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# Evaluating loss functions for extreme streamflow predictions

Georgia Papacharalampous, Francesco Marra, Eleonora Dallan, and Marco Borga

✉ [georgia.papacharalampous@unipd.it](mailto:georgia.papacharalampous@unipd.it), [papacharalampous.georgia@gmail.com](mailto:papacharalampous.georgia@gmail.com)



**TESAF**



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# Designing “fit-for-purpose” hydrological models (1)

- **General focus:** Calibration and validation of hydrological models
- **Core concept:**

$$z = \mathcal{H}\mathcal{M}(\mathbf{x}_p; \boldsymbol{\theta})$$

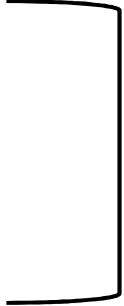
( $z$  = statistical functional of the conditional streamflow distribution  $\underline{y}|\underline{\mathbf{x}}_p$ ,

$\mathcal{H}\mathcal{M}$  = hydrological model,  $\mathbf{x}_p$  = predictor variables,  $\boldsymbol{\theta}$  = parameters)

- **Core choice:** Loss function that is strictly consistent for the target functional

# Designing “fit-for-purpose” hydrological models (2)

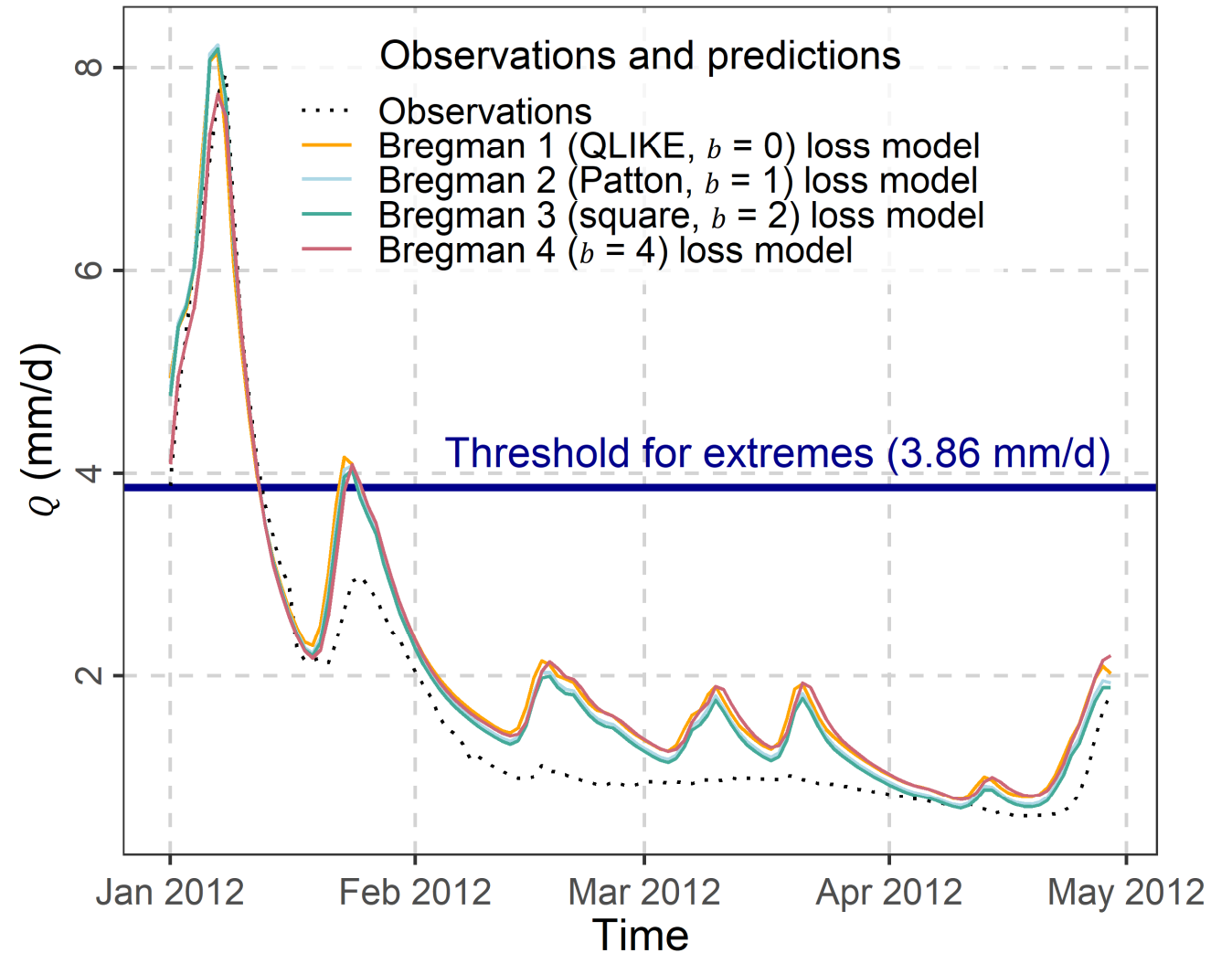
- **Specific focus:** Variable transformations (e.g.,  $\log(y)$  instead of  $y$ ) in strictly consistent loss functions for:

