Heat diffusion distance processes:
a statistical method to analyze graph data

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Datashape Seminar

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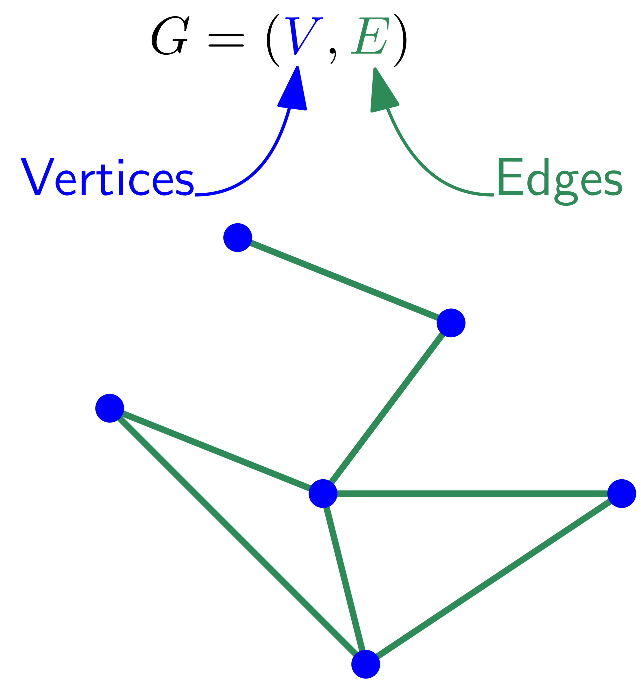
Introduction

Goals :

- analysis of graph samples

$$(G_1, \ldots, G_N)$$

- theoretical results (asymptotic in N)
- useable in practice



Requirements :

- take into account topological information
- graphs can be weighted
- graph sizes (same/different)
- node correspondance (known/unknown)

Outline

1. Tools
   - Heat Kernel Diffusion Processes
   - Heat Persistence Diffusion Processes

2. Theoretical Results
   - Functional Central Limit Theorem
   - Gaussian Approximation Rates

3. Simulations
   - Confidence Bands
   - Two-sample Tests
   - Neural Networks

Comparing graphs

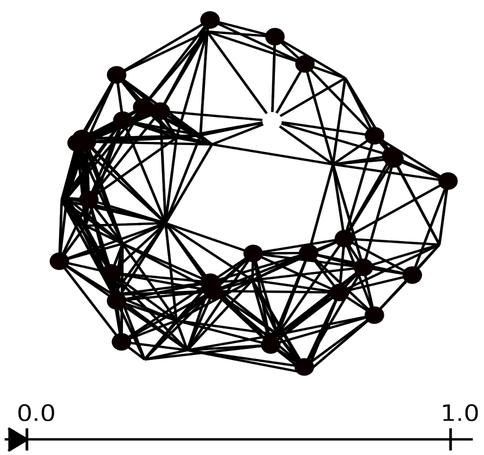
Assumption :
same sizes n & known node correspondance.

Heat Diffusion :

W, weight matrix, $W_{i,j}$: weight of $\{i,j\}$,
0 if $\{i,j\}$ is not in G.

D, degree matrix, $D_{i,i} = \sum_{j=1}^{n} W_{i,j}$

L = D - W, laplacian.



Initial heat distribution $u_0 \in \mathbb{R}^n$

$$\frac{d}{dt} u_t = -L u_t, \quad t \geq 0$$

e^{-tL}, heat kernel at time t :

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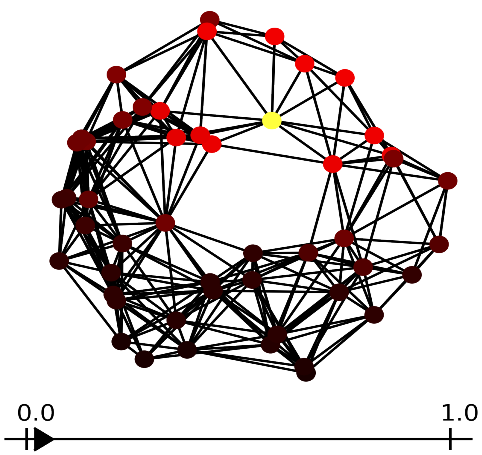

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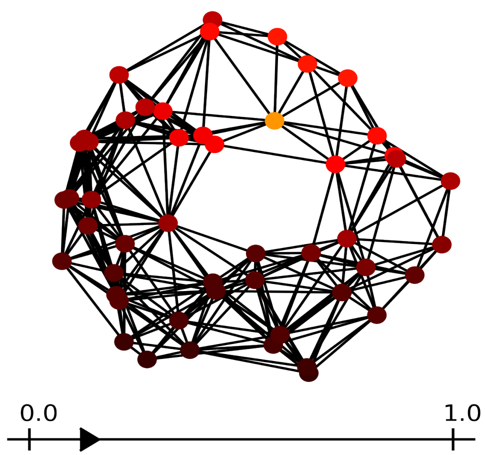

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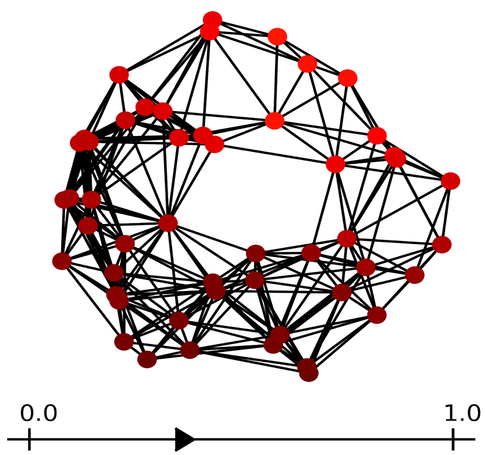

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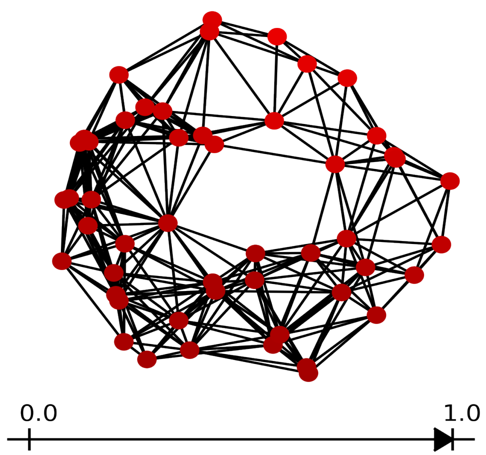

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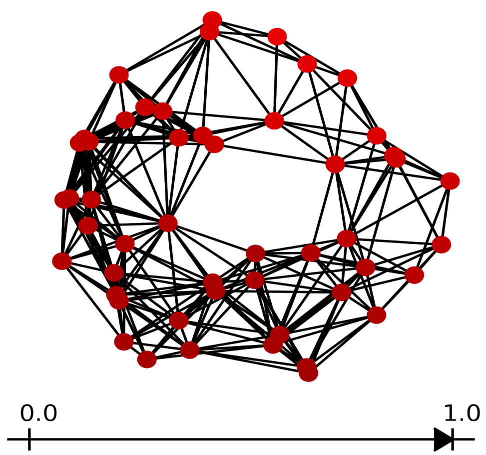

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e^{-tL}, heat kernel at time t :

Heat Kernel Distance : $D_t(G, G') = \|e^{-tL} - e^{-tL'}\|_F$ [HGJ13]

- respectful of the topology ✓
- t : scale parameter ✓

[HGJ13] : Graph diffusion distance: A difference measure for weighted graphs based on the graph Laplacian exponential kernel, Hammond, Gur, Johnson, 2013

Comparing graphs

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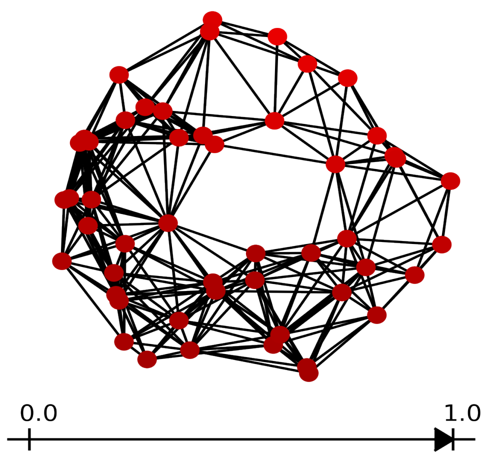

