Evaluating Sensitivity to the Stick Breaking Prior in Bayesian Nonparametrics

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Collaborators

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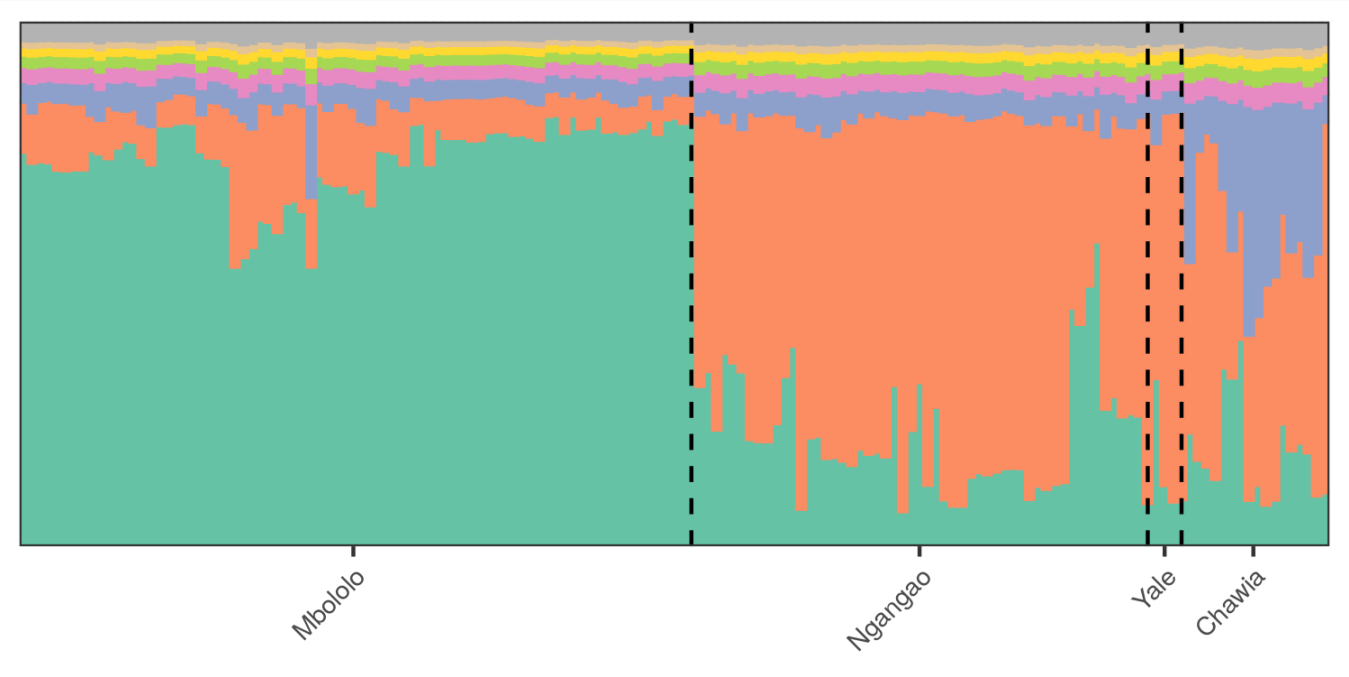
MIT

Motivation

Inferring population structure from genomic sequences.

- Genetic data from *Turdus helleri*, an endagered bird species (Pritchard et al. 2011).
- Microsatellites sequences of 155 individiuals at 7 loci.



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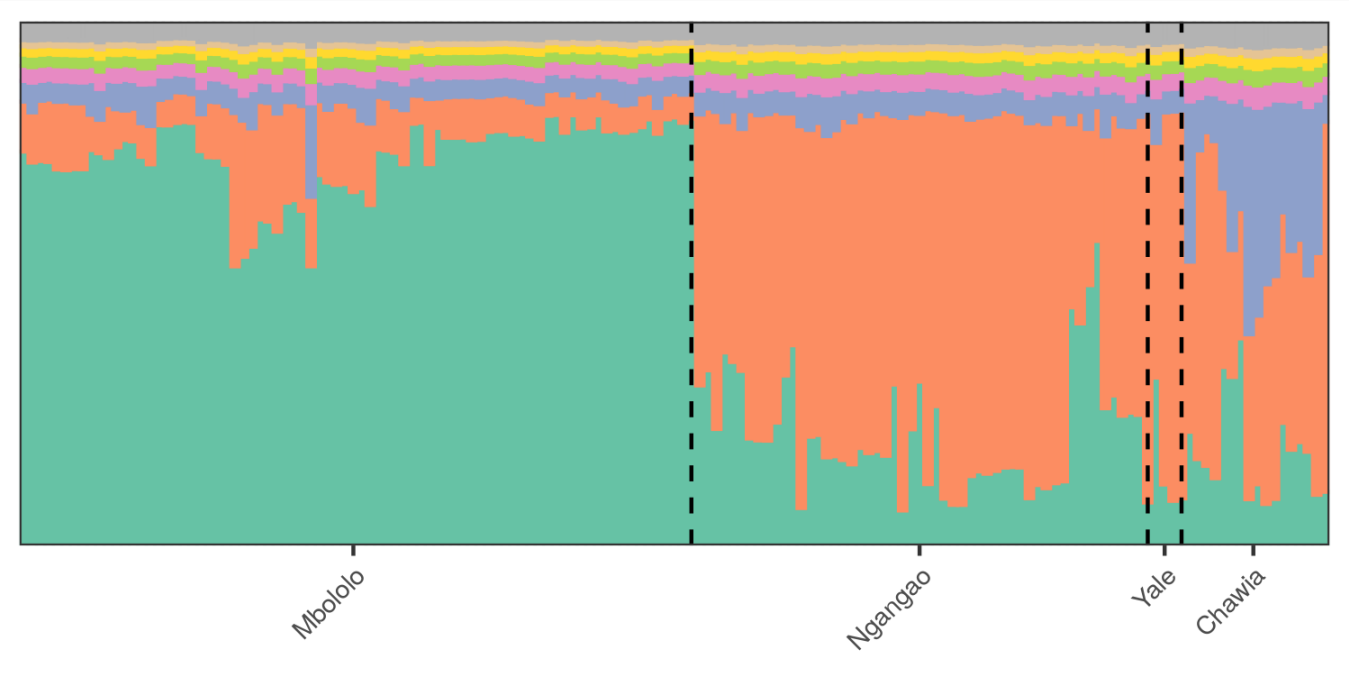

Possible questions of interest:

1. How many latent populations—aka clusters—are present in the data set?

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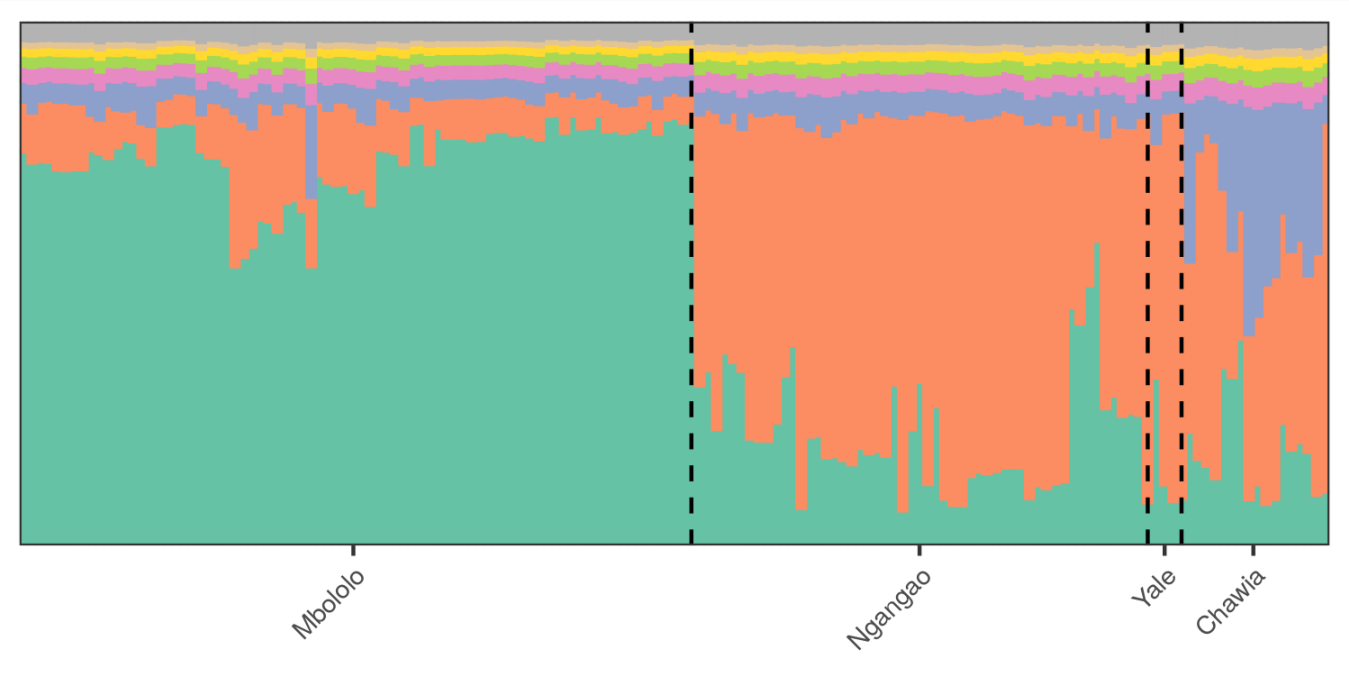

