Handling factors in variable selection problems arxiv.org/abs/1709.07238 Gonzalo Garcia-Donato¹ and Rui Paulo²

¹ Universidad de Castilla-La Mancha (Spain), ² Universidad de Lisboa (Portugal)

Workshop Métodos Bayesianos'17. 8/11/17

Workshop Métodos Bayesianos'17. 8/11/17

- 1 Basics of variable selection
- 2 Considering factors
- 3 The big problem

1 Basics of variable selection

2 Considering factors

3 The big problem

Competing models

• Main uncertainty concerns which (numerical) variables of a given set

 $\{x_1, x_2, \ldots, x_k\}$

explain a response variable y. Other variables are known to explain y (eg. the constant). Focus here is on linear models and the response y is Gaussian.

Competing models

• Main uncertainty concerns which (numerical) variables of a given set

```
\{x_1, x_2, \ldots, x_k\}
```

explain a response variable y. Other variables are known to explain y (eg. the constant). Focus here is on linear models and the response y is Gaussian.

• The formal Bayesian answer considers all possible models that arise when different combination of the potential variables are chosen.

• There are a total of 2^k models, that normally are notated through the use of a binary vector γ .

$$M_{\gamma}: y_i = lpha + eta_1 x_{i1} + eta_7 x_{i7} + \epsilon_i, \ \epsilon_i \sim N(0, \sigma^2), \ i = 1, \dots, n,$$

or

$$M_{\gamma^{\star}}: y_i = \alpha + \beta_1 x_{i1} + \beta_4 x_{i4} + \epsilon_i, \ \epsilon_i \sim N(0, \sigma^2), \ i = 1, \ldots, n.$$

Competing models (cont')

• The simplest possible model (null model) is

$$M_{(0,\ldots,0)}: y_i = \alpha + \epsilon_i, \ \epsilon_i \sim N(0,\sigma^2), \ i = 1,\ldots,n.$$

and the most complex model (full model) is

$$M_{(1,\ldots,1)}: y_i = \alpha + \sum_{j=1}^k \beta_j x_{ij} + \epsilon_i, \ \epsilon_i \sim N(0,\sigma^2), \ i = 1,\ldots,n.$$

Competing models (cont')

• The simplest possible model (null model) is

$$M_{(0,\ldots,0)}: y_i = \alpha + \epsilon_i, \ \epsilon_i \sim N(0,\sigma^2), \ i = 1,\ldots,n.$$

and the most complex model (full model) is

$$M_{(1,\ldots,1)}: y_i = \alpha + \sum_{j=1}^k \beta_j x_{ij} + \epsilon_i, \ \epsilon_i \sim N(0,\sigma^2), \ i = 1,\ldots,n.$$

ullet In general, model M_γ can be compactly expressed as

$$M_{\gamma}: \boldsymbol{y} = \boldsymbol{1}\alpha + \boldsymbol{X}_{\gamma}\boldsymbol{\beta}_{\gamma} + \boldsymbol{\epsilon},$$

where X_{γ} is the design matrix (assume columns centered) that has k_{γ} columns.

Competing models (cont')

• The simplest possible model (null model) is

$$M_{(0,\ldots,0)}$$
: $y_i = \alpha + \epsilon_i, \ \epsilon_i \sim N(0,\sigma^2), \ i = 1,\ldots,n.$

and the most complex model (full model) is

$$M_{(1,\ldots,1)}: y_i = \alpha + \sum_{j=1}^k \beta_j x_{ij} + \epsilon_i, \ \epsilon_i \sim N(0,\sigma^2), \ i = 1,\ldots,n.$$

ullet In general, model M_γ can be compactly expressed as

$$M_{\gamma}: \boldsymbol{y} = \boldsymbol{1}\alpha + \boldsymbol{X}_{\gamma}\boldsymbol{\beta}_{\gamma} + \boldsymbol{\epsilon},$$

where X_{γ} is the design matrix (assume columns centered) that has k_{γ} columns.

