How to tune your simulator

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Overview

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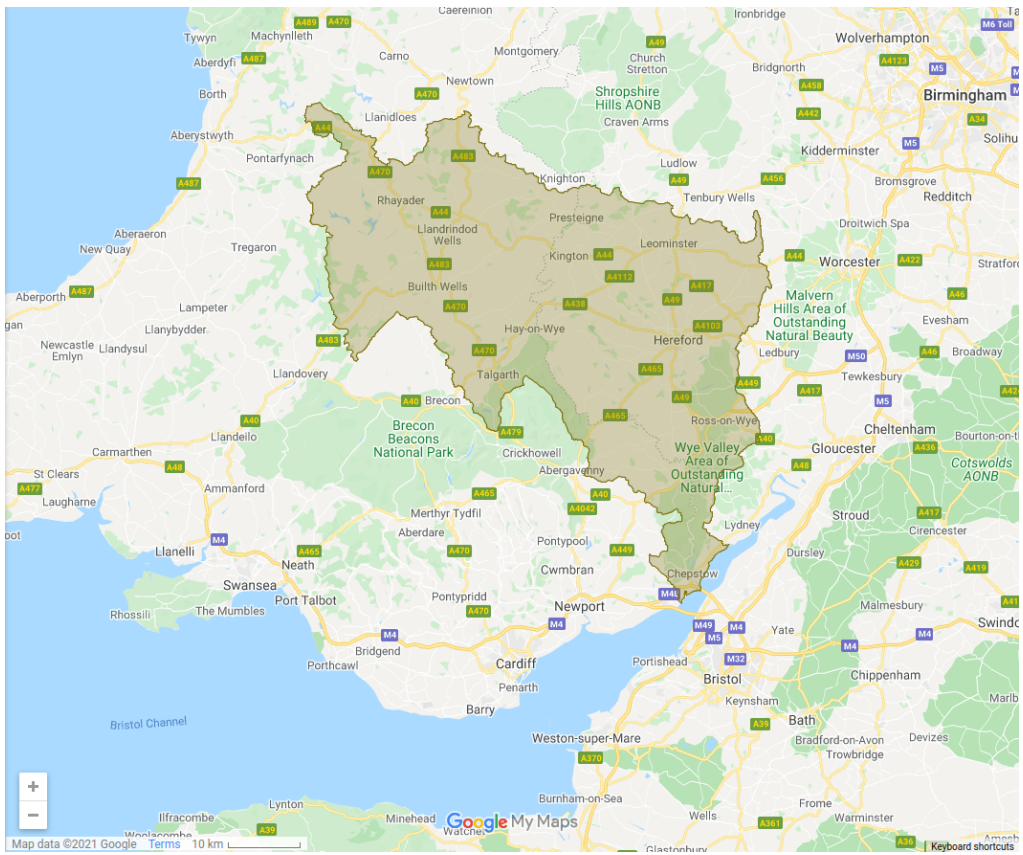
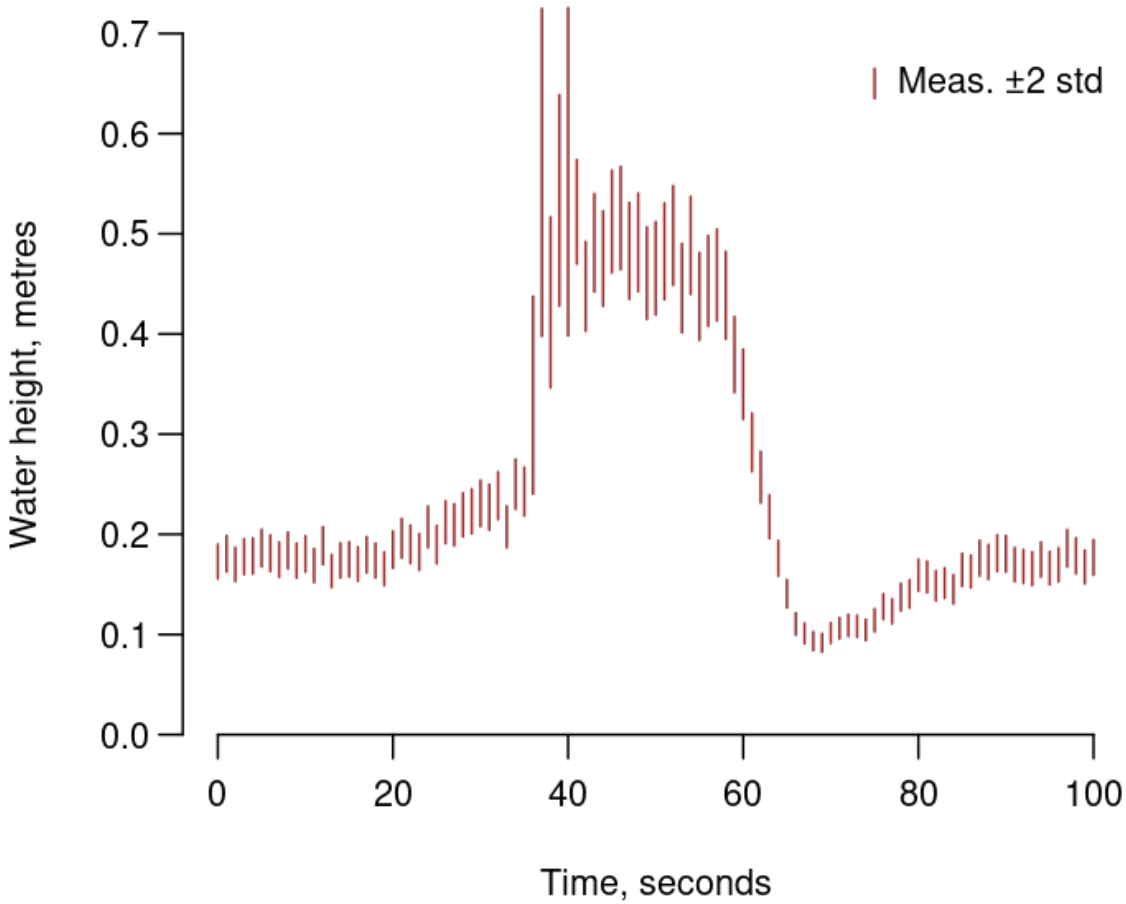
The Wye catchment and Hereford



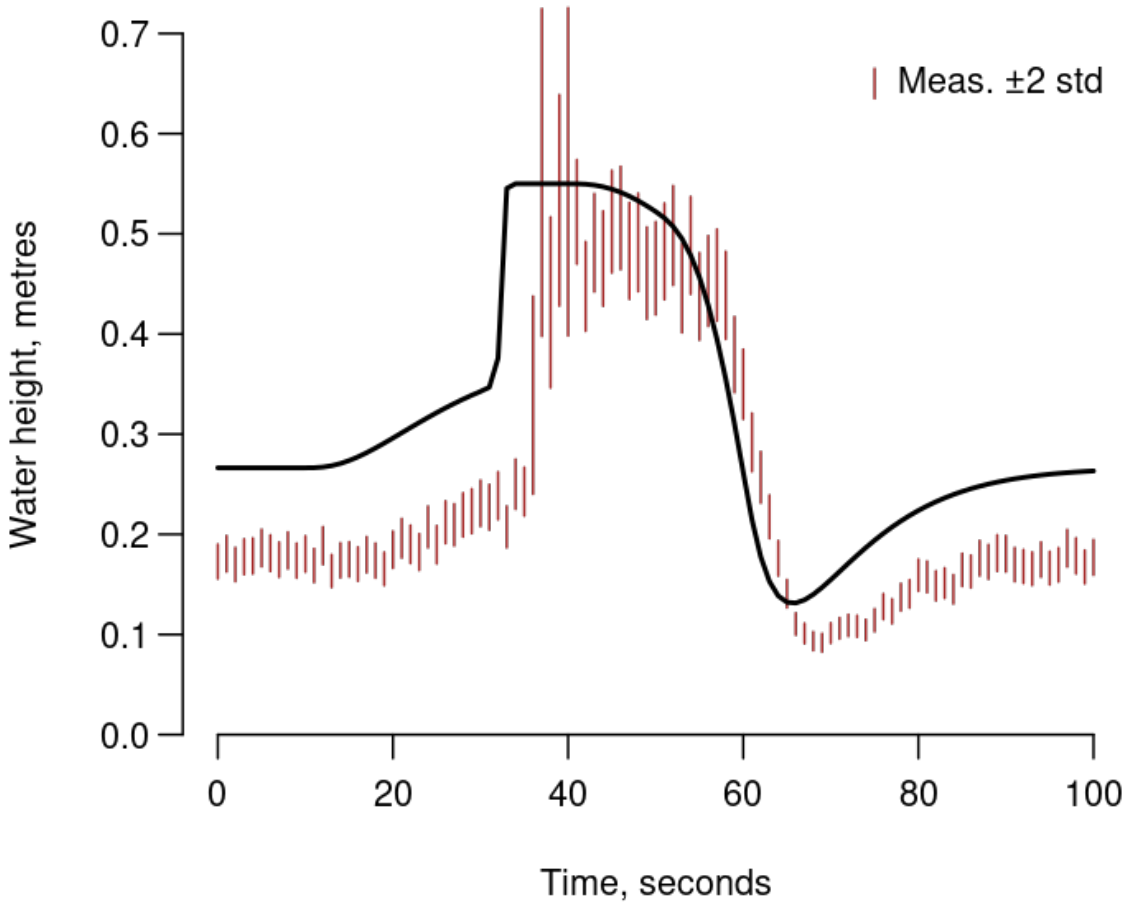
Outline of our application

Nature gives us this 😕



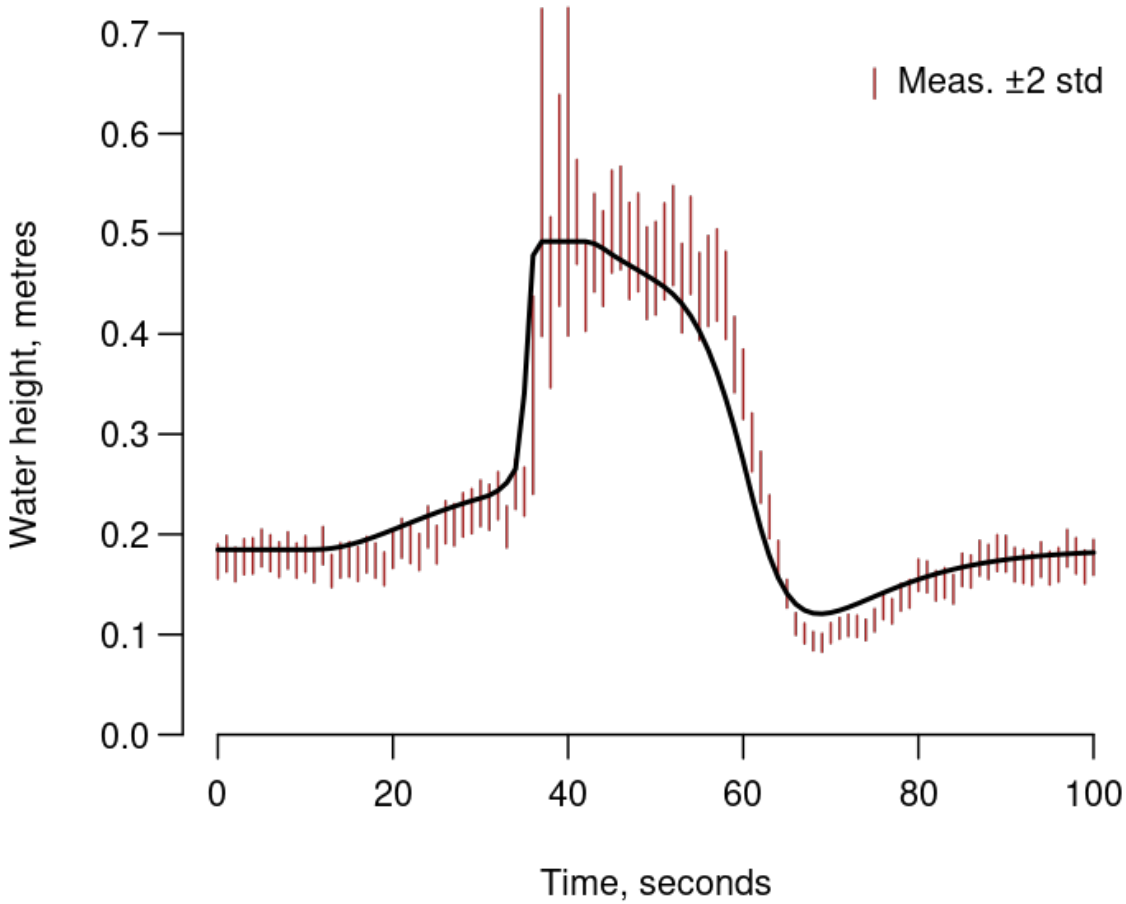
Outline of our application

Our first run of the simulator gives us this 😱



Outline of our application

So how do we efficiently get to this? 😌



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A. In a statistical approach we link the simulator parameters and the observations in a statistical model, which explicitly allows for limitations in the simulator.

B. This produces a smoother objective function, and then we can use statistical optimization to manage the trade-off between 'explore' and 'exploit' with only a limited number of simulator runs.

A little notation

- f is the simulator, with a scalar output.
- Its inputs comprise control variables x and parameters θ.
- Collectively, $\boldsymbol{x} := (x_1, \ldots, x_n)$ and

$$f(\boldsymbol{x}; \theta) := \begin{pmatrix} f(x_1; \theta) \\ \vdots \\ f(x_n; \theta) \end{pmatrix} = \begin{pmatrix} f_1(\theta) \\ \vdots \\ f_n(\theta) \end{pmatrix} = \boldsymbol{f}(\theta).$$

- Similarly,

$$Y(\boldsymbol{x}) := \begin{pmatrix} Y_1 \\ \vdots \\ Y_n \end{pmatrix} = \boldsymbol{Y}, \quad Z(\boldsymbol{x}) := \begin{pmatrix} Z_1 \\ \vdots \\ Z_n \end{pmatrix} = \boldsymbol{Z}$$

are actual system values, and observables, respectively.

The Normal model

- Assume a transformation of $\boldsymbol{Z}$, $\boldsymbol{Y}$, and $\boldsymbol{f}$ after which

$$\boldsymbol{Z} \mid \boldsymbol{Y}, \theta^*, \alpha, K \sim \mathrm{N}\left(\boldsymbol{Y}, D\right)$$
$$\boldsymbol{Y} \mid \theta^*, \alpha, K \sim \mathrm{N}\left(\alpha \mathbf{1} + \boldsymbol{f}(\theta^*), K\right)$$

is an acceptable implementation of the ▸ 'best input' model.

  - $D := \mathrm{diag}(\sigma_1^2, \ldots, \sigma_n^2)$, a diagonal matrix of reported measurement errors,
  - θ^* is the best value of the parameters,
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- Integrating out $\boldsymbol{Y}$,

$$\boldsymbol{Z} \mid \theta^*, \alpha, K \sim \mathrm{N}\Big(\alpha \mathbf{1} + \boldsymbol{f}(\theta^*), K + D\Big),$$

  from which derive $L(\theta^*, \alpha, K)$, based on measurements $\boldsymbol{z}^{\mathrm{obs}}$.

The Normal model (cont)

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- The 'engineering' approach eliminates the nuisance parameters by setting them to zero,

$$-2 \log L^{\text{eng}}(\theta^*) := -2 \log L(\theta^*, 0, \mathbf{0}) = \sum_{i=1}^{n} \frac{\left(z_i^{\text{obs}} - f_i(\theta^*)\right)^2}{\sigma_i^2},$$

apparently hoping that treating the simulator as perfect will make its limitations go away 😬

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- Treat K as stationary, and thin z^{obs} to the point where $K_{\mathcal{I},\mathcal{I}} \approx \kappa^2 I$, where $\mathcal{I} \subset \{1, \ldots, n\}$ are the retained outputs:

$$-2 \log L_{\mathcal{I}}(\theta^*, \alpha, \kappa) \approx \sum_{i \in \mathcal{I}} \frac{\{z_i^{\text{obs}} - (\alpha + f_i(\theta^*))\}^2}{\kappa^2 + \sigma_i^2} + \sum_{i \in \mathcal{I}} \log(\kappa^2 + \sigma_i^2),$$

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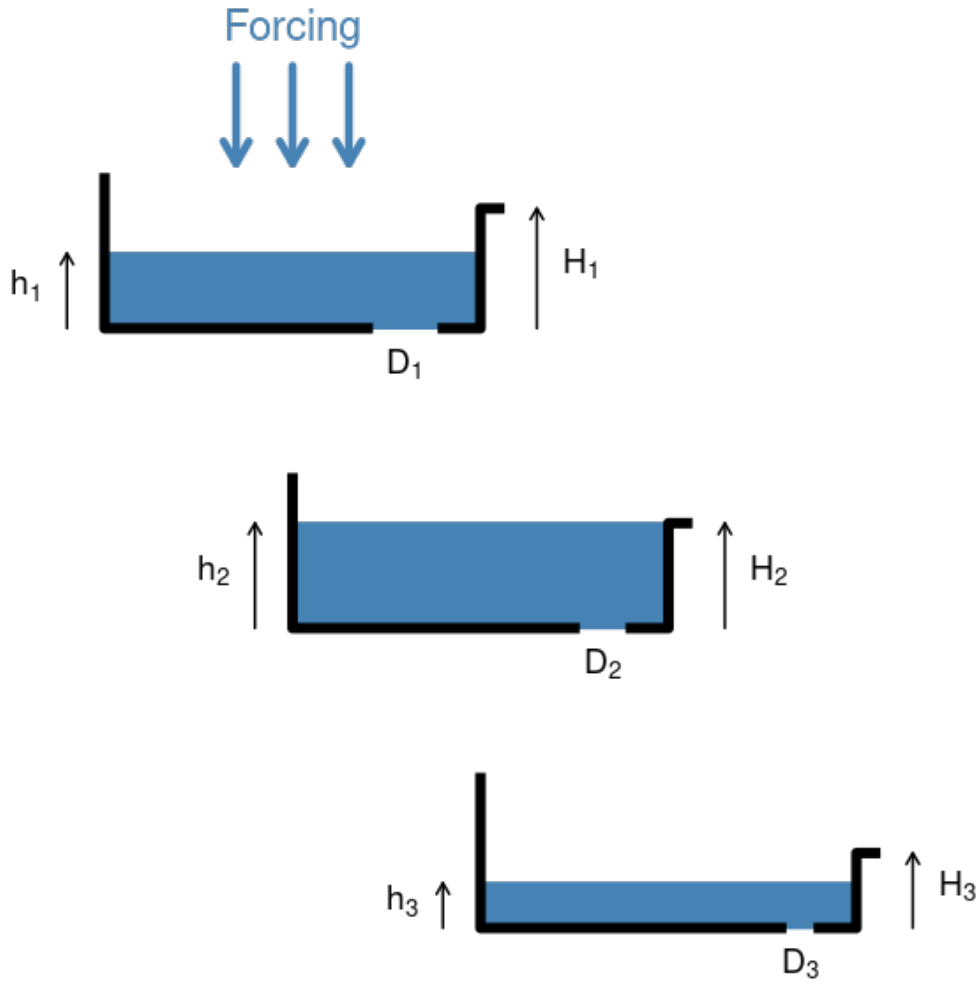
- I'm not claiming that this is awesome statistics (indeed, profile likelihood is a bit mysterious). But $L_{\mathcal{I}}^{\text{prf}}$ is an attainable incremental improvement on current practice.

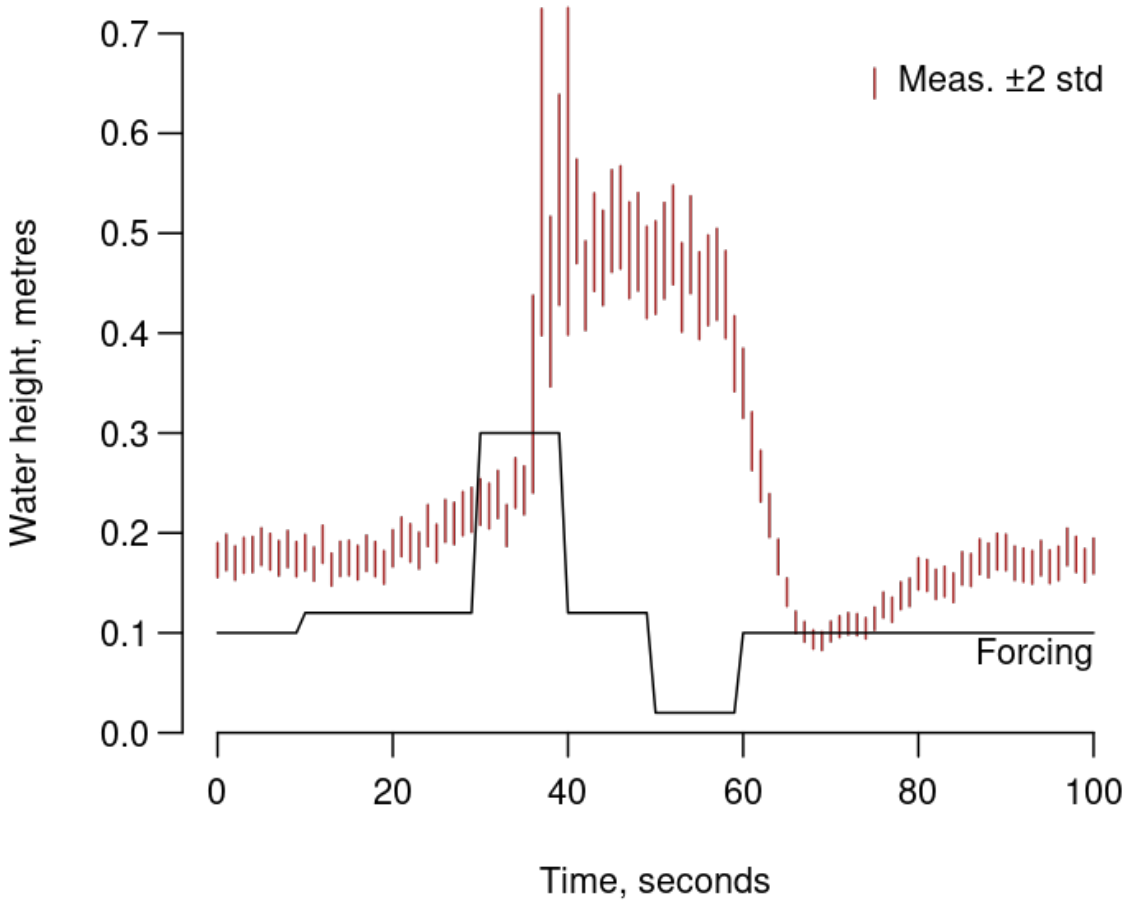
The buckets simulator



Parameters are (D_i, H_i) for each bucket. A time-series for forcing is specified, the outputs are a time-series for each h_i.

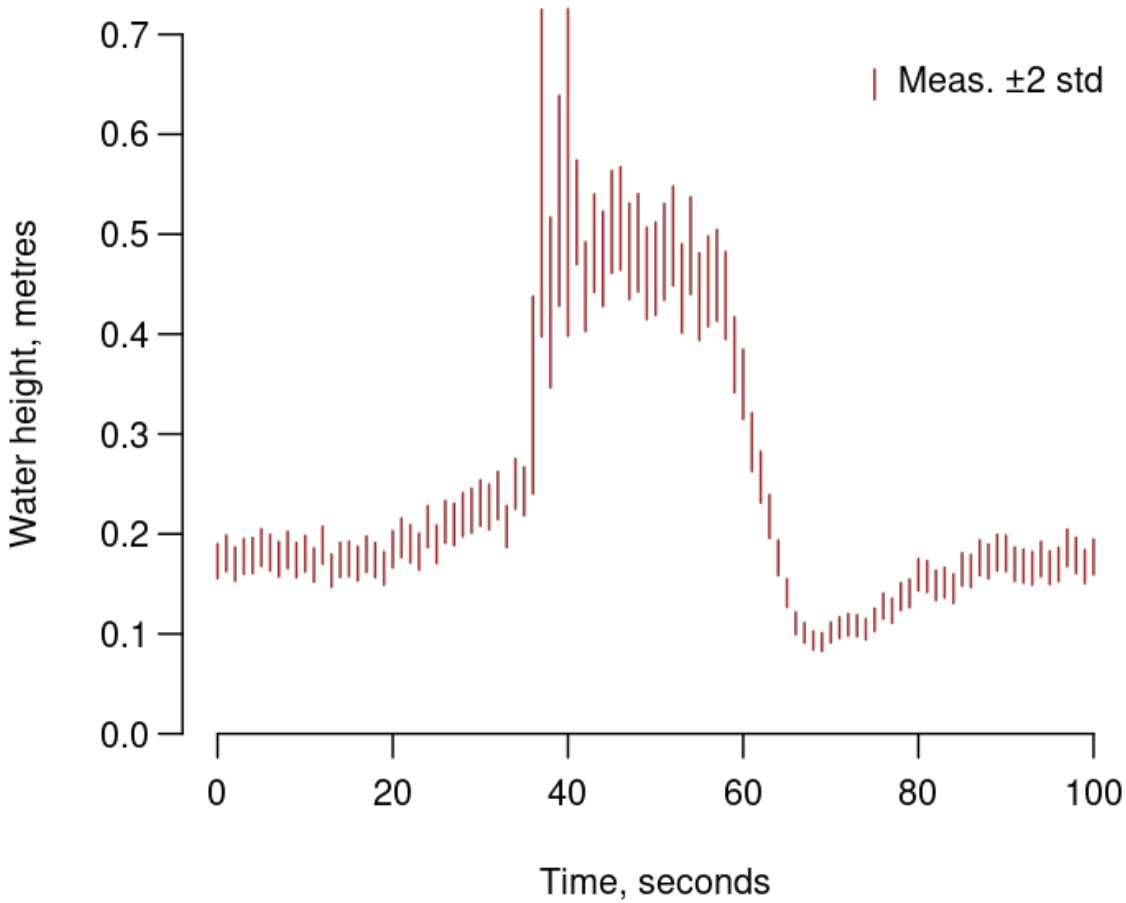
The system

Nature is running a five-bucket system, with $D_i = 0.3$, $H_i = 0.5$.
Observe h_5 with a known state-dependent measurement error.



Thinning = 'feature extraction'

All of the observations



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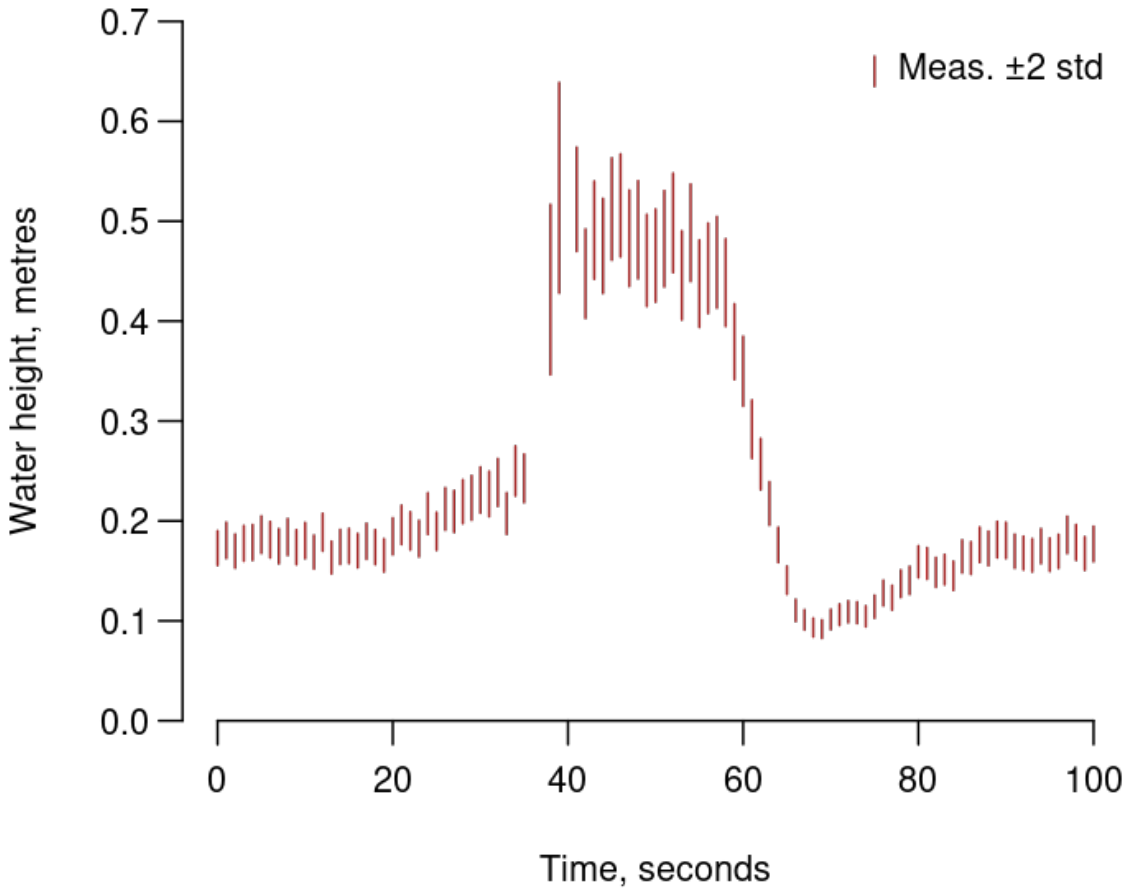

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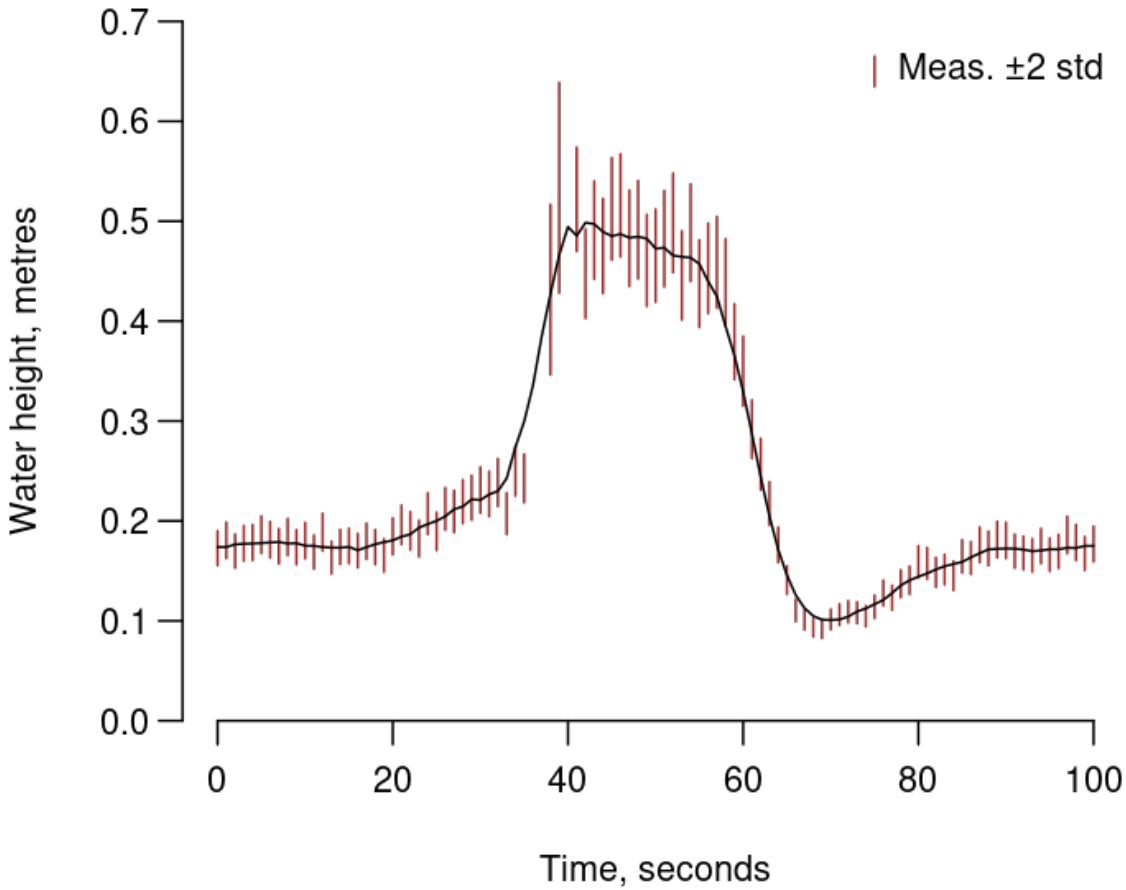
Add a moving average



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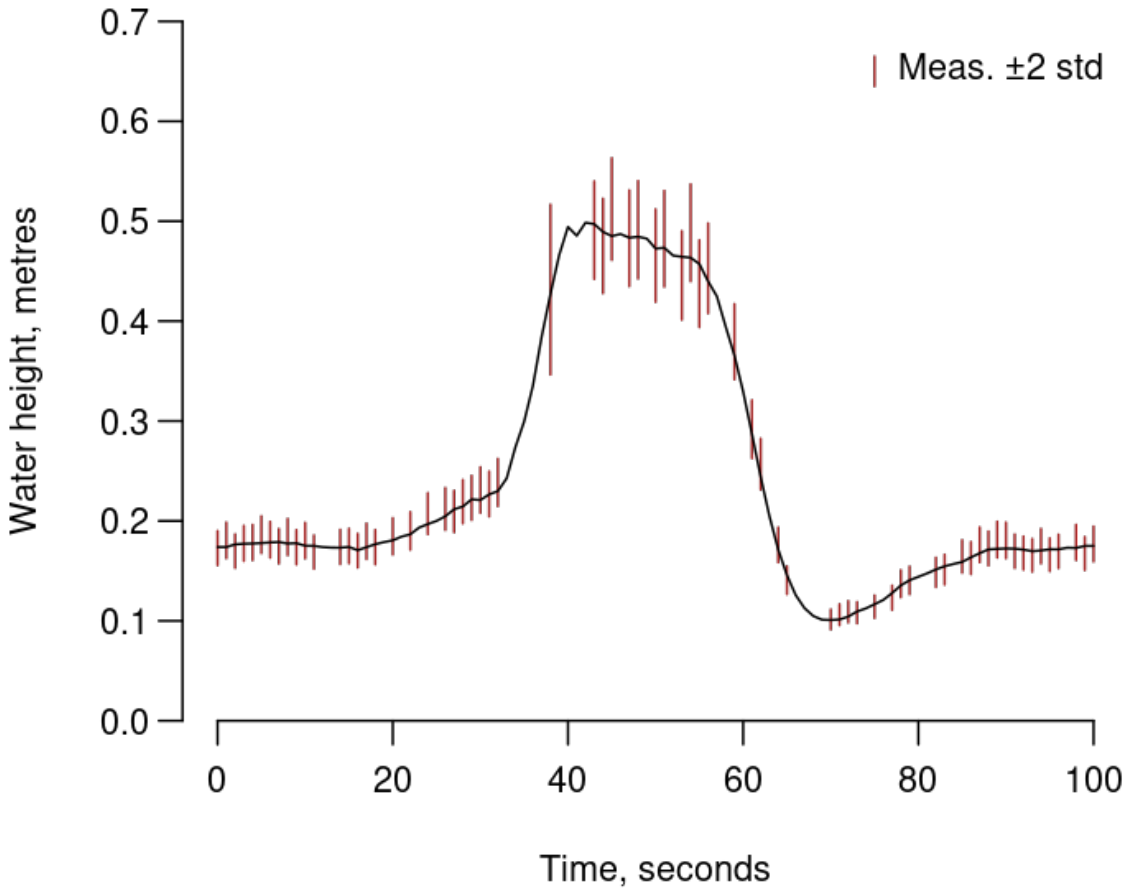
Drop the outliers



