Edgeworth and confidence interval correction in spiked PCA

lain Johnstone & Jeha Yang

Statistics & Biomedical Data Science, Stanford & Two Sigma

Shanghai, December 10, 2019

▲□▶ ▲□▶ ▲ 三▶ ▲ 三▶ 三 のへぐ

Edgeworth and confidence interval correction in spiked PCA

lain Johnstone & Jeha Yang

Statistics & Biomedical Data Science, Stanford & Two Sigma

Shanghai, December 10, 2019



Viral protein mutations and spiked models



Quadeer et. al. PLOS Comp. Bio. 2018

(日) (四) (日) (日) (日)

Viral protein mutations and spiked models





A suggestive simulation on correlation matrices

[David Morales, Matt McKay]

▲□▶ ▲□▶ ▲□▶ ▲□▶ □ のQで

 $\rho_1 = 0.2$; $\rho_2 = 0.1$

2nd eigenvalue



Theoretical variance is pretty accurate, but there seems to be a shift in the mean (similar to what we've seen before in the eigenvector projections of sample covariance when spikes were close to each other)

Outline

- Background on spiked covariance model
- Edgeworth correction single spike
- Edgeworth for multiple spikes
- Explaining the repulsion correction
- Confidence intervals after selection

▲□▶ ▲□▶ ▲□▶ ▲□▶ ■ ●の00

High dimensional spiked PCA model

• Data :
$$X = [x_1 \cdots x_n]'$$
 with

$$x_1, \cdots, x_n \overset{i.i.d.}{\sim} N_{p+1}(0, \Sigma)$$

• Large dimensional asymptotic regime : as $n \to \infty$,

$$\gamma_{n} := p/n \rightarrow \gamma \in (0,\infty)$$

Spiked eigenstructure of Σ : for a fixed r,

$$\underbrace{\ell_1 > \dots > \ell_r}_{\textit{Spikes}} > 1 = \ell_{r+1} = \dots = \ell_{p+1}$$

Statistics : eigenvalues of sample covariance matrix X'X/n

$$\hat{\rho}_1 \geq \cdots \geq \hat{\rho}_{p+1}$$

▲□▶ ▲□▶ ▲□▶ ▲□▶ ■ ●の00

 \rightarrow w.l.o.g. Σ is diagonal

Largest Eigenvalue $\hat{\rho}_1$: Numerical illustration p = 200, n = 800 [i.e. $\gamma_n = p/n = 0.25$] subcritical critical supercritical Spike $h = \ell - 1$: 0, 0.25, $h_+ = 0.5$, 0.75, 1.



▲□▶ ▲□▶ ▲ 三▶ ▲ 三▶ 三 のへぐ

Finite rank model, K = 1: phase transition

$$\Sigma = \operatorname{diag}(\ell_1, 1, \ldots, 1) \qquad p/n \to \gamma$$

Interior point transition at $\ell_1 = 1 + \sqrt{\gamma}$:

[Baik-Ben Arous-Peché,05]

▲□▶ ▲□▶ ▲三▶ ▲三▶ 三三 のへで



Finite rank model, K = 1: phase transition

$$\Sigma = \operatorname{diag}(\ell_1, 1, \ldots, 1) \qquad p/n \to \gamma$$

Interior point transition at $\ell_1 = 1 + \sqrt{\gamma}$:

[Baik-Ben Arous-Peché,05]

▲□▶ ▲□▶ ▲ 三▶ ▲ 三▶ 三 のへぐ



Largest Eigenvalue $\hat{\rho}_1$: Numerical illustration

subcritical critical supercritical
Spike
$$h = 0, 0.25, h_+ = 0.5, 0.75, 1.$$

p = 200, n = 800 [i.e. $\gamma_n = p/n = 0.25$]



◆□▶ ◆□▶ ◆三▶ ◆三▶ 三三 - のへで

Largest eigenvalue: Phase transition

Different rates, limit distributions:

