Conformal Prediction Interval for Dynamic Time-Series

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Layout

- 1. Introduction
- 2. Problem Setup and Algorithm
- 3. Theoretical Analyses
- 4. Experiment
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1. Introduction

- **Goal**: Construct Prediction Intervals for Time-series to address Uncertainty Quantification.
- **Challenges**:
    1. Dynamic data
    2. Spatio-Temporal Correlation
    3. Ensemble ML Models
    4. Distribution-Free

1. Introduction

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    2. Benefit: have exact marginal coverage guarantee.
    3. Limitation: guarantee only holds for exchangeable data.
- **Our Contribution**
    1. Proposes **EnbPI**, an efficient wrapper around any ensemble model that has been trained.
    2. Theoretically, prediction intervals enjoy approximate marginal coverage, which is exact asymptotically.
    3. Empirically, **EnbPI** ensures exact marginal coverage and even conditional coverage on many tasks.
       Modification can handle missing data in graph networks and anomaly detection.

2. Problem Setup—Data and Objective

- Assume $Y_t = f(X_t) + \epsilon_t, t \geq 1$. $Y_t \in \mathbb{R}, X_t \in \mathbb{R}^d, \epsilon_t \sim F$ (CDF).
    1. Training data $\{(X_t, Y_t)\}_{t=1}^{T}$ are available.

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  1. Training data $\{(X_t, Y_t)\}_{t=1}^{T}$ are available.
  2. For each $t > T$, we build $(1-\alpha)$-level prediction intervals $C_{T,t}^{\alpha}$ so that

$$P\left(Y_t \in C_{T,t}^{\alpha}\right) \geq 1 - \alpha, \tag{1}$$

  where $C_{T,t}^{\alpha}$ indicates previous T data are used to construct the interval at level $1-\alpha$.
  We call (1) as marginal coverage.
  Meanwhile, if X_t lies in a subspace $\mathcal{X} \subset \mathbb{R}^d$, conditional coverage requires

$$P\left(Y_t \in C_{T,t}^{\alpha} | X_t \in \mathcal{X}\right) \geq 1 - \alpha, \tag{2}$$

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  which has been shown impossible to achieve without distributional assumption.
  Our method can empirically achieve (2) in some cases.
  3. Further assume $\{Y_t\}_{t>T}$ are observable feedback after constructing $\{C_{T,t}^{\alpha}\}_{t>T}$, but not immediately (e.g. construct a batch of s intervals before observing all of these…).

2. Problem Setup—Prediction

- For prediction, fix $\mathscr{A} : \{\mathbb{R}^d \times \mathbb{R}\}^N \to (\mathbb{R}^d \to \mathbb{R})$ as a regression algorithm that trains on N data and outputs a predictor $\hat{f}$ that approximates f.

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$$C^{\alpha}_{T,t} := \hat{f}_{-t}\left(X_t\right) \pm (1-\alpha) \text{ quantile of } \left\{\hat{\epsilon}_i\right\}_{i=t-1}^{t-T}, \tag{3}$$

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  where $\hat{f}_{-j}$ implies 1) predictor $\hat{f}$ can differ at each index 2) datum (X_j, Y_j) is never used to train $\hat{f}_{-j}$.
- In ensemble learning (e.g., bootstrap aggregation), multiple bootstrap models $\hat{f}^b$ are then aggregated via ϕ (e.g., mean, median, trimmed mean) to improve prediction accuracy.

2. Algorithm—Big Picture

- Our ayAlgorithm will:
  1. Efficiently compute each $\hat{f}_{-t}, t \geq 1$ as an ensemble predictor. Importantly, doing so only requires the computational power of training one ensemble.
  2. Under mild assumptions, show $C^{\alpha}_{T,t}$ approximately satisfies (1) at each $t > T$.

$$P\left(Y_t \in C^{\alpha}_{T,t}\right) \geq 1 - \alpha \qquad (1)$$

2. Algorithm—Training

- Our **EnbPI** is designed for bagging estimators, with three parts:
- **Part 1**: Train bootstrap models. Typical bootstrap estimation, but this is the only time $\mathscr{A}$ is ever used.