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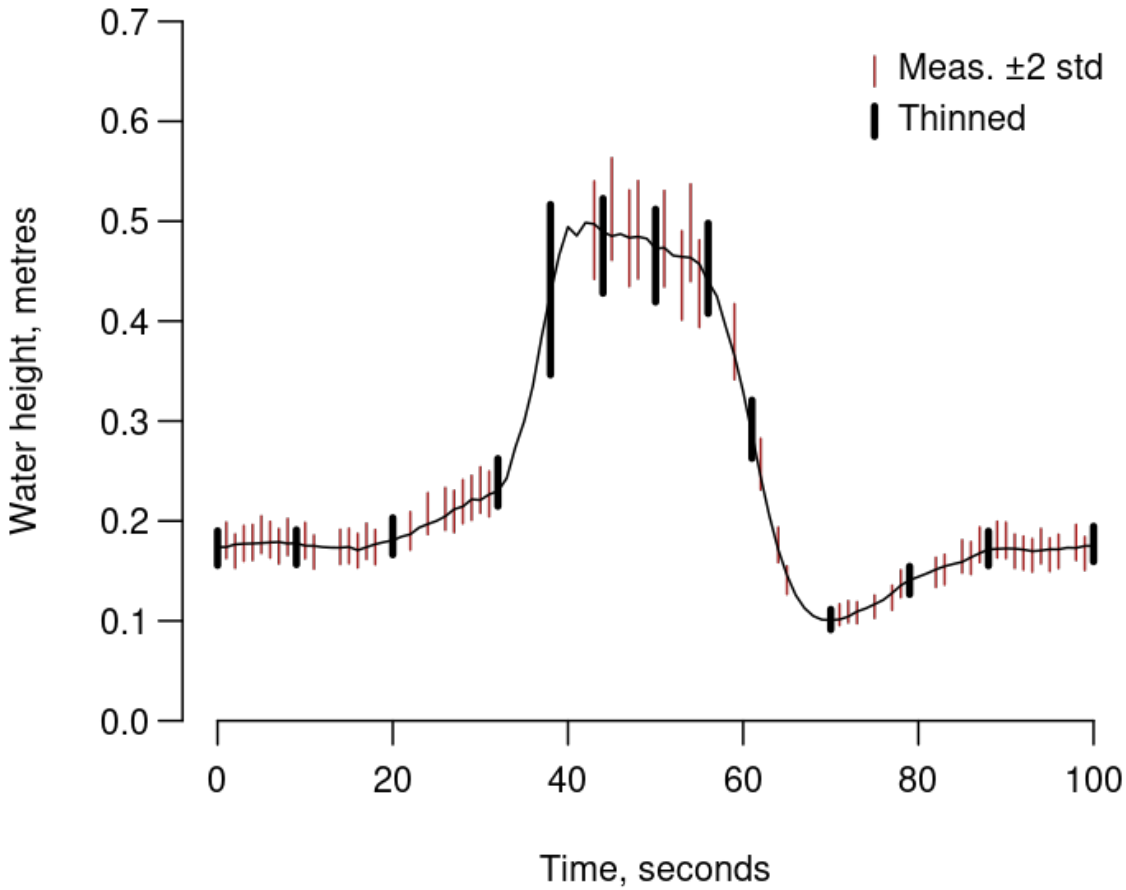
Thin the survivors



Our simulator

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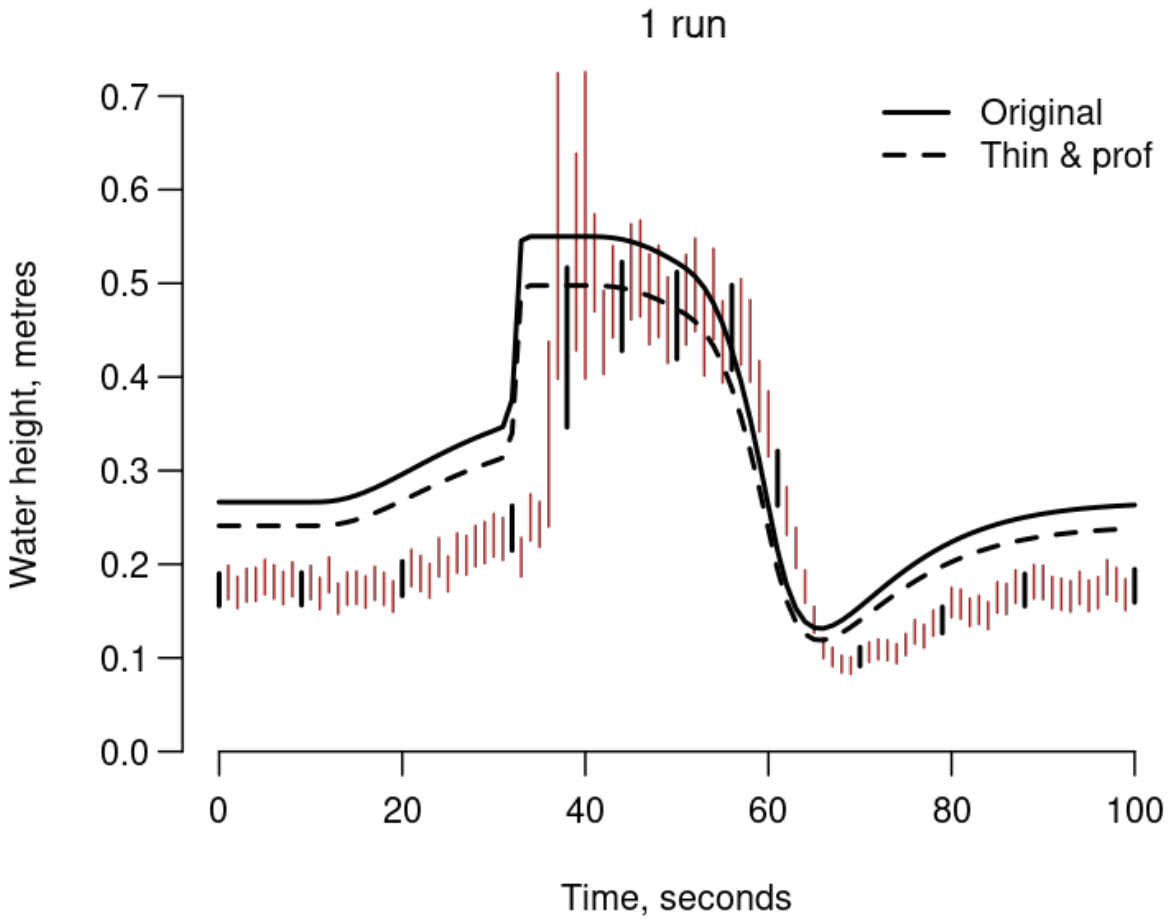

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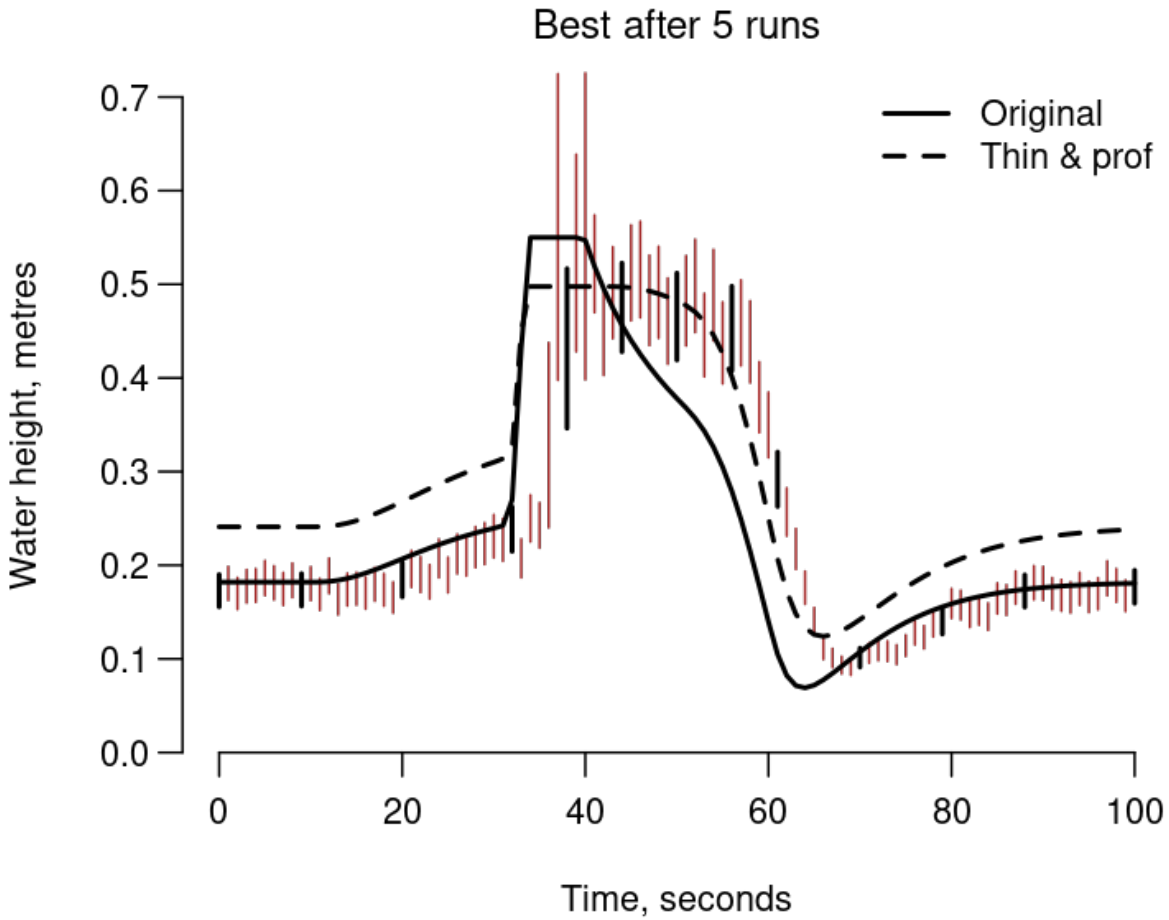

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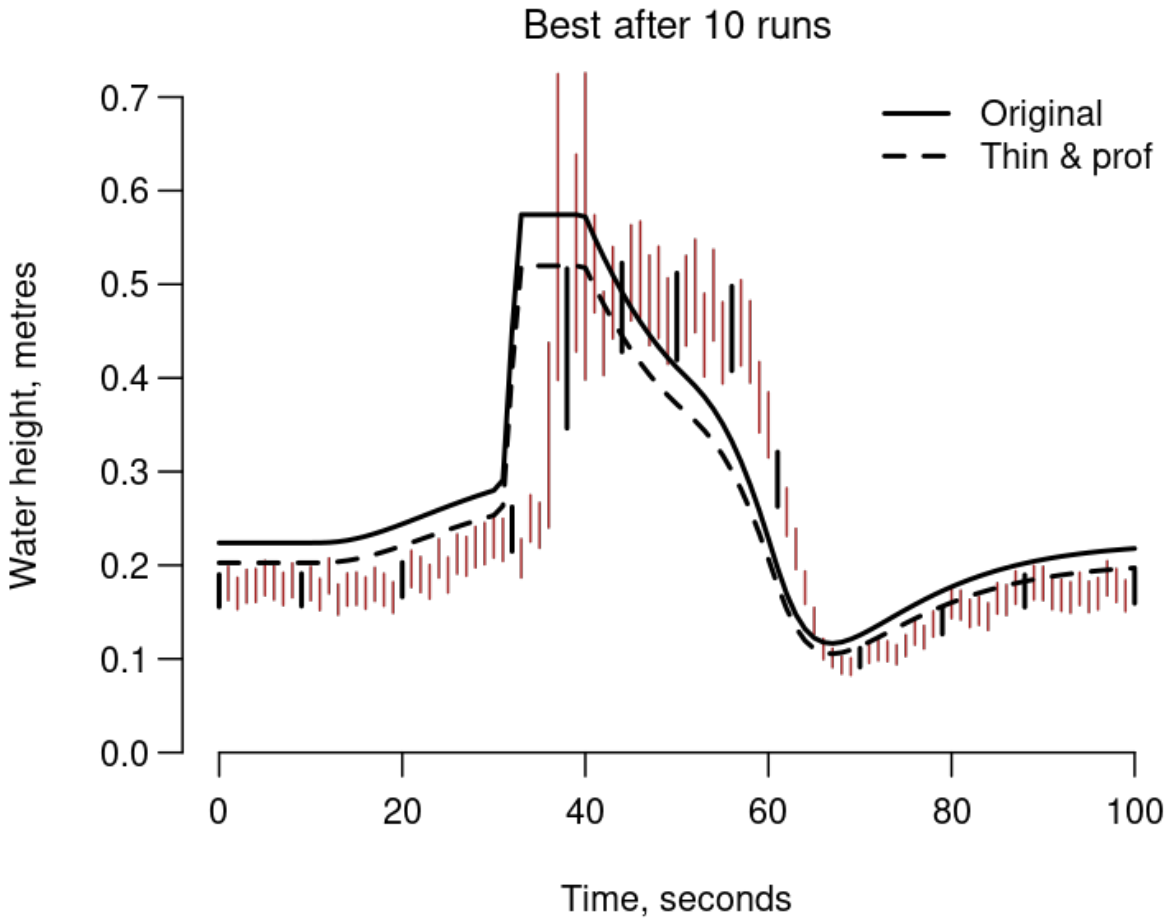

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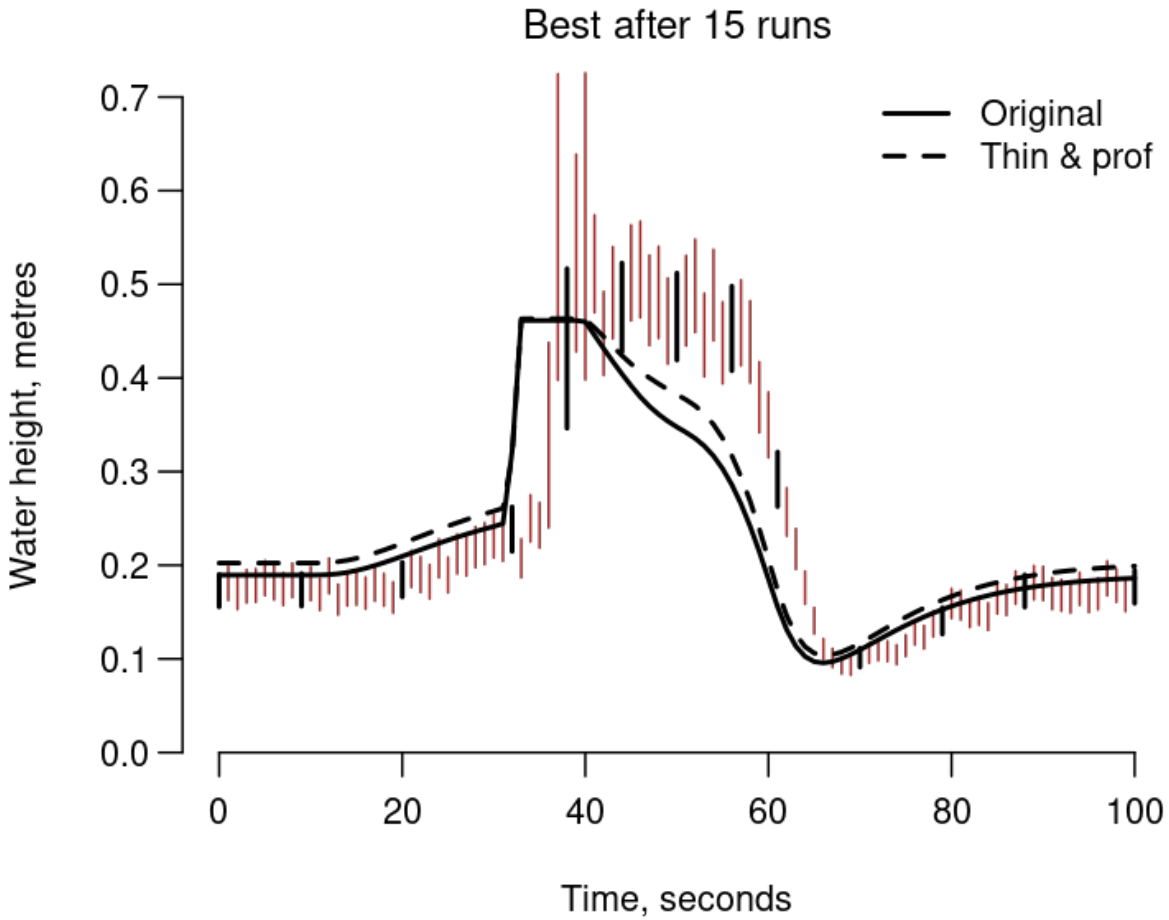

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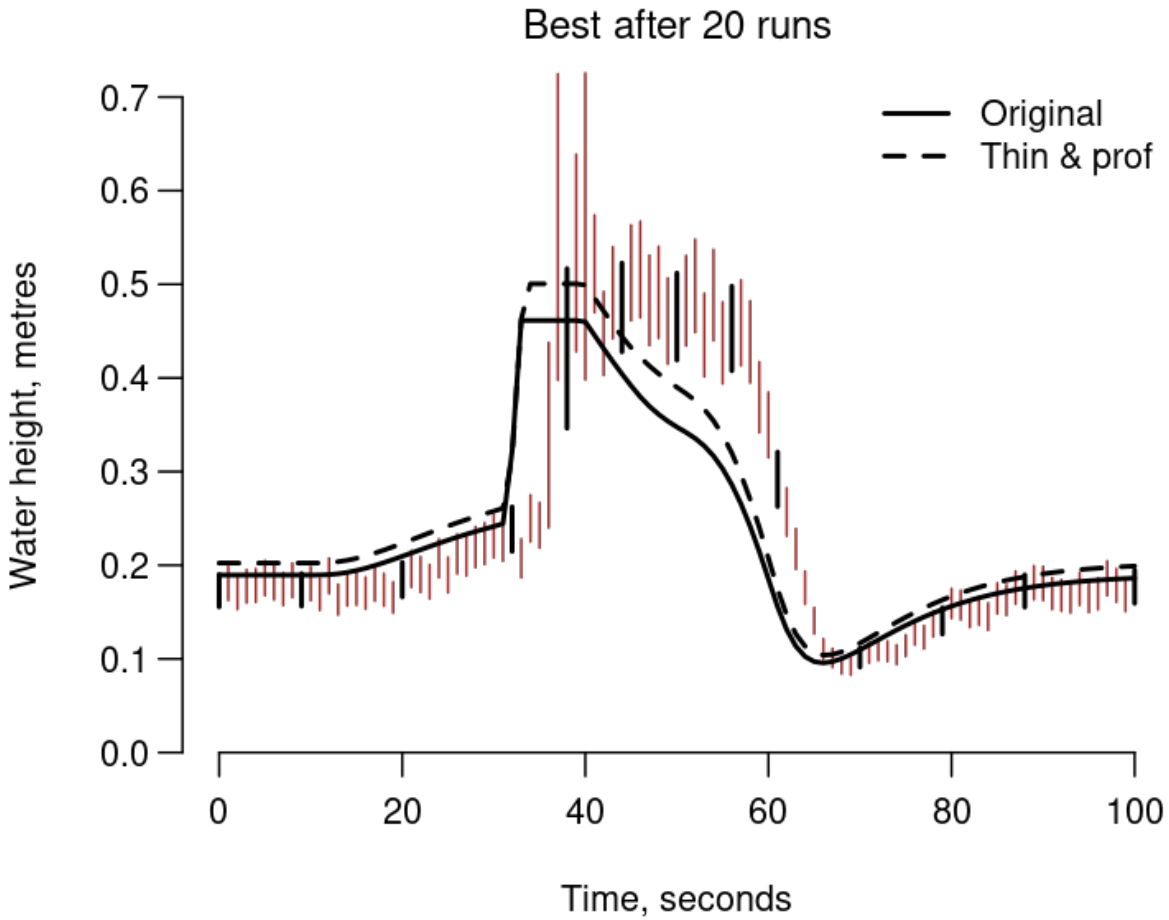

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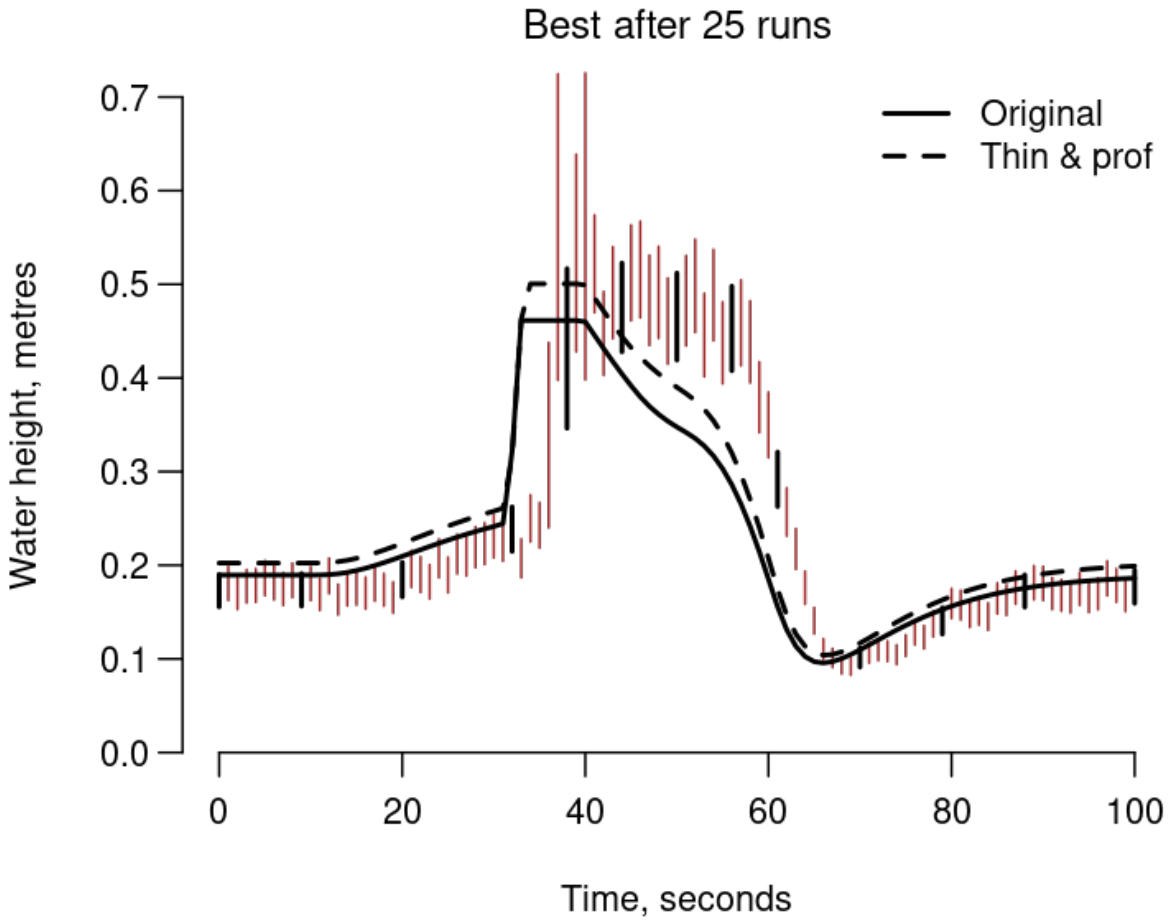

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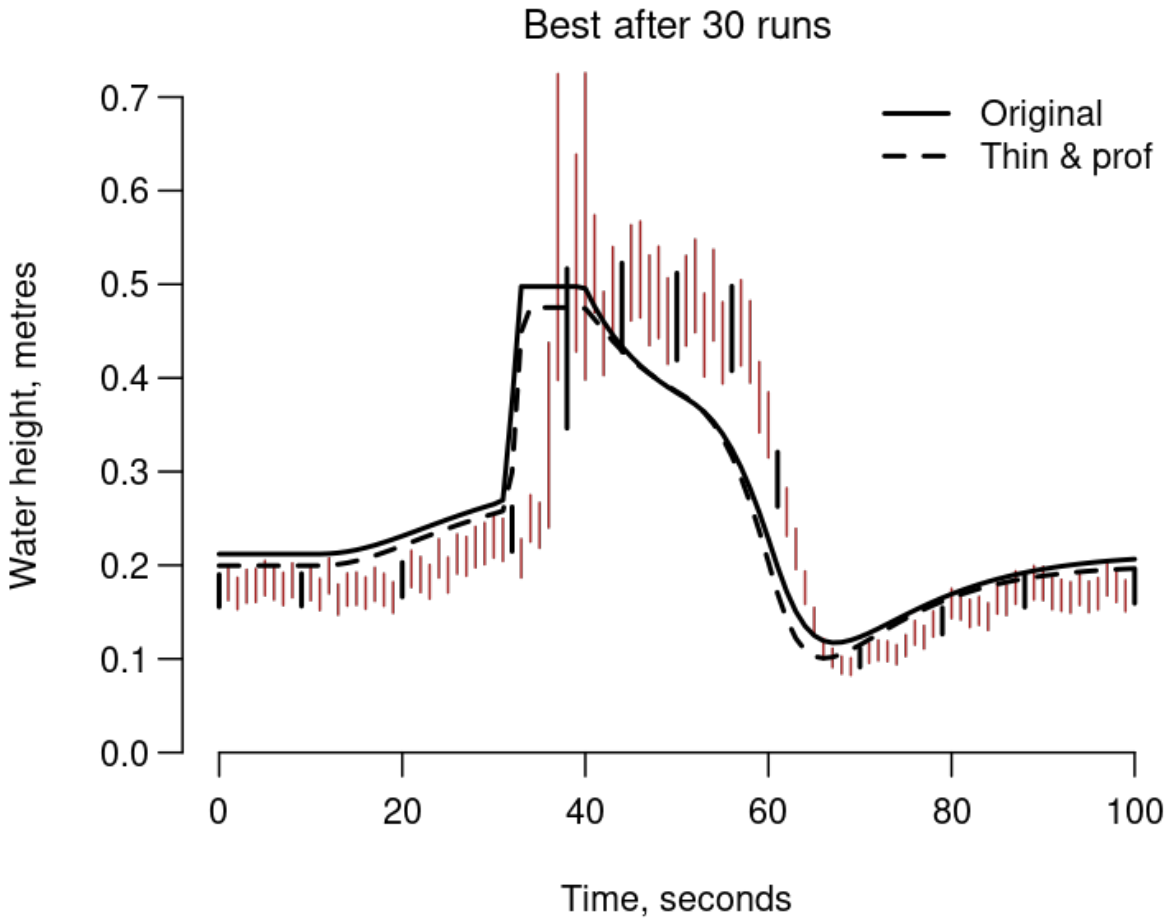

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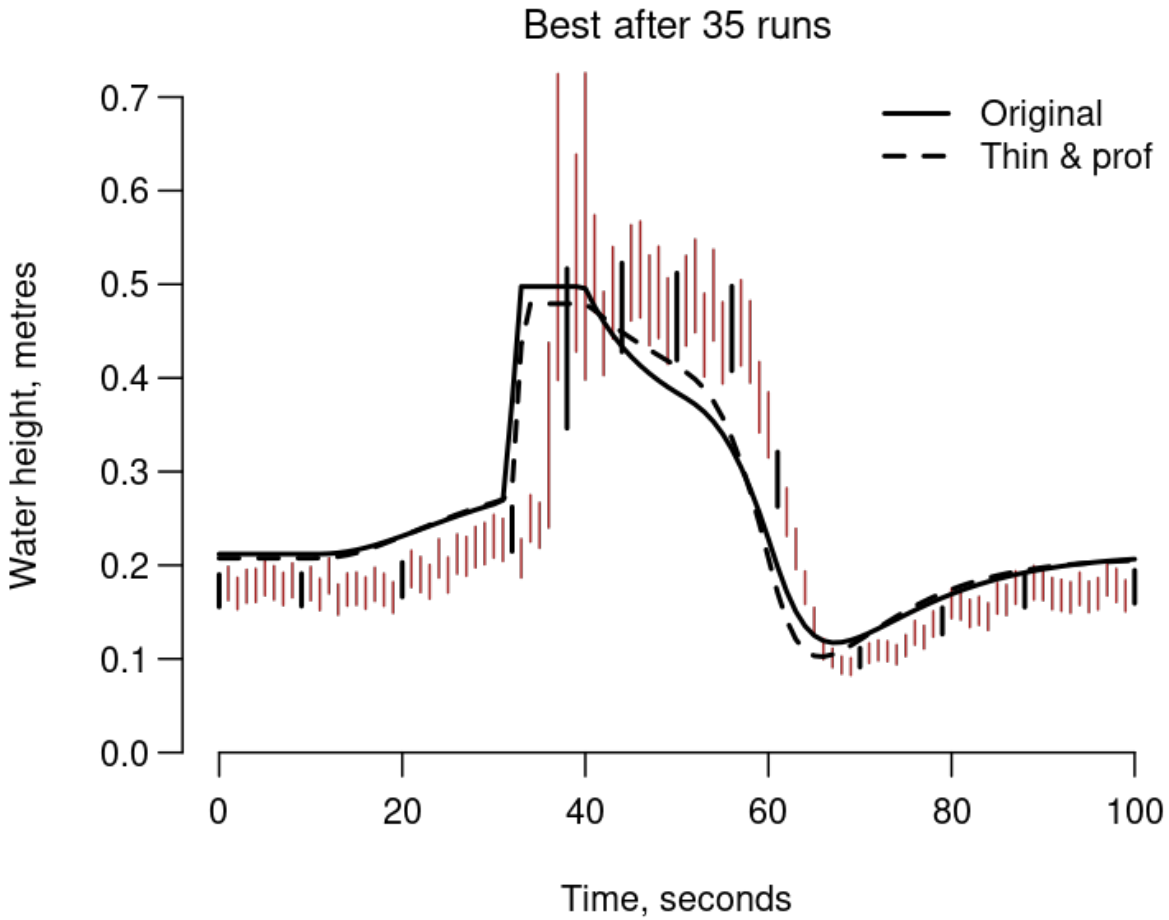

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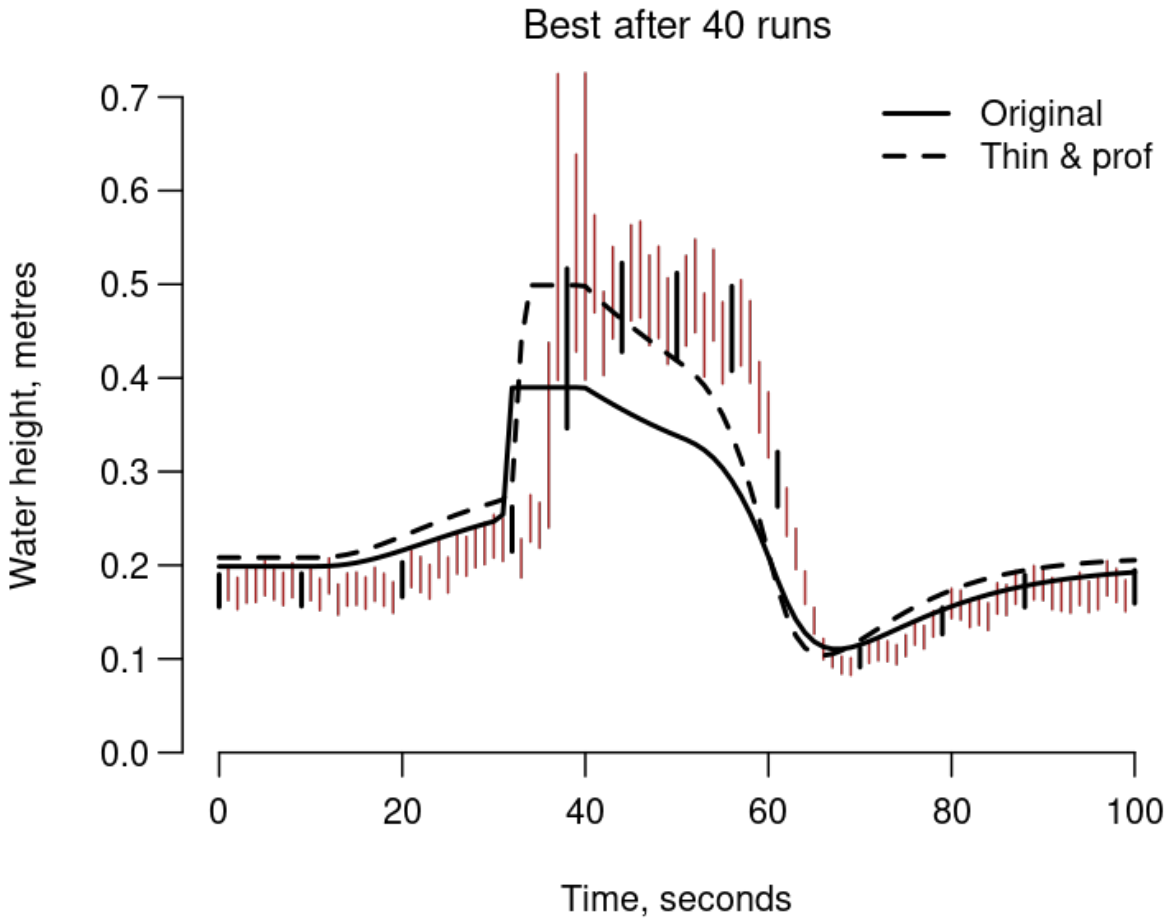

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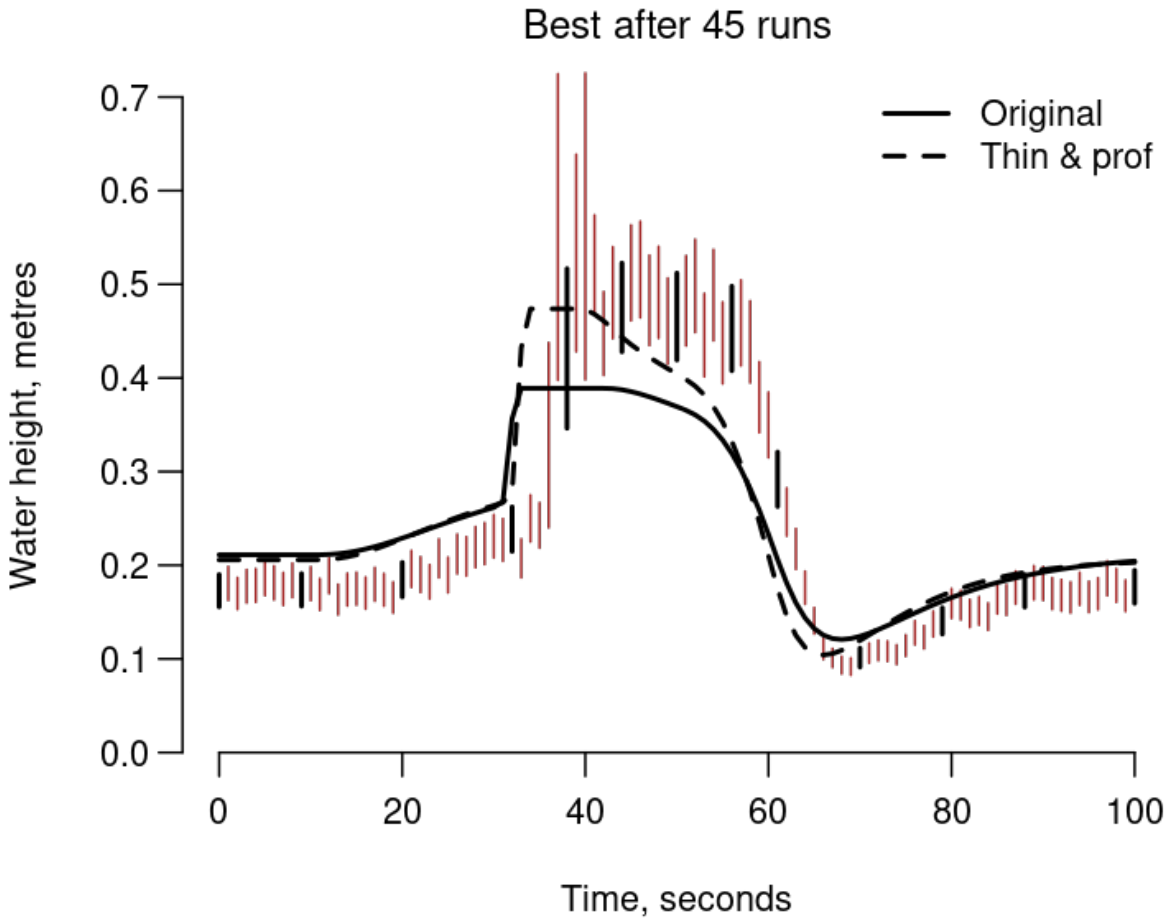