- ✓ Mean
  - ✓ Median
  - ✓ Other quantiles
- 
- Functionals  
of interest

- **Key target:** Extreme streamflow predictions

# Progress so far and next steps

- **Now:** GR4J + 3 functionals ×  
5 loss functions + 1 case study
- **Next:** Large-sample dataset →  
Generalized findings across  
hydroclimatic regimes



# Foundations and domain

- $z$ : prediction
- $y$ : observation
- $\mathbf{z}_n = (z_1, \dots, z_n)^T$ : vector of predictions in train or test set
- $\mathbf{y}_n = (y_1, \dots, y_n)^T$ : vector of observations in train or test set
- $L(z, y)$ : loss function when we predict  $z$  and  $y$  realizes
- $\bar{L}(\mathbf{z}_n, \mathbf{y}_n) = (1/n) \sum_{i=1}^n L(z_i, y_i)$ : average loss in train or test set when we predict  $\mathbf{z}_n$  and  $\mathbf{y}_n$  realizes
- $V(z, y)$ : identification function when we predict  $z$  and  $y$  realizes
- $\bar{V}(\mathbf{z}_n, \mathbf{y}_n) = (1/n) \sum_{i=1}^n V(z_i, y_i)$ : empirical identification function in train or test set when we predict  $\mathbf{z}_n$  and  $\mathbf{y}_n$  realizes
- With monotonicity and convexity hereinafter referring to the domain  $z, y > 0$

# Loss and identification functions for the mean (1)

- Bregman loss function:

$$L_{\text{Br}}(z, y; \varphi) = \varphi(y) - \varphi(z) - \varphi'(z)(y - z), \text{ with:}$$

$\varphi$  convex implying  $L$  consistent and  $\varphi$  strictly convex implying  $L$  strictly consistent

- For  $\varphi(t) = |t|^b, t > 0$ , we have the following family of loss functions:

$$L_{\text{Br}}(z, y; b) = (1/b(b - 1))(y^b - z^b) - (1/(b - 1))z^{b-1}(y - z), b \in \mathbb{R} \setminus \{0, 1\}$$

- Special cases arise for specific values of  $b$ :

$$L_{\text{Br}}(z, y) = \begin{cases} L_{\text{Bregman 1 (QLIKE)}}(z, y) = (y/z) - \log(y/z) - 1, b = 0 \\ L_{\text{Bregman 2 (Patton)}}(z, y) = y \log(y/z) - y + z, b = 1 \\ L_{\text{Bregman 3 (square)}}(z, y) = (1/2)(z - y)^2, b = 2 \\ L_{\text{Bregman 4}}(z, y) = (1/12)(y^4 - z^4) - (1/3)z^3(y - z), b = 4 \end{cases}$$