1: **for** $b = 1, \ldots, B$ **do**
2: Sample with replacement an index set $S_b = (i_1, \ldots, i_T)$ from indices $(1, \ldots, T)$.
3: Compute $\hat{f}^b = \mathcal{A}(\{(x_i, y_i) \mid i \in S_b\})$.
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- **Part 2**: Compute LOO residuals $\hat{\epsilon}_i$ from LOO ensemble models.
- Remarks:
  1. Choice of B: concentration inequality, J+aB (Kim et al. 2020).
  2. Compared with split conformal: no data-splitting or overfitting.
  3. Efficiency: no more fitting $\mathscr{A}$.

5: Initialize $\boldsymbol{\epsilon} = \{\}$
6: **for** $i = 1, \ldots, T$ **do**
7: $\hat{f}^{\phi}_{-i}(x_i) = \phi(\{\hat{f}^b(x_i) \mid i \notin S_b\})$
8: Compute $\hat{\epsilon}^{\phi}_i = |y_i - \hat{f}^{\phi}_{-i}(x_i)|$
9: $\boldsymbol{\epsilon} = \boldsymbol{\epsilon} \cup \{\hat{\epsilon}^{\phi}_i\}$
10: **end for**

2. Algorithm—Interval Construction

- **Part 3**: Construct prediction intervals with sliding.
- Remarks
  1. Adaptive width
  2. When $s \to \infty$
  3. Importance of Sliding
- Overall, **EnbPI** adopts a natural idea with simple implementation for real-world applications.

for $t = T+1, \ldots, T+T_1$ **do**
  Let $\hat{f}^{\phi}_{-t}(x_t) = (1-\alpha)$ quantile of $\{\hat{f}^{\phi}_{-i}(x_t)\}_{i=1}^{T}$
  Let $w_t^{\phi} = (1-\alpha)$ quantile of $\boldsymbol{\epsilon}$.
  Return $C^{\phi,\alpha}_{T,t}(x_t) = [\hat{f}^{\phi}_{-t}(x_t) \pm w_t^{\phi}]$
  if $t - T = 0 \bmod s$ **then**
    for $j = t-s, \ldots, t-1$ **do**
      Compute $\hat{\epsilon}_j^{\phi} = |y_j - \hat{f}^{\phi}_{-j}(x_t)|$
      $\boldsymbol{\epsilon} = (\boldsymbol{\epsilon} - \{\hat{\epsilon}_1^{\phi}\}) \cup \{\hat{\epsilon}_j^{\phi}\}$ and reset index of $\boldsymbol{\epsilon}$.
    end for
  end if
end for

3. Theoretical Guarantee

- WLOG, we analyze the coverage at $t = T + 1$, but Theorem holds at any $t > T$. Drop ϕ for notation simplicity.
- **Assumptions**:
  1. Data Regularity: The error process $\{\epsilon_t\}_{t \geq 1}$ is stationary, strongly mixing, with bounded sum of mixing coefficients. Their common CDF F is Lipschitz with $L > 0$.
  2. Estimation Quality: There exists a real sequence $\{\delta_T\}_{T \geq 1}$ that converges to zero such that $\sum_{t=1}^{T} (\hat{\epsilon}_t - \epsilon_t)^2 / T \leq \delta_T^2$.

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- **Theorem** *(Informally): For any* $\alpha \in (0,1)$, *the prediction interval* $C^{\alpha}_{T,T+1}(X_t)$ *from* ***EnbPI*** *satisfies*

$$\left| P\left(Y_{T+1} \notin C^{\alpha}_{T,T+1}\right) - \alpha \right| \leq C\left((\log T/T)^{1/3} + \delta_T^{2/3} \right)$$

- C can be identified under assumptions above.

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1. RHS Rate

1. Factor $(\log T/T)^{1/3}$ comes from assuming strongly mixing errors; different error assumptions (e.g., independent, stationary, etc.) yield different rates (Xu and Xie, 2021a, Corollary 1—3).
2. It is a worst-case analysis; empirical coverage is almost always $1-\alpha$ over all test points.