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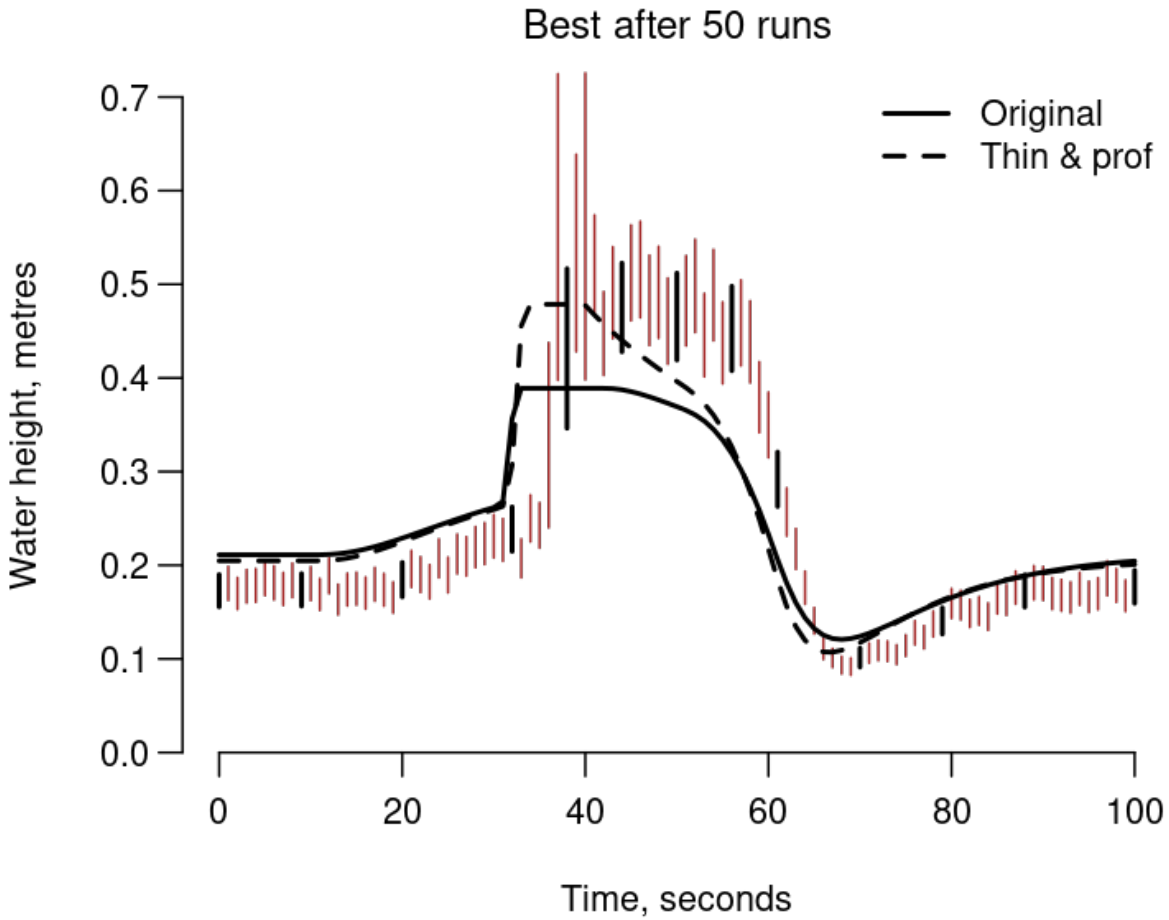

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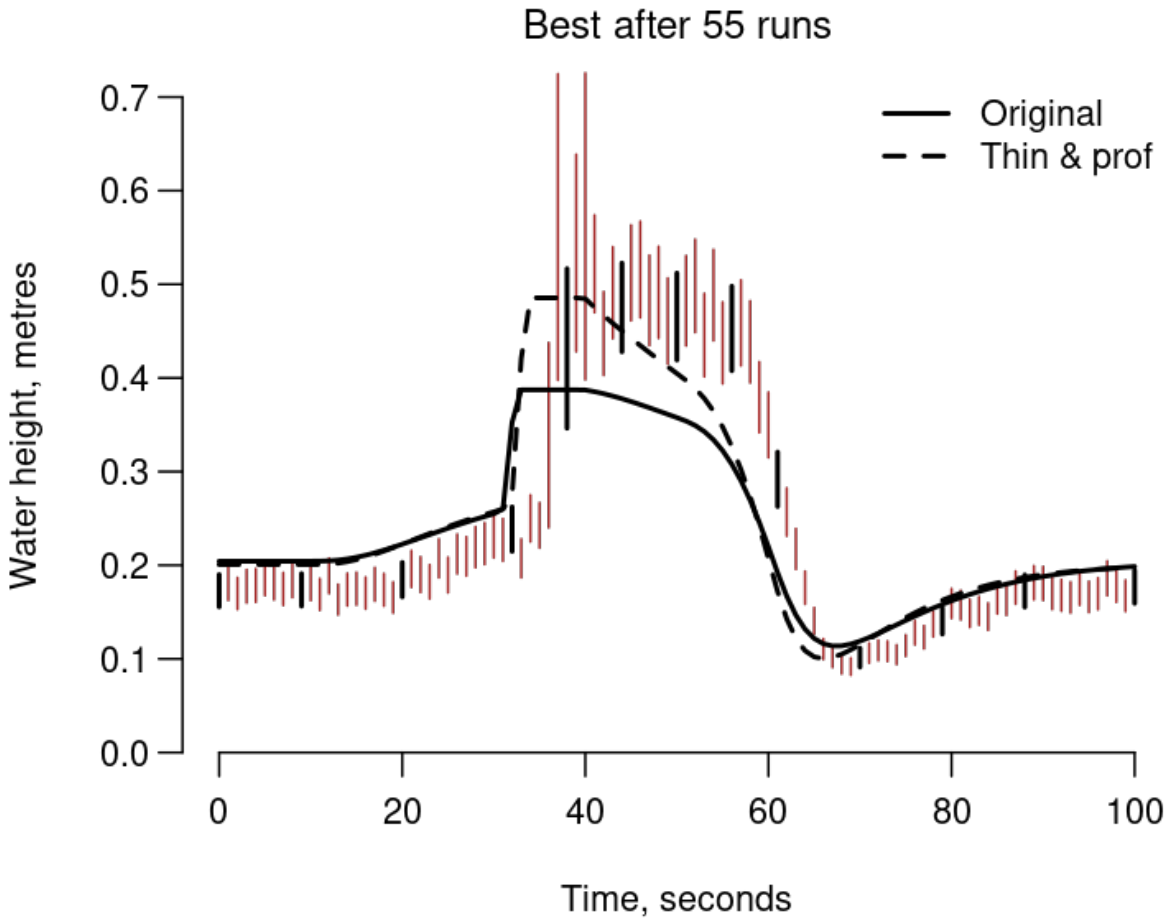

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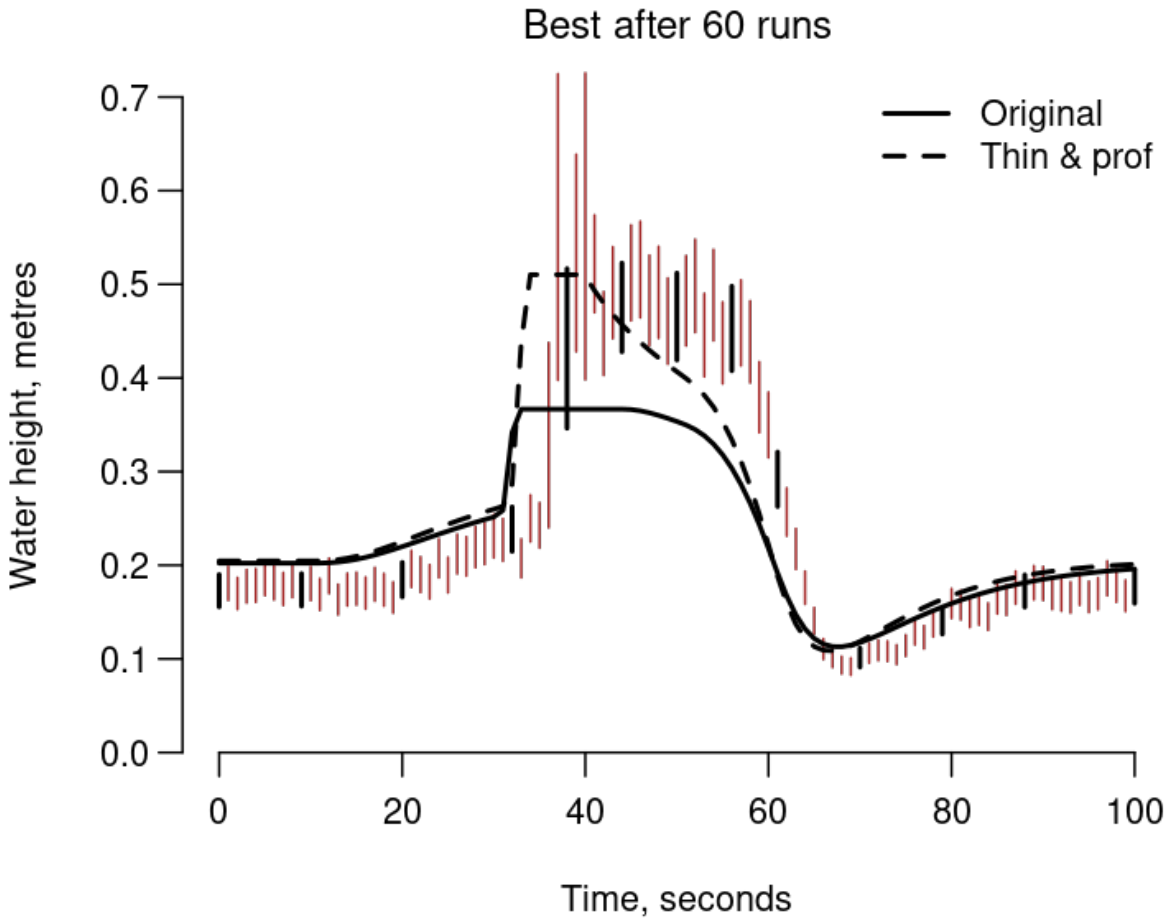

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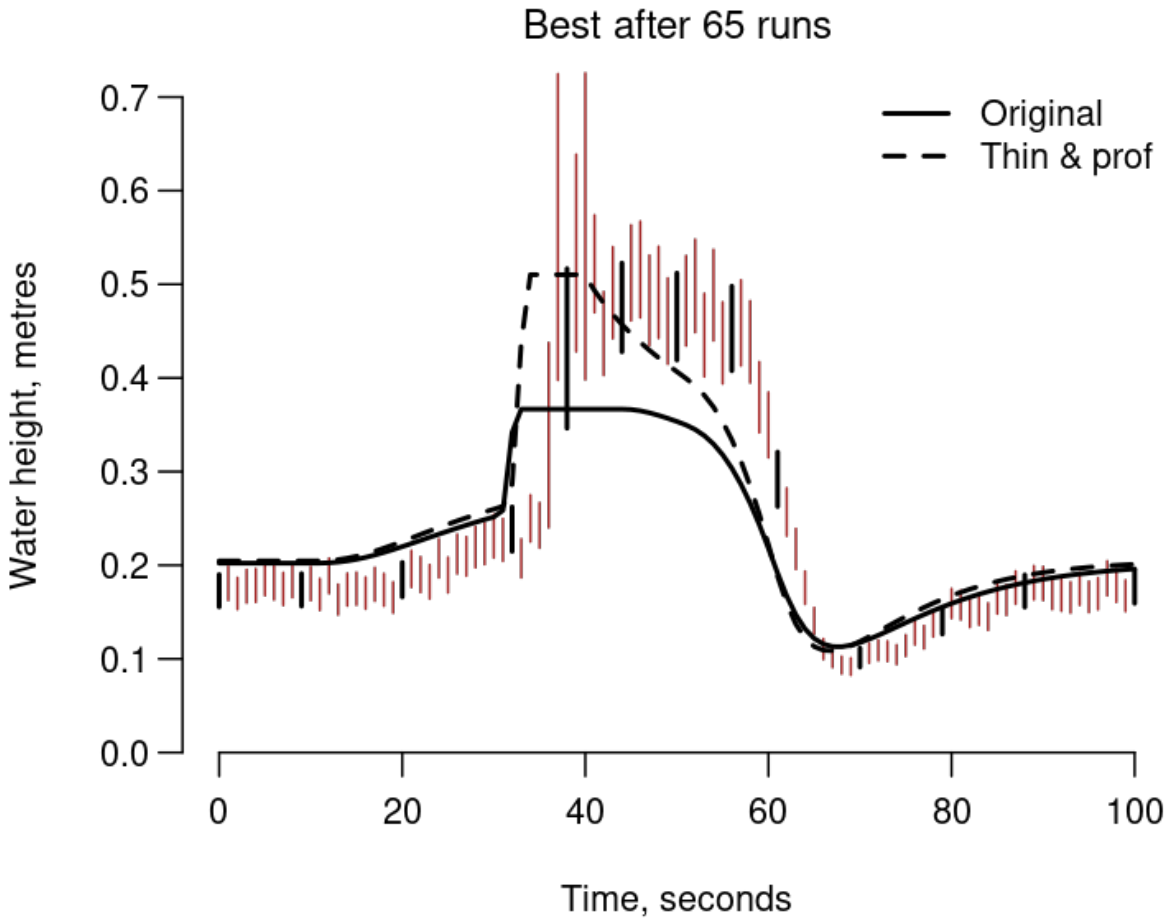

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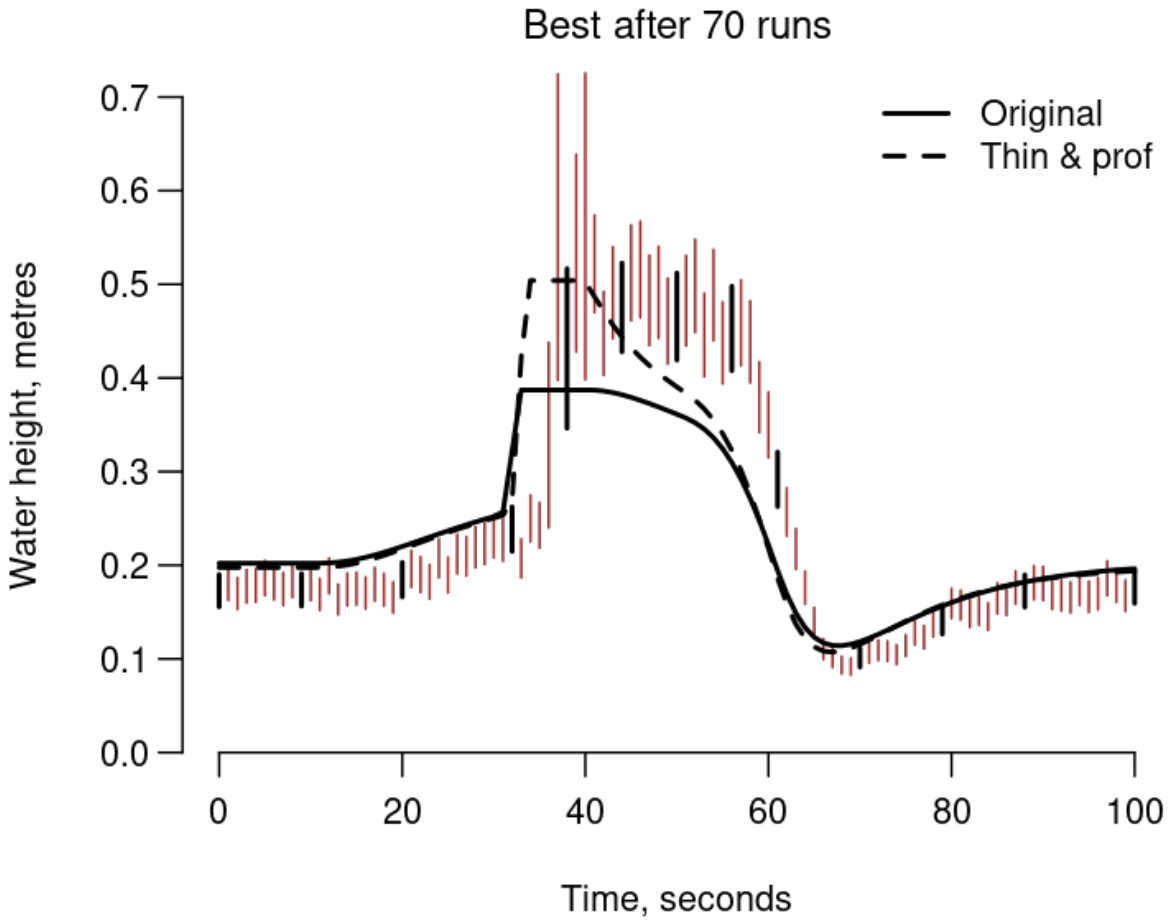
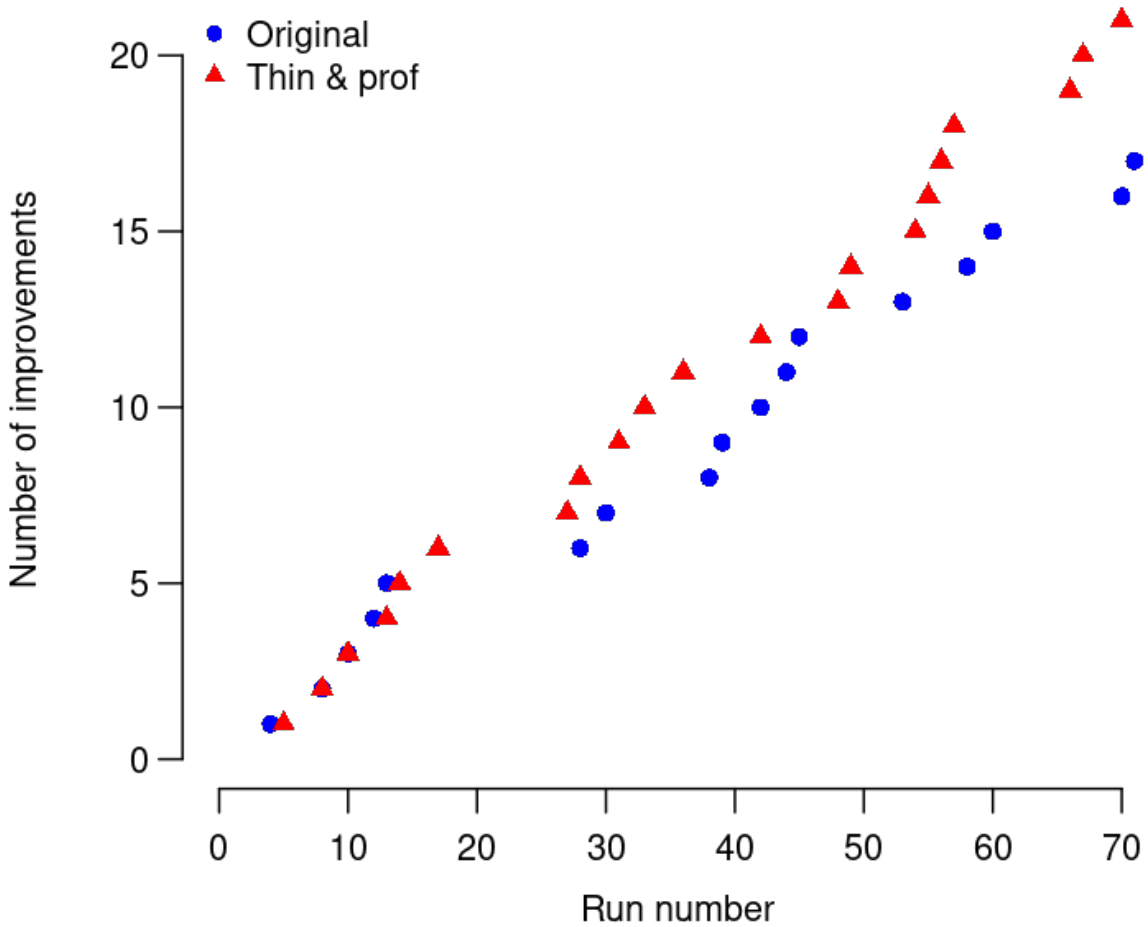


What's going on?

The original likelihood function is lumpy (Rougier, 2013), and it is hard for the optimiser to make progress. Not so the thin & prof likelihood:



Where next?

The thin & prof log-likelihood function ought to be smooth-ish, especially near to the global maximum. This seems like a good candidate for Bayesian optimization, to squeeze out a better fit than the best so far.

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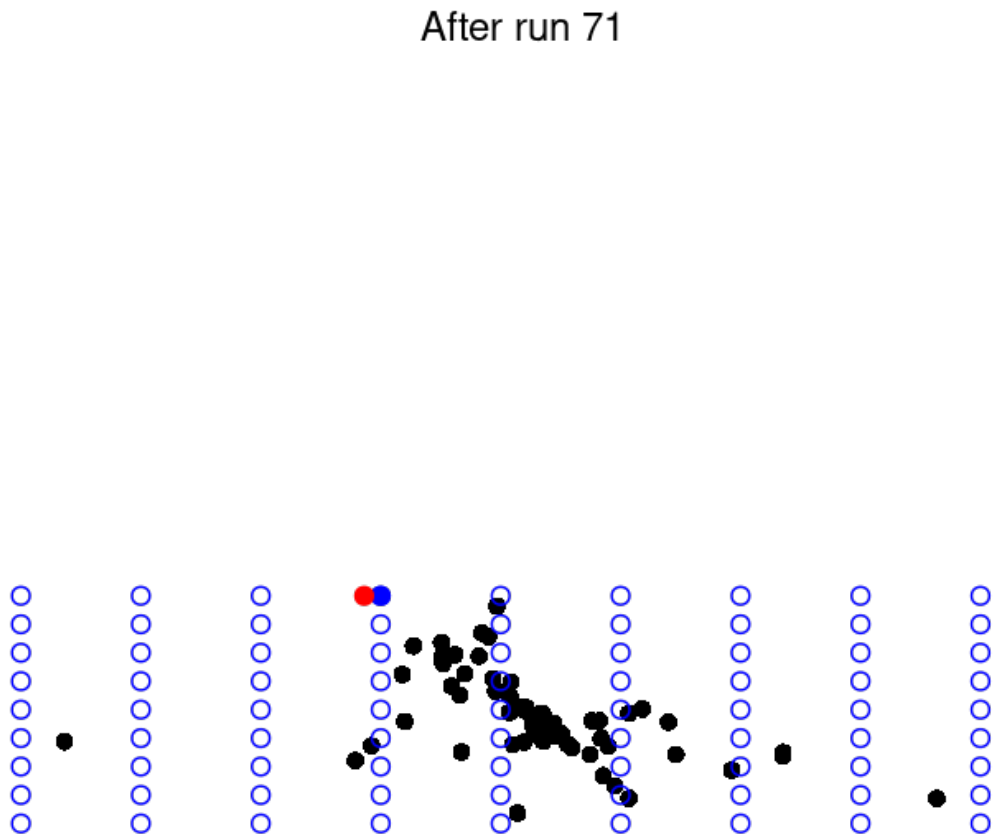
- Some algebra shows that

$$\mathbb{E}\{\lambda(L_\theta)\} = \ell^{\text{best}} + (m(\theta) - \ell^{\text{best}})\Phi(\ell^{\text{best}}) - v(\theta)\phi(\ell^{\text{best}}),$$

  where L_θ is the unknown value of ℓ_θ, Φ and ϕ are the Gaussian distribution function and density function, evaluated with $m(\theta)$ and $v(\theta)$.

Bayesian optimization (cont)

Simple adaptive search:



▸ More details

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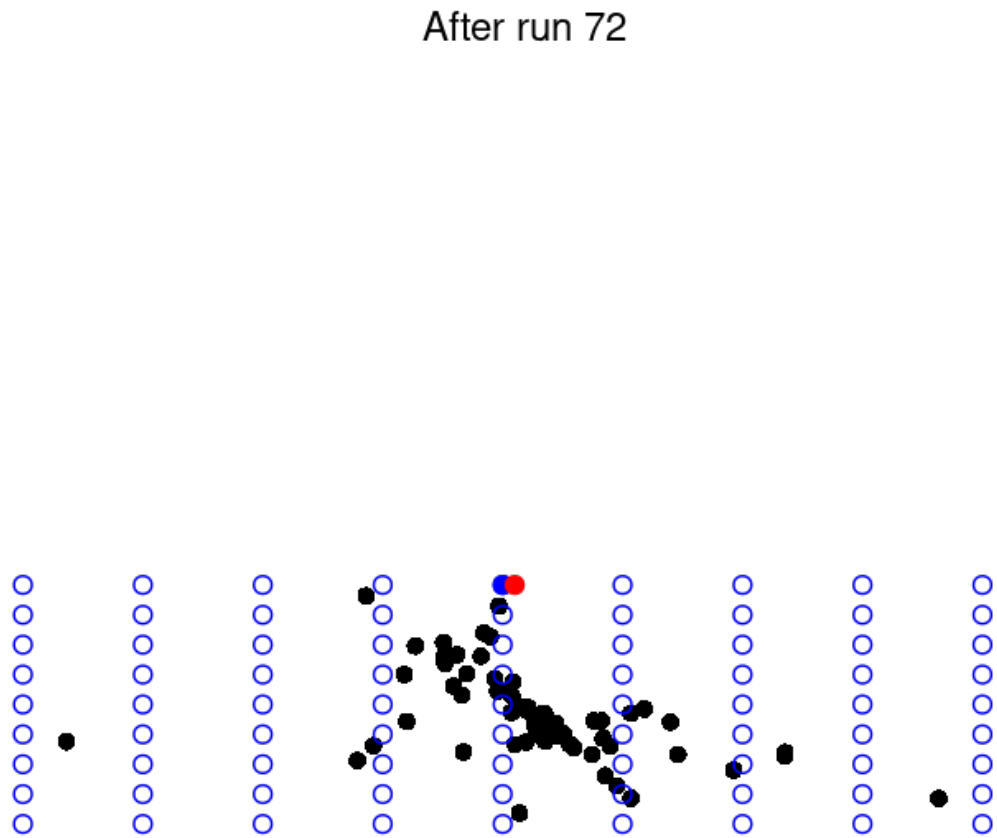

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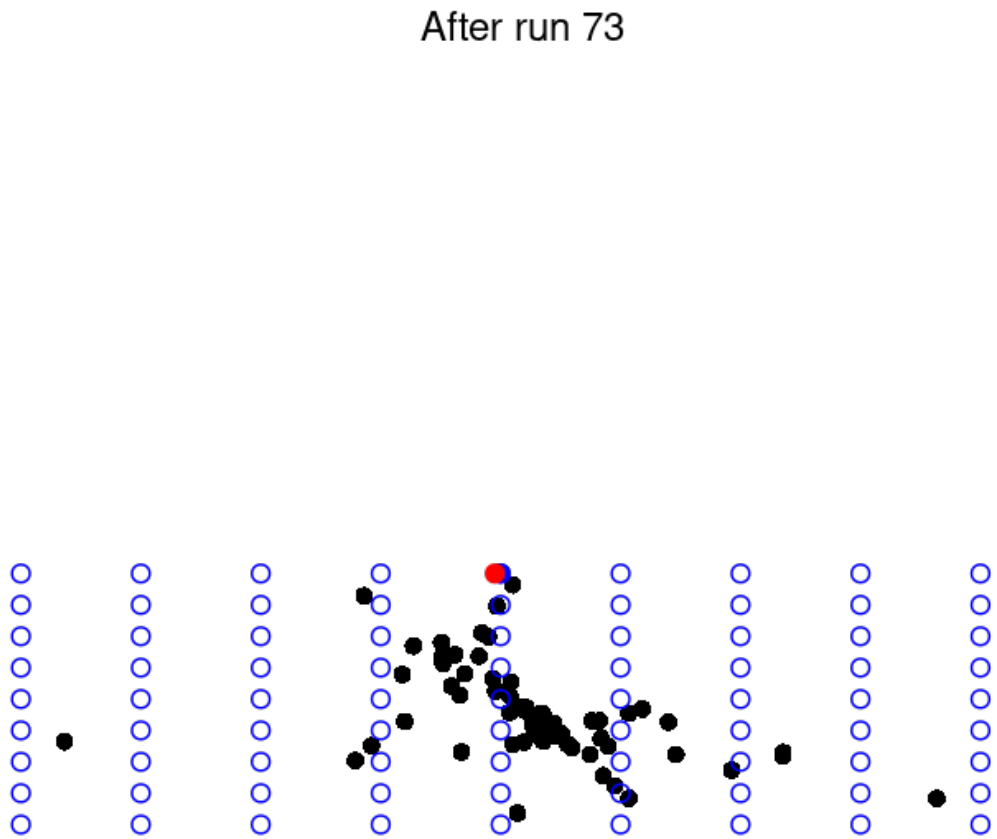

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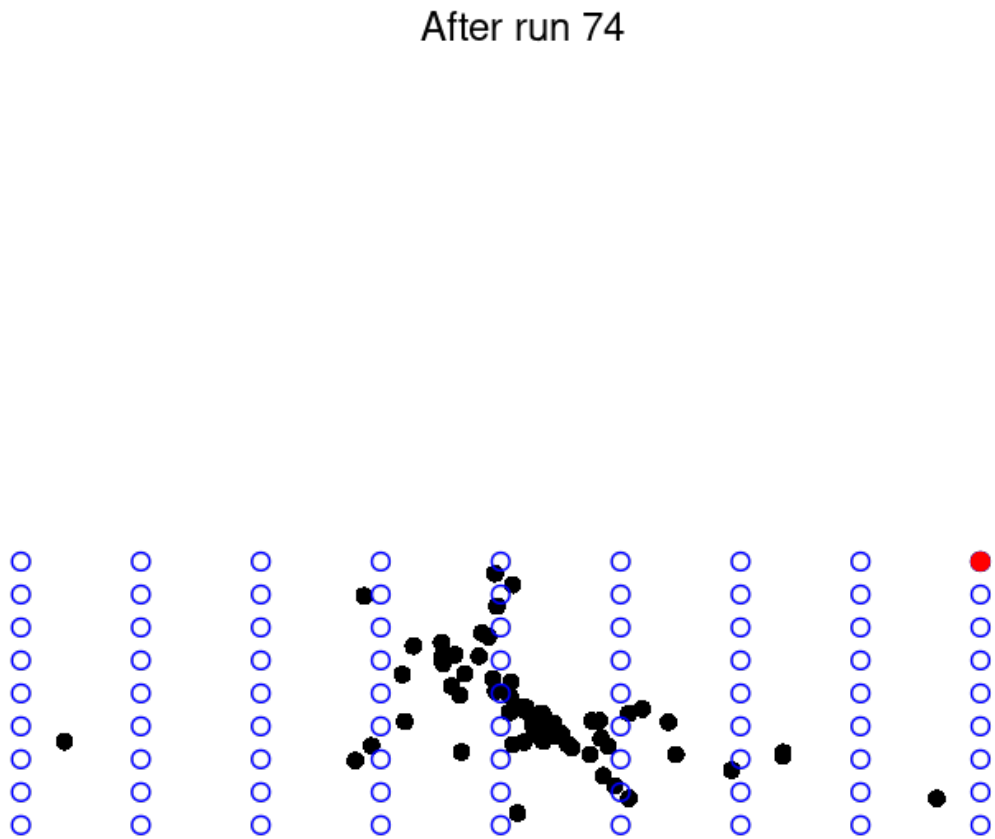

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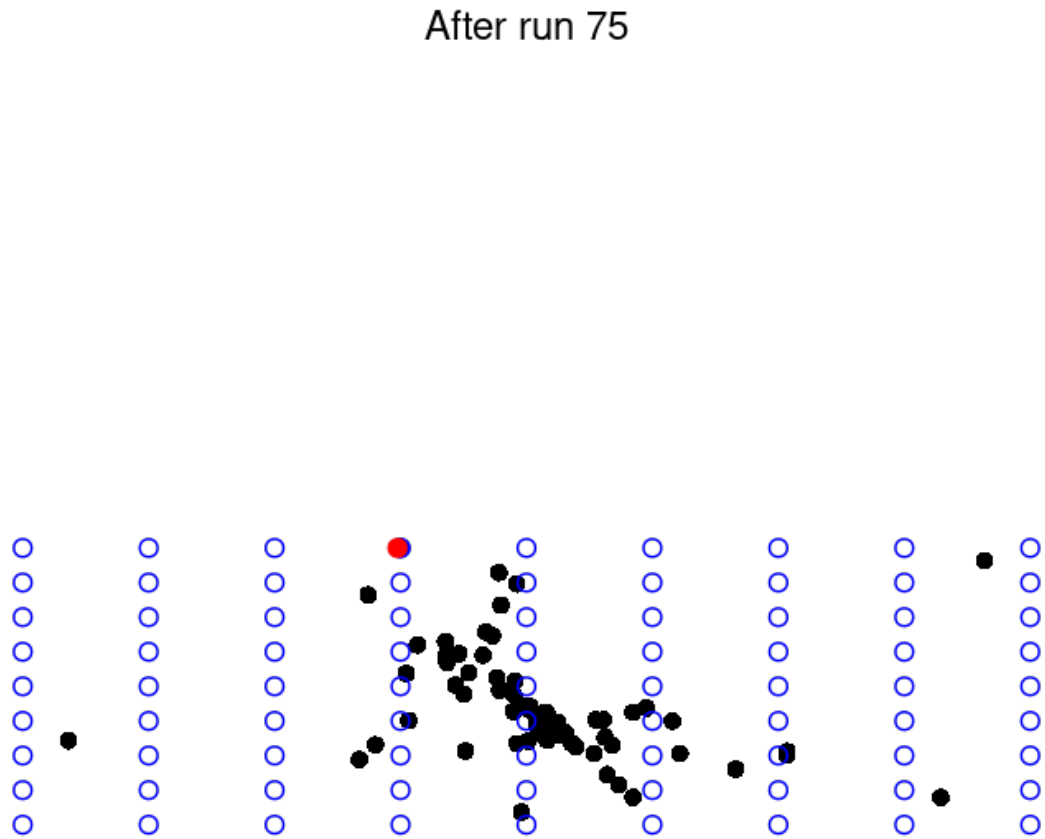

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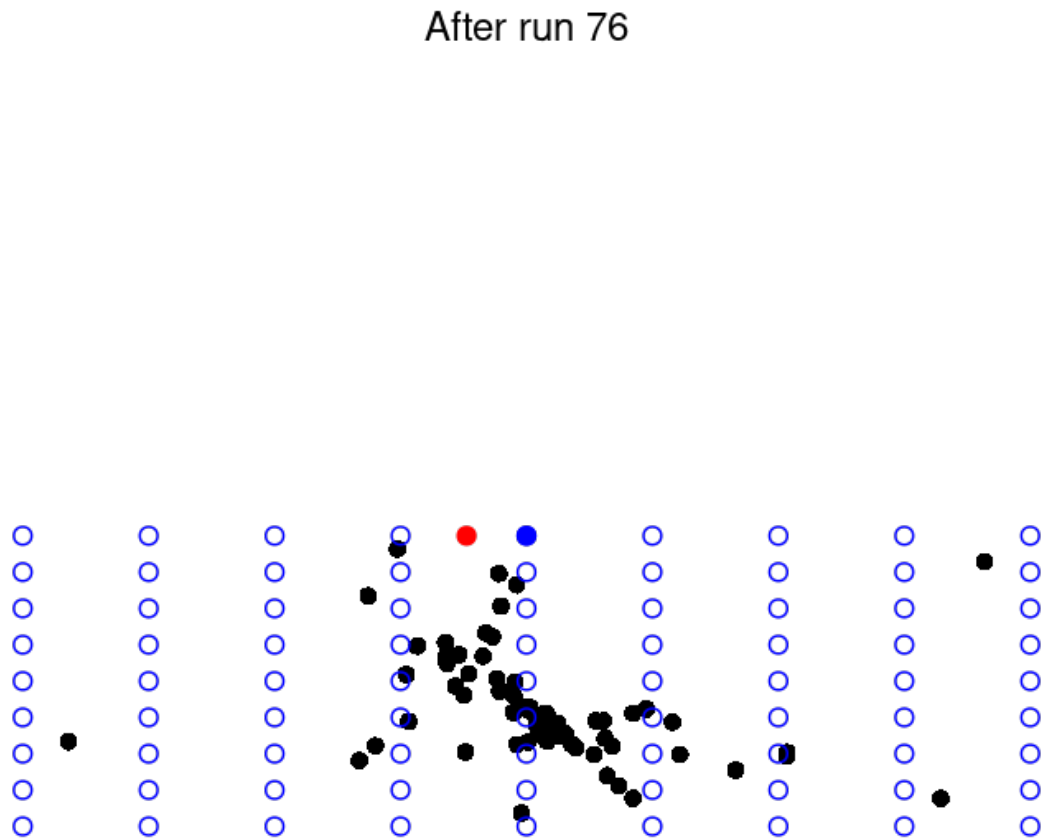

