 1)$  and  $\alpha = (10, 10, 10)$  have the exact same *a priori* means
- BUT the larger the alphas are, the more weight they have (tighter prior)

# Effect of increasing alpha

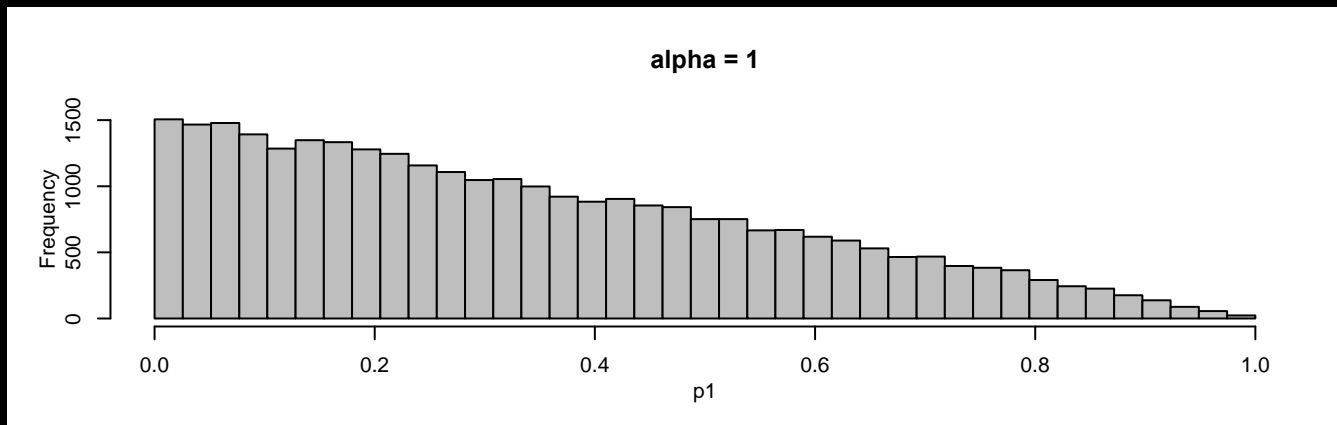


# Rough guide to interpretation

- Alphas can roughly be interpreted as effective sample size
- e.g. we're interested in a mixing model using salmon as consumers. We have 300 sampled items from 43 stomachs that we'd like to use as a prior. How to construct alphas?
- Relative ps = 0.1, 0.2, 0.7
- Sample size = 10, alpha = c(1, 2, 7)
- Sample size = 43, alpha = c(4.3 8.6 30.1)

# Dirichlet: why '1' is the default prior

- The marginal distribution of the previous example doesn't look uniform or 'uninformative'

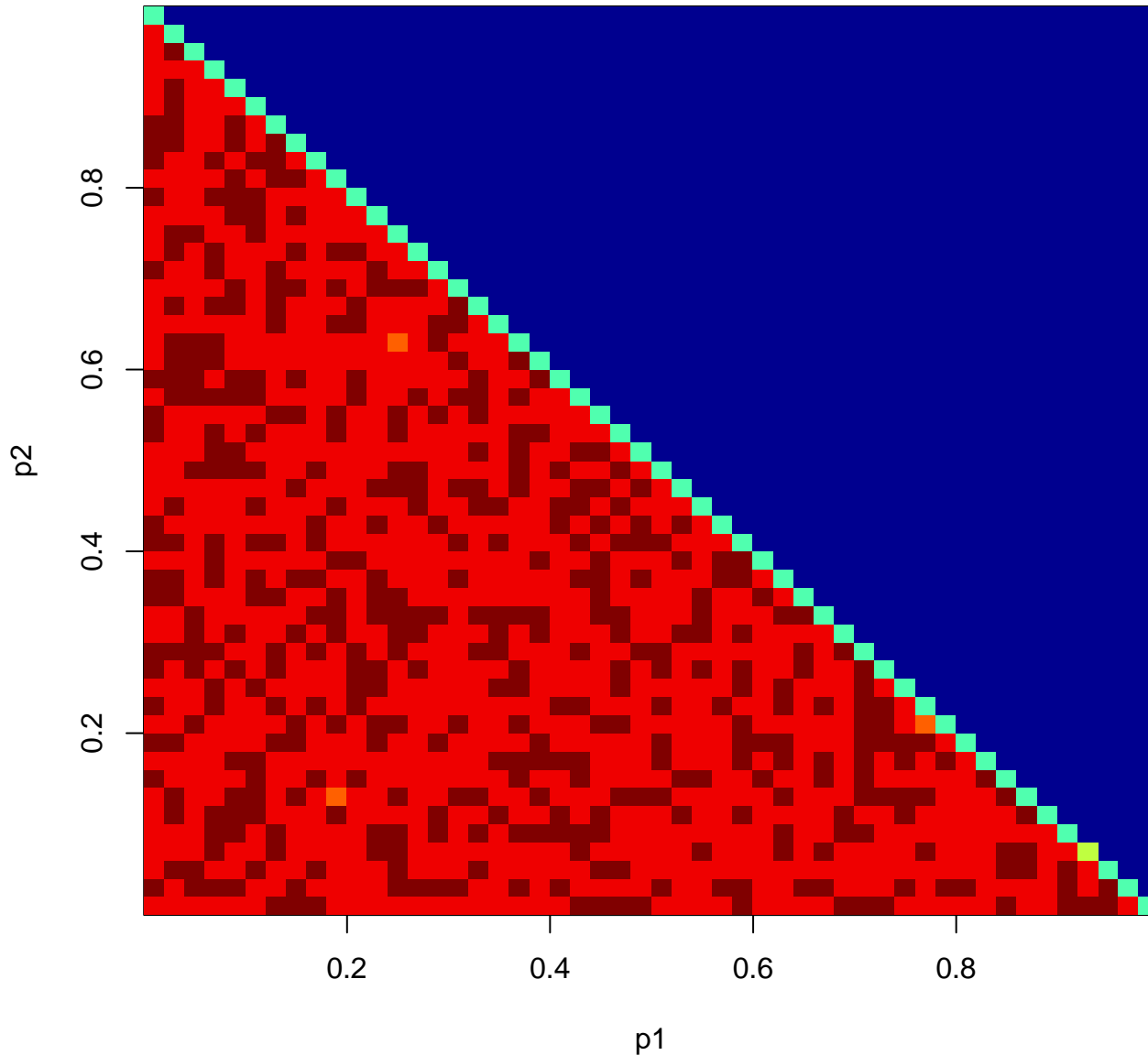


- Very confusing, but this prior is uniform on the entire compositional simplex
  - In other words, all diet combinations are equally likely