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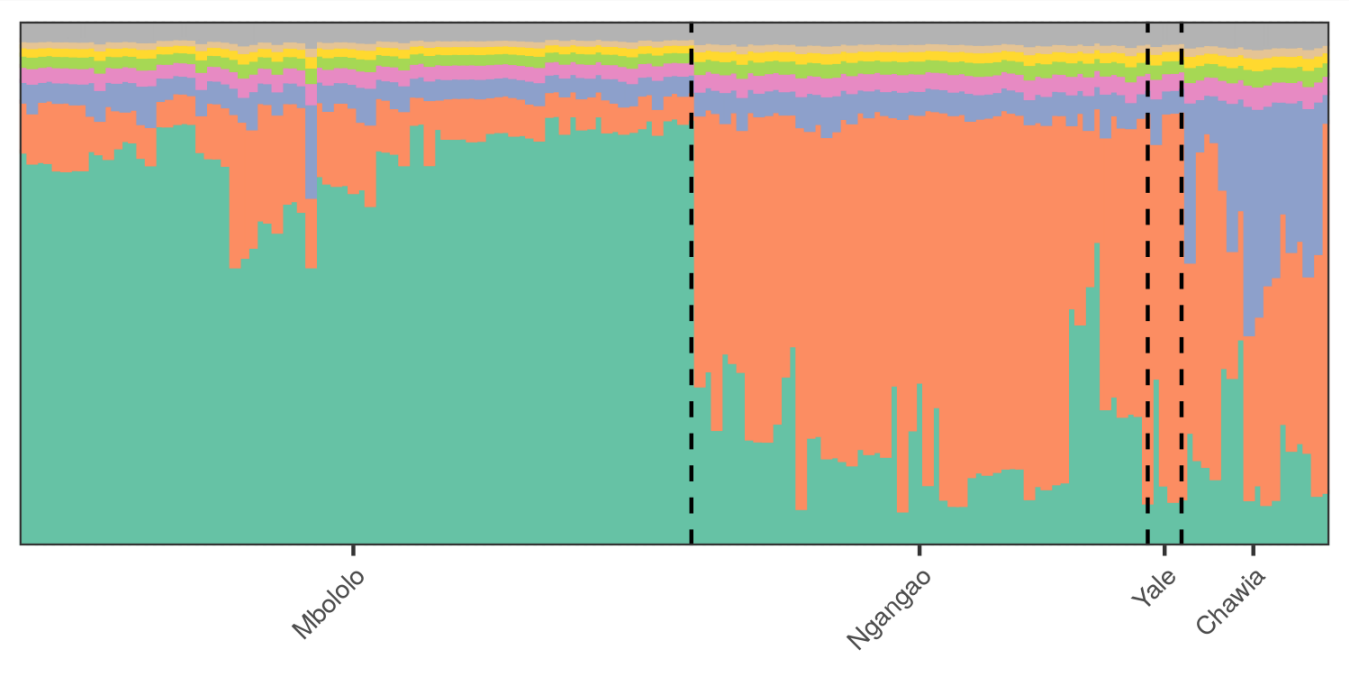

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1. How many latent populations—aka clusters—are present in the data set?
2. Which individuals cluster together?
3. What are the unique characterstics of each cluster?

Research problem

A Bayesian nonparametric (BNP) model makes inferring the number of clusters amenable to Bayesian inference.

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Problem: re-running VB for multiple model choices is expensive.

We propose: a linear approximation to efficiently estimate BNP sensitivity from a single run of VB (to avoid expensive refitting).

Outline

- The BNP model
- The variational approximation
- Hyperparameter sensitivity
- Functional sensitivity and influence functions
- Results on data

The BNP Model

A **Dirichlet process prior** allows for an infinite number of components.

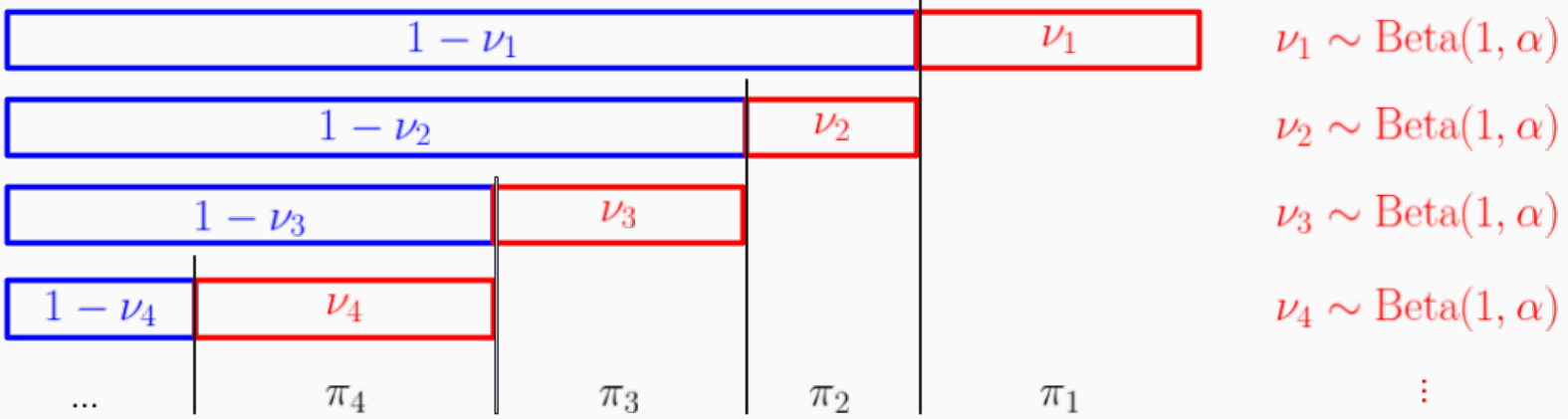

Figure 2: A schematic of the Dirichlet process prior

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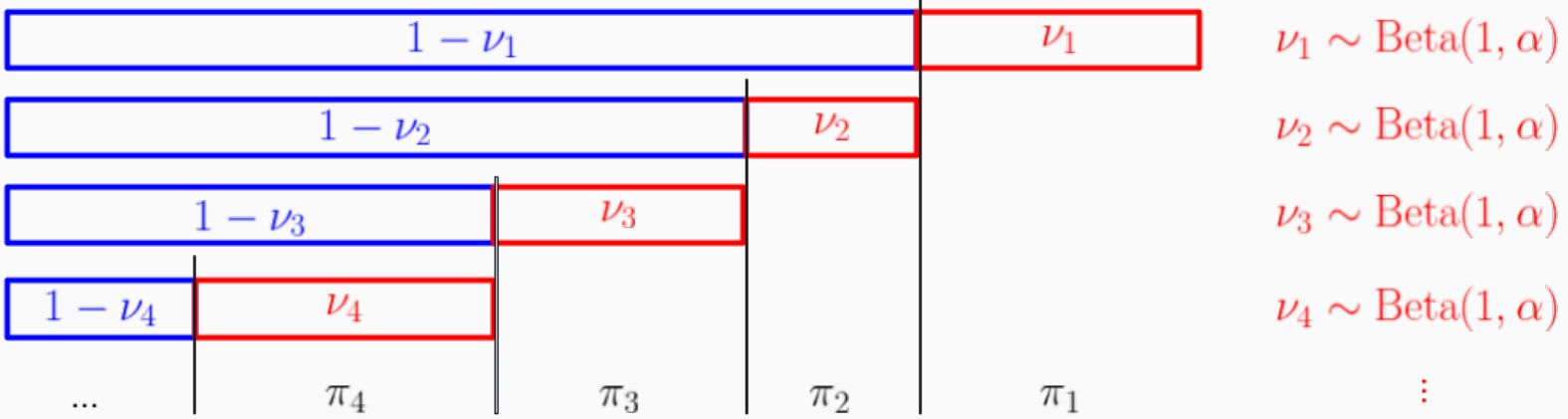

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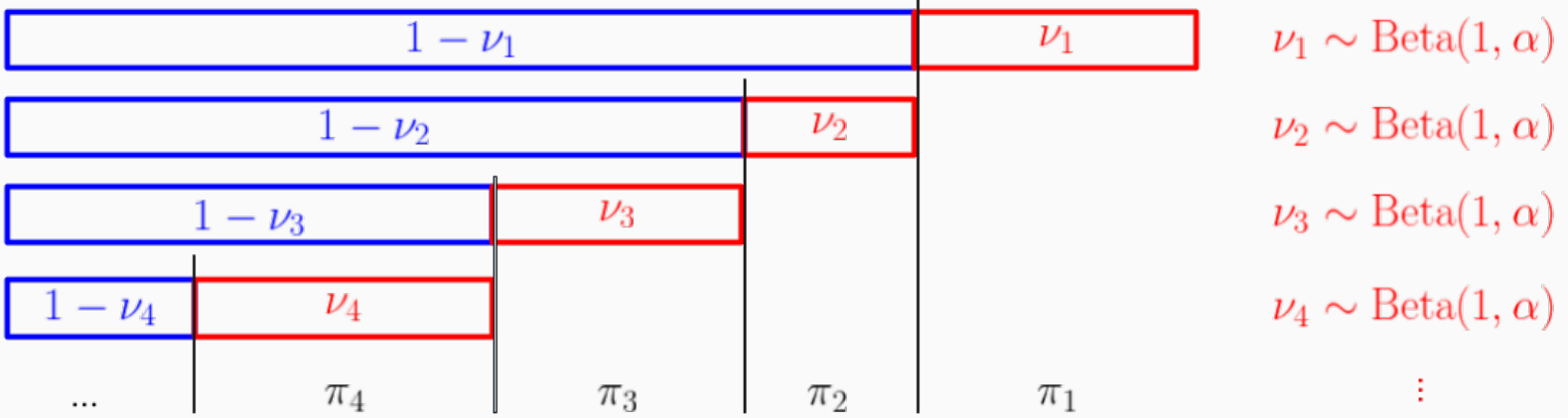

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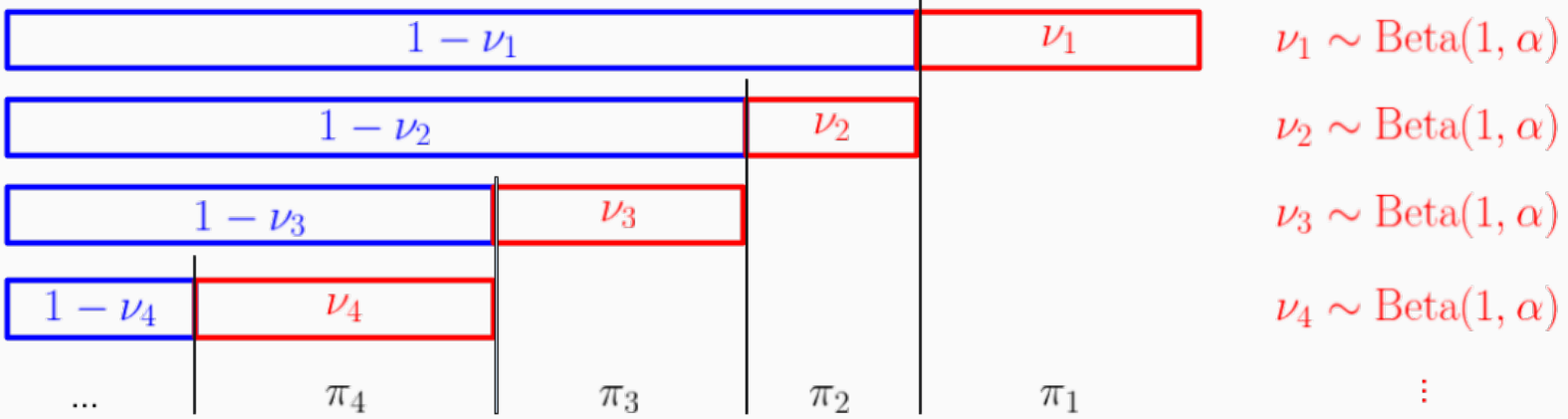