For
$$h < \sqrt{\gamma}$$
: $n^{2/3} \left[\frac{\hat{\rho}_1 - \mu(\gamma_n)}{\tau(\gamma_n)} \right] \stackrel{\mathcal{D}}{\Rightarrow} TW_{\beta}$,
For $h > \sqrt{\gamma}$: $n^{1/2} \left[\frac{\hat{\rho}_1 - \rho(h, \gamma_n)}{\sigma(h, \gamma_n)} \right] \stackrel{\mathcal{D}}{\Rightarrow} N(0, 1)$

▲□▶ ▲□▶ ▲ 三▶ ▲ 三▶ 三三 - のへぐ

Largest eigenvalue: Phase transition

Different rates, limit distributions:

For
$$h < \sqrt{\gamma}$$
: $n^{2/3} \left[\frac{\hat{\rho}_1 - \mu(\gamma_n)}{\tau(\gamma_n)} \right] \stackrel{\mathcal{D}}{\Rightarrow} TW_{\beta}$,
For $h > \sqrt{\gamma}$: $n^{1/2} \left[\frac{\hat{\rho}_1 - \rho(h, \gamma_n)}{\sigma(h, \gamma_n)} \right] \stackrel{\mathcal{D}}{\Rightarrow} N(0, 1)$

with

$$\rho(\mathbf{h},\gamma) = (1+\mathbf{h})\left(1+\frac{\gamma}{\mathbf{h}}\right) \qquad \sigma^2(\mathbf{h},\gamma) = 2(1+\mathbf{h})^2\left(1-\frac{\gamma}{\mathbf{h}^2}\right)$$



Statistical physics lit, 94-Baik-Ben Arous-Peche(05) , Paul (07) Baik-Silverstein (06), Bloemendal-Virag (11) Mo (11) , Wang (12) Benaych-Georges-Guionnet-Maida (11)

・ロット (雪) ・ (日) ・ (日) ・ (日)

Normal approximation – multiple spikes

Assume that all spikes are simple, supercritical :

$$\ell_1 > \dots > \ell_r > 1 + \sqrt{\gamma}$$

Asymptotic mutual independence:

with
$$\rho_{kn} := \rho(\ell_k, \gamma_n), \quad \sigma_{kn} := \sigma(\ell_k, \gamma_n),$$

$$(\hat{z}_{kn})_{k=1,\cdots,r} := \left(n^{1/2} \frac{(\hat{\rho}_k - \rho_{kn})}{\sigma_{kn}}\right)_{k=1,\cdots,r} \Rightarrow N(0, I_r)$$

Shi (2013)

▲□▶ ▲□▶ ▲ 三▶ ▲ 三▶ 三 のへぐ

Edgeworth approximations

Inaccuracy of approximations : \hat{z}_{kn} associated with $\ell_k = 2.7$



◆□▶ ◆□▶ ◆三▶ ◆三▶ 三三 - のへで

Traditional Edgeworth

(Smooth function of) means model: Petrov, 1975, Hall, 1992

$$S_n = \frac{1}{\sqrt{n\kappa_{2n}}} \sum_{i=1}^n X_{ni} \quad \text{indep, mean } 0, \in \mathbb{R}^d, \quad d \text{ fixed}$$
$$\kappa_{jn} = \frac{1}{n} \sum_{1}^n \mathbb{E} X_{ni}^j \quad \text{moments}$$

First order expansion:

$$\mathbb{P}\left(S_n \le x\right) = \Phi(x) + n^{-1/2} p(x)\phi(x) + o(n^{-1/2})$$
$$p(x) = \frac{-\kappa_{3n}}{\kappa_{2n}^{3/2}} \frac{H_2(x)}{6}, \qquad H_2(x) = x^2 - 1.$$

skewness correction

▲□▶ ▲□▶ ▲ 三▶ ▲ 三▶ 三三 - のへぐ

Single spike, first order expansion for $\hat{\rho}_1$

$$\hat{z}_{1n} = n^{1/2} (\hat{
ho}_1 -
ho_{1n}) / \sigma_{1n}$$

Theorem In spiked model, $h_1 = \ell_1 - 1 > \sqrt{\gamma}$, $\gamma_n = p/n$,

$$\mathbb{P}(\hat{z}_{1n} \leq x) = \Phi(x) + n^{-1/2} p_{1n}(x) \phi(x) + o(n^{-1/2}),$$

