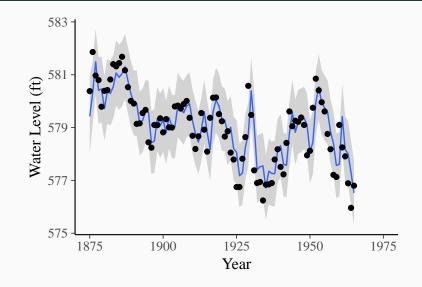
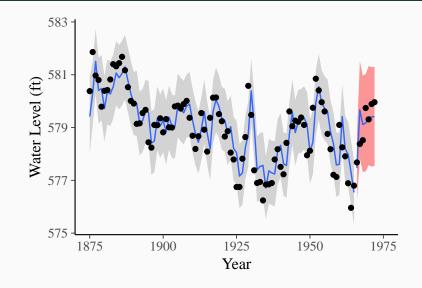
# Approximate leave-future-out cross-validation for Bayesian time series models

Paul Bürkner, Jonah Gabry, Aki Vehtari

## Water Level of Lake Huron



#### Water Level of Lake Huron: Predictions



# Leave-Future-Out Cross-Validation (LFO-CV)

Perform M-step-ahead predictions (M-SAP) at observation i

$$p(y_{i+1},...,y_{i+M} | y_1,...,y_i) =: p(y_{i+1:M} | y_{1:i})$$

Estimate expected M-SAP performance via LFO-CV

$$ELPD_{LFO} = \sum_{i=L}^{N-M} \log p(y_{i+1:M} \mid y_{1:i})$$

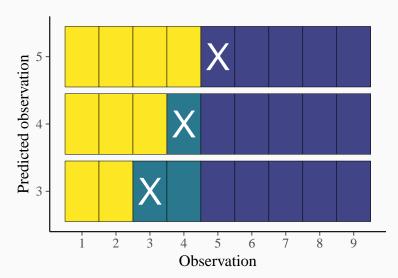
This requires fitting a separate model for each i

$$p(y_{i+1:M} | y_{1:i}) = \int p(y_{i+1:M} | y_{1:i}, \theta) p(\theta | y_{1:i}) d\theta$$

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# **Approximate M-Step-Ahead Predictions**

We are moving **backwards** in time!



# Pareto Smoothg Importance Sampling (PSIS) for LFO-CV

PSIS approximation of M-SAP:

$$p(y_{i+1:M} \mid y_{1:i}) \approx \frac{\sum_{s=1}^{S} w_i^{(s)} p(y_{i+1:M} \mid y_{1:i}, \theta^{(s)})}{\sum_{s=1}^{S} w_i^{(s)}}$$

Let's call  $J_i$  the index set of observations included in the approximating model but **not** in the target model

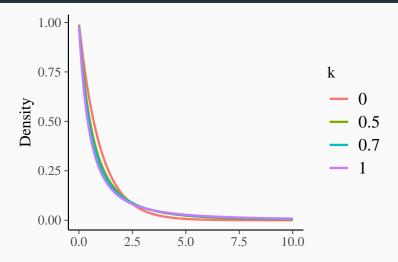
For observation i and posterior sample s we compute the importance ratio as

$$r_i^{(s)} = \frac{1}{\prod_{j \in J_i} p(y_j \mid \theta^{(s)})}$$

Stabilize  $r_i^{(s)}$  via Pareto smoothing to obtain weights  $w_i^{(s)}$ 

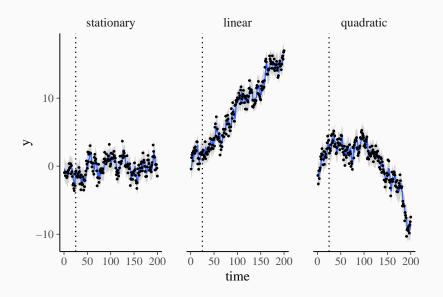
At what point do we have to refit the model?

