Testing Many Possibly Irregular Polynomial Constraints

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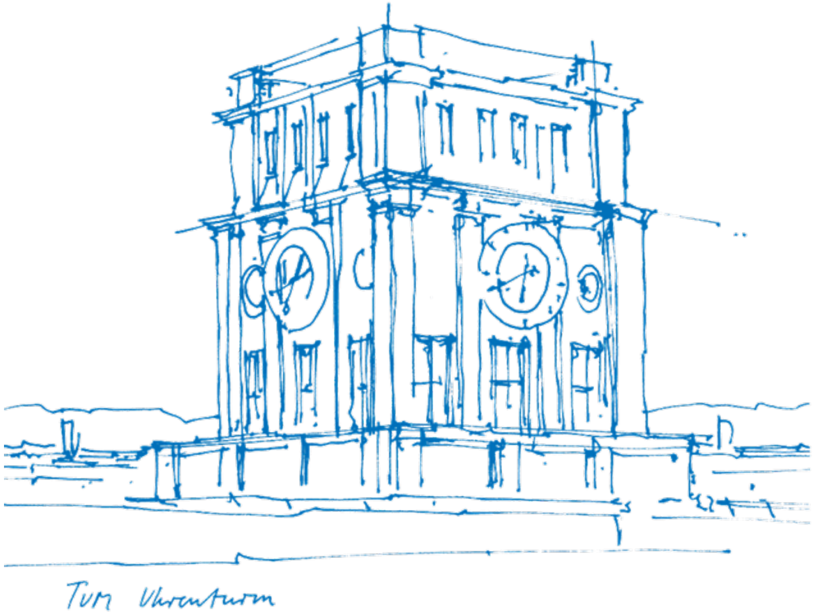
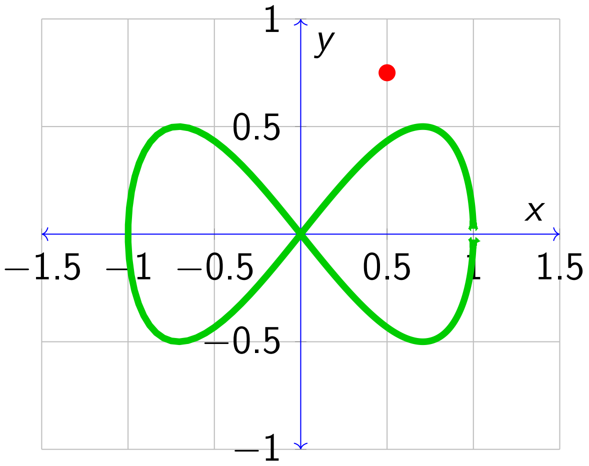
(joint work with Mathias Drton and Dennis Leung)



Curve with a Singular Point: Lemniscate of Gerono



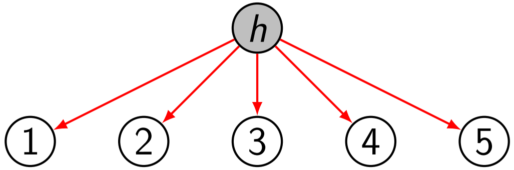
Parametrization

$$x = \frac{t^2 - 1}{t^2 + 1}, \qquad y = \frac{2t(t^2 - 1)}{(t^2 + 1)^2}$$

Characterization by Constraints

$$x^4 - x^2 + y^2 = 0$$

Statistical Example: One-Factor Analysis Model



$$X \sim N_k(0, \Sigma)$$

Parametrization

$$\Sigma = \Omega + \Gamma\Gamma^\top,$$

where $\Omega > 0$ diagonal and $\Gamma \in \mathbb{R}^{k \times 1}$.

Characterization by Constraints

Equality constraints (tetrads):

$$\sigma_{uv}\sigma_{wz} - \sigma_{uw}\sigma_{vz} = 0.$$

Inequality constraints:

$$-\sigma_{uv}\sigma_{vw}\sigma_{uw} \leq 0, \qquad \sigma_{uv}^2\sigma_{vw}^2 - \sigma_{vv}^2\sigma_{uw}^2 \leq 0.$$

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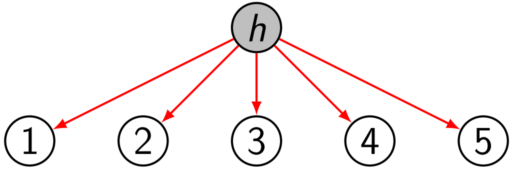

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Topic of the talk: Testing the goodness-of-fit based on samples $X_1, \ldots, X_n \sim N_k(0, \Sigma)$.

