ESC Final 22-Fall
Drug Consumption

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from BIC to Bayes Factor

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1. Model Selection

1. AIC (Akaike Information Criterion)
2. BIC (Bayesian Information Criterion)

$$AIC_M = -2log\,L_M + 2p_M$$
$$BIC_M = -2log\,L_M + (log\,n) * p_M$$

- log L_M: model M의 log-likelihood
- p_M: Penalty Term. model M의 parameter 개수

$$AIC_M = -2log\,L_M + 2p_M$$
$$BIC_M = -2log\,L_M + (log\,n) * p_M$$

1. AIC 혹은 BIC의 값이 낮을수록 "상대적으로 좋은" 모델이다.

2. model M이 복잡해질수록(= parameter의 개수 증가) AIC 혹은 BIC의 값이 높아져 모델이 "좋지 않게" 된다. [Law of Parsimony]

3. log n ≥ 2 일 때, AIC에 비해 BIC의 penalty term 효과가 커진다.

2. Why Bayesian?

"n이 충분히 클 때" 두 모델 M1과 M2의 BIC를 비교하면,
두 모델 사이의 "Bayes Factor"인 bayesian model selection 기준을 approximate할 수 있다.

approximation 공식

$$BF_{12} \approx exp(\frac{BIC_1}{-2} - \frac{BIC_2}{-2})$$

3. Bayesian Factor

BF_{12} 공식

$$\frac{P(M_1|\mathbf{Y})}{P(M_2|\mathbf{Y})} = \frac{P(\mathbf{Y}|M_1)}{P(\mathbf{Y}|M_2)} * \frac{P(M_1)}{P(M_2)}$$

$P(M_1)$과 $P(M_2)$는 model 자체에 대한 prior로, parameter에 prior와 혼동해서는 안 된다. 예를 들어, 우리의 사전 지식에 따라 두 모델이 비슷하게 보인다면 P(M1) = P(M2) = 0.5과 같이 assign할 수 있다.

3. Bayesian Factor

$$\frac{P(M_1|\mathbf{Y})}{P(M_2|\mathbf{Y})} = \frac{P(\mathbf{Y}|M_1)}{P(\mathbf{Y}|M_2)} * \frac{P(M_1)}{P(M_2)}$$

1. Bayesian Factor: M_1과 M_2의 Posterior Model Probabillity인 $P(M_1|Y)$과 $P(M_2|Y)$ 사이의 비율. 이 비율 값이 클수록 M_1에게 유리하게 작용한다.

2. Rules of Thumb: 비율 값이 100이상이면 M_2 대신 M_1을 선택해야 한다는 강력한 증거.

3. Bayesian Factor

Typically, we will deal with parametric models M_k, which are described through model parameters, such as $\boldsymbol{\theta}_k$. So the marginal likelihoods $P(\boldsymbol{Y}|M_k)$ are evaluated using

$$P(\boldsymbol{Y}|M_k) = \int P(\boldsymbol{Y}|\boldsymbol{\theta}_k, M_k)P(\theta_k|\, M_k)d\theta_k, \tag{2}$$

where $P(\boldsymbol{Y}|\theta_k, M_k)$ is the likelihood under M_k, and $P(\theta_k|M_k)$ is the prior distribution of θ_k. A closed form analytical expression of the marginal likelihoods is difficult to obtain, even with completely specified priors (unless they are conjugate priors). Moreover, in most cases $\boldsymbol{\theta}_k$ will be high-dimensional and a direct numerical integration will be computationally intensive, if not impossible. For this reason we turn to a way to approximate this integral given in (2).

실제 상황에서 conjugacy 등이 성립하지 않는 이상 위 적분을 analytical하게 구할 수 있는 경우가 많지 않아서, Bayes Factor의 정확한 값을 구하기 어렵다.

4. Why Utilize BF?

Bayesian Model Averaging

여러 candidate model이 있을 때, 그 중 하나만을 선택하는 것이 아니라 각 모델에게 가중치를 부여해 모든 모델을 종합적으로 고려하는 "averaging". 일종의 Bayesian ensemble을 가능하게 한다

각 모델에게 부여되는 weight는 BF의 분자와 분모를 이뤘던 Posterior Model Probability (PMP) 이다.