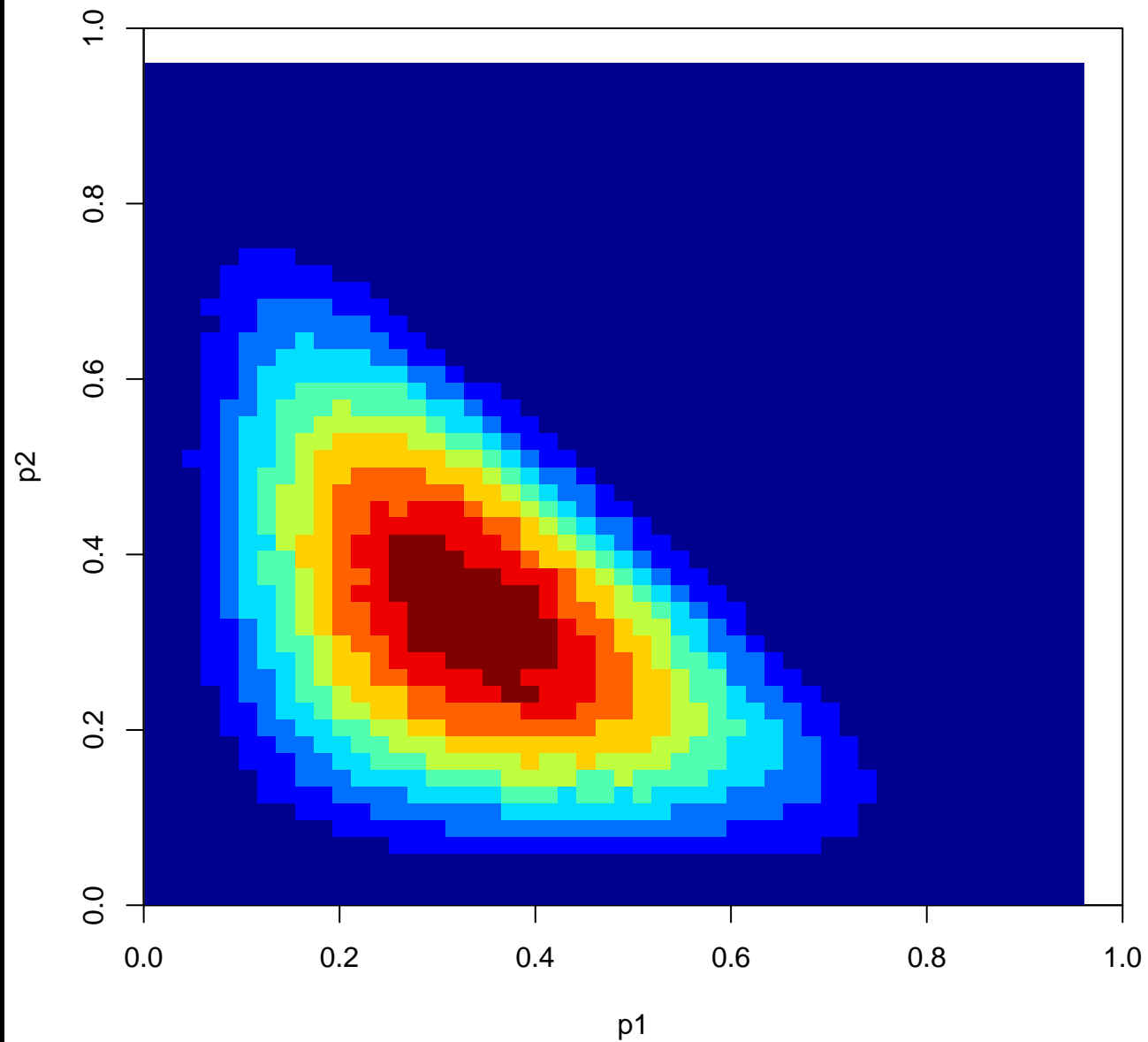
# Let's look at this in $> 1$ dimension

3 source model,  $\alpha = 1$



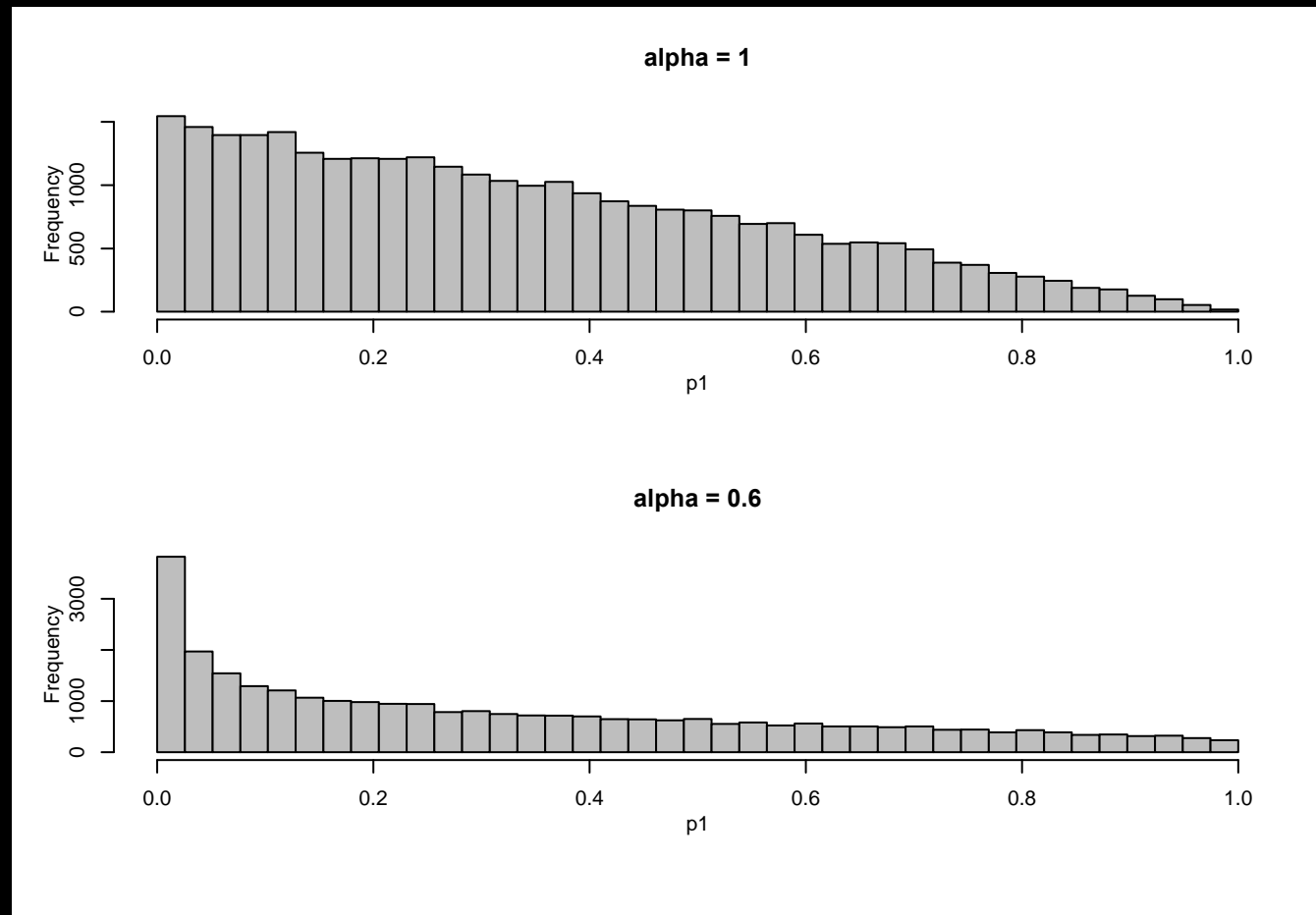
- Imagine we have 3 sources (= 2 parameters)