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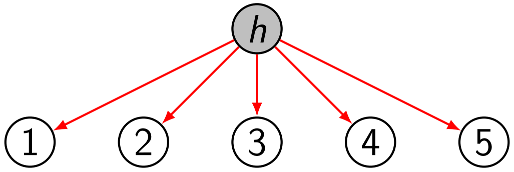
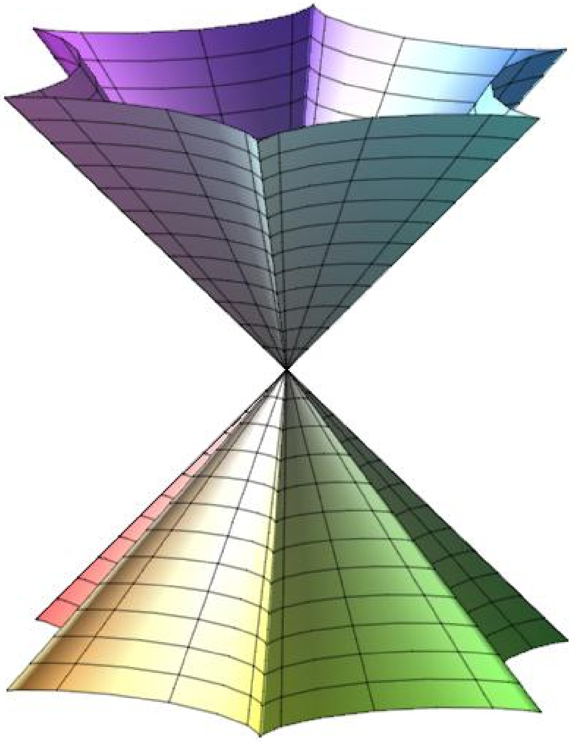
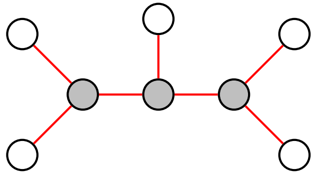




Further Examples

- Gaussian Latent Tree Models



Characterized by vanishing of certain tetrads and inequality constraints on the covariance matrix. (Long paths $\longrightarrow$ small correlations)

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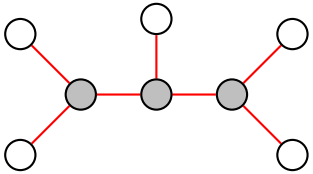

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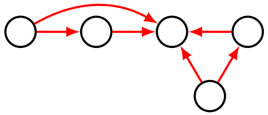
- Linear Non-Gaussian Structural Equation Models



$$X = \Lambda^\top X + \varepsilon$$

Denote $S = (s_{ij})$ and $T = (t_{ijl})$ the second and third order moments of X.

$$\text{rk}\begin{pmatrix} s_{11} & s_{12} & \cdots & s_{1k} & s_{22} & s_{23} & \cdots & s_{kk} \\ t_{111} & t_{112} & \cdots & t_{11k} & t_{122} & t_{123} & \cdots & t_{1kk} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ t_{11k} & t_{12k} & \cdots & t_{1kk} & t_{22k} & t_{23k} & \cdots & t_{kkk} \end{pmatrix} = k$$

$$t_{111}t_{222}t_{333}t_{123} - (t_{222}t_{333}t_{112}t_{113} + t_{333}t_{111}t_{122}t_{223} + t_{111}t_{222}t_{333}t_{233}) - t_{123}(t_{111}t_{223}t_{233} + t_{222}t_{133}t_{113} + t_{333}t_{112}t_{122}) + \ldots = 0 \quad \text{(Aronhold invariant)}$$

Master Thesis Daniela Schkoda (2022).
Goodness-of-fit tests for non-Gaussian linear causal models.

- ...

General Setup: Testing Constraints on Statistical Models

Parametric family:

$$\mathcal{P} = \{P_\theta : \theta \in \Theta\}, \text{ where } \Theta \in \mathbb{R}^d.$$

Model:

$$\Theta_0 = \{\theta \in \Theta : \ f_j(\theta) \leq 0 \text{ for all } 1 \leq j \leq p\}.$$

Our main interest: Polynomial constraints f_j.

