# LTCC: Selective Inference

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## Structure of the course

- 1. Introduction.
- 2. Unconditional inference.
  - Fixed design.
  - Random design.
- 3. Conditional inference.
  - Most powerful conditional inference.
  - Information-splitting methods.
- 4. Bayesian approaches.
- 5. Other topics.

## Key references

Review papers:

- Zhang, Khalili, Asgharian (2022). "Post-model-selection inference in linear regression models: an integrated review", *Statistics Surveys*.
- Kuchibhotla, Kolassa, Kuffner (2022). "Post-selection inference", Annual Review of Statistics and Its Application.

Week 1:

- Berk, Brown, Buja, Zhang, Zhao (2013). "Valid post-selection inference", *Annals of Statistics*.
- Bachoc, Preinerstorfer, Steinberg (2020). "Uniformly valid confidence intervals post-model-selection", *Annals of Statistics*.

The classical approach to statistical inference assumes that all the models to fit and all the inferential objectives are fixed prior to the data analysis.

For example, a common regression problem assumes observation of a vector  $Y \sim N(X\beta, \sigma^2 I)$  and seeks inference for  $\beta$ .

However, this is not how statistics operates in practice.

Typically, the practitioner **interacts with the data** in order to select a suitable model to fit and/or a set of relevant inferential questions to address—the **selection stage**.

Such data exploration allows the practitioner to **focus only on the most relevant aspects** of the data-generating process.

**BUT** it invalidates the assumptions of a fixed model or inferential objectives, leading to a (possible) loss of the inferential guarantees indicated by classical theory.

The further **sampling variability** introduced in the pre-analysis stage often leads to:

- Overstatement of statistical significance (exaggerated *p*-values).
- Confidence intervals with low coverage.
- Overestimation of effect sizes.
- Underestimation of variances.

Selection effects are **regularly overlooked in statistical practice**, and are often cited as one of the main causes of the replicability crisis in science.

Famously, Breiman (1992) referred to this issue as a "quiet scandal in the statistical community".

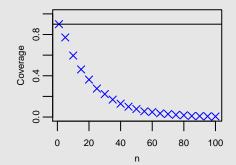
 $\rightarrow$  The goal of selective inference is to restore validity of inference after selection.

#### Example: inference on winners

Let  $Y_i \sim N(\theta_i, 1)$  independently for i = 1, ..., n, and suppose a confidence interval is required for the mean of the largest observation,  $\theta_I(Y)$ , where

$$I(Y) = \underset{i=1,\ldots,n}{\arg \max} Y_i.$$

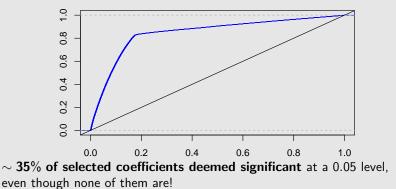
Plot shows the coverage of conventional 90% confidence intervals  $[y_{l(Y)} - 1.64, y_{l(Y)} + 1.64]$  for the case  $\theta_1 = \ldots = \theta_n$  as  $n \to \infty$ .



#### Example: inference after model selection

 $Y \sim N(\mathbf{0}, I_{80})$  and  $X \in \mathbb{R}^{80 \times 20}$  with N(0, 1) entries independent of Y.

A forward stepwise algorithm minimising the AIC is used to select a linear submodel, and a marginal *p*-value is computed to test significance for each variable in the selected model.



CDF of p-values

Selective inference has a long and rich history.

Many approaches have been advocated to estimate/control selection effects, such as

- Simultaneous inference (Bonferroni, BH, ...).
- Bayesian methods: model averaging, empirical Bayes.
- Bootstrap.
- Differential privacy.

The goal of this course is to give an overview of recent proposals and describe how they fit within the general framework.

#### Framework

Data matrix denoted by [Y, X], where

Y = (Y<sub>1</sub>,...,Y<sub>n</sub>)<sup>T</sup> ∈ ℝ<sup>n</sup> is a quantitative response vector.
 X = [X<sub>1</sub>,...,X<sub>p</sub>] ∈ ℝ<sup>n×p</sup> is a n×p design matrix, containing observations of p covariates. For now assume **design is fixed**.