3 source model,  $\alpha = 3$

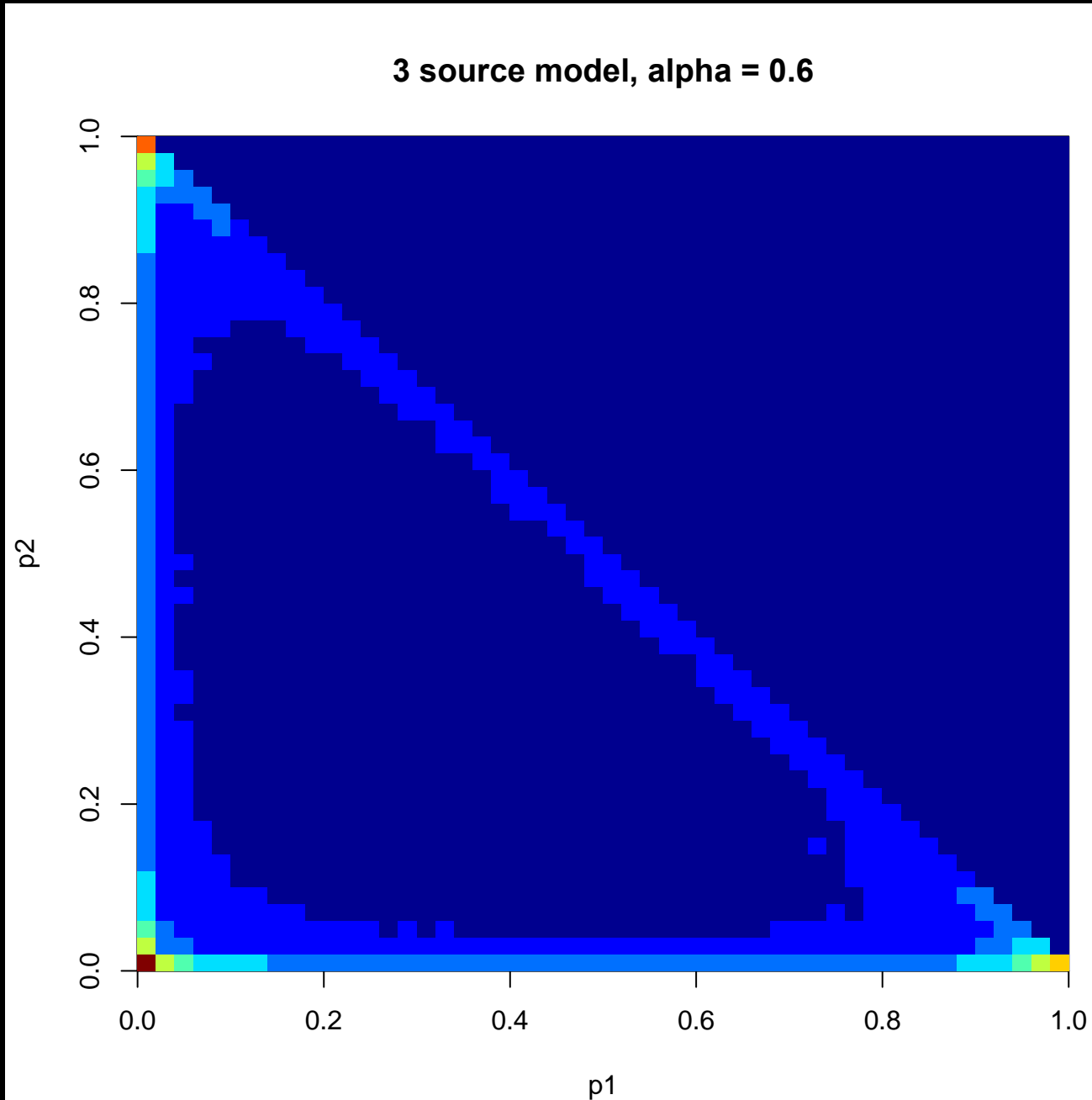


# BUT we can also make the Dirichlet marginals look more $\sim$ uniform

- Wouldn't that be better than  $\alpha = 1$ ?