Based on samples $X_1, \ldots, X_n \sim P_\theta$ test

$$H_0 : \theta \in \Theta_0 \text{ vs. } H_1 : \theta \in \Theta \setminus \Theta_0.$$

Likelihood-Ratio Test

$$\lambda_n = -2 \log \left(\frac{\sup_{\theta \in \Theta_0} \mathcal{L}_n(\theta)}{\sup_{\theta \in \Theta} \mathcal{L}_n(\theta)} \right).$$

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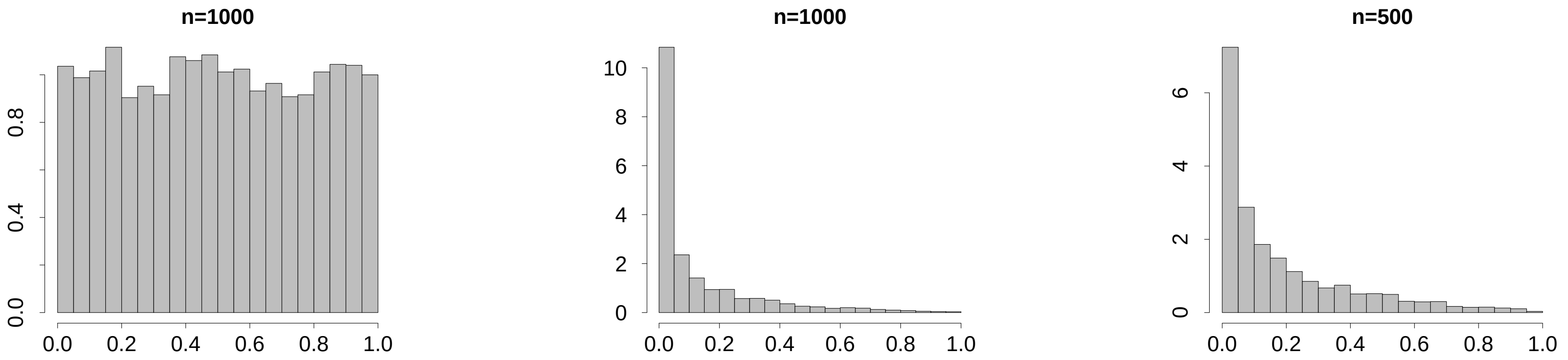
Simulated p-values (one-factor analysis model, Bartlett correction):



$k = 15$ observed variables, Σ **regular point**.

$k = 15$ observed variables, Σ close to a **singular point**.

$\mathbf{k = 200}$ observed variables, Σ regular point.

Wald Test

Tetrad: $f_1(\Sigma) = \sigma_{13}\sigma_{24} - \sigma_{23}\sigma_{14}$.

$$W_n = \frac{f_1(\hat{\Sigma})^2}{\widehat{\text{var}}[f_1(\hat{\Sigma})]} = \frac{n\, f_1(\hat{\Sigma})^2}{(\nabla f_1(\hat{\Sigma}))^\top V(\hat{\Sigma}) \nabla f_1(\hat{\Sigma})}, \qquad \text{where } \hat{\Sigma} = \frac{1}{n}\sum_{i=1}^{n} X_i X_i^\top.$$

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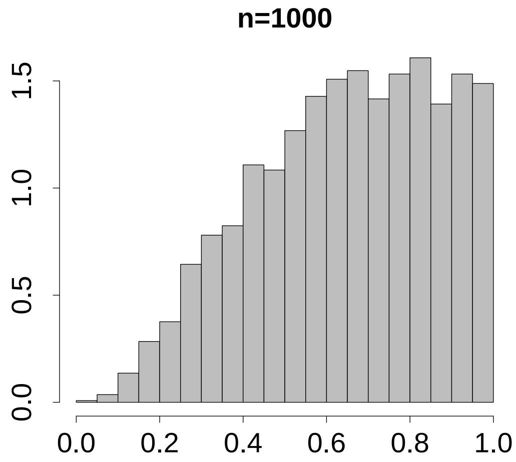
Limitations

- ✗ Invalid at singular points ($\nabla f_1(\Sigma) = 0$).