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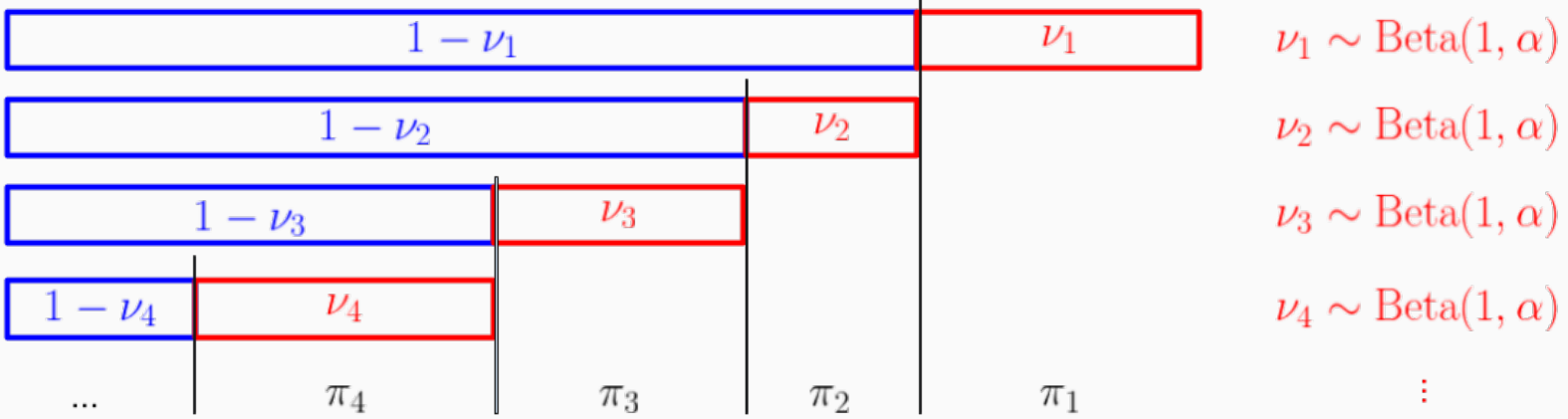

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What makes this stick-breaking prior a reasonable one?

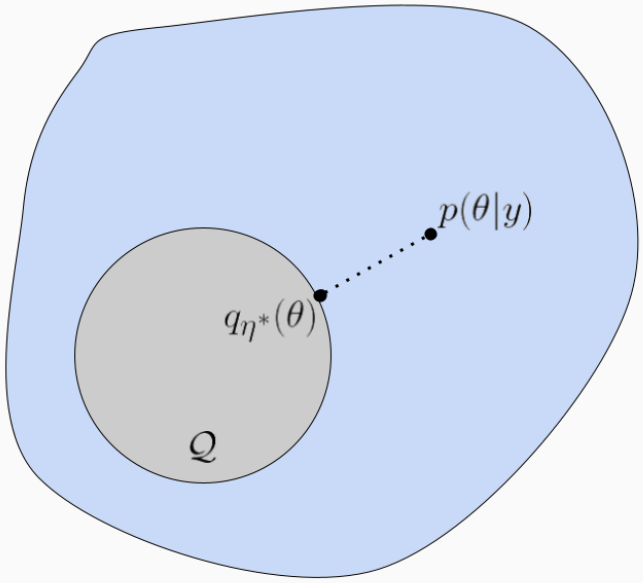
The Variational Approximation

Let θ be latent variables and y the observed data.

We posit a class of mean-field distributions parameterized by a real vector η.

We solve

$$\eta^* = \arg\min_{\eta} KL\left(q(\theta|\eta)\middle\|p(\theta|y)\right)$$



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Note that

- The optimal variational parameters η^* depend on the prior through optimizing the KL objective.
- The approximate posterior quantities are then functions of η^*, e.g.

$$\eta^* \mapsto \mathbb{E}_{q_{\eta^*}}[\#\text{clusters}] \quad \text{or} \quad \eta^* \mapsto \mathbb{E}_{q_{\eta^*}}\left[\#\left\{\begin{smallmatrix}\text{clusters in}\\ \text{new dataset}\end{smallmatrix}\right\}\right].$$

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How do these approximate posterior quantities depend on the DP prior?

Hyperparameter Sensitivity

Let ϵ be a real-valued hyperparameter for the stick-breaking distribution (e. g., this could be the α concentration parameter, or it could parameterize a functional shape).

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Main idea: We approximate the dependence of η^* on ϵ with a first-order Taylor expansion:

$$\eta^*(\epsilon) \approx \eta^*(0) + \frac{d\eta^*(\epsilon)}{d\epsilon^T}\Big|_{\epsilon=0} \epsilon$$

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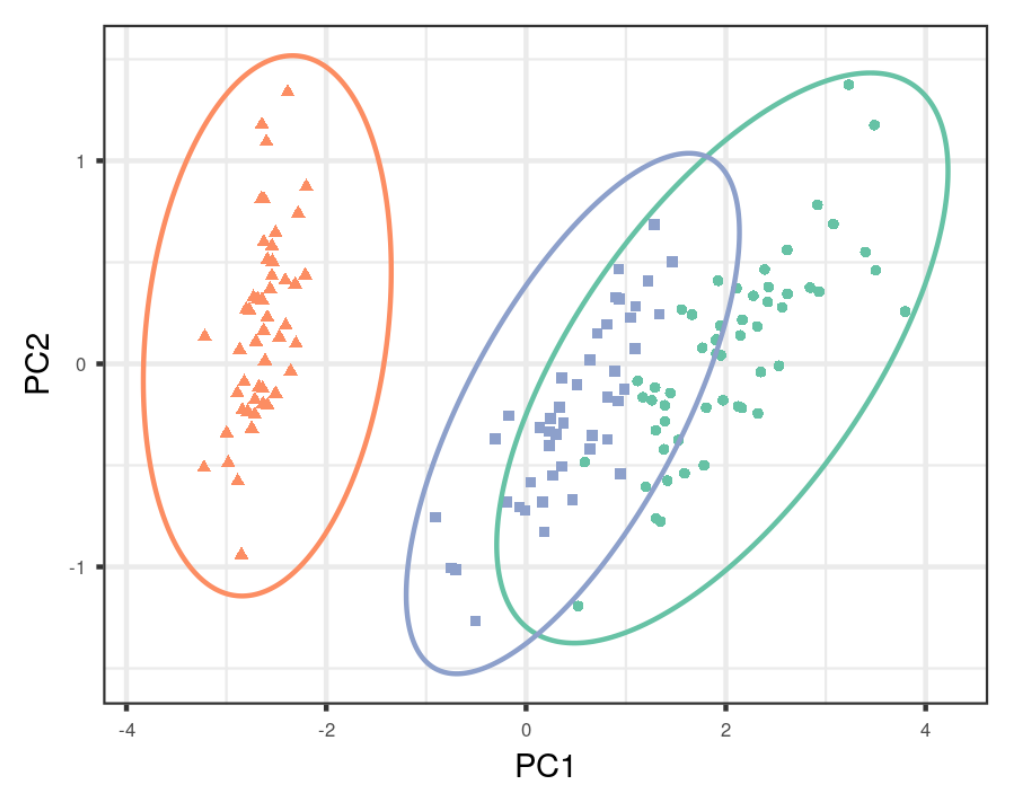
Notes:

- Evaluation of the derivative can be done efficiently using formulas from Giordano et al. 2018 and modern automatic differentiation tools.
- We only use a linear approximation for the map $\epsilon \mapsto \eta^*(\epsilon)$. We retain nonlinearities in the map $\eta^* \mapsto \mathbb{E}_{q_{\eta^*}}$ [#clusters].

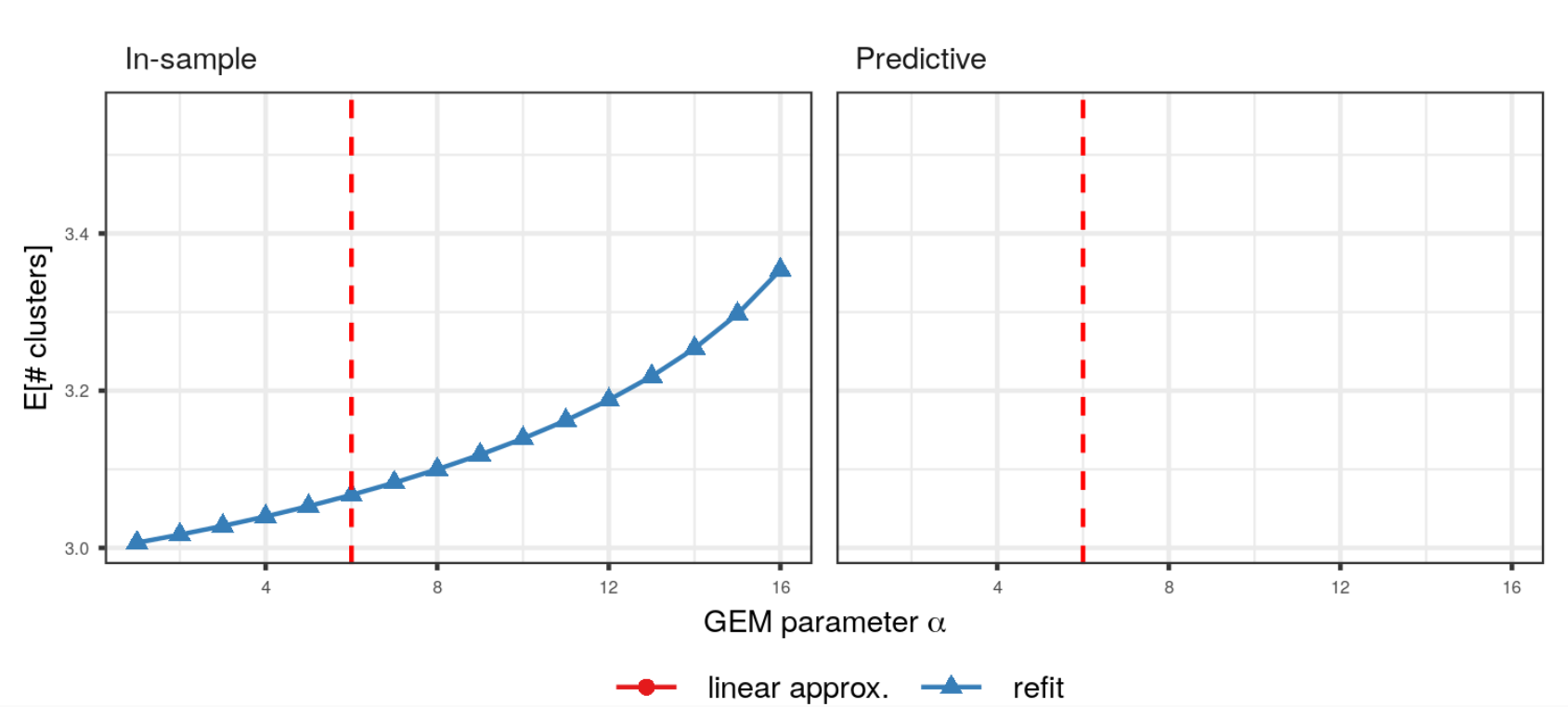
A simple example: iris data

We fit a Gaussian mixture model with a DP prior to the iris data.



The iris data in principal component space and GMM fit at $\alpha = 6$.

iris data: parametric sensitivity



The expected number of posterior clusters in the iris data as α varies.