$$Pr(M_{\gamma} \mid \boldsymbol{y}) \propto m_{\gamma}(\boldsymbol{y}) Pr(M_{\gamma}), \ m_{\gamma}(\boldsymbol{y}) = \int M_{\gamma}(\boldsymbol{y} \mid \boldsymbol{\beta}_{\gamma}, \sigma, \alpha) \pi_{\gamma}(\boldsymbol{\beta}_{\gamma}, \sigma, \alpha) d\boldsymbol{\beta}_{\gamma} d\sigma d\alpha.$$

The Bayesian method then proceeds computing posterior probabilities of all 2^k the models:

$$Pr(M_{\gamma} \mid \boldsymbol{y}) \propto m_{\gamma}(\boldsymbol{y}) Pr(M_{\gamma}), \ m_{\gamma}(\boldsymbol{y}) = \int M_{\gamma}(\boldsymbol{y} \mid \boldsymbol{\beta}_{\gamma}, \sigma, \alpha) \pi_{\gamma}(\boldsymbol{\beta}_{\gamma}, \sigma, \alpha) d\boldsymbol{\beta}_{\gamma} d\sigma d\alpha.$$

• The ratio $\frac{m_{\gamma}(\mathbf{y})}{m_0(\mathbf{y})} \equiv B_{\gamma}$ is called the Bayes factor of M_{γ} to the null model.

$$Pr(M_{\gamma} \mid \boldsymbol{y}) \propto m_{\gamma}(\boldsymbol{y}) Pr(M_{\gamma}), \ m_{\gamma}(\boldsymbol{y}) = \int M_{\gamma}(\boldsymbol{y} \mid \boldsymbol{\beta}_{\gamma}, \sigma, \alpha) \pi_{\gamma}(\boldsymbol{\beta}_{\gamma}, \sigma, \alpha) d\boldsymbol{\beta}_{\gamma} d\sigma d\alpha.$$

- The ratio $\frac{m_{\gamma}(\mathbf{y})}{m_0(\mathbf{y})} \equiv B_{\gamma}$ is called the Bayes factor of M_{γ} to the null model.
- The method is parsimonious since the Bayes factor automatically penalizes complexity.

$$Pr(M_{\gamma} \mid \boldsymbol{y}) \propto m_{\gamma}(\boldsymbol{y}) Pr(M_{\gamma}), \ m_{\gamma}(\boldsymbol{y}) = \int M_{\gamma}(\boldsymbol{y} \mid \boldsymbol{\beta}_{\gamma}, \sigma, \alpha) \pi_{\gamma}(\boldsymbol{\beta}_{\gamma}, \sigma, \alpha) d\boldsymbol{\beta}_{\gamma} d\sigma d\alpha.$$

- The ratio $\frac{m_{\gamma}(\mathbf{y})}{m_0(\mathbf{y})} \equiv B_{\gamma}$ is called the Bayes factor of M_{γ} to the null model.
- The method is parsimonious since the Bayes factor automatically penalizes complexity. Of great importance is the specification of
 - Prior for parameters under each model: $\pi_\gamma(m{eta}_\gamma,lpha,\sigma)$, and

$$Pr(M_{\gamma} \mid \boldsymbol{y}) \propto m_{\gamma}(\boldsymbol{y}) Pr(M_{\gamma}), \ m_{\gamma}(\boldsymbol{y}) = \int M_{\gamma}(\boldsymbol{y} \mid \boldsymbol{\beta}_{\gamma}, \sigma, \alpha) \pi_{\gamma}(\boldsymbol{\beta}_{\gamma}, \sigma, \alpha) d\boldsymbol{\beta}_{\gamma} d\sigma d\alpha.$$

- The ratio $\frac{m_{\gamma}(\mathbf{y})}{m_0(\mathbf{y})} \equiv B_{\gamma}$ is called the Bayes factor of M_{γ} to the null model.
- The method is parsimonious since the Bayes factor automatically penalizes complexity. Of great importance is the specification of
 - Prior for parameters under each model: $\pi_{\gamma}(m{eta}_{\gamma}, lpha, \sigma)$, and
 - prior over the model space $Pr(M_{\gamma})$.

