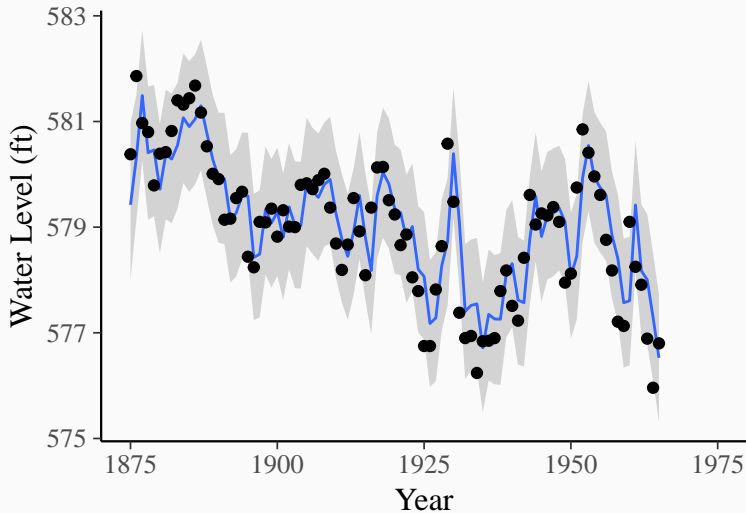


# Approximate leave-future-out cross-validation for Bayesian time series models

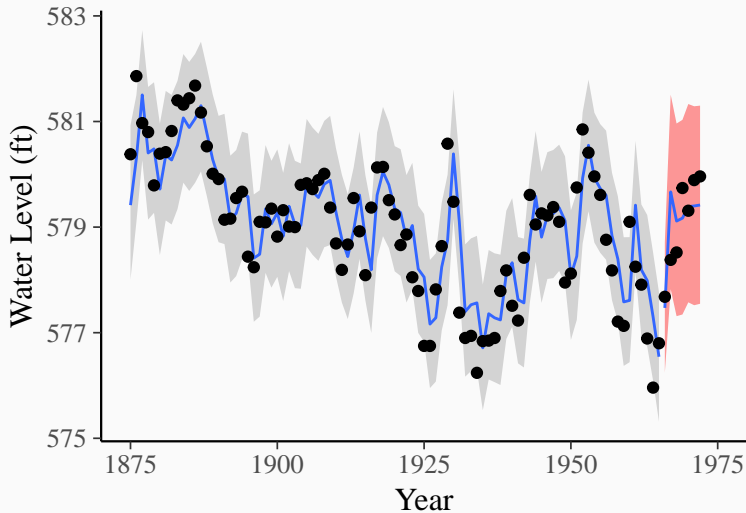
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Paul Bürkner, Jonah Gabry, Aki Vehtari

# 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  $i$

$$p(y_i, \dots, y_{i+M-1} \mid y_1, \dots, y_{i-1}) =: p(y_{i+1:M} \mid y_{1:i})$$

Estimate expected M-SAP performance via LFO-CV

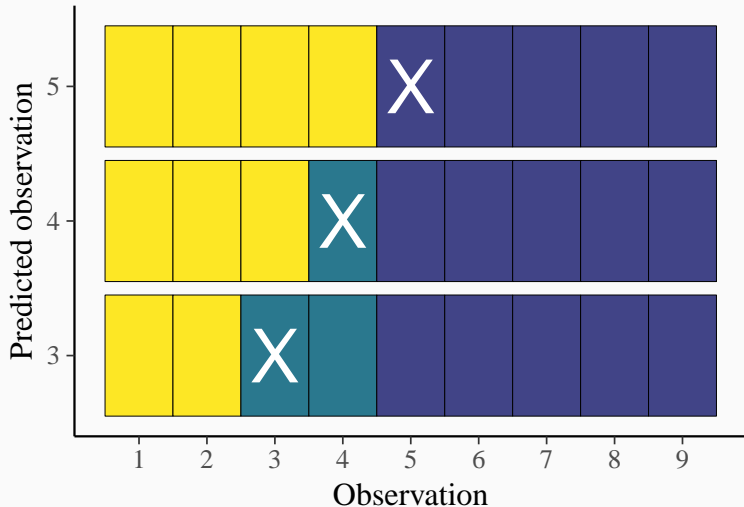
$$\text{ELPD}_{\text{LFO}} = \sum_{i=L+1}^{N-M+1} \log p(y_{i+1:M} \mid y_{1:i})$$

This requires fitting a separate model for each  $i$

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

# Approximate M-Step-Ahead Predictions

We are moving **backwards** in time!



