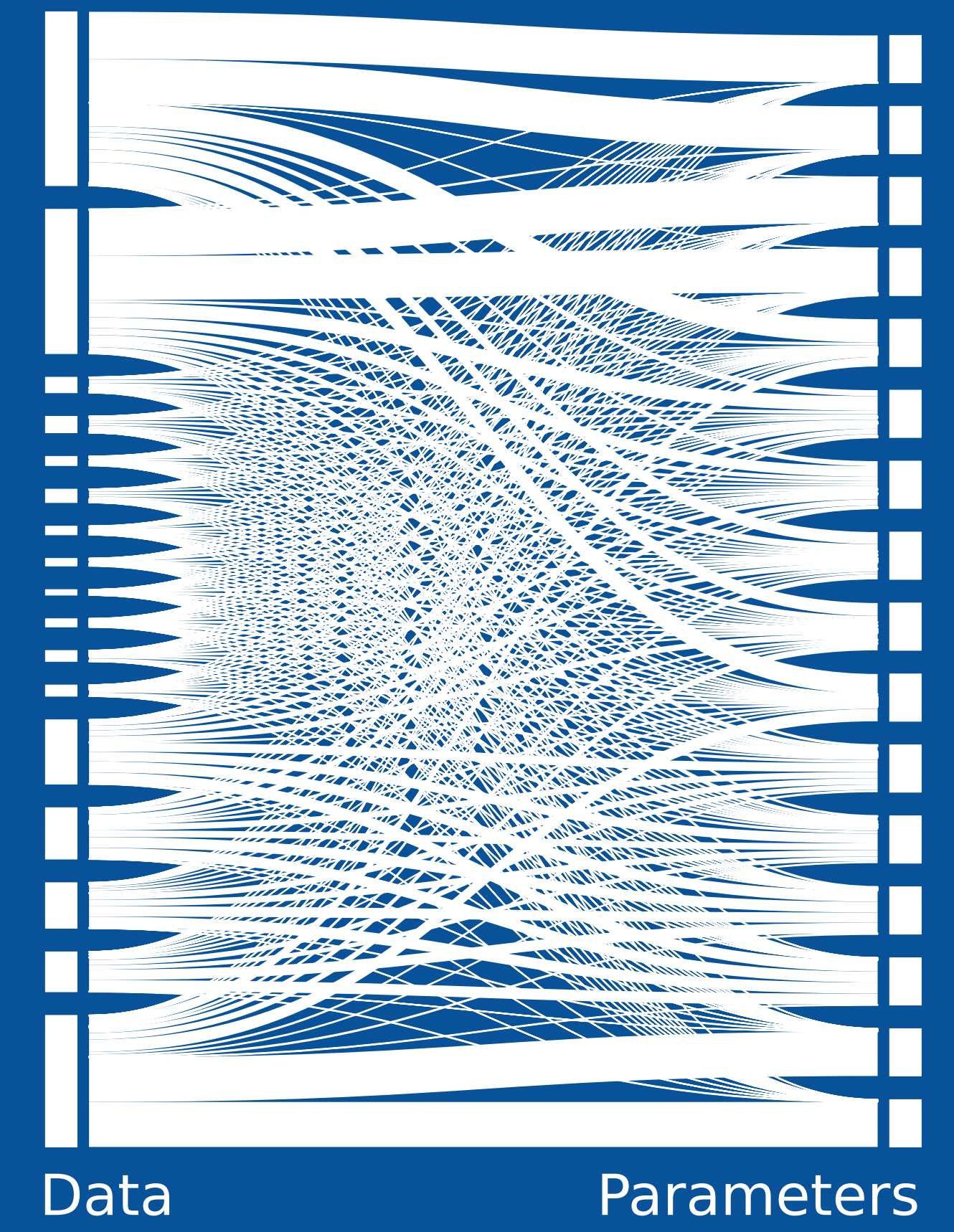


Robustly account for informativeness in ABC via inverse ML models.