In general (provided finite expectation), one can write

$$Y = \mu + \varepsilon$$
, where  $\mu = E[Y]$  and  $\varepsilon = Y - \mu$ . (1)

Often  $\mu$  is assumed to belong to a parametric class, such as the linear model  $\{X\beta \colon \beta \in \mathbb{R}^p\}$ , and inference is sought for the corresponding parameter.

If  $p \sim n$  or p > n it is common to seek a smaller model due to identifiability issues and lack of interpretability of the larger model.

An index set  $M = \{i_1, \ldots, i_m\} \subseteq \{1, \ldots, p\}$  will denote a **linear** submodel containing only the covariates in M, where m = |M|.

If  $X_M = [X_{i_1}, \ldots, X_{i_m}]$  denotes the submatrix of X that contains only the covariates in M, the linear submodel corresponding to M posits

$$Y = X_M \beta^M + \varepsilon, \quad \beta^M \in \mathbb{R}^m.$$
<sup>(2)</sup>

### The projection parameter

In selective inference one normally treats **models as approximations** of a (potentially very complex) true underlying distribution.

This aligns more naturally with the model-selection framework and is considerably more realistic.

Even if  $\mu \notin \operatorname{span}(X_M) = \{X_M b \colon b \in \mathbb{R}^m\}$  for some M, one can still define a meaningful model-dependent parameter, the **projection parameter**:

$$\beta_M = \arg\min_{b \in \mathbb{R}^p} E \|Y - X_M b\|^2 = (X_M^T X_M)^{-1} X_M^T \mu = X_M^\dagger \mu \in \mathbb{R}^m, \quad (3)$$

for all M with m < n and  $\operatorname{rank}(X_M) = m$ , where  $A^{\dagger} := (A^T A)^{-1} A^T$ .

 $\rightarrow$  It is the **best linear predictor** of  $\mu$  in *M* with respect to the squared error loss.

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The entries of the projection parameter, denoted by  $\beta_{jM}$ ,  $j \in M$ , have a different interpretation to the conventional regression coefficients.

 $\rightarrow$  If  $Y = X_M \beta^M + \varepsilon$ ,  $\beta_j^M$  is the average difference in the response for a unit difference in  $X_{i_i}$ , ceteris paribus in the model M.

 $\rightarrow$  In the non-linear case,  $\beta_{jM}$  is the average difference in the response approximated in the submodel M.

Naturally, if the selected model is in fact correct, then  $\beta_M = \beta^M$  and the usual interpretation holds.

#### Interpretation of the projection parameter

For  $j \in M$ , let  $X_{jM}$  be the corresponding column of  $X_M$ , and define

$$r_{jM} = \left\{ I_n - X_{M \setminus \{j\}} X_{M \setminus \{j\}}^{\dagger} \right\} X_{jM}, \tag{4}$$

the residual vector of the regression of  $X_{iM}$  on the other predictors in M.

We can rewrite the *j*-th coefficient of  $\beta_M$  as

$$\beta_{jM} = \frac{1}{\|r_{jM}\|^2} r_{jM}^T \mu,$$
 (5)

so  $\beta_{jM}$  is a **measure the relevance** of the *j*-th covariate once we have adjusted for the other covariates in *M*.

#### Interpretation of the projection parameter

More specifically, denote by  $P_M = X_M X_M^{\dagger}$  the projection matrix onto span $(X_M)$ .

We can decompose it as

$$P_M = P_{M \setminus \{j\}} + (r_{jM}^T X_{jM}) r_{jM} r_{jM}^T.$$
(6)

 $\rightarrow$  The **null hypothesis**  $H_0: \beta_{iM} = 0$  is equivalent to

$$P_M \mu = P_{M \setminus \{j\}} \mu. \tag{7}$$

PoSl<sup>1</sup> (**Post Selection Inference**) is a framework for **selective inference** for projection parameters with

- Finite sample guarantees for any dimension (n, p).
- Universal validity over (virtually) all model selection procedures.

Seminal work; introduced ideas which constitute the basis of much of the contemporary work on selective inference.

Crucially, it requires very strong distributional assumptions.

Extensions with less restrictive assumptions will be considered later.