About $\pi_\gamma(oldsymbol{eta}_\gamma, lpha, \sigma)$ and the conventional approach

What we call 'conventional' approach are a family of priors of the form:

$$\pi_{\gamma}(\alpha,\boldsymbol{\beta}_{\gamma},\sigma) = \sigma^{-1} \int N_{k_{\gamma}}(\boldsymbol{\beta} \mid \boldsymbol{0}, g\sigma^{2}(\boldsymbol{X}^{t}\boldsymbol{X})^{-1}) h(g) dg,$$

where h(g) is a mixing function and for the null

$$\pi_0(\alpha,\sigma)=\sigma^{-1}.$$

• Conventional priors follow the tradition of Jeffreys-Zellner-Siow (60's and 80's), followed by many others (90's and 00's) and recently formally endorsed by Bayarri et al (2012).

About $\pi_\gamma(oldsymbol{eta}_\gamma, lpha, \sigma)$ and the conventional approach

What we call 'conventional' approach are a family of priors of the form:

$$\pi_{\gamma}(\alpha,\boldsymbol{\beta}_{\gamma},\sigma)=\sigma^{-1}\int N_{k_{\gamma}}(\boldsymbol{\beta}\mid\boldsymbol{0},g\sigma^{2}(\boldsymbol{X}^{t}\boldsymbol{X})^{-1})\,\boldsymbol{h}(g)\,dg,$$

where h(g) is a mixing function and for the null

$$\pi_0(\alpha,\sigma)=\sigma^{-1}.$$

• Conventional priors follow the tradition of Jeffreys-Zellner-Siow (60's and 80's), followed by many others (90's and 00's) and recently formally endorsed by Bayarri et al (2012).

• You obtain

$$B_{\gamma} = \mathcal{B}\Big(\frac{SSE_{\gamma}}{SSE_0}, 1, k_{\gamma} + 1, n\Big),$$

where SSE_{γ} is the sum of squared errors and \mathcal{B} is a univariate integral.

Basics of variable selection

About $Pr(M_{\gamma})$ and the multiplicity issue

• The Bayes factor already penalizes complexity so this should not be done through $Pr(M_{\gamma})$.

- The Bayes factor already penalizes complexity so this should not be done through $Pr(M_{\gamma})$.
- The standard default prior over the model space is

$$Pr(M_{\gamma})=1/2^{k},$$

but this tends to favor models of dimension $\approx k/2$, particularly if k is large.

- The Bayes factor already penalizes complexity so this should not be done through $Pr(M_{\gamma})$.
- The standard default prior over the model space is

$$Pr(M_{\gamma})=1/2^{k},$$

but this tends to favor models of dimension $\approx k/2$, particularly if k is large. • Our preferred prior is

$$Pr(M_{\gamma} \mid \tau) = \tau^{k_{\gamma}} (1-\tau)^{k-k_{\gamma}}, \tau \sim U(0,1),$$

which was studied by Scott and Berger (2010), who argued adjusts for multiplicity.

- The Bayes factor already penalizes complexity so this should not be done through $Pr(M_{\gamma})$.
- The standard default prior over the model space is

$$Pr(M_{\gamma})=1/2^{k},$$

but this tends to favor models of dimension $\approx k/2$, particularly if k is large. • Our preferred prior is

$$Pr(M_{\gamma} \mid \tau) = \tau^{k_{\gamma}} (1-\tau)^{k-k_{\gamma}}, \tau \sim U(0,1),$$

which was studied by Scott and Berger (2010), who argued adjusts for multiplicity. This adjustment effect becomes clear with the alternative form:

$$Pr(M_{\gamma}) = 1/\{\# \text{ of models of dimension } k_{\gamma}\}$$

which has also the form

1 Basics of variable selection

2 Considering factors

3 The big problem

Factors

A factor, Λ , is a categorical variable (eg. nationality, sex, etc) and for each sample unit takes only one of several, ℓ , categories or levels (eg. "Español/a", "Francés/a", "Argentino/a").

Factors

A factor, Λ , is a categorical variable (eg. nationality, sex, etc) and for each sample unit takes only one of several, ℓ , categories or levels (eg. "Español/a", "Francés/a", "Argentino/a").

• In many applied problems, factors are considered as possible explanatory variables jointly with perhaps numerical variables.

Factors

```
A factor, \Lambda, is a categorical variable (eg. nationality, sex, etc) and for each sample unit takes only one of several, \ell, categories or levels (eg. "Español/a", "Francés/a", "Argentino/a" ).
```

• In many applied problems, factors are considered as possible explanatory variables jointly with perhaps numerical variables.