uniformly in $x \in \mathbb{R}$, with

$$p_{1n}(x) = -\alpha_{2n}H_2(x) - \alpha_{0n}$$

$$\alpha_{2n} = \alpha_2(h_1, \gamma_n) = \frac{\sqrt{2}}{3} \frac{h_1^3 + \gamma_n}{(h_1^2 - \gamma_n)^{3/2}}$$

$$\alpha_{0n} = \alpha_0(h_1, \gamma_n) = \frac{\gamma_n}{\sqrt{2}} \frac{h_1 + 1}{(h_1^2 - \gamma_n)^{3/2}}$$

◆□▶ ◆□▶ ◆三▶ ◆三▶ 三三 のへぐ

Coefficients of Edgeworth expansion for single-spike

$$\alpha_2(h_1,\gamma_n) = \frac{\sqrt{2}}{3} \frac{h_1^3 + \gamma_n}{(h_1^2 - \gamma_n)^{3/2}}, \qquad \alpha_0(h_1,\gamma_n) = \frac{\gamma_n}{\sqrt{2}} \frac{h_1 + 1}{(h_1^2 - \gamma_n)^{3/2}}$$

• Larger for "harder" cases i.e. larger γ and smaller $h \ (> \sqrt{\gamma})$

► Larger than the fixed *p* case i.e. $\gamma = 0$, $\alpha_2 = \sqrt{2}/3$, $\alpha_0 = 0$ Muirhead-Chikuse (1975)

Empirically reasonable if

$$\frac{9}{2}\frac{\alpha_2^2}{n} = \frac{(h_1^3 + \gamma)^2}{n(h_1^2 - \gamma)^3} \le 0.2$$

◆□▶ ◆□▶ ◆ 臣▶ ◆ 臣▶ 三臣 - ∽ � � �

Single Spike Simulation



◆□▶ ◆□▶ ◆三▶ ◆三▶ 三三 - のへで

Edgeworth for multiple spikes

Eigenvalues are repulsive!



▶ joint density of $(\hat{\rho}_1, \cdots, \hat{\rho}_{n \land (p+1)})$ has a Jacobian factor

$$\prod_{i < j} |\hat{
ho}_i - \hat{
ho}_j|$$

 \rightarrow pushes eigenvalues apart

But, not visible at leading order (for supercritical spikes:)

$$(\hat{z}_{kn})_{k=1,\cdots,r} \Rightarrow N(0,I_r)$$

A D > A P > A B > A B >

3

Multi spike, first order expansion for $\hat{\rho}_k$

$$\hat{z}_{kn} = n^{1/2} (\hat{\rho}_k - \rho_{kn}) / \sigma_{kn}$$

Theorem In spiked model, $h_k = \ell_k - 1 > \sqrt{\gamma}$, $\gamma_n = p/n$,

$$\mathbb{P}(\hat{z}_{kn} \le x) = \Phi(x) + n^{-1/2} p_{kn}(x) \phi(x) + o(n^{-1/2}),$$

uniformly in $x \in \mathbb{R}$, with

$$p_{kn}(x) = -\alpha_2(h_k, \gamma_n)H_2(x) - \alpha_{0,k}(\mathbf{h}, \gamma_n)$$
$$\alpha_2(h_k, \gamma_n) = \frac{\sqrt{2}}{3} \frac{h_k^3 + \gamma_n}{(h_k^2 - \gamma_n)^{3/2}},$$
$$\alpha_{0,k}(\mathbf{h}, \gamma) = \frac{1}{\sqrt{2}} \frac{h_k + 1}{(h_k^2 - \gamma)^{1/2}} \Big[\frac{\gamma}{h_k^2 - \gamma} + \sum_{j \neq k} \frac{h_j}{h_k - h_j} \Big]$$