<sup>&</sup>lt;sup>1</sup>Berk, Brown, Buja, Zhang, Zhao (2013). "Valid post-selection inference", *Ann. Stat.* 

Assume a Gaussian response  $Y \sim N(\mu, \sigma^2 I_n)$ , with  $\mu \in \mathbb{R}^n$  and  $\sigma^2 > 0$ .

PoSI requires an estimator  $\hat{\sigma}$  which is **independent** of all estimates  $\hat{\beta}_{jM}$ , and such that

$$\hat{\sigma}^2 \sim \sigma^2 \frac{\chi_r^2}{r}.$$
(8)

We write  $r = \infty$  if  $\sigma^2$  is known.

Distributional requirements constitute a major practical limitation of the approach.

However, they are only needed for finite-sample validity; asymptotic guarantees can be derived under much weaker conditions, as we shall see.

A valid variance estimator will be available if p < n and the full model  $Y \sim N(X\beta, \sigma^2 I_n)$  is (at least approximately) valid.

#### PoSI

For a **fixed** submodel *M*, a natural estimator of  $\beta_M$  is

$$\hat{\beta}_M = X_M^{\dagger} Y \sim \mathcal{N}(\beta_M, \sigma^2 (X_M^T X_M)^{-1}).$$
(9)

If a suitable estimate of  $\sigma^2$  is available, confidence sets and testing procedures for  $\beta_M$  are provided by classical normal theory.

Introduce the *t*-values relative to submodel *M*:

$$t_{jM} = \frac{\beta_{jM} - \hat{\beta}_{jM}}{\left[ (X_M^T X_M)^{-1} \right]_{jj}^{1/2} \hat{\sigma}} \sim t_r, \quad j \in M.$$

$$(10)$$

A valid  $1 - \alpha$  valid confidence interval for  $\beta_{iM}$  is given by

$$CI_{jM}(K) = [\hat{\beta}_{jM} \pm K[(X_M^T X_M)^{-1}]_{jj}^{1/2} \hat{\sigma}], \quad K = t_{r,1-\alpha/2}.$$
(11)

In the selective context, however, the submodel M is allowed to depend on the data, i.e. it is **random**, which invalidates the previous CI.

Write a random submodel as  $\hat{M} \equiv \hat{M}(Y) \subseteq \{1, \dots, p\}.$ 

Think of  $\hat{M}$  as the result of some variable-selection procedure such as LASSO, stepwise regression, visual diagnostics, etc.

In principle,  $\hat{M}: \mathbb{R}^n \to \mathcal{M}_{all}$  can be any *measurable* map, where

$$\mathcal{M}_{\mathsf{all}} = \{ M \subseteq \{1, \dots, p\} \colon \mathsf{rank}(X_M) = |M| \}, \tag{12}$$

i.e. the projection parameter needs to be identifiable.

#### PoSI

Associated with a random model  $\hat{M}$  there is a random projection parameter  $\beta_{\hat{M}} = X^{\dagger}_{\hat{M}}\mu$ , which constitutes the **moving target of inference**.

Note that

- $\beta_{\hat{M}}$  has random dimension  $|\hat{M}|$ .
- For a fixed j, it might not be the case that  $j \in \hat{M}$ .
- Conditionally on  $j \in \hat{M}$ , the parameter  $\beta_{\hat{M}}$  is random.

Furthermore, the corresponding estimator

$$\hat{\beta}_{\hat{M}} = X_{\hat{M}}^{\dagger} Y \tag{13}$$

is **not normally distributed** due to the extra variability from the selection step, so classical normal theory does not apply.

Given the stochastic nature of the parameter, what constitutes a valid inferential procedure this setting?

In the fixed-*M* setting, the  $1 - \alpha$  confidence interval  $CI_{jM}(K)$  for  $\beta_{jM}$  satisfies

$$P\left(\beta_{jM} \in CI_{jM}(K)\right) = 1 - \alpha.$$
(14)

In the random-model setting, the **PoSI** (Post-Selection Inference) framework seeks a value of K such that

$$P\left(\beta_{j\hat{M}} \in Cl_{j\hat{M}}(K) \;\forall \; j \in \hat{M}\right) \ge 1 - \alpha, \tag{15}$$

for any selection procedure  $\hat{M}$ . K is called the **PoSI constant**.