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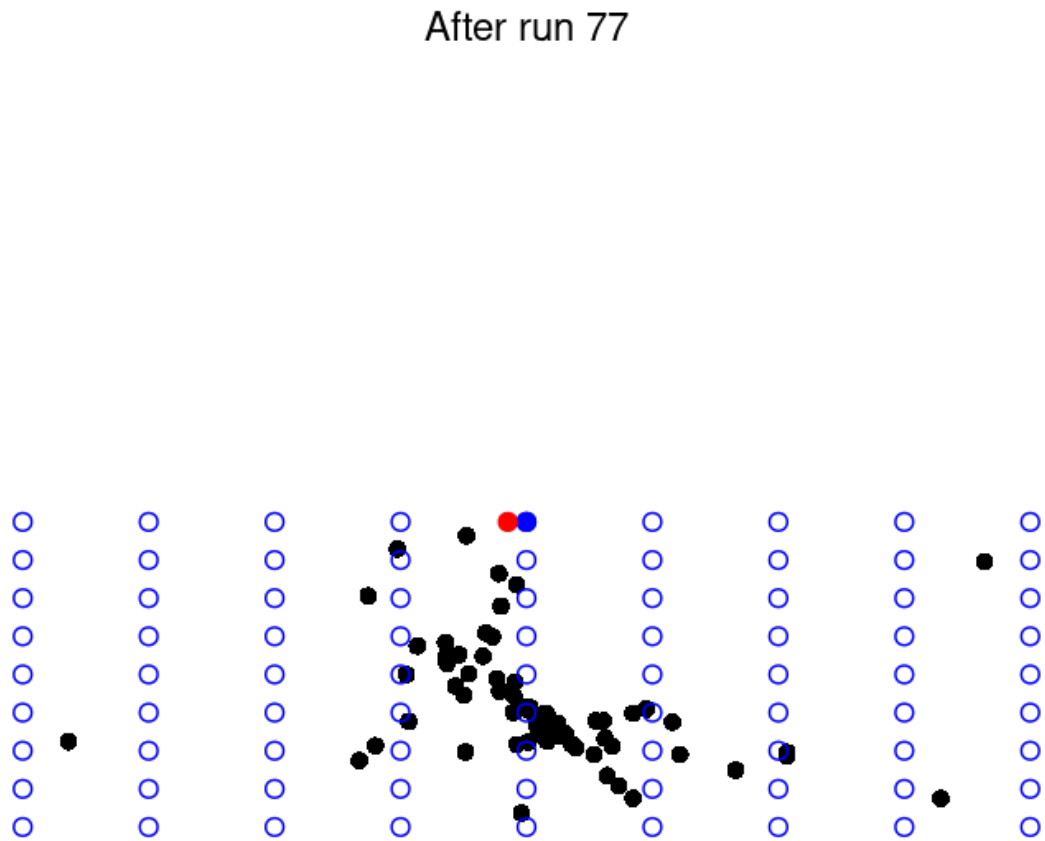

▸ More details

Bayesian optimization (cont)

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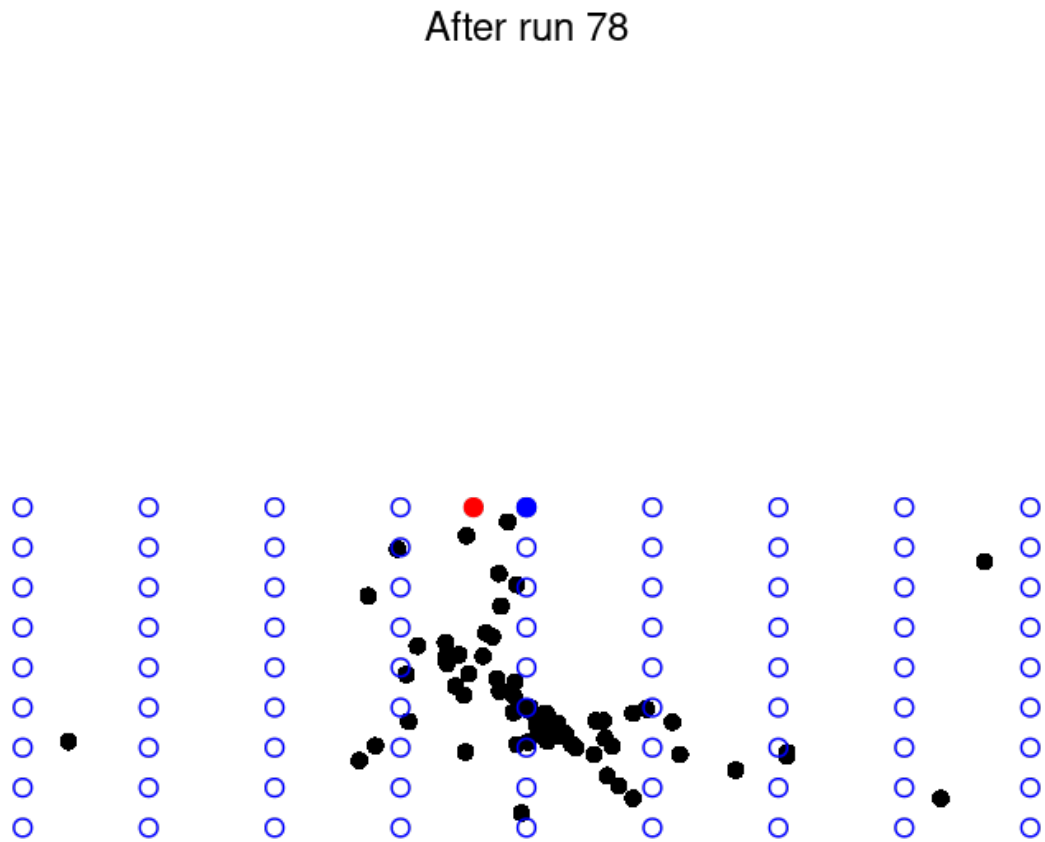

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Bayesian optimization (cont)

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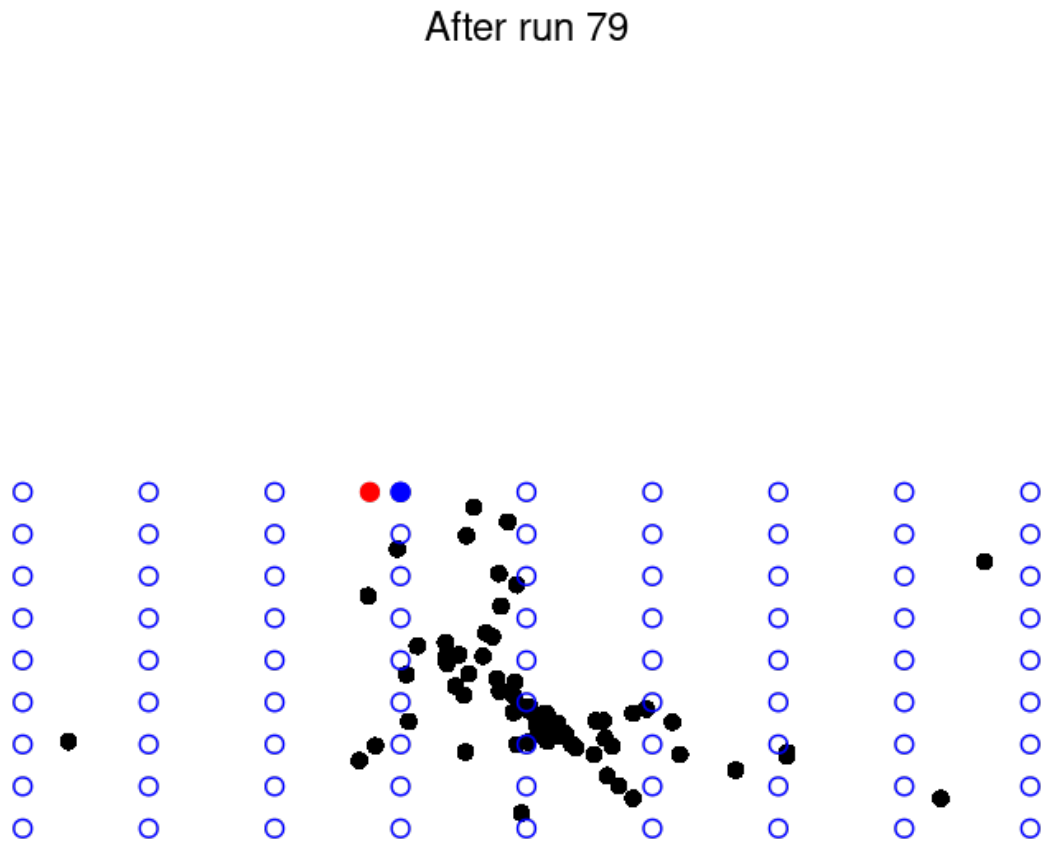

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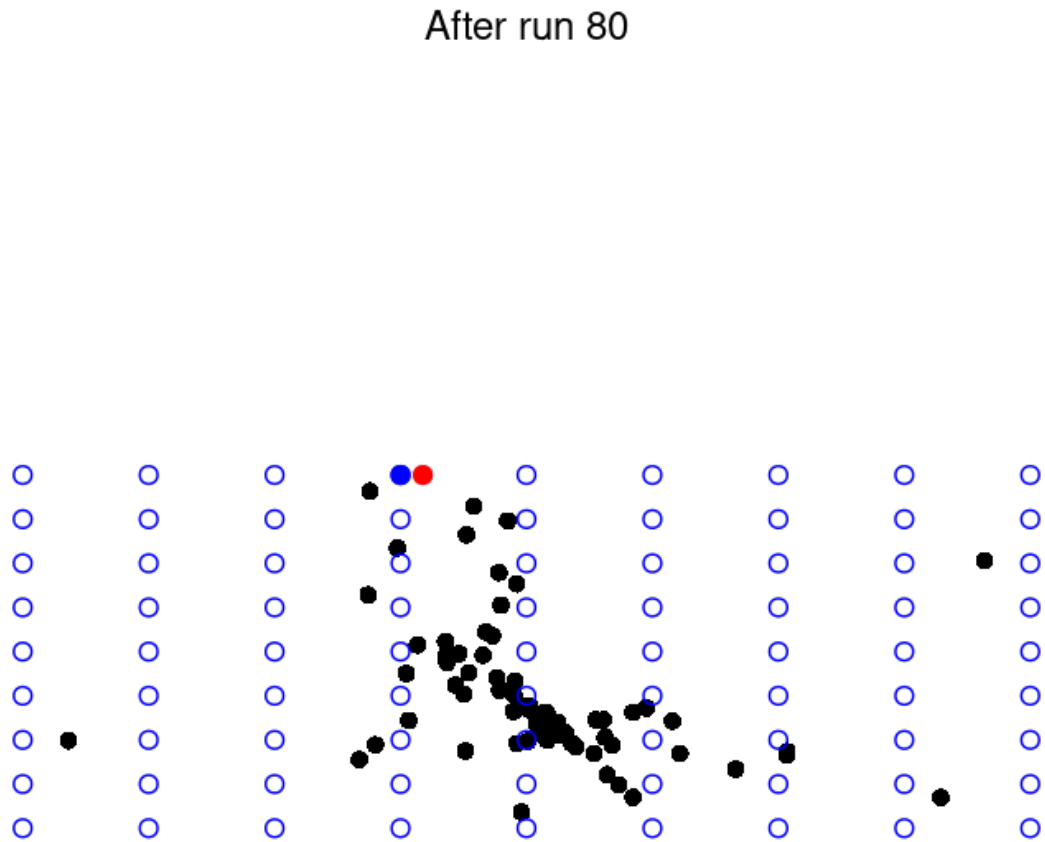

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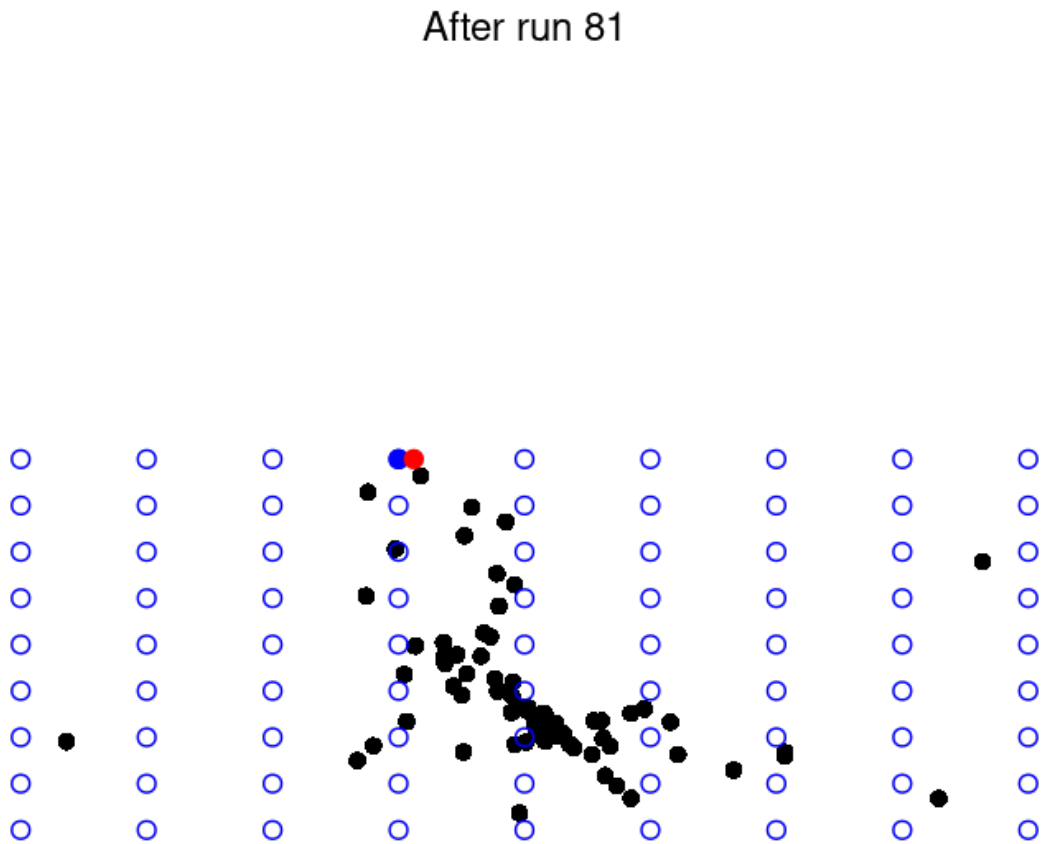

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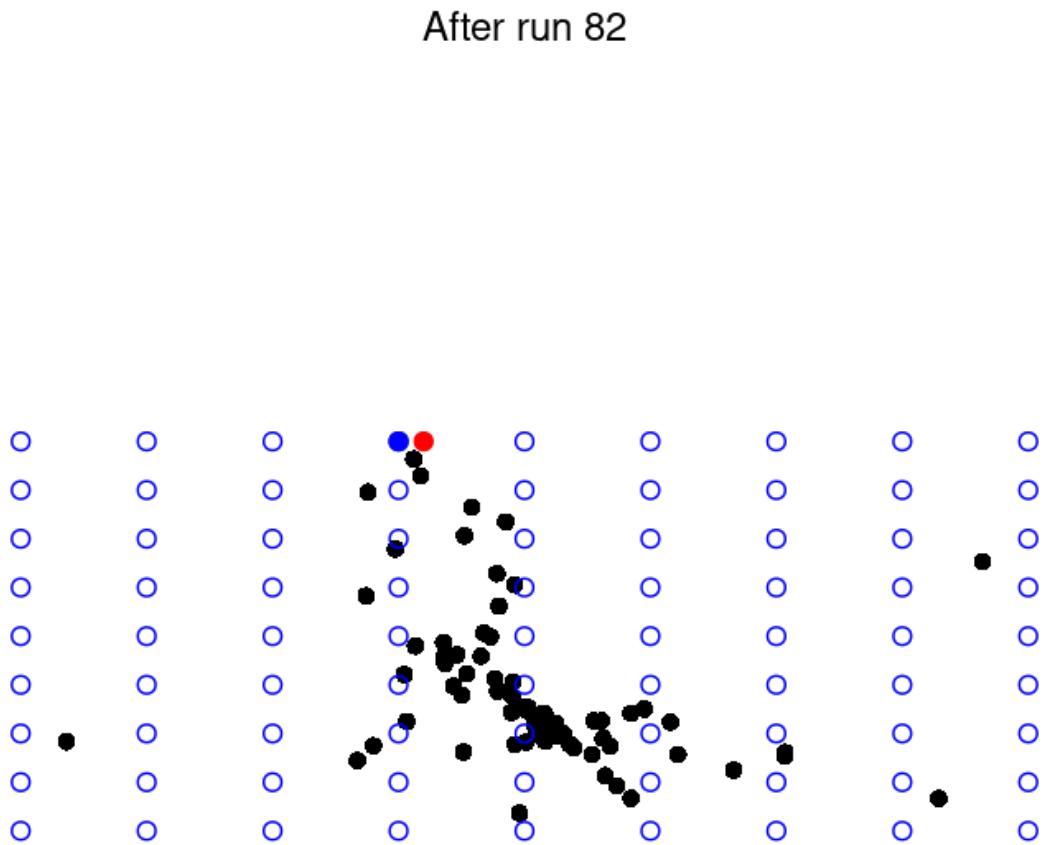

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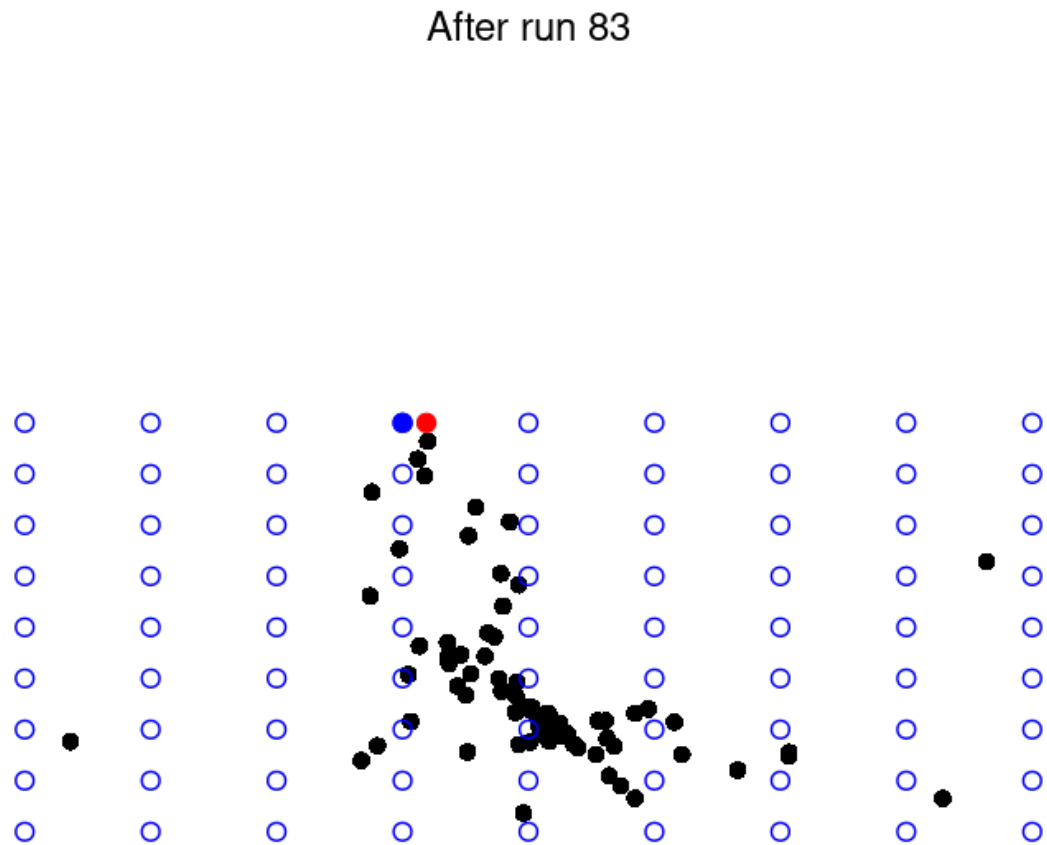

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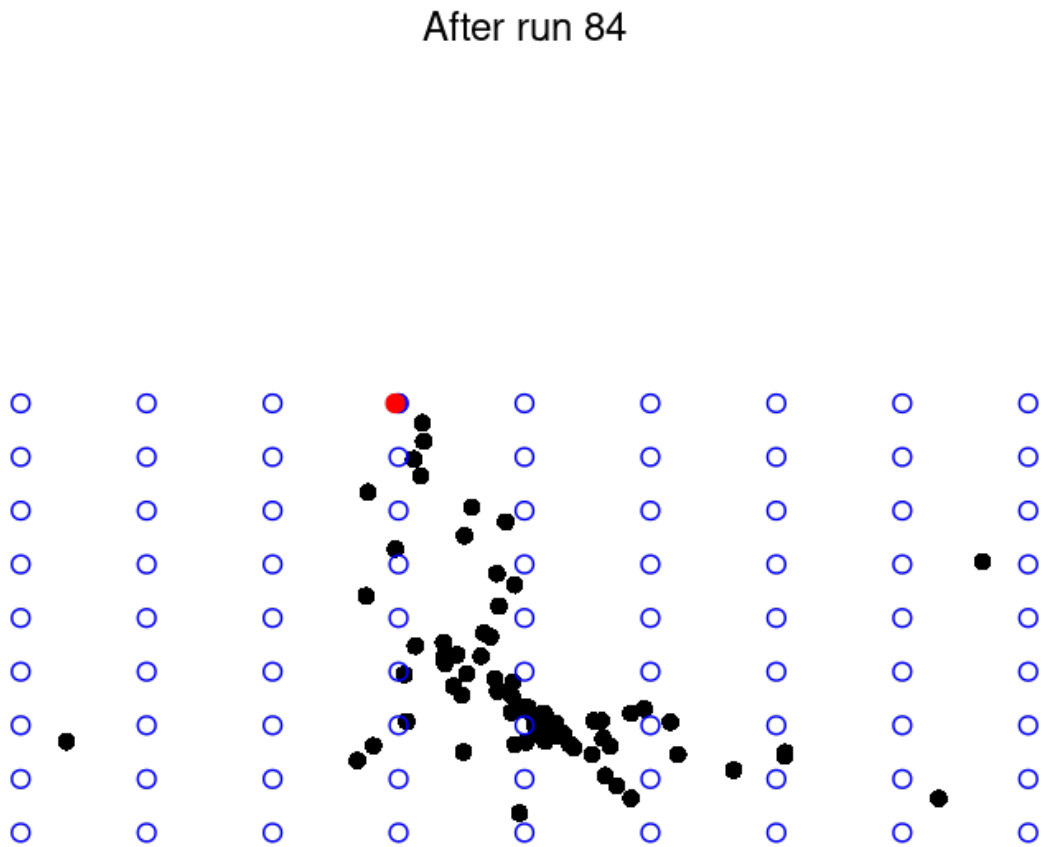

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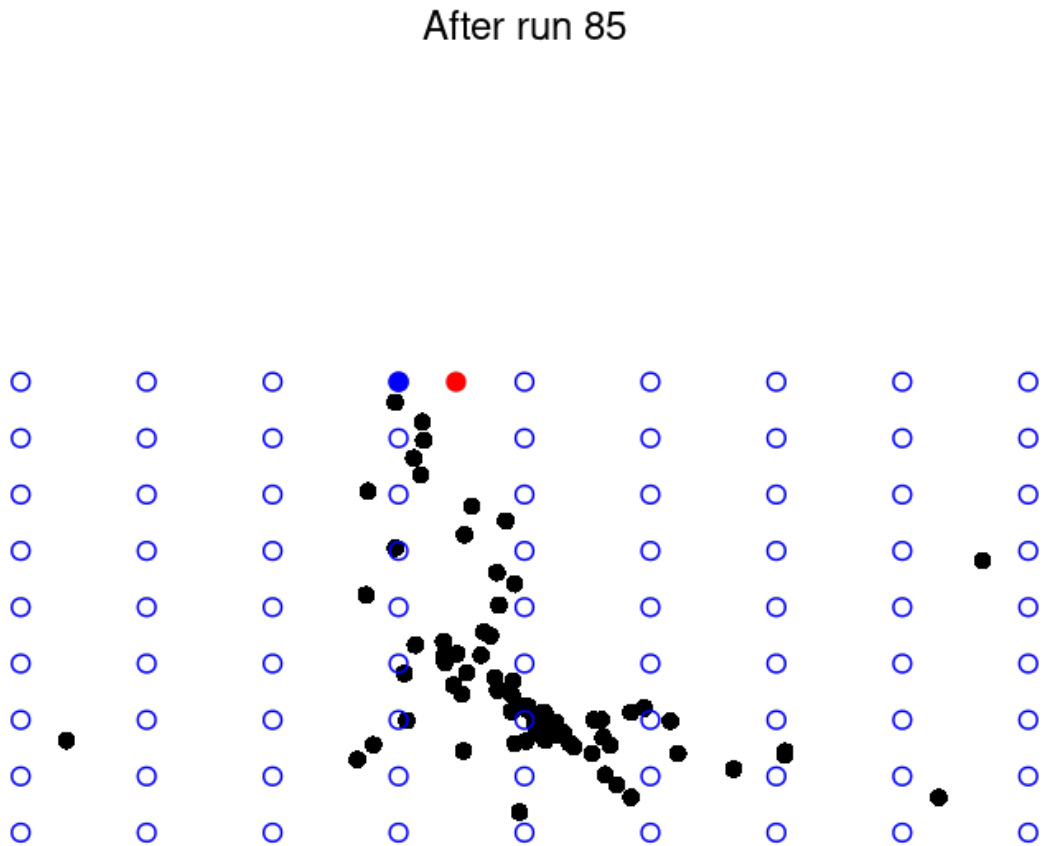

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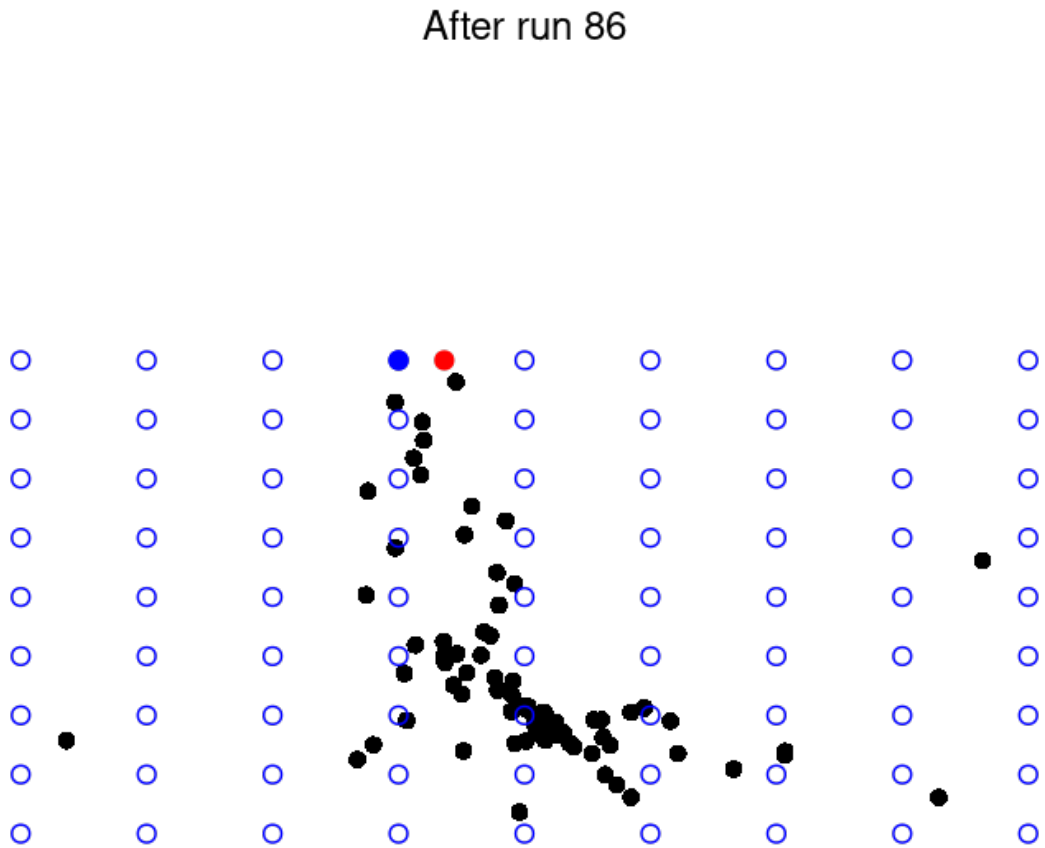

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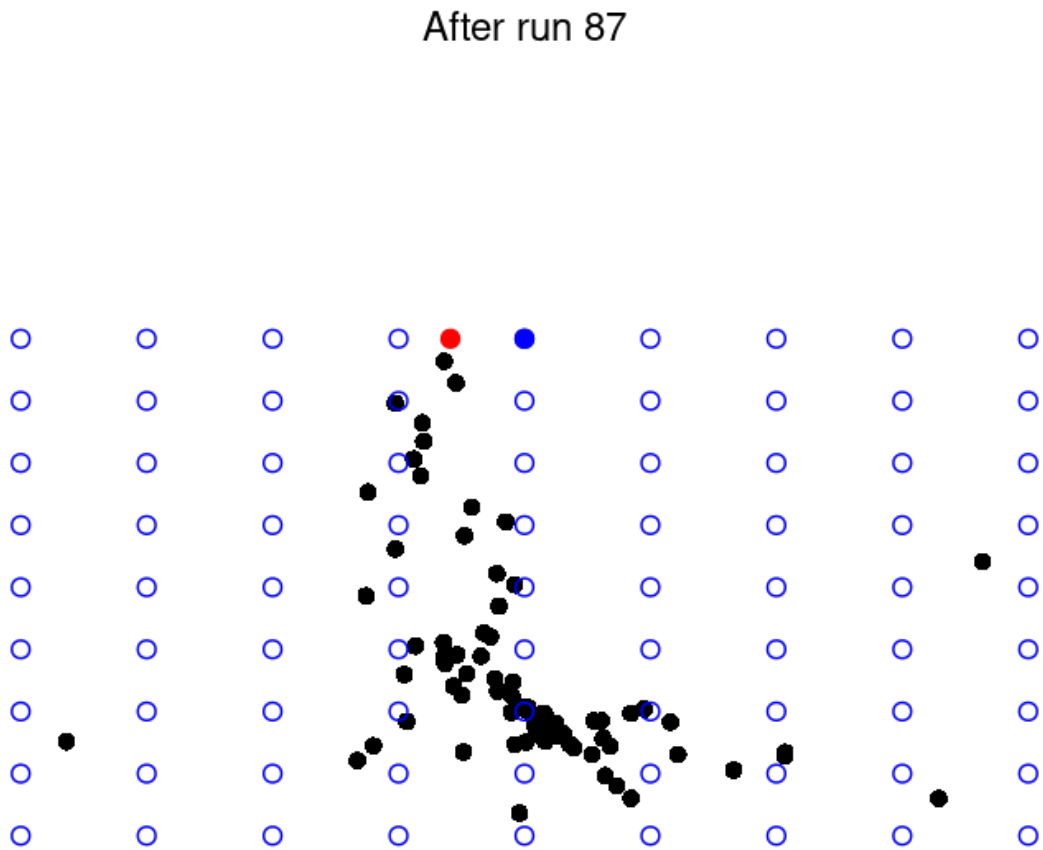

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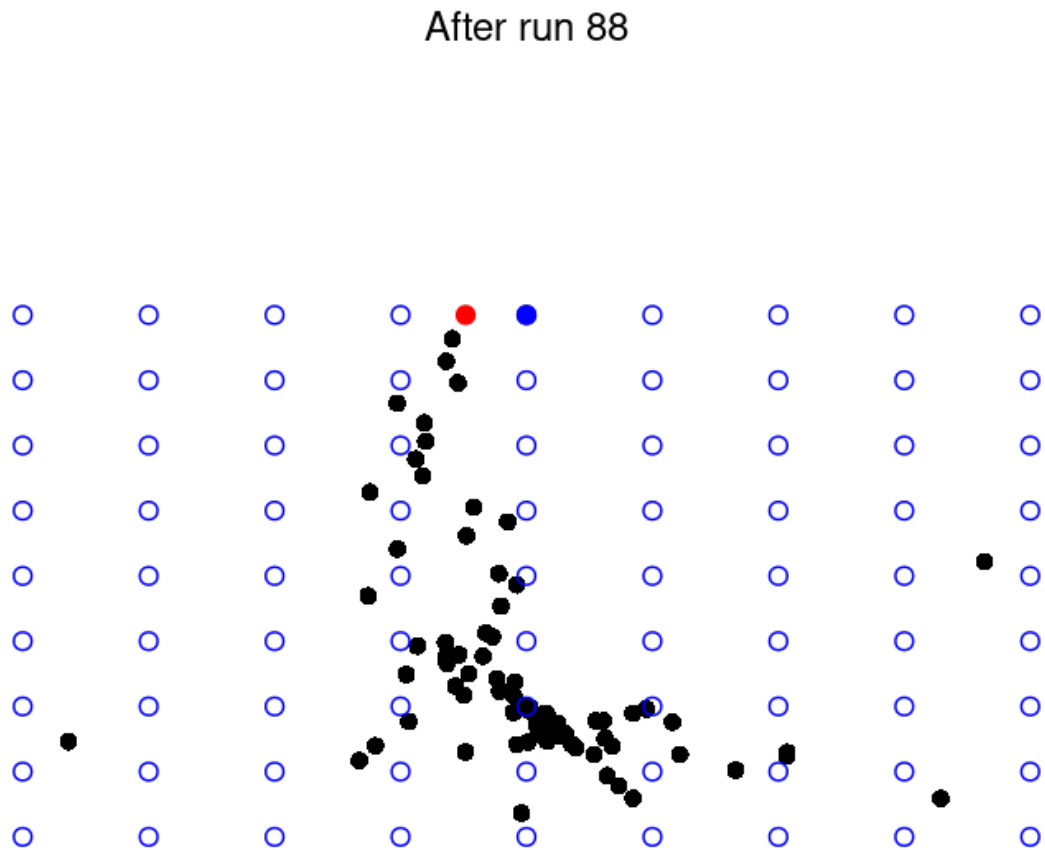

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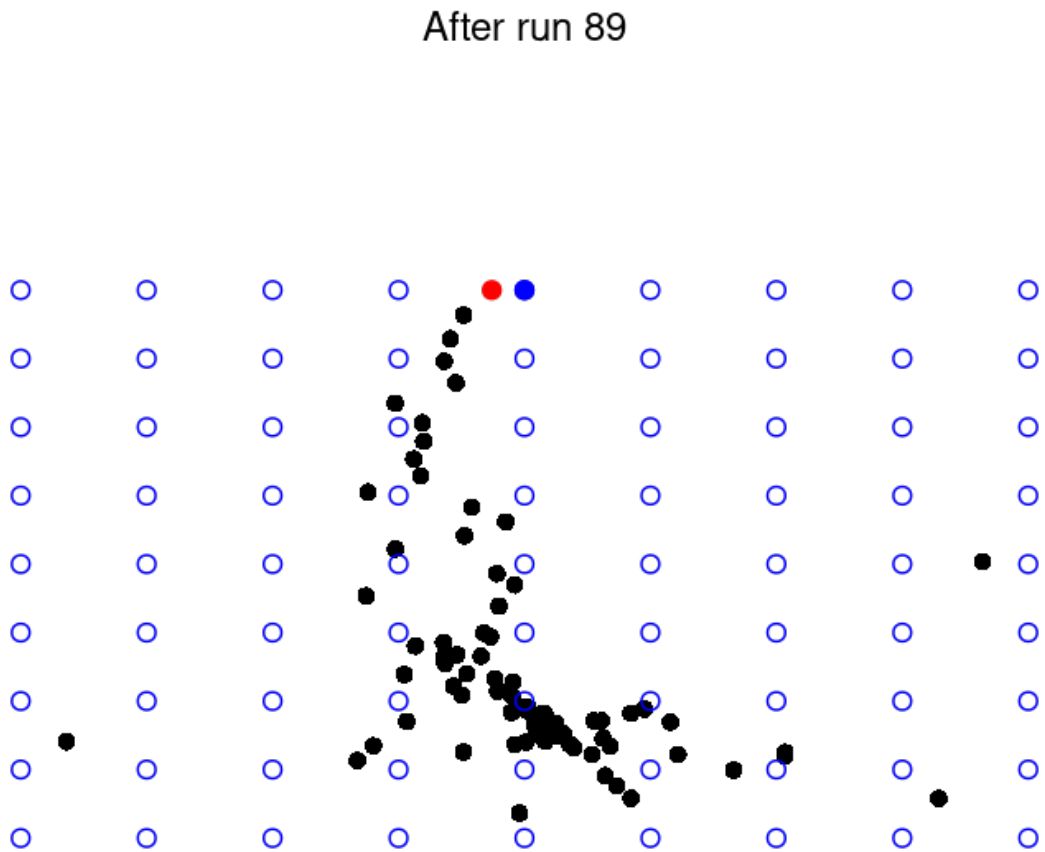