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2. **Assumption Implications:**

1. Assumption 1 allows arbitrary data dependency.
2. Assumption 2 holds true for many classes of f and algorithms $\mathscr{A}$ (Xu and Xie, 2021a, Section 4.2).
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      In general, Assumption 2 requires asymptotically exact approximation of $\hat{f}$ to f.
3. **Theorem Applicability:** holds for split conformal (Papadopoulos et al., 2007), but
   1. T in the Theorem becomes the size of calibration data.
   2. LOO ensemble predictor $\hat{f}_{-i}$ are in general better function approximators.

3. Theoretical Analyses—Proof Sketch

- Define $\hat{p}_{T+1} := T^{-1} \sum_{i=1}^{T} \mathbf{1}\left\{\hat{\epsilon}_i > \hat{\epsilon}_{T+1}\right\}$, whereby $Y_{T+1} \notin C^{\alpha}_{T,T+1}\left(X_{T+1}\right)$ iff $\hat{p}_{T+1} \leq \alpha$.

  The proof then analyzes how quickly $\hat{F}(x) := T^{-1} \sum_{i=1}^{T} 1\{\hat{\epsilon}_i \leq x\}$ $(\hat{F}(\hat{\epsilon}_{T+1}) = 1 - \hat{p}_{T+1})$ converges to $F(\epsilon_{T+1}) \sim \text{Unif}[0,1]$, whereby $\left| P\left(Y_{T+1} \notin C^{\alpha}_{T,T+1}\right) - \alpha \right|$ is also bounded.

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- **Lemma 1:**

  Define $\tilde{F}(x) := T^{-1} \sum_{i=1}^{T} \mathbf{1}\left\{\epsilon_i \leq x\right\}$. Under Assumption 1, there is an event A_T in the probability space of $\{\epsilon_t\}_{t=1}^{T}$, such that conditional on A_T, $\sup_x |\tilde{F}(x) - F(x)| \leq C(\log T/T)^{1/3}$. Moreover, $P(A_T^C) \leq C(\log T/T)^{1/3}$.

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- **Lemma 2:**

  Under Assumption 1 and 2, $\sup_x |\hat{F}(x) - \tilde{F}(x)| \leq C\delta_T^{2/3} + 2 \sup_x |\tilde{F}(x) - F(x)|$

- Together with Lemma 1 & 2, basic algebraic manipulation and triangle inequality prove the Theorem.

Experiment—Setup

- **Key Questions: EnbPI** on marginal coverage, conditional coverage (with missing data on networks), and anomaly detection.
- **Data:** Primarily use renewable energy data (e.g., solar and wind). Each time-series contains hourly data for a whole year. See Fig (a) & (b). We have marginal coverage results on data from other domains (Xu and Xie 2021a, Section 8.4).