Information



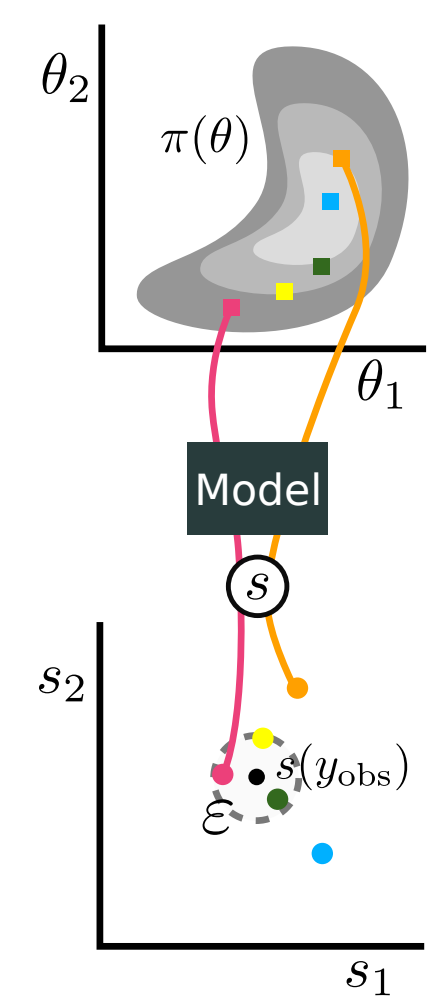
Yannik Schaelte^{1,2,3}, Jan Hasenauer^{1,2,3}

2022-05

1: Helmholtz Center Munich, Institute of Computational Biology, 2: Technical University Munich, Center for Mathematics, 3: University Bonn, Faculty of Mathematics and Natural Sciences

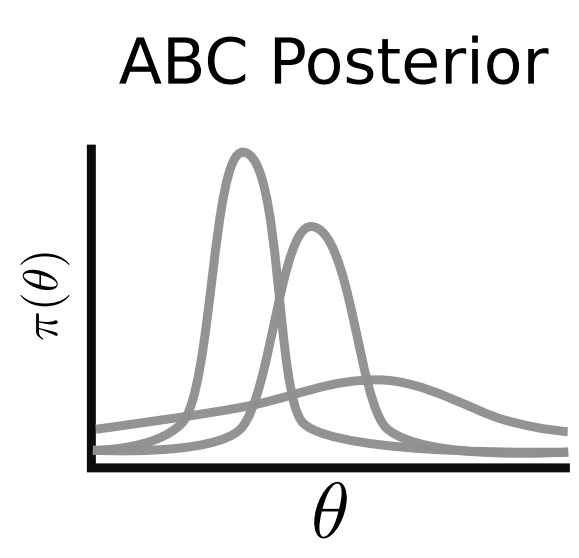
Mini-Intro: ABC

- Parameter inference method that doesn't need to evaluate the likelihood function
- until N acceptances:
 - sample parameters $\theta \sim \pi(\theta)$
 - simulate data $y \sim \pi(y|\theta)$
 - accept if $d(s(y), s(y_{obs})) < \epsilon$
- often combined with an SMC scheme



The problem

- ABC Posterior
- ABC **easily gives bad results** if summary statistics and distance are not properly calibrated
- ABC posteriors can look very **different**, depending on the **method**