K개의 후보 모델이 있을 때 k^{th} 모델의 PMP

$$p(M_k|\boldsymbol{Y}) = \frac{p(\boldsymbol{Y}|M_k)p(M_k)}{\sum_{k=1}^{K} p(\boldsymbol{Y}|M_k)p(M_k)}$$

$$p(\boldsymbol{Y}|M_k) = \int p(\boldsymbol{Y}|\theta_k, M_k)p(\theta_k|M_k)d\theta_k$$

이며, 이때 활용가능한 approximation이

$$p(\boldsymbol{Y}|M_k) = exp(\frac{BIC_k}{-2}) \quad (\text{assuming n is "large"})$$

4. Why Utilize BF?

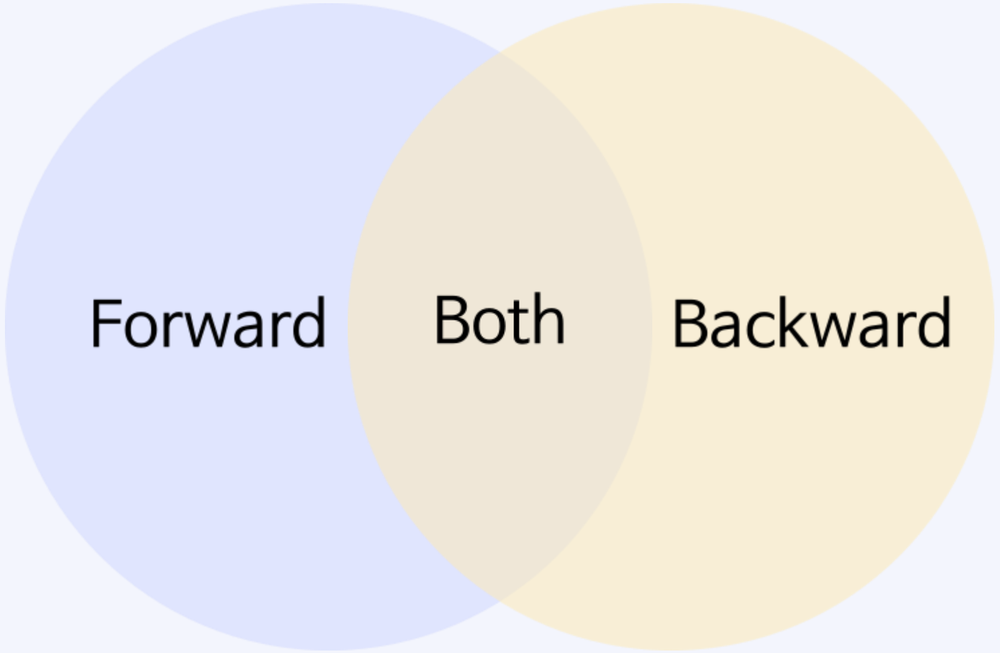
Then the BMA estimate of prediction at unobserved $\boldsymbol{Y}^*$ is

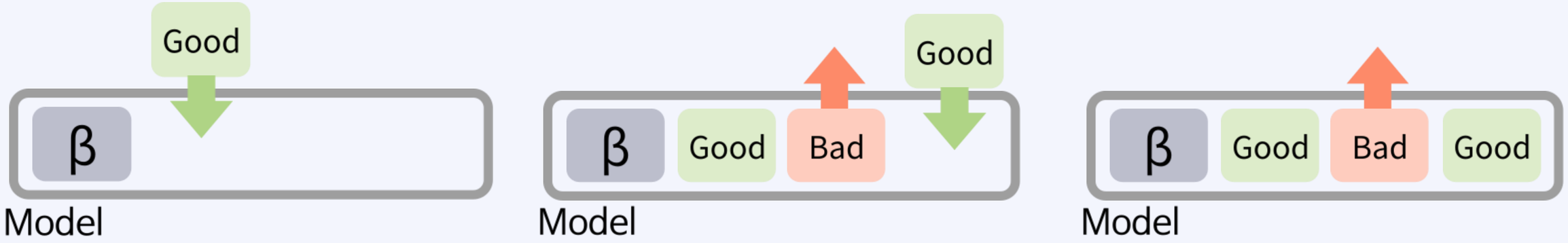
$$\boldsymbol{Y}^* = \sum_{k=1}^{K} \boldsymbol{Y}_k^* p(\mathcal{M}_k | \boldsymbol{Y})$$