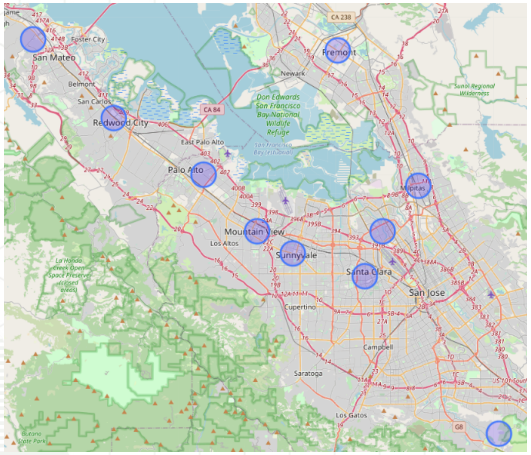

Fig (a): California non-uniform solar radiation sensors

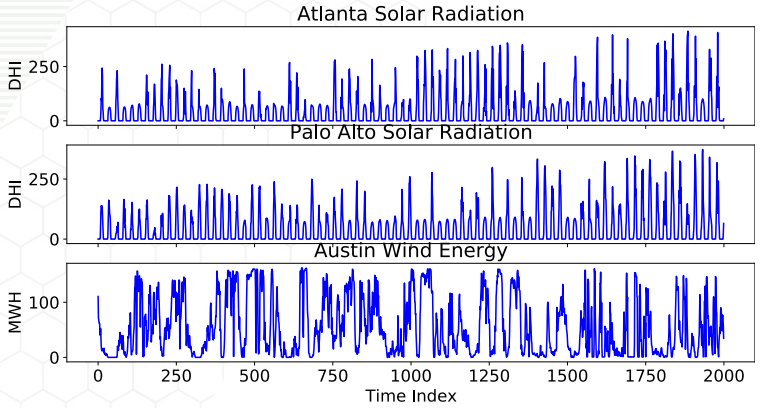

Fig (b): First 2000 Y_t of each time-series

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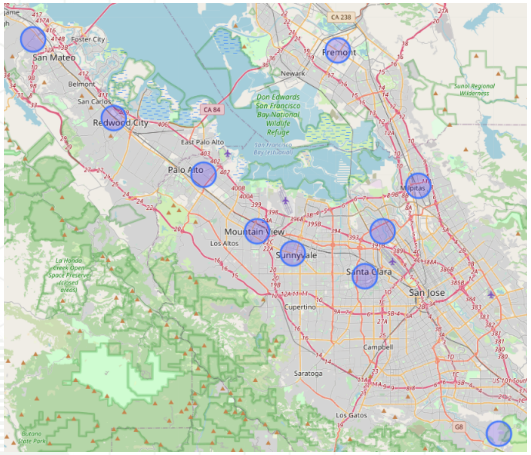
  We have marginal coverage results on data from other domains (Xu and Xie 2021a, Section 8.4).
- **Features:** X_t is either univariate (past history of Y_t) or multivariate (other time series).
- **Regression** $\mathscr{A}$: Ridge, Random Forest (RF), Neural Network (NN), and RNN.
- **Competing Methods:** ARIMA(10,1,10), ICP, WeightedICP.
- Unless otherwise specified, we set ϕ=mean, B =30, and use the first 20% of total data for training (e.g., $T = 0.2(T + T_1)$). The stride s varies depending on our interests.



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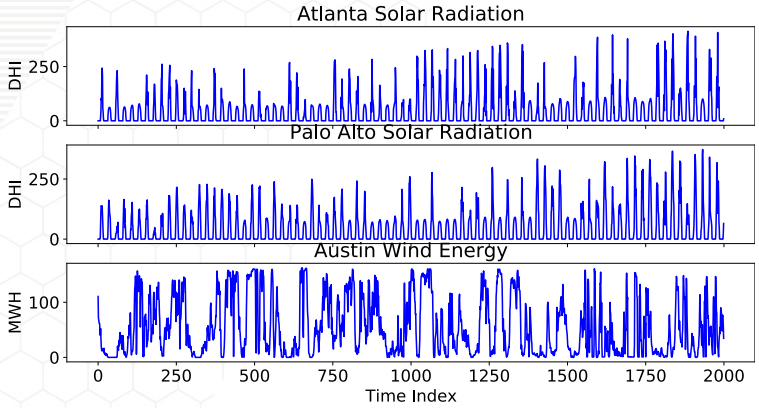

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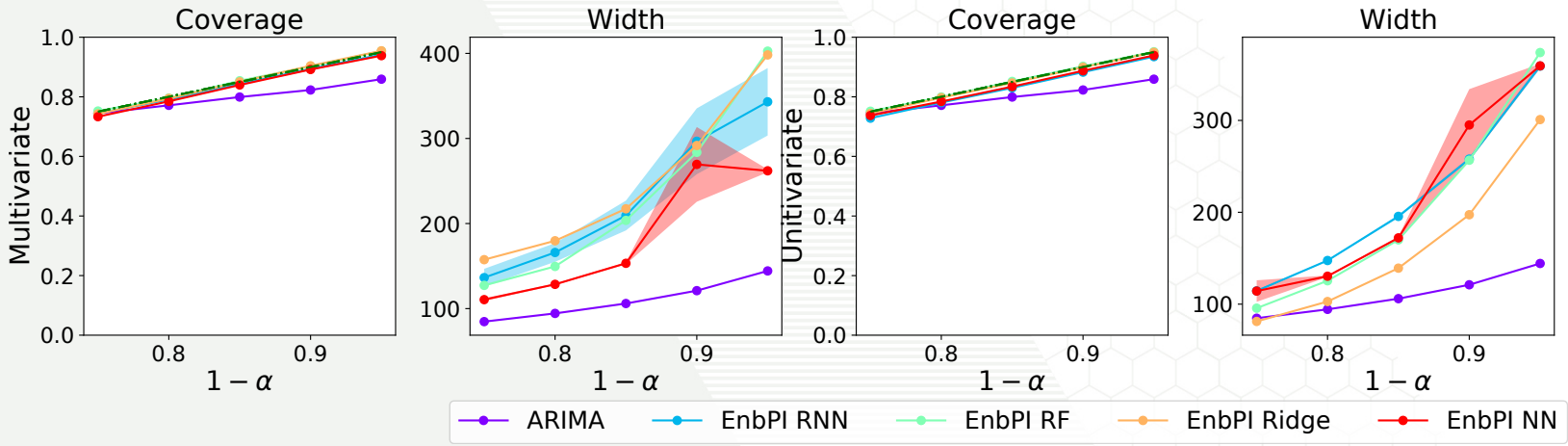