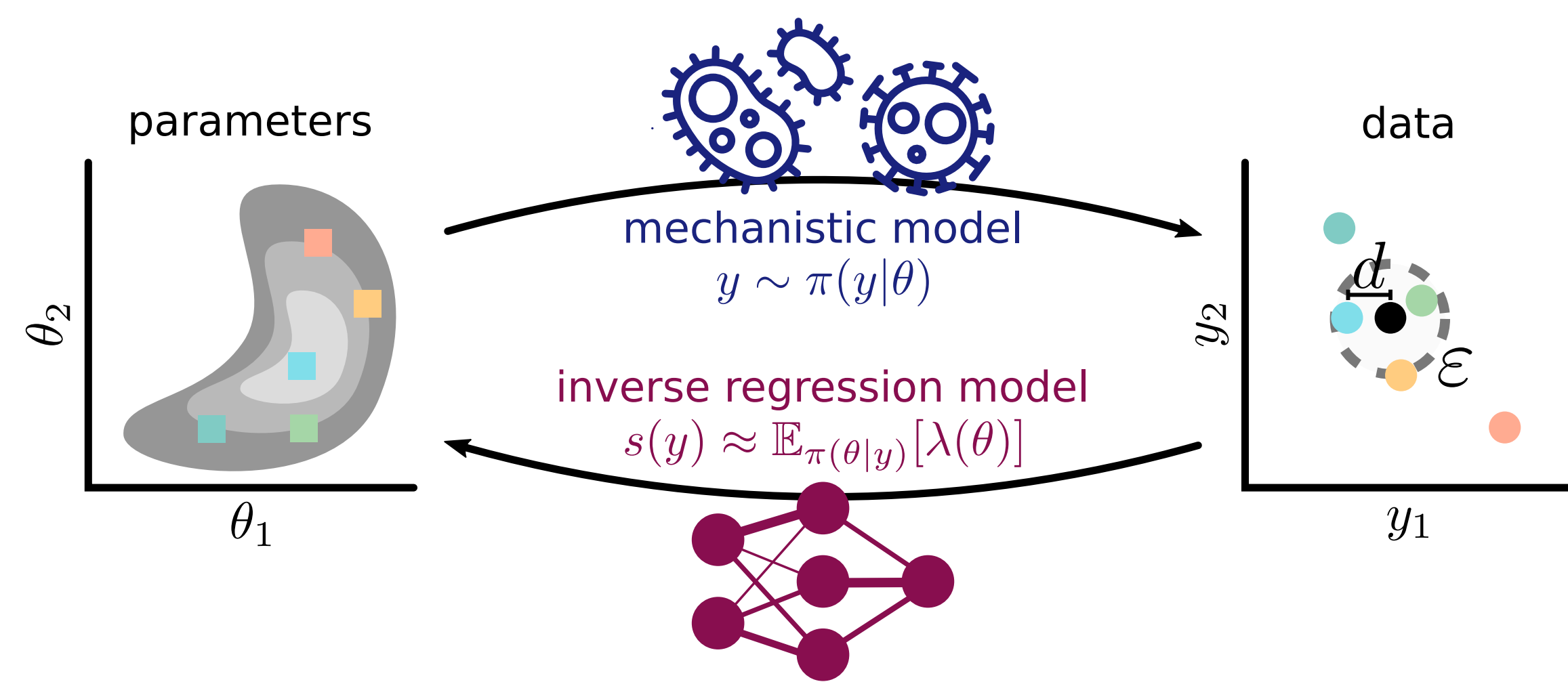


Method: Robust adaptive distances

- Use **robust norms** with **adaptive weights** to normalize for **scale** and down-weight **outliers**