Some key aspects of this approach:

- Universality: Cls are valid regardless of the selection procedure, even if this involves subjective and informal decisions; the practitioner is even allowed to change their mind and report a different model post-hoc.
- Intervals tend to be very conservative as a result: the actual coverage can be well above the nominal one for some selection rules.
- However, there exists a selection procedure that requires full protection: unless there is a strong reason for discarding certain ill-behaved selection rules, PoSI is optimal.
- It provides only **unconditional** guarantees (more on this later).
- Implemented via simulation (computationally demanding if  $p \approx 20$ ).

The conservative nature of PoSI can be partially alleviated under the assumption that not all models in  $\mathcal{M}_{\mathsf{all}}$  are being searched.

In many applications, there is a priori knowledge about the set of plausible selected models, e.g.

- A subset of the covariates is forced into the model (e.g. an intercept).
- There is a size restriction on the model:  $|M| \le k$  (sparsity).
- Hierarchical restrictions: polynomial regression, interactions, etc.

If such assumption can be made, we denote by  $\mathcal{M}\subseteq\mathcal{M}_{\mathsf{all}}$  the *pre-specified* set of allowed models.

With sufficiently strong restrictions on  $\mathcal{M}$  (particularly the sparsity one), the PoSI approach becomes **computationally manageable for large** *p*.

Further reduction can be achieved by discarding variables ignoring the response, e.g. if there is collinearity.

#### PoSI: the selection-adjusted constant

The PoSI constant K is formally defined as

$$\mathcal{K}(\mathcal{X}, \mathcal{M}, \alpha, r) = \min\left\{\mathcal{K} > 0 \colon \mathbb{P}\left(\max_{\mathcal{M} \in \mathcal{M}} \max_{j \in \mathcal{M}} |t_{j\mathcal{M}}| \le \mathcal{K}\right) \ge 1 - \alpha\right\},\tag{16}$$

where, recall,

$$t_{jM} = \frac{\beta_{jM} - \hat{\beta}_{jM}}{[(X_M^T X_M)^{-1}]_{jj}^{1/2} \hat{\sigma}} = \frac{e_j^T X_M^{\dagger} (Y - \mu)}{[(X_M^T X_M)^{-1}]_{jj}^{1/2} \hat{\sigma}}.$$
 (17)

 $T = \max_{M \in \mathcal{M}} \max_{j \in M} |t_{jM}|$  is **distribution constant**, so K is computable.

For any measurable model-selection procedure  $\hat{M} : \mathbb{R}^n \to \mathcal{M}$ , we have the trivial bound

$$\max_{j\in\hat{M}}|t_{j\hat{M}}| \leq \max_{M\in\mathcal{M}}\max_{j\in M}|t_{jM}|.$$
(18)

#### Thus,

$$\mathbb{P}\left(\max_{j\in\hat{M}}|t_{j\hat{M}}|\leq K\right)\geq \mathbb{P}\left(\max_{M\in\mathcal{M}}\max_{j\in M}|t_{jM}|\leq K\right)\geq 1-\alpha,$$
(19)

where  $K = K(X, \mathcal{M}, \alpha, r)$ .

Among all possible model-selection procedures, there is one for which the nominal covarage is achieved, i.e. for which the PoSI constant is **sharp**.

It is the **significance-hunting procedure**, which seeks the model with the most significant observed effect:

$$\hat{M}^{*}(Y) = \arg\max_{M \in \mathcal{M}} \max_{j \in M} |t_{jM}|.$$
(20)

Although it is generally not advisable to select a model via  $\hat{M}^*$ , protection against it is a **guarantee against bad practice**.

## PoSI: computation of the PoSI constant

**Closed-form expressions** for *K* are **not available**.

Brute force Monte Carlo used to approximate the  $1 - \alpha$  quantile of

$$T = \max\{|t_{jM}| \colon M \in \mathcal{M}, j \in M\}.$$
(21)

 $\rightarrow$  If rank(X) = p and  $\mathcal{M} = \mathcal{M}_{all}$ , need to evaluate  $p2^{p-1}$  t-values.