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

PSIS approximation of M-SAP:

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

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

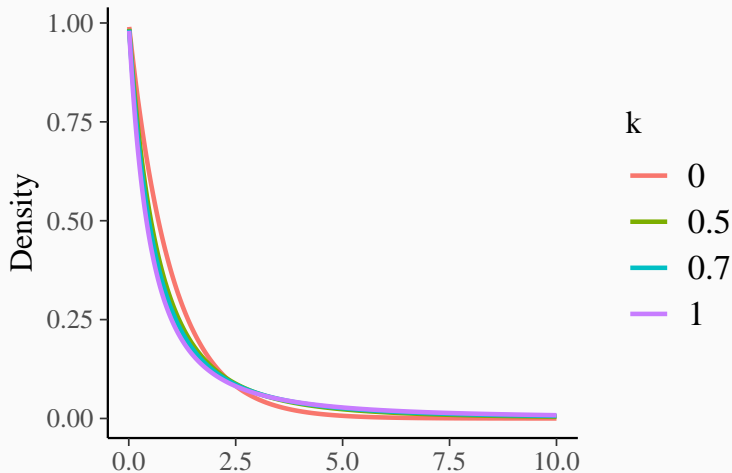
For observation  $i$  and posterior sample  $s$  we compute the importance ratio as

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

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

At what point do we have to refit the model?

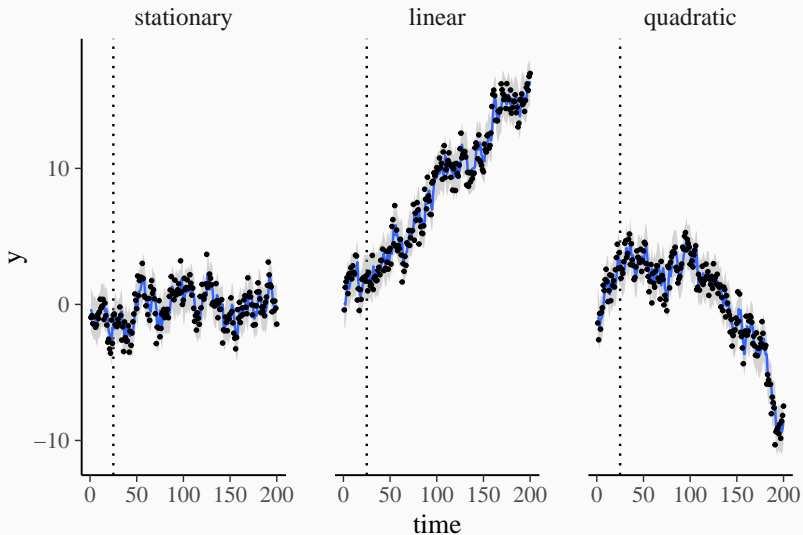
# The Generalized Pareto Distribution



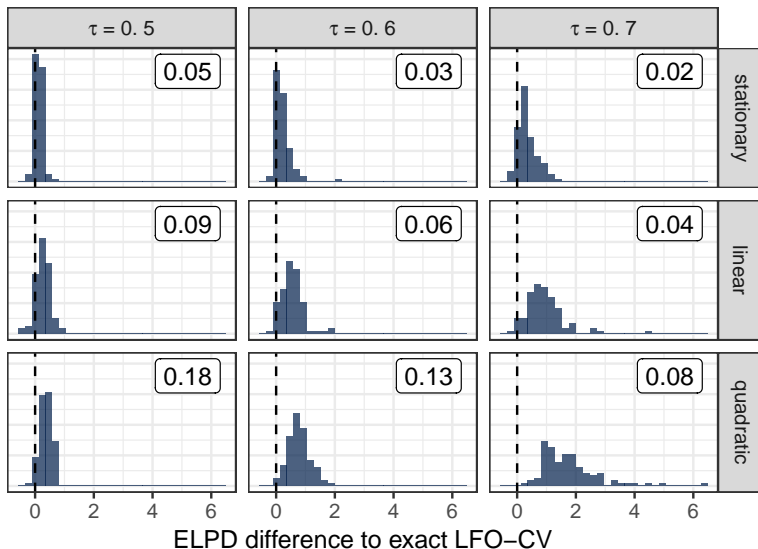
Refit the model if  $k$  exceeds a given threshold  $\tau$