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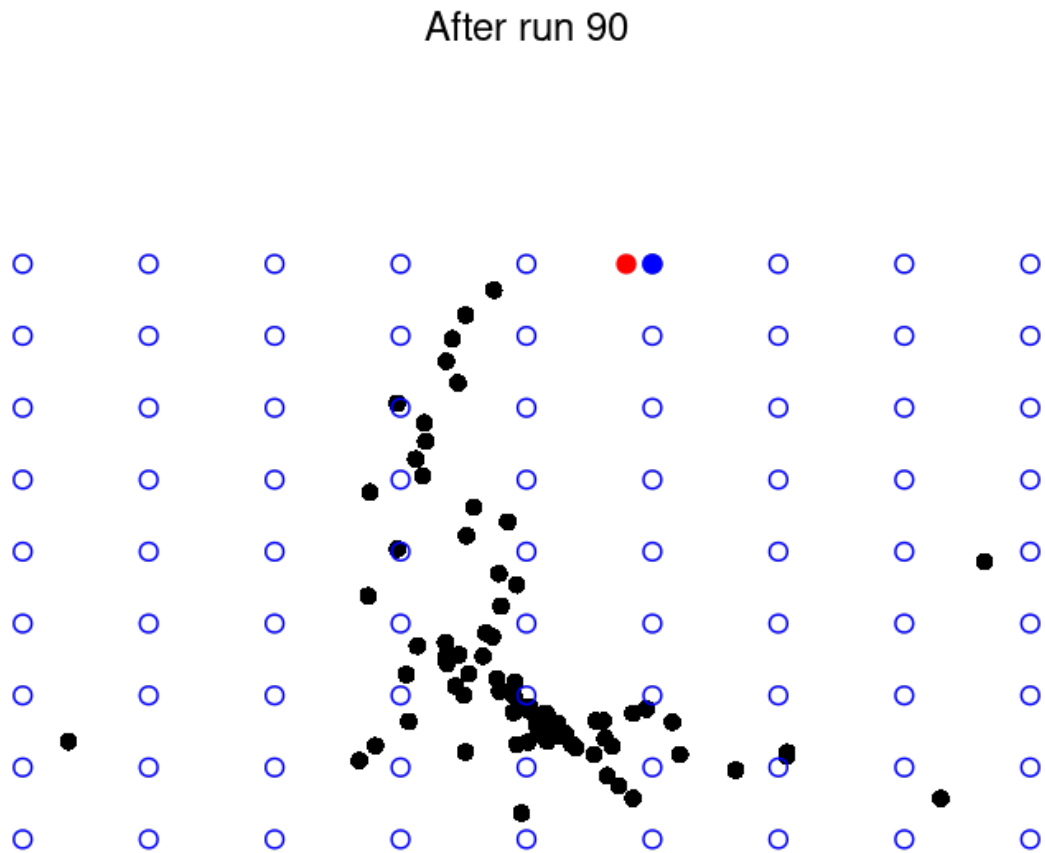

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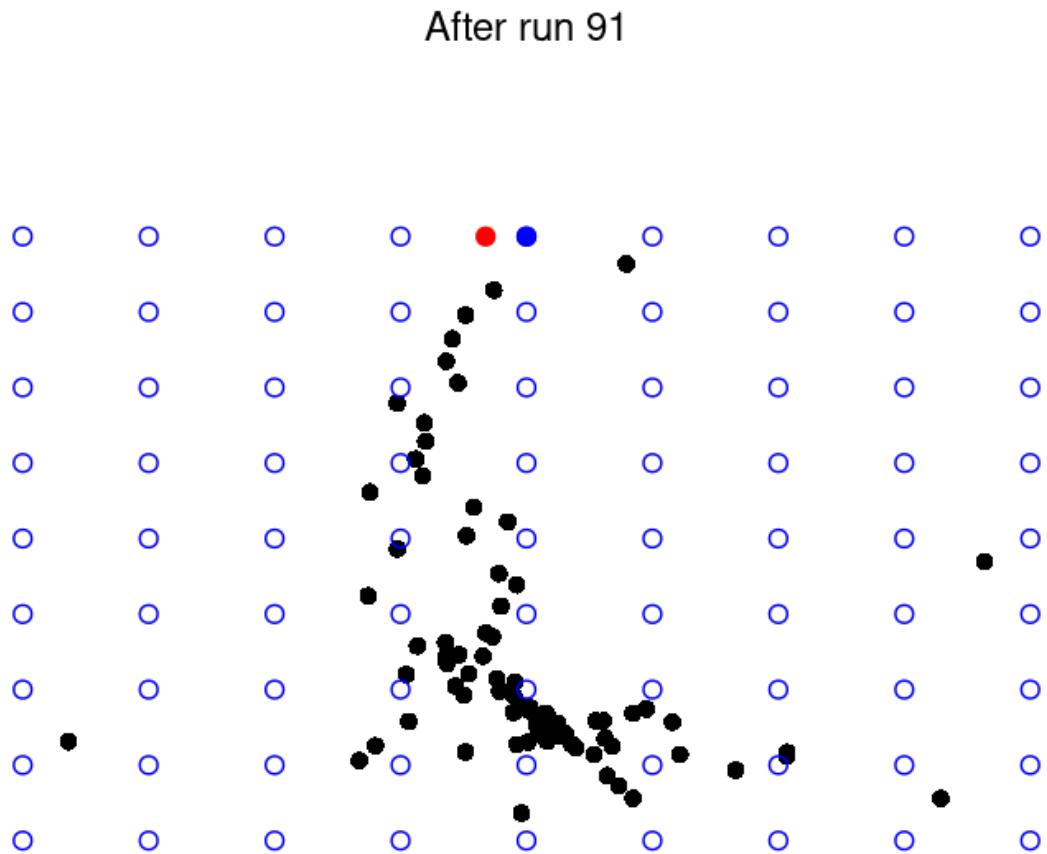

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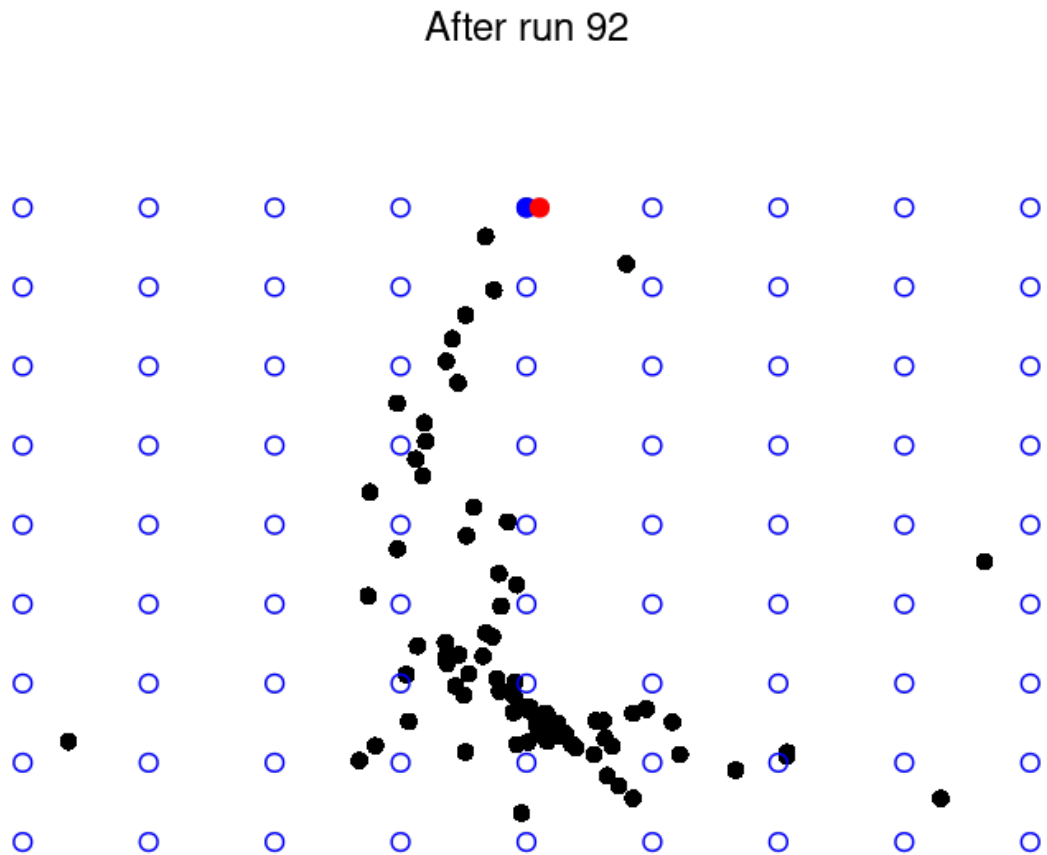

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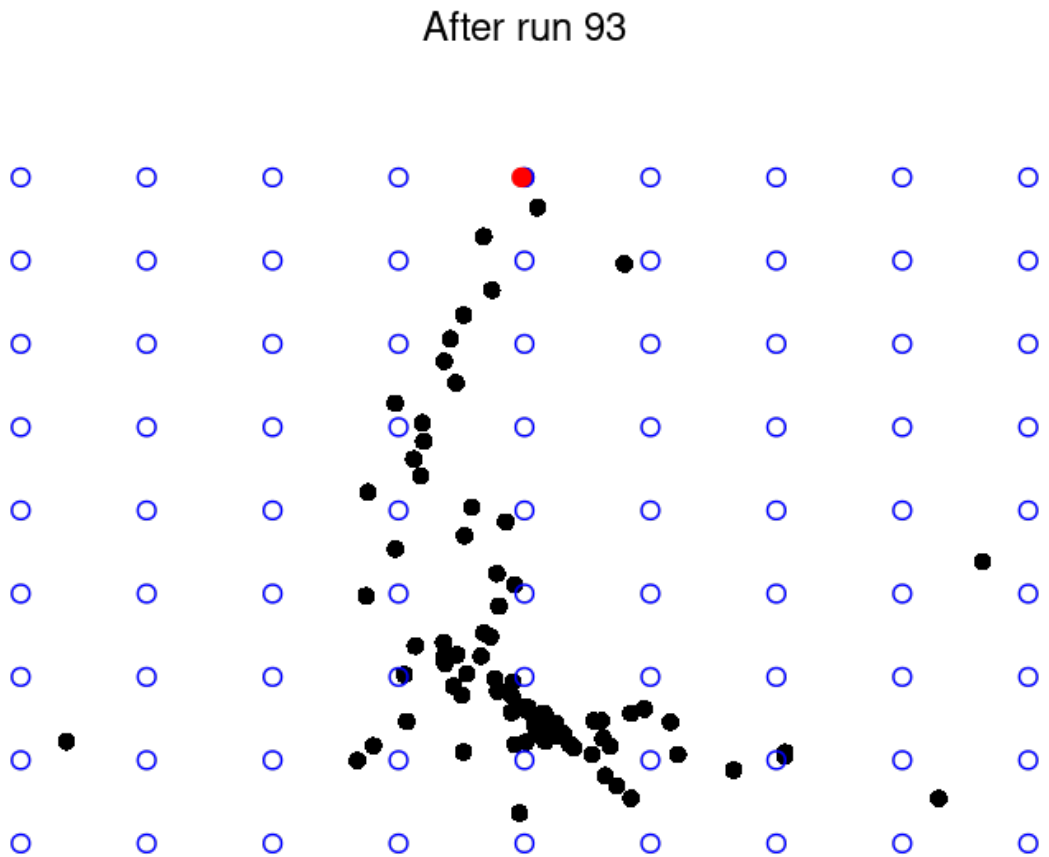

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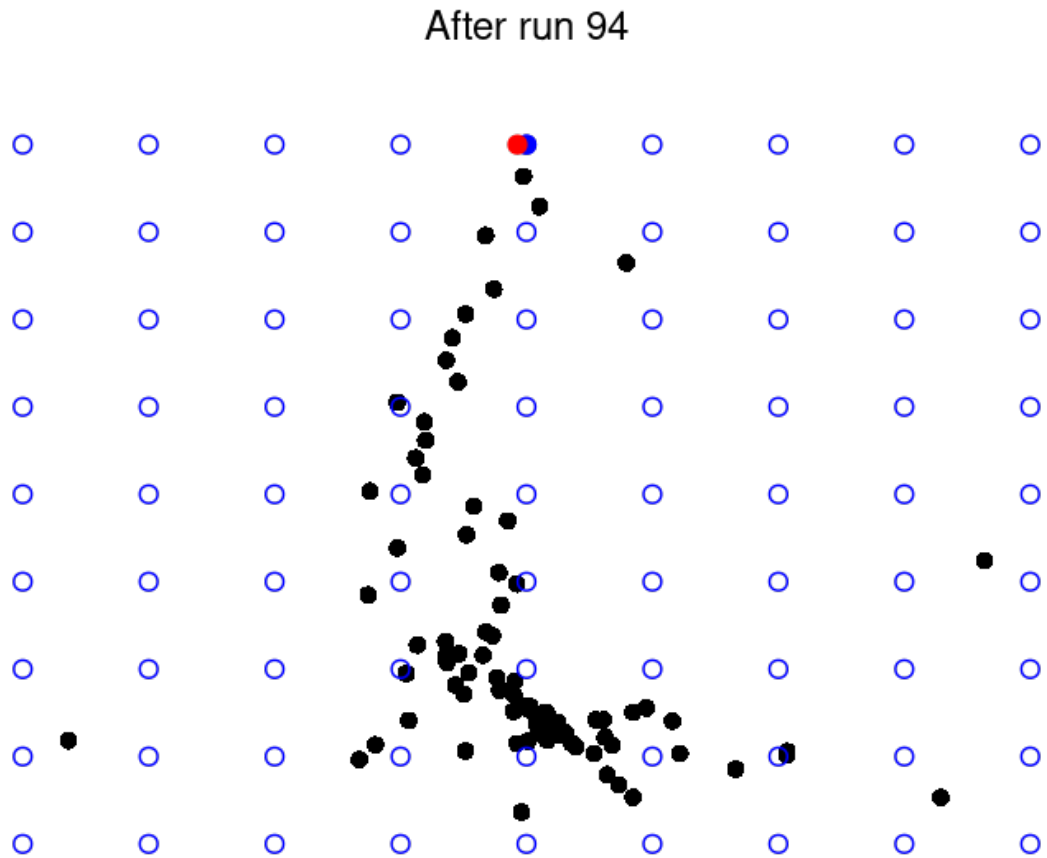

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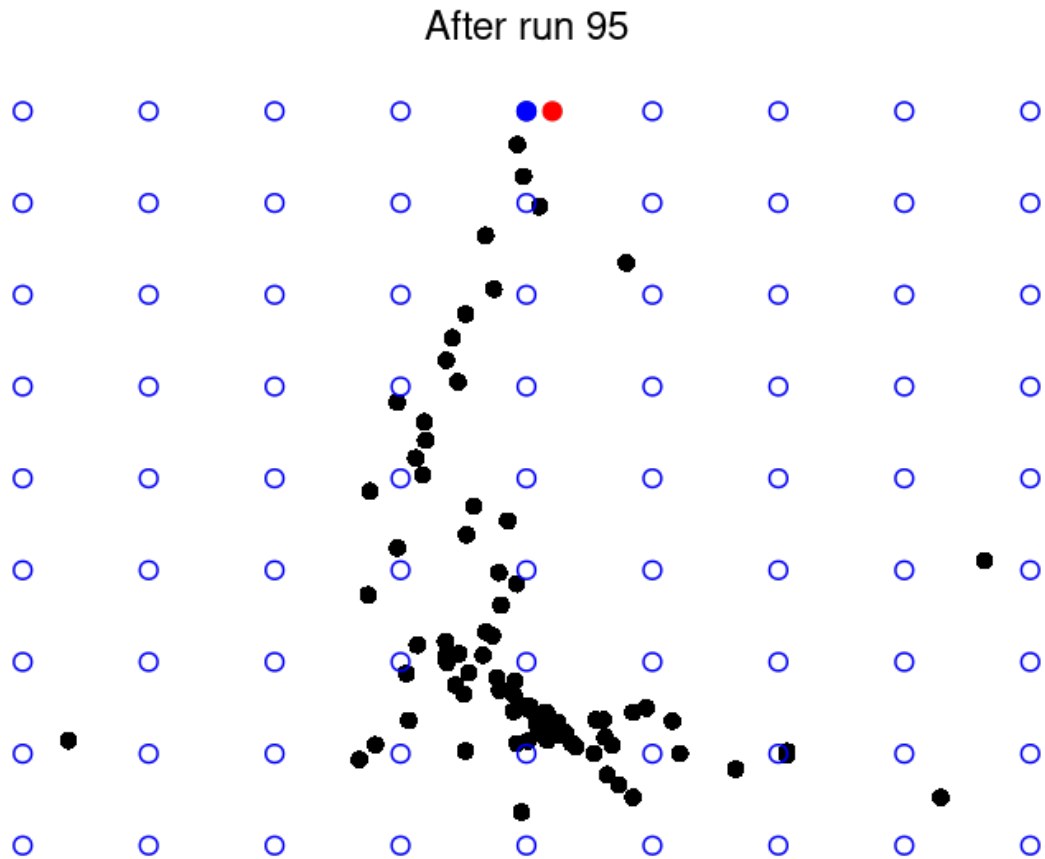

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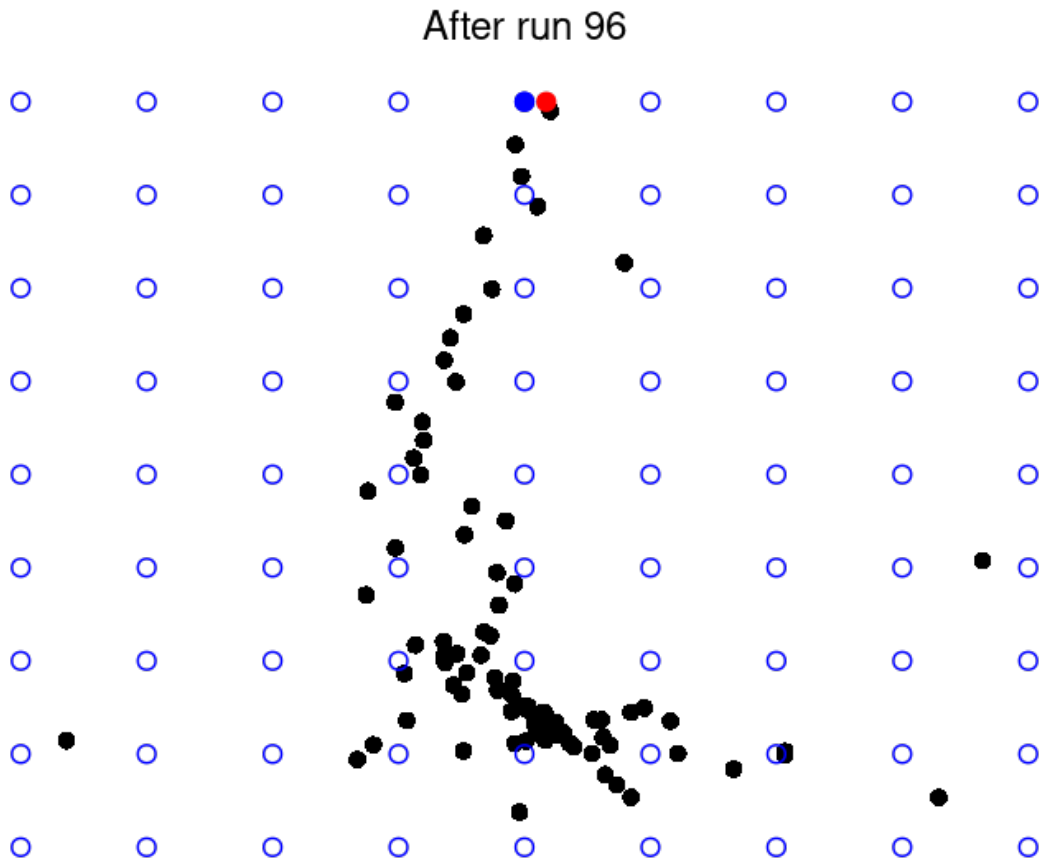

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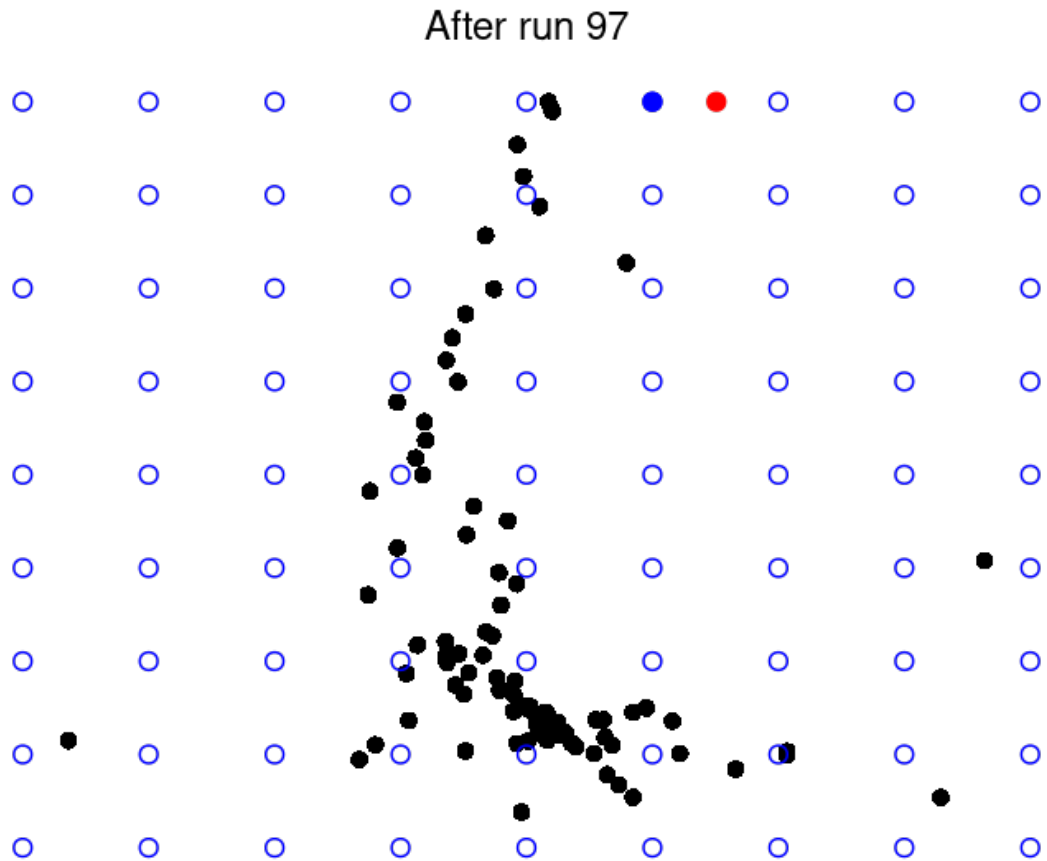

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Bayesian optimization (cont)

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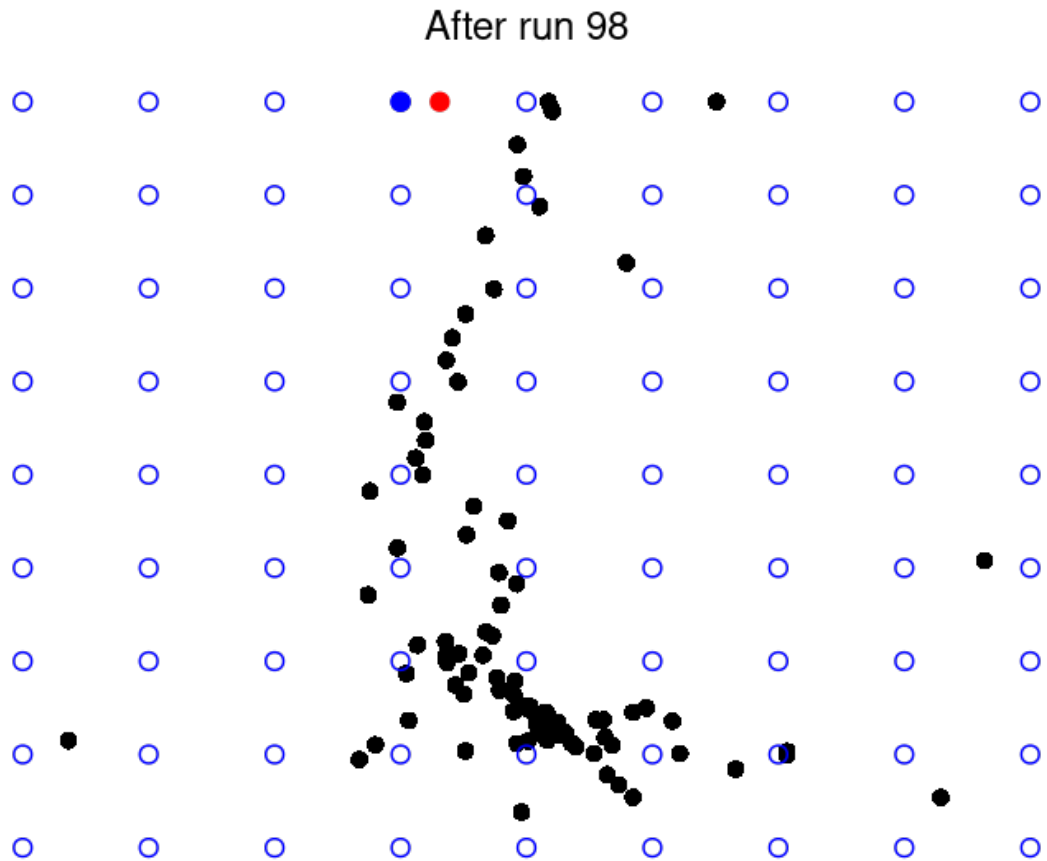

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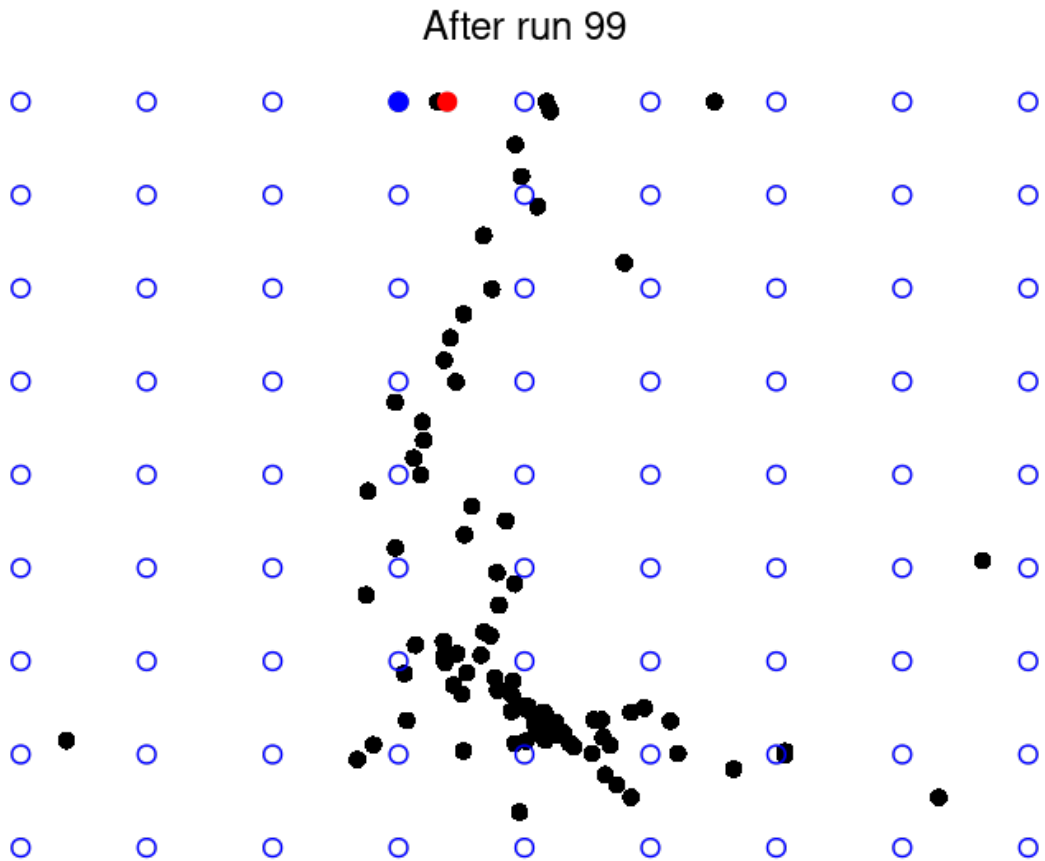

▸ More details

Results

I use the `RobustGaSP` emulator (Gu et al., 2018) with linear and quadratic trend (centred), a 9^6-point grid for $\mathcal{S}^+$ (half a million points), and `optim(method = "L-BFGS-B")` for the quasi-Newton method.

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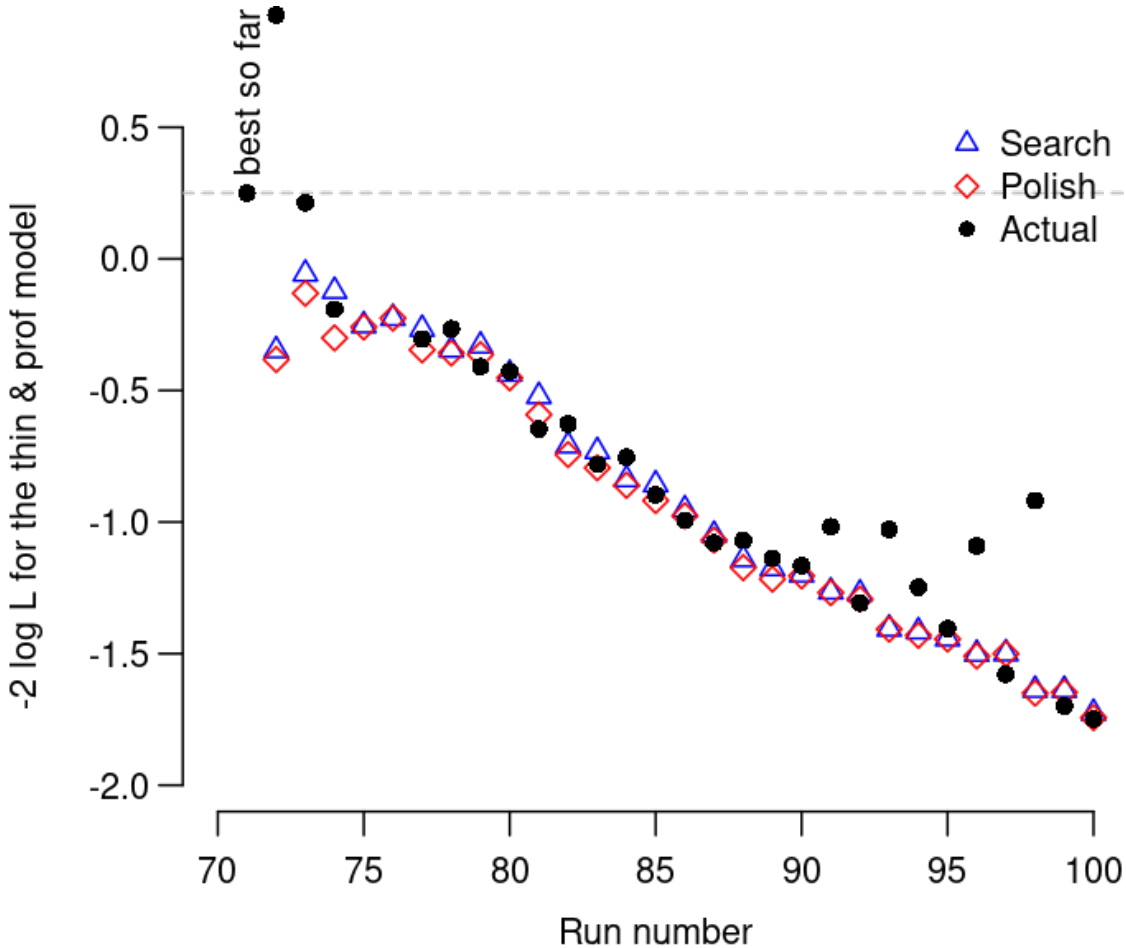

Second phase of runs

Original continues with Downhill Simplex. Thin & prof switches to Bayesian optimization.