Method: Inverse ML models

- Idea: learn an **inverse regression model** $s: y \rightarrow \theta$



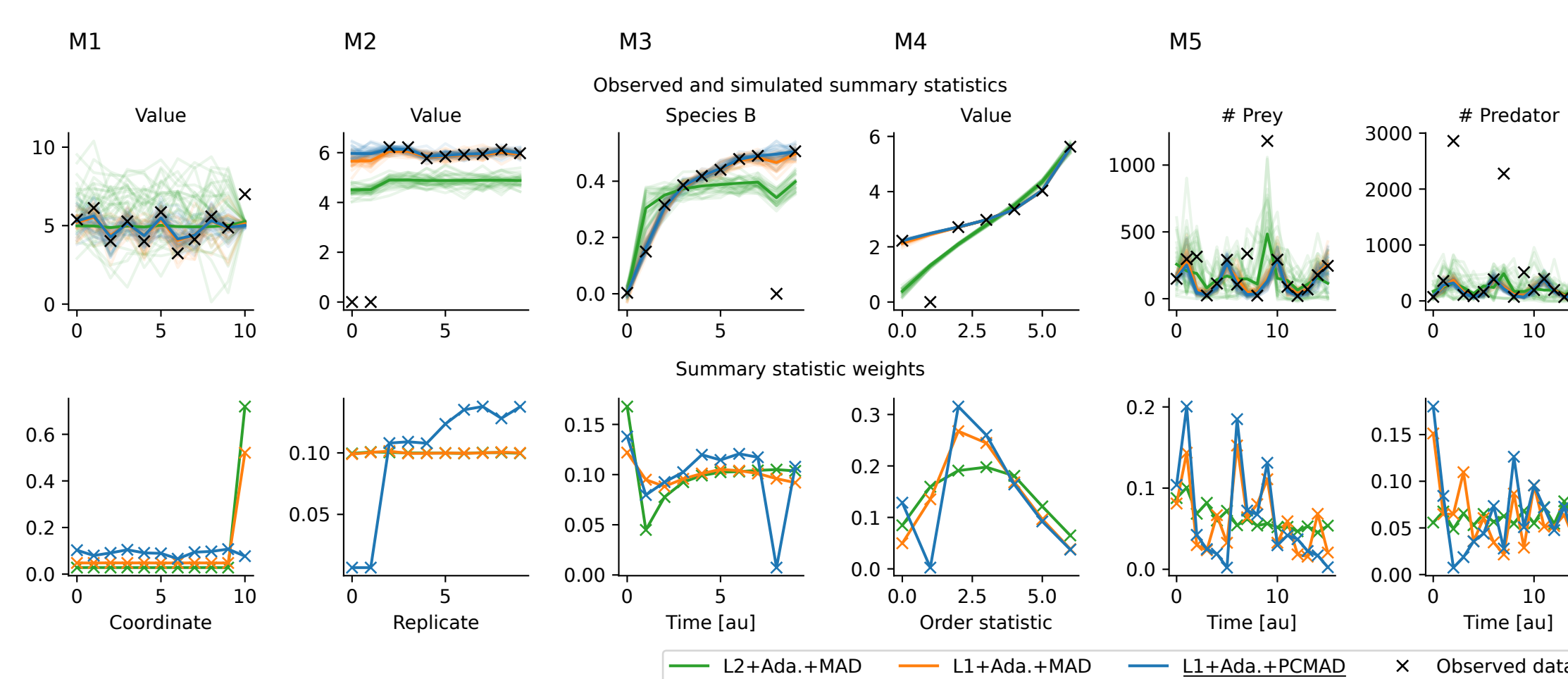
- use that model
 - to construct low-dimensional **summary statistics** ("Summarize all information of data on each parameter in a single value per parameter")
 - to define additional **informativeness weights** given via normalized sensitivities ("If the data were perturbed, how much would the optimal parameters change?")
- learn functions of parameters to capture **higher-order moments**, $s: y \rightarrow \lambda(\theta)$

Results

Robustness

the new robust adaptive distances **substantially outperform** established methods, on a variety of test problems with different model and data types