# Loss and identification functions for the mean (2)

- A special case of the Bregman loss function for evaluating predictions of extremes:

$$L_{\text{Bregman 5 (Taggart)}} [\alpha \in \mathbb{R}](z, y) = (y - a)^2 \mathbb{1}\{y \geq a\} + [(y - z)^2 - (y - a)^2] \mathbb{1}\{z \geq a\}$$

- An intuitive interpretation of this loss function follows:

- Both observation and prediction are in the extreme region ( $z \geq a$  and  $y \geq a$ ):  
The  $(y - a)^2$  terms cancel out, leaving exactly the standard squared error:

$$L_{\text{Bregman 5 (Taggart)}} [\alpha \in \mathbb{R}](z, y) = (y - z)^2$$

- False alarm ( $z \geq a$  and  $y < a$ ): The first term is zero, leaving:

$$L_{\text{Bregman 5 (Taggart)}} [\alpha \in \mathbb{R}](z, y) = (y - z)^2 - (y - a)^2$$

- Missed extreme ( $z < a$  and  $y \geq a$ ): The second term is zero, leaving:

$$L_{\text{Bregman 5 (Taggart)}} [\alpha \in \mathbb{R}](z, y) = (y - a)^2$$

# Loss and identification functions for the mean (3)

- Neither is in the extreme region ( $z < a$  and  $y < a$ ): Both indicator functions are zero, meaning no penalty is applied:

$$L_{\text{Bregman 5 (Taggart)}}[\alpha \in \mathbb{R}](z, y) = 0$$

- Mean identification function:

$$V_{\text{mean}}(z, y) = z - y$$

# Loss and identification functions for the median (1)

- GPL loss function for the median:

$$L_{\text{GPL } [\tau=0.5]}(z, y; g) = |g(z) - g(y)|, \text{ with:}$$

$g$  non-decreasing implying  $L$  consistent and  $g$  strictly increasing implying  $L$  strictly consistent

- Special cases arise for specific functions  $g$ :

$$L_{\text{GPL } 1 [\tau = 0.5]}(z, y; g = \log(t)) = |\log(z) - \log(y)|$$

$$L_{\text{GPL } 2 [\tau = 0.5] \text{ (absolute)}}(z, y; g = t) = |z - y|$$

$$L_{\text{GPL } 3 [\tau = 0.5]}(z, y; g = t^2) = |z^2 - y^2|$$

$$L_{\text{GPL } 4 [\tau = 0.5]}(z, y; g = t^3) = |z^3 - y^3|$$

# Loss and identification functions for the median (2)

- A special case of the GPL loss function for the median for evaluating predictions of extremes:

$$L_{\text{GPL } 5 \text{ (Taggart)}} [\tau = 0.5, a \in \mathbb{R}](z, y) = |(z - a)\mathbb{1}\{z \geq a\} - (y - a)\mathbb{1}\{y \geq a\}|$$

- An intuitive interpretation of this loss function follows:
  - Both in the extreme region ( $z \geq a$  and  $y \geq a$ ): The score is exactly the standard absolute error:

$$L_{\text{GPL } 5 \text{ (Taggart)}} [\tau = 0.5, a \in \mathbb{R}](z, y) = |z - y|$$

- False alarm ( $z \geq a$  but  $y < a$ ): The observation term becomes zero. The penalty is strictly how far the forecast pushed into the extreme zone:

$$L_{\text{GPL } 5 \text{ (Taggart)}} [\tau = 0.5, a \in \mathbb{R}](z, y) = (z - a)$$

# Loss and identification functions for the median (3)

- Missed extreme ( $z < a$  but  $y \geq a$ ): The forecast term becomes zero. The penalty is how far the observation pushed into the extreme zone:

$$L_{\text{GPL 5 (Taggart)}} [\tau = 0.5, a \in \mathbb{R}] (z, y) = (y - a)$$

- Neither is extreme ( $z < a$  and  $y < a$ ): Both terms are zero, yielding:

$$L_{\text{GPL 5 (Taggart)}} [\tau = 0.5, a \in \mathbb{R}] (z, y) = 0$$

No penalty is applied because the event occurred entirely outside the region of interest.