  $W_n \to_d F$ where $\frac{1}{4}\chi^2_1 \prec_{st} F \prec_{st} \chi^2_1$ (D. & Xiao, 2016)

- ✗ Only allows for low number of constraints ($p \leq d$).

- ✗ Difficult to handle inequality constraints.



Testing single tetrad,
Σ close to a **singular point**.

Connection to U-statistics

Tetrad: $f_1(\Sigma) = \sigma_{13}\sigma_{24} - \sigma_{23}\sigma_{14}$.

Observation:

$\widehat{f}_1 = \frac{n}{n-1} f_1(\hat{\Sigma}_n) = \frac{1}{\binom{n}{2}} \sum_{i<j} h_1(X_i, X_j)$ is a U-statistic with kernel

$$h_1(X_i, X_j) = \frac{1}{2}\{(X_{i1}X_{i3}X_{j2}X_{j4} - X_{i2}X_{i3}X_{j1}X_{j4}) + (X_{j1}X_{j3}X_{i2}X_{i4} - X_{j2}X_{j3}X_{i1}X_{i4})\}.$$

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Asymptotics (one dimensional):

Gaussian approximation: $\sqrt{n}(\widehat{f}_1 - f_1(\Sigma)) \longrightarrow N(0, m^2\sigma_{g_1}^2)$

where m is the degree of the kernel h_1 and $\sigma_{g_1}^2$ is the variance of the Hájek projection

$$g_1(X_i) = \mathbb{E}[h_1(X_i, X_j)|X_i] = \frac{1}{2}\left\{(X_{i1}X_{i3}\sigma_{24} - X_{i2}X_{i3}\sigma_{14}) + (\sigma_{13}X_{i2}X_{i4} - \sigma_{23}X_{i1}X_{i4})\right\}.$$

Irregular points: $\sigma_{g_1}^2 = 0 \implies$ U-statistic is degenerate $\implies$ Gaussian approximations fails.

Estimable Constraints and U-statistics

Assumption: $f(\theta) = (f_1(\theta), \ldots, f_p(\theta))^\top$ is *estimable*.

That is, for some integer m there exists a measurable, symmetric function $h : \mathbb{R}^m \to \mathbb{R}^p$ such that

$$\mathbb{E}[h(X_1, \ldots, X_m)] = f(\theta) \quad \text{for all } \theta \in \Theta,$$

whenever $X_1, \ldots, X_m$ are i.i.d. with distribution P_θ.

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U-statistics: $U_n = \frac{1}{\binom{n}{m}} \sum_{(i_1,\ldots,i_m) \in I_{n,m}} h(X_{i_1}, \ldots, X_{i_m})$, where $I_{n,m} = \{(i_1, \ldots, i_m) : 1 \le i_1 < \ldots < i_m \le n\}$.

$\longrightarrow$ Reject for "large" values of $\max_{1 \le j \le p}(\sqrt{n}\, \hat{\sigma}_j^{-1}) U_{n,j}$.

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Asymptotics: $\sqrt{n}\,(U_n - f(\theta)) \longrightarrow N_p(0, \Gamma_g)$, where $\Gamma_g = \mathrm{Cov}[g(X_1)]$ and g Hájek projection.

U-statistic is degenerate at irregular points $\Longrightarrow$ Gaussian approximation fails.

Independent Sums

Observation: $h(X_{(i-1)m+1}, \ldots, X_{im})$ are independent.

$$H_n = \frac{m}{n} \sum_{i=1}^{m} h(X_{(i-1)m+1}, \ldots, X_{im}).$$

Test statistic:

$$\max_{1 \le j \le p} (\sqrt{n}\ \hat{\sigma}_j^{-1}) H_{n,j}.$$

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Asymptotics: $\sqrt{n/m}\,(H_n - f(\theta)) \longrightarrow N(0, \Gamma_h)$, where $\Gamma_h = \mathrm{Cov}[h(X_1, \ldots, X_m)]$.

- ✔ High-dimensional approximation of test statistic ($p \gg n$). (Chernozhukov et al., 2013)
- ✔ Non-degenerate limit at every parameter.
- ✗ inefficient . . . sum is only over $\frac{n}{m}$ elements.

Independent sums guard against degeneracy, but can we do better/use more kernel evaluations?

