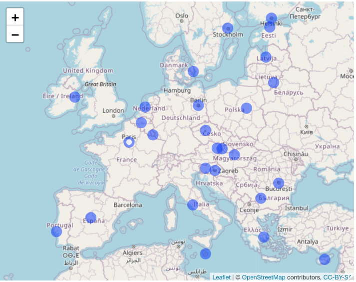
Wasserstein multivariate auto-regressive models for modeling distributional time series and its application in graph learning

Yiye JIANG

Univ. Grenoble Alpes, CNRS, Inria, Grenoble INP, LJK, 38000 Grenoble, France
yiye.jiang@inria.fr

Multivariate distributional time series



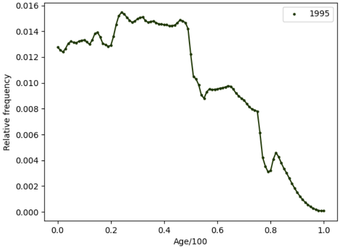


Figure 1: *Observations of the age distributions across European union countries over years* 1995 *to* 2035 *(projected).*

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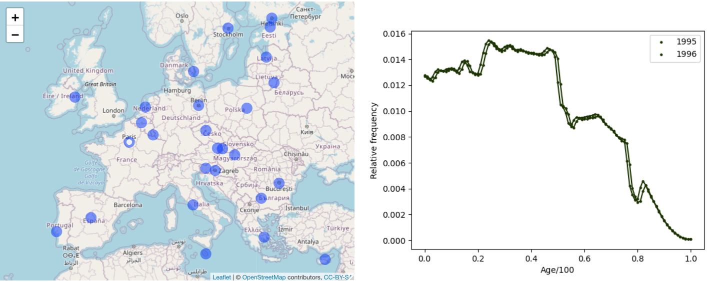

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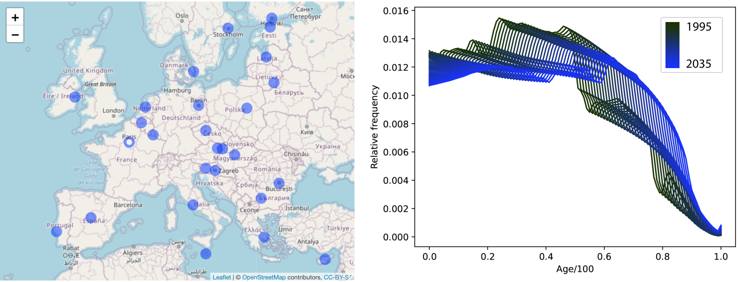
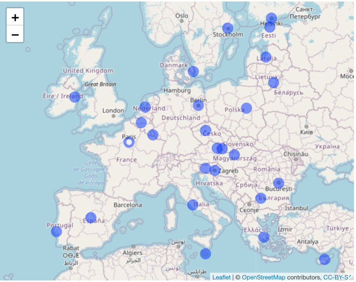
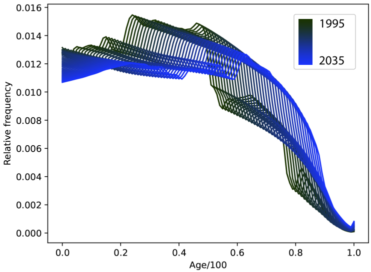


Figure 3: *Observations of the age distributions across European union countries over years* 1995 *to* 2035 *(projected).* On the right are the observations $(\boldsymbol{\mu}_{it})_t \in \mathcal{P}([0,1])$ along time recorded at $i =$ France. Lighter curves correspond to more recent years.





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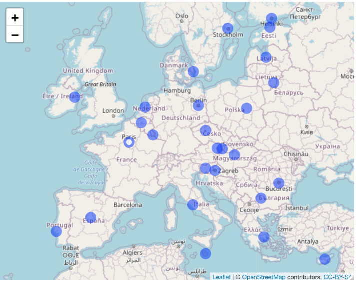
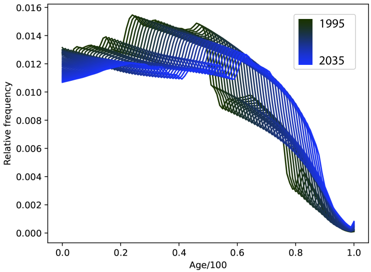
1. A model to describe the new time series type:

$$\boldsymbol{\mu}_{it} \in \mathcal{P}(\mathbb{R}), i = 1...N, t \in \mathbb{Z}.$$