- Quantile identification function for the median:

$$V_{\text{GPL}} [\tau=0.5] (z, y) = \mathbb{1}\{z \geq y\} - 0.5$$

# Loss and identification functions for the $\tau$ -quantile (1)

- GPL loss function:

$$L_{\text{GPL}}(z, y; g, \tau) = (\mathbb{1}\{z \geq y\} - \tau)(g(z) - g(y)), \text{ with:}$$

$g$  non-decreasing implying  $L$  consistent and  $g$  strictly increasing implying  $L$  strictly consistent

- Special cases arise for specific functions  $g$ :

$$L_{\text{GPL } 1 [\tau]}(z, y; g = \log(t)) = (\mathbb{1}\{z \geq y\} - \tau)(\log(z) - \log(y))$$

$$L_{\text{GPL } 2 \text{ (pinball) } [\tau]}(z, y; g = t) = (\mathbb{1}\{z \geq y\} - \tau)(z - y)$$

$$L_{\text{GPL } 3 [\tau]}(z, y; g = t^2) = (\mathbb{1}\{z \geq y\} - \tau)(z^2 - y^2)$$

$$L_{\text{GPL } 4 [\tau]}(z, y; g = t^3) = (\mathbb{1}\{z \geq y\} - \tau)(z^3 - y^3)$$

# Loss and identification functions for the $\tau$ -quantile (2)

- A special case of the GPL loss function for evaluating predictions of extremes:

$$L_{\text{GPL 5 (Taggart)}} [\tau, \alpha \in \mathbb{R}] (z, y) = (\mathbb{1}\{z \geq y\} - \tau) \left( (z - a) \mathbb{1}\{z \geq a\} - (y - a) \mathbb{1}\{y \geq a\} \right)$$

- An intuitive interpretation of this loss function follows:

- Both in the extreme region ( $z \geq a$  and  $y \geq a$ ): The score is exactly the standard pinball loss:

$$L_{\text{GPL 5 (Taggart)}} [\tau, \alpha \in \mathbb{R}] (z, y) = (\mathbb{1}\{z \geq y\} - \tau)(z - y)$$

- False alarm ( $z \geq a$  but  $y < a$ ): The observation term becomes zero. The penalty is strictly how far the forecast pushed into the extreme zone:

$$L_{\text{GPL 5 (Taggart)}} [\tau, \alpha \in \mathbb{R}] (z, y) = (\mathbb{1}\{z \geq y\} - \tau)(z - a)$$

# Loss and identification functions for the $\tau$ -quantile (3)

- Missed extreme ( $z < a$  but  $y \geq a$ ): The forecast term becomes zero. The penalty is how far the observation pushed into the extreme zone:

$$L_{\text{GPL 5 (Taggart)}} [\tau, \alpha \in \mathbb{R}] (z, y) = (\mathbb{1}\{z \geq y\} - \tau)(y - a)$$

- Neither is extreme ( $z < a$  and  $y < a$ ): Both terms are zero, yielding:

$$L_{\text{GPL 5 (Taggart)}} [\tau, \alpha \in \mathbb{R}] (z, y) = 0$$

No penalty is applied because the event occurred entirely outside the region of interest.

- Quantile identification function:

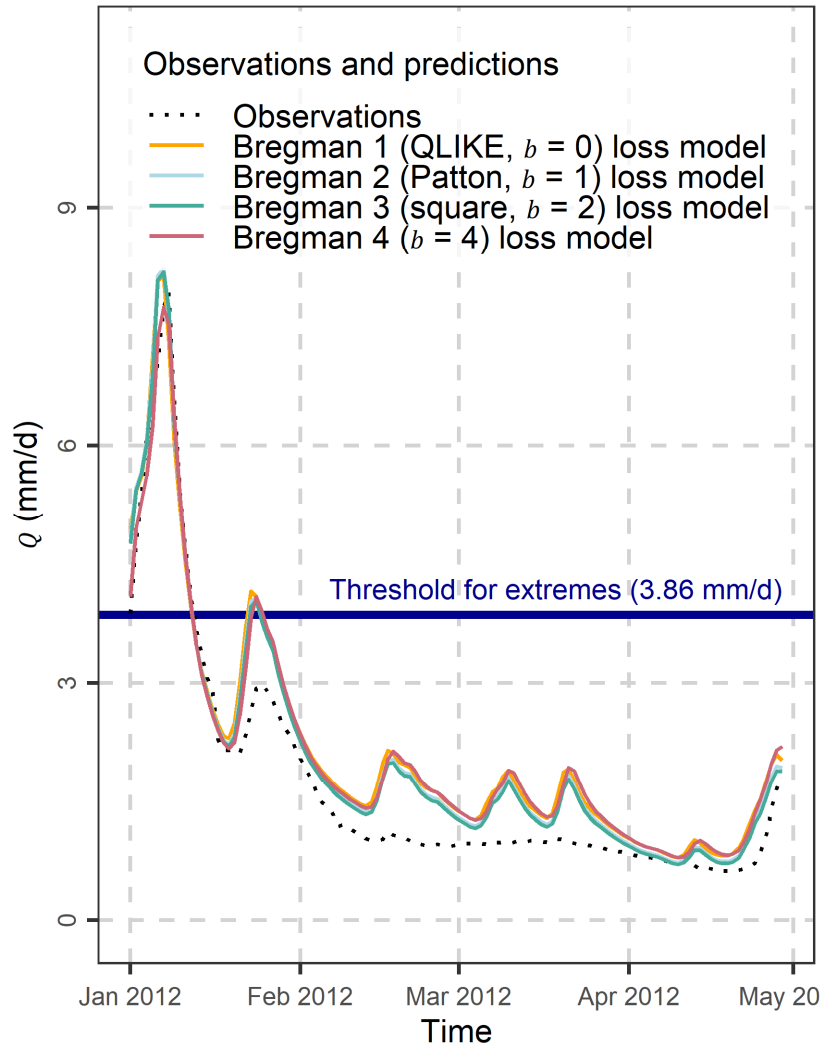
$$V_{\text{quantile}}(z, y; \tau) = \mathbb{1}\{z \geq y\} - \tau$$

# Case study design

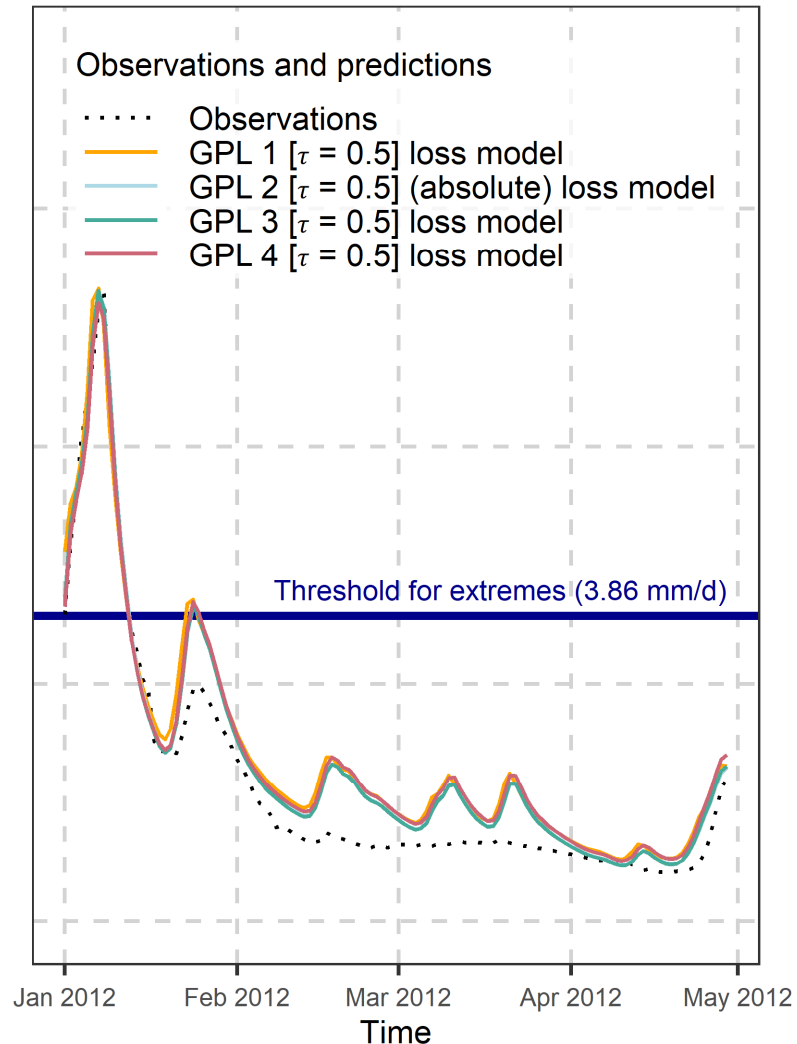
- **Model:** GR4J via `airGR`
- **Dataset:** 20-year daily rainfall-runoff dataset from `airGRdatasets`
- **Target functionals:** Mean, median, 0.90-quantile
- **Loss functions:** Subcases of the Bregman and Generalized Piecewise Linear (GPL) loss functions; five per functional
- **Calibration:** Using the non-extreme loss functions per functional
- **Evaluation:** Using all loss and identification functions per functional; extremes defined via the Taggart loss threshold (here set to the 95<sup>th</sup> percentile in the train set)