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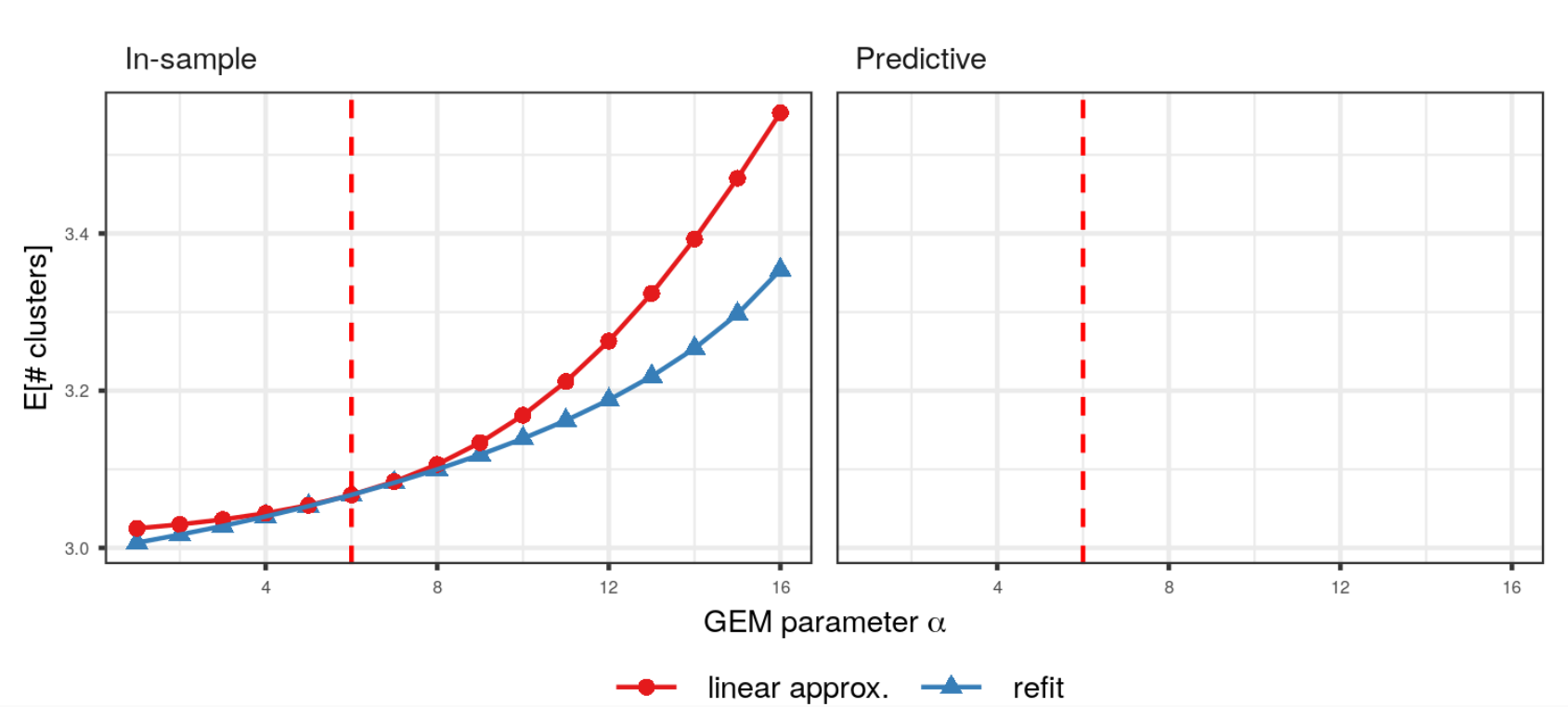

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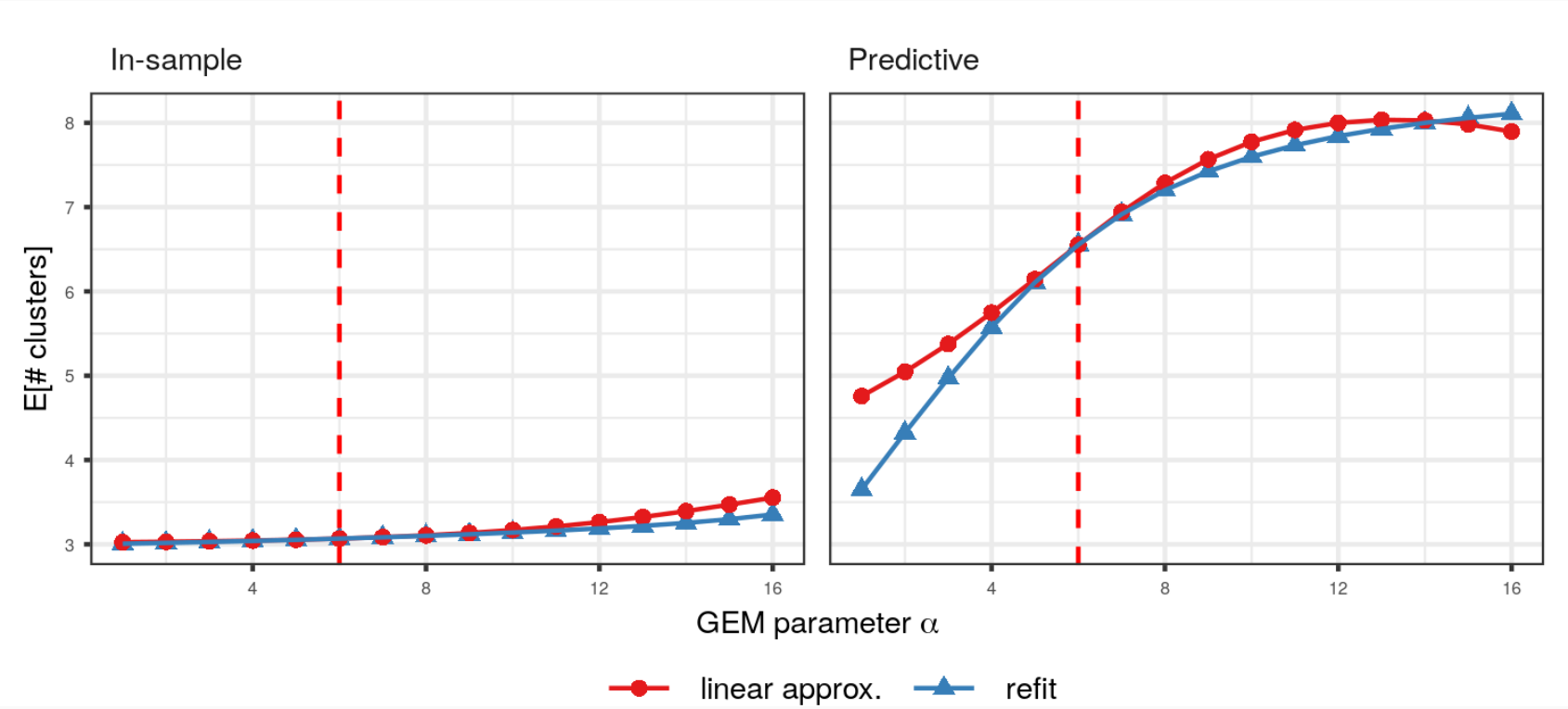

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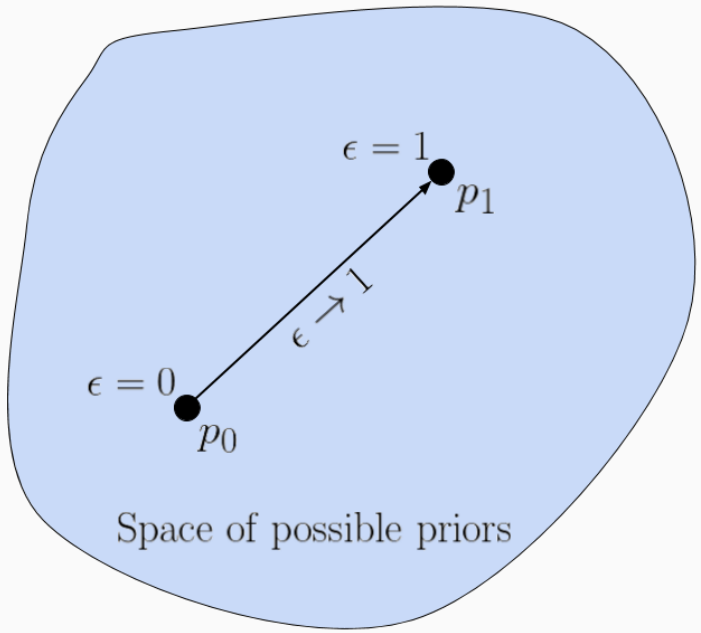
Functional sensitivity

Let $p_0(\nu_k)$ be the original Beta prior on sticks.

Suppose we wish to replace p_0 with another distribution p_1. Define the "contaminated" prior as:

$$p_c(\nu_k|\epsilon) \propto p_0(\nu_k) \exp(\epsilon\phi(\nu_k))$$

where $\phi(\nu_k) = \log p_1(\nu_k) - \log p_0(\nu_k)$.



Functional sensitivity: influence functions

Consider a posterior statistic of interest $g(\eta)$, e.g.