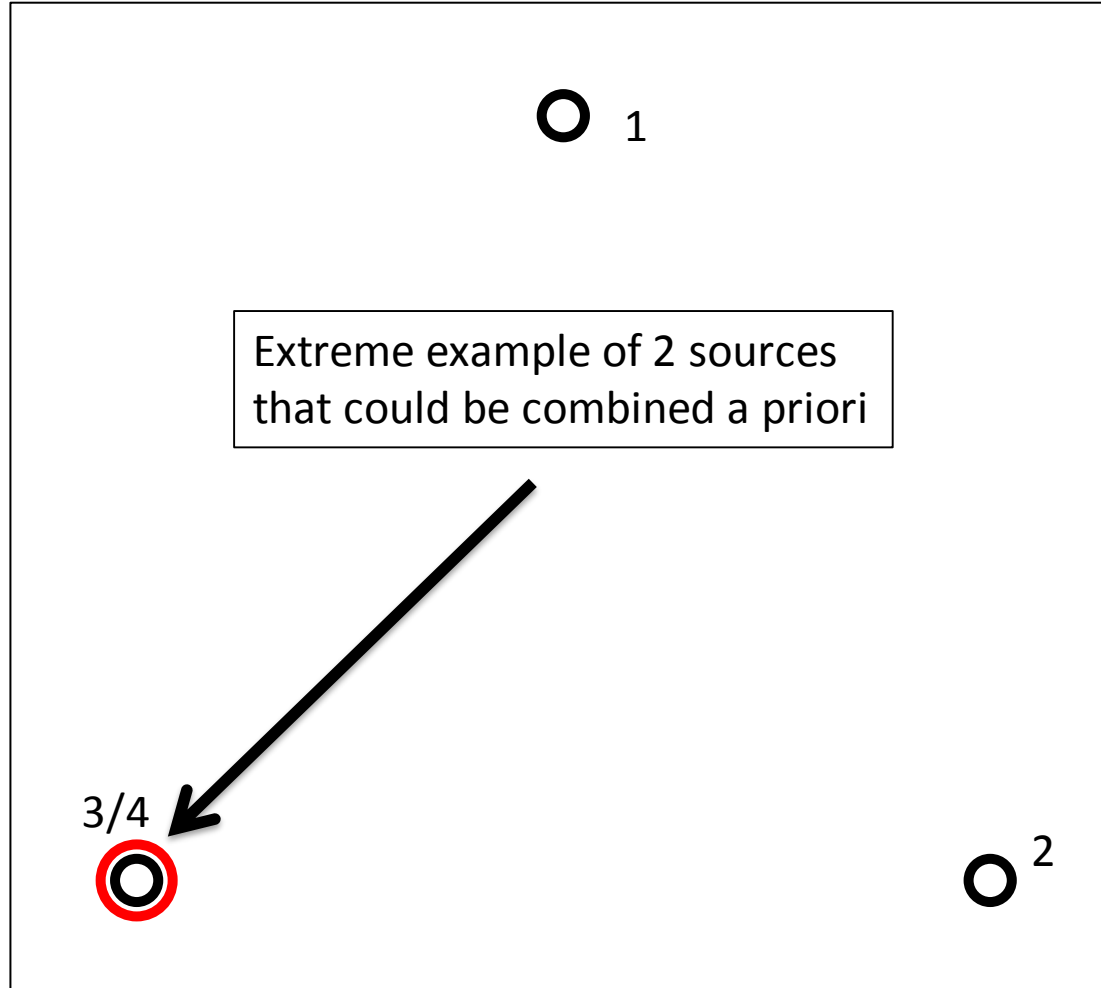
# Nope! In 2D, extreme values given high weight



# Dirichlet: impact of source geometry

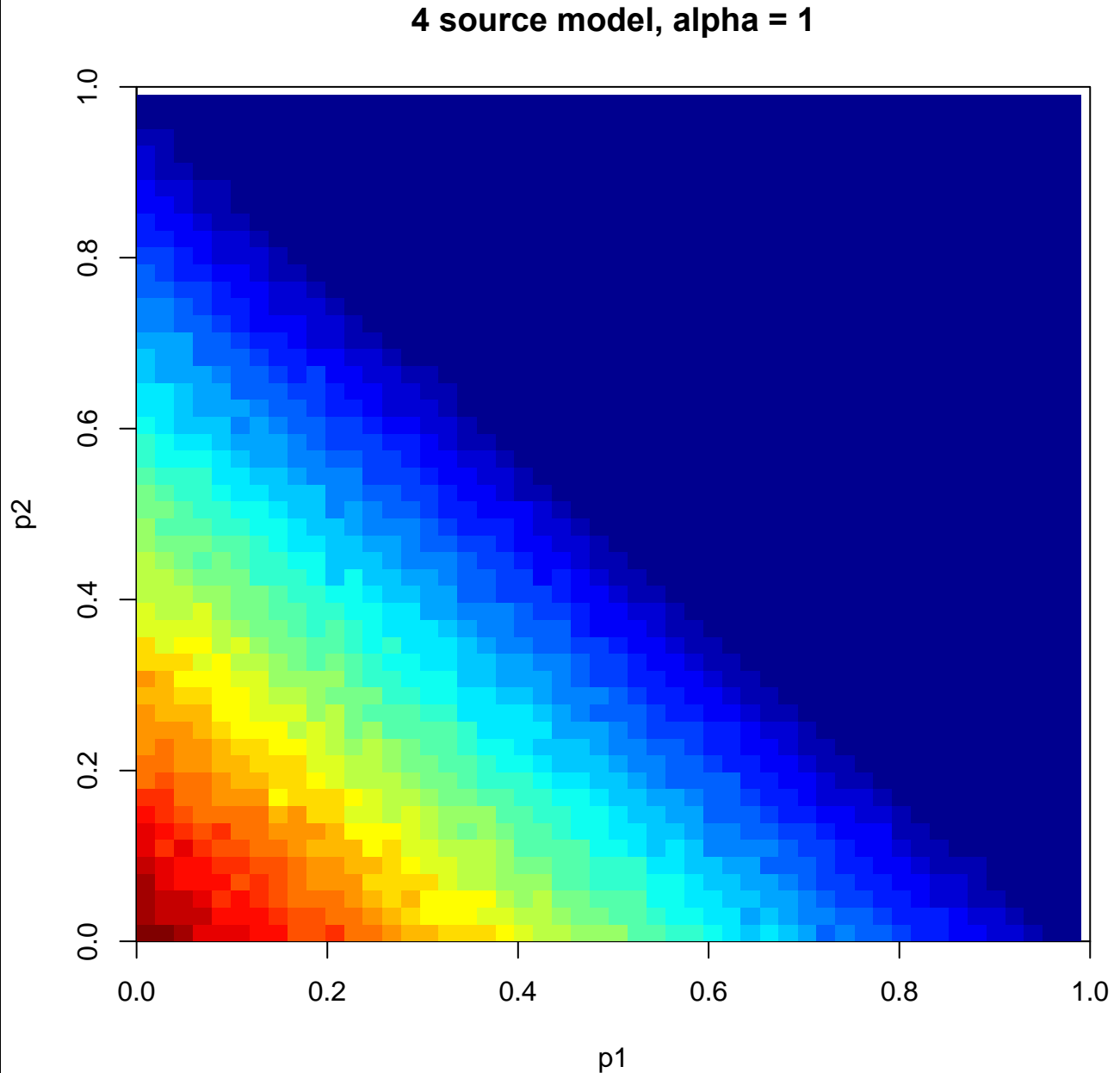
- In Bayesian statistics, we think of our estimates (posterior distribution) as  $\Pr(\theta \mid \text{data})$ , but it should really be  $\Pr(\theta \mid \text{data}, \text{model})$
- model includes source geometry
- Bad geometry can impact the prior

