Simulation-based Time Series Analysis:

Likelihood-free Estimation, Testing for Structure, and Prediction with Transformers using Synthetic Data

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Overview of presentation

- Introduction to time series

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- Conditional independence testing

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- Simulation-based estimation

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- Simulation-based estimation
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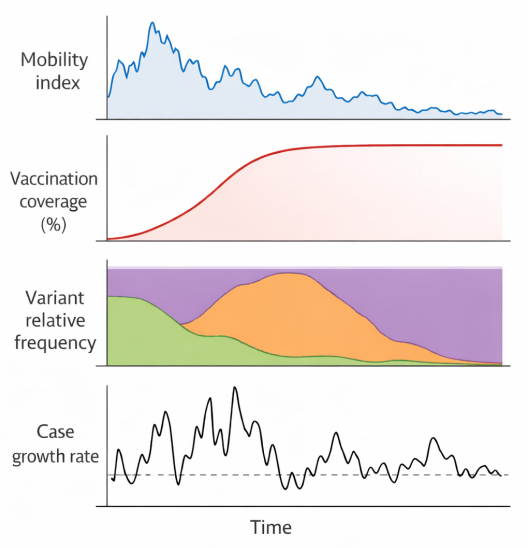
- Example: time series in epidemiology

COVID-19 time series May 2020–2022 (n=365x2=730, d=4)



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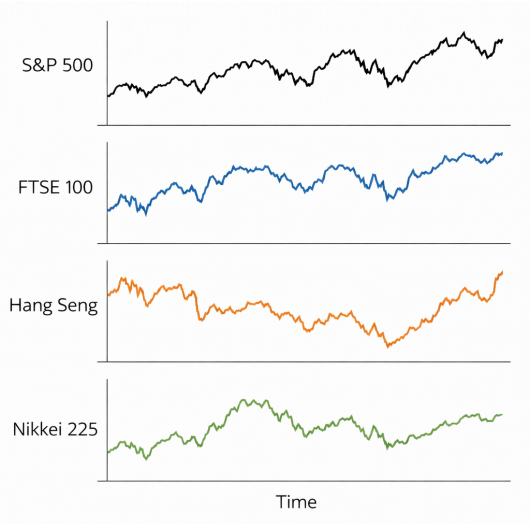
- We show a subset of the results based on BH-adjusted p-values

Closing prices of each stock index over time



Independence testing reveals same day returns are dependent

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- We reject *every* null hypothesis at the significance level $\alpha = 0.05$

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- Next, we present the testing procedure

Dynamic generalized covariance measure test (1/2)

- **Inputs:** Data $X_{1:n}$, $Y_{1:n}$, $Z_{1:n}$, significance level α, number of simulations s, $p \in [2, \infty]$ for norm in test statistic, and method for selecting the window size L

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- Obtain residual products $\hat{R}_t = \mathrm{vec}(\hat{\varepsilon}_t \hat{\xi}_t^\top)$, $t \in [n]$
- Calculate test statistic on time series of residual products

$$T(\hat{R}_{1:n}) = \max_{j \in [n]} \left\| \frac{1}{\sqrt{n}} \sum_{t \leq j} \hat{R}_t \right\|_p$$

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- Reject null hypothesis at level α if $T(\hat{R}_{1:n}) > \hat{q}_{1-\alpha}^{\text{boot}}$, else retain

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- Let Θ be a parameter space, which can be infinite-dimensional
- Let $G_t^{(n)} : \mathbb{R}^\infty \times \Theta \to \mathbb{R}^d$ be some measurable function, $t, n, d \in \mathbb{N}$

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- Denote the collections by $\mathcal{P}_n = \{P_{\theta,n} : \theta \in \Theta\}$ and $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$

Key assumption: Decaying influence of noise inputs (Wu 2005)

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- There exist $\Psi, \rho > 0$ such that, for some $q > 2$ and all $j \in \mathbb{N}$, we have

$$\sup_{\theta\in\Theta}\sup_{\ell\in\mathbb{Z}}\sup_{i\in\mathbb{N}}\sup_{t\in\mathbb{N}} \left\| G_t^{(i)}(\boldsymbol{\epsilon}_\ell, \theta) - G_t^{(i)}(\tilde{\boldsymbol{\epsilon}}_{\ell,j}, \theta)\right\|_{L^q(\theta)} \leq \Psi(j \vee 1)^{-\rho}$$

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where $\|\cdot\|_{L^q(\theta)} = \mathbb{E}_\theta\left(\|\cdot\|_2^q\right)^{1/q}$, $\mathbb{E}_\theta(\cdot)$ is expectation w.r.t. θ-dependent distribution

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  where $\|\cdot\|_{L^q(\theta)} = \mathbb{E}_\theta \left(\|\cdot\|_2^q\right)^{1/q}$, $\mathbb{E}_\theta(\cdot)$ is expectation w.r.t. θ-dependent distribution