◆□▶ ◆□▶ ◆三▶ ◆三▶ 三三 のへぐ

Interpretation

Edgeworth corrected density

$$\phi + n^{-1/2} (\alpha_2 H_3 + \alpha_0 H_1) \phi$$

Relative to single spike case: α_2 unchanged, but

$$\Delta \alpha_0 = \alpha_{0,k}(\boldsymbol{h}, \gamma_n) - \alpha_0(\boldsymbol{h}_k, \gamma_n) = \frac{1}{\sqrt{2}} \frac{\boldsymbol{h}_k + 1}{(\boldsymbol{h}_k^2 - \gamma_n)^{1/2}} \sum_{j \neq k} \frac{\boldsymbol{h}_j}{\boldsymbol{h}_k - \boldsymbol{h}_j}$$

► $\Delta \alpha_0 > 0$, e.g. smaller spikes $h_j < h_k$, push density to right, conversely for $\Delta \alpha_0 < 0$

▲□▶ ▲□▶ ▲□▶ ▲□▶ ■ ●の00

• additive in
$$\ell_j$$
, $j \neq k$

Repulsion example 1 : \hat{z}_{kn} associated with $\ell_k = 2.7$



Figure: Density of \hat{z}_{kn} associated with $\ell_k = 2.7$

596

ж

ヘロト 人間ト 人間ト 人間ト

Repulsion example 2 : histograms of $(\hat{\rho}_k)_{k=1,\dots,r}$ together



Blue, red, green vertical lines correspond to $\rho_{1n}, \rho_{2n}, \rho_{3n}$, respectively.

≣ જવભ

(日)

Explaining the Repulsion Correction

▲□▶ ▲□▶ ▲ 三▶ ▲ 三▶ 三三 - のへぐ

Perturbation setup

 $\mathsf{Recall} \quad \ell_1 > \dots > \ell_r > 1 + \sqrt{\gamma} > 1 = \ell_{r+1} = \dots = \ell_{p+1}$

Focus on ℓ_k : $n^{-1}X'Xv_k = \hat{\rho}_k v_k$,

$$\hat{\rho}_k \to \rho_{kn} = \rho(\ell_k, \gamma_n) = \ell_k + \gamma \frac{\ell_k}{\ell_k - 1}$$

Permute columns:

$$X = [\sqrt{\ell_k} Z_1, \ Z_2 \Sigma_2^{1/2}] \qquad \Sigma_2 = \mathsf{diag}(\ell_{(k)}, 1, \cdots, 1)$$

Population eigenvalues of Σ_2 :

$$H_{(k)} = \left(1 - \frac{r-1}{p}\right)\delta_1 + \frac{1}{p}\sum_{j\neq k}\delta_{\ell_j} = \delta_1 + p^{-1}H^{\Delta}$$

(ロト (母) (主) (主) の(())

Standard first steps

$$\begin{split} n^{-1}X'Xv_k &= \hat{\rho}_k v_k & X = [\sqrt{\ell_k}Z_1, \ Z_2 \Sigma_2^{1/2}] \\ n^{-1}Z_2 \Sigma_2 \Sigma_2' &= U \Lambda U' & U \in O(n), \ \Lambda = \text{diag}(\lambda_1 \ge \cdots \lambda_n) \\ z &= U'Z_1 \sim N(0, I_n) \quad z \perp \Lambda \quad (\text{Gaussian assumptions!}) \end{split}$$

Schur complement, Woodbury formula, resolvent,...

$$R(x) = (\Lambda - xI_n)^{-1}$$

 \Rightarrow Key equation:

$$(\hat{\rho}_{k} - \rho_{kn})[1 + \ell_{k}n^{-1}z'\tilde{R}_{kn}z] = -\ell_{k}\rho_{kn}[n^{-1}z'R(\rho_{kn})z + \ell_{k}^{-1}]$$