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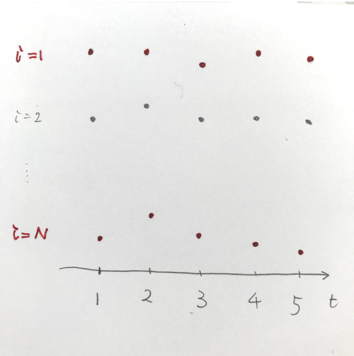
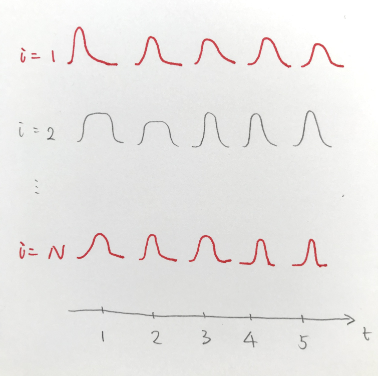
2. Represent the series dependencies by a graph.

Vector auto-regressive model (VAR)





N scalar TS (data for VAR) N distributional TS (our data)

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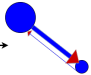
$A \rightarrow \mathcal{G}$

1.8	0.05
1.2	-0.4

$\longrightarrow$



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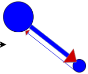

$$Extension: \quad \boldsymbol{x}_{it} \in \mathbb{R} \longrightarrow \boldsymbol{\mu}_{it} \in \mathcal{W}_2(\mathbb{R}).$$

Backgrounds on statistics in $W_2(\mathbb{R})$

$$\mathcal{W}_2(\mathbb{R}) = \left\{ \mu \in \mathcal{P}(\mathbb{R}) \middle| \int_{\mathbb{R}} x^2 d\mu(x) < \infty \right\},$$

endowed with the 2-Wasserstein distance

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Extension of VAR models: $\mathcal{W}_2 := \mathcal{W}_2(\mathbb{R})$ is not linear.

Enable again linear methods - Tangent space

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Let $\gamma \in \mathcal{W}_2$ be an atomless measure (it possesses a continuous cdf F_γ), the tangent space at γ is defined as

$$\mathrm{Tan}_\gamma = \overline{\{t(T_\gamma^\mu - i) : \mu \in \mathcal{W}_2,\ t > 0\}}^{\mathcal{L}_\gamma^2},$$

where $T_\gamma^\mu = F_\mu^{-1} \circ F_\gamma$ is the optimal transport map, that pushes γ forward to μ.

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$$\langle f, g \rangle_\gamma := \int_{\mathbb{R}} f(x) g(x)\, d\gamma(x),\ f, g \in \mathcal{L}_\gamma^2(\mathbb{R}),$$

and the induced norm $\| \cdot \|_\gamma$.

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Definition

The logarithmic map $\mathrm{Log}_\gamma : \mathcal{W}_2 \to \mathrm{Tan}_\gamma$ is defined as

$$\mathrm{Log}_\gamma \mu = T_\gamma^\mu - i.$$

The exponential map $\mathrm{Exp}_\gamma : \mathrm{Tan}_\gamma \to \mathcal{W}_2$ is defined as

$$\mathrm{Exp}_\gamma g = (g + id)\#\gamma,$$

where $T\#\mu$ is the measure pushforwarded by function T, defined as $[T\#\mu](A) = \mu(\{x : T(x) \in A\})$.

Tangent space and Geodesic

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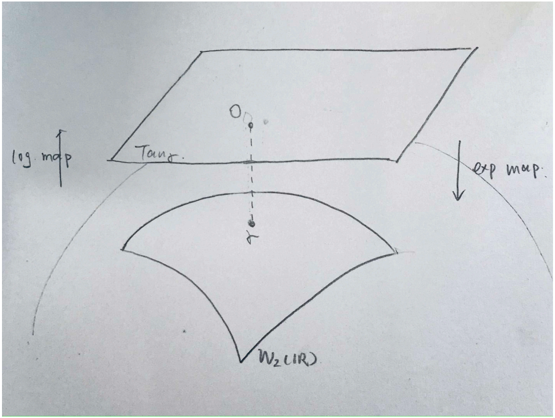