- We make this assumption for $X_{1:n}$, $Y_{1:n}$, and $Z_{1:n}$

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Theorem (Informal)

Recall the test statistic $T(\hat{R}_{1:n})$ and estimated quantile $\hat{q}_{1-\alpha}^{\mathrm{boot}}$. We have

$$\limsup_{n \to \infty} \sup_{P \in \mathcal{P}_n^*} \mathbb{P}_P \left(T(\hat{R}_{1:n}) > \hat{q}_{1-\alpha}^{\mathrm{boot}} \right) \leq \alpha.$$

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- **Key assumption:** We know $G_t^{(n)}$ and can simulate from it at any value of $\theta \in \Theta$

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- For nonstationary time series, need rolling-window estimator (not discussed here)

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- Takes time to find good features
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- Automatic feature selection, computationally efficient, little knowledge needed

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- If physical dependence measure (Wu 2005) decays uniformly over Θ, we can estimate $\Phi(\theta)$, $\theta \in \Theta$, via time-averages of $2p+1$ random features

$$\frac{1}{n-m} \sum_{t=m+1}^{n} \varphi\left([X_t(\theta), \ldots, X_{t-m}(\theta)]^\top\right)$$

Example: Mean of Gaussian

- **Goal:** Estimate $\theta_0 = 0$ given $X_1^{\text{obs}}, \ldots, X_n^{\text{obs}} \overset{\text{iid}}{\sim} \mathcal{N}(\theta_0, 1)$ with $\Theta = [-3, 3]$

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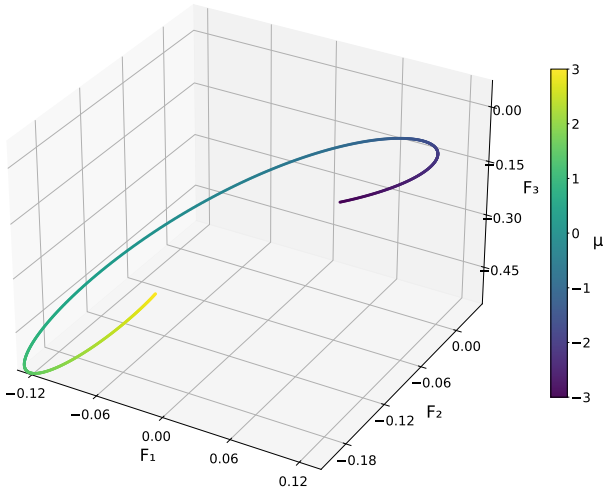
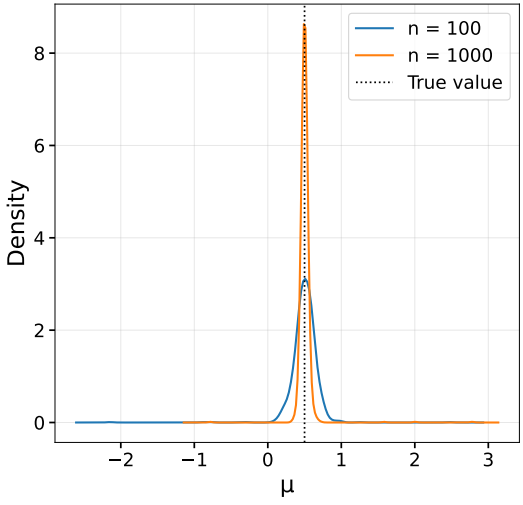
- We will compare our random feature estimator $\hat{\theta}$ with $\hat{\theta}^{\text{MLE}} = \frac{1}{n} \sum_{t=1}^{n} X_t$

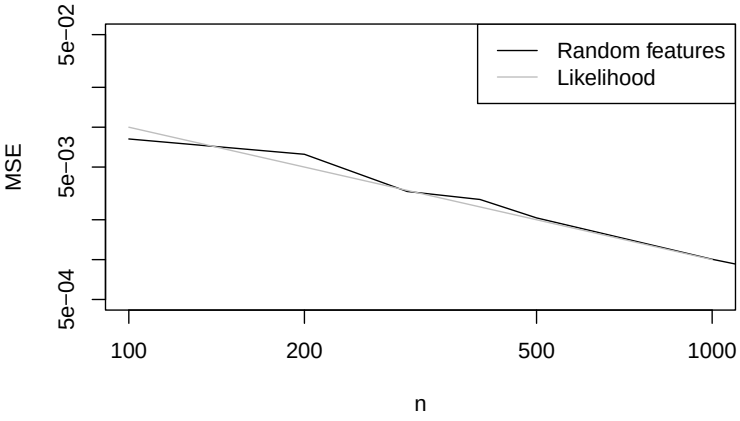
Time-average of 3 features, colored by parameter value ($n = 1000$, $s = 10$)