▲□▶ ▲□▶ ▲目▶ ▲目▶ 目 のへぐ

The Forward Map $H \rightarrow F_{\gamma,H}$

Silverstein equation: H probability measure on \mathbb{R} , $\gamma > 0$,

$$z(\mathsf{m}) = -rac{1}{\mathsf{m}} + \gamma \int rac{t}{1+t\mathsf{m}} dH(t), \qquad \mathsf{m} \in \mathbb{C}^+$$

 $z(\mathsf{m})=z$ has unique solution $\mathsf{m}(z)$ for $z\in\mathbb{C}^+$, and

$$\mathsf{m}(z) = \int \frac{1}{\lambda - z} d\mathsf{F}(\lambda) = m_{\mathsf{F}}(z)$$

defines (Stieltjes transform of) a probability distribution $F = F_{\gamma,H}$.

Population: Σ_p $H_p = F^{\Sigma_p} = \frac{1}{p} \sum \delta_{\sigma_i}$ Sample: $B_n = n^{-1} Z_p \Sigma_p Z'_p$ $F^{B_n} = \frac{1}{n} \sum \delta_{\lambda_i}$ If $H_p \Rightarrow H, \ p/n \rightarrow \gamma$ $F^{B_n} \Rightarrow F_{\gamma,H}$

(Marcenko-Pastur-Bai-Silverstein)

▲ロ ▶ ▲周 ▶ ▲ 国 ▶ ▲ 国 ▶ ● の Q @

Stochastic Decomposition

 \Rightarrow

$$n^{-1}z'f(\Lambda)z = n^{-1}\sum f(\lambda_i)z_i^2 = n^{-1}\sum f(\lambda_i) + n^{-1/2}S_n(f)$$
$$S_n(f) = n^{-1/2}\sum f(\lambda_i)(z_i^2 - 1) \qquad (\Lambda \perp z)$$

$$n^{-1}\sum_{i} f(\lambda_{i}) = \int f(\lambda_{i}) d\mathsf{F}_{\gamma_{n},H_{n}}(\lambda) + n^{-1} \left[\sum_{i} f(\lambda_{i}) - n \int f d\mathsf{F}_{\gamma_{n},H_{n}}\right]$$
$$= \mathsf{F}_{\gamma_{n},H_{n}}(f) + n^{-1}G_{n}(f)$$

deterministic equiv. Bai-Silverstein CLT

(ロ)、(型)、(E)、(E)、 E) の(()

$$n^{-1}z'f(\Lambda)z = \mathsf{F}_{\gamma_n, H_n}(f) + n^{-1/2}S_n(f) + n^{-1}G_n(f)$$

Perturbing the centering

 $H = \delta_1 + p^{-1} H^{\Delta}$ From Wang-Silverstein-Yao, 2014 $F_{\gamma,H}(f) = F_{\gamma}(f) + n^{-1} A(f) + O(n^{-2})$

$$A(f) = \frac{1}{2\pi i} \int_{\mathcal{C}} f(z_0(\mathsf{m})w(\mathsf{m})d\mathsf{m})$$

$$z_0(\mathsf{m}) = -rac{1}{\mathsf{m}} + rac{\gamma}{1+\mathsf{m}}$$
 $w(\mathsf{m}) = \int rac{t}{1+t\mathsf{m}} dH^{\Delta}(t)$



Evaluating $A_n(g_{kn})$

In WSY 14, set $H \leftarrow H_{(k)n} = \delta_1 + \frac{1}{p} \sum_{j \neq k} (\delta_{\ell_j} - \delta_1)$

$$f(z) \leftarrow g_{kn}(z) = (\rho_{kn} - z)^{-1}, \quad w(m) = \sum_{j \neq k} \left(\frac{\ell_j}{1 + \ell_j m} - \frac{1}{1 + m} \right)$$

$$A_n(g_{kn}) = \frac{1}{2\pi i} \int_{\mathcal{C}} \sum_{j \neq k} t_j(\mathsf{m}) d\mathsf{m} = \frac{h_k}{(h_k^2 - \gamma)} \sum_{j \neq k} \frac{h_j}{h_k - h_j}$$

