Network Two-Sample Test

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Introduction and motivation

Networks: relational data



Figure: Plot of some socical network (Fortunato & Newman: 20 years of network community detection, Nature, 2022)

Introduction and motivation

Networks: relational data



Figure: Internet network (Zook et al., 2004)

- Relational nature: no direct observations on individuals
- Research interests (on one network)
 - Clustering nodes (community detection) Zhao et al. (2012); Zhang & Zhou (2015); Gao et al. (2018)
 - Learning node representation Young & Scheinerman (2007); Cape et al. (2018); Lei (2021); Xie (2022+)
 - Denoising and link prediction *Chatterjee (2015); Gao et al. (2015); Z et al. (2017); Xu (2018)*
 - And many, many more...

Levin & Levina (2019) says well:

"A core problem in statistical network analysis is to develop network analogues of classical techniques."

Today's topic: network two-sample test

- Given two sets of networks $A^{(1)}, \ldots, A^{(N_A)}; B^{(1)}, \ldots, B^{(N_B)}$
- Question: Compare the models behind networks A and B
- Motivating applications:
 - Sociology: compare structural roles of two nodes through their ego-networks
 - Biomedical studies: compare brain imaging networks for diagnosis and disease sub-type discovery

Two-sample test: $A^{(1)}, \ldots, A^{(N_A)}$ vs. $B^{(1)}, \ldots, B^{(N_B)}$

Problem difficulty depends on:

 1. Multiple observations: N_A, N_B → ∞? Ginestet et al. (2017); Ghoshdastidar & Von Luxburg (2018); Kolaczyk et al. (2020); Ghoshdastidar et al. (2020); Chen et al. (2022); Maugis et al. (2020); Bravo-Hermsdorff et al. (2021); Yuan & Wen (2021)

With diverging N_A, N_B , one can:

- Easily denoise A and B
- Easily estimate the variability of your test statistic

Issue:

• Within-group heterogeneity (e.g., schizophrenia data)

Two-sample test: $A^{(1)}, \ldots, A^{(N_A)}$ vs. $B^{(1)}, \ldots, B^{(N_B)}$

Problem difficulty depends on:

• 2. Known node registration?

Ghoshdastidar and Von Luxburg (2018); Li and Li (2018); Ghoshdastidar et al. (2020); Chen et al. (2022).

With known node registration, one can:

• Perform edge-wise comparison

But node correspondence...

- may not exist (e.g., Google+ ego-network data)
- may not be known (e.g., person ↔ social media accounts)

Introduction and motivation



Figure: The same network plotted with three different node orders (*Olhede & Wolfe, 2014*)

Two-sample test: $A^{(1)}, \ldots, A^{(N_A)}$ vs. $B^{(1)}, \ldots, B^{(N_B)}$

Assumption 1: Multiple observations Assumption 2: Known node registration

- Many existing works assume both: Ghoshdastidar and Von Luxburg (2018); Ghoshdastidar et al. (2020); Chen et al. (2022).
- Some assume neither, but usually need other significant assumptions (low-rankness, degree monotonicity i.e. identification by degree):

Tang et al. (2017); Agterberg et al. (2020); Yang et al. (2014); Sabanayagam et al. (2021)

(graph-matching-based methods)

Goals:

- No multiple observations: $N_A = N_B = 1$
- No/Unknown node registration
- Avoid strong structural assumptions
- Scalable and memory-parsimonious algorithm
- Handle potentially very different network sizes and sparsity levels
- Finite-sample higher-order accuracy

Input data:

• Adjacency matrices: $A \in \{0,1\}^{m \times m}$, $B \in \{0,1\}^{n \times n}$

Base model:

• Adjacency matrix: $A \in \{0,1\}^{m \times m}$

$$A_{ij} = A_{ji} = \begin{cases} 1 & i \leftrightarrow j \\ 0 & \text{otherwise} \end{cases}$$

• Symmetric edge probability matrix: $W^{(A)} \in \mathbb{R}^{m \times m}$:

$$A_{ij}|W^{(A)} \overset{\text{independent}}{\sim} \text{Bernoulli}(W^{(A)}_{ij})$$