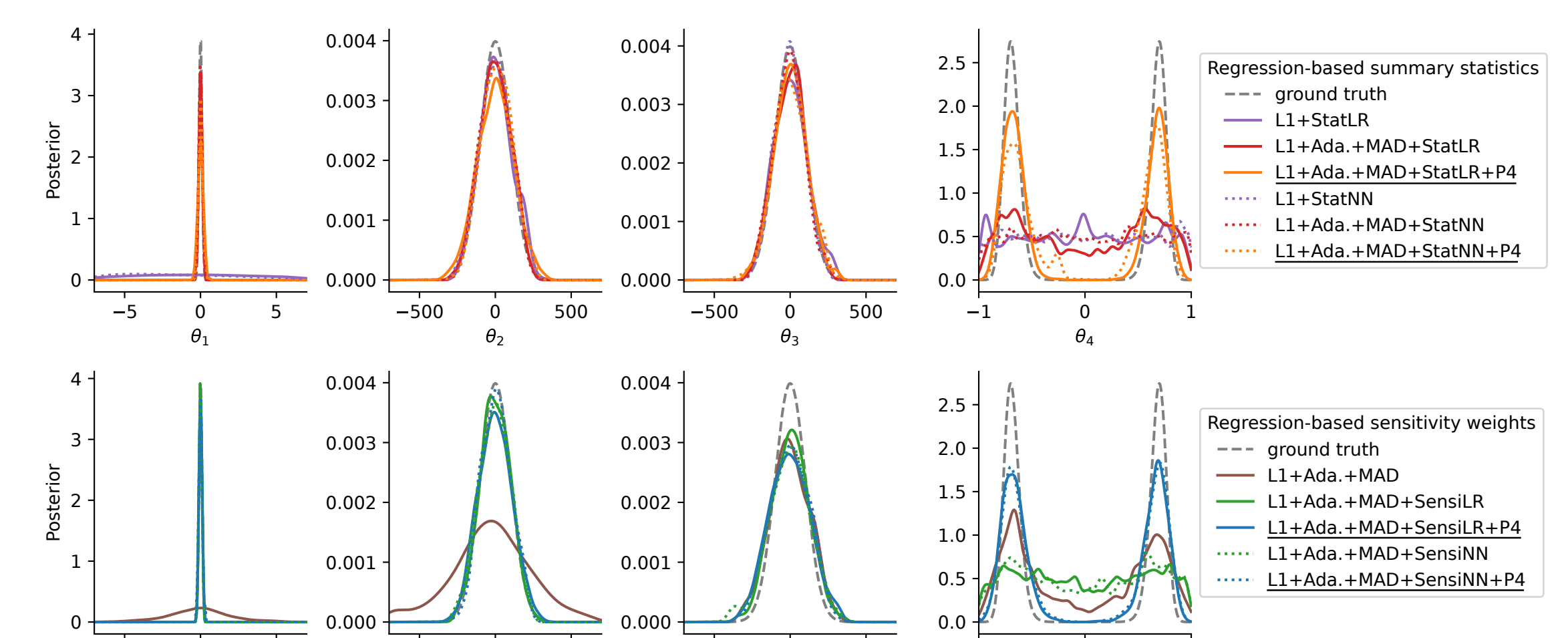
	M1	M2	M3	M4	M5
L2+Cal.+MAD	0.530	0.098	0.073	0.151	0.042
L2+Ada.+MAD	2.414	1.215	0.199	0.541	1.113
L2+Ada.+CMAD	0.502	0.096	0.053	0.087	0.036
L2+Ada.+PCMAD	0.490	0.097	0.052	0.085	0.036
L1+Cal.+MAD	0.504	0.116	0.057	0.099	0.035
L1+Ada.+MAD	0.540	0.098	0.065	0.118	0.041
L1+Ada.+CMAD	0.527	0.148	0.073	0.131	0.055
L1+Ada.+PCMAD	0.496	0.098	0.052	0.085	0.037
	0.494	0.112	0.059	0.104	0.020
	0.495	0.098	0.052	0.085	0.037
	0.499	0.114	0.058	0.101	0.039