Main goal

"Repeat" the variable selection exercise but now selecting among certain set of potential covariates and/or factors

$$\{x_1,\ldots,x_k,\Lambda_1,\ldots,\Lambda_p\}$$

Factors

```
A factor, \Lambda, is a categorical variable (eg. nationality, sex, etc) and for each sample unit takes only one of several, \ell, categories or levels (eg. "Español/a", "Francés/a", "Argentino/a" ).
```

• In many applied problems, factors are considered as possible explanatory variables jointly with perhaps numerical variables.

Main goal

"Repeat" the variable selection exercise but now selecting among certain set of potential covariates and/or factors

$$\{x_1,\ldots,x_k,\Lambda_1,\ldots,\Lambda_p\}$$

In principle the problem is solved using dummies, but we will see that certain aspects are not well understood and may lead to unexpected results and accompanying challenges.

Factors

```
A factor, \Lambda, is a categorical variable (eg. nationality, sex, etc) and for each sample unit takes only one of several, \ell, categories or levels (eg. "Español/a", "Francés/a", "Argentino/a" ).
```

• In many applied problems, factors are considered as possible explanatory variables jointly with perhaps numerical variables.

Main goal

"Repeat" the variable selection exercise but now selecting among certain set of potential covariates and/or factors

$$\{x_1,\ldots,x_k,\Lambda_1,\ldots,\Lambda_p\}$$

In principle the problem is solved using dummies, but we will see that certain aspects are not well understood and may lead to unexpected results and accompanying challenges. These can be better understood in the simplest scenario with only one factor (ℓ levels) and no numerical covariates:

Workshop Métodos Bayesianos'17. 8/11/17

The null model M_0 only contains the intercept, but

Question

What does it mean that the factor Λ is a relevant predictor?

The null model M_0 only contains the intercept, but

Question

What does it mean that the factor Λ is a relevant predictor?

• Answer 1. All levels of the factor are important, or

The null model M_0 only contains the intercept, but

Question

What does it mean that the factor Λ is a relevant predictor?

- Answer 1. All levels of the factor are important, or
- Answer 2. any level of the factor is important.

The null model M_0 only contains the intercept, but

Question

What does it mean that the factor Λ is a relevant predictor?

- Answer 1. All levels of the factor are important, or
- Answer 2. any level of the factor is important.

Answer 1 implies comparing only two models:

$$M_0, M_1: y_{ij} = \alpha + a_j + \epsilon_{ij}, j = 1, \ldots, \ell,$$

but has two severe drawbacks:

• If M_1 is accepted, we do not know which levels are relevant

The null model M_0 only contains the intercept, but

Question

What does it mean that the factor Λ is a relevant predictor?

- Answer 1. All levels of the factor are important, or
- Answer 2. any level of the factor is important.

Answer 1 implies comparing only two models:

$$M_0$$
, $M_1: y_{ij} = \alpha + a_j + \epsilon_{ij}$, $j = 1, \ldots, \ell$,

but has two severe drawbacks:

- If M_1 is accepted, we do not know which levels are relevant
- M_1 is highly penalized due to its complexity (particularly if $\ell >>$).

The null model M_0 only contains the intercept, but

Question

What does it mean that the factor Λ is a relevant predictor?

- Answer 1. All levels of the factor are important, or
- Answer 2. any level of the factor is important.

Answer 1 implies comparing only two models:

$$M_0$$
, $M_1: y_{ij} = \alpha + a_j + \epsilon_{ij}$, $j = 1, \ldots, \ell$,

but has two severe drawbacks:

- If M_1 is accepted, we do not know which levels are relevant
- M_1 is highly penalized due to its complexity (particularly if $\ell >>$).

We prefer (and use in what follows) Answer 2, implying that there are 2^{ℓ} competing models:

$$M_0, M_{\gamma}: y_{ij} = \alpha + a_j \gamma_j + \epsilon_{ij}, \gamma \in \{0,1\}^{\ell},$$

we will see other advantages of this approach later.

Question

How to specify $Pr(M_{\gamma})$?

Question

How to specify $Pr(M_{\gamma})$?