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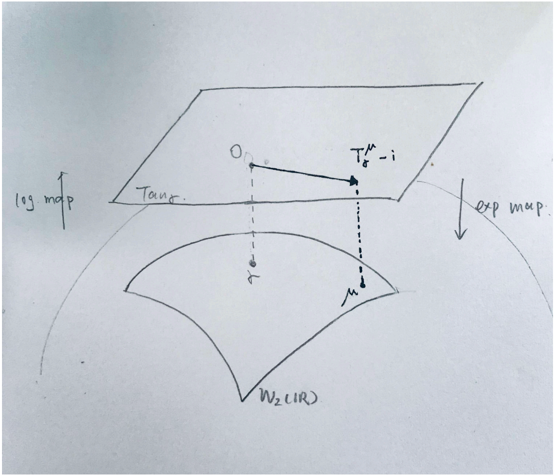

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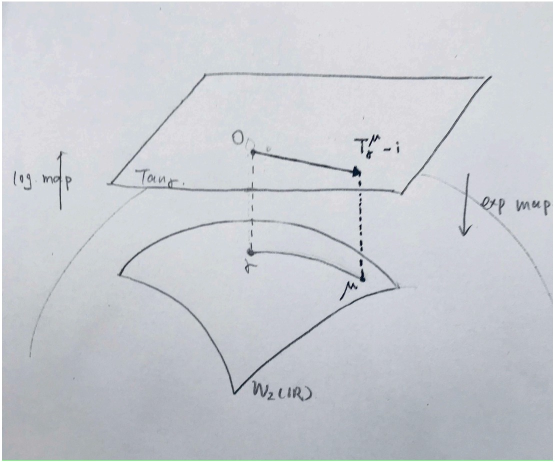

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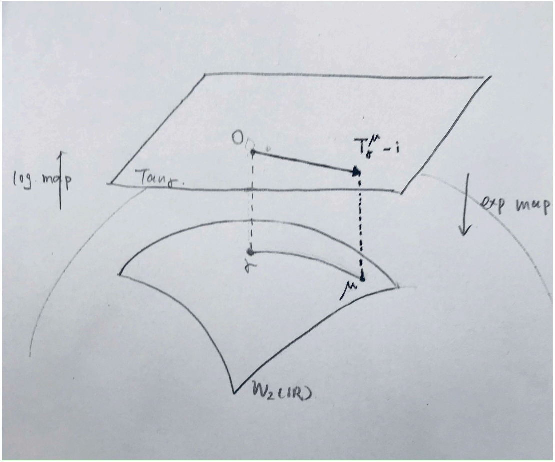
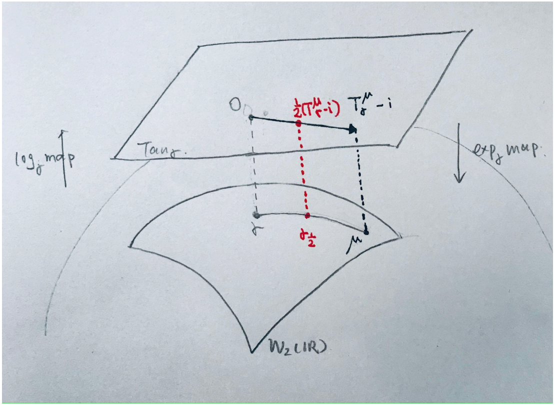


The geodesic (McCann's interpolant) between γ and μ

$$\mathrm{Exp}_\gamma[\alpha(T_\gamma^\mu - i)],\ \alpha : 0 \to 1,$$

Constant-speed Geodesic



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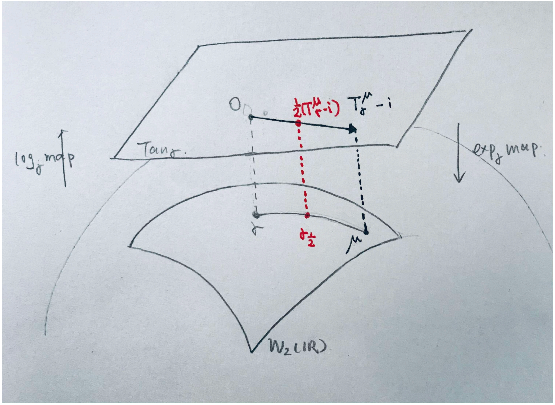

$$d_W(\gamma, \gamma_{\frac{1}{2}}) = \frac{1}{2} d_W(\gamma, \mu)$$

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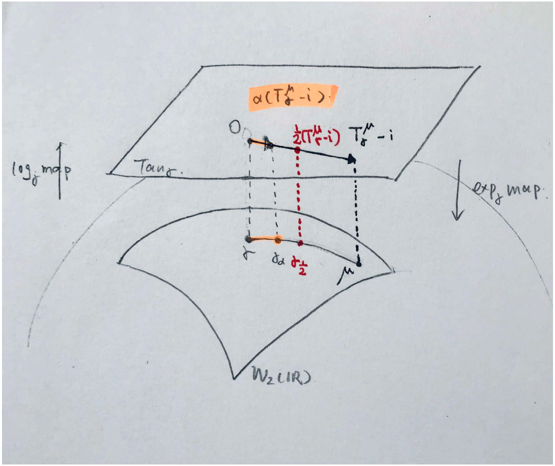