repulsion term



Back to $n^{-1}z'R(\rho_{kn})z$

$$-R(\rho_{kn}) = -(\Lambda - \rho_{kn}I_n)^{-1} = g_{kn}(\Lambda)$$

Decomposition:

$$-n^{-1}z'R(\rho_{kn})z\approx F_{\gamma_n}(g_{kn})+n^{-1/2}S_n(g_{kn})+n^{-1}D_n(g_{kn})$$

$$D_n(g_{kn}) = G_n(g_{kn}) + A_n(g_{kn}) + O(n^{-1})$$
$$= \tilde{\alpha}_{0,k}(\mathbf{h}, \gamma_n) + Z_{kn},$$

since, from Bai-Silverstein CLT

$$G_n(g_{kn}) = \mu_{\gamma_n}(g_{kn}) + Z_{kn},$$

$$\mu_{\gamma_n}(g_{kn}) = \frac{\gamma_n h_k}{(h_k^2 - \gamma_n)^2}$$

<mark>bulk term</mark> ৰ □ > ৰি ≥ ৰ ই > ৰ ই > ৩৫৫

Key linearization

$$\hat{z}_{kn} = \frac{n^{1/2}(\hat{\rho}_k - \rho_{kn})}{\sigma_{kn}} \approx \frac{S_n(g_{kn}) + n^{-1/2}D_n(g_{kn})}{\sigma_{kn}\mathsf{F}_{\gamma_n}(g_{kn}^2) + h.o.t.}$$

Delta method for Edgeworth expansion, + conditioning

$$\mathbb{P}\{\hat{z}_{kn} \leq x\} = \mathbb{E}\left\{\mathbb{P}\{S_n(g_{kn}) \leq \frac{y_n(x)}{|h|}\}\right\} + o(n^{-1/2})$$

▲□▶ ▲□▶ ▲ □▶ ▲ □▶ □ のへぐ

Final steps:

Edgeworth expansion (conditional on Λ)

uncondition; identify terms

Edgeworth (conditional on Λ)

$$S_n(g_{kn}) = n^{-1} \sum X_{ni}$$
 $X_{ni} = c_{ni}(z_i^2 - 1)$ $c_{ni} = g_{kn}(\lambda_i)$

From e.g. Petrov 1975, n.i.d. case:

$$\mathbb{P}\left\{\frac{1}{\bar{\kappa}_{2n}\sqrt{n}}\sum X_{ni} \leq y \left|\Lambda\right\} = \Phi(y) - \frac{\bar{\kappa}_{jn}}{\bar{\kappa}_{2n}^{3/2}\sqrt{n}} \frac{H_2(y)}{6} \phi(y) + o(n^{-1/2})\right\}$$

Cumulants:
$$\bar{\kappa}_{jn} = \kappa_j n^{-1} \sum_{1}^n c_{ni}^j = \kappa_j \mathsf{F}_{\gamma_n}(g_{kn}^j) + O(n^{-1/2})$$

quadratic term:

$$\frac{\bar{\kappa}_{jn}}{\bar{\kappa}_{2n}^{3/2}} = \frac{\sqrt{2}}{3} \frac{h_k^3 + \gamma_n}{(h_k^2 - \gamma_n)^{3/2}} + O(n^{-1/2}) = \alpha_2(h_k, \gamma_n) + O(n^{-1/2})$$

◆□ ▶ ◆□ ▶ ◆ 臣 ▶ ◆ 臣 ▶ ○ 臣 ○ の Q @

Assembling pieces

$$\mathbb{P}\{\hat{z}_{kn} \leq x\} = \mathbb{E}\left[\Phi(y_n) - \frac{\alpha_2(h_k, \gamma_n)}{\sqrt{n}} \frac{H_2(y_n)}{6} \phi(y_n) + o(n^{-1/2})\right]$$
$$y_n = y_n(x) = x - \frac{1}{\bar{\kappa}_{2n}\sqrt{n}} D_n(g_{kn}) \quad \text{repulsive shift}$$
$$= x - \frac{1}{\bar{\kappa}_{2n}\sqrt{n}} [\tilde{\alpha}_{0,k}(\boldsymbol{h}, \gamma_n) + Z_{kn}]$$
$$\mathbb{E}\Phi(y_n) \approx \Phi(x) - \frac{\alpha_{0k}(\boldsymbol{h}, \gamma_n)}{\sqrt{n}} \phi(x)$$