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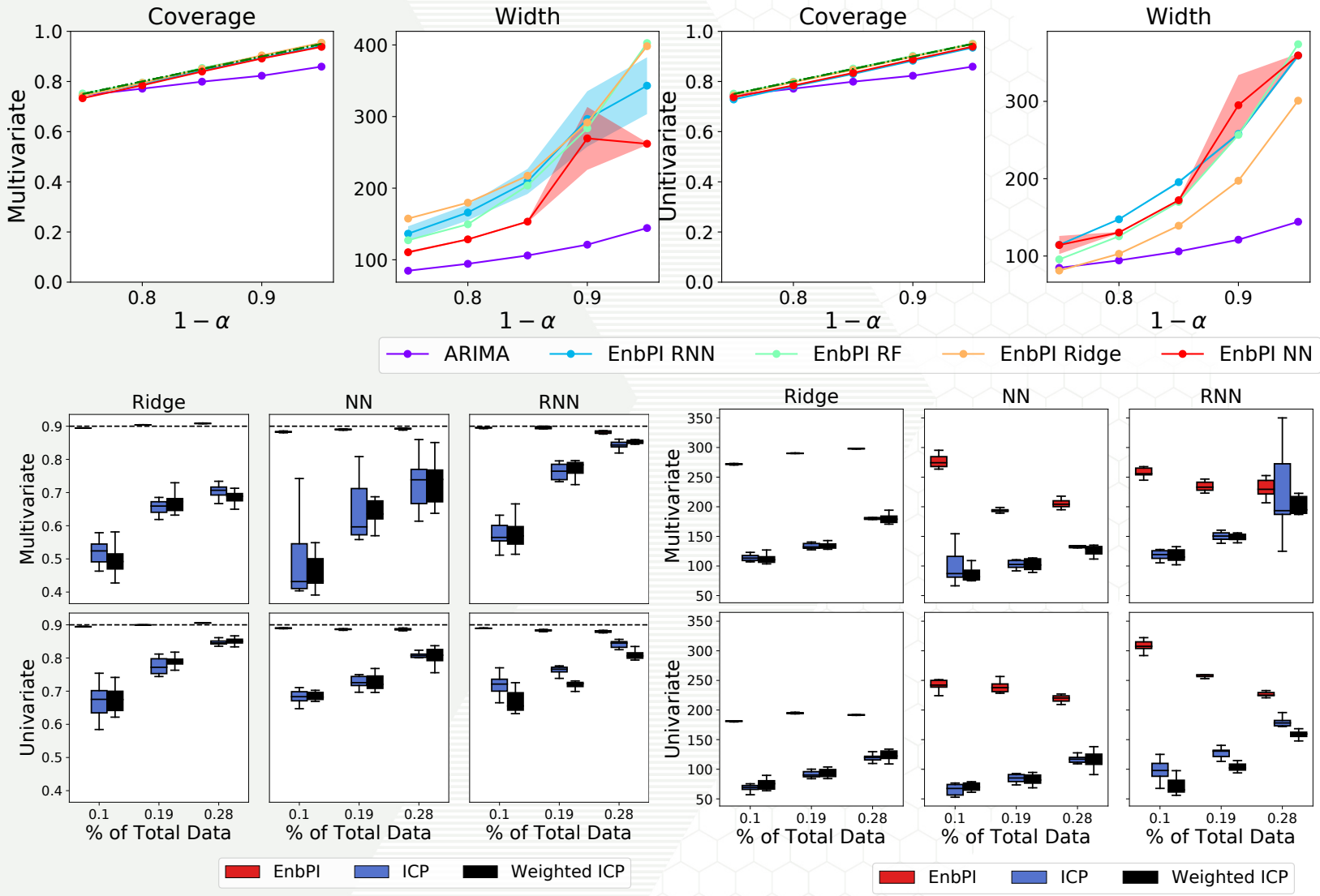
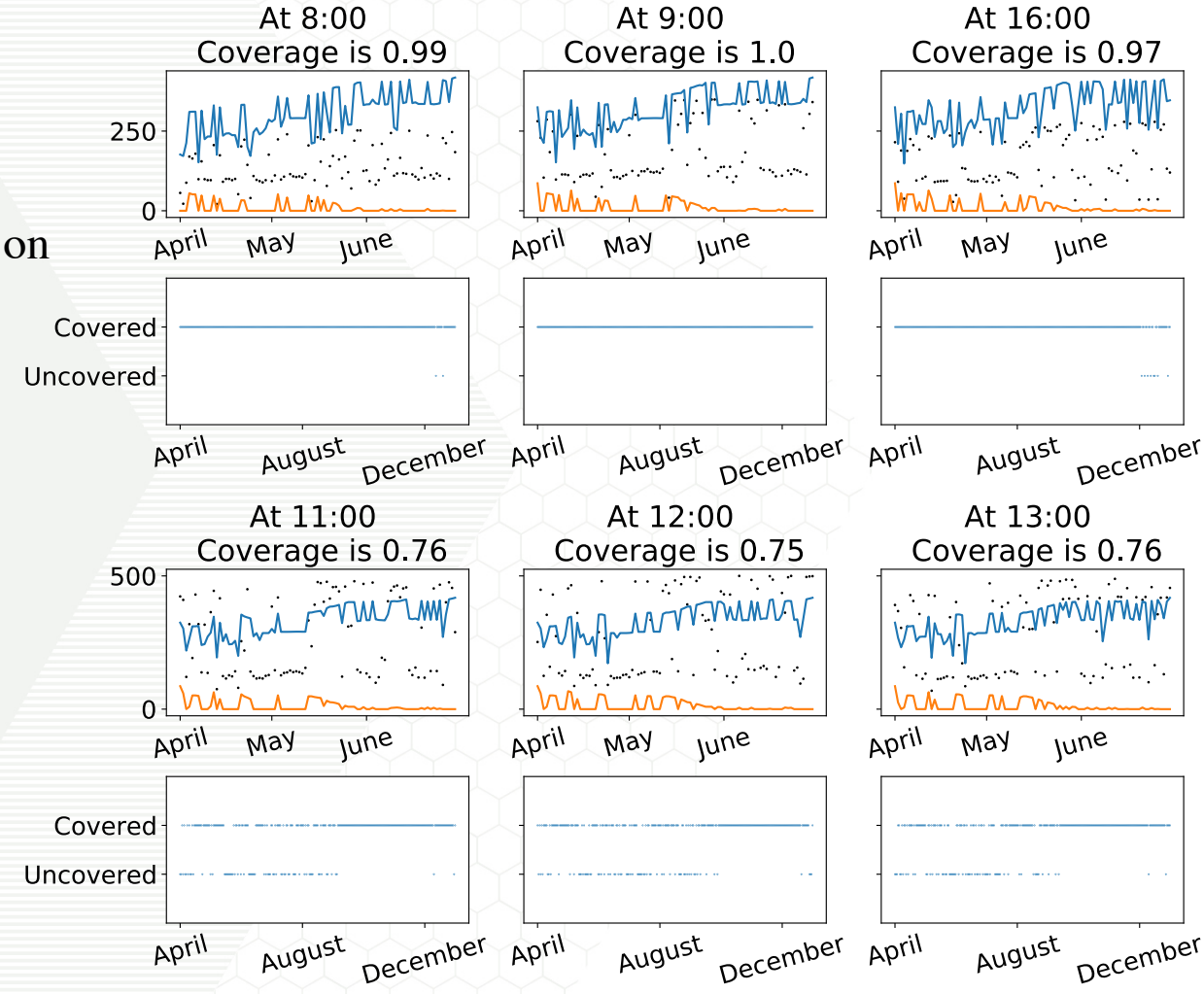