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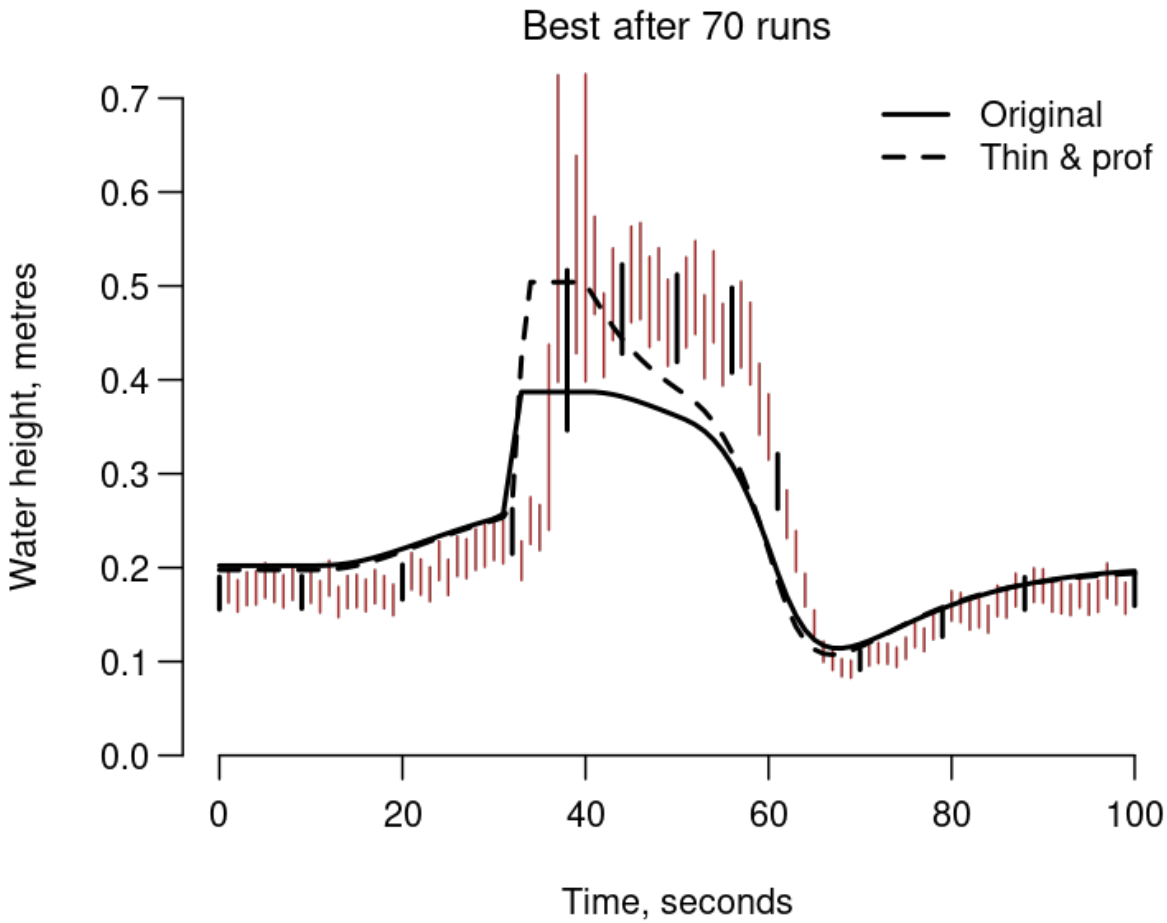

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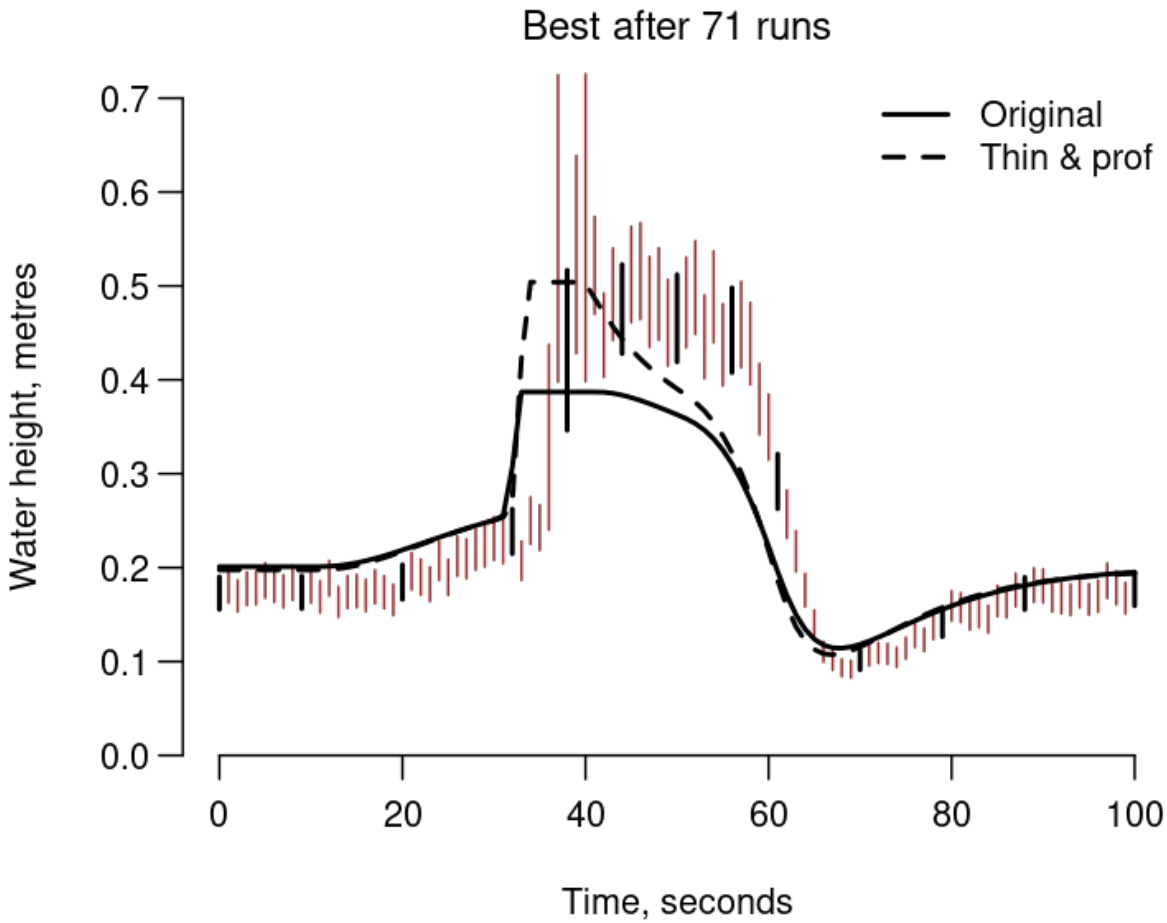

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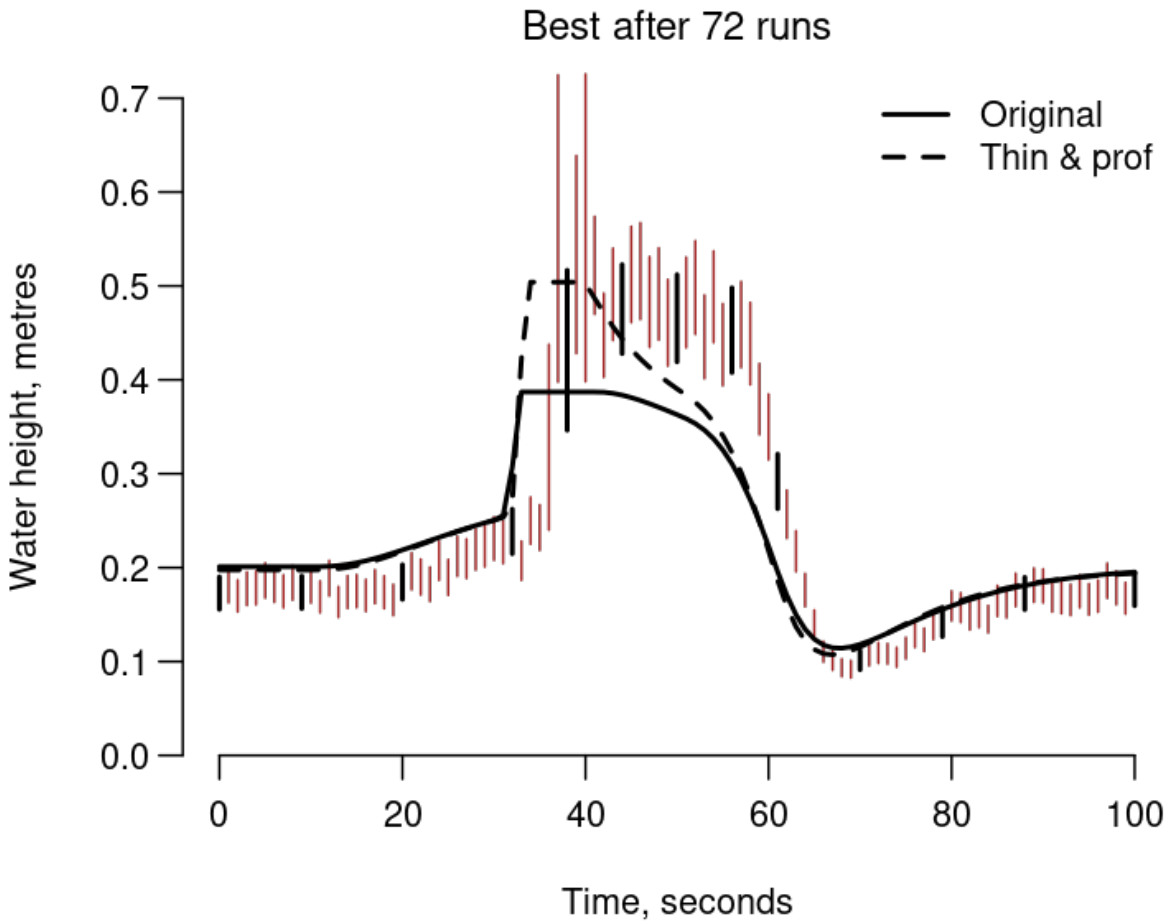

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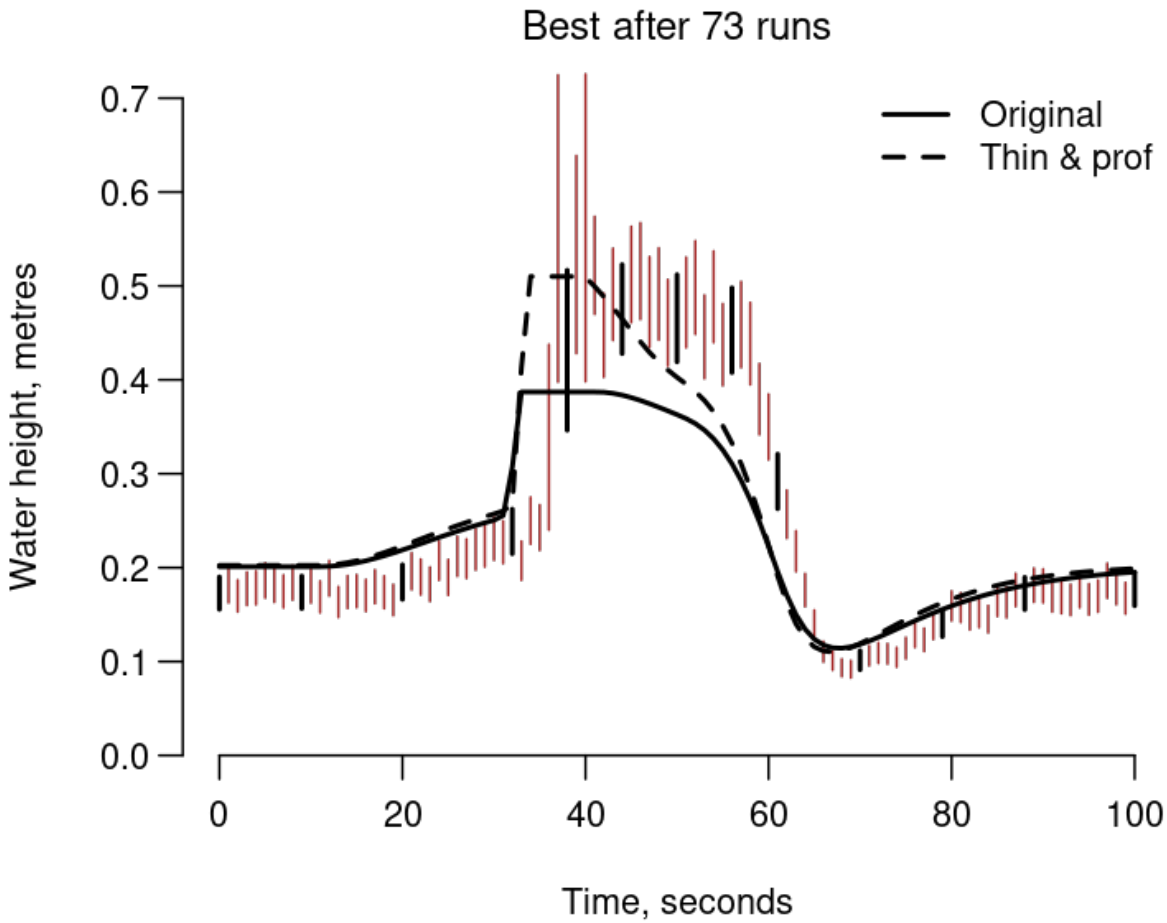

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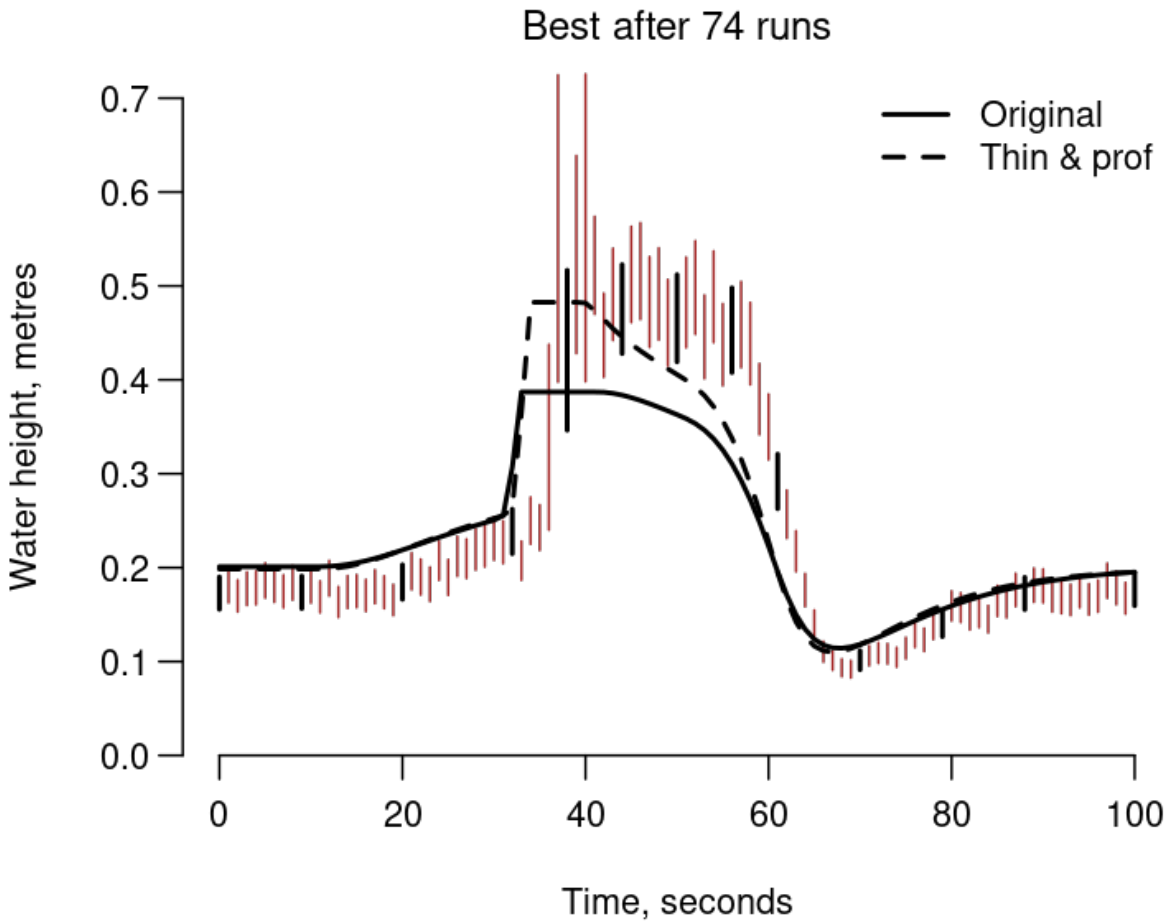

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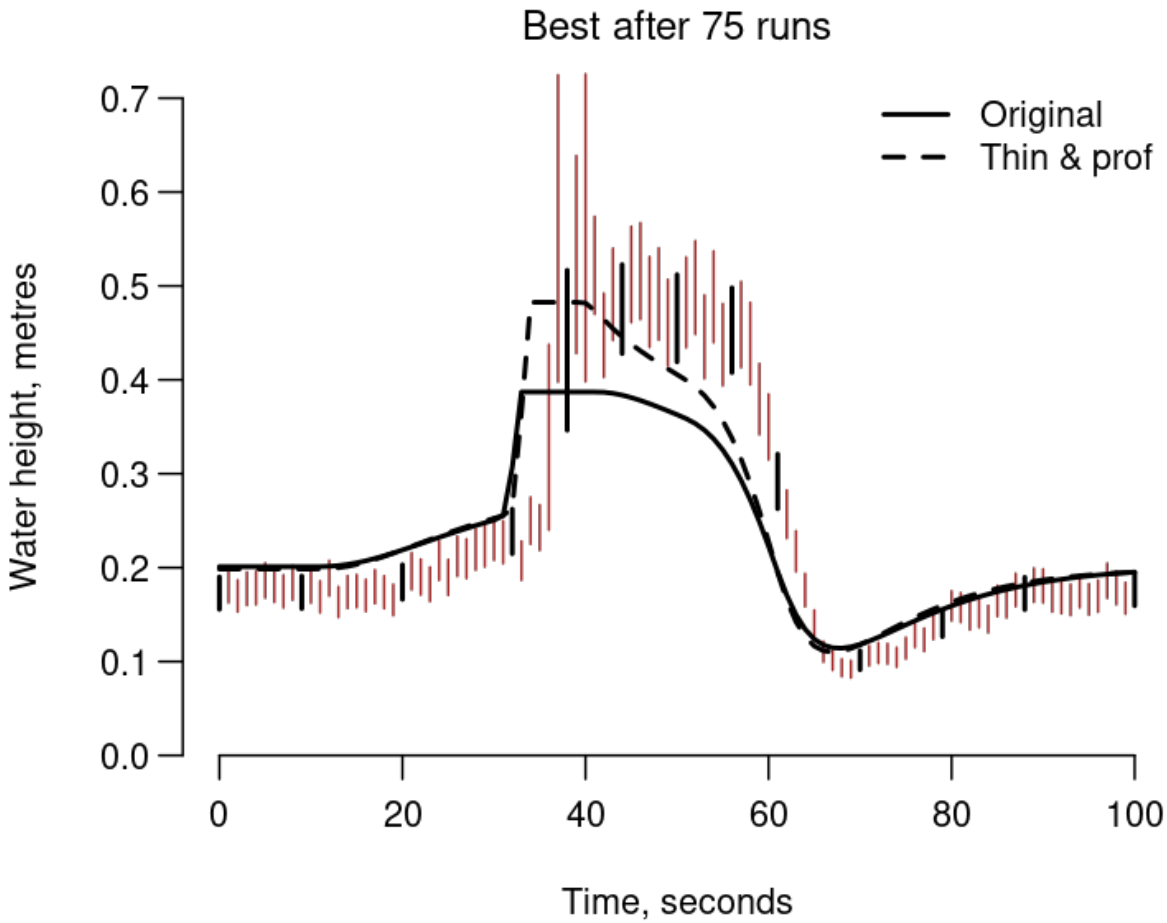

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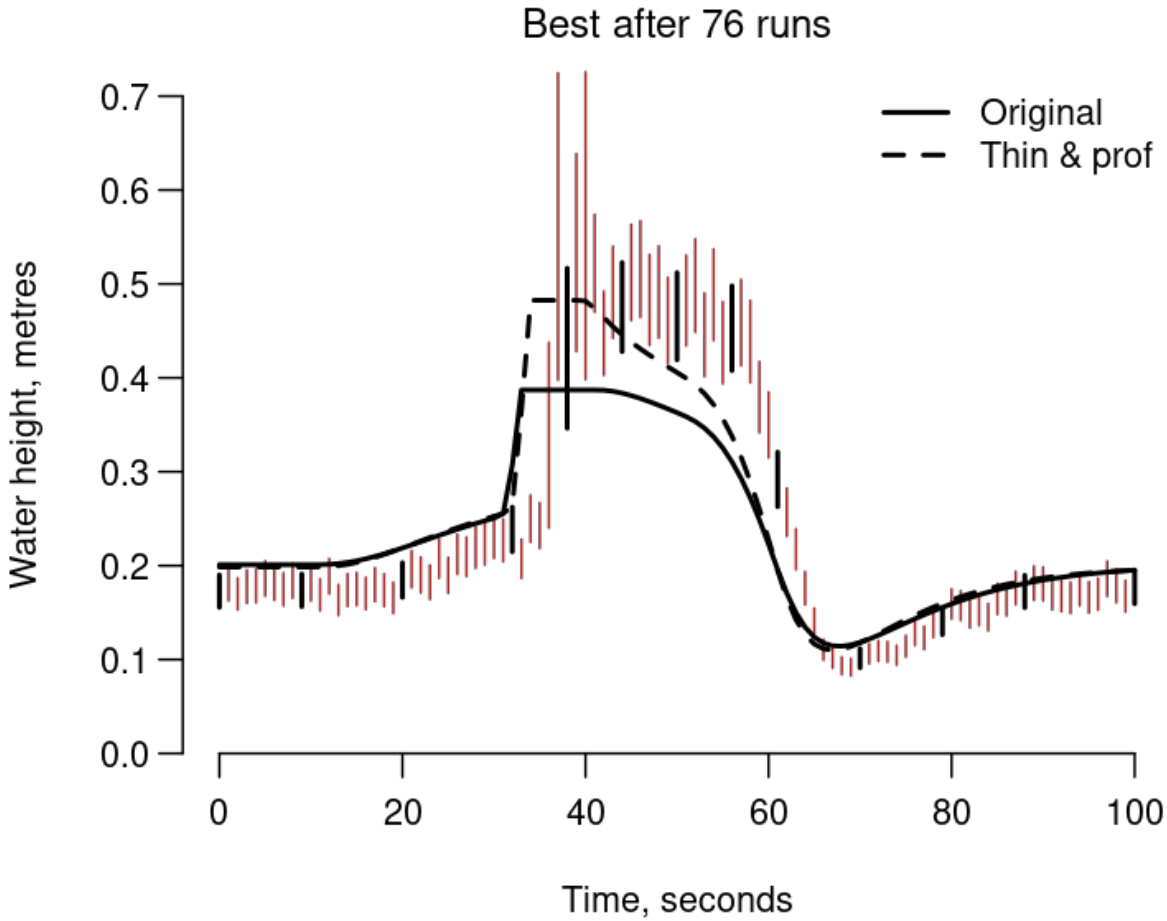

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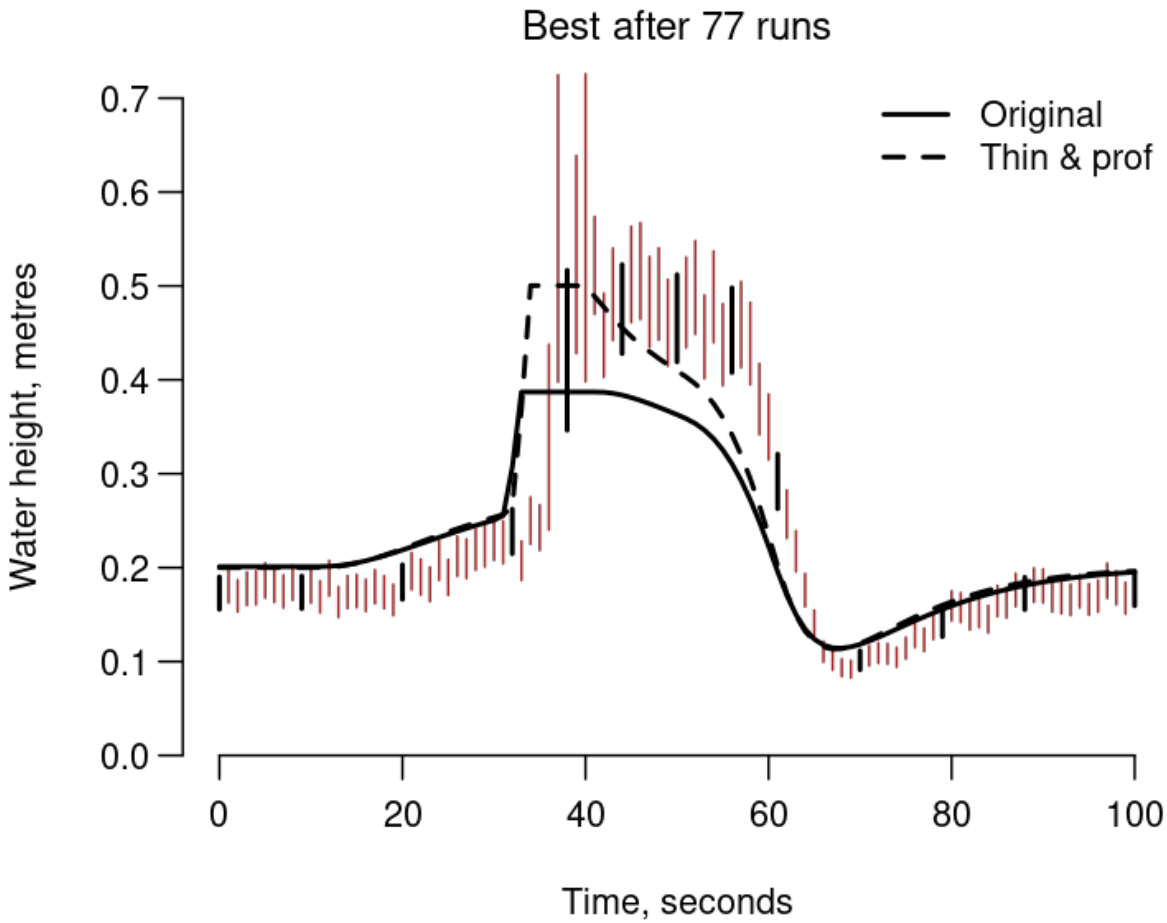

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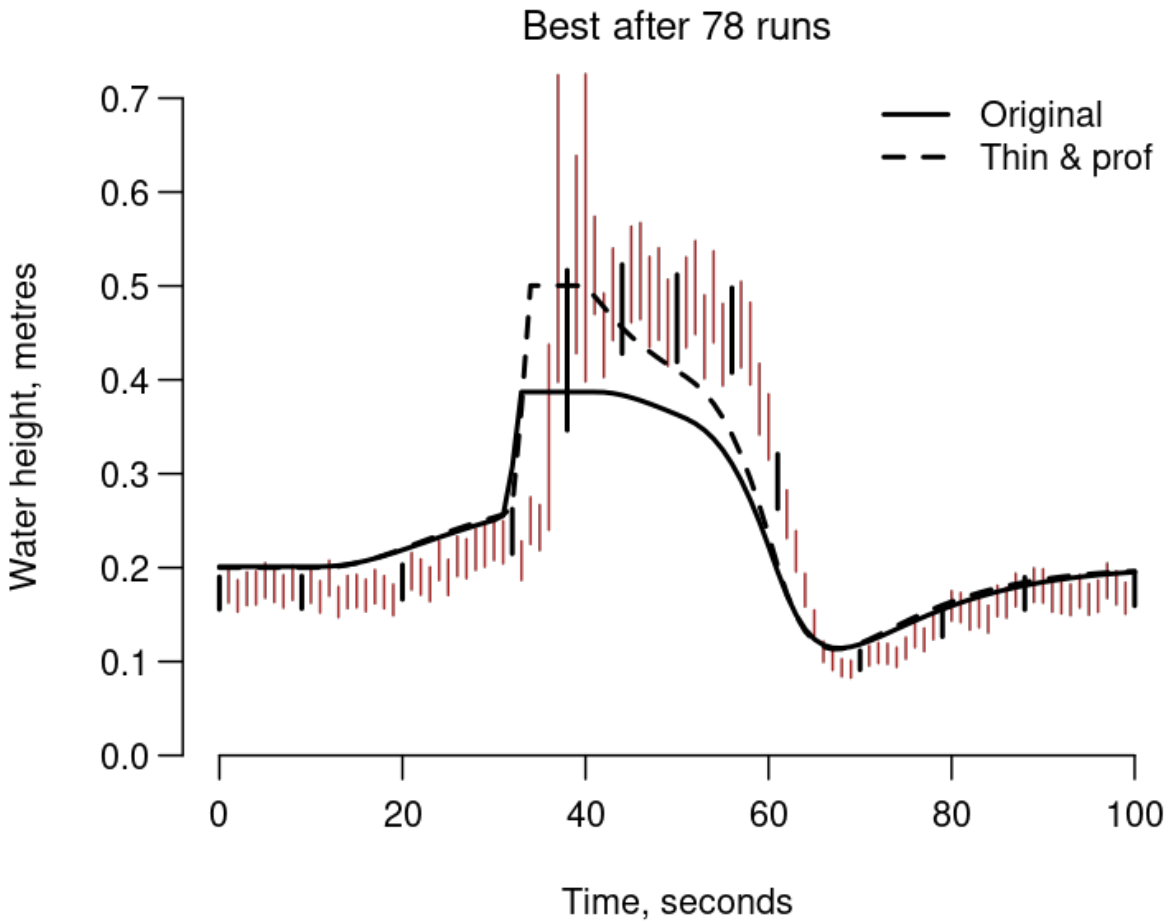

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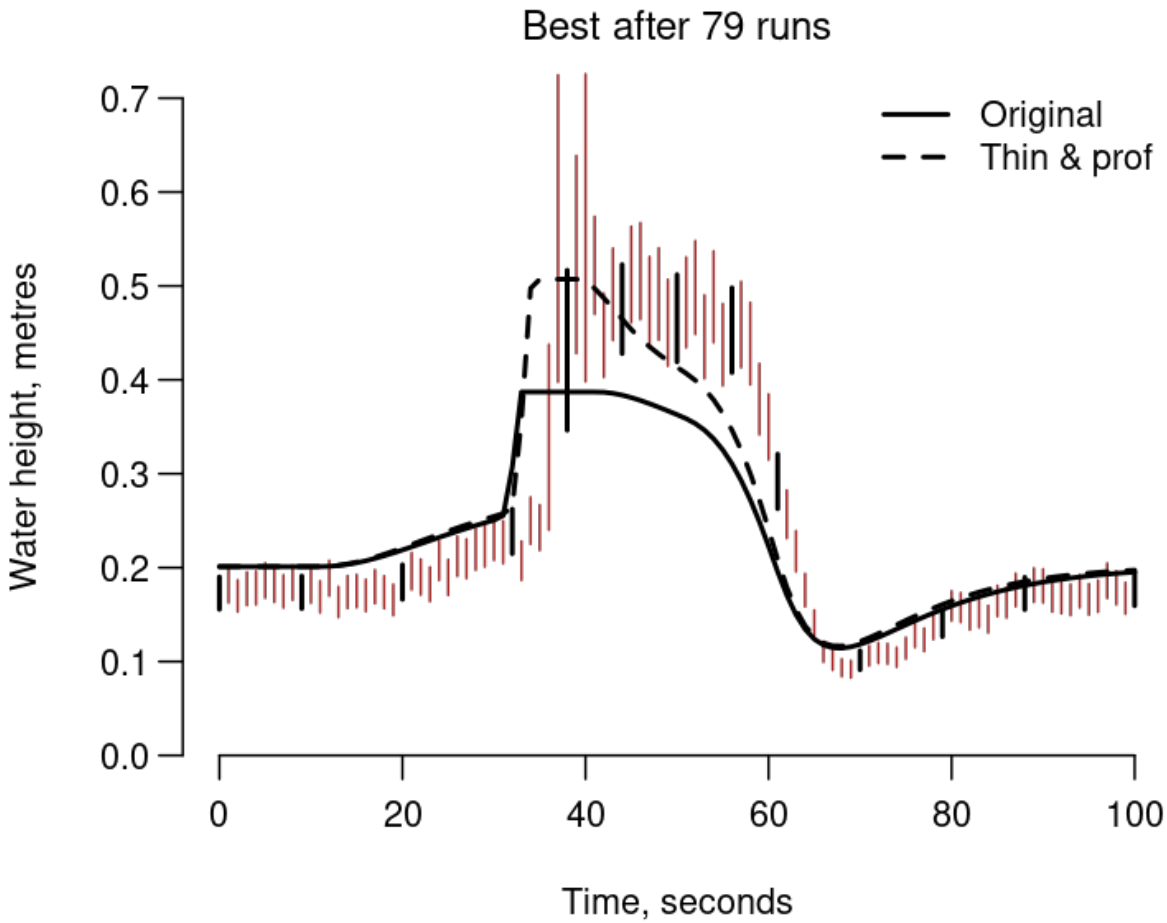

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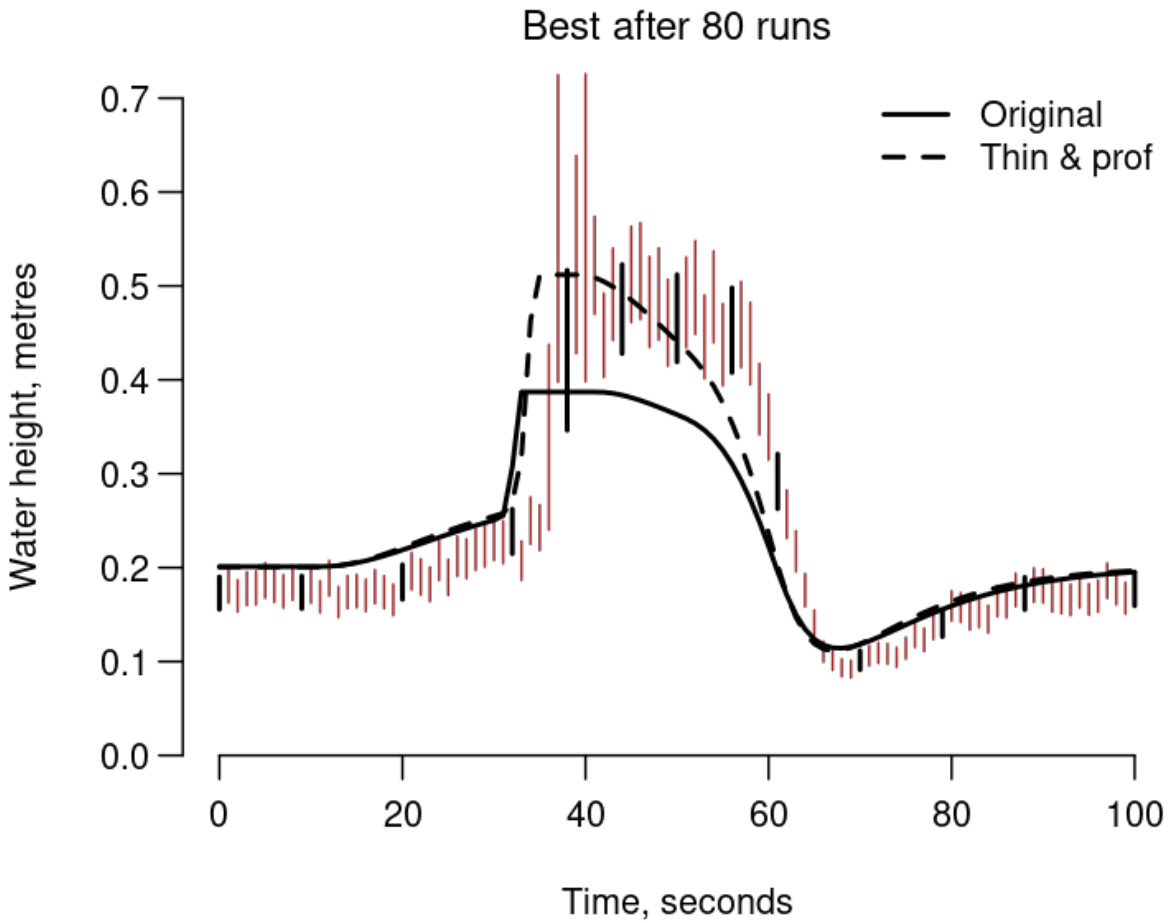

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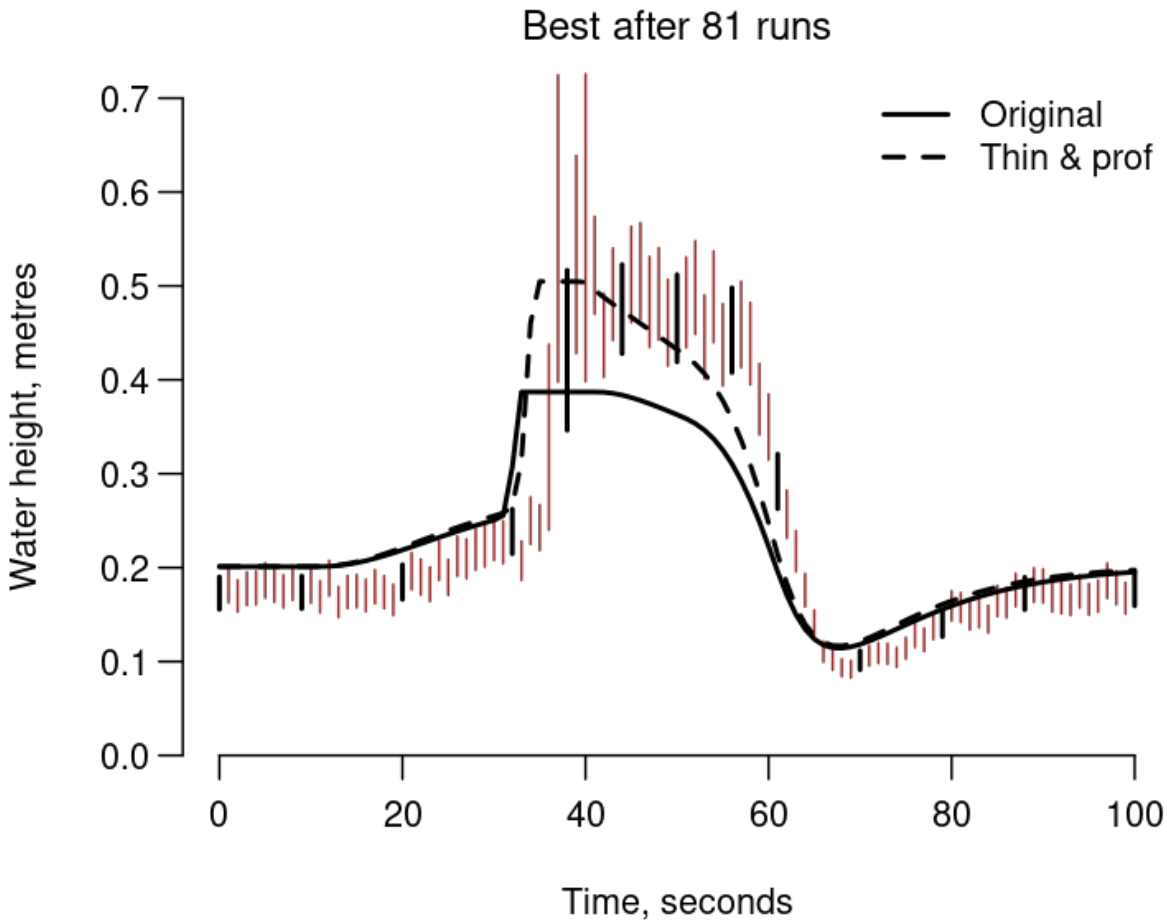