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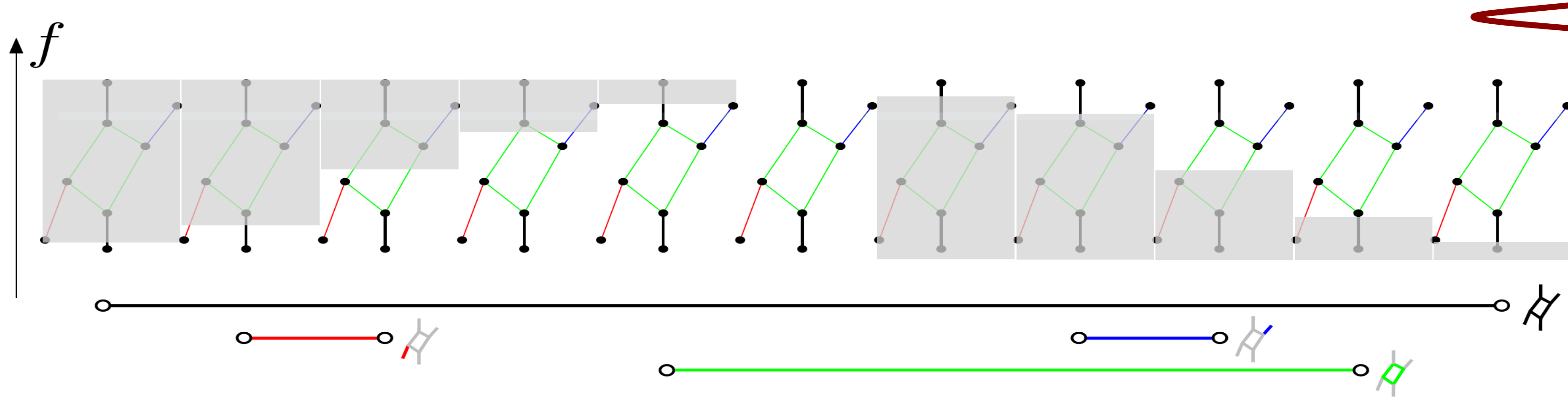
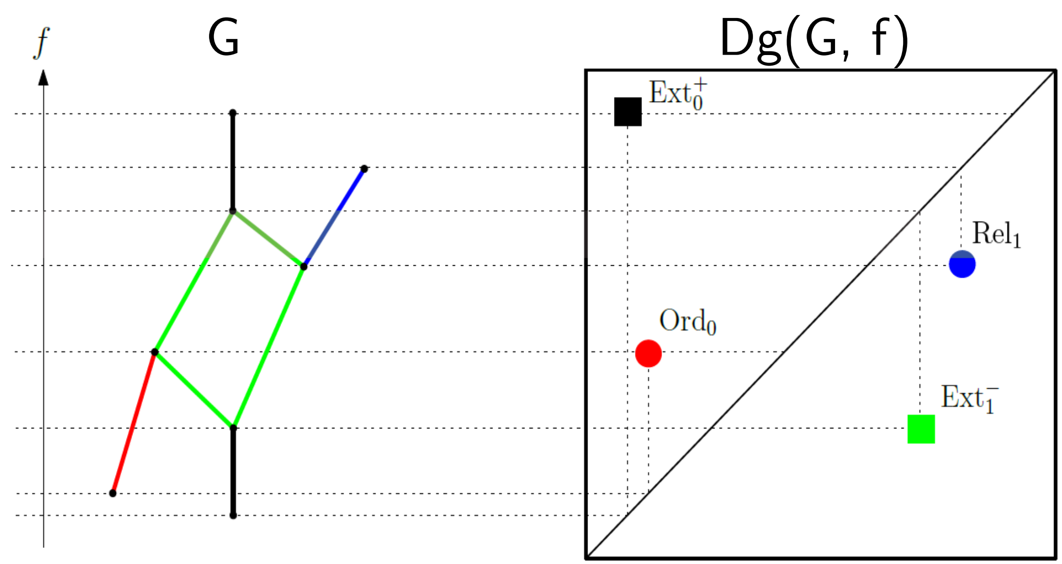
Using Topological Data Analysis

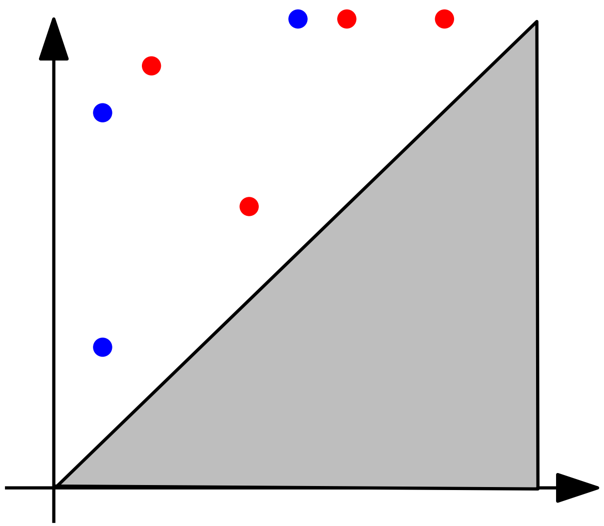




Figures from [CCIL+19]

[CCIL+19]: Perslay : A Neural Network Layer for Persistence Diagrams and New Graph Topological Signatures, Carriere, Chazal, Ike, Lacombe, Royer, Umeda, 2019

Comparing persistence diagrams



μ, ν : finite multisets of points in $\mathbb{R}^2$.
$\Delta = \{(a,a), \forall a \in \mathbb{R}\}$: diagonal

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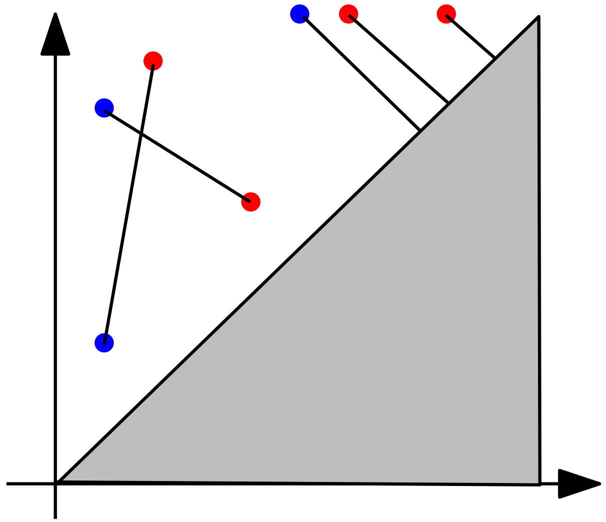

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π : a matching from $\mu \cup \Delta$ to $\nu \cup \Delta$

$$\sup_{x \in \mu \cup \Delta} \|x - \pi(x)\|_\infty$$

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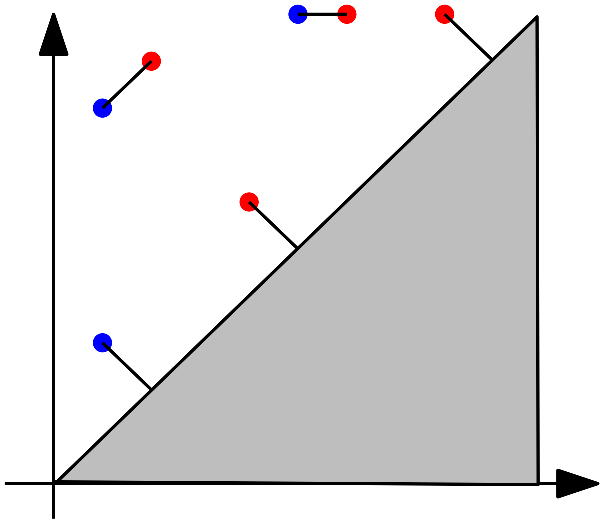

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π : a matching from $\mu \cup \Delta$ to $\nu \cup \Delta$

$\Pi(\mu,\nu)$: set of all matchings

Bottleneck Distance :

$$d_B(\mu,\nu) := \inf_{\pi \in \Pi(\mu,\nu)} \sup_{x \in \mu \cup \Delta} \|x - \pi(x)\|_\infty$$

Choice of f

Heat Kernel Signature (HKS) : [SOG09] [HRG14]

$$h_t(G) : i \to (e^{-tL})_{i,i}$$

"Remaining heat at node i"

[SOG09]: A concise and provably informative multiscale signature based on heat diffusion, Sun, Ovsjanikov, Guibas, 2009

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Heat Persistence Distance (HPD) :

$$\boxed{H_t(G, G') = \max_{D_g} \; d_B\left(Dg\left(G, h_t(G)\right), Dg\left(G', h_t(G')\right)\right)}$$

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How choose t ?

Don't Choose !

Functional Point of View

$$D.(G,G') : \begin{array}{ccc} [0,T] & \mapsto & \mathbb{R} \\ t & \mapsto & D_t(G,G') \end{array} \quad \text{or} \quad H.(G,G') : \begin{array}{ccc} [0,T] & \mapsto & \mathbb{R} \\ t & \mapsto & H_t(G,G') \end{array}$$

Empirical Process Point of View

$$\{D_t((G,G')), \quad t \in [0,T]\} \quad \text{or} \quad \{H_t((G,G')), \quad t \in [0,T]\}$$

$$\mathcal{F}_{HKD} = \{D_t(\cdot), \quad t \in [0,T]\} \quad \text{or} \quad \mathcal{F}_{HPD} = \{H_t(\cdot), \quad t \in [0,T]\}$$

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(G_0, G'_0) (G_1, G'_1)

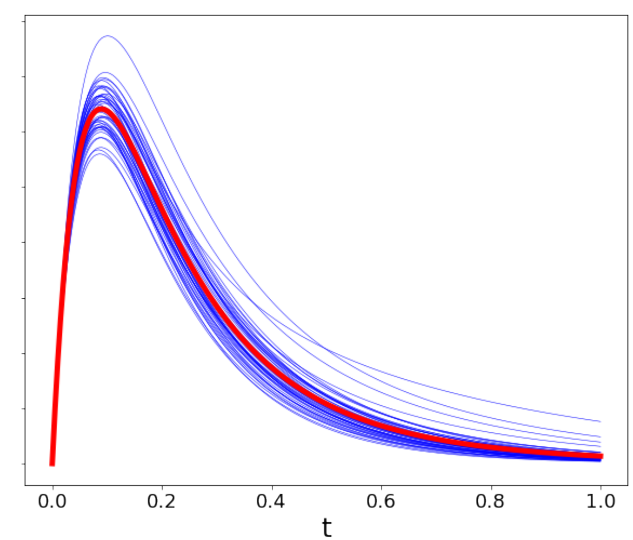
(G_2, G'_2) $(G_{\dots}, G'_{\dots})$

(G_N, G'_N)

Dataset

$D_\cdot(\cdot)$

or $H_\cdot(\cdot)$



Lipschitz continuity

$\forall (G, G')$ of size n with bounded positive weights,
$t \rightarrow D_t(G, G')$ is k-lipschitz continuous.

$\forall (G, G')$ of size at most n with bounded positive weights,
$t \rightarrow H_t(G, G')$ is k-lipschitz continuous.

Remark
k is independent of (G, G')
k depends on n

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$\forall(G,G')$ of size n with bounded positive weights,
$t \to D_t(G,G')$ is k-lipschitz continuous.