 $\rightarrow$  Computations are specific to the design X.

 $\rightarrow$  Universal bounds needed in high-dimensional problems.

## PoSI: one primary predictor

Sometimes the analysis is centred on a predictor of interest,  $X_j$ , while the other predictors in M act as controls, so that

- The submodel space is  $\mathcal{M}_j = \{ M \in \mathcal{M}_{all} : j \in M \}.$
- Only the *t*-statistic associated with  $X_j$  is relevant.

In this context, the PoSI constant is defined differently:

$$\mathcal{K}_{j}(X, \mathcal{M}, \alpha, r) = \min \left\{ \mathcal{K} > 0 \colon \mathbb{P}\left( \max_{\mathcal{M} \in \mathcal{M}_{j}} |t_{j\mathcal{M}}| \le \mathcal{K} \right) \ge 1 - \alpha 
ight\}.$$
 (22)

As in the unrestricted case, exact coverage with this constant is achieved by the significance-hunting procedure

$$\hat{M}_{j}^{*}(Y) = \arg\max_{M \in \mathcal{M}_{j}} |t_{jM}|.$$
(23)

PoSI provides simultaneous inference for up to  $p2^{p-1}$  linear contrasts  $\beta_{jM}$ .

Scheffé's method provides simultaneous protection for all linear combinations without all the computational burden.

Write

$$t_{x} = \frac{(Y - \mu)^{T} x}{\hat{\sigma} \|x\|}, \quad x \in \operatorname{span}(X) \setminus \{\mathbf{0}\}.$$
(24)

Recall that for  $x \propto r_{jM} \in \text{span}(X)$ ,  $t_x = t_{jM}$ , so simultaneous inference for all the directions in the column space of X is an overkill for our problem.

Scheffé's constant, explicitly given by  $K_S(\alpha, d, r) = \sqrt{dF_{d,r,1-\alpha}}$ , with  $d = \dim{\text{span}(X)}$ , satisfies

$$\mathbb{P}\left(\sup_{x\in \text{span}(X)}|t_x|\leq K_S\right)=1-\alpha,$$
(25)

and thus it provides valid selective intervals regardless of the design.

Naturally  $K \leq K_S$  for any X, and often the **difference is substantial**, but provides a valid solution when simulation of PoSI constant is too costly.

### PoSI: size of the PoSI constant

Asymptotic bounds for  $n \ge p$ ,  $p \to \infty$  and  $\mathcal{M} = \mathcal{M}_{\mathsf{all}}$ :

- Lower bound:  $K = \Omega(\sqrt{\log p})$ , achieved by orthogonal designs.
- **Upper bound**:  $K = O(\sqrt{p})$ , achieved by equicorrelated designs.

 $\rightarrow$  For orthogonal X,  $\beta_{jM} \equiv \beta_j$  for all (j, M), so only p directions need to be covered.

- $\rightarrow$  Large range  $(\sqrt{\log p}, \sqrt{p})$  suggests strong dependence on X.
- $\rightarrow$  Scheffé constant has  $K_S \sim \sqrt{p}$ , so its optimality is case-dependent.

For sparse model spaces,  $\mathcal{M}_s = \{M \subseteq \{1, \dots, p\} \colon |M| \leq s\}$ ,

$$K = O\left(\sqrt{s\log(p/s)}\right). \tag{26}$$

#### PoSI: other universal bounds

A general upper bound for K is given by

$$Q_{T}\{g(\mathcal{M}, X), r, 1 - \alpha/2\} \le \frac{g(\mathcal{M}, X) + A}{1 - Br^{-1/2}}$$
(27)

for some known constants A, B > 0, where  $Q_T(x, r, \alpha)$  is the  $\alpha$  quantile of a non-central t distribution with r degrees of freedom and non-centrality parameter x, and

$$g(\mathcal{M}, X) = \mathbb{E}\left[\max_{M \in \mathcal{M}} \max_{j \in M} |w_{jM}^{T}Z|\right], Z \sim N(0, I_n), w_{jM}^{T} = e_{jM}^{T}X_{M}^{\dagger}/\|e_{jM}^{T}X_{M}^{\dagger}\|.$$
(28)

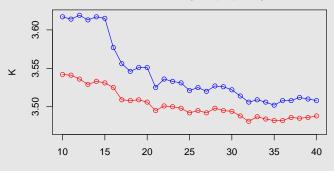
Two important cases:

- Orthogonal designs:  $g(\mathcal{M}, X) = \sqrt{2\log(2p)}$ .
- Sparse models,  $\mathcal{M}_s = \{M \colon |M| \le s\}$ :  $g(\mathcal{M}, X) = \sqrt{2s \log(6p/s)}$ .