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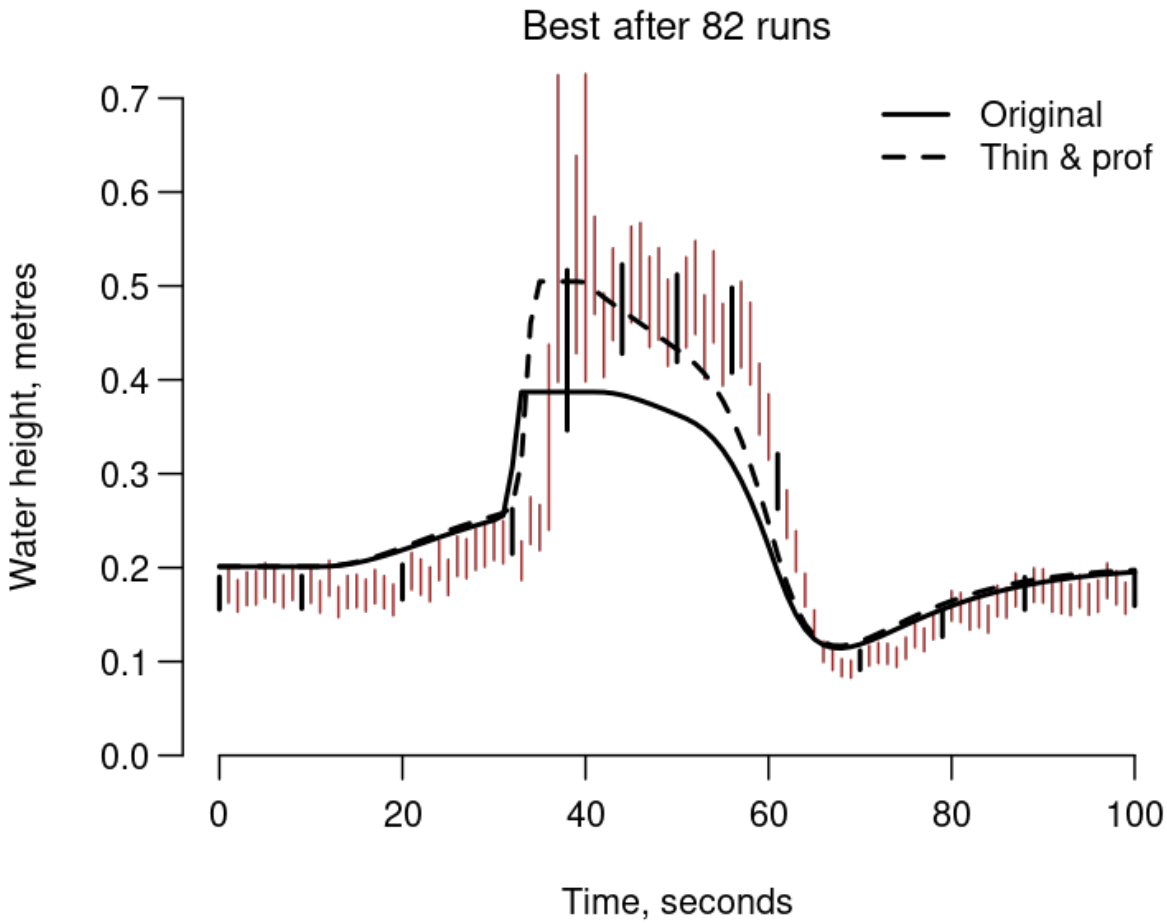

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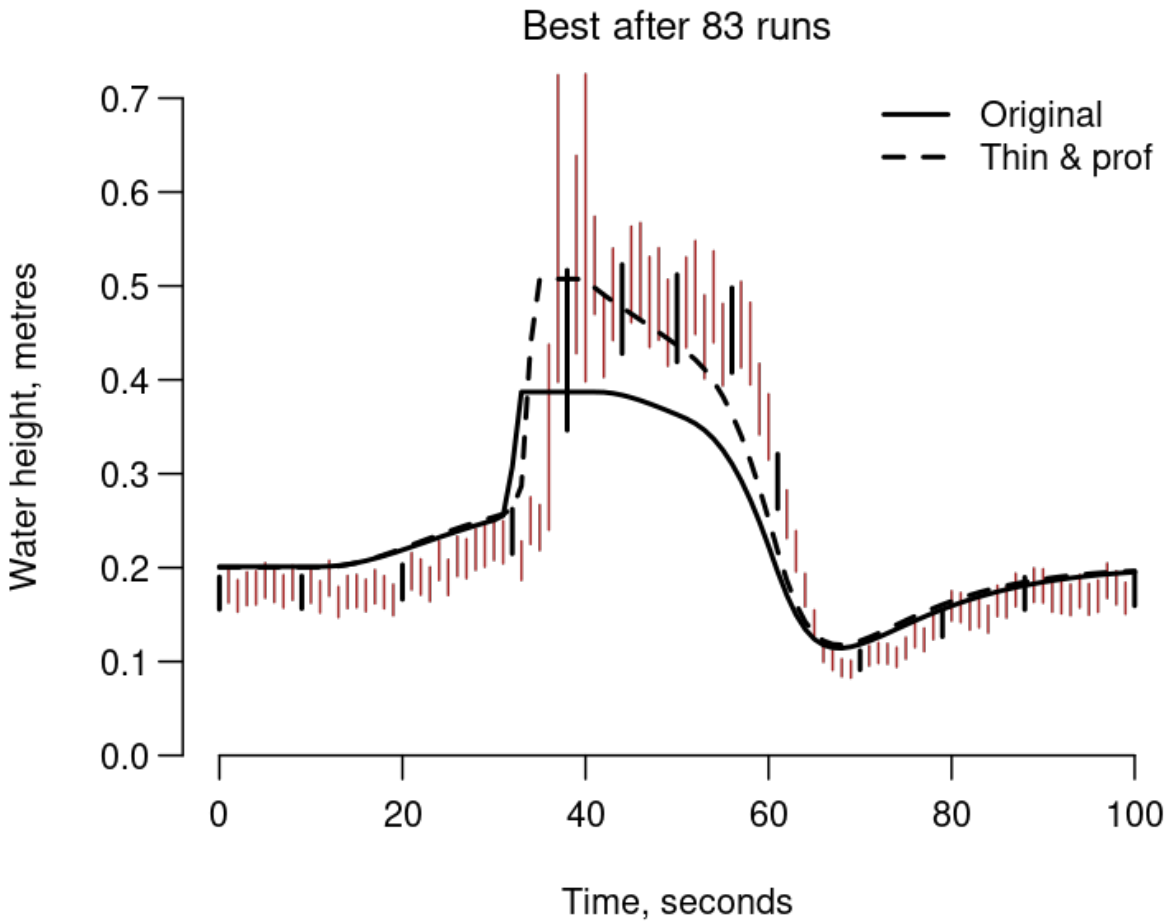

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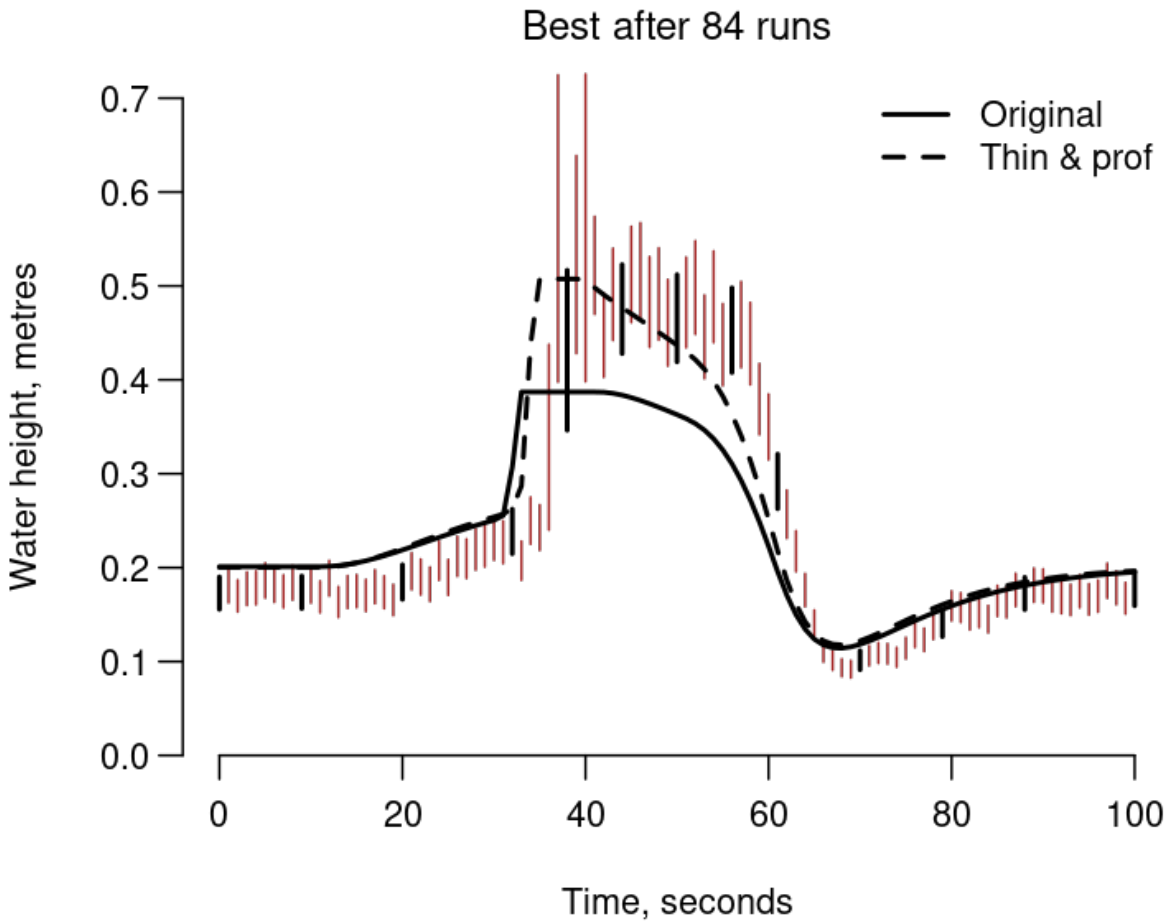

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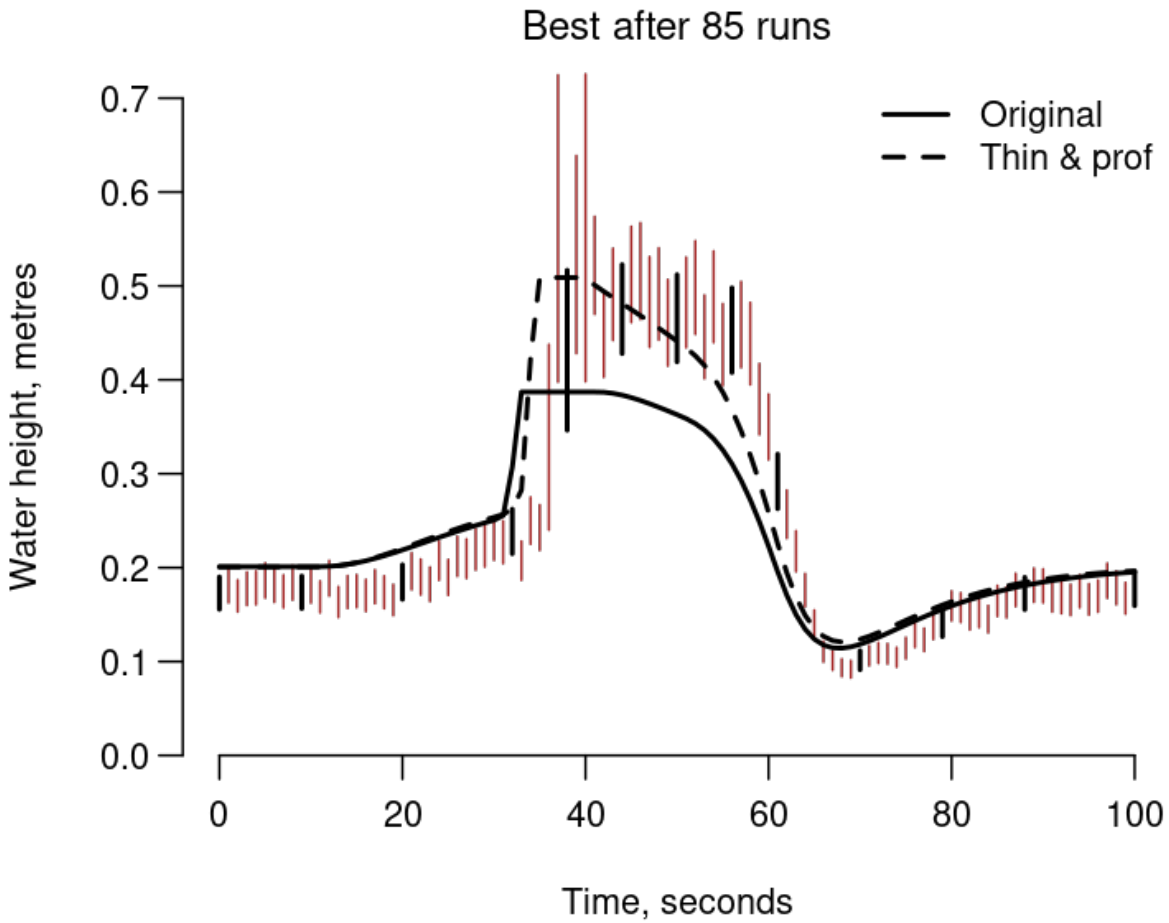

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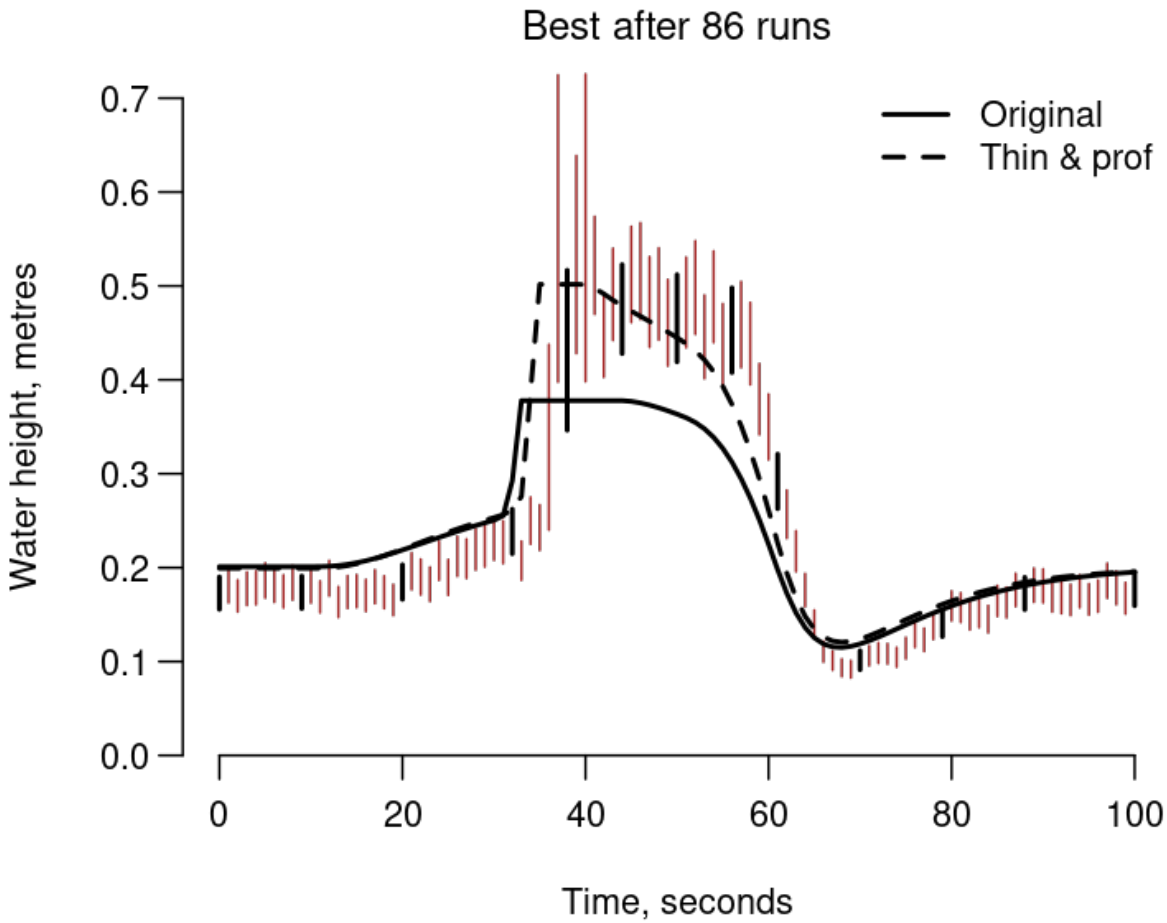

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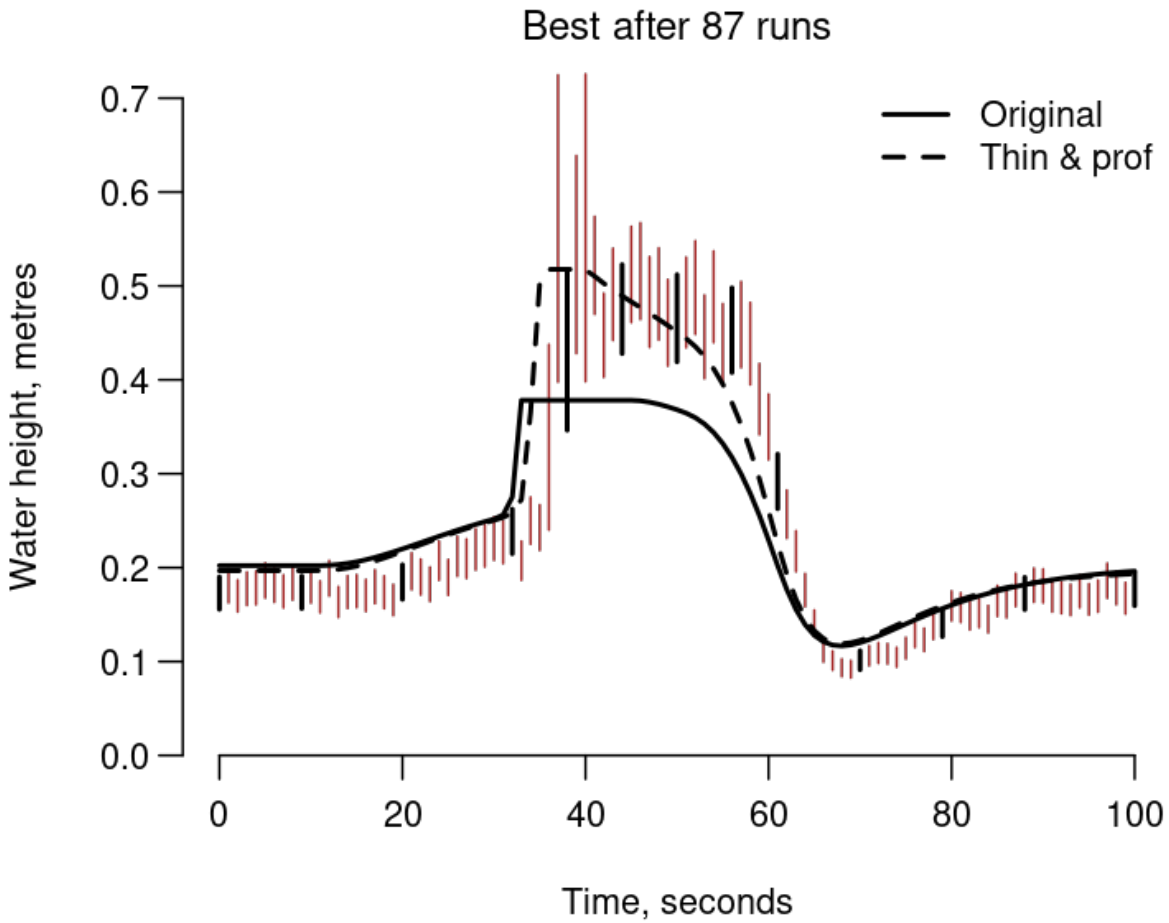

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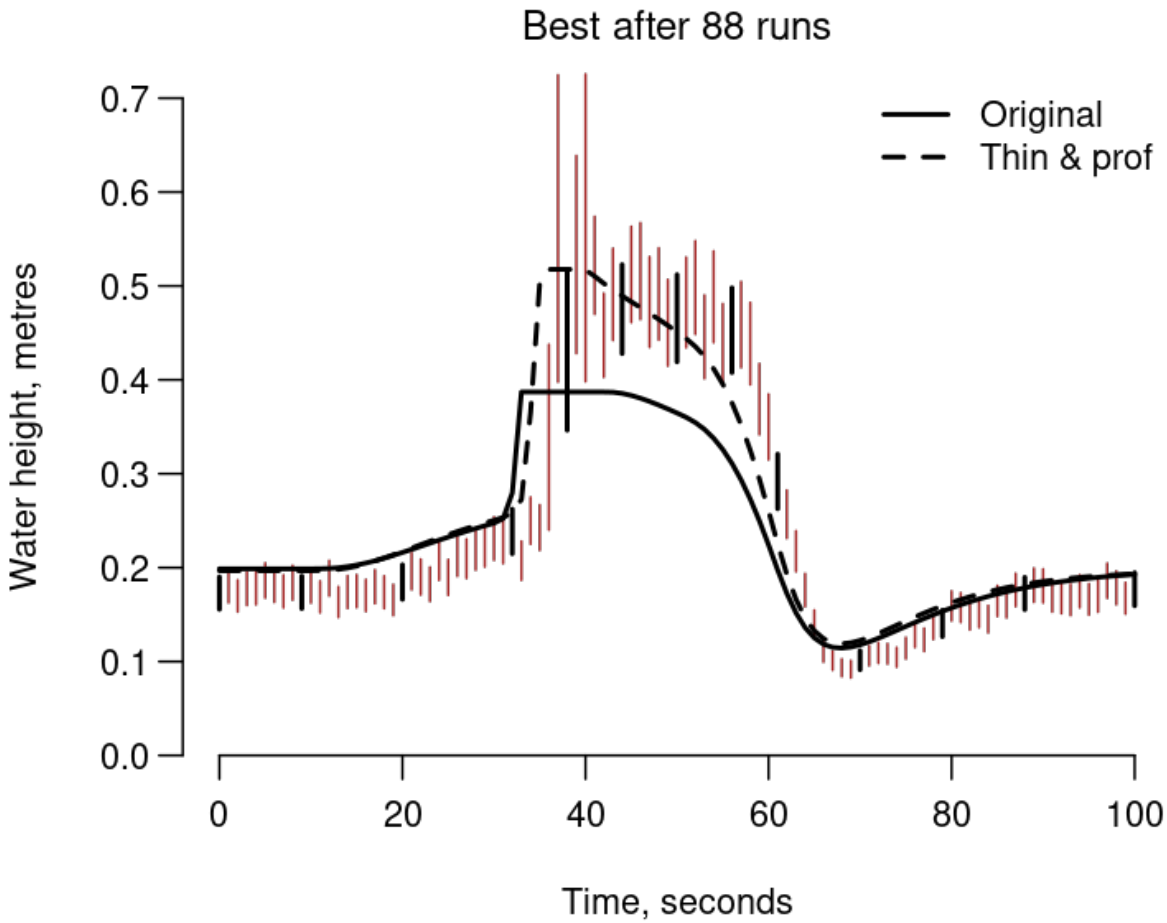

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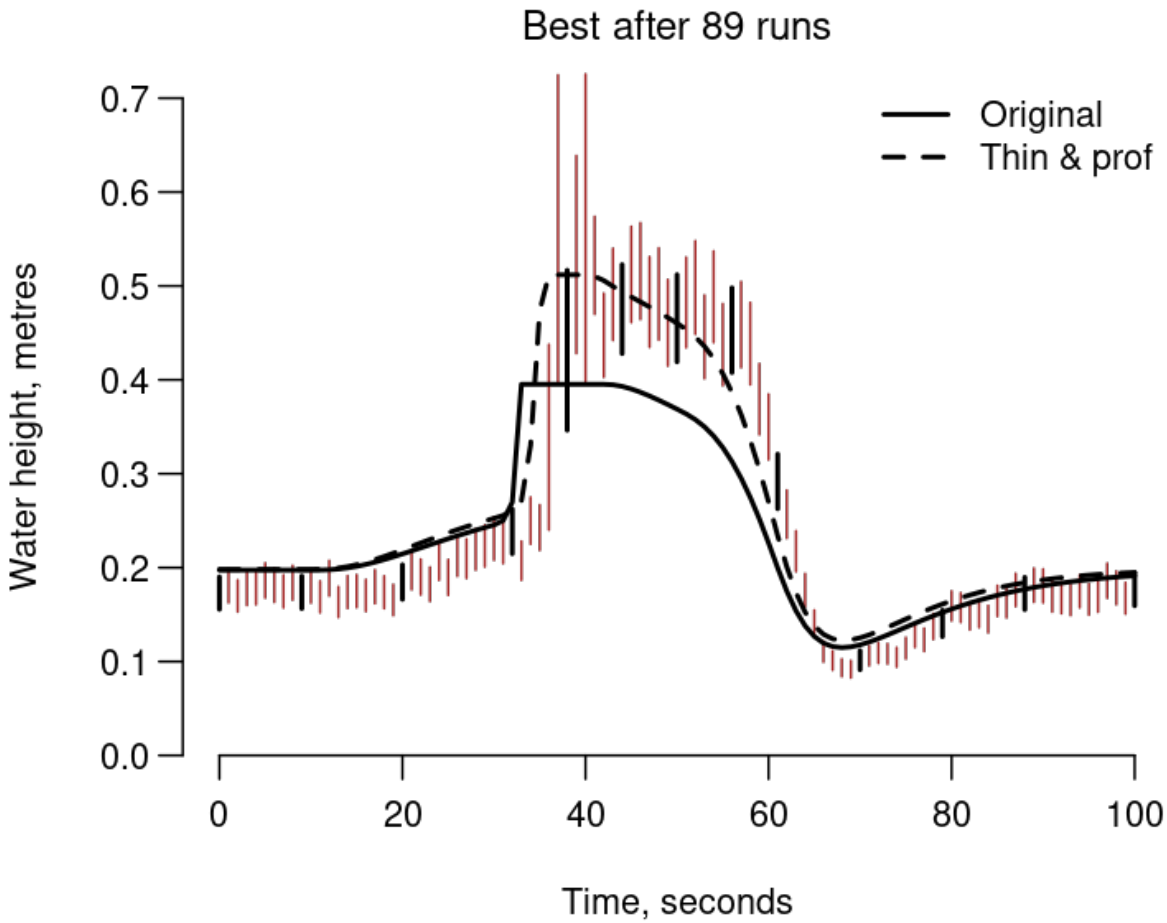

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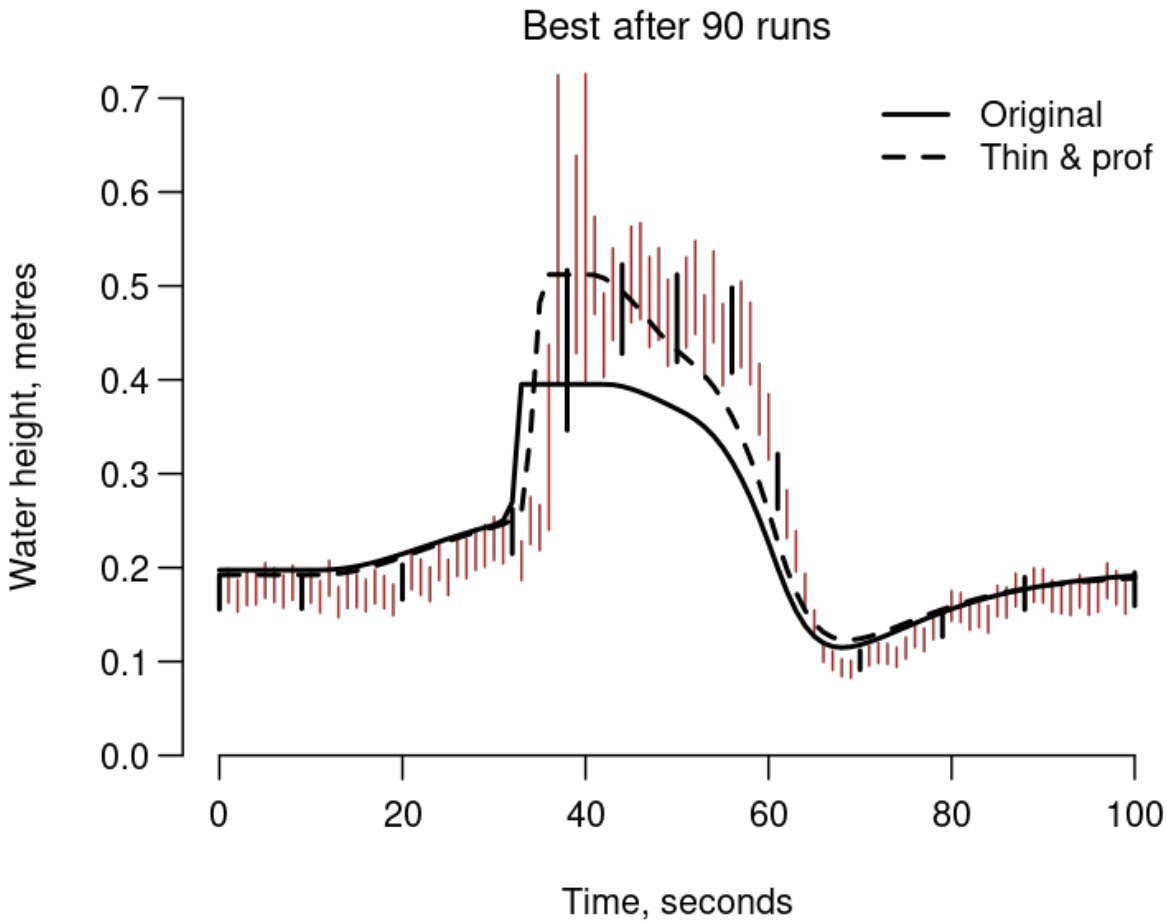

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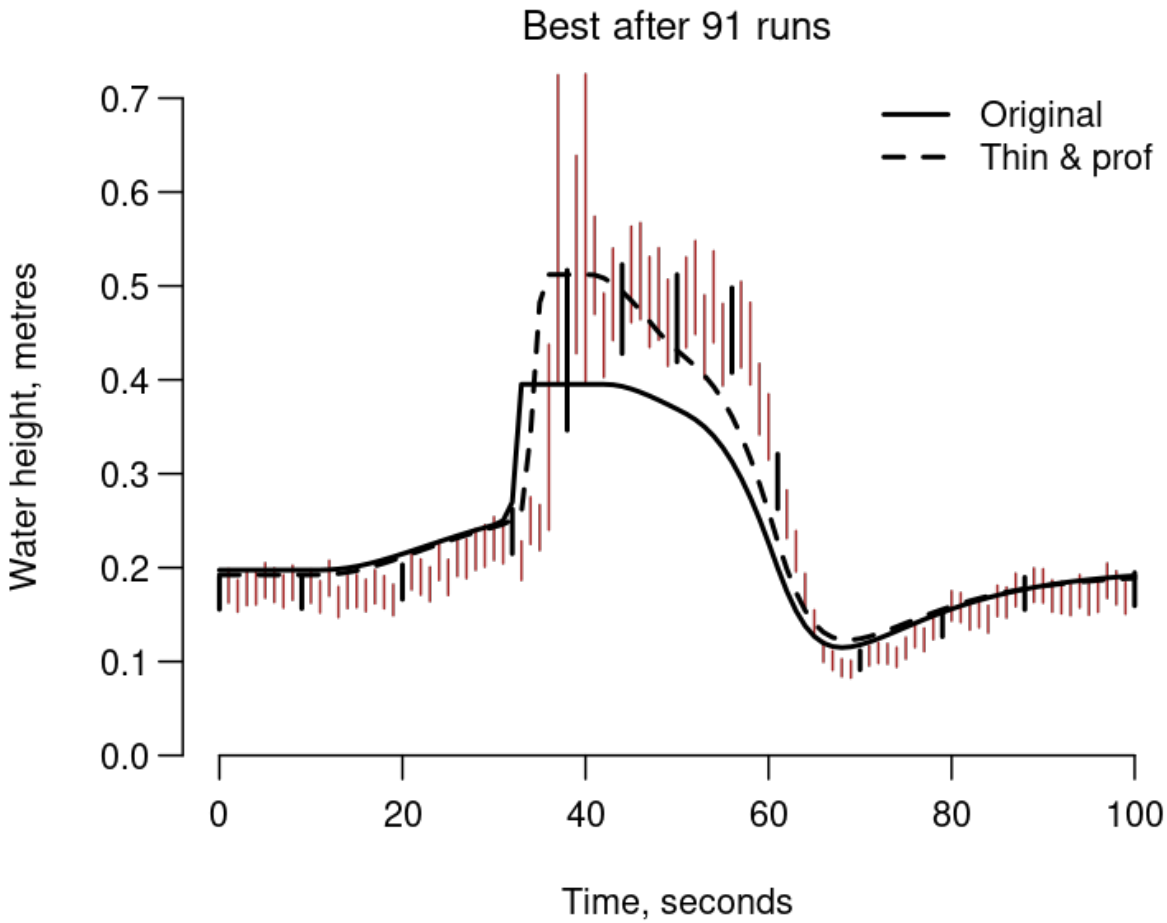

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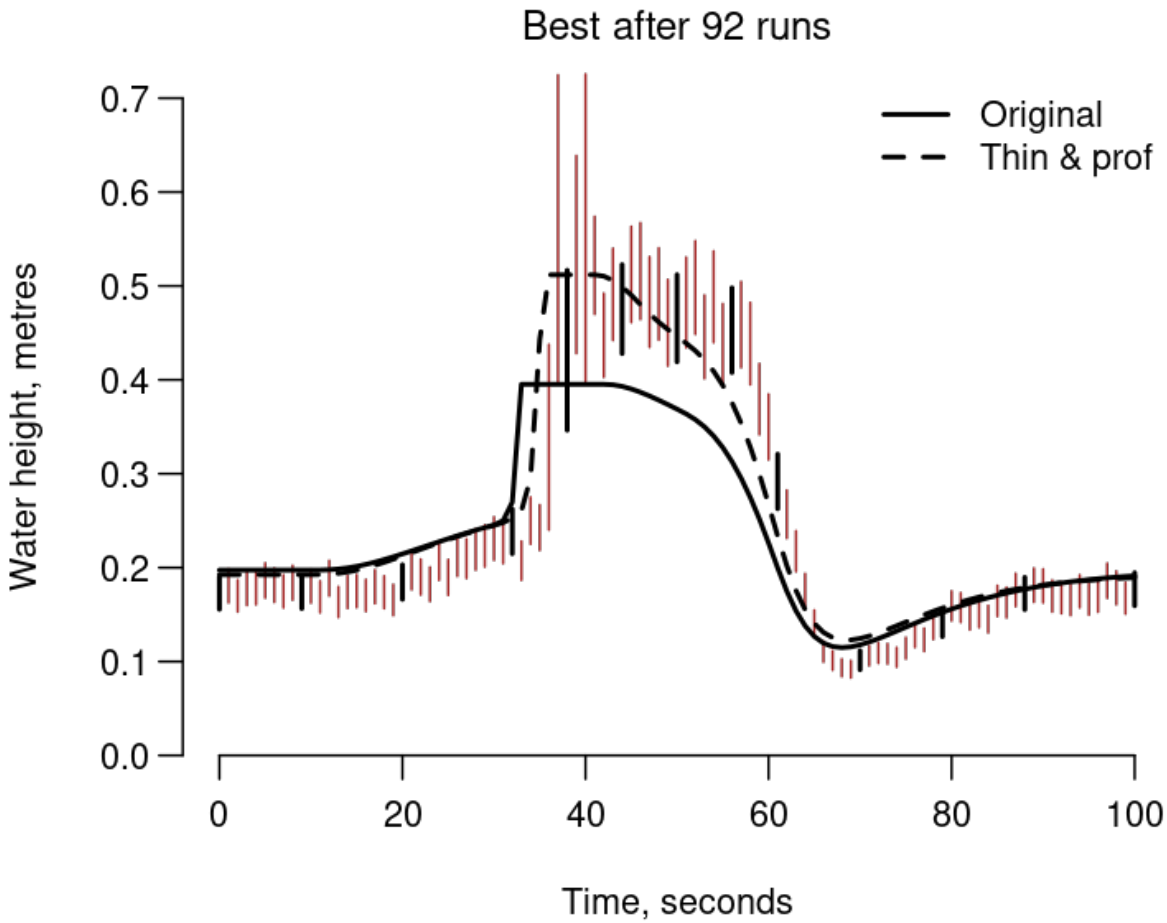