$n^{3/2}w_{\max}$

$\forall(G,G')$ of size at most n with bounded positive weights,
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$2nw_{\max}$

Remark
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Functional central limit theorem

- $(G_1, G'_1), \ldots, (G_N, G'_N) \sim P$ (i.i.d sample)
- P_N : empirical measure

t fixed, $\sqrt{N}(P_N - P)D_t = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \Big(D_t((G_i, G'_i)) - \mathbb{E}_P \left[D_t((G, G')) \right] \Big)$

$$\xrightarrow{\mathcal{D}} \mathcal{N}(0, \sigma_t^2)$$

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The families $\mathcal{F}_{HKD} = \{D_t(\cdot),\ t \in [0,T]\}$ and $\mathcal{F}_{HPD} = \{H_t(\cdot),\ t \in [0,T]\}$ are **Donsker**.

$$\{\sqrt{N}(P_N - P)D_t,\ t \in [0,T]\} \xrightarrow{weak} \text{Gaussian Process } \mathbb{G}$$

$\forall h : \mathcal{C}([0,T]) \to \mathbb{R}$, continuous and bounded

$$\lim_{N \to \infty} \mathbb{E}\left[h\Big(\sqrt{N}(P_N - P)D_. \Big) \right] = \mathbb{E}\left[h(\mathbb{G}) \right]$$

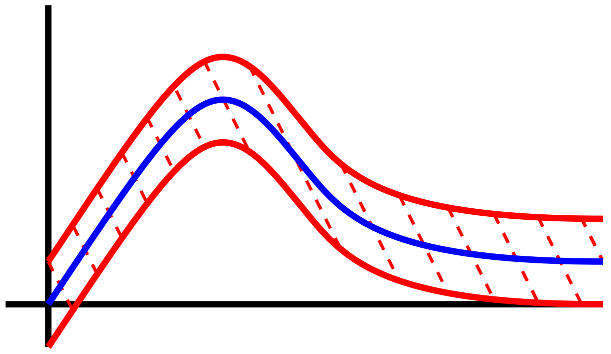
Consequences: consistent confidence bands and two-sample tests

Confidence bands

$\mathcal{D} = (G_1, G'_1), \ldots, (G_N, G'_N) \sim P$
$P_N = N^{-1} \sum_i \delta_{(G_i, G'_i)}$
$\alpha \in]0, 1[$

$$\mathbb{P}\left(\|P_N D. - P D.\|_\infty \geq T_{\alpha,P} \right) \leq \alpha$$

unknown



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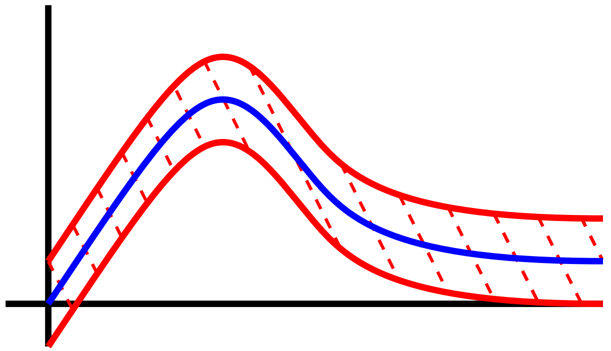

From the Donsker property:

$$\sqrt{N}(P_N D. - PD.) \xrightarrow{weak} \mathbb{G} \xleftarrow{weak} \sqrt{N}(\hat{P}_N D. - P_N D.) \mid \mathcal{D}$$

$\tilde{c}_\alpha$ Monte Carlo estimator of c_α, s.t

$$\mathbb{P}\left(\|\hat{P}_N D. - P_N D.\|_\infty \geq c_\alpha/\sqrt{N} \mid \mathcal{D}\right) \leq \alpha.$$

$$\lim_{N\to\infty} \mathbb{P}\left(\|P_N D. - PD.\|_\infty \geq \tilde{c}_\alpha/\sqrt{N}\right) \leq \alpha$$

Two-sample Tests

$X_1, \ldots, X_N \sim P$ a sample
$P_N = N^{-1} \sum_i \delta_{X_i}$

$Y_1, \ldots, Y_M \sim Q$ a sample
$Q_M = M^{-1} \sum_i \delta_{Y_i}$

$$\mathcal{H}_0 : P = Q \quad \text{or} \quad \mathcal{H}_1 : P \neq Q$$

Idea : compute $T_{N,M} = \|P_N D. - Q_M D.\|_\infty$.

- reject $\mathcal{H}_0$, if $T_{N,M} > T$
- accept $\mathcal{H}_0$, otherwise

$\boxed{\mathbb{P}_{\mathcal{H}_0}(T_{N,M} > T) \leq \alpha}$

$\tilde{c}$: Monte-Carlo estimator of c, s.t.

$$\mathbb{P}\left(\|\hat{P}_N D. - \hat{Q}_M D.\|_\infty \geq c \frac{\sqrt{N+M}}{\sqrt{NM}} \mid \mathcal{D}\right) \leq \alpha.$$

resampled from
$Z = (X_1, \ldots, X_N, Y_1, \ldots, Y_M)$

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$Z = (X_1, \dots, X_N, Y_1, \dots, Y_M)$

$$\boxed{\lim_{N,M \to \infty} \mathbb{P}_{\mathcal{H}_0}\left(T_{N,M} \geq \tilde{c} \frac{\sqrt{N+M}}{\sqrt{NM}} \right) \leq \alpha}$$

$$\boxed{\text{if } PD. \neq QD., \quad \lim_{N,M \to \infty} \mathbb{P}_{\mathcal{H}_1}\left(T_{N,M} \geq \tilde{c} \frac{\sqrt{N+M}}{\sqrt{NM}} \right) = 1}$$

Results

Gaussian Approximation with rate r_N :

$\forall\lambda > 1$, $\exists C$ s.t. $\forall N \geq 1$,
one can construct on the same probability space both X_N and a version of the Gaussian process $\mathbb{G}^{(N)}$, s.t.

$$\mathbb{P}\left(\|X_N - \mathbb{G}^{(N)}\|_\infty > C.r_N\right) \leq N^{-\lambda}.$$

$\left\{\sqrt{N}(P_N - P)D_t, \quad t \in [0,T]\right\}$ and $\left\{\sqrt{N}(P_N - P)H_t, \quad t \in [0,T]\right\}$
admit Gaussian Approximations with rate :

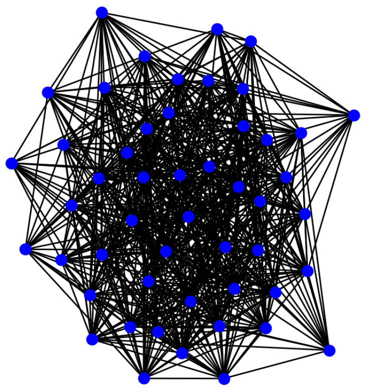
$$r_N = N^{-1/7} \log N^{9/14}.$$

Simulations : Stochastic Models

Erdös-Renyi (ER)

$n = 50$

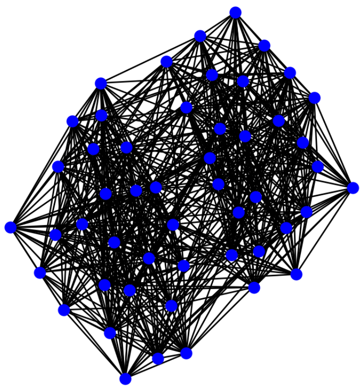
$p = 0.5$



Stochastic Block Model (SBM)

$n_1 = n_2 = 25$

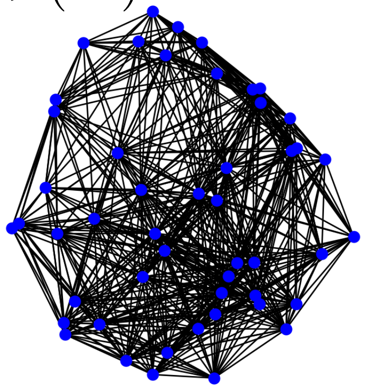
$p = \begin{pmatrix} 0.75, & 0.25 \\ 0.25 & 0.75 \end{pmatrix}$



Geometric (Disk)

$n = 50$ or $\mathcal{P}(50)$

$p = 0.5$



Geometric (Annulus)