Proposal: Randomized Incomplete U-statistics

$$U'_{n,N} = \frac{1}{\hat{N}} \sum_{\iota=(i_1,\ldots,i_m)\in I_{n,m}} Z_\iota h(X_{i_1},\ldots,X_{i_m})$$

- $I_{n,m} = \{(i_1,\ldots,i_m) : 1 \le i_1 < \ldots < i_m \le n\}$.
- Computational budget parameter $N \le \binom{n}{m}$.
- $\{Z_\iota : \iota \in I_{n,m}\}$ are i.i.d. $\mathrm{Ber}(p_n)$ with $p_n = N/\binom{n}{m}$.
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Asymptotics: $\sqrt{n}(U'_{n,N} - f(\theta)) \approx N(0, m^2\Gamma_g + \frac{n}{N}\Gamma_h)$.

Choose $N = \mathcal{O}(n)$ to guard against degeneracy!

Proposed Test

Test statistic

$$\mathcal{T} = \max_{1\leq j\leq p}(\sqrt{n}\,\widehat{\sigma}_j^{-1})U'_{n,N,j}.$$

Critical value

1. Approximate distribution of $\mathcal{T}$ by maximum of Gaussian random vector $Y \sim N_p(0,\Gamma)$, where $\Gamma = m^2\Gamma_g + \frac{n}{N}\Gamma_h$.
2. Construct an estimate $\widehat{\Gamma}$ of the true asymptotic covariance matrix Γ in a Gaussian multiplier bootstrap method. Then $W \sim N_p(0,\widehat{\Gamma})$ is "close" to $Y \sim N_p(0,\Gamma)$.
3. Critical value: Quantile $c_{W_0}(1-\alpha)$ of $W_0 = \max_{1\leq j\leq p}\widehat{\sigma}_j^{-1}W_j$.

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Our analysis. . .

If $N = \mathcal{O}(n)$ then the proposed test based on an incomplete U-statistic is asymptotically valid (controls type I error) in high dimensions $p \gg n$ and under *mixed degeneracy*:

$$P(\mathcal{T} > c_{W_0}(1-\alpha)) \le \alpha.$$

Mixed Degeneracy

Background on high-dimensional Gaussian approximation

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Mixed degeneracy assumption

Let $p_1, p_2 \in \mathbb{N}$ such that $p_1 + p_2 = p$ and assume:

(A) There exists $c > 0$ such that $\sigma_{g_j}^2 \geq c$ for all $j = 1, \ldots, p_1$.

(B) There exists $k > 0$ and $\beta > 0$ such that $\|g_j(X_1) - f_j(\theta)\|_{\psi_\beta} \leq Cn^{-k}$ for all $j = p_1 + 1, \ldots, p$.

$\implies \sigma_{g_j}^2 \leq \tilde{C} n^{-2k}$

High-dimensional Gaussian Approximation

Theorem

Under mixed degeneracy (and additional moment conditions on h), we have the ***Gaussian approximation*** *on the hyperrectangles*

$$\sup_{R \in \mathbb{R}^p_{\mathrm{re}}} |P(\sqrt{n}(U'_{n,N} - f(\theta)) \in R) - P(Y \in R)| \leq C\{\omega_{n,1} + \omega_{n,2} + \omega_{n,3}\},$$

where $Y \sim N_p(0, m^2\Gamma_g + \frac{n}{N}\Gamma_h)$ *and*

$$\omega_{n,1} = \left(\frac{m^{2/\beta} \log(pn)^{1+6/\beta}}{n \wedge N}\right)^{1/6}, \qquad \omega_{n,2} = \frac{N^{1/2} m^2 \log(pn)^{1/2+2/\beta}}{n^{\min\{1/2+k,\, 5/6\}}}, \qquad \omega_{n,3} = \left(\frac{Nm^2 \log(p)^2}{n^{\min\{1+k, m\}}}\right)^{1/3}.$$

Note:

If $N = \mathcal{O}(n)$ and $k \geq 1/3$ is fixed, then the bound vanishes asymptotically if $\log(pn)^{3/2+6/\beta} = o(n)$.

High-dimensional Bootstrap Approximation

Recall: $Y = m\, Y_g + \sqrt{n/N}\, Y_h,$ where $Y_g \sim N_p(0, \Gamma_g)$ and $Y_h \sim N_p(0, \Gamma_h)$ are independent.