### The Generalized Pareto Distribution

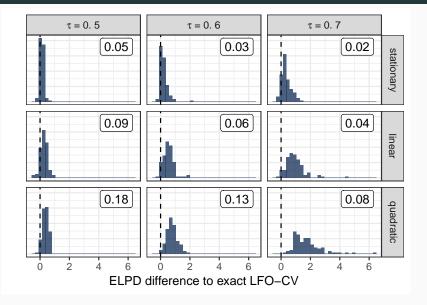


Refit the model if k exceeds a given threshold  $\tau$ 

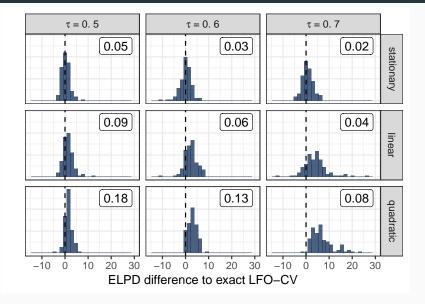
#### **Simulation Conditions**



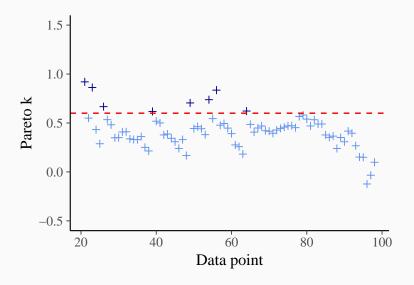
#### Simulation Results: ELPD of 1-SAP



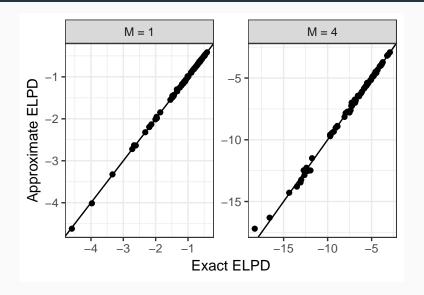
#### Simulation Results: ELPD of 4-SAP



## Lake Huron Model: Pareto k Estimates



## Lake Huron Model: ELPD Estimates



#### Conclusion

- CV has to respect the model's prediction task
- LFO-CV seems reasonable for time series models
- We can approximate LFO-CV via PSIS
- PSIS-LFO-CV provides a close approximation to exact LFO-CV
- PSIS-LFO-CV improves speed by an order of magnitude

#### Resources:

- Preprint: https://arxiv.org/abs/1902.06281
- GitHub: https://github.com/paul-buerkner/LFO-CV-paper
- Email: paul.buerkner@gmail.com

Thank You!

# Importance Sampling

All we care about are expectations (over f):

$$\mathbb{E}_f[h(\theta)] = \int h(\theta) f(\theta) d\theta$$

Switch the distribution (from f to g) over which to integrate:

$$\mathbb{E}_f[h(\theta)] = \frac{\int h(\theta) r(\theta) g(\theta) d\theta}{\int r(\theta) g(\theta) d\theta}$$

with importance ratios

$$r(\theta) = \frac{f(\theta)}{g(\theta)}$$

# Pareto Smoothed Importance Sampling (PSIS)

Suppose we can obtain samples  $\theta^{(s)}$  from g and compute importance ratios  $r(\theta^{(s)}) =: r^{(s)}$ . Then we can approximate

$$\mathbb{E}_f[h(\theta)] \approx \frac{\sum_{s=1}^{S} r^{(s)} h(\theta^{(s)})}{\sum_{s=1}^{S} r^{(s)}}$$

Problem: The importance ratios  $r^{(s)}$  tend to be highly unstable

Solution: Stabilize  $r^{(s)}$  by applying Pareto Smoothing

- PSIS weights  $w^{(s)}$  that replace  $r^{(s)}$
- Diagnose accuracy via the Pareto shape parameter k

# **Approximate Block M-Step-Ahead Predictions**