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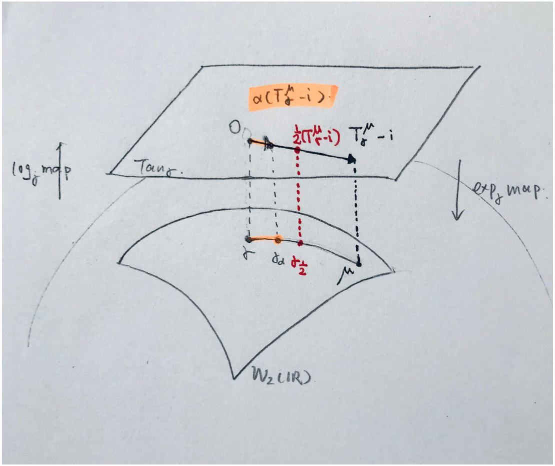

$$d_W(\gamma, \gamma_\alpha) = \alpha d_W(\gamma, \mu)$$

Related work: Univariate Wasserstein AR model

Vector AR models with $N = 1$:

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Chen et al. (2021); Zhang et al. (2021); Zhu and Müller (2021) extended the univariate AR model by **interpreting the regressive dependency from a geometric point of view.**

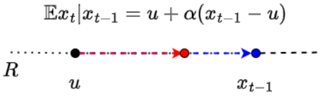

Figure 4: *Geometric interpretation of regressive dependency of AR models.*

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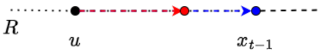

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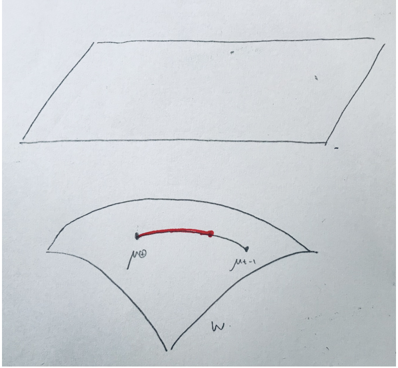

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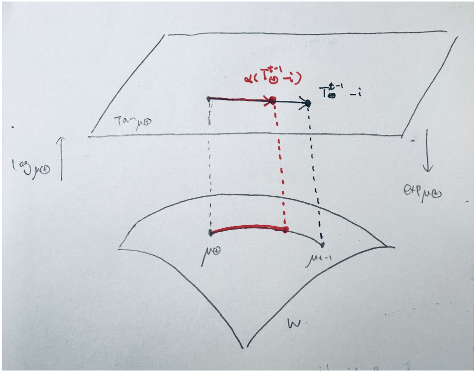
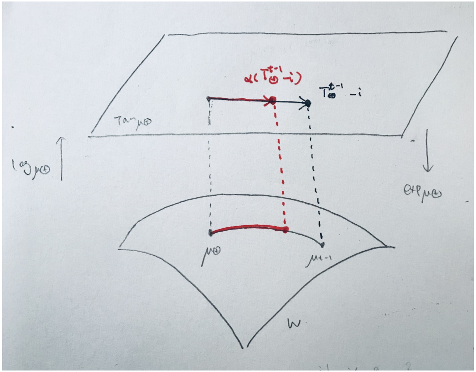


$$\mathbb{E}\boldsymbol{x}_t|\boldsymbol{x}_{t-1} = u + \alpha(\boldsymbol{x}_{t-1} - u) \Longrightarrow \mathbb{E}_{\oplus}\boldsymbol{\mu}_t|\boldsymbol{\mu}_{t-1} = \mathrm{Exp}_{\mu_\oplus}\left\{\alpha(\boldsymbol{T}_{\oplus}^{t-1} - i)\right\}$$