Further refinements are available in the literature combining these two cases under the **Restricted Isometry Property**.

#### PoSI: size of the PoSI constant (empirical)

Set p = 10,  $n \in \{10, ..., 40\}$ ,  $r = \infty$  and  $\alpha = 0.05$ ; predictors generated as Gaussian vectors with covariance  $\Sigma_{ii} = 1$ ,  $\Sigma_{ij} = 0.5$ ; Nsim =  $5 \times 10^4$ .



 $\mathcal{M} = \mathcal{M}_{\mathsf{all}}; \ \mathcal{M} = \{M \colon |M| \leq 5\}.$ 

n

 $\rightarrow$  The Scheffé constant for this problem is 4.28.

## PoSI: coverage

Empirical coverages of 95% CIs over 5000 samples; setting as before.

Data generated as  $Y = X\beta + N(\mathbf{0}, I_n)$  under two parameters:

$$- \beta^{(1)} = \mathbf{0}. - \beta^{(2)} = (1, 1, -1, -1, 0, \dots, 0)^{T}.$$

Variable-selection rules:

- Lasso with cross-validation.
- Screening: a predictor is selected iff its significance *p*-value in the full linear model  $\mu = X\beta$  is below 0.05.

$$p = 10, n = 30$$

 $\mathbf{p}=\mathbf{10}, \mathbf{n}=\mathbf{1000}$ 

		Lasso	Screen.
	PoSI	97.6	97.2
$\beta^{(1)}$	Scheffé	99.8	99.8
	Unadj.	63.6	62.5
	PoSI	99.5	99.5
$\beta^{(2)}$	Scheffé	99.9	100
	Unadj.	93.4	92.8

	Lasso	Screen.
PoSI	95.7	95.4
Scheffé	99.7	99.8
Unadj.	50.5	50.4
PoSI	99.2	99.1
Scheffé	100	99.9
Unadj.	92.5	88.7

#### PoSI: extensions

The original PoSI framework has some practical limitations, most notably the restrictive distributional assumptions

$$Y \sim N(\mu, \sigma^2 I_n), \quad \hat{\sigma}^2 \sim \sigma^2 \frac{\chi_r^2}{r}.$$
 (29)

Bachoc et al.<sup>2</sup> develop a more general framework that

- Provides asymptotically valid (but fixed-p) confidence intervals without parametric assumptions on the errors ε.
- Does not require a consistent estimator of  $\sigma$ .
- Is applicable with other types of data (e.g. binary).

<sup>&</sup>lt;sup>2</sup>Bachoc, Preinerstorfer, Steinberg (2020). "Uniformly valid confidence intervals post-model-selection". *Ann. Stat.* 

# Generalised PoSI: framework

- Data  $Y = (Y_1, \ldots, Y_n)^T \sim \mathbb{P}_n$  has independent but not necessarily identically distributed components.
- $\mathbb{P}_n \in \mathbf{P}_n$ , where  $\mathbf{P}_n$  is a large non-parametric family of distributions.
- Statistician has a set of models  $\mathcal{M}_n = \{M_{1,n}, \ldots, M_{d,n}\}$ , possibly misspecified, where each  $M_{j,n}$  is a set of distributions over  $\mathcal{B}(\mathbb{R}^n)$ .
- For each model M ∈ M<sub>n</sub> there is a prespecified parameter of interest, θ<sub>M,n</sub>(ℙ<sub>n</sub>) ≡ θ<sub>M,n</sub>, of dimension m(M), and a corresponding estimator θ̂<sub>M,n</sub>. Typically θ<sub>M,n</sub> is a projection of P<sub>n</sub> onto P<sub>n</sub>.