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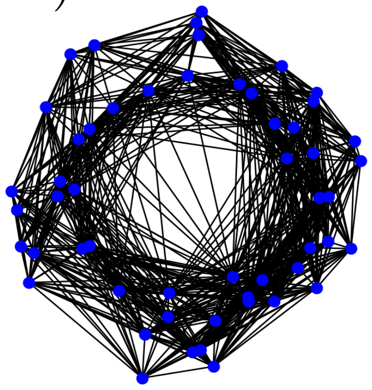
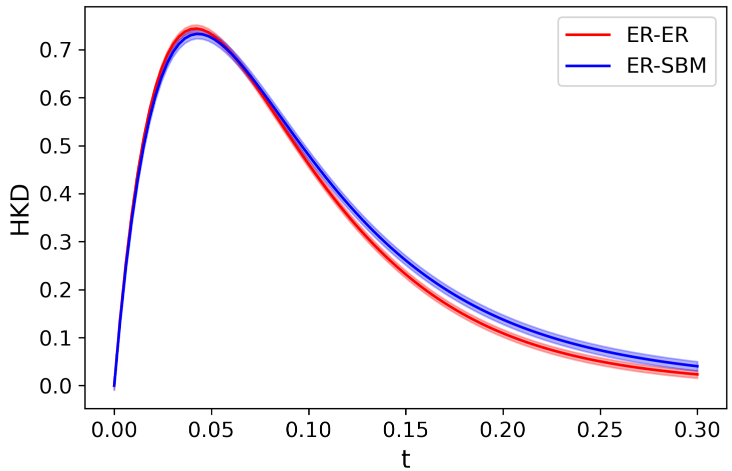
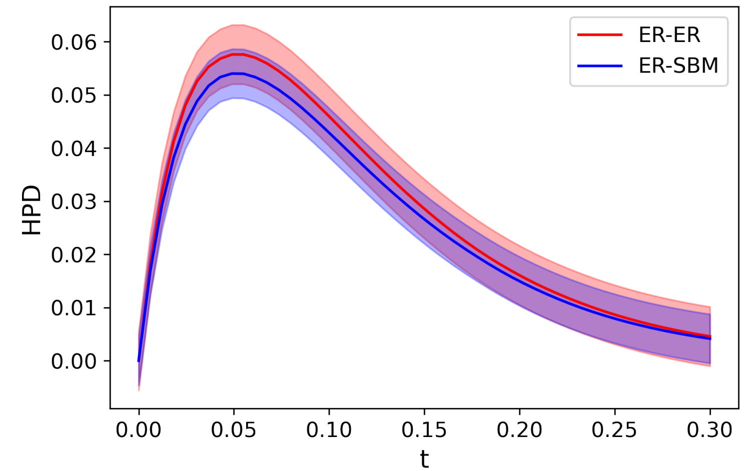
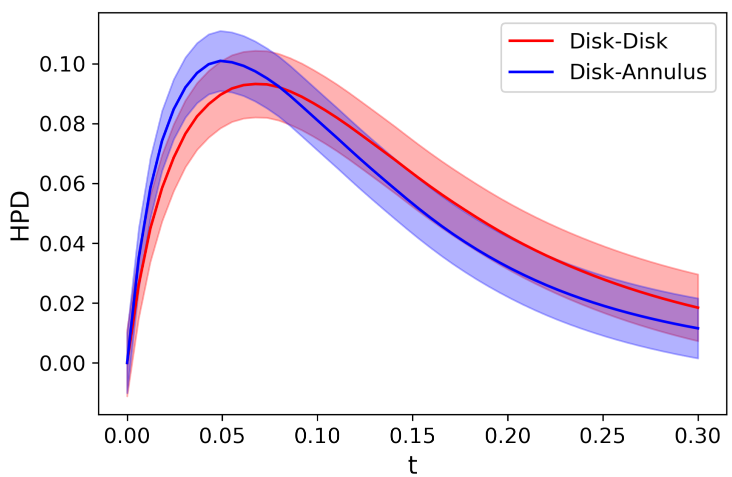
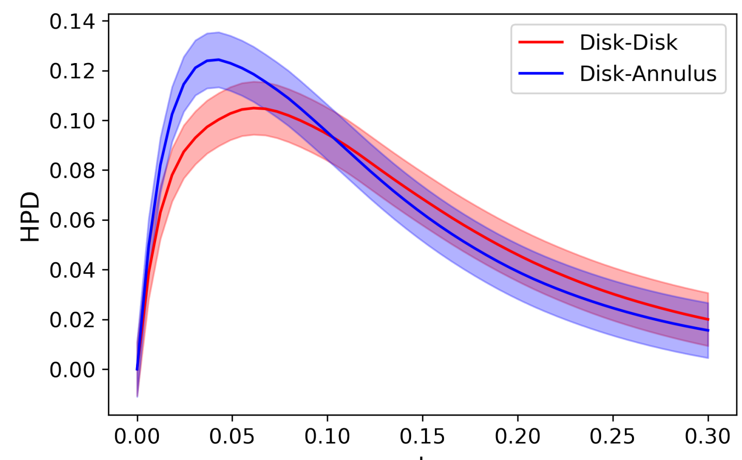


Simulations : Confidence Bands







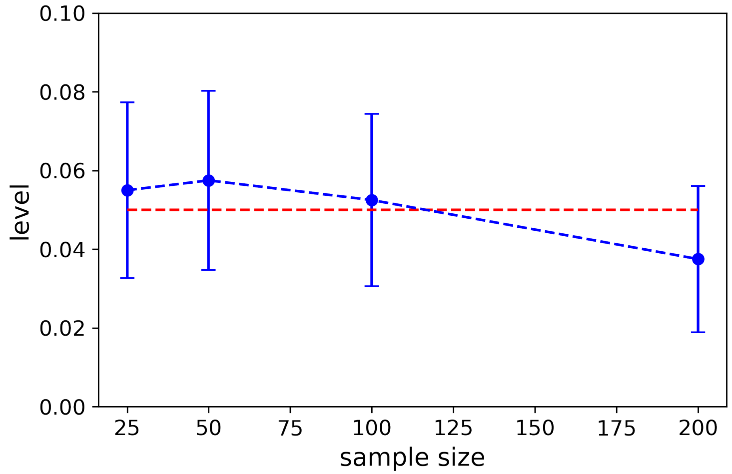


Graphs with random size.

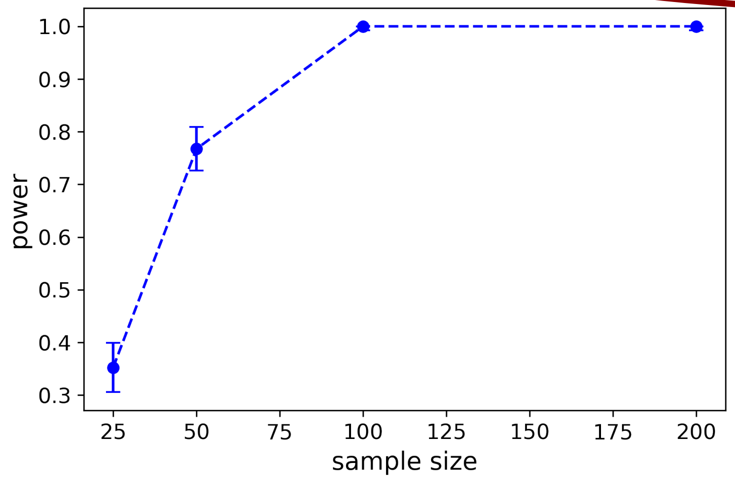
Confidence level 99%, sample size : 100, bootstrap sample size : 1000.

Simulations : Two-sample Tests

HKD



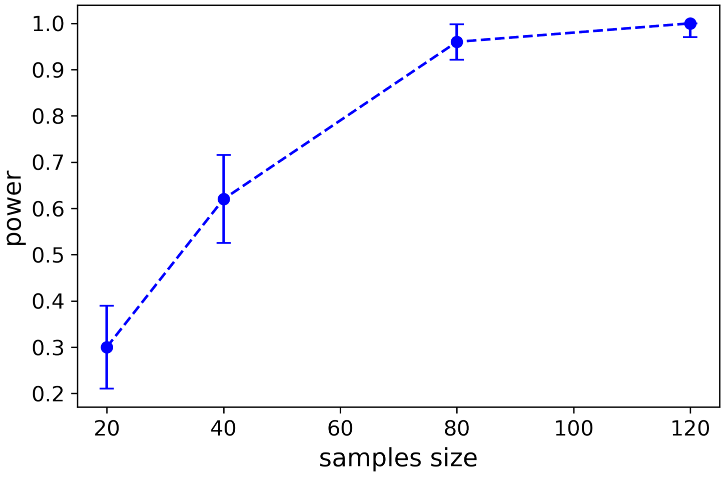
ER-ER



ER-ER vs ER-SBM

Level 95%, bootstrap sample size : 1000, number of tests : 400

HPD



Disk-Disk vs Disk-Annulus

Level 95%, bootstrap sample size : 1000, number of tests : 100

Simulations : Two-sample Tests

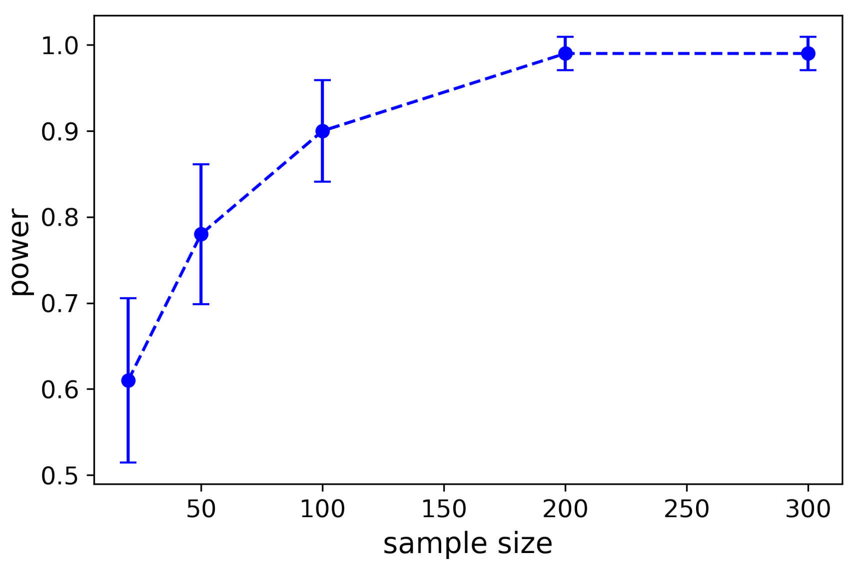
Neyman-Pearson regime :

sample of size N

Neyman-Pearson test : $ER(p_1(N))$ vs $ER(p_2(N))$

$$|p_1(N) - p_2(N)| \gg 1/\sqrt{N}$$

$$n = 50 \qquad \begin{matrix} p_1(N) \searrow \\ \qquad 0.5 \\ p_2(N) \nearrow \end{matrix} \qquad |p_1(N) - p_2(N)| \sim \log(N)/\sqrt{N}$$