Graphon model: two-stage data generation

- Latent node positions $X_1, \ldots, X_m \stackrel{\text{i.i.d.}}{\sim}$ Uniform[0,1]
- 2 Edge probabilities:

$$W_{ij}^{(A)} = \boldsymbol{\rho}_A \cdot f_A(X_i, X_j)$$

where:

- Latent graphon function $f_A: [0,1]^2 \rightarrow [0,1]$, s.t. $\int_0^1 \int_0^1 f_A(u,v) \, du \, dv = 1$
- *ρ_A*: sparsity multiplier

Problem set up

$$W_{ij}^{(A)} = \rho_A \cdot f_A(X_i, X_j)$$

Remarks:

- *f_A* encodes all network structures
- X_i encodes node's role
- Both are inestimable





Goal: compare f_A vs f_B , using just A and B

Is this even doable?

Idea: compare network summary statistics

- Question 1: which statistics to compare?
- Question 2: similar summary statistics $\stackrel{?}{\Leftrightarrow}$ similar network models

Question 1: which statistics to compare?

Network moment: frequency of the corresponding motif



Figure: Network motifs (Jayavelu & Bar, 2014)

- Network motif: *R* with *r* nodes and *s* edges
- Empirical network moment

$$\widehat{U}_m := \binom{m}{r}^{-1} \sum_{1 \le i_1 < \dots < i_r \le m} h(A_{i_1,\dots,i_r})$$

where the kernel $h(\cdot)$ is

$$h(A_{i_1,\ldots,i_r}) := \begin{cases} 1, & \text{if } A_{i_1,\ldots,i_r} \text{ contains } R\\ 0, & \text{otherwise} \end{cases}$$

• **Example:** *R* = Triangle:

$$\widehat{U}_m := \binom{m}{3}^{-1} \sum_{1 \le i_1 < i_2 < i_3 \le m} A_{i_1, i_2} A_{i_2, i_3} A_{i_3, i_1} \tag{1}$$

Define population network moment: μ_m := E[Û_m]
Similarly define V_n and ν_n for B

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Network Two-Sample Test

Question 2: similar summary statistics $\stackrel{?}{\Leftrightarrow}$ similar network models

• Goal: Horvitz-Thompson estimator (population version)

$$d_{m,n,\rho_A,\rho_B} := \rho_A^{-s} \cdot \mu_m - \rho_B^{-s} \cdot \nu_n$$

 Similar network moments ≈ similar network models! (Borgs et al, 2008)

Theorem 1 (Inverse Counting Lemma, [7]). Suppose the graphon functions f_A and f_B are measurable and bounded by 1. For any k_0 , if $|d_{m,n,\rho_A,\rho_B}| \leq 3^{-k_0^2}$ holds for all motifs with at most k_0 nodes, then the cut distance, denoted by $\delta_{\Box}(\cdot, \cdot)$, satisfies

$$\delta_{\square}(f_A, f_B) := \inf_{\sigma} \sup_{S, T \subset [0,1]} \Big| \int_{S \times T} \Big\{ f_A(x, y) - f_B(\sigma(x), \sigma(y)) \Big\} \, \mathrm{d}x \, \mathrm{d}y \Big| \le \frac{22}{\sqrt{\log k_0}}$$

where $\sigma : [0,1] \rightarrow [0,1]$ ranges over all invertible measure-preserving maps.

• Goal: Horvitz–Thompson estimator (population version)

$$d_{m,n,\rho_A,\rho_B} := \rho_A^{-s} \cdot \mu_m - \rho_B^{-s} \cdot \nu_n$$

• Sample version (point estimator)

$$\widehat{D}_{m,n} := \widehat{\rho}_A^{-s} \cdot \widehat{U}_m - \widehat{\rho}_B^{-s} \cdot \widehat{V}_n$$

- Next steps:
 - i. estimate $\operatorname{Var}(\widehat{D}_{m,n})$ and studentize $\widehat{D}_{m,n}$ into $\widehat{T}_{m,n}$
 - ii. distribution approximation for $\widehat{T}_{m,n}$
- Let's analyze \widehat{U}_m

Analysis of \widehat{U}_m : take R = Triangle as an example, assuming $\rho_A = 1$

$$\binom{m}{3}\widehat{U}_{m} = \sum_{\substack{i,j,k \\ \vdots=U_{m}, \text{ Randomness due to } X_{i}'s}} \sum_{\substack{i=U_{m}, \text{ Randomness due to } X_{i}'s}} \sum_{\substack{i,j \\ i=(\widehat{U}_{m}, -U_{m}), \text{ Randomness due to observational error}}} \sum_{i=(\widehat{U}_{m}-U_{m}), \text{ Randomness due to observational error}}$$
(2)

where:

• Recall $W_{i,j} = f(X_i, X_j)$, then U_m is a U-statistic

•
$$\eta_{i,j} = A_{i,j} - W_{i,j}^{(A)}$$

• Θ 's: coefficients, functions of X_i 's

Decomposition of \widehat{U}_m :

$$\widehat{U}_m = \underline{U}_m + (\widehat{U}_m - \underline{U}_m)$$

where

- $U_m = U_m(X_1, ..., X_m)$: randomness in $W^{(A)}$, driven by random latent node positions
- $\hat{U}_m U_m$: observational errors in $A|W^{(A)}$, driven by Bernoulli edge realization
- "Non-degenerate" case: $Var(U_m) \gg Var(\widehat{U}_m U_m)$, focus on U_m

• $U_m := \mathbb{E}[\widehat{U}_m | W^{(A)}]$ admits Hoeffding's ANOVA decomposition

$$U_{m} - \mu_{m} = \underbrace{\frac{r}{m} \sum_{i=1}^{n} g_{A;1}(X_{i})}_{\text{Linear part, main term}} + \underbrace{\frac{r(r-1)}{m(m-1)} \sum_{1 \le i < j \le m} g_{A;2}(X_{i}, X_{j})}_{\text{Quadratic part, correction}} + (\text{Remainder})$$
(3)

where all $g_{A;k}$'s are **uncorrelated** • Other terms $(\hat{\rho}_A, \hat{V}_n, \hat{\rho}_B)$ can be analyzed similarly

Recall:

$$\widehat{D}_{m,n} := \widehat{\rho}_A^{-s} \cdot \widehat{U}_m - \widehat{\rho}_B^{-s} \cdot \widehat{V}_n$$

• Variance estimation:

$$\widehat{S}_{m,n}^2 := \frac{1}{m^2} \widehat{\alpha}_1^2(X_i) + \frac{1}{n^2} \widehat{\beta}_1^2(Y_j)$$

where

$$\widehat{\alpha}_{1}(X_{i}) := r\widehat{\rho}_{A}^{-s}\widehat{g}_{A;1}(X_{i}) - \underbrace{2s\widehat{\rho}_{A}^{-(s+1)}\widehat{U}_{m}\widehat{g}_{\rho_{A};1}(X_{i})}_{\text{Plug-in error}}$$

and β defined similarly

• Studentization:

$$\widehat{T}_{m,n} := \widehat{S}_{m,n}^{-1} \{ \widehat{D}_{m,n} - (\rho_A^{-s} \cdot \mu_m - \rho_B^{-s} \cdot \nu_n) \}$$

• Distribution of $\widehat{T}_{m,n}$?

• Edgeworth expansion approximates $F_{\widehat{T}_{mn}}(u)$ by

$$G_{m,n}(u) := \Phi(u) - \varphi(u) \cdot \{Q_1 + Q_2(u^2 + 1) + I_0\},\$$

where

- Φ: CDF of N(0,1)
- *φ*: PDF of *N*(0,1)
- I_0, Q_1 and Q_2 are estimable coefficients :

$$I_0 \asymp Q_1 \asymp Q_2 \asymp (m \wedge n)^{1/2} \cdot (m^{-1} + n^{-1})$$

(Lengthy details omitted, see paper ArXiv: 2208.07573)

If you're curious...