# Adding 4<sup>th</sup> source to our example



# What this means for prior

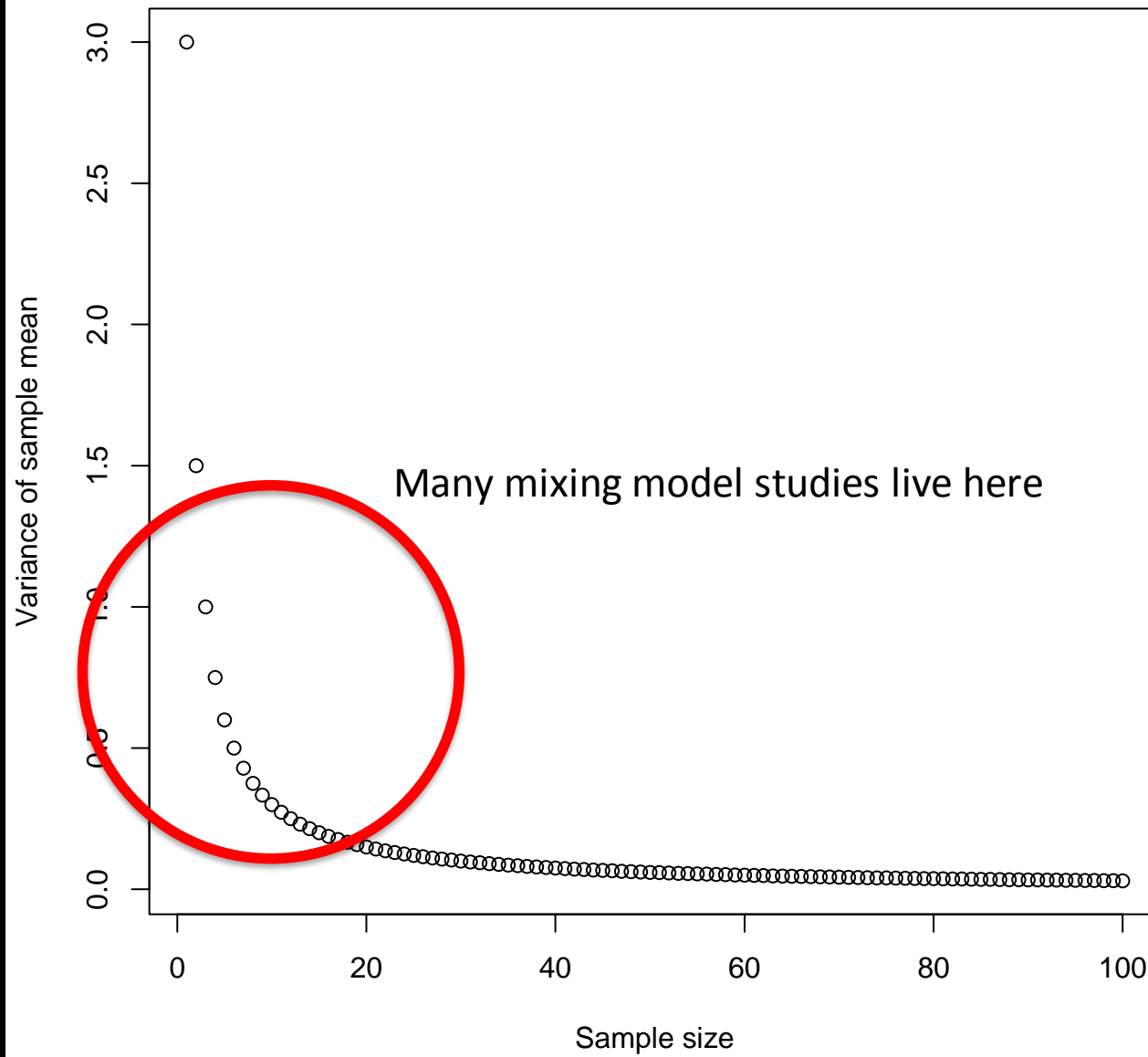
This means that sources 1/2 are getting down weighted, and sources 3/4 receive much more prior mass



# Priors on source means / variances

- Ward et al. 2010 (“fully Bayesian model”)
- Motivation: mixing model applications often have different #s of samples / source
- Sample processing can be expensive, making sample sizes small
- $\text{Var}(\text{sample mean}) = \sigma^2 / n$