# Examples of predictions and threshold for extremes

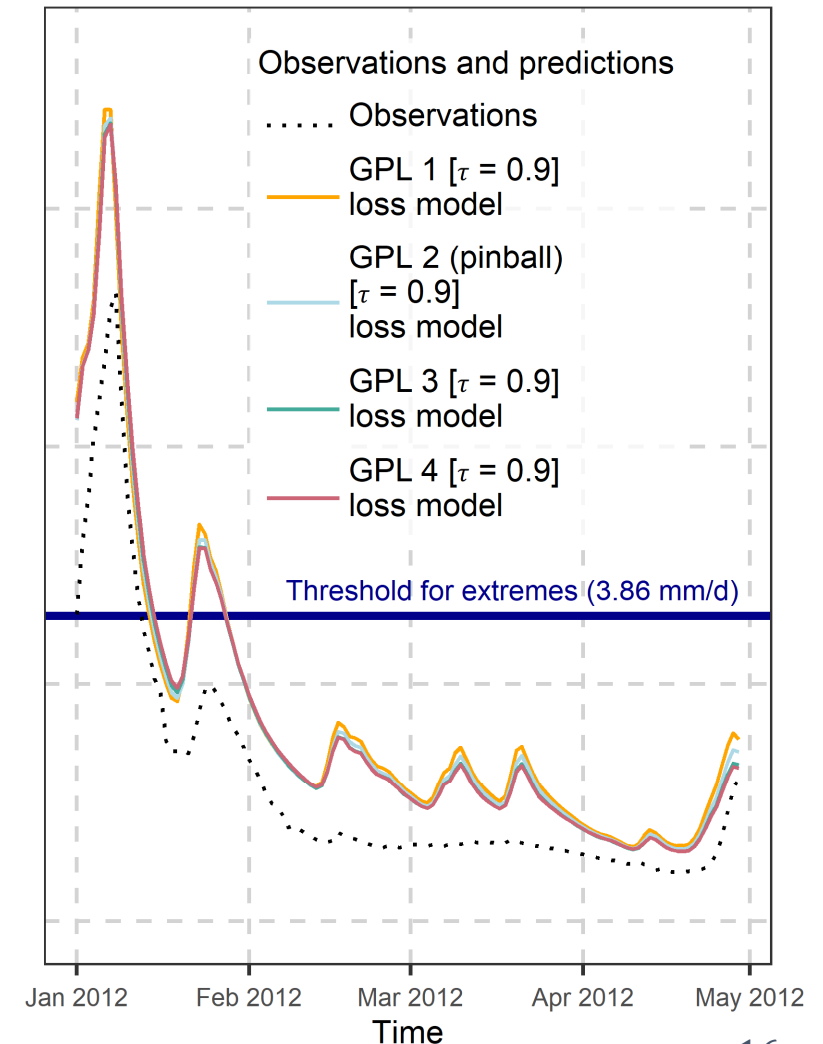
## Predictive mean



## Predictive median



## Predictive 0.90-quantile



# Predictive performance (1)

## Predictive mean

Loss or identification function

	Train				Test				
Bregman 1 (QLIKE, $b = 0$ ) loss	0.03	0.04	0.04	0.04	0.04	0.04	0.04	0.04	Rank (1 = best)
Bregman 2 (Patton, $b = 1$ ) loss	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	
Bregman 3 (square, $b = 2$ ) loss	0.16	0.16	0.16	0.16	0.18	0.17	0.17	0.18	
Bregman 4 ( $b = 4$ ) loss	0.99	0.99	0.99	0.93	2.07	1.83	1.81	1.97	
Bregman 5 (Taggart) loss	0.04	0.04	0.04	0.04	0.06	0.05	0.05	0.06	
Mean identification	0.06	0.01	-0.01	0.04	0.02	-0.03	-0.06	-0.01	
Quantile identification [ $\tau = 0.5$ ]	0.08	-0.01	-0.06	0.06	0.05	-0.03	-0.07	0.04	
	Bregman 1 (QLIKE, $b = 0$ ) loss model	Bregman 2 (Patton, $b = 1$ ) loss model	Bregman 3 (square, $b = 2$ ) loss model	Bregman 4 ( $b = 4$ ) loss model	Bregman 1 (QLIKE, $b = 0$ ) loss model	Bregman 2 (Patton, $b = 1$ ) loss model	Bregman 3 (square, $b = 2$ ) loss model	Bregman 4 ( $b = 4$ ) loss model	
	Model				Model				



# Predictive performance (3)

## Predictive 0.90-quantile

Loss or identification function	Train				Test				Rank (1 = best)
	Model 1	Model 2	Model 3	Model 4	Model 1	Model 2	Model 3	Model 4	
GPL 1 [ $\tau = 0.9$ ] loss	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	1