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Approach: Construct W_g, W_h such that, given the data, both are independent and approximate Y_g, Y_h.

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Gaussian Multiplier Bootstrap:

$$W_h = \frac{1}{\sqrt{\hat{N}}} \sum_{\iota=(i_1,\ldots,i_m)\in I_{n,m}} \xi_\iota\, Z_\iota\, (h(X_{i_1},\ldots,X_{i_m}) - U'_{n,N}),$$

where $\{\xi_\iota : \iota \in I_{n,m}\}$ are a collection of independent $N(0,1)$ r.v.'s.

$\Longrightarrow$ Given the data, we have $W_h \approx Y_h$.

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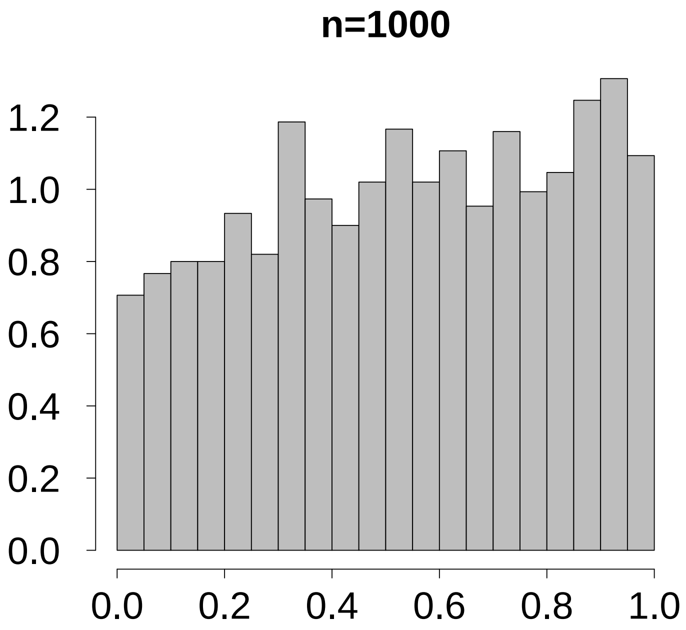
$\Longrightarrow$ Given the data, we have $W_h \approx Y_h$.

1. Similarly, we construct W_g, such that, given the data, $W_g \approx Y_g$.
2. Finite sample Berry Esseen type bound for the approximation $Y \approx W = m\, W_g + \sqrt{n/N}\, W_h$.
3. Control studentization.
4. Establish asymptotic validity (control of type I error).

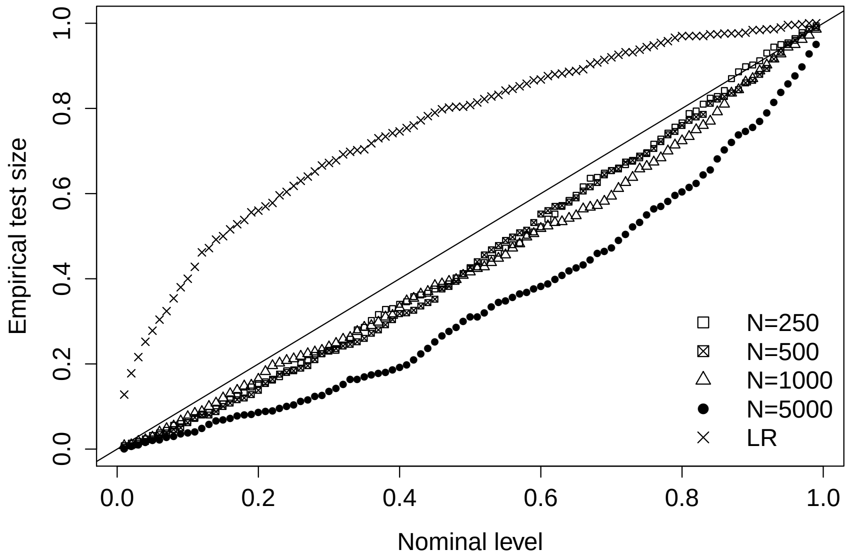
Our Test at Irregular Points



Simulated p-values for testing tetrads with $k = 15$ observed variables close to a singular point.
Computational budget parameter $N = 2n$.