**Note**: We can phrase the original PoSI problem as a special case of this framework with  $\mathbb{P}_n = N(\mu_n, \sigma^2 I_n)$ ,  $M = \{N(X_M \beta^M, \sigma^2 I_n): \beta^M, \sigma^2\}$ , and  $\theta_{M,n} = X_M^{\dagger} \mu_n$ .

# Generalised PoSI: objective

For a fixed  $\alpha \in (0, 1)$ , define a family of intervals for  $\theta_{M,n}^{(j)}$ ,

$$\{Cl_{1-\alpha,M}^{(j)}: M \in \mathcal{M}_n, 1 \le j \le m(M)\},\tag{30}$$

satisfying

$$\liminf_{n \to \infty} \mathbb{P}_n \left( \theta_{M,n}^{(j)} \in CI_{1-\alpha,M}^{(j)} \text{ for all } 1 \le j \le m(M), M \in \mathcal{M}_n \right) \ge 1 - \alpha.$$
(31)

It then follows that

$$\liminf_{n \to \infty} \mathbb{P}_n \left( \theta_{\hat{M}_n, n}^{(j)} \in Cl_{1-\alpha, \hat{M}_n}^{(j)} \text{ for all } 1 \le j \le m(\hat{M}_n) \right) \ge 1 - \alpha$$
(32)

for any model-selection procedure  $\hat{M}_n \colon \mathbb{R}^n \to \mathcal{M}_n$ .

## Generalised PoSI: notation

Let 
$$\theta_n = (\theta_{M_1,n}^T, \dots, \theta_{M_d,n}^T)^T$$
 and  $\hat{\theta}_n = (\hat{\theta}_{M_1,n}^T, \dots, \hat{\theta}_{M_d,n}^T)^T$ .

Assume regularity conditions such that

$$d\left\{\operatorname{diag}(V_n)^{\dagger/2}(\hat{\theta}_n - \theta_n), N(0, \operatorname{corr}(V_n))\right\} \to 0 \quad \text{as } n \to \infty.$$
(33)

for a sequence of covariances  $V_n$ , where  $d\{\cdot\}$  is any distance metrising convergence in distribution, and

- diag(A) is the diagonal matrix sharing the diagonal with A.
- $A^{1/2}$  is the square root of a SPD matrix A.

$$-A^{\dagger/2} = (A^{\dagger})^{1/2}$$

$$-\operatorname{corr}(A) = \operatorname{diag}(A)^{\dagger/2}A\operatorname{diag}(A)^{\dagger/2}$$

Define  $\mathcal{K}_{1-\alpha}(\Sigma)$  as the  $1-\alpha$  quantile of  $||Z||_{\infty}$ , where  $Z \sim \mathcal{N}(0, \Sigma)$ .

This new "PoSI constant" is based on a Gaussian distribution because the guarantees of this method are asymptotic for fixed p.

The original PoSI constant in the known- $\sigma^2$  case  $(r = \infty)$  can be written as  $K_{1-\alpha}(\operatorname{corr}(\Gamma_X))$ , where the  $|M_i| \times |M_j|$  block of  $\Gamma_X$  is given by

$$X_{M_i}^{\dagger}(X_{M_j}^{\dagger})^T, \qquad (34)$$

for  $M_i, M_j \in \mathcal{M}$ .

# Generalised PoSI: consistent variance estimation

#### Theorem

(**Bachoc et al., Theorem 2.3**) Let  $\hat{V}_n$  be a consistent estimator of  $V_n$ . Under certain asymptotic conditions on  $\hat{\theta}_n$  and  $\hat{V}_n$ , the intervals

$$CI_{1-\alpha,M}^{(j)} = \hat{\theta}_{M,n}^{(j)} \pm \sqrt{[\hat{V}_n]_{\rho(M)+j}} \mathcal{K}_{1-\alpha}(\operatorname{corr}(\hat{V}_n))$$
(35)

are asymptotically valid post-selection  $1 - \alpha$  confidence intervals for  $\theta_{jM}$ , where for  $M = M_{j,n}$ ,  $\rho(M) = \sum_{l=1}^{j-1} m(M_{l,n})$ .