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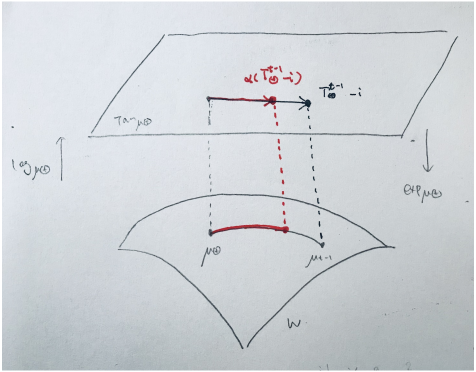
Let $\boldsymbol{\mu}, \boldsymbol{\gamma}$ be two random measures from $(\Omega, \mathcal{F}, \mathbb{P})$ to $\mathcal{W}_2$,

$$\mathbb{E}_{\oplus}\boldsymbol{\mu} = \underset{\nu\in\mathcal{W}_2}{\arg\min}\,\mathbb{E}\left[d_W^2(\boldsymbol{\mu},\nu)\right], \; \mathbb{E}_{\oplus}\boldsymbol{\mu}|\boldsymbol{\gamma} := \underset{\nu\in\mathcal{W}_2}{\arg\min}\,\mathbb{E}\left[d_W^2(\boldsymbol{\mu},\nu)|\boldsymbol{\gamma}\right]$$



Multivariate Wasserstein AR model

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We proposed a centering for random measures so that the centered measures always have $U[0,1]$ as population Fréchet mean.

Multivariate Wasserstein AR model

For a multivariate distributional time series $\boldsymbol{\mu}_{it}$, $i = 1, \ldots, N, t \in \mathbb{Z}$, we define the regressive dependency on their centered versions $\tilde{\boldsymbol{\mu}}_{it} \leftrightarrow \tilde{\boldsymbol{F}}_{it}^{-1} := \boldsymbol{F}_{it}^{-1} \circ [F_{i,\oplus}^{-1}]^{-1}$ as

$$\mathbb{E}_{\oplus}\widetilde{\boldsymbol{\mu}}_{it}|\widetilde{\boldsymbol{\mu}}_{j,t-1} = \mathrm{Exp}_{Leb}\left(\sum_{j=1}^{N} A_{ij}(\widetilde{\boldsymbol{T}}_{Leb}^{j,t-1} - i)\right),$$

where $\widetilde{\boldsymbol{T}}_{Leb}^{j,t-1} - i$ is the tangent vector of $\widetilde{\boldsymbol{\mu}}_{j,t-1}$.

Multivariate Wasserstein AR model

For a multivariate distributional time series $\boldsymbol{\mu}_{it}$, $i = 1, \ldots, N, t \in \mathbb{Z}$, we define the regressive dependency on their centered versions $\tilde{\boldsymbol{\mu}}_{it} \leftrightarrow \tilde{\boldsymbol{F}}_{it}^{-1} := \boldsymbol{F}_{it}^{-1} \circ [F_{i,\oplus}^{-1}]^{-1}$ as

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3. Theoretically, we proved the stationarity under assumptions.

Constrained least-square estimation

Given the observations $\boldsymbol{\mu}_{it}, t = 0, ..., T, i = 1, ..., N$ (thus the centered observations $\widetilde{\boldsymbol{\mu}}_{it}$), we propose the estimator of A as

$$\widetilde{\boldsymbol{A}} = \underset{\substack{A \text{ satisfies the} \\ \text{model assumptions}}}{\arg\min}{}^{1} \; \frac{1}{T} \sum_{t=1}^{T} d_{\mathcal{W}}^{2} \left(\widetilde{\boldsymbol{\mu}}_{it}, \; \mathbb{E}_{\oplus} \widetilde{\boldsymbol{\mu}}_{it} | \widetilde{\boldsymbol{\mu}}_{j,t-1} \right),$$

[1] The details see Jiang (2022).

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$\widetilde{\boldsymbol{A}}$ is sparse and $0 \leqslant \widetilde{\boldsymbol{A}}_{ij} \leqslant 1$.

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We proved that $\widetilde{\boldsymbol{A}}$ is consistent.

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Age distributions of countries

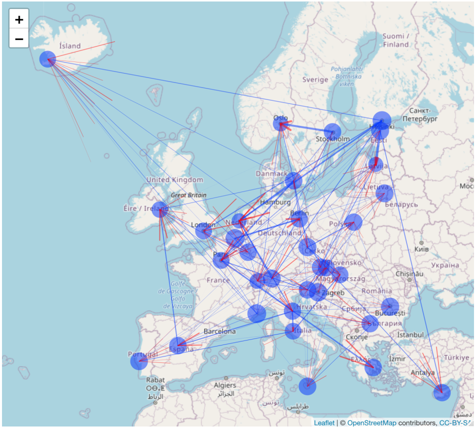

Figure 6: *Visualization of* $\widetilde{\boldsymbol{A}}$. $\widetilde{\boldsymbol{A}}_{ij}$ are represented by the weighted directed edges from node j to node i.