$$\begin{split} \mathcal{I}_{0} &:= \sigma_{m,n}^{-1}(m^{-1}\alpha_{0} - n^{-1}\beta_{0}), \\ Q_{m,n,\rho_{A},\rho_{B};1} &:= \frac{1}{2}\sigma_{m,n}^{-3} \Big\{ -m^{-2}\mathbb{E}[\alpha_{4}(X_{1},X_{2})\alpha_{1}(X_{2})] - m^{-2}\mathbb{E}[\alpha_{1}(X_{1})\alpha_{3}(X_{1})] \\ &\quad + n^{-2}\mathbb{E}[\beta_{1}(Y_{1})\beta_{3}(Y_{1})] + n^{-2}\mathbb{E}[\beta_{4}(Y_{1};Y_{2})\beta_{1}(Y_{2})] \Big\}, \\ Q_{m,n,\rho_{A},\rho_{B};2} &:= \sigma_{m,n}^{-3} \Big\{ m^{-2} \Big(\mathbb{E}[\alpha_{1}^{3}(X_{1})/6 \\ &\quad + \alpha_{1}(X_{1})\alpha_{1}(X_{2})\alpha_{2}(X_{1},X_{2})] \Big) - n^{-2} \Big(\mathbb{E}[\beta_{1}^{3}(Y_{1})/6 + \beta_{1}(Y_{1})\beta_{1}(Y_{2})\beta_{2}(Y_{1},Y_{2})]) \Big\} \\ &\quad + \frac{1}{2} \sigma_{m,n}^{-5} \Big\{ \Big(-m^{-3}\xi_{\alpha;1}^{2} - m^{-2}n^{-1}\xi_{\beta;1}^{2} \Big) \cdot \mathbb{E}[\alpha_{1}(X_{1})\alpha_{3}(X_{1}) + \alpha_{4}(X_{1};X_{2})\alpha_{1}(X_{2})] \\ &\quad + \Big(m^{-1}n^{-2}\xi_{\alpha;1}^{2} + n^{-3}\xi_{\beta;1}^{2} \Big) \cdot \mathbb{E}[\beta_{1}(Y_{1})\beta_{3}(Y_{1}) + \beta_{4}(Y_{1};Y_{2})\beta_{1}(Y_{2})] \Big\}. \end{split}$$

Inference procedures:

• Hypothesis testing:

$$H_0: d_{m,n,\rho_A,\rho_B} = 0, \quad \text{vs} \quad H_a: d_{m,n,\rho_A,\rho_B} \neq 0.$$
 (10)

The empirical p-value produced by our method is

$$\widehat{p}_{\text{val}} := 2 \cdot \min\left\{\widehat{G}_{m,n}(\widehat{T}_{m,n}^{(\text{obs})}), 1 - \widehat{G}_{m,n}(\widehat{T}_{m,n}^{(\text{obs})})\right\}$$

where we define the observed statistic by $\widehat{T}_{m,n}^{(\mathrm{obs})} := \widehat{D}_{m,n} / \widehat{S}_{m,n} + \delta_T.$ Given a significance level α ,

• Cornish-Fisher CI:

$$\left(\widehat{D}_{m,n}-\left(\widehat{q}_{\widehat{T}_{m,n};1-\alpha/2}-\delta_{T}\right)\cdot\widehat{S}_{m,n},\ \widehat{D}_{m,n}-\left(\widehat{q}_{\widehat{T}_{m,n};\alpha/2}-\delta_{T}\right)\cdot\widehat{S}_{m,n}\right).$$

where $\widehat{q}_{\widehat{T}_{m,n};\alpha} := z_{\alpha} + \widehat{I}_0 + \widehat{Q}_1 + \widehat{Q}_2(z_{\alpha}^2 - 1)$ and z_{α} is N(0,1) quantile

Theory

Higher-order accuracy (simplified version):

- Conditions:
 - $\bigcirc \log(m \lor n) / (m \land n) \to 0$
 - Similar conditions for *B*-index terms $\rho_A^{r/2}m \to \infty$;
- Define error bound:

$$M_A := \begin{cases} (\rho_A m)^{-1}, & \text{Acyclic } R\\ \rho_A^{-r/2} m^{-1}, & \text{Cyclic } R \end{cases}$$
(4)

W.h.p., we have

$$\left\|F_{\widehat{T}_{m,n}}(u) - \widehat{G}_{m,n}(u)\right\|_{\infty} \lesssim (m \wedge n)(m^{-1}M_A + n^{-1}M_B),\tag{5}$$

where $\widehat{G}_{m,n}(u)$: empirical Edgeworth expansion (EEE)

Larger and more cyclic motifs requires denser networks

Power optimality:

• Under regularity conditions, our test achieves consistency:

(Type-I error rate) + (Type-II error rate) $\rightarrow 0$

when

$$d_{m,n,\rho_A,\rho_B} \gg m^{-1/2} + n^{-1/2}$$

• No method is consistent when $d_{m,n,\rho_A,\rho_B} \lesssim m^{-1/2} + n^{-1/2}$