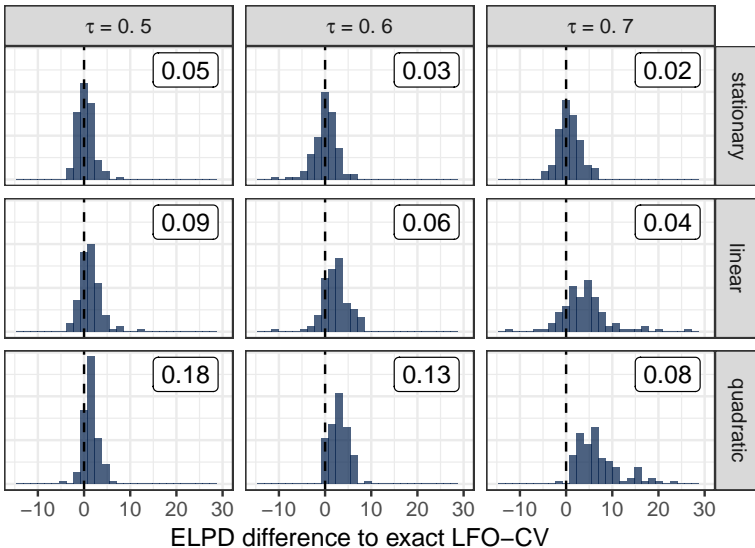
# Simulation Conditions



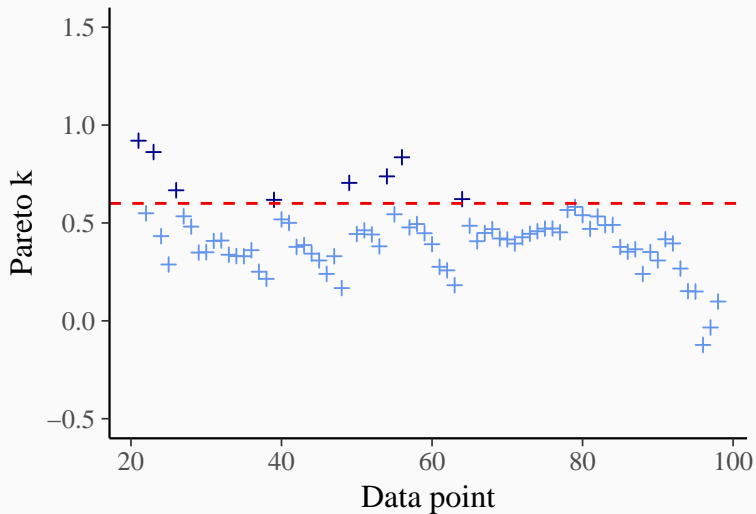
# Simulation Results: ELPD of 1-SAP



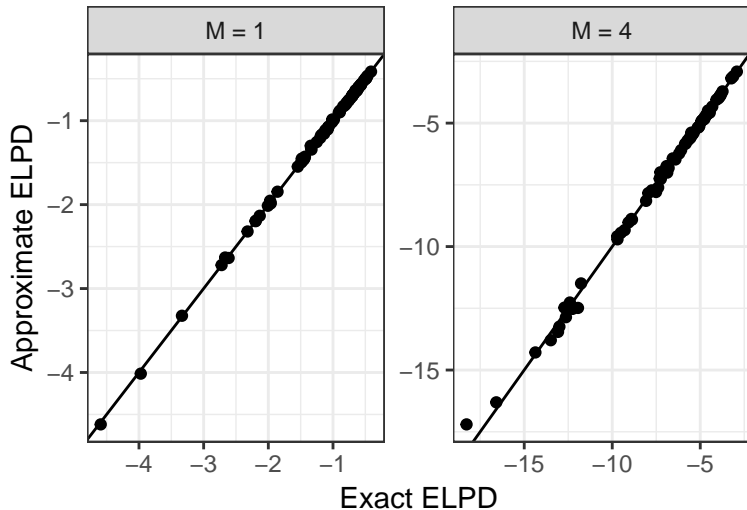
# Simulation Results: ELPD of 4-SAP



## 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](mailto: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