Age distributions of countries

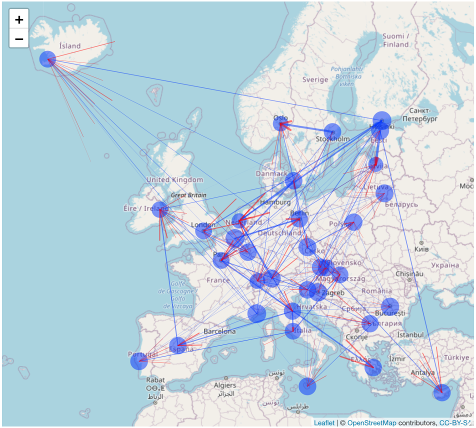

Figure 7: *Visualization of $\widetilde{\boldsymbol{A}}$.* $\widetilde{\boldsymbol{A}}_{ij}$ are represented by the weighted directed edges from node j to node i. Thicker edges correspond to larger values.

Age distributions of countries

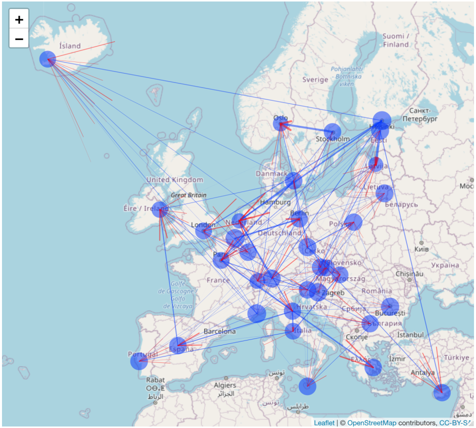

Figure 8: *Visualization of $\widetilde{\boldsymbol{A}}$.* $\widetilde{\boldsymbol{A}}_{ij}$ are represented by the weighted directed edges from node j to node i. Thicker edges correspond to larger values. The blue circles around nodes represent $\widetilde{\boldsymbol{A}}_{ii}$.

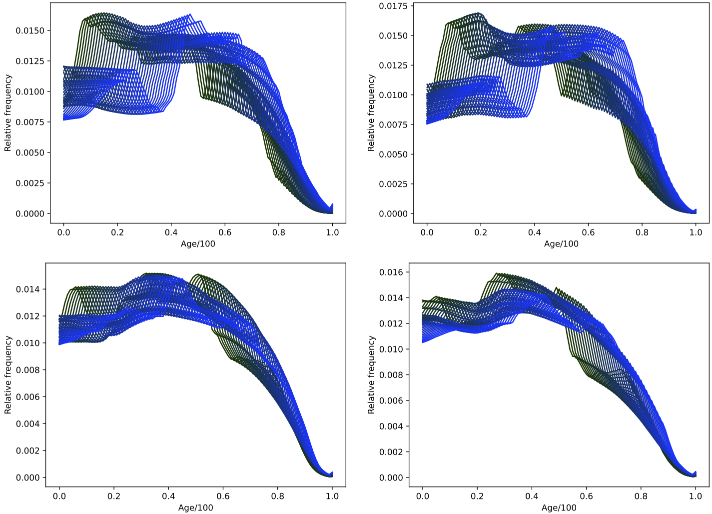

Figure 9: *Evolution of age structure from* 1996 *to* 2036 *(projected). Estonia (top left), Latvia(top right), Sweden (bottom left) versus Norway (bottom right).*

Age distributions of countries

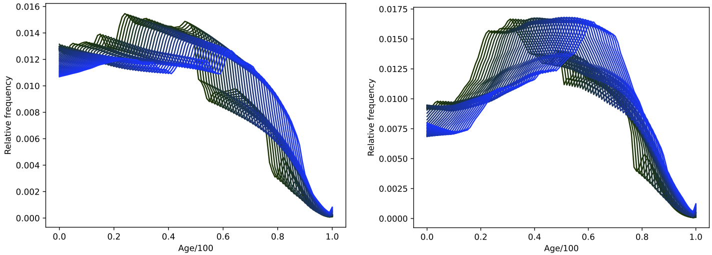

Figure 10: *Evolution of age structure from* 1996 *to* 2036 *(projected) of France (left) versus Italy (right).*

Thanks for your attention !

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Assumption

$\boldsymbol{\mu}$ is supported on $[0,1]$.