GPL 2 (pinball) [ $\tau = 0.9$ ] loss	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	2
GPL 3 [ $\tau = 0.9$ ] loss	0.30	0.29	0.28	0.28	0.38	0.36	0.38	0.38	3
GPL 4 [ $\tau = 0.9$ ] loss	1.67	1.56	1.53	1.53	2.98	2.80	2.94	2.96	4
GPL 5 (Taggart) [ $\tau = 0.9$ ] loss	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.02	NA
Quantile identification [ $\tau = 0.9$ ]	0.01	-0.02	-0.03	-0.02	-0.01	-0.03	-0.04	-0.03	NA
	GPL 1 [ $\tau = 0.9$ ] loss model	GPL 2 (pinball) [ $\tau = 0.9$ ] loss model	GPL 3 [ $\tau = 0.9$ ] loss model	GPL 4 [ $\tau = 0.9$ ] loss model	GPL 1 [ $\tau = 0.9$ ] loss model	GPL 2 (pinball) [ $\tau = 0.9$ ] loss model	GPL 3 [ $\tau = 0.9$ ] loss model	GPL 4 [ $\tau = 0.9$ ] loss model	
	Model				Model				

# Key takeaways

- When the data-generating process is unknown, both the target functional and the specific loss function of interest must be specified to reach optimal performance.
- To better predict extremes, consider transformations in loss functions.
- The transformation should be introduced into the Bregman and GPL loss functions.
- To assess extreme predictions, consider specialized loss functions.
- Uncertainties might notably affect case study results, especially in the test set.
- Therefore, moving toward large-sample datasets is necessary.

# Related toy experiments



## **Communicating hydrological model calibration with toy examples**

EGU26-5507 poster (Wed, 06 May, 14:00–15:45 at Hall X5 | X5.224)