$$g_{\mathrm{cl}}(\eta) = \mathbb{E}_{q_\eta}\left[\#\text{clusters}\right]$$

Let S_g be the *local sensitivity* of g with respect to a hyper-parameter ϵ

$$S_g := \frac{d}{d\epsilon}\, g(\eta(\epsilon))$$

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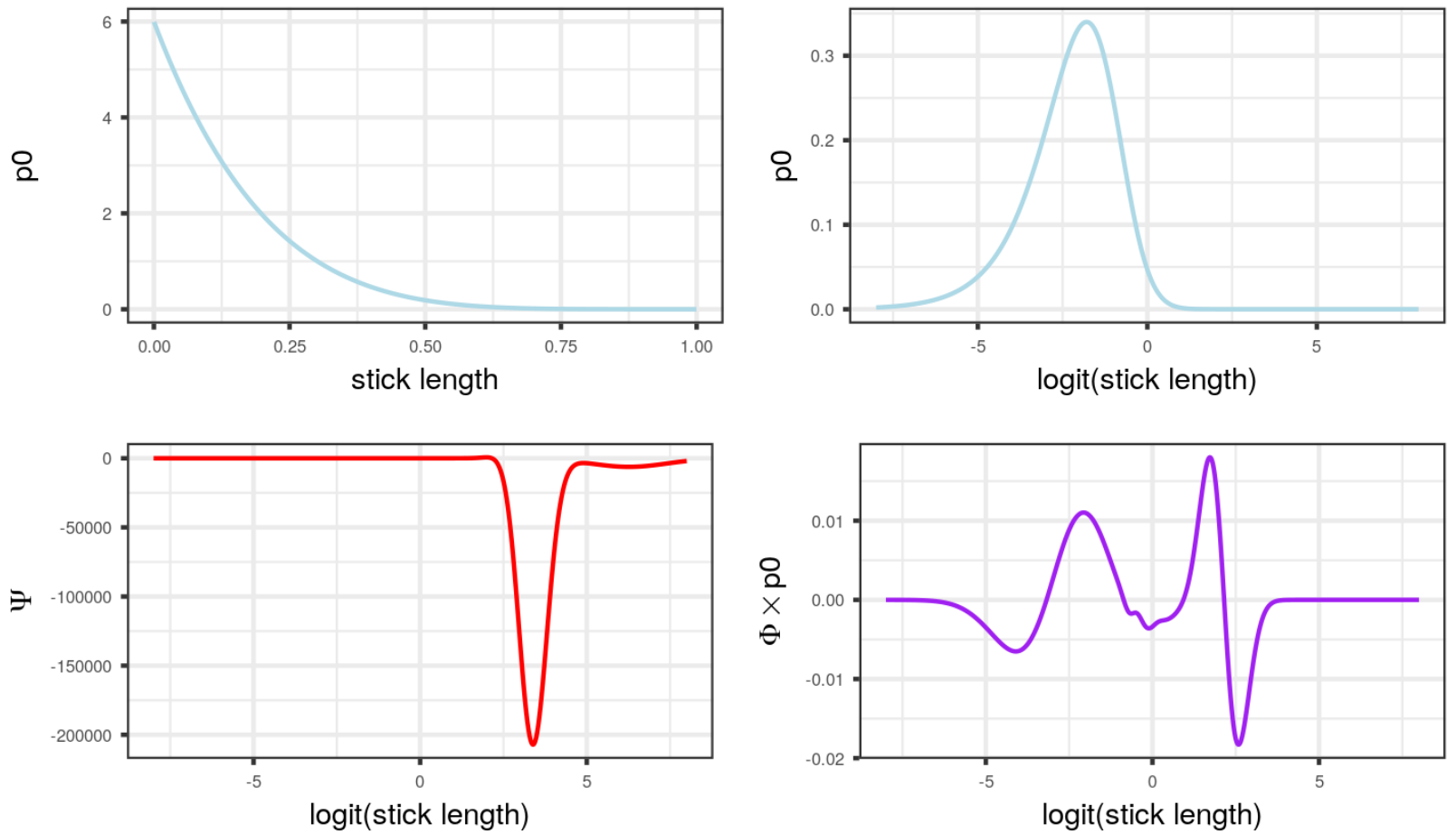
The local sensitivity can be expressed as an inner-product between an *influence function* Ψ and the functional perturbation ϕ in an appropriate Hilbert space:

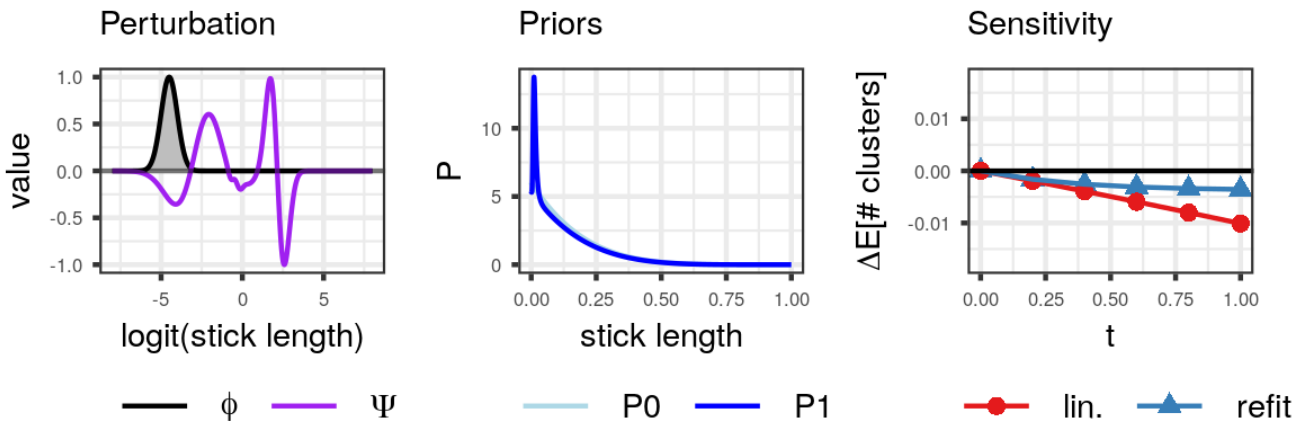
$$\begin{aligned} S_g &= \langle \Psi, \phi \rangle \\ &= \int \Psi(\nu)\phi(\nu)p_0(\nu)\, d\nu \end{aligned}$$

Iris data: influence functions



The influence function for the number of clusters, g_{cl}.

Iris data: functional perturbations



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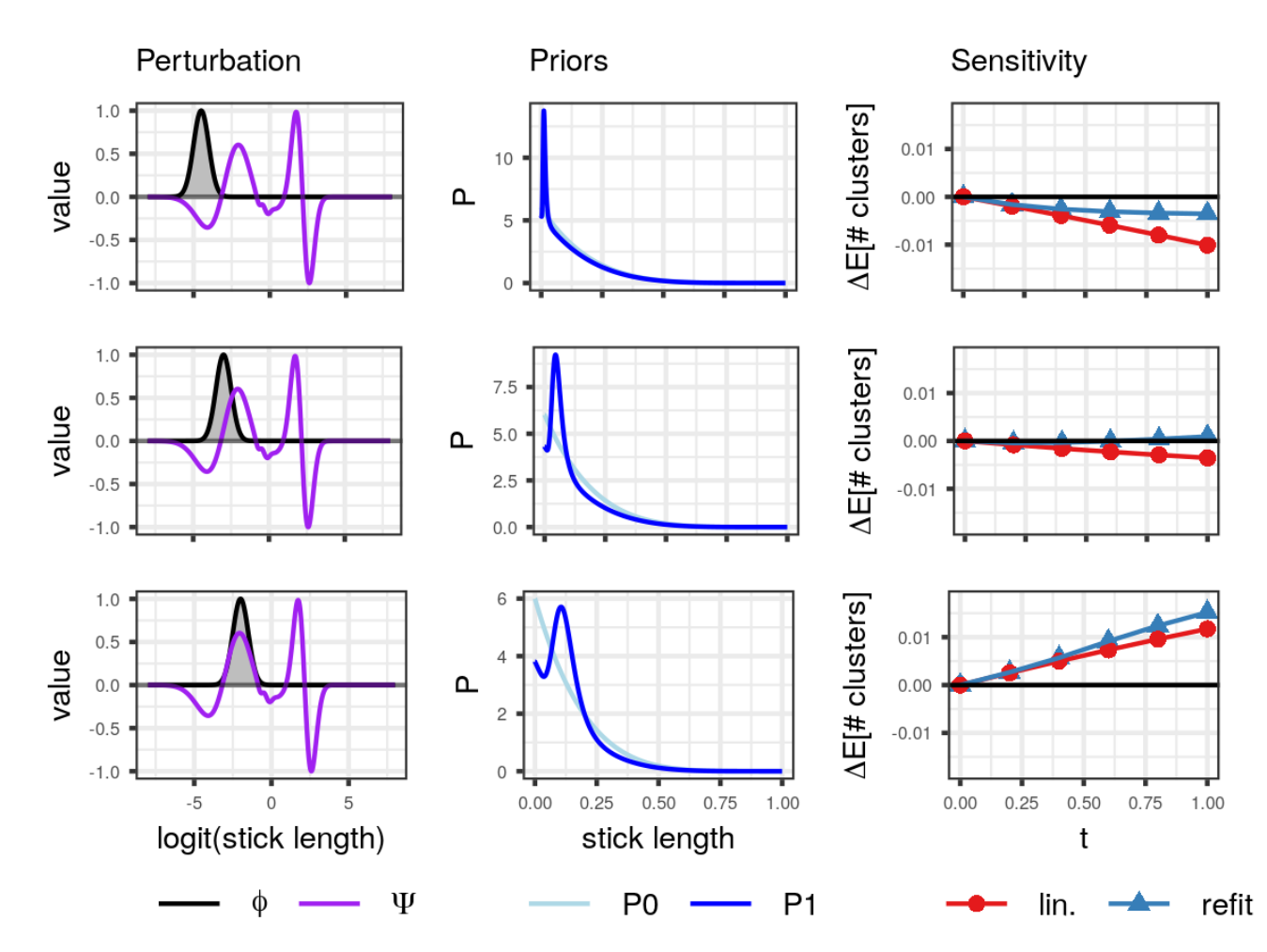
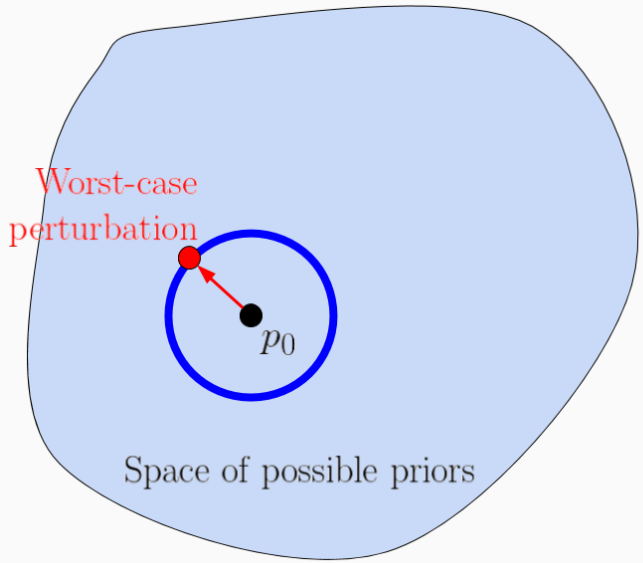


Functional perturbations: worst-case

There are many possible choices for p_1.