Final result:

$$\mathbb{P}\{\hat{z}_{kn} \leq x\} = \Phi(x) - \frac{1}{\sqrt{n}} \left[\alpha_2(h_k, \gamma_n) \frac{H_2(y)}{6} + \alpha_{0k}(h, \gamma_n) \right] \phi(x) + o(n^{-1/2})$$

◆□▶ ◆□▶ ◆臣▶ ◆臣▶ 臣 の�?

Confidence intervals after selection

Inference for supercritical spikes

Below bulk edge:

Even for supercritical ℓ_k , $\mathbb{P}\{\hat{\rho}_k < b(\gamma)\}\$ can be significant!



 \rightarrow inference after selection of supercritical spikes

Selection rule: select all $\hat{\rho}_k, k = 1, \cdots, \hat{r}$ such that

$$\hat{\rho}_k > \theta_n := b(\gamma_n) + n^{-1/3} \sqrt{\gamma_n}$$

Consistent: $\mathbb{P}(\hat{r}=r)=1-o(n^{-m}), m \in \mathbb{N}$

Minimal conditioning: Liu-Markovic-Tibshirani (2018)

 $\hat{\rho}_k \mid \hat{\rho}_k > \theta_n$

Pivots

Exact distribution of $\hat{\rho}_k$:

$$\overline{F}_{kn}(x,\ell) = \mathbb{P}_{\ell}(\hat{\rho}_k > x)$$

Exact pivot given $\hat{\rho}_k > \theta_n$:

$$u_{kn}(\hat{
ho}_k, \ell) := rac{\overline{F}_{kn}(\hat{
ho}_k, \ell)}{\overline{F}_{kn}(heta_n, \ell)} \sim U(0, 1) \qquad ext{for all } \ell$$

Approach:

- 1. Approximate \overline{F}_{kn} by Gaussian, Edgeworth, ...
- 2. Form approximate pivots $u_{kn}^{A}(\hat{\rho}_{k}, \ell) \approx U(0, 1)$
- 3. Confidence intervals: $\{\ell_k > 1 + \sqrt{\gamma} : u_{kn}^A(\hat{\rho}_k, \ell) \in I\}$

▲□▶ ▲□▶ ▲□▶ ▲□▶ ■ ● ●

Pivots ctd.

$$\begin{split} \{\boldsymbol{\ell}_{\boldsymbol{k}} > 1 + \sqrt{\gamma} : \boldsymbol{u}_{\boldsymbol{k}\boldsymbol{n}}^{A}(\hat{\rho}_{\boldsymbol{k}}, \boldsymbol{\ell}) \in \boldsymbol{I} \} \\ \boldsymbol{I} = \begin{cases} [0, 1 - \alpha] & \text{upper} \\ [\alpha/2, 1 - \alpha/2] & \text{two-sided...} \end{cases} \end{split}$$

Usually $\ell_k
ightarrow u_{kn}^A(\hat{
ho}_k, \ell)$ is monotone \nearrow



▲□▶ ▲□▶ ▲三▶ ▲三▶ 三三 のへで

Pivots ctd.

$$\{\ell_k > 1 + \sqrt{\gamma} : u_{kn}^A(\hat{\rho}_k, \ell) \in I\}$$

$$I = \begin{cases} [0, 1 - \alpha] & \text{upper} \\ [\alpha/2, 1 - \alpha/2] & \text{two-sided...} \end{cases}$$
Usually $\ell_k \rightarrow u_{kn}^A(\hat{\rho}_k, \ell)$ is monotone \nearrow

Gaussian example:

$$\overline{F}_{kn}(x,\boldsymbol{\ell}) \approx \overline{\Phi}(z_n(x,\boldsymbol{\ell}_k)), \qquad z_n(x,\boldsymbol{\ell}) = n^{1/2} \frac{x - \rho(\boldsymbol{\ell},\gamma_n)}{\sigma(\boldsymbol{\ell},\gamma_n)}$$