 $\rightarrow$  Since guarantees are only aymptotic, the PoSI constant is computed from a multivariate Gaussian instead of a multivariate *t* distribution.

 $\rightarrow$  In a fully non-parametric setting consistent estimation of the variance is rarely possible, so this construction is still of limited use.

# Generalised PoSI: variance overestimation

#### Theorem

(Bachoc et al., Theorem 2.5) Suppose there exists estimators  $\hat{v}_{j,n}^2$  of  $[V_n]_j$ , and an estimator  $\hat{K}_n$  of  $K_{1-\alpha}(corr(V_n))$  such that

$$\mathbb{P}\left(\frac{K_{1-\alpha}(\operatorname{corr}(V_n))}{\hat{K}_n}\max_j \sqrt{\frac{[V_n]_j}{\hat{v}_{j,n}^2}} > 1+\varepsilon\right) \to 0 \text{ for all } \varepsilon > 0.$$
(36)

Then, under the same conditions as before, the intervals

$$CI_{1-\alpha,M}^{(j)} = \hat{\theta}_{M,n}^{(j)} \pm \sqrt{\hat{v}_{\rho(M)+j,n}^2} \hat{K}_n$$
(37)

are asymptotically valid post-selection  $1 - \alpha$  confidence intervals for  $\theta_{jM}$ .

- $\rightarrow$  Estimators  $\hat{v}_{i,n}^2$  are possible to construct in a variety of settings.
- $\rightarrow$  Widely applicable upper bounds for  $K_{1-\alpha}(\operatorname{corr}(V_n))$  are available.

#### Generalised PoSI: homoskedastic quantitative data

Consider a misspecified version of original PoSI, where

– The true distribution of Y is such that the entries are independent, have identical variance  $\sigma_n^2$ , and

$$\max_{i=1,\dots,n} \left[ \mathbb{E} \left( |Y_i - \mathbb{E}(Y_i)|^{2+\delta} \right) \right]^{\frac{2}{2+\delta}} \le \tau \sigma_n^2$$
(38)

for some  $\delta >$  0,  $\tau \geq 1.$ 

- The set of working models  $\mathcal{M}_n$  for Y contains homoskedastic linear models  $\mathbb{E}(Y) = X_M \beta_M$ ,  $M \subseteq \{1, \ldots, p\}$ , with p fixed.

Asymptotically valid selective CIs for projection parameters are given by

$$CI_{1-\alpha,M}^{(j)} = \hat{\beta}_{M,n}^{(j)} \pm \sqrt{\hat{\sigma}_{M,n}^{2} [(X_{M}^{T} X_{M})^{-1}]_{jj}} K_{1-\alpha}(\operatorname{corr}(\Gamma_{X})); \quad (39)$$
$$\hat{\sigma}_{M,n}^{2} = \frac{\|(I_{n} - P_{M})Y\|^{2}}{n - |M|}. \quad (40)$$

# Generalised PoSI: homoskedastic quantitative data

The resulting intervals are very similar to original PoSI intervals, but there are two key differences:

- The variance is estimated using the residual sum of squares from the fit of the selected model. This will in general overestimate the true variance, but adapts to misspecification.
- Since validity is guaranteed only asymptotically, the PoSI constant is computed from a multivariate Gaussian (rather than *t*) distribution.

This framework can be applied to heteroskedastic and binary data.

Diabetes dataset of Hastie and Efron (2012).

442 patients, 10 covariates.

Response: quantitative measure of disease progression.

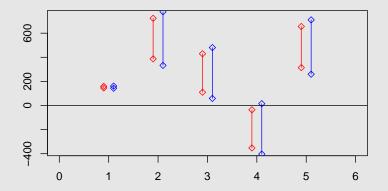
<u>Covariates</u>: age, sex, BMI, blood pressure, and 6 blood serum measurements.

We run the LASSO with penalty selected by cross-validation to identify the most significant predictors, obtaining:

BMI MAP HDL LTG

#### Data example

Comparison of unadjusted intervals with PoSI intervals at 95% level.



HDL is deemed significant (within the selected model) if the selection step is ignored, but when the appropriate adjustment is made there is no ground for rejection.

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