# Freeing up mean / variance

- Including this uncertainty in sample mean / variance can lead to better fits to the data
- It also allows us to include prior information from other studies / systems (Ward et al. 2010)
- Caution: because this is so flexible, very small sample sizes may result in source geometry shifting to fit the data better
  - Sample means / variance treated as parameters along with the proportions (and any other terms, like residual errors)

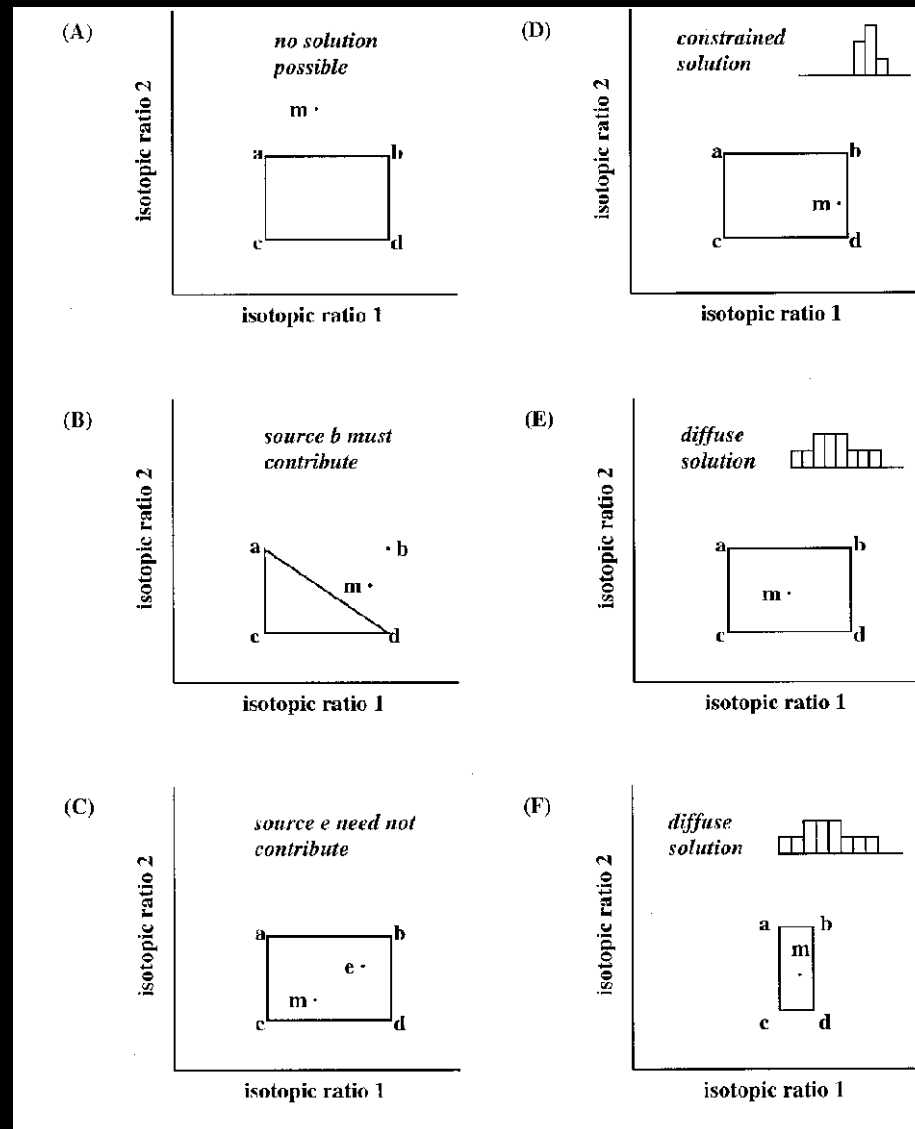


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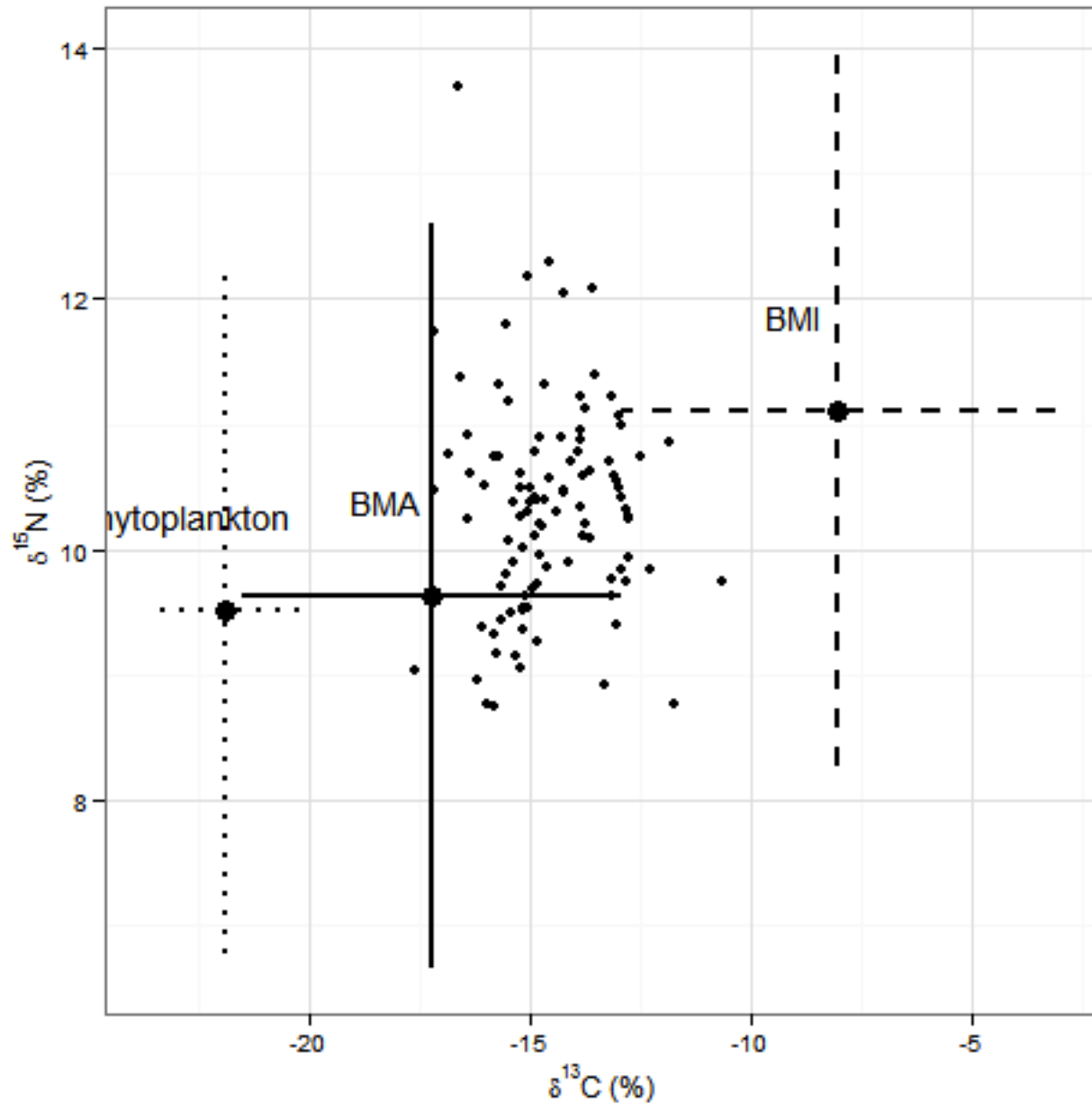
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- “MixSIR / SIAR / MixSIAR” don’t work right for my dataset – PLEASE HELP!
- You can only fit models as complex as your data will allow
- Do the data violate any of the basic assumptions of mixing models?
- Most mixing models are underdetermined (Sources > isotopes + 1; Fry 2013)