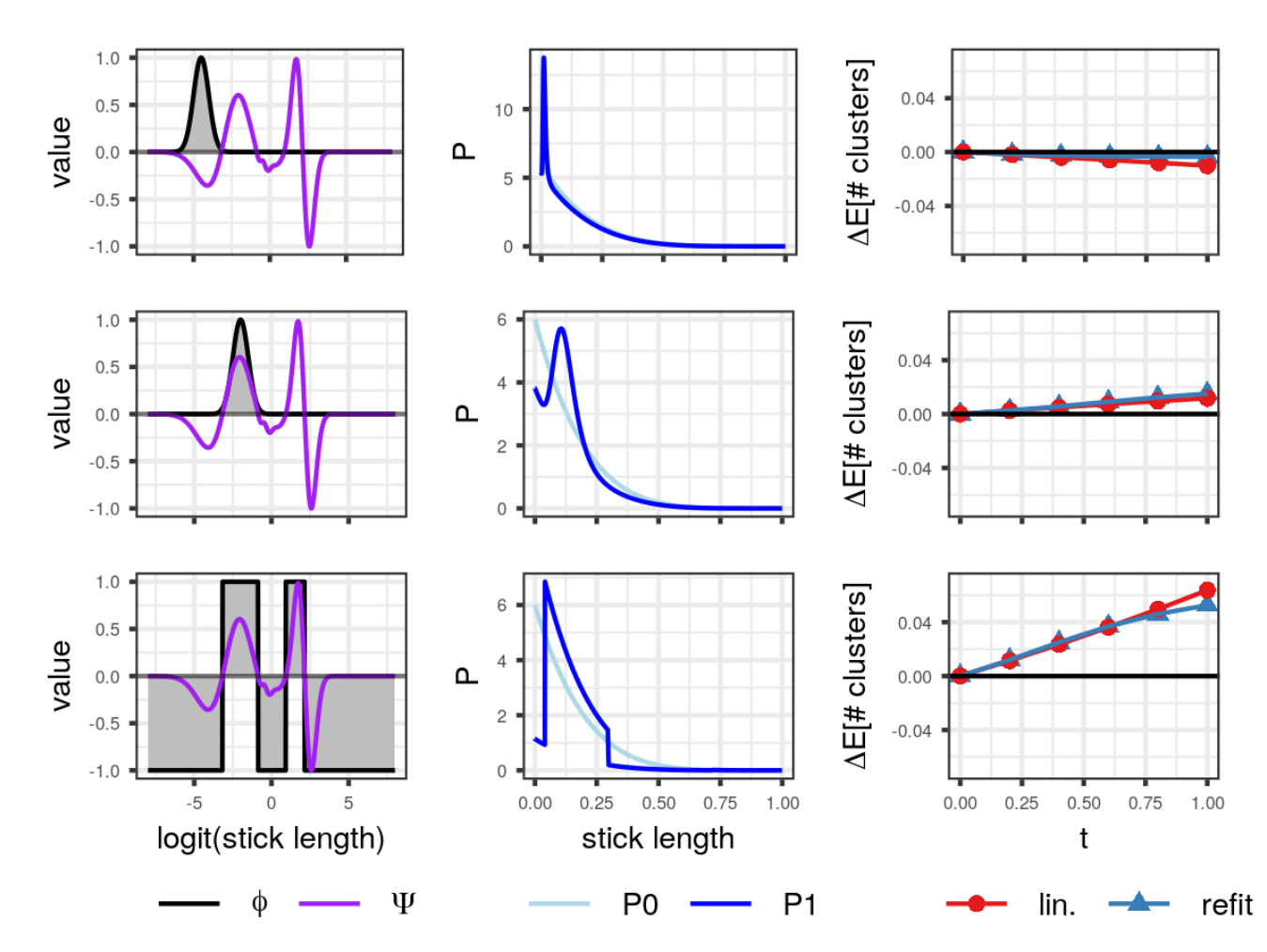
Given a posterior quantity g, we can find the *worst-case* perturbation in a ball of radius δ, that is, find the direction such that $|S_g|$ is maximized.



Specifically, we consider the L-infinity ball of radius δ:

$$B_\delta := \{\phi : \|\phi\|_\infty < \delta\}$$

Iris data: worst-case perturbation



Results on STRUCTURE

We adapt STRUCTURE (Pritchard et al. 2011; Raj et al. 2014) , a Bayesian model for population genetics, to include a BNP prior.

We study genetic data from the Taita thrush, an endagered bird species. The data consists of microsatellites sequences of 155 individiuals at 7 loci.

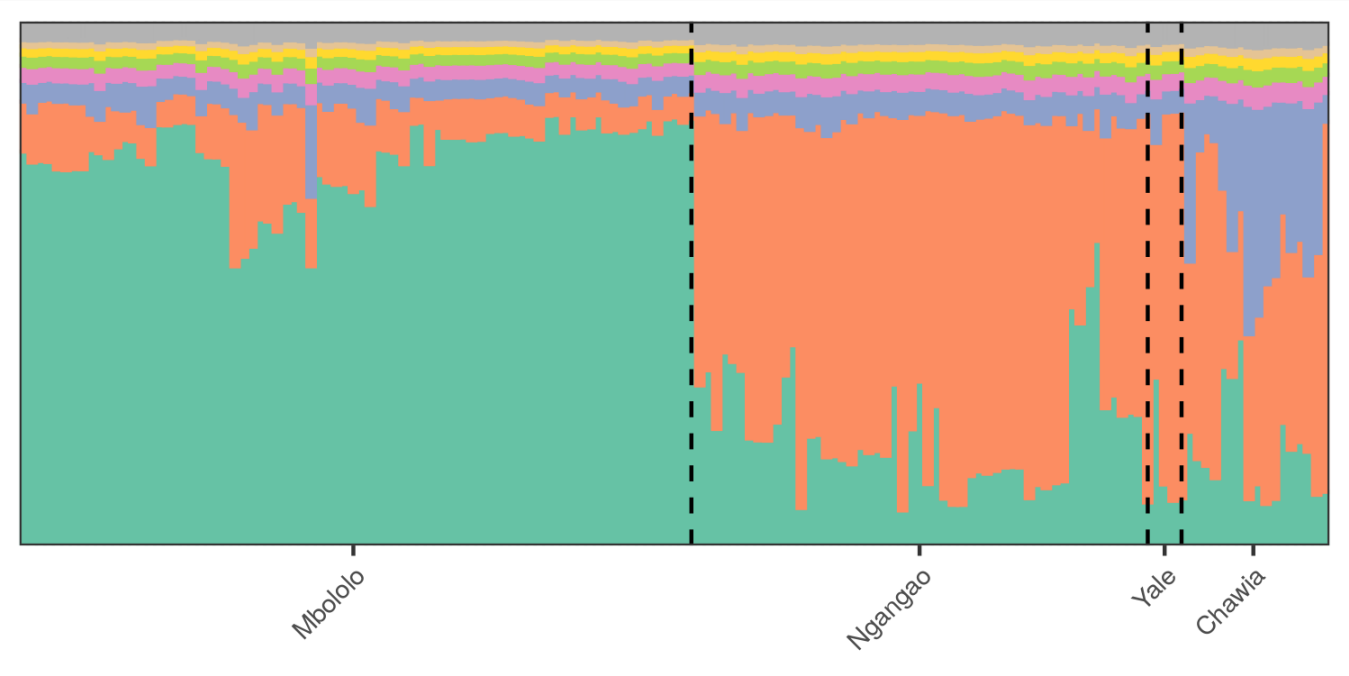
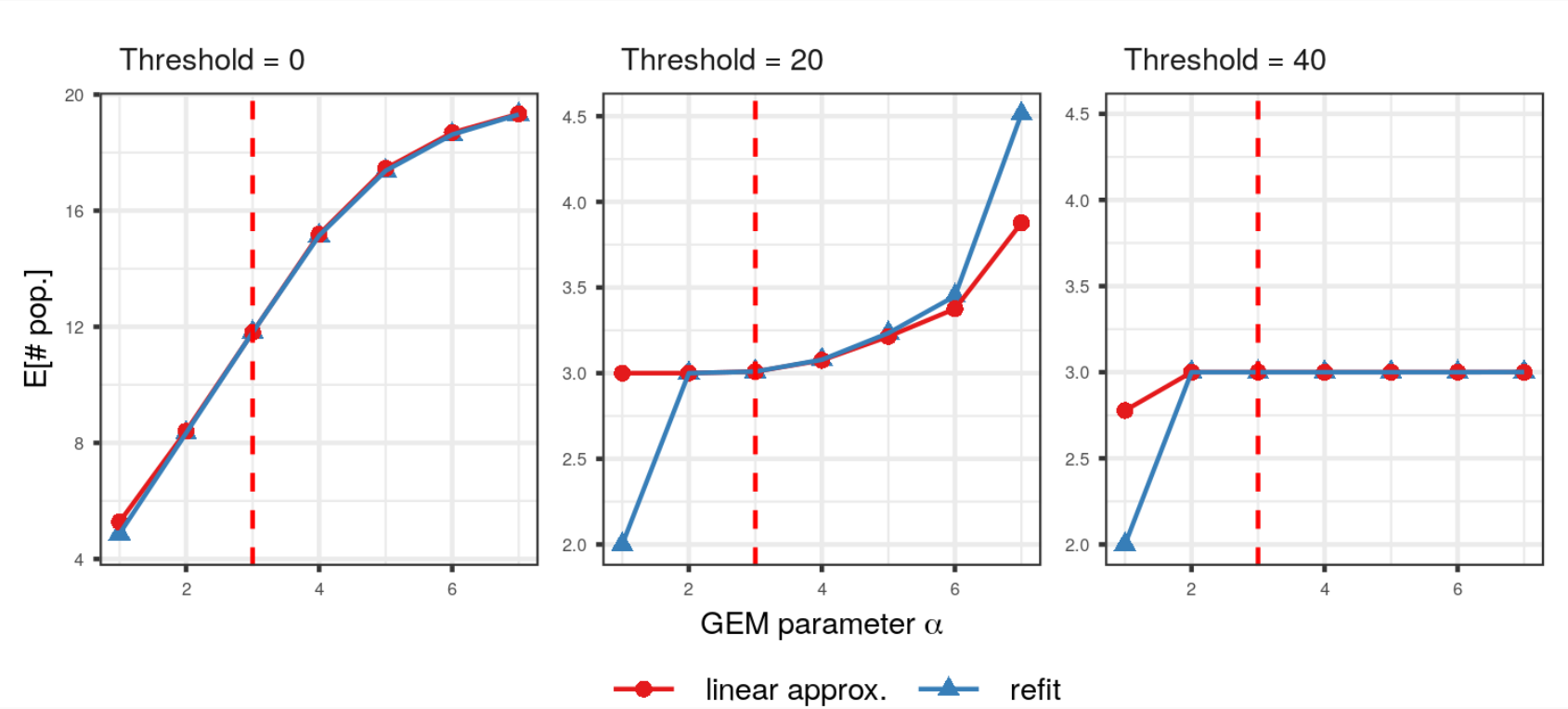


Figure 3: The intitial fit at $\alpha = 3$.

STRUCTURE: parametric sensitivity



The expected number of posterior in-sample clusters in the thrush data as α varies.