Density plot based on 1,000 independent estimates



Theoretical MSE of MLE vs MSE of our estimator (100 replicates per n)



Theoretical guarantees for random feature estimators

- We prove consistency $\hat{\theta} \xrightarrow{p} \theta_0$ and asymptotic normality

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- Examples: ODEs observed through dependent noise, nonstationary state-space models, and structural time series models

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- We develop theory, and propose methods for smoothing and forecasting

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for some scaling factor $\kappa > 0$ and autoregressive coefficient $\phi \in (-1, 1)$, with $X_0 \sim N(0, \frac{\sigma_X^2}{1-\phi^2})$ and $\varepsilon_t^X \overset{\text{iid}}{\sim} N(0, \sigma_X^2)$, $\varepsilon_t^Y \overset{\text{iid}}{\sim} N(0, \sigma_Y^2)$ for some $\sigma_X, \sigma_Y > 0$

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- Seasonality: linear combination of sines, cosines (weekly, monthly, yearly periods)
- Trend: product of linear trend and exponential trend
- Our rolling-window estimator can be used (consistent and asymptotically normal)

Unifying framework: Simulation-and-regression with parameter uncertainty

- We propose minimizing the Monte Carlo approximation to

$$R_{P_{\widehat{\text{mix}}}}(f) = \mathbb{E}_{P_{\widehat{\text{mix}}}}\left[\sum_{t\in\mathcal{T}} L\left(X_t - [f(Y)]_t\right)\right] = \mathbb{E}_{\theta\sim\widehat{\text{CD}}_n}\left[\mathbb{E}_{P_\theta}\left[\sum_{t\in\mathcal{T}} L\left(X_t - [f(Y)]_t\right)\right]\right]$$

for some loss L, where the expectation is w.r.t. the mixture distribution $P_{\widehat{\text{mix}}} = \int_\Theta P_\theta d\widehat{\text{CD}}_n(\theta)$ of sequences X, Y corresponding to some *estimated confidence distribution* $\widehat{\text{CD}}_n$ over $\Theta \subset \mathbb{R}^p$ for θ_0 (D. Liu, R. Y. Liu, and Xie 2022)

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- When $\widehat{\text{CD}}_n$ is uniform over Θ, this is like TSFM pre-training (no information)
- When $\widehat{\text{CD}}_n$ is Dirac delta at $\hat{\theta}$, this is like classical simulation-and-regression, which aims to minimize the Monte Carlo approximation to

$$R_{P_{\hat{\theta}}}(f) = \mathbb{E}_{P_{\hat{\theta}}}\left[\sum_{t\in\mathcal{T}} L(X_t - [f(Y)]_t)\right]$$

  where expectation is w.r.t. distribution $P_{\hat{\theta}}$ of sequences X, Y corresponding to $\hat{\theta}$

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Questions we aim to answer

- **Calibration:** Does accounting for parameter uncertainty improve the calibration of pre-trained/untrained transformers that output multiple conditional quantiles?
- **Pre-training:** When does a pre-trained transformer fine-tuned with our method outperform a transformer trained from scratch with our method?
- **Fine-tuning and simulation-and-regression:** When does accounting for parameter uncertainty improve on simulation-and-regression methods and TSFM fine-tuning methods that are based on parameter point estimates?

Thank you!

Questions or comments?

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Does accounting for parameter uncertainty improve the calibration of pre-trained/untrained transformers that output conditional quantiles?

- For untrained transformers, see answer to question: "In the context of simulation-and-regression, does accounting for parameter uncertainty achieve better performance than using parameter estimate?"

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In the context of simulation-and-regression, does accounting for parameter uncertainty achieve better performance than using parameter estimate?

- When does this inequality hold:

$$\mathbb{E}_{P_{\theta_0}}\left[\sum_{t\in\mathcal{T}} L\left(X_t - [f^*_{P_{\widehat{\text{mix}}}}(Y)]_t\right)\right] < \mathbb{E}_{P_{\theta_0}}\left[\sum_{t\in\mathcal{T}} L\left(X_t - [f^*_{P_{\hat{\theta}}}(Y)]_t\right)\right]$$

where both expectations are with respect to the distribution P_{θ_0} of the sequences corresponding to the unknown true parameter θ_0, $f^*_{P_{\widehat{\text{mix}}}}$ is the minimizer in the function class of $R_{P_{\widehat{\text{mix}}}}(f)$, and $f^*_{P_{\hat{\theta}}}$ is the minimizer in the function class of $R_{P_{\hat{\theta}}}(f)$

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- Intuitively, this occurs when the following conditions hold
- Large parameter uncertainty, e.g., when the sample size of the observed time series is small relative to the noise
- The distributions used in the pre-training phase are close to the true distribution, e.g., when we have domain knowledge or we have previously observed time series with similar distributions

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