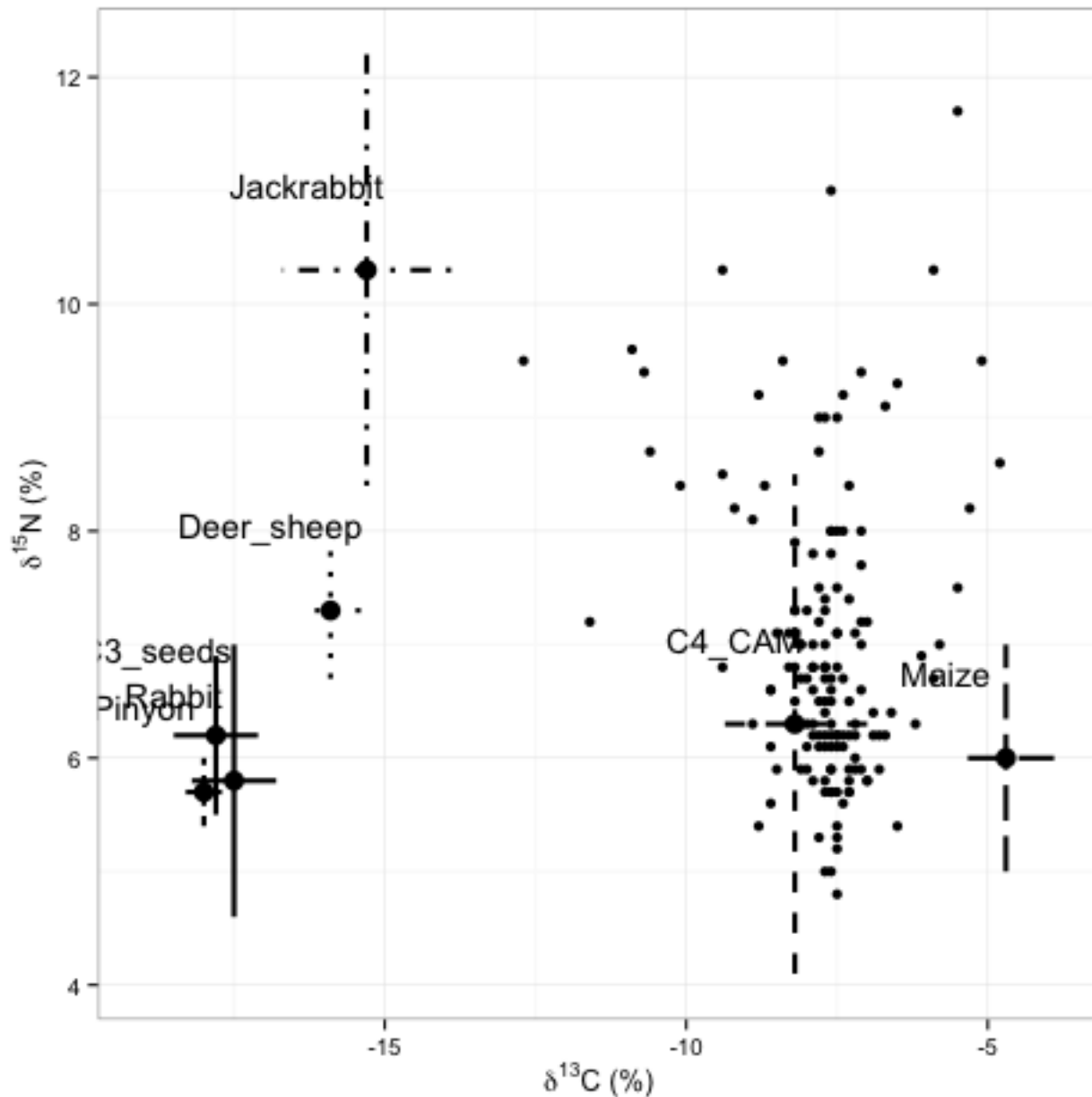
# Geometry is critical & mixing models won't solve problems (Phillips and Gregg 2003)