Our method simultaneously achieves:

- Higher-order accurate control of "risks"
- Rate-optimal "power"

It is not hard to achieve just one, but difficult to achieve both

Network hashing

Recall:

$$G_{m,n}(u) := \Phi(u) - \varphi(u) \cdot \{Q_1 + Q_2(u^2 + 1) + I_0\},\$$

where

$$\begin{split} \mathcal{I}_{0} &:= \sigma_{m,n}^{-1}(m^{-1}\alpha_{0} - n^{-1}\beta_{0}), \\ Q_{m,n,\rho_{A},\rho_{B};1} &:= \frac{1}{2}\sigma_{m,n}^{-3} \Big\{ -m^{-2}\mathbb{E}[\alpha_{4}(X_{1},X_{2})\alpha_{1}(X_{2})] - m^{-2}\mathbb{E}[\alpha_{1}(X_{1})\alpha_{3}(X_{1})] \\ &\quad + n^{-2}\mathbb{E}[\beta_{1}(Y_{1})\beta_{3}(Y_{1})] + n^{-2}\mathbb{E}[\beta_{4}(Y_{1};Y_{2})\beta_{1}(Y_{2})] \Big\}, \\ Q_{m,n,\rho_{A},\rho_{B};2} &:= \sigma_{m,n}^{-3} \Big\{ m^{-2} \big(\mathbb{E}[\alpha_{1}^{3}(X_{1})/6 \\ &\quad + \alpha_{1}(X_{1})\alpha_{1}(X_{2})\alpha_{2}(X_{1},X_{2})] \big) - n^{-2} \big(\mathbb{E}[\beta_{1}^{3}(Y_{1})/6 + \beta_{1}(Y_{1})\beta_{1}(Y_{2})\beta_{2}(Y_{1},Y_{2})] \big) \Big\} \\ &\quad + \frac{1}{2}\sigma_{m,n}^{-5} \Big\{ \big(-m^{-3}\xi_{\alpha;1}^{2} - m^{-2}n^{-1}\xi_{\beta;1}^{2} \big) \cdot \mathbb{E}[\alpha_{1}(X_{1})\alpha_{3}(X_{1}) + \alpha_{4}(X_{1};X_{2})\alpha_{1}(X_{2})] \\ &\quad + \big(m^{-1}n^{-2}\xi_{\alpha;1}^{2} + n^{-3}\xi_{\beta;1}^{2} \big) \cdot \mathbb{E}[\beta_{1}(Y_{1})\beta_{3}(Y_{1}) + \beta_{4}(Y_{1};Y_{2})\beta_{1}(Y_{2})] \Big\}. \end{split}$$

No cross terms (e.g., sth. like $\mathbb{E}[\gamma(X_1, Y_1)])!$

Suppose you "Google" a keyword network *A* in a huge network database B_1, \ldots, B_K :

- **(1)** Network hashing: each network \rightarrow a few summary statistics
- **Past query:** compare *A* to each *B_k* using only summary statistics! **Benefits:**
 - Easy indexing and maintenance for network database curators, memory efficient
 - Enhanced privacy protection
 - Query is lightning fast, much faster than existing methods
 - Our method can serve as a screening stage for other methods (to test exact equality of models, under additional assumptions)

Simulations

Benchmarks:

- Normal approximation
- Node sub-sampling (variant of *Bhattacharyya & Bickel, (2015)*)
- Node re-sampling (variant of Green & Shalizi, (2022))

Motifs:

- Triangle (cyclic)
- V-shape (acyclic)

Performance evaluation criteria:

- Simulation 1: Accuracy: K-S distance $\|\widehat{F}_{\widehat{T}_{m,n}}(u) F_{\widehat{T}_{m,n}}(u)\|_{\infty}$
- Simulation 2: Accuracy of CI level control
- Simulation 3: database query accuracy
- All simulations: Time cost

Simulation 1

A, B from two different smooth graphons



Figure: Green: our method; black: N(0,1); orange: node sub-sampling; violet: node re-sampling; cyan (left panel): true distribution Monte Carlo emulation

Simulation 2



Simulation 3

Database: 10 different models, each generate 100 networks; Keyword networks: one from a database model, one from outside



Figure: Comparison of query accuracy and speed. All networks are size *n*. Incomplete curves indicate benchmark went timeout.