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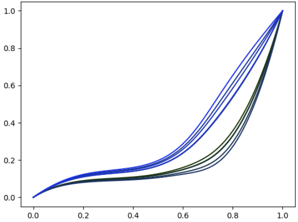

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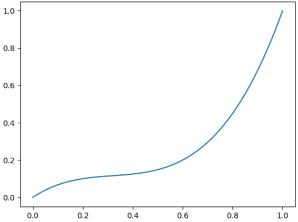

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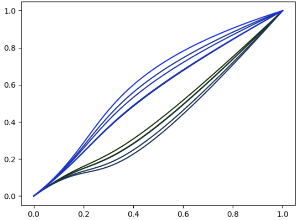

Multivariate Wasserstein AR model

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1. identifiable: $\begin{cases} A \rightarrow \mathbb{E}_{\oplus}\widetilde{\boldsymbol{\mu}}_{it}|\widetilde{\boldsymbol{\mu}}_{j,t-1} \\ A' \rightarrow \mathbb{E}_{\oplus}\widetilde{\boldsymbol{\mu}}_{it}|\widetilde{\boldsymbol{\mu}}_{j,t-1} \end{cases}$

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For $\boldsymbol{\mu}_{it}$, $t \in \mathbb{Z}, i = 1, \ldots, N$, we propose the Wasserstein multivariate AR Model

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Quantile function representation

$$\widetilde{\boldsymbol{F}}_{i,t}^{-1} = \boldsymbol{\epsilon}_{i,t} \circ \left[\sum_{j=1}^{N} A_{ij} \left(\widetilde{\boldsymbol{F}}_{j,t-1}^{-1} - i \right) + id \right],$$

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Iterated random function system: TS analysis in metric space

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$\boldsymbol{\Phi}_{\epsilon_t}$ contractive at exp decay rate in expectation $\rightarrow$ *stability*

$$\rightarrow existence \xrightarrow{\text{add str}} stationarity.$$

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$$\Rightarrow (\mathcal{X}, d) := (\mathcal{T}, \|\cdot\|_{Leb})^{\otimes N},$$

for any $\mathbf{X} = (\mathbf{X}_i)_{i=1}^N, \mathbf{Y} = (\mathbf{Y}_i)_{i=1}^N \in (\mathcal{T}, \|\cdot\|_{Leb})^{\otimes N}$

$$d(\mathbf{X}, \mathbf{Y}) := \sqrt{\sum_{i=1}^{N} \|\mathbf{X}_i - \mathbf{Y}_i\|_{Leb}^2}.$$

Existence, uniqueness

$$\widetilde{\boldsymbol{F}}_{i,t}^{-1} = \boldsymbol{\epsilon}_{i,t} \circ \left[\sum_{j=1}^{N} A_{ij} \left(\widetilde{\boldsymbol{F}}_{j,t-1}^{-1} - i \right) + id \right], \quad i = 1, \ldots, N. \quad (1)$$

Contraction of system (at exp decay rate)

1. $\mathbb{E} \left[\boldsymbol{\epsilon}_{i,t}(x) - \boldsymbol{\epsilon}_{i,t}(y) \right]^2 \leqslant L^2 (x-y)^2, \ \forall x, y \in [0,1], t \in \mathbb{Z}, \ i = 1, \ldots, N,$
2. $\|A\|_2 < \frac{1}{L}$.

Theorem

Under the assumptions above, the IRF system (1) almost surely admits a solution $\boldsymbol{X}_t$, $t \in \mathbb{Z}$, with $\boldsymbol{X}_t \overset{d}{=} \pi$, $\forall\, t \in \mathbb{Z}$. Moreover, if there exists another solution $\boldsymbol{S}_t$, $t \in \mathbb{Z}$, then for all $t \in \mathbb{Z}$

$$\boldsymbol{X}_t \overset{d}{=} \boldsymbol{S}_t, \quad \textit{almost surely.}$$

Stationarity

Stationarity

Definition: A random process $\{\mathbf{V}_t\}_t$ in a separable Hilbert space $(\mathcal{H}, \langle\cdot,\cdot\rangle)$ is said to be stationary if

1. $\mathbb{E}\left\|\mathbf{V}_t\right\|^2 < \infty$
2. The Hilbert mean $U := \mathbb{E}\left[\mathbf{V}_t\right]$ does not depend on t.
3. The auto-covariance operators defined as

$$\mathcal{G}_{t,t-h}(V) := \mathbb{E}\left\langle \mathbf{V}_t - U, V\right\rangle \left(\mathbf{V}_{t-h} - U\right), \quad V \in \mathcal{H},$$

do not depend on t, that is $\mathcal{G}_{t,t-h}(V) = \mathcal{G}_{0,-h}(V)$ for all t.