# Essentially 1-D problem

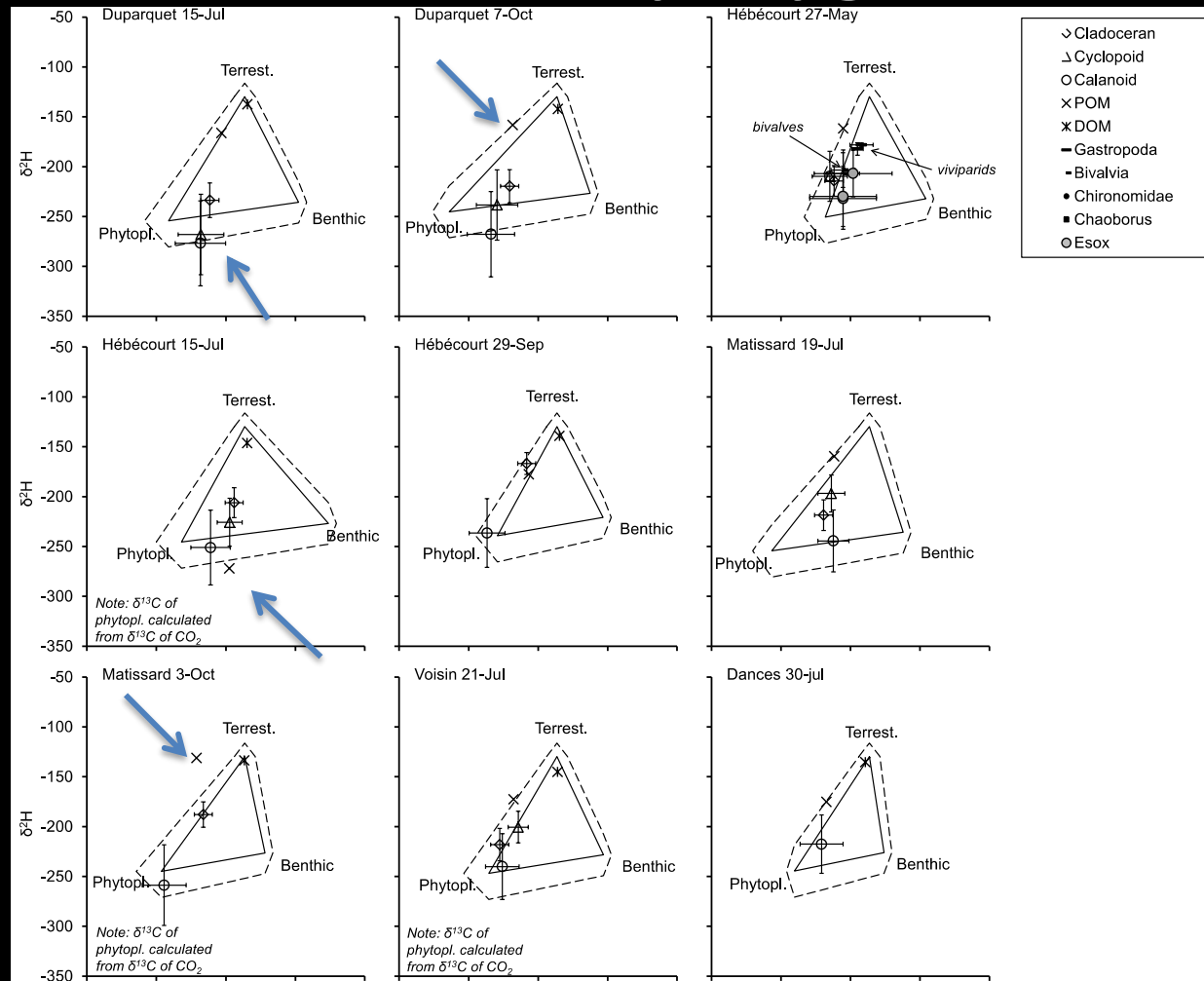


# Confounded sources



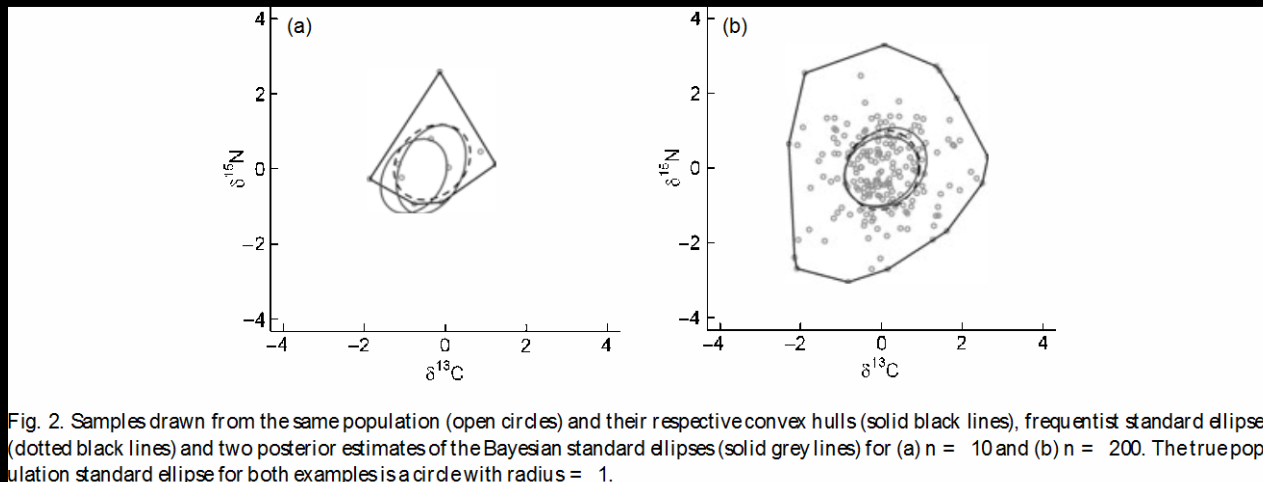


# Consumer signatures falling outside of resource polygon



# If mixing models aren't appropriate (bad geometry, other reasons)

- SIBER (Jackson et al. 2011)



- Test for differences among groups (e.g. Bodey et al. 2014 JAE)

# Ongoing research

- Including more than one data type in prior
  - Genetics, observational data, etc. (E. Ward)
- Incorporating multiple data types in likelihood
  - ‘fastinR’ FAs and SIs (Neubauer & Jensen 2014)
- Quantifying bias in different models to experimental / real data (Brett, Galloway, others)
- Using mixing models to estimate / infer movement (Carlisle et al. 2012, Phills et al.)
- Simulating effect of missing sources on estimates (Phillips, Inger, etc)
- More mechanistic mixing models (Stock & Semmens)