The standard approaches imply that prior probability of M_0 is largely affected by ℓ . This effect is very severe for constant prior:

$Pr(H_0)$				
	$\ell = 3$	$\ell = 7$		
Constant	1/8	1/128		
Scott-Berger	1/4	1/8		

Question

How to specify $Pr(M_{\gamma})$?

The standard approaches imply that prior probability of M_0 is largely affected by ℓ . This effect is very severe for constant prior:

$Pr(H_0)$				
	$\ell = 3$	$\ell = 7$		
Constant	1/8	1/128		
Scott-Berger	1/4	1/8		

Our proposal is a two-stage (hierarchical) specification: $Pr(H_0) = Pr(\Lambda) = 1/2$ and then

 $Pr(M_{\gamma} \mid \Lambda) = Constant,$

Question

How to specify $Pr(M_{\gamma})$?

The standard approaches imply that prior probability of M_0 is largely affected by ℓ . This effect is very severe for constant prior:

$Pr(H_0)$				
	$\ell = 3$	$\ell = 7$		
Constant	1/8	1/128		
Scott-Berger	1/4	1/8		

Our proposal is a two-stage (hierarchical) specification: $Pr(H_0) = Pr(\Lambda) = 1/2$ and then

 $Pr(M_{\gamma} \mid \Lambda) = \text{Constant},$

or (better) the Scott-Berger in this second stage:

$${\it Pr}(M_\gamma \mid \Lambda) = rac{1}{\ell {\ell \choose k_\gamma}} \; .$$

Which automatically controls for the multiplicity issue that arises due to the ℓ dummy variables used, a potential pitfall already observed by Chipman (1996).

Perhaps someone has realized that the full model is rank deficient (many more models with more than one factor).

Perhaps someone has realized that the full model is rank deficient (many more models with more than one factor). This is quite uncomfortable but also the conventional priors cannot be used.

Idea!

Perhaps someone has realized that the full model is rank deficient (many more models with more than one factor). This is quite uncomfortable but also the conventional priors cannot be used.

Idea!

Reparametrize the problem from a full rank (eg. choosing one level as the baseline) expression of the full model.

We could have the illusory perception that parameterizations do not have either any impact in testing composed hypotheses. But this turned out to be quite wrong:

Perhaps someone has realized that the full model is rank deficient (many more models with more than one factor). This is quite uncomfortable but also the conventional priors cannot be used.

Idea!

Reparametrize the problem from a full rank (eg. choosing one level as the baseline) expression of the full model.

We could have the illusory perception that parameterizations do not have either any impact in testing composed hypotheses. But this turned out to be quite wrong:

Real example 1

y is body mass index of n = 1002 obese children aged 3-11 (Zurriaga et al, 2011).

• Potential factor: Sports (coded 0 to 5).

Perhaps someone has realized that the full model is rank deficient (many more models with more than one factor). This is quite uncomfortable but also the conventional priors cannot be used.

Idea!

Reparametrize the problem from a full rank (eg. choosing one level as the baseline) expression of the full model.

We could have the illusory perception that parameterizations do not have either any impact in testing composed hypotheses. But this turned out to be quite wrong:

Real example 1

y is body mass index of n = 1002 obese children aged 3-11 (Zurriaga et al, 2011).

• Potential factor: Sports (coded 0 to 5).

 $\begin{array}{c} Pr(H_0 \mid \mathbf{y}) \\ base = 0 \quad base = 1 \end{array}$

Perhaps someone has realized that the full model is rank deficient (many more models with more than one factor). This is quite uncomfortable but also the conventional priors cannot be used.

Idea!

Reparametrize the problem from a full rank (eg. choosing one level as the baseline) expression of the full model.

We could have the illusory perception that parameterizations do not have either any impact in testing composed hypotheses. But this turned out to be quite wrong:

Real example 1

y is body mass index of n = 1002 obese children aged 3-11 (Zurriaga et al, 2011).

• Potential factor: Sports (coded 0 to 5).

 $\begin{array}{c} Pr(H_0 \mid \mathbf{y})\\ base = 0 \quad base = 1\\ \hline 0.440 \quad 0.002 \end{array}$

Issue 3: Reparameterizations? (cont')

• Since parameterizations are so influential, the safest alternative is not doing any!