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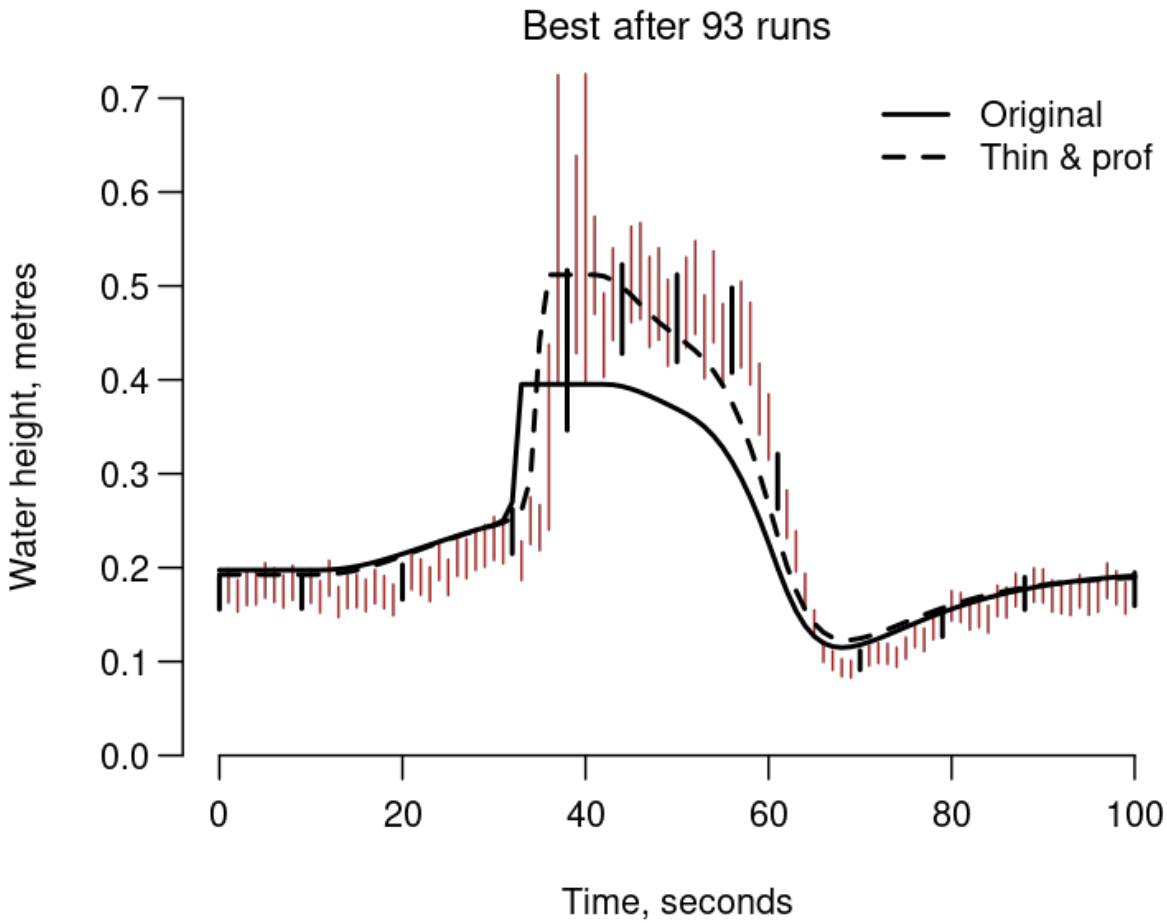

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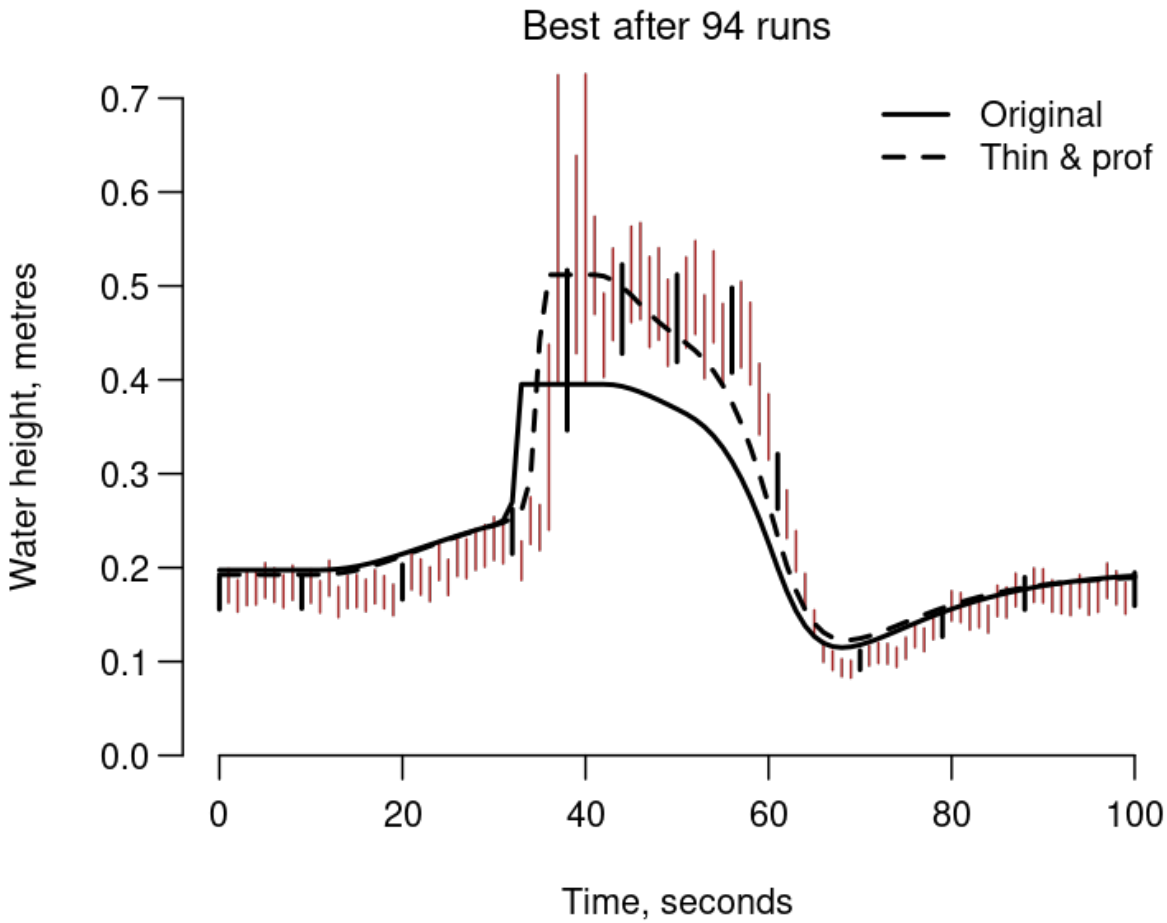

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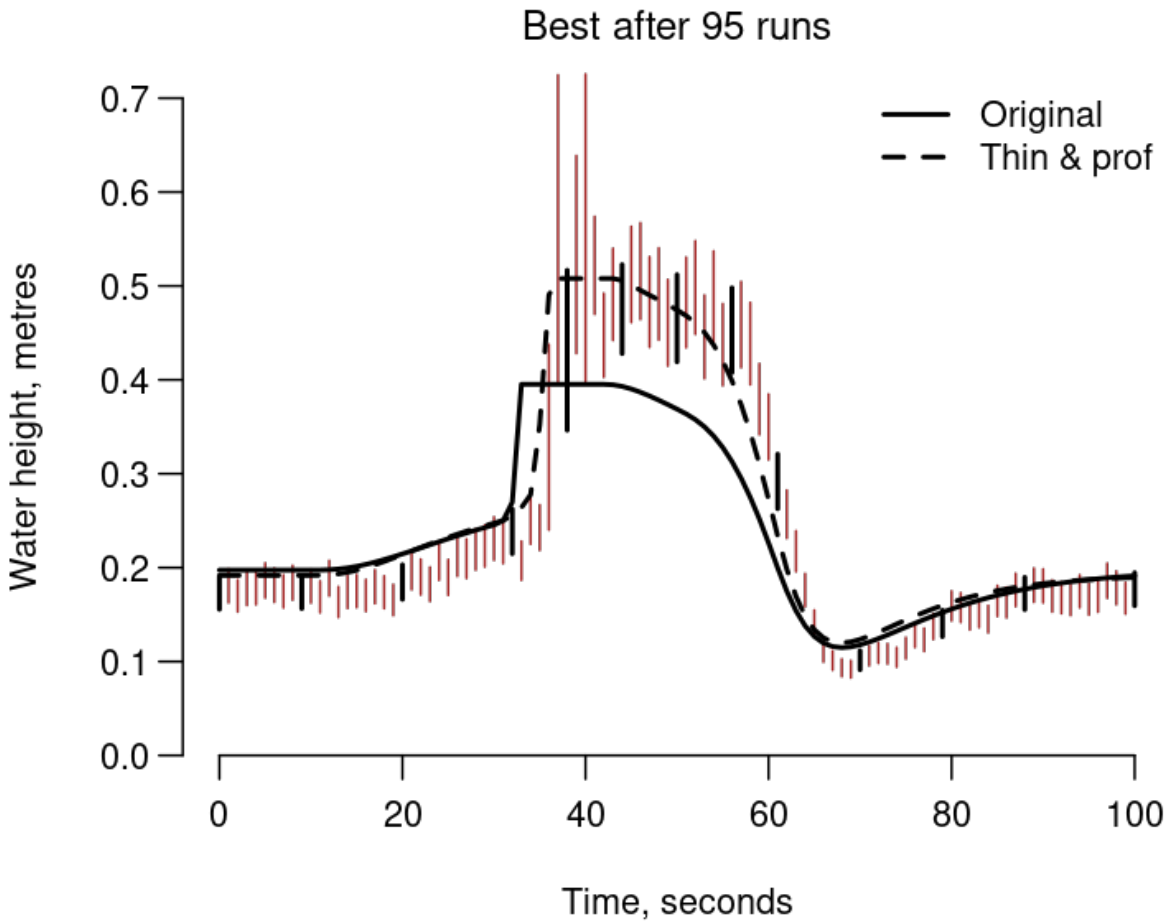

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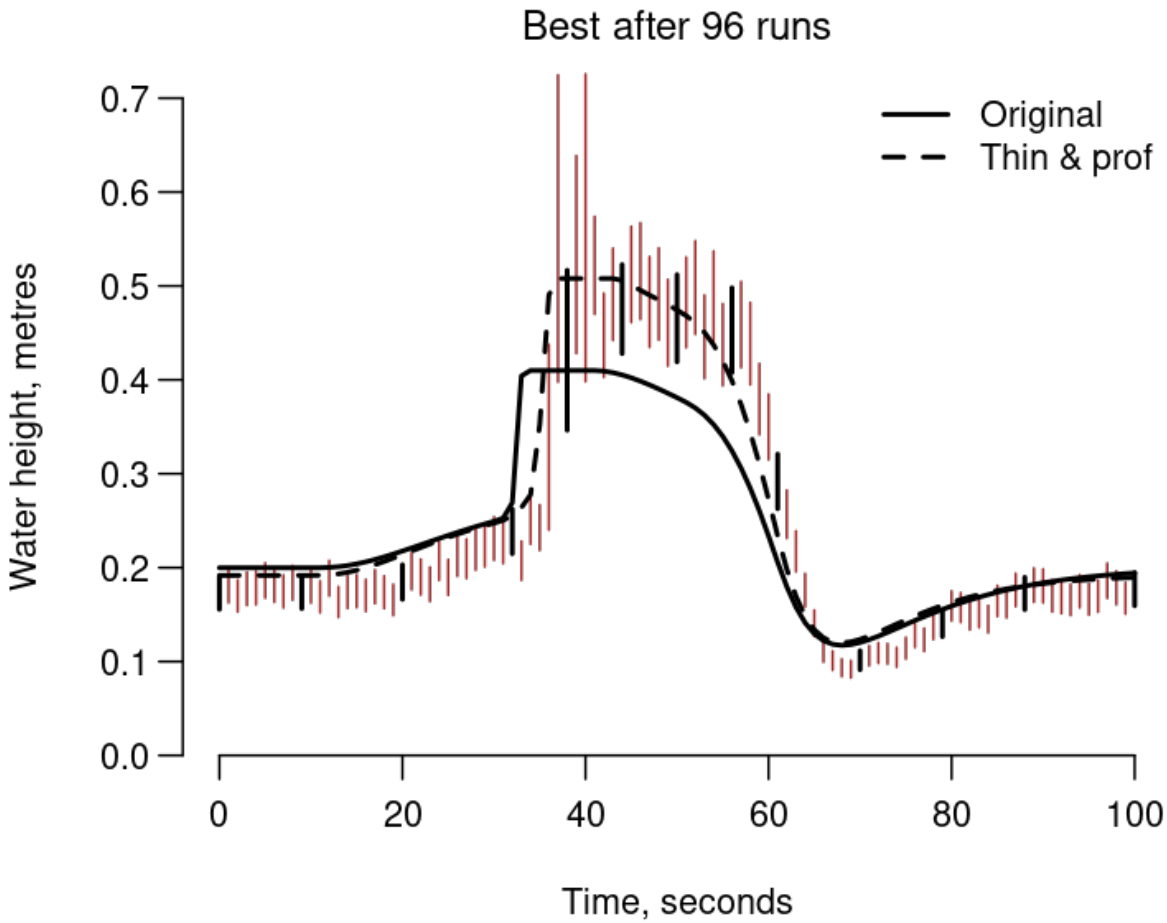

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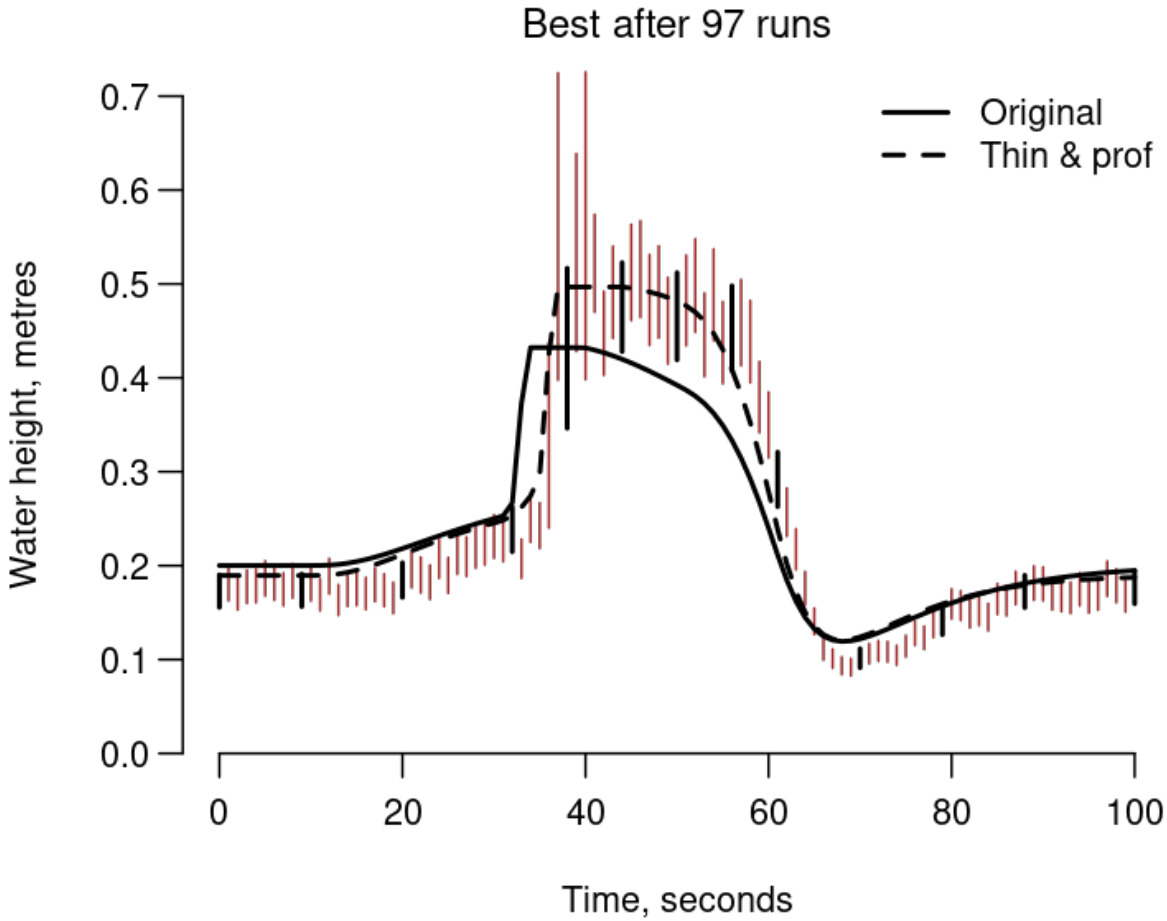

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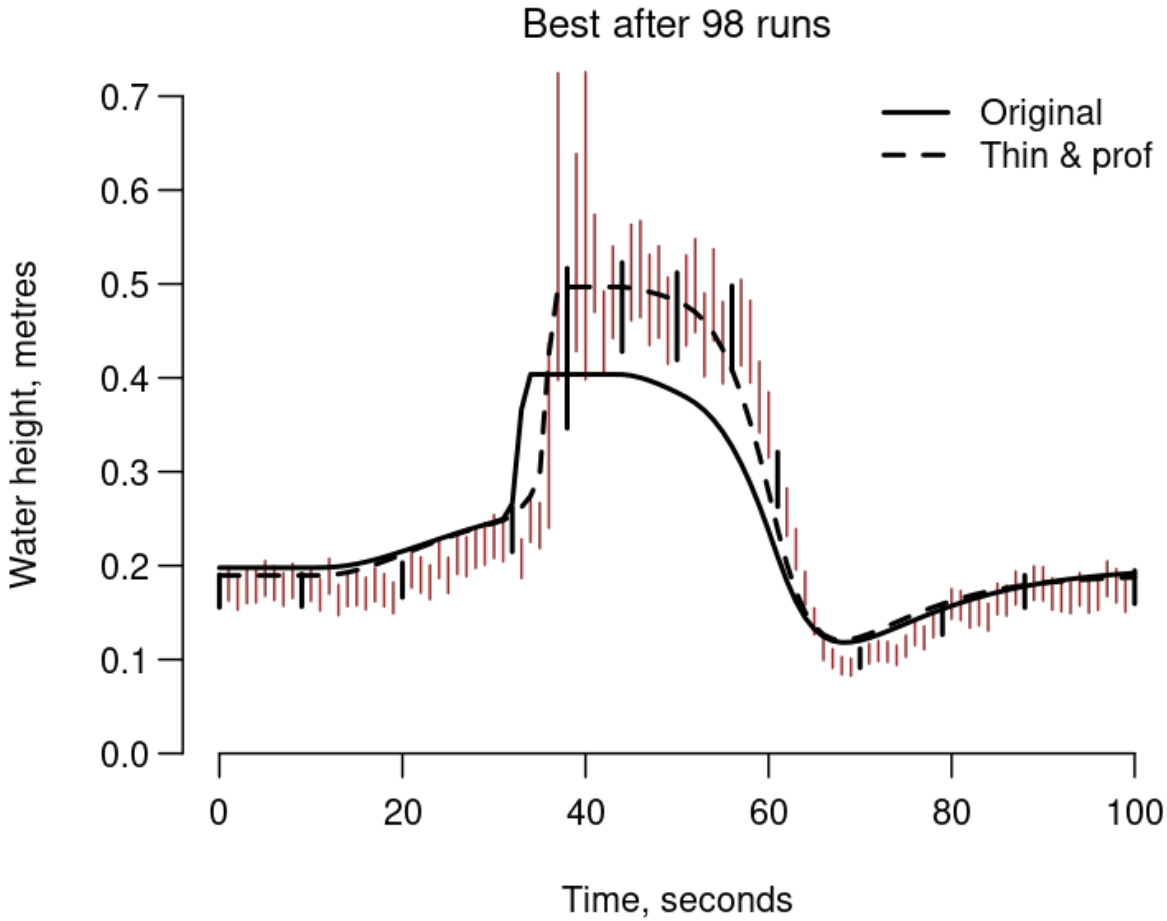

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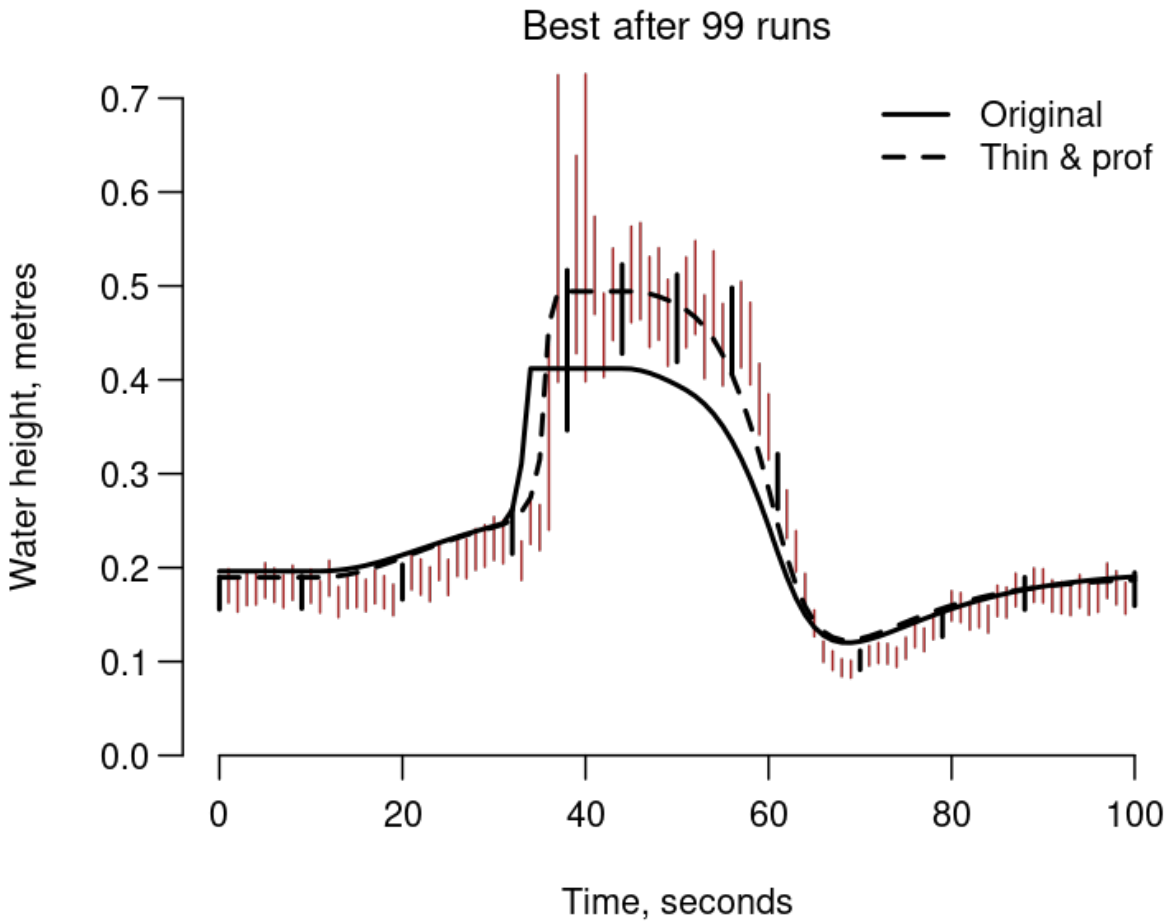

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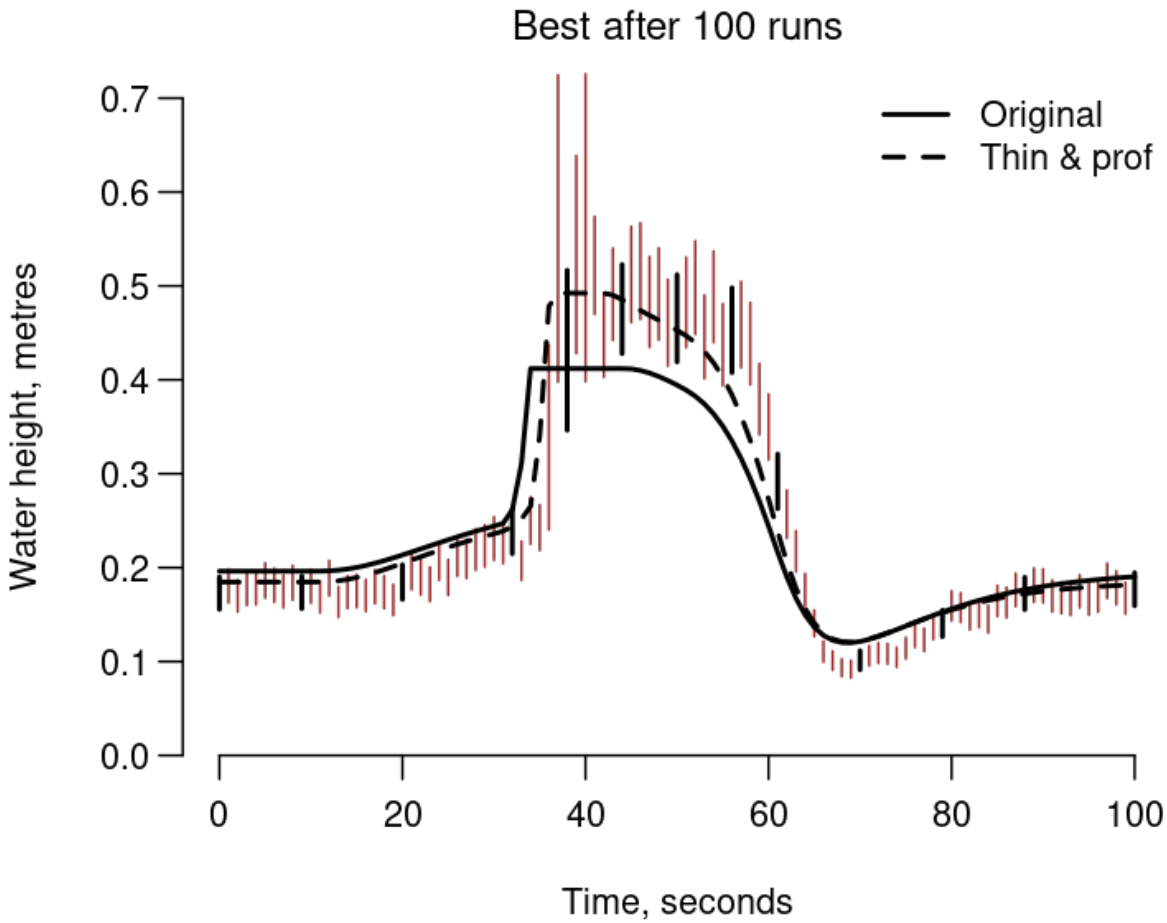
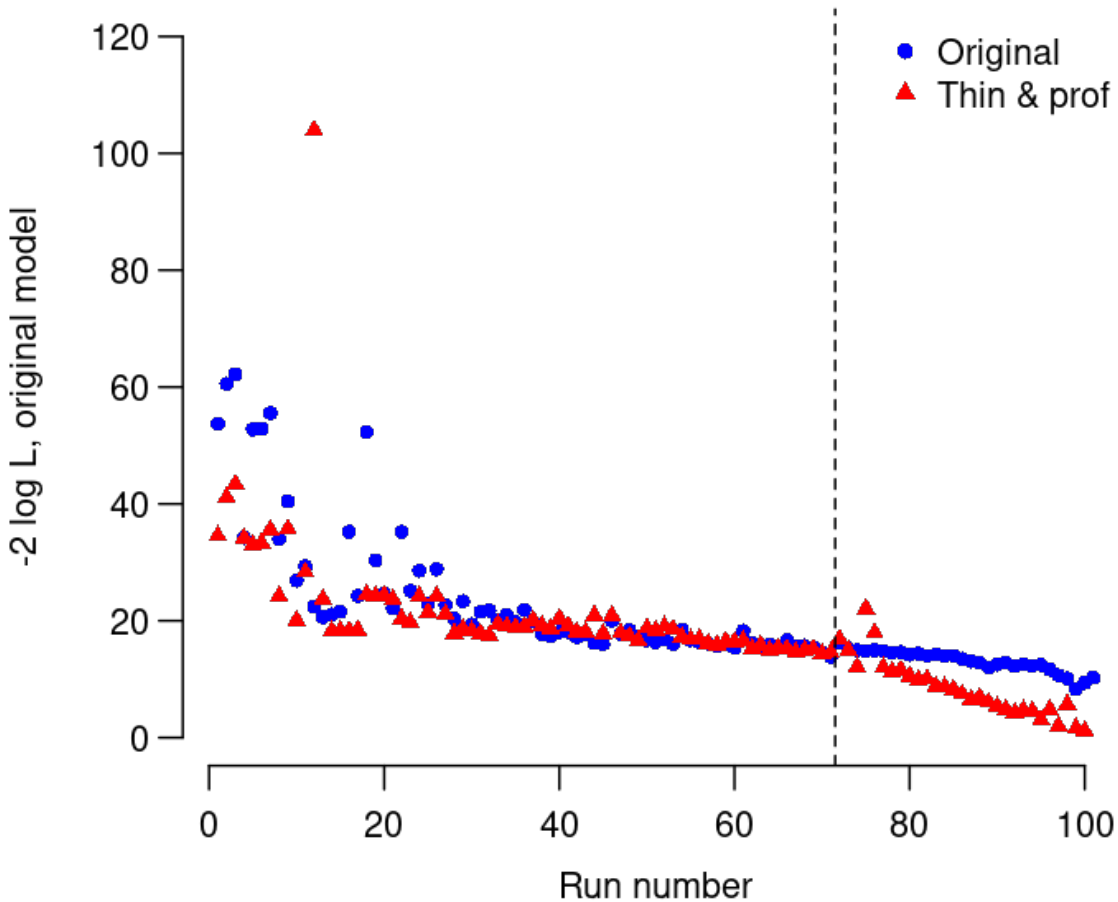


A gratifying result

The optimized thin & prof model typically performs better than the optimized original model, *even according to the original model log-likelihood* (α plugged in).



Extensions

Other structural outputs; e.g., spatial

Exactly the same approach: thin and profile.

Two or more time-series

Need to choose one of:

1. Same α and κ for both/all time-series?
2. Different α, same κ?
3. Same α, different κ? (this one seems odd)
4. Different α, different κ?

Prediction

As well as θ^*, need to carry information about α and κ through into the prediction: possibly just plug-in. We get pointwise approximate 95% confidence intervals for the predicted time-series under new forcing.

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4. We switch to Bayesian optimization to finish the job efficiently, emulating the log-likelihood with a Gaussian Process, and using adaptive search.
5. While there are no guarantees, we hope this approach produces a better estimate of the best input, for the same number of simulator runs.

T H E E N D

Time for questions and discussion.

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The 'best input' model

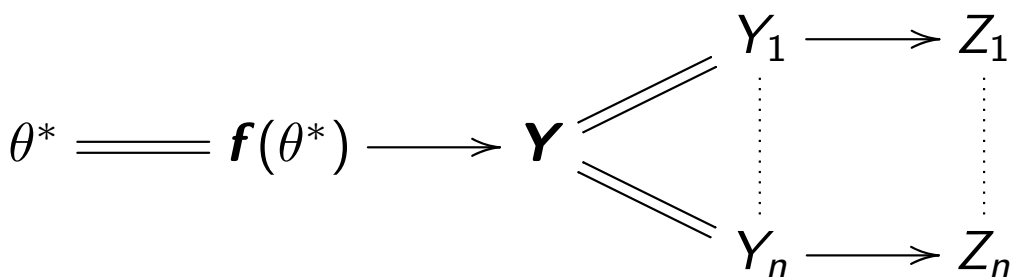
See Goldstein and Rougier (2004, 2009), Rougier (2007), Rougier and Goldstein (2014). This is the ubiquitous model for linking simulator runs, the system, and observables.

- There is a 'best' value of the parameters, θ^*, such that $\boldsymbol{Y} \perp\!\!\!\perp \theta^* \mid \boldsymbol{f}(\theta^*)$, or, as a DAG,

$$\theta^* \Longrightarrow \boldsymbol{f}(\theta^*) \longrightarrow \boldsymbol{Y}$$

  where $\Longrightarrow$ denotes a deterministic edge.
  If we knew θ^*, we'd run the simulator just once to predict $\boldsymbol{Y}$, no matter what the value of θ^* happened to be.

- Also ubiquitous is to add on a simple error structure for the observables



Return

Can we do better? (cont)

- We can profile out α directly

$$L_{\mathcal{J}}(\theta, \kappa) := \max_{\alpha \in [-\alpha_{\max}, \alpha_{\max}]} L_{\mathcal{J}}(\theta, \alpha, \kappa) = L_{\mathcal{J}}(\theta, \tilde{\alpha}(\theta, \kappa), \kappa)$$

where

$$\hat{\alpha}(\theta, \kappa) := \sum_{i \in \mathcal{J}} w_i (z_i^{\text{obs}} - f_i(\theta)), \quad w_i := \frac{(\kappa^2 + \sigma_i^2)^{-1}}{\sum_j (\kappa^2 + \sigma_j^2)^{-1}}$$

$$\tilde{\alpha}(\theta, \kappa) := -\alpha_{\max} \vee \hat{\alpha}(\theta, \kappa) \wedge \alpha_{\max}.$$

- Then we can profile out κ using a 1D numerical optimization,

$$L_{\mathcal{J}}(\theta) := \max_{\kappa \in [0, \kappa_{\max}]} L_{\mathcal{J}}(\theta, \tilde{\alpha}(\theta, \kappa), \kappa).$$

- Computing $L_{\mathcal{J}}(\theta)$ only requires one run of the simulator, plus a quick numerical optimization; i.e., its cost is comparable to computing the original $L(\theta)$.

Can we do better? (cont)

- The bounds on α and κ in the profile likelihoods are not just for show. Profile likelihood is a notoriously tricky approach for estimating variances, and we want to keep α and κ fairly close to their default values of 0 and 0 in order to stop the profile running off to a statistical but not plausible solution.

  I have been using

$$\alpha_{\max} = \kappa_{\max} = 2\,\text{median}\{\sigma_1, \ldots, \sigma_n\}.$$

- In summary, we have (at least) two approaches:

  1. Original model, which is just the scaled sum of squared deviations over all outputs, i.e. no discrepancy.
  2. Thin & prof model, where the outputs have been thinned, and the discrepancy parameters have been profiled out.

Return

Bayesian optimization (cont)

A myopic adaptive approach (simple, room for improvement):

0a. Find the bounding box of all inputs so far, $\mathcal{B}$.

0b. Expand by 10% from the centroid to give $\mathcal{B}^+$ (don't overshoot the parameter limits).

0c. Fill $\mathcal{B}^+$ with a grid to give $\mathcal{S}^+$.

1. Build a GP emulator of ℓ using all runs so far.
2. Evaluate $\mathbb{E}\{\lambda(L_\theta)\}$ at every point in $\mathcal{S}^+$.
3. Improve the best point on $\mathcal{S}^+$ using a quasi-Newton method, staying inside $\mathcal{B}^+$, to give θ^{new}.
4. Run the simulator at θ^{new} and compute the profile likelihood $\ell_{\theta^{\text{new}}}$.
5. If θ^{new} is outside $\mathcal{B}$, go back to 0, otherwise go back to 1.

▸ Return