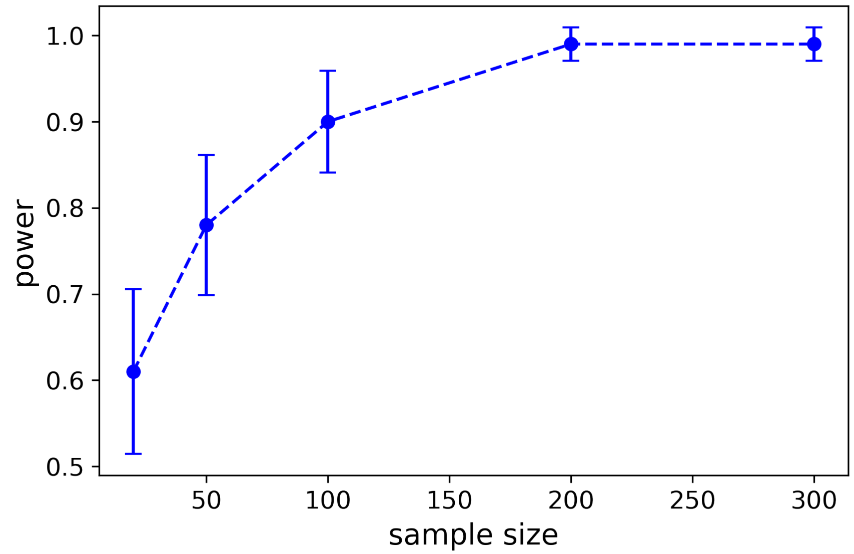
Simulations : Two-sample Tests

Neyman-Pearson regime :

sample of size N
Neyman-Pearson test : $ER(p_1(N))$ vs $ER(p_2(N))$

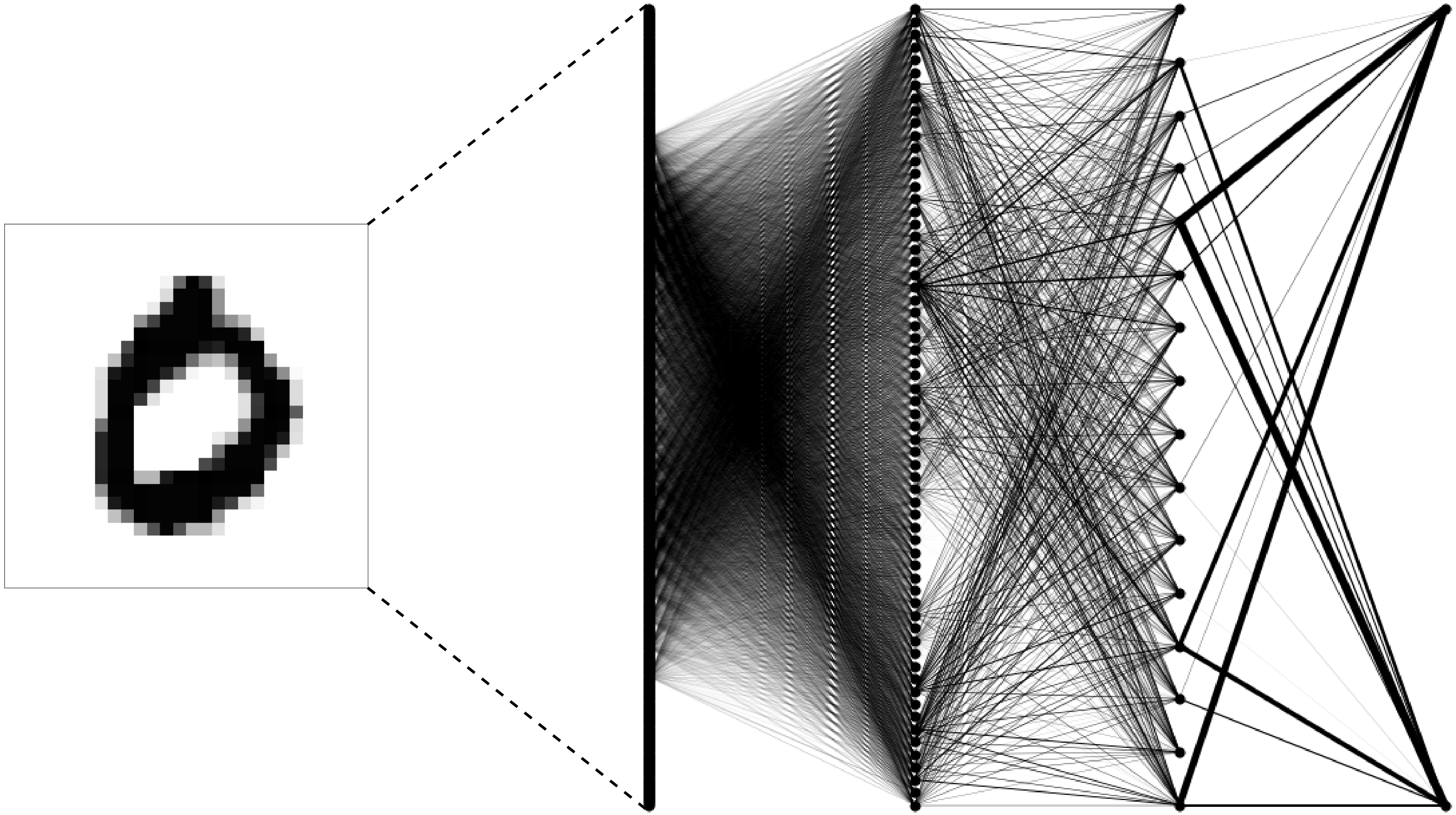
$$|p_1(N) - p_2(N)| \gg 1/\sqrt{N}$$

$$n = 50 \qquad \begin{array}{l} p_1(N) \searrow \\ p_2(N) \nearrow \end{array} 0.5 \qquad |p_1(N) - p_2(N)| \sim \log(N)/\sqrt{N}$$

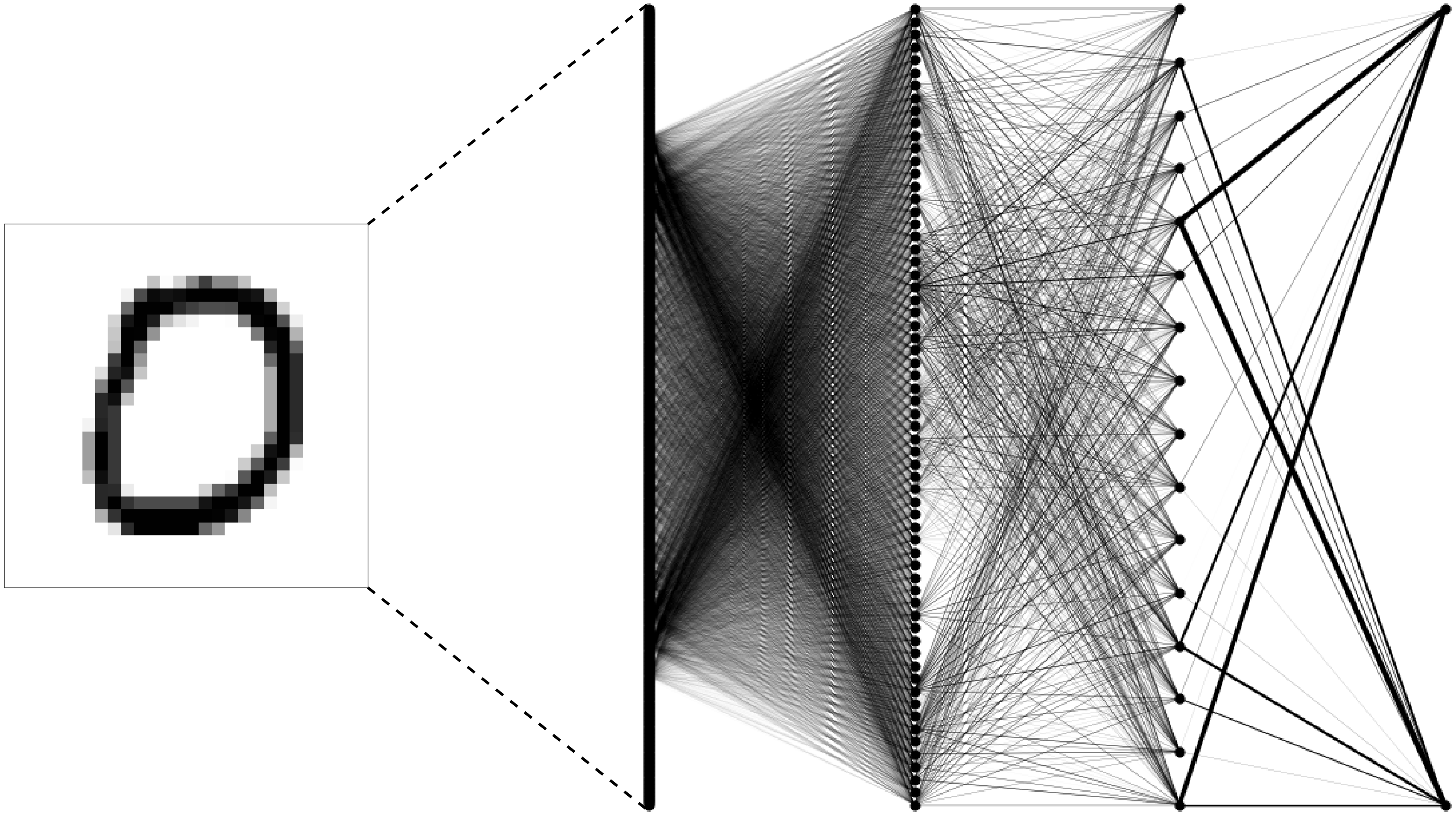


L. (2021) Heat diffusion distance processes: a statistically founded method to analyze graph data sets. arXiv preprint arXiv:2109.13213.