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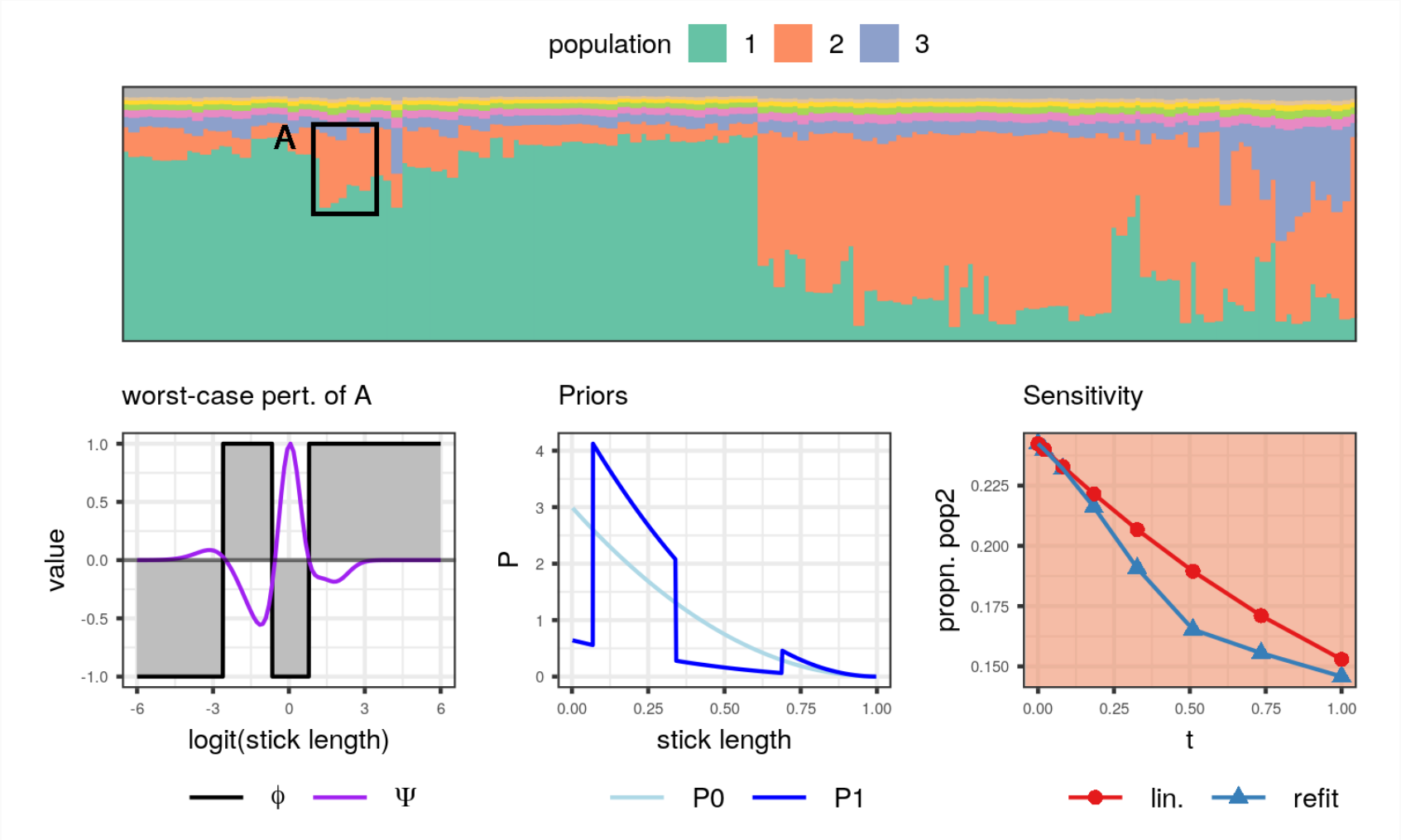

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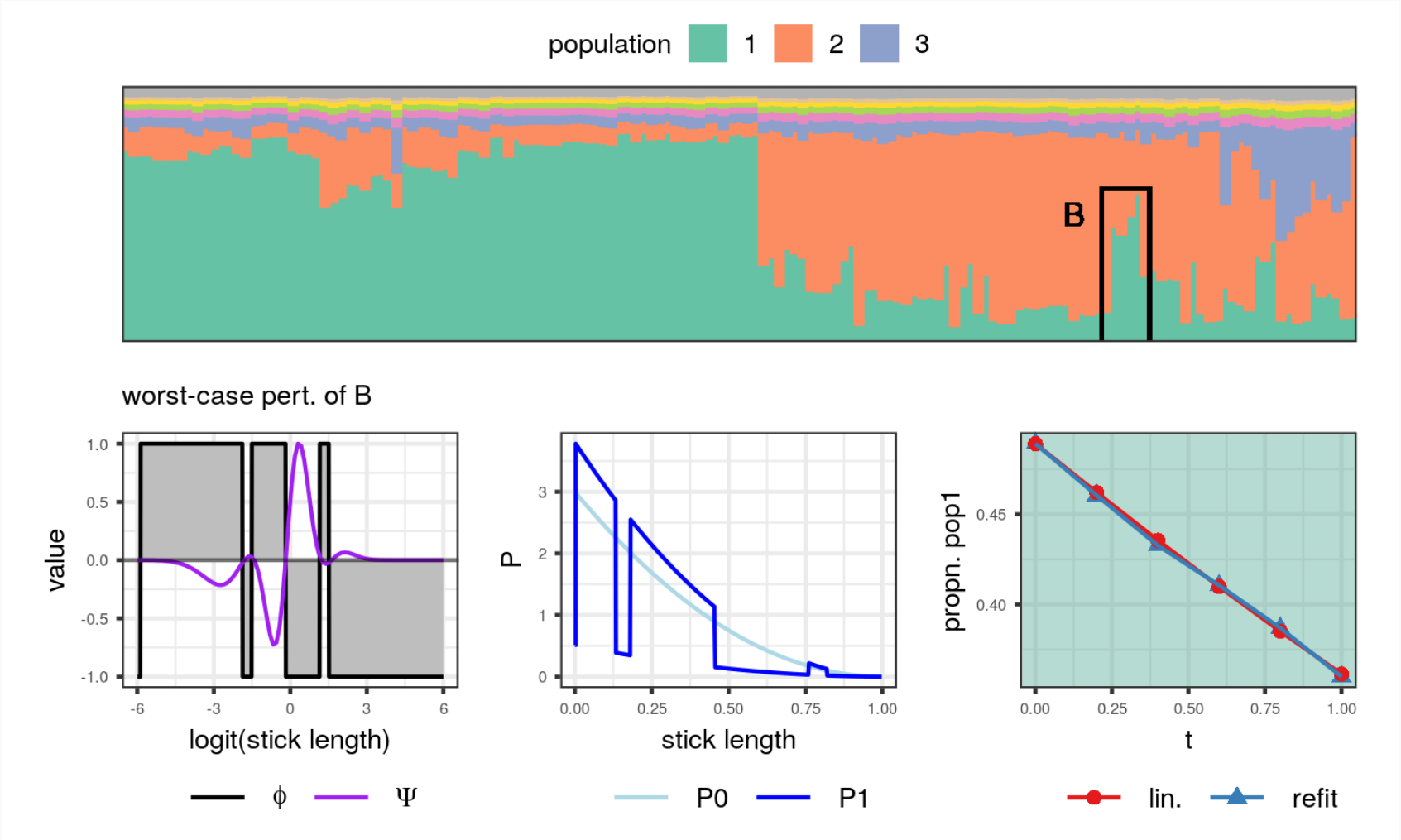

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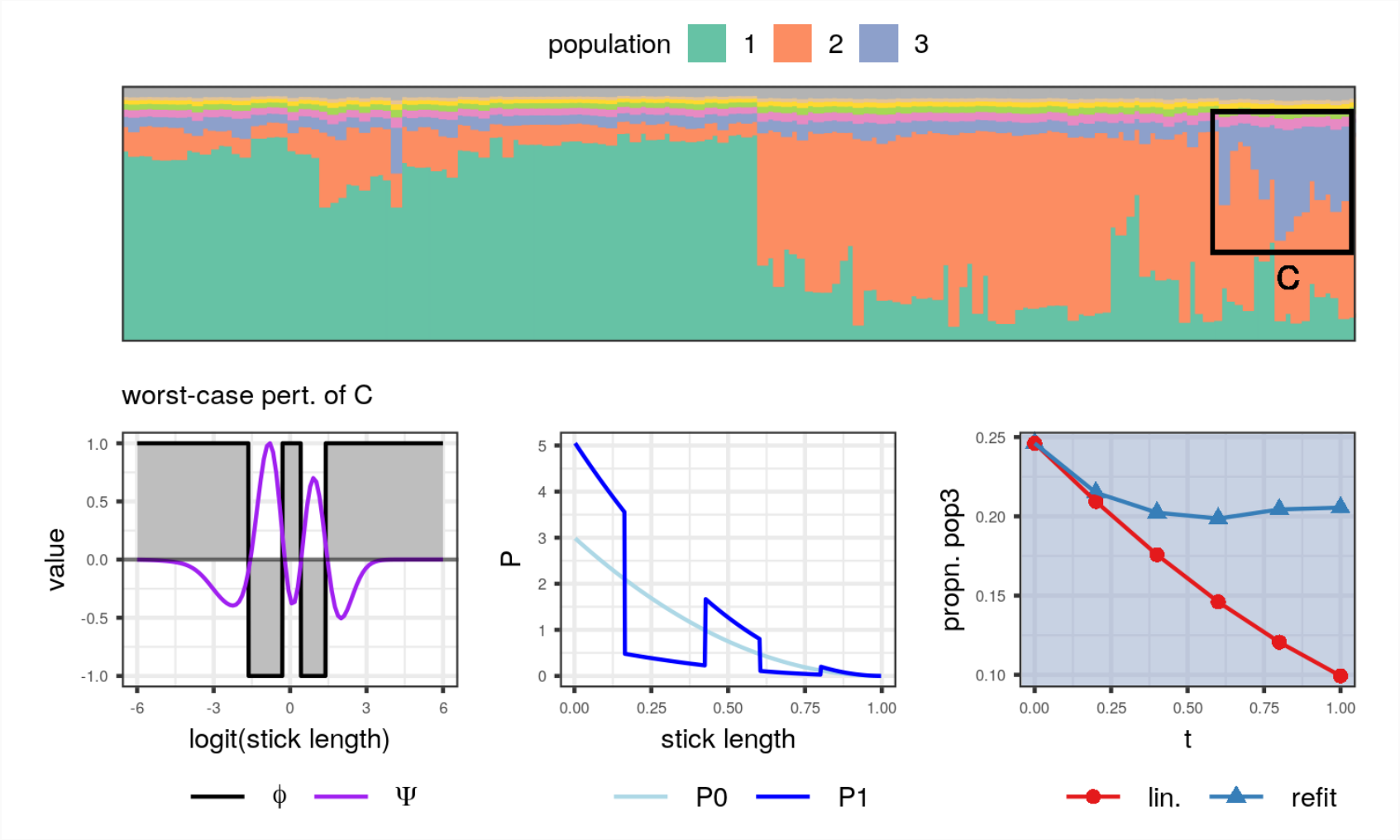
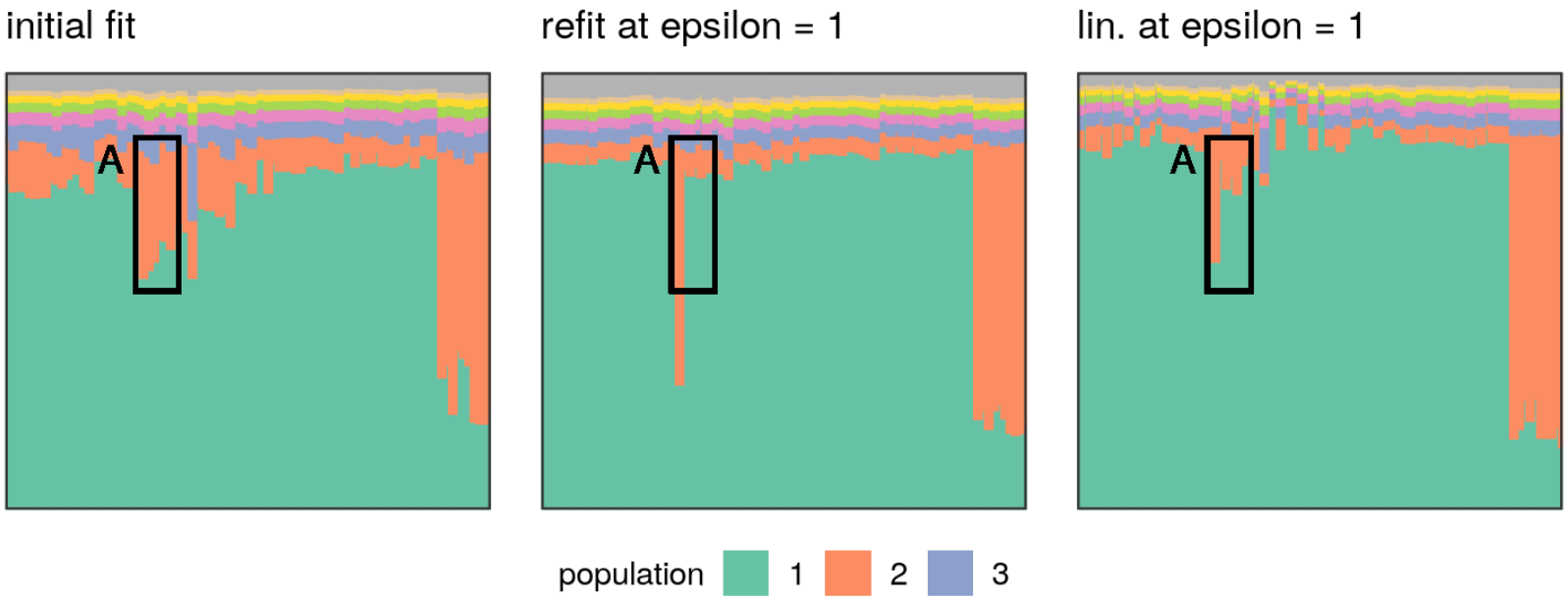