Size vs. Power

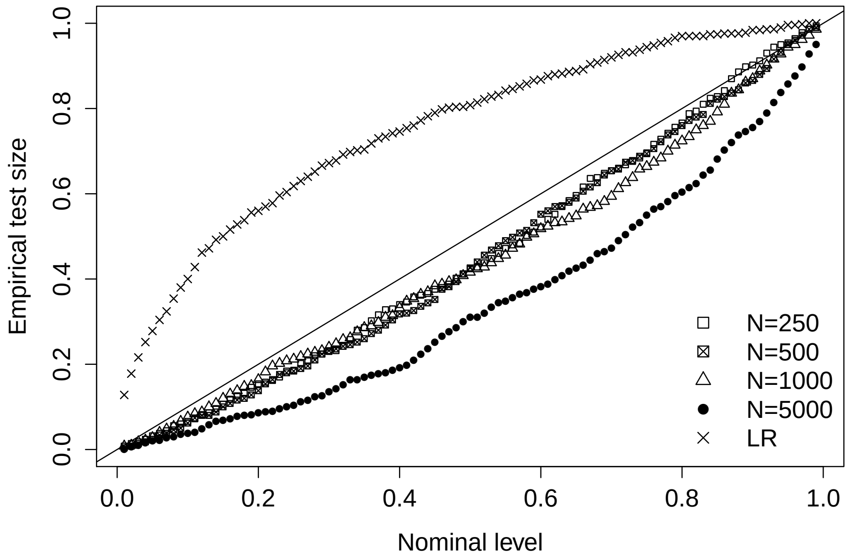
$n = 500$



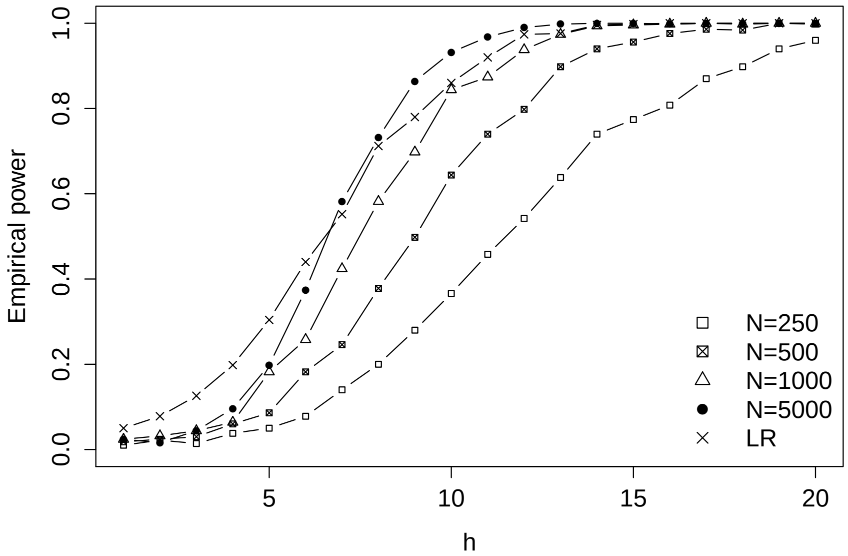
Empirical sizes vs. nominal levels for testing tetrads with $k = 15$ observed variables. True parameter is close to a **singular point**.

Size vs. Power

$n = 500$



Empirical sizes vs. nominal levels for testing tetrads with $k = 15$ observed variables. True parameter is close to a **singular point**.



Empirical power for different local alternatives for testing tetrads with $k = 15$ observed variables ($\alpha = 0.05$). True parameter is a **regular point**.

Trade-off between efficiency and guarding against singularities.

Conclusion

- ✔ General strategy for simultaneous testing of many constraints ($p \gg n$).
- ✔ Equality and inequality constraints.
- ✔ Optimization free.
  Although computationally demanding for large p and large computational budget N.
- ✔ Accommodate irregular settings where the incomplete U-statistics is mixed degenerate via $N = \mathcal{O}(n)$.

Our paper and background reading:

Sturma, Drton, Leung (2022).
Testing Many and Possibly Singular Polynomial Constraints. arXiv:2208.11756.

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Algebraic tests of general Gaussian latent tree models. NeurIPS 2018.

Drton (2009).
Likelihood ratio tests and singularities. Ann. Statist., 37(2):979–1012

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