 \rightarrow Selective Z pivot:

$$u_n^z(\hat{\rho}_k, \ell_k) := \frac{\overline{\Phi}(z_n(\hat{\rho}_k, \ell_k))}{\overline{\Phi}(z_n(\theta_n, \ell_k))}$$

◆□▶ ◆□▶ ◆三▶ ◆三▶ 三三 のへぐ

Edgeworth pivots

Edgeworth approximation

$$\Phi_{kn}^{E}(x,\boldsymbol{\ell}) = \Phi(x) + n^{-1/2} p_{k}(x;\boldsymbol{\ell},\gamma_{n})\phi(x)$$

 \rightarrow Selective *E* pivot: [estimated $\hat{\ell}$: $\hat{\ell}_j = \rho_n^{-1}(\hat{\rho}_j)$]

$$u_{kn}^{E}(\hat{\rho},\ell_{k}) := \frac{\overline{\Phi}_{kn}^{E}(z_{n}(\hat{\rho}_{k},\ell_{k}),\hat{\ell})}{\overline{\Phi}_{kn}^{E}(z_{n}(\theta_{n},\ell_{k}),\hat{\ell})}$$

Positive (E) pivot:

$$u_{kn}^{P}(\hat{\boldsymbol{\rho}}, \boldsymbol{\ell}_{k}) := \begin{cases} u_{kn}^{E}(\hat{\boldsymbol{\rho}}, \boldsymbol{\ell}_{k}) & \text{if } \overline{\Phi}_{kn}^{E}(z_{n}(\hat{\boldsymbol{\rho}}_{k}, \boldsymbol{\ell}_{k}), \hat{\boldsymbol{\ell}}) > 0\\ u_{n}^{z}(\hat{\boldsymbol{\rho}}, \boldsymbol{\ell}_{k}) & \text{otherwise} \end{cases}$$

▲□▶ ▲□▶ ▲ 三▶ ▲ 三▶ 三 のへぐ

Coverage accuracy

Theorem: Uniformly in $\alpha \in [0, 1]$, for any $1 \le k \le r$,

$$\mathbb{P}\{u(\hat{\boldsymbol{\rho}}) \leq \alpha \mid \hat{\rho}_k > \theta_n\} - \alpha$$

=
$$\begin{cases} O(n^{-1/2}) & \text{for } u(\hat{\boldsymbol{\rho}}) = u_n^z(\hat{\rho}_k, \ell_k), \\ o(n^{-1/2}) & \text{for } u(\hat{\boldsymbol{\rho}}) = u_{kn}^E(\hat{\boldsymbol{\rho}}, \ell_k), u_{kn}^P(\hat{\boldsymbol{\rho}}, \ell_k) \end{cases}$$

▲□▶ ▲□▶ ▲□▶ ▲□▶ ▲□ ● ● ●

- Consequence of the Edgeworth expansion
- ▶ also holds for clipped pivots $((u(\hat{\rho}) \lor 0) \land 1)$

Numerical coverage - 2 spikes



◆□ > ◆□ > ◆豆 > ◆豆 > ̄豆 = のへで

Numerical coverage - 2 spikes



▶ Repulsion stronger for closer spikes → worse approximations

▶ selective E(o) has $\overline{\Phi}^E < 0$ with prob > 5% in tough cases: h = (2.0, 1.5), (2.5, 2.0)

Positive pivot(+) usually fixes this!

Future work

Other models, e.g. low rank denoising

$$X = \sum_{k=1}^{r} \ell_k \boldsymbol{u}_k \boldsymbol{u}_k' + Z$$

- non-Gaussian data
- second order expansions: LSS obstacle

Reference: (single spike) Yang & J., *Statistica Sinica* 2018. (multispike) in preparation.

▲□▶ ▲□▶ ▲ □▶ ▲ □▶ □ のへぐ

THANK YOU!