Issue 3: Reparameterizations? (cont')

• Since parameterizations are so influential, the safest alternative is not doing any!

How to use the conventional priors?

For rank-deficient models M_{γ} use a particular family of $(\mathbf{X}_{\gamma}^{t}\mathbf{X}_{\gamma})^{-}$ which is regular.

Issue 3: Reparameterizations? (cont')

• Since parameterizations are so influential, the safest alternative is not doing any!

How to use the conventional priors?

For rank-deficient models M_{γ} use a particular family of $(X_{\gamma}^{t}X_{\gamma})^{-}$ which is regular. Priors are not unique, but the Bayes factor is:

$$B_{\gamma} = \mathcal{B}\Big(\frac{SSE_{\gamma}}{SSE_0}, 1, r_{\gamma} + 1, n\Big),$$

where r_{γ} is the rank of X_{γ} ($r_{\gamma} < k_{\gamma}$).

Basics of variable selection

2 Considering factors





full problem

Recall:

 $\{x_1,\ldots,x_k,\Lambda_1,\ldots,\Lambda_p\}.$

full problem

Recall:

$$\{x_1,\ldots,x_k,\Lambda_1,\ldots,\Lambda_p\}.$$

Our proposal can be summarized as:

• Do not reparameterize,

full problem

Recall:

$$\{x_1,\ldots,x_k,\Lambda_1,\ldots,\Lambda_p\}.$$

Our proposal can be summarized as:

- Do not reparameterize,
- use hierarchical-SB prior:

$$P(\{x_{i_1}, \dots, x_{i_{m_1}}, \Lambda_{j_1}, \dots, \Lambda_{j_{m_2}}\}) = \left[(k+p+1) \binom{k+p}{m_1+m_2} \right]^{-1}$$
(1)
$$P(M_{\gamma} \mid \{x_{i_1}, \dots, x_{i_{m_1}}, \Lambda_{j_1}, \dots, \Lambda_{j_{m_2}}\}) = \left[\prod_{h=1}^{m_2} \ell_h \binom{\ell_h}{k_{\gamma}^h}\right]^{-1} ,$$
(2)

where, in (2), $m_2 \ge 1$ (otherwise, it is equal to one), and $1 \le k_{\gamma}^h \le \ell_h$ is the number of levels of factor Λ_h active in M_{γ} .

Application: childhood Obesity

Real example

y is body mass index of n = 1002 obese children aged 3-11 (Zurriaga et al, 2011).

- 4 Fixed covariates: Intercept, WeightBorn, HeightBorn and Age;
- 2 Potential covariates: HrsScrDay and HrsSleep;
- 2 Potential factors: Sports (coded 0 to 5) and HealthyFood (0-2). In both cases smaller codes correspond to negative habits.

Application: childhood Obesity

Real example

y is body mass index of n = 1002 obese children aged 3-11 (Zurriaga et al, 2011).

- 4 Fixed covariates: Intercept, WeightBorn, HeightBorn and Age;
- 2 Potential covariates: HrsScrDay and HrsSleep;
- 2 Potential factors: Sports (coded 0 to 5) and HealthyFood (0-2). In both cases smaller codes correspond to negative habits.

$Sports(\ell = 6)$	$HealthyFood(\ell=3)$	HrsScrDay	HrsSleep
0.995	0.998	0.999	0.622

Table: Inclusion probabilities of factors and covariates.

Application: childhood Obesity

Real example

y is body mass index of n = 1002 obese children aged 3-11 (Zurriaga et al, 2011).

- 4 Fixed covariates: Intercept, WeightBorn, HeightBorn and Age;
- 2 Potential covariates: HrsScrDay and HrsSleep;
- 2 Potential factors: Sports (coded 0 to 5) and HealthyFood (0-2). In both cases smaller codes correspond to negative habits.

$Sports(\ell = 6)$	$HealthyFood(\ell=3)$	HrsScrDay	HrsSleep
0.995	0.998	0.999	0.622

Table: Inclusion probabilities of factors and covariates.

Sports				He	althyFo	od		
0	1	2	3	4	5	0	1	2
0.99	0.08	0.25	0.09	0.14	0.09	0.82	0.76	0.78

Table: Inclusion probabilities of levels of factors.

The big problem

Thanks!