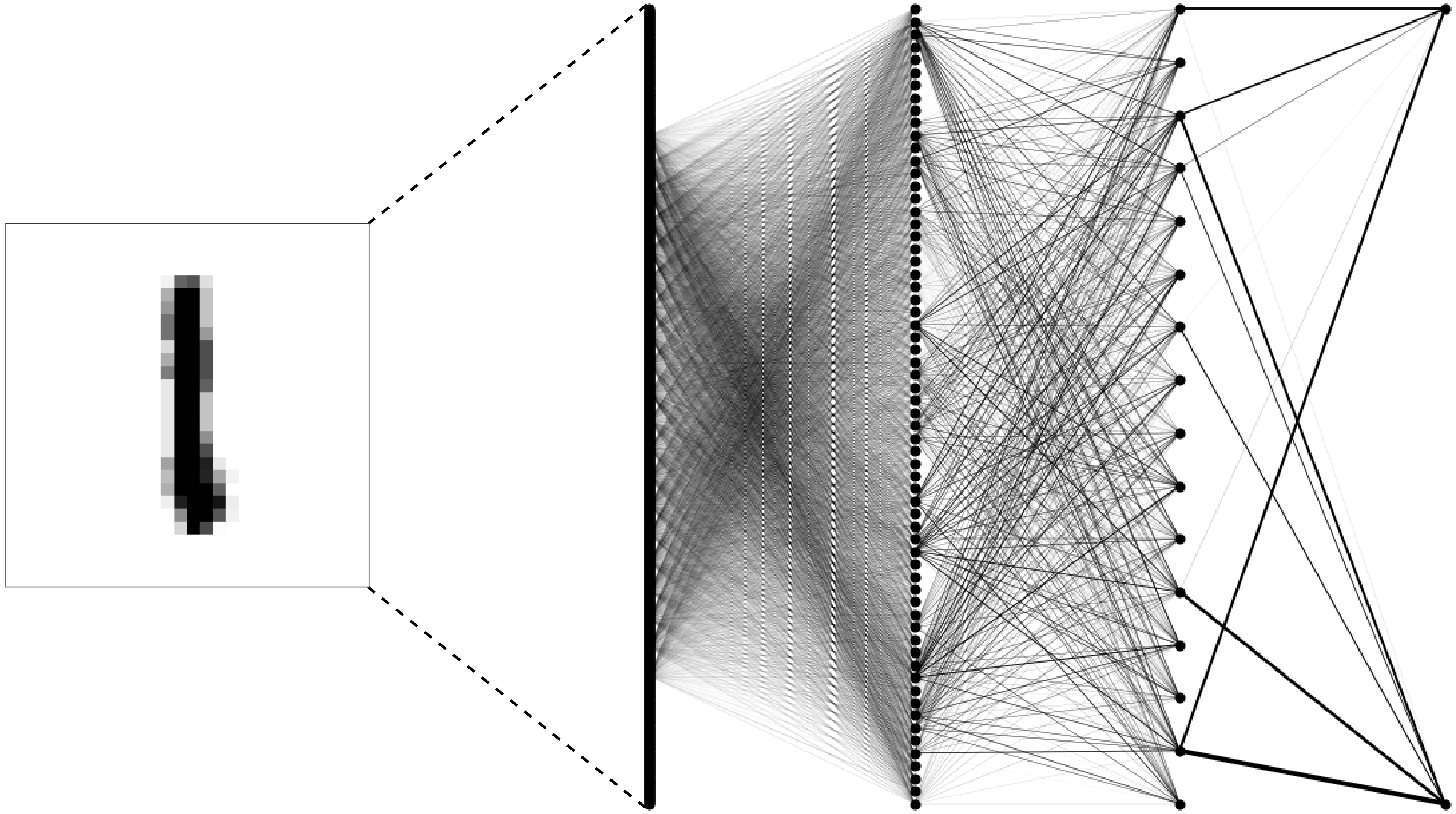
Neural Network (on MNIST)



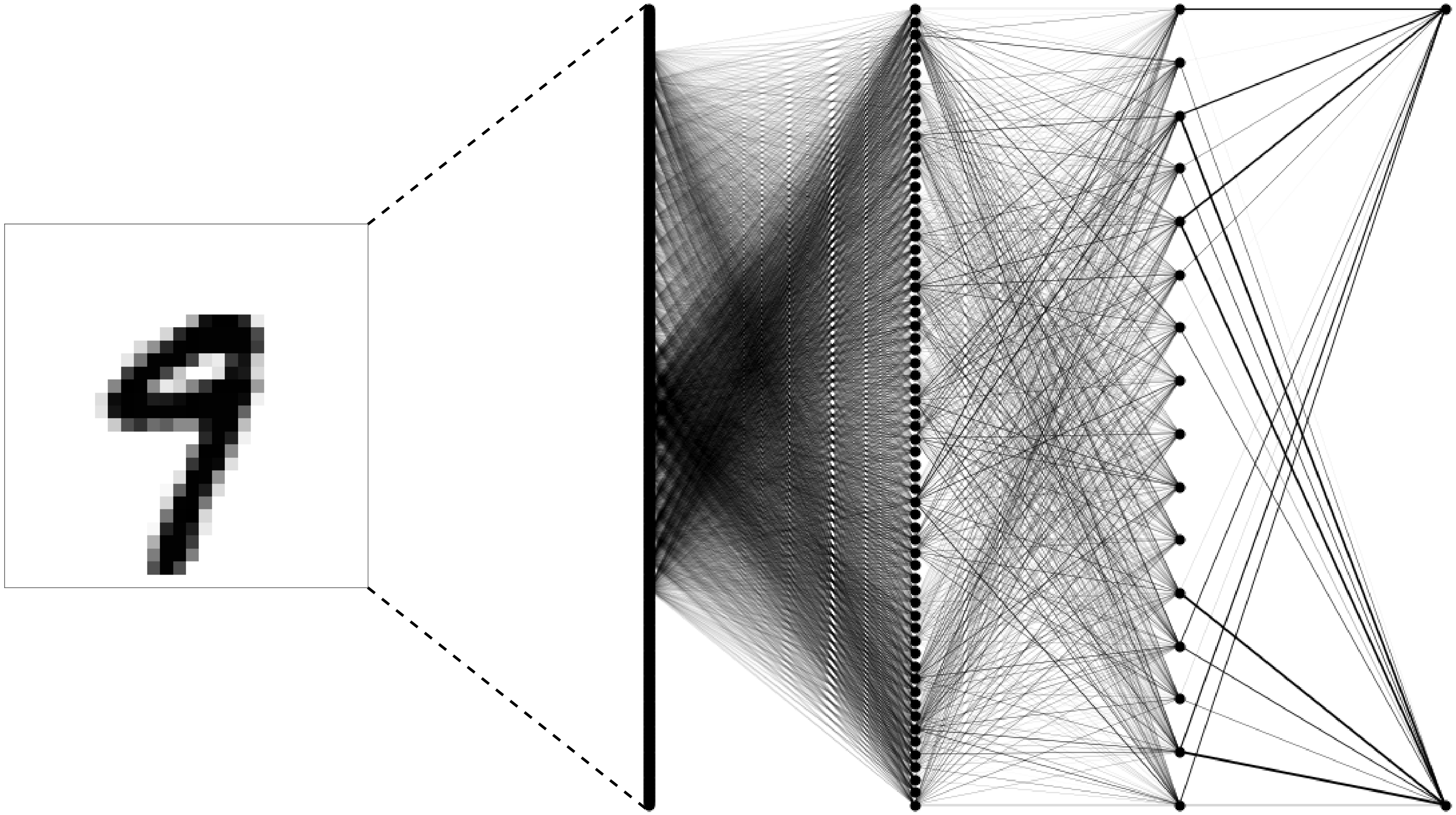
Neural Network (on MNIST)



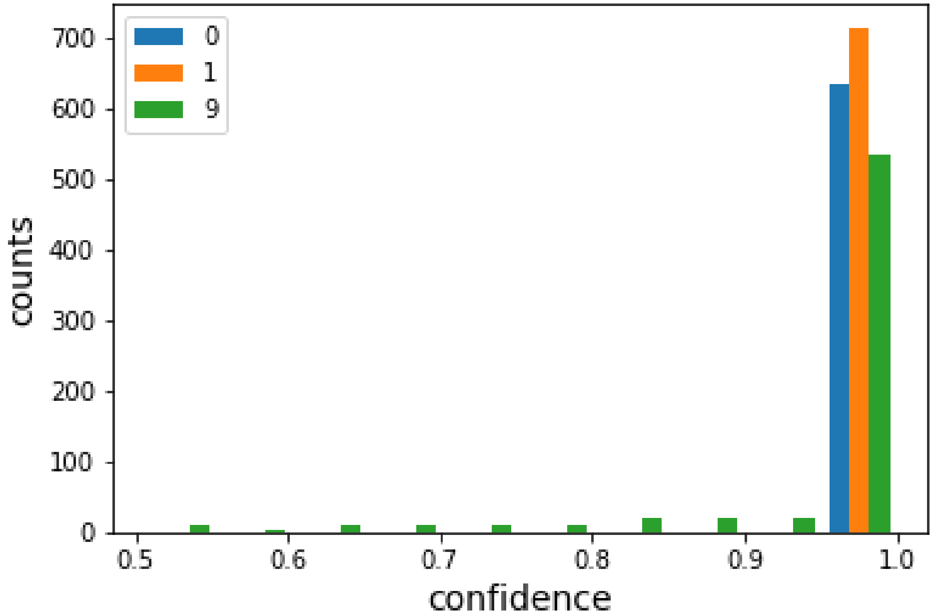
Neural Network (on MNIST)



Neural Network (on MNIST)