Computational times

Compute time of results on the Taita thrush dataset.

	time (seconds)
Initial fit	7
Hessian solve for α sensitivity	0.3
Linear approx. $\eta^{lin}(\alpha)$ for $\alpha = 1, ..., 7$	0.006
Refits $\eta(\alpha)$ for $\alpha = 1, ..., 7$	30
The influence function	0.6
Hessian solve for worst-case ϕ	0.4
Linear approx. $\eta^{lin}(\epsilon)\|_{\epsilon=1}$ for worst-case ϕ	0.001
Refit $\eta(\epsilon)\|_{\epsilon=1}$ for worst-case ϕ	10

Limitations of local sensitivity



Inferred admixtures after the worst-case perturbation to individuals A. Individual $n = 26$ had a large increase in admixture proportion of population 2 after the refit.

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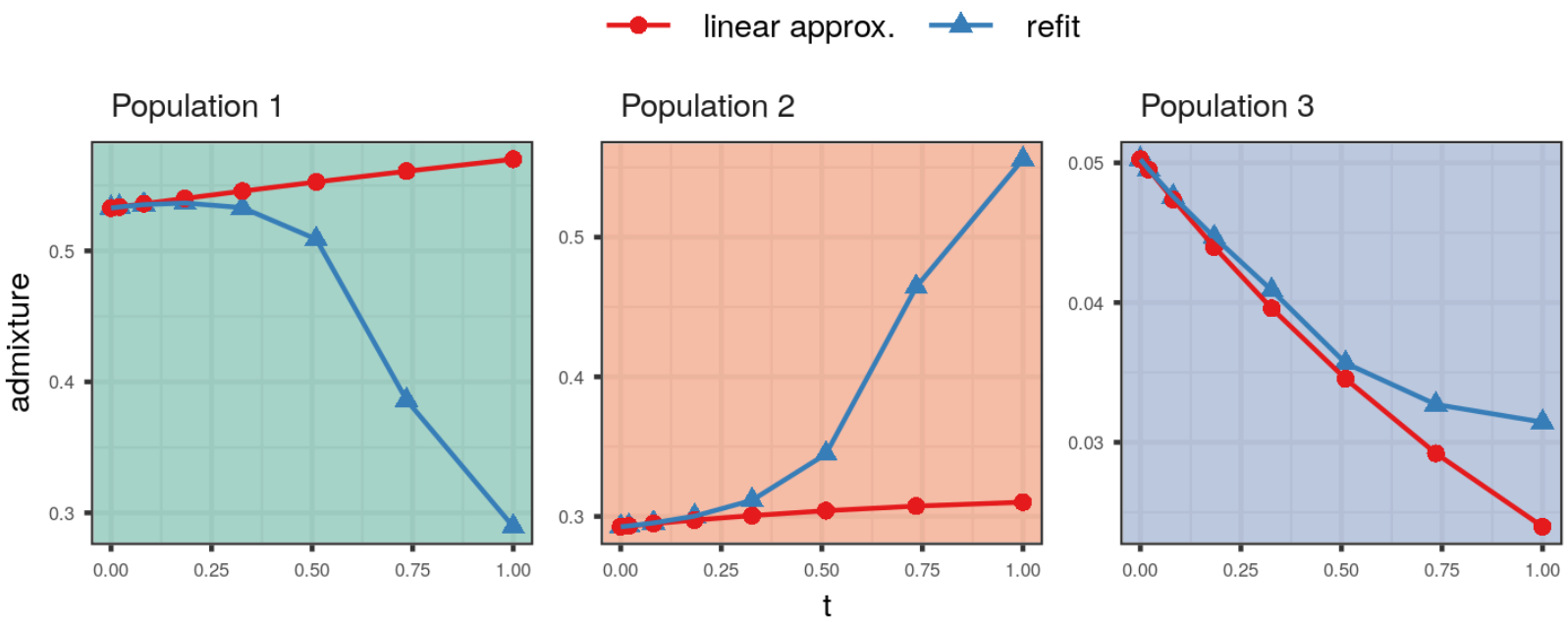

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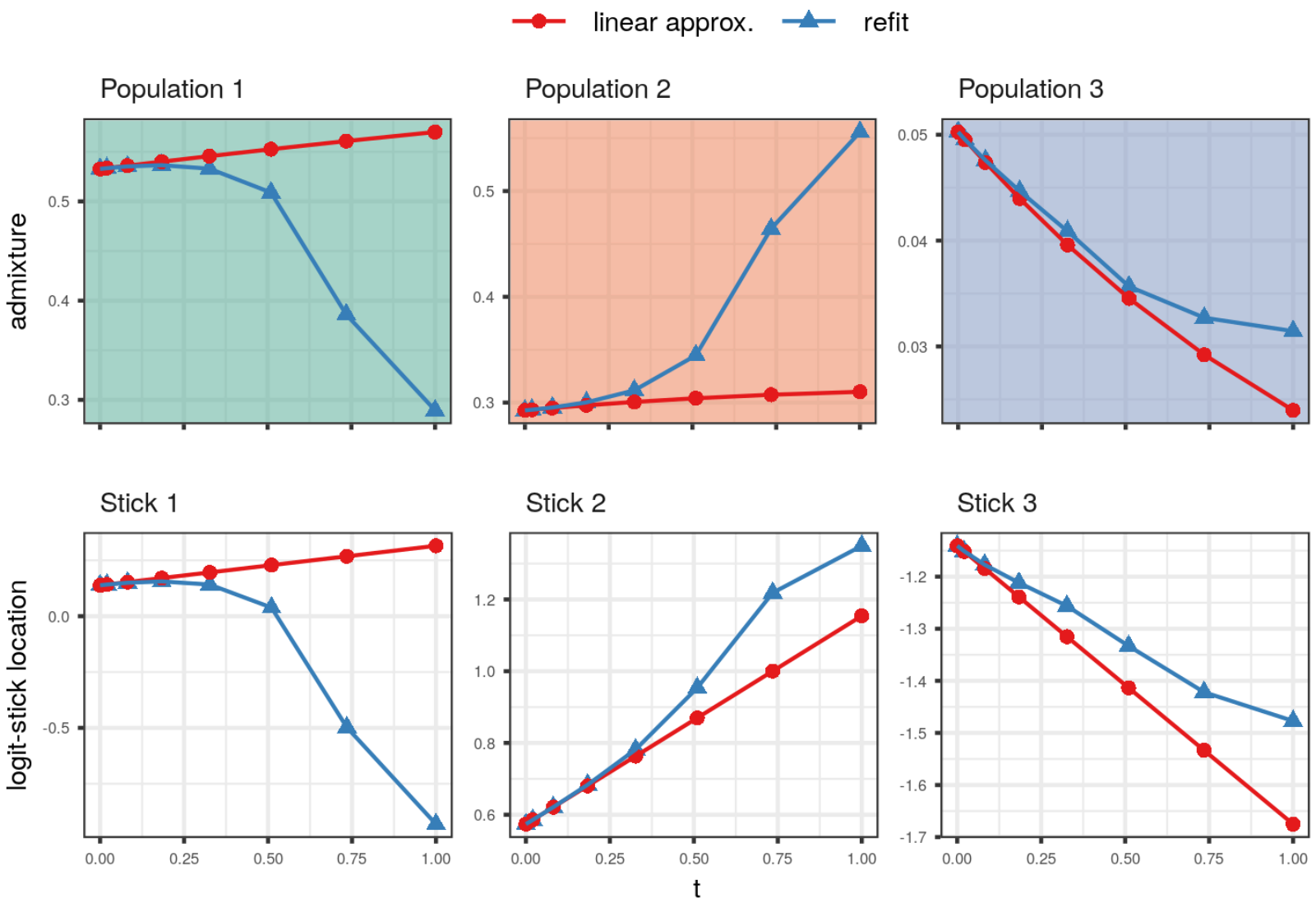

Conclusions

- We provide a tool to efficiently evaluate the sensitivity of the variational posterior to prior chioces.
- Linearizing the variational parameters provides a reasonable alternative re-optimizing the variational approximation after model perturbations.
- The influence function can provide guidance to find particularly sensitive model perturbations.

References

A workshop paper:

Runjing Liu, Ryan Giordano, Michael I. Jordan, Tamara Broderick. "Evaluating Sensitivity to the Stick Breaking Prior in Bayesian Nonparametrics."

https://arxiv.org/pdf/1810.06587.pdf

Code:

Paragami: parameter folding and flattening for optimization problems

https://github.com/rgiordan/paragami

Vittles: library for sensitivity analysis in optimization problems

https://pypi.org/project/vittles/

JAX: composable transformations of Python+NumPy programs

https://github.com/google/jax