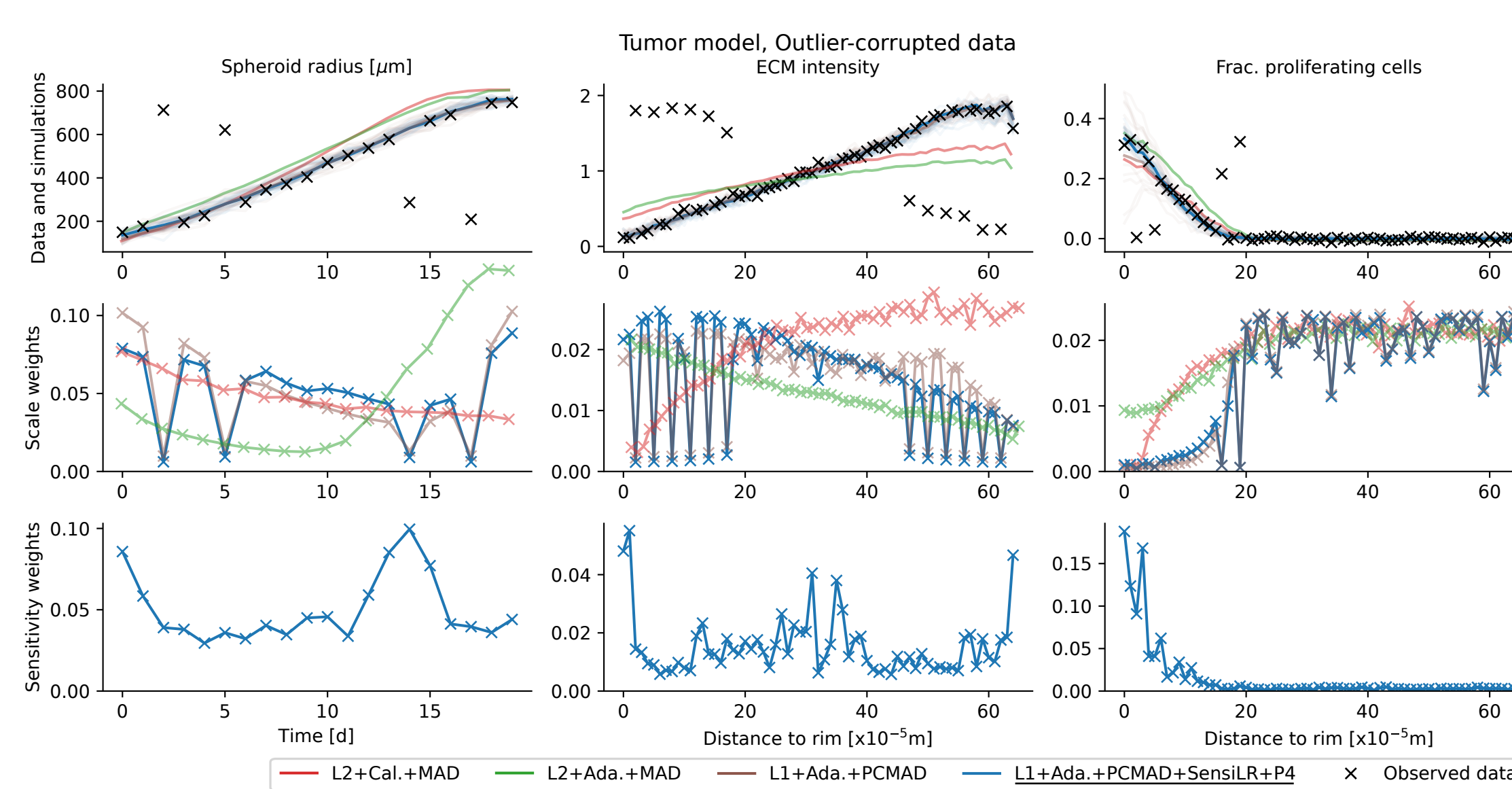
they reliably **identify outliers** and yield accurate fits with **low bias** and **tight confidence intervals**

Informativeness

established methods perform badly and can yield **wrong interpretations**; only the **combination** of the new methods (accounting for informativeness; adaptive weighting; assessing higher-order moments) allows to tackle more **challenging problems**



we are able to **simultaneously** robustly detect outliers and account for informativeness also on **complex application problems** (here: an agent-based model of tumor spheroid growth)

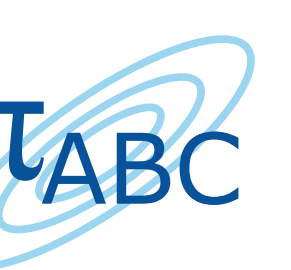


Further information

Robust adaptive distance functions for approximate Bayesian inference on outlier-corrupted data. Schälte et al., 2021

Informative and adaptive distances and summary statistics in sequential approximate Bayesian computation. Schälte et al., 2022

pyABC: Efficient and robust easy-to-use approximate Bayesian computation. Schälte et al., 2022



github.com/yannikschaelte
yannik.schaelte@gmail.com
@yannik_schaelte



Helmholtz Zentrum münchen
German Research Center for Environmental Health