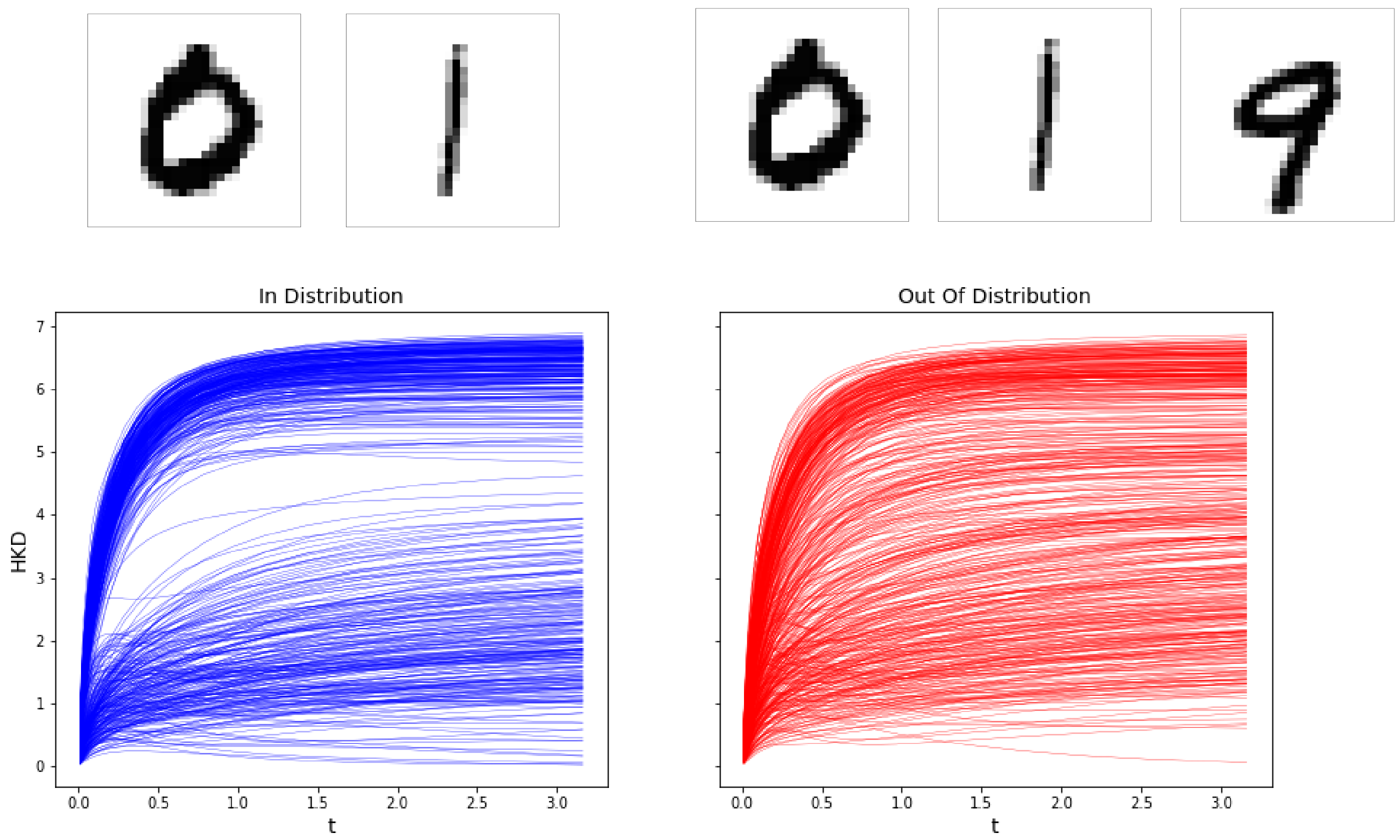


Network confidence



most 9's : confidence $\geq 95\%$.

Out of distribution detection

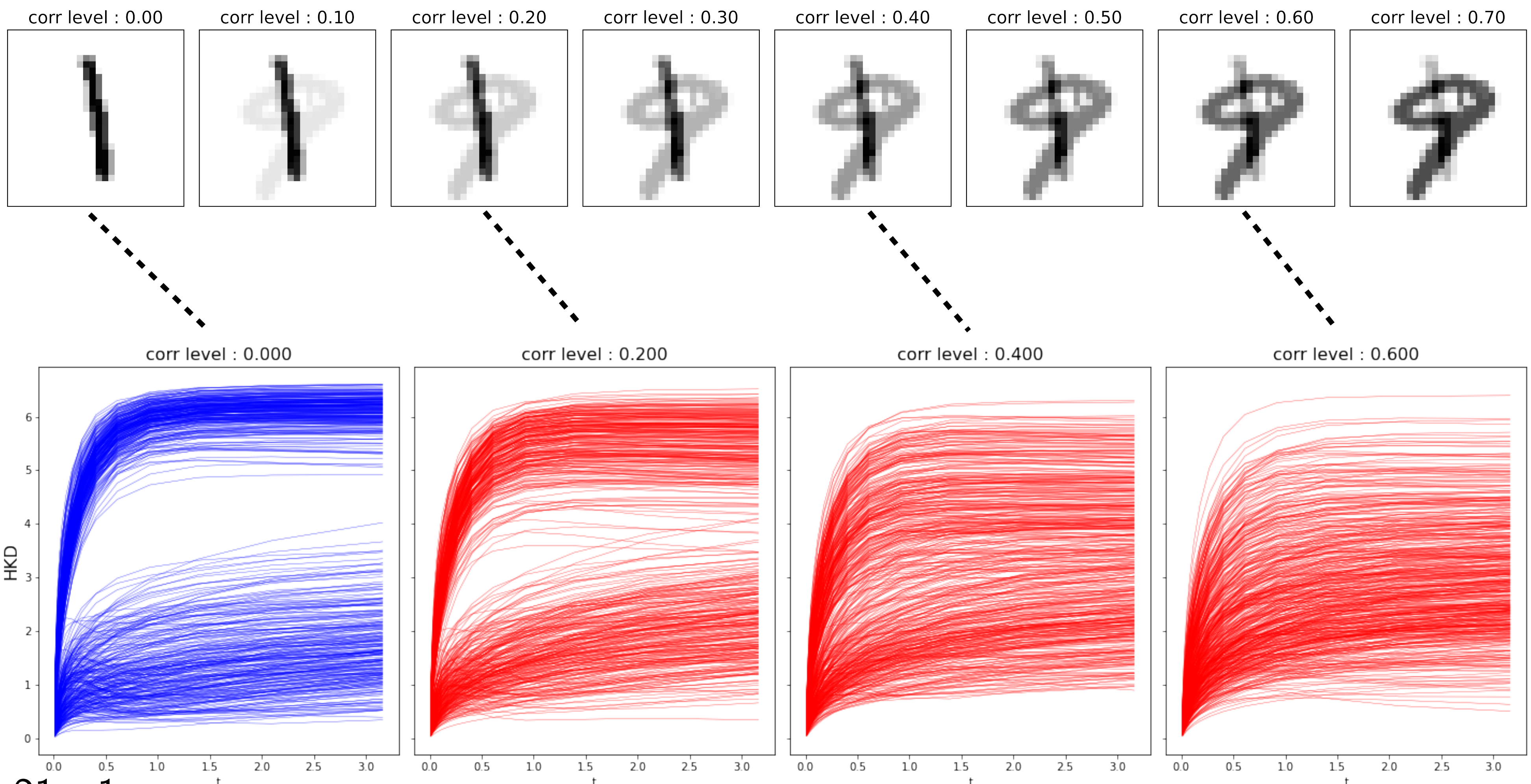


two-sample test : ✓

Corrupted distribution (interpolation)

Training with digits : 0, 1.

Testing with corrupted digits.