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$d(X,Y) = \sqrt{\sum_{i=1}^{N} \|X_i - Y_i\|_{Leb}^2}$ is induced by the inner product:

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Stationarity

Theorem

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The model we propose is justified, thus it is a valid TS model.

Constrained least-square estimation

For auto-regressive model

$$\widetilde{\boldsymbol{F}}_{i,t}^{-1} = \boldsymbol{\epsilon}_{i,t} \circ \left[\sum_{j=1}^{N} A_{ij} \left(\widetilde{\boldsymbol{F}}_{j,t-1}^{-1} - i \right) + id \right],$$

Given the centered observations $\widetilde{\boldsymbol{F}}_{t}^{-1}$, $t = 0, 1, \ldots, T$, we propose

$$\widetilde{\boldsymbol{A}}_{i:} = \underset{A_{i:} \in B_{+}^{1}}{\arg\min} \frac{1}{T} \sum_{t=1}^{T} \left\| \widetilde{\boldsymbol{F}}_{i,t}^{-1} - \sum_{j=1}^{N} A_{ij} \left(\widetilde{\boldsymbol{F}}_{j,t-1}^{-1} - i \right) - i \right\|_{Leb}^{2},$$

where B_{+}^{1} is the constraint set of N-simplex.

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$$\widetilde{\boldsymbol{F}}_{i,t}^{-1} := \boldsymbol{F}_{i,t}^{-1} \circ (F_{i,\oplus}^{-1})^{-1},$$

where the population Fréchet mean $\mu_{i,\oplus}$ is also an unknown parameter so is $F_{i,\oplus}^{-1}$, we estimate by the empirical Fréchet mean

$$\bar{\boldsymbol{\mu}}_i := \underset{\nu \in \mathcal{W}_2}{\arg\min} \frac{1}{T} \sum_{t=1}^{T} d_W^2(\boldsymbol{\mu}_{i,t}, \nu), \quad \text{with } \boldsymbol{F}_{\bar{\mu}_i}^{-1} = \frac{1}{T} \sum_{t=1}^{T} \boldsymbol{F}_{\mu_{i,t}}^{-1}$$

Constrained least-square estimation

In practice, we center $\boldsymbol{\mu}_{i,t}$ by $\boldsymbol{F}_{\bar{\mu}_i}^{-1}$

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The optimization problem (1) can be solved by the accelerated projected gradient descent (Parikh and Boyd, 2014, Chapter 4.3). The projection onto B_+^1 is given in Thai et al. (2015).

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Note that the N-simplex constraint promotes the **sparsity** in $\widehat{\boldsymbol{A}}$.

Constrained least-square estimation

Theorem

Assume[a] *the transformed sequence* $\widetilde{\boldsymbol{F}}_t^{-1}, t = 0, 1, \ldots, T$ *checks Model* (1) *with Assumption* N*-simplex true. Suppose additionally* $\widetilde{\boldsymbol{F}}_0^{-1} \stackrel{d}{=} \pi$ *with* π *the stationary distribution defined in Theorem 2. Given Assumption contraction of regression operation holds true. Then given the true coefficient* A *satisfies Assumption* N*-simplex, we have*

$$\widehat{\boldsymbol{A}} - A \xrightarrow{p} 0.$$

[a] The complete assumption sees Jiang (2022).

Related work: Univariate Wasserstein AR model

Describe this regressive dependencyship with

AR model of optimal transport (Zhu and Müller, 2021):

$$\boldsymbol{T}_{t+1} = \boldsymbol{\epsilon}_t \circ (\alpha(\boldsymbol{T}_t - i) + id), \quad 0 < \alpha < 1$$

AR model of tangent vector (Zhang et al., 2021):

$$\boldsymbol{T}_{t+1} - i = \alpha(\boldsymbol{T}_t - i) + \boldsymbol{\epsilon}_t, \qquad 0 < |\alpha| < 1,$$

Tangent vector with regression operator (Chen et al., 2021)

$$\boldsymbol{T}_{t+1} - i = \Gamma(\boldsymbol{T}_t - i) + \boldsymbol{\epsilon}_t, \quad \Gamma : Log_{\mu_\oplus}(\mathcal{W}) \rightarrow Log_{\mu_\oplus}(\mathcal{W})$$

the model in tangent space than is the ordinary AR model for functional TS in Hilbert space, expect the log image issue