Experiment—Conditional Coverage

- We condition on each hourly coverage, by letting $s = 24$. Missing data are present.
- **Why this is conditional:** train on all hourly data but examine coverage by hour.
- **Handle missing flows:** We sample from empirical flows. More discussions see (Xu and Xie 2021a, Section 3.2)



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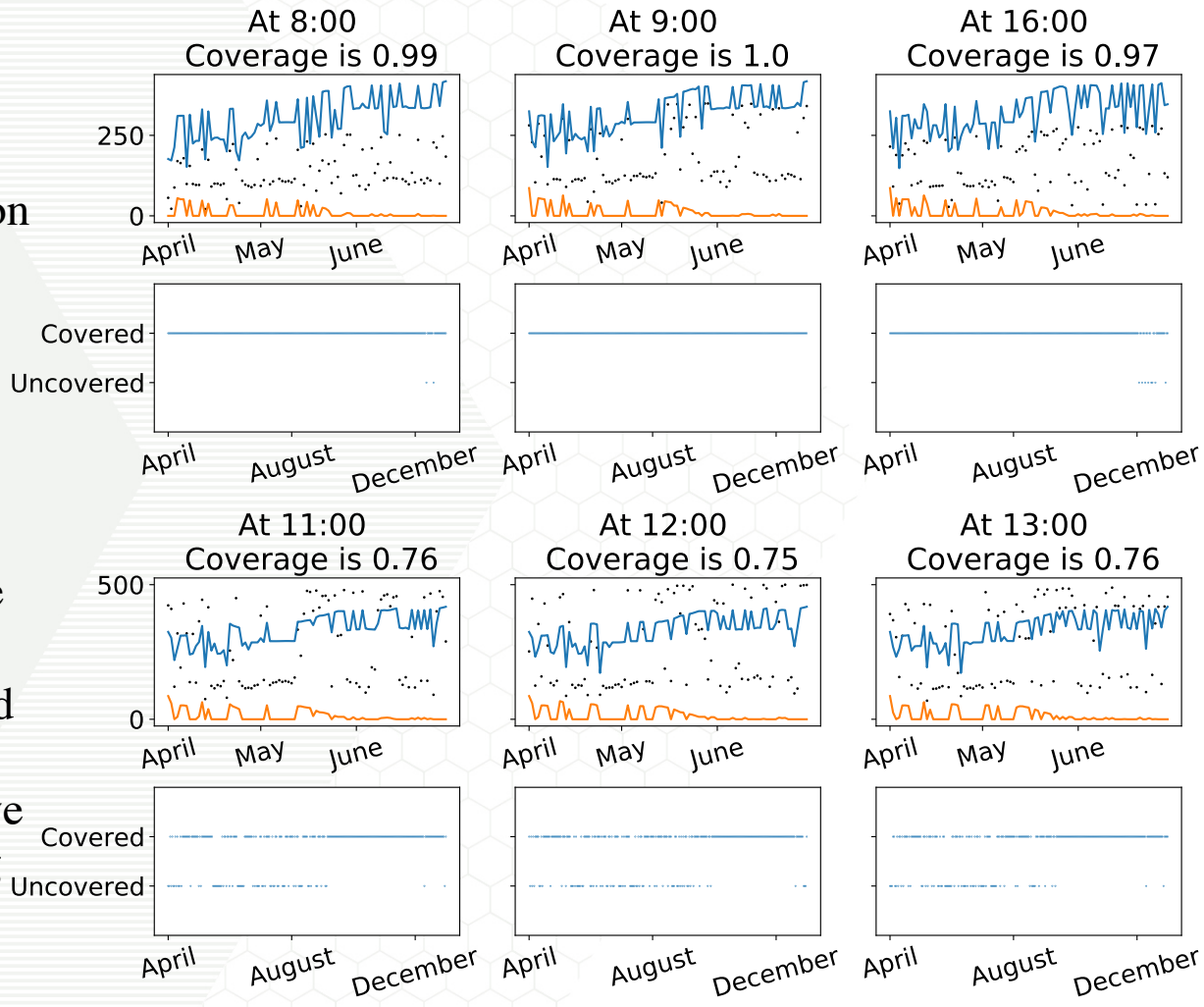
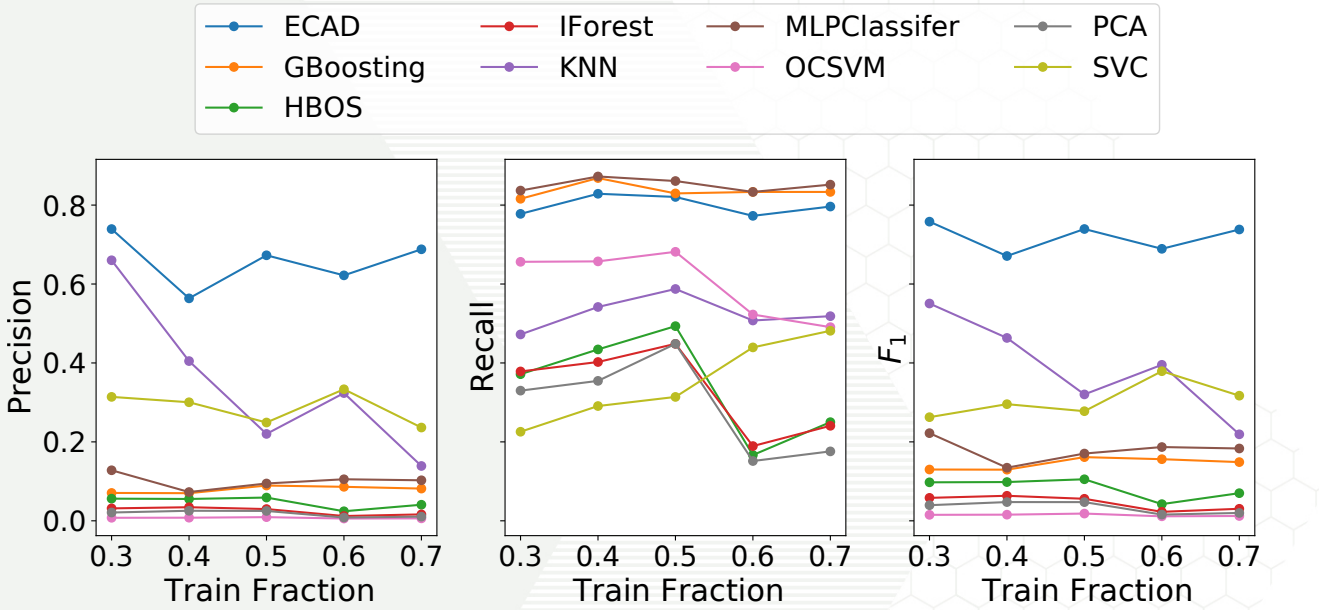
- **How to improve coverage:** See (Xu and Xie 2021a, Figure 8)
- Results on network data (Xu and Xie 2021a, Section 8.3)
  The primary difference is that we define X_t to contain neighboring values as well.



Experiment—Anomaly Detection



- Use Financial Crime Data.
- The detector wraps around classification algorithms. Details see (Xu and Xie 2021a, Section 8.5).
- Significant improvement over other supervised and unsupervised detectors.

Conclusion

- Present a predictive inference method for dynamic time-series, useful in uncertainty quantification.
- Theoretically, **EnbPI** intervals are approximately marginally valid without assuming data exchangeability.
- Computationally, it is an efficient ensemble-based wrapper for many regression algorithms, including deep neural networks.
- Empirically, it is versatile on a wide range of time-series, including network data and data with missing entries, and maintains validity when traditional methods fail. It can even work well for anomaly detection.

Extension

- **Methodologically**,
  1. Adapt **EnbPI** for classification problems, especially those in computer vision.
  2. Better connect **EnbPI** with other applications, such as anomaly detection and sequential change-point detection
     See our latest work on conformal anomaly detection (Xu and Xie, 2021b).
- **Theoretically**,
  1. How and why LOO ensemble predictors are better function approximators than those in split conformal.
  2. Move towards conditional coverage analyses.
  3. Analyze widths of prediction intervals.

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