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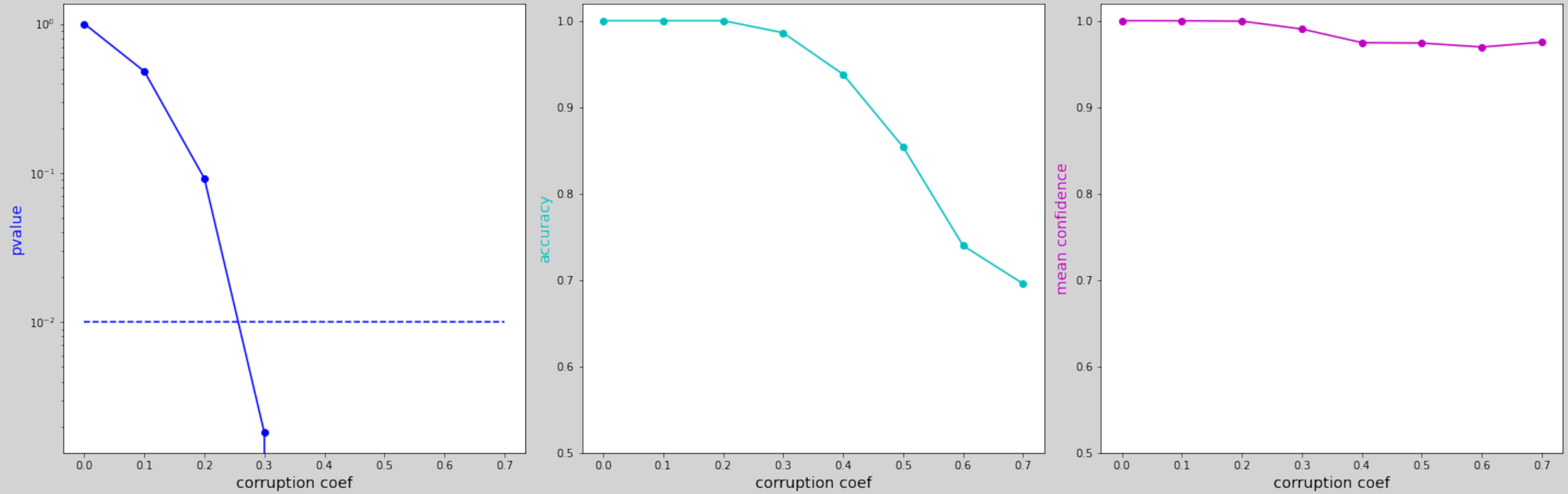
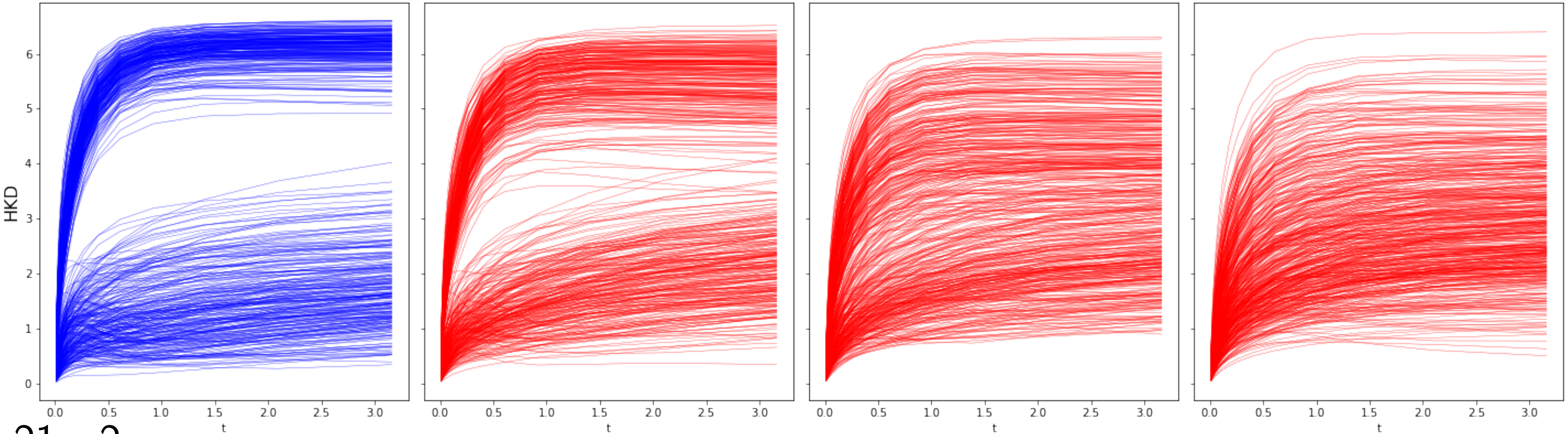
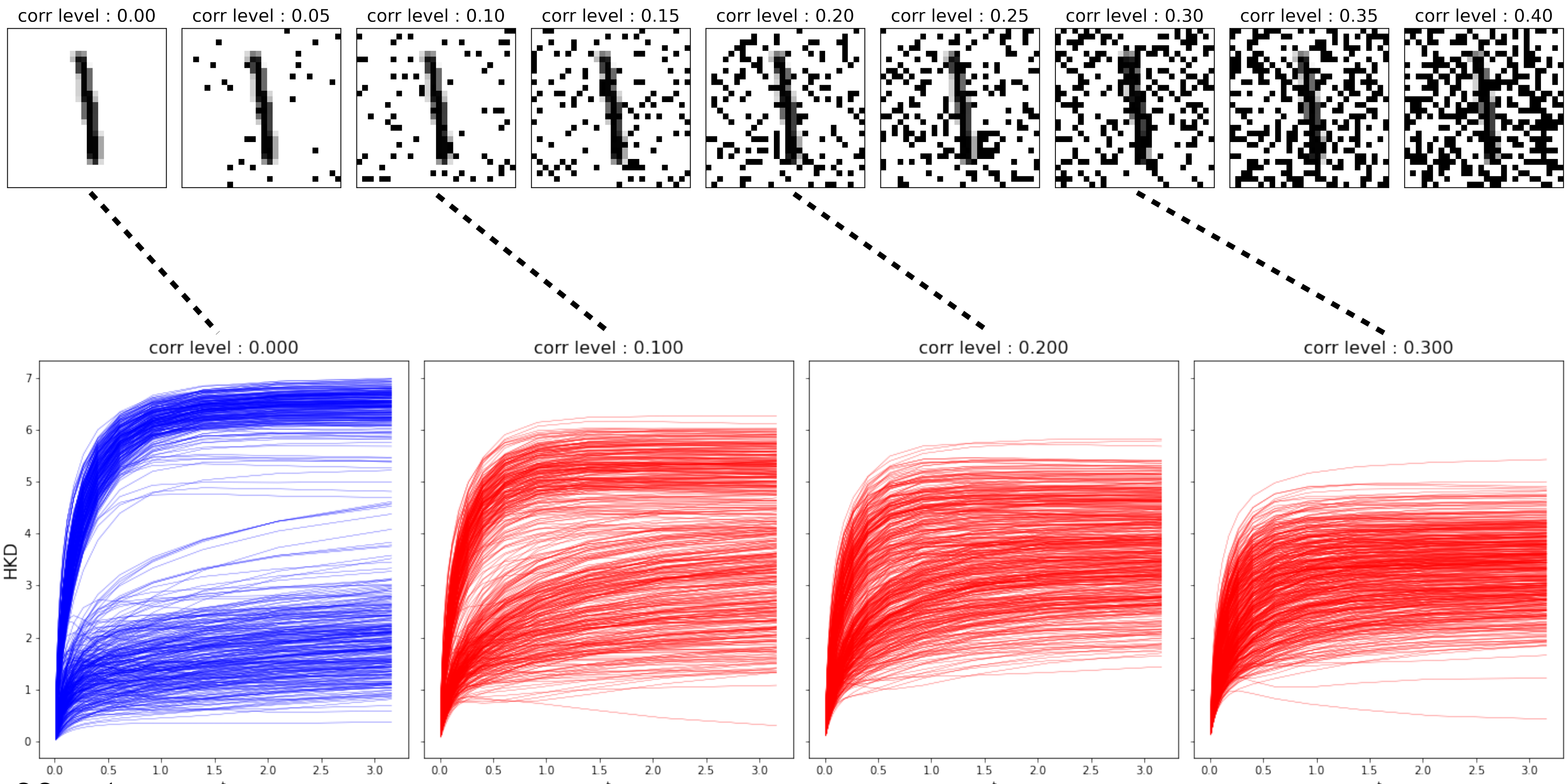




Corrupted distribution (random pixels)

Training with digits : 0, 1.

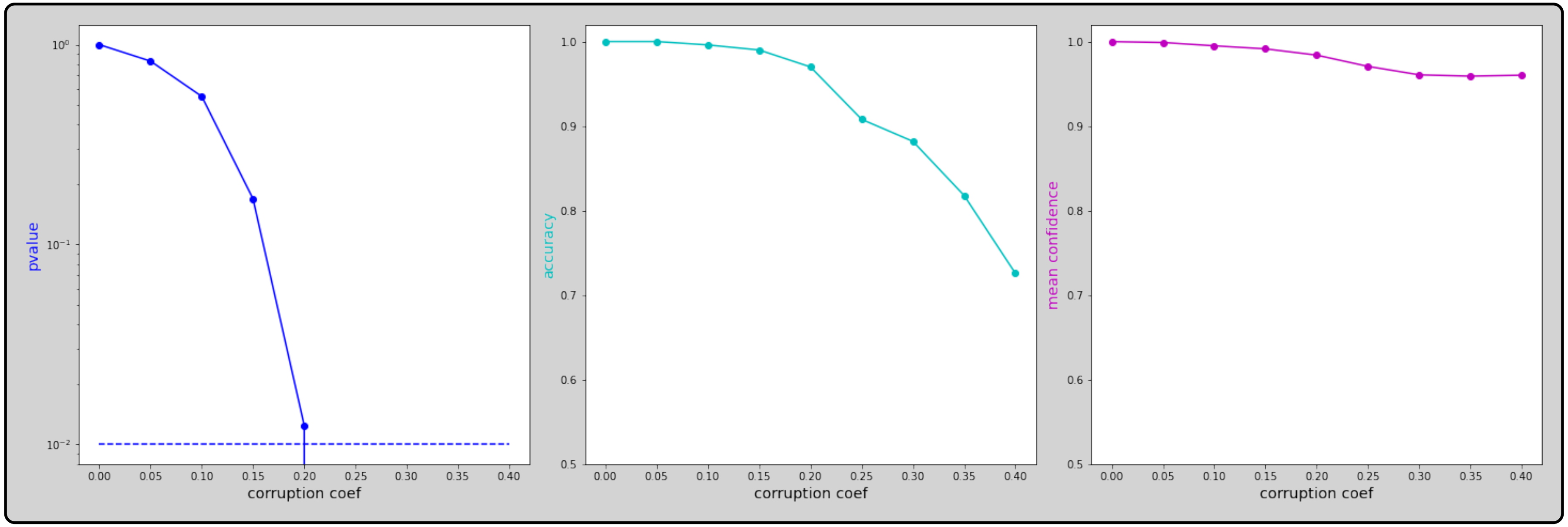
Testing with corrupted digits.

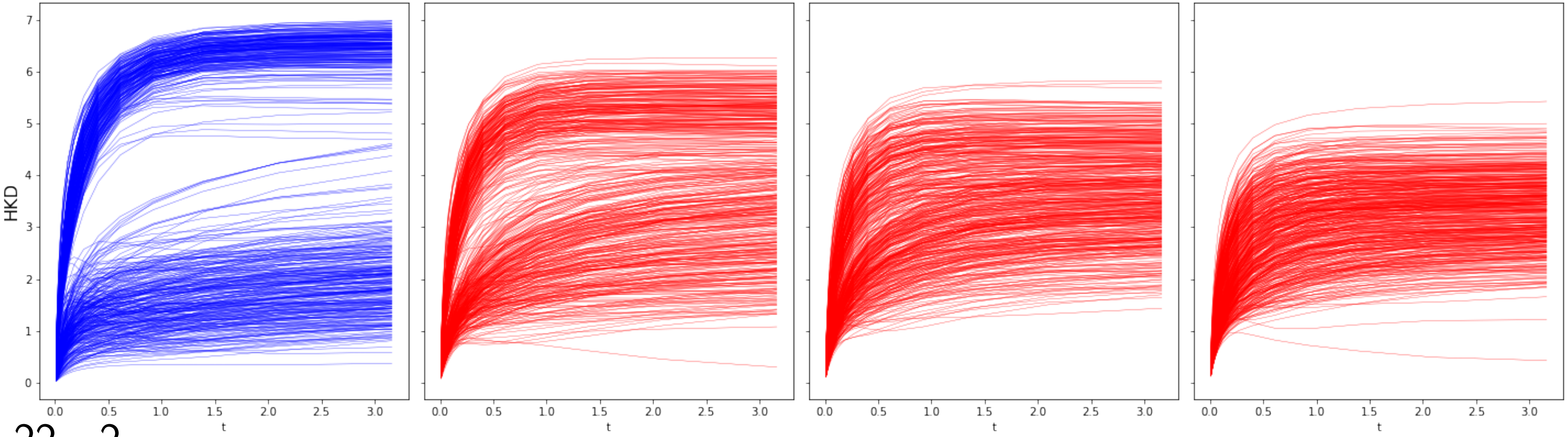


Corrupted distribution (random pixels)

Training with digits : 0, 1.

Testing with corrupted digits.





Perspectives

- Applications to real datasets
- Learning tasks : classification, change point detection, ...
- Relationship between n and N

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Thank you for your attention!