Data examples



Figure: Data set 1: Google+ ego-networks

Data examples



Figure: Data set 2: Schizophrenia brain image networks

Table 2: Time cost comparison table. Unit is second. Timeout is 12 hours = 43200 seconds.

	Our method (hash)	Our method (test)	Subsample	Resample
Data example 1	116.39	18.81	10884.62	(Timeout)
Data example 2	3.60	64.36	2488.21	(Timeout)
	NonparGT	NetLSD	NetComp	
Data example 1	(Execution error)	(Timeout)	(Timeout)	
Data example 2	4327.09	(Execution error)	4304.51	

Figure: Time cost comparison

Extensions

What if I do have multiple observations? $A^{(1)}, \ldots, A^{(N_A)}; B^{(1)}, \ldots, B^{(N_B)}, N_A, N_B > 1.$

• If nodes are matched (same set of nodes):

Pool (average over) all adjacency matrices in one group

$$A^{\text{pool}} := N_A^{-1} \sum_{\ell=1}^{N_A} A^{(\ell)}$$

Apply our algorithm to pooled *A*, *B* with no formula change
If nodes are independently generated:

Ompute $\widehat{U}_m^{(\ell)}$ for each network ℓ in Group A, then average:

$$\widehat{U}_m^{\text{pool}} := N_A^{-1} \sum_{\ell=1}^{N_A} \widehat{U}_m^{(\ell)}$$

Do the same for $\hat{\rho}_A$, \hat{V}_n , $\hat{\rho}_B$ and all emp. Edgeworth expansion coef. **Source Formula changes:** (assuming equal network sizes)

- A new variance estimator
- Edgeworth expansion formula: $m \rightarrow mN_A$, $n \rightarrow nN_B$

Extensions

Degenerate U-statistics:

- Reducing the U-statistic reinstates normality (Weber, 1981; Chen & Kato, 2019; Shao et al, 2023)
- **Example:** $Z_1, \ldots, Z_n \stackrel{\text{i.i.d.}}{\sim} N(0,1)$, then:

$$\sum_{1 \le i < j \le n} Z_i Z_j \not\xrightarrow{d} \mathsf{Normal}$$

However, $Z_1 Z_2 + Z_3 Z_4 + \cdots \xrightarrow{d} \mathsf{Normal}$

- Reduced statistic also computes faster, but inflates variance
- We proposed a novel test statistic, automatically adaptive to potential degeneracy (see paper)

Extensions

FDR control for query:

- Recall set up: test A vs each of B_1, \ldots, B_K
- Vector of test statistics: $\widehat{T} \approx \iota + \gamma W + \mathcal{K}$, where
 - $W \sim N(0,1)$
 - $\mathscr{K} \sim N(0, \Psi)$
- \mathscr{K} has "weak dependence" (*Fan et al, 2012*), i.e., $\Psi \approx \text{diag}(\Psi)$
- Conditional on W, \widehat{T} produces nearly independent p-values

Theorem 6. Suppose the conditions of Theorem 2 hold for all networks (keyword and database entries). Additionally, assume $\lim_{K,m,n_{\min}\to\infty} \frac{\log(mK)}{m} + \frac{\log(n_{\min}K)}{n_{\min}} + \frac{\log^{1/2}(mK)}{\rho_{A}m} + \max_{j\in[1:K]} \frac{\log^{1/2}(n_{j}K)}{\rho_{B_{j}}n_{j}} = 0,$ where $n_{\min} := \min_{k\in[1:K]} n_{k}$. Then, we have $FDP(t) - \frac{\sum_{k\in\{\text{true nulls}\}} \left[\Phi(a_{k}(z_{t/2} + \eta_{k})) + \Phi(a_{k}(z_{t/2} - \eta_{k}))\right]}{\sum_{k\in[1:K]} \mathbb{I}\left[\widehat{p}_{k} \leq t\right]} \to 0,$ (16)

as $K, m, n_{\min} \to \infty$, where $a_k := \left(1 - \gamma_k^2\right)^{-1/2}$, $z_t := \Phi^{-1}(t)$, and $\eta_k := \gamma_k W$ with $W \sim N(0, 1)$.

Thank you!

Questions?