where $\boldsymbol{Y}_k^*$ predicted response from $\mathcal{M}_k$

이처럼 BMA 앙상블 기법을 활용해 관측되지 않는 Y^* 값의 prediction이 가능하다

5. R 실습


Forward
Both
Backward


Good
β
Model
Good
β
Good
Bad
Model
Good
β
Good
Bad
Good
Model

step: Choose a model by AIC in a Stepwise Algorithm 함수

R Code

step(object, scope, scale = 0,

direction = c("both", "backward", "forward"),

trace = 1, keep = NULL, steps = 1000, k = 2, ...)

```
null=glm(Coke~1, data=overdose)
full=glm(Coke~., data=overdose)
step(null, scope=list(lower=null, upper=full), direction="forward", k=log(nrow(overdose)))
step(full, data=overdose, direction="backward", k=log(nrow(overdose)))
step(null, scope = list(upper=full), data=overdose, direction="both", k=log(nrow(overdose)))
```

https://www.rdocumentation.org/packages/stats/versions/3.6.2/topics/step

5. R 실습

Step1 Step2 Step3 Step4

```
Start:  AIC=2601.9
Coke ~ 1

             Df Deviance    AIC
+ Ectasy      1   261.48 1643.0
+ Amphet      1   289.82 1836.9
+ Mushrooms   1   335.98 2115.6
+ Cannabis    1   347.13 2177.1
+ Ketamine    1   348.54 2184.7
+ legath      1   350.01 2192.7
+ LSD         1   351.28 2199.5
+ Benzos      1   356.71 2228.4
+ Heroin      1   361.69 2254.6
+ Crack       1   368.17 2288.0
+ Amyl        1   373.36 2314.4
+ Nicotine    1   380.16 2348.4
+ Meth        1   382.95 2362.2
+ SS          1   388.67 2390.1
+ VSA         1   403.18 2459.2
+ Country     1   404.93 2467.4
+ Impulsive   1   408.96 2486.1
+ Age         1   413.08 2505.0
+ Oscore      1   419.80 2535.4
+ Cscore      1   419.94 2536.0
+ Ascore      1   423.64 2552.6
+ Gender      1   425.21 2559.5
+ Nscore      1   429.04 2576.4
+ Education   1   430.79 2584.1
+ Alchol      1   431.24 2586.1
+ Caff        1   432.32 2590.8
+ Ethnicity   1   433.70 2596.8
<none>           436.62 2601.9
+ Semer       1   435.30 2603.7
+ Escore      1   436.37 2608.3
+ Choc        1   436.60 2609.4
```

```
Step:  AIC=1643.01
Coke ~ Ectasy

             Df Deviance    AIC
+ Amphet      1   233.87 1440.2
+ Heroin      1   237.38 1468.3
+ Crack       1   238.81 1479.6
+ Benzos      1   243.91 1519.4
+ Meth        1   250.46 1569.4
+ Ketamine    1   252.22 1582.5
+ Amyl        1   252.42 1584.1
+ Cannabis    1   252.47 1584.5
+ Nicotine    1   253.53 1592.4
+ Mushrooms   1   254.56 1600.0
+ VSA         1   257.31 1620.2
+ Impulsive   1   257.50 1621.6
+ Ascore      1   257.50 1621.6
+ legath      1   257.82 1624.0
+ SS          1   258.28 1627.3
+ LSD         1   258.79 1631.0
+ Nscore      1   259.34 1635.0
+ Country     1   259.90 1639.1
+ Cscore      1   260.13 1640.8
<none>           261.48 1643.0
+ Alchol      1   260.61 1644.2
+ Ethnicity   1   260.78 1645.5
+ Semer       1   260.93 1646.6
+ Caff        1   261.05 1647.4
+ Choc        1   261.32 1649.4
+ Gender      1   261.39 1649.9
+ Age         1   261.43 1650.1
+ Oscore      1   261.43 1650.2
+ Escore      1   261.47 1650.5
+ Education   1   261.48 1650.5
```

5. R 실습

Step1 Step2 Step3 Step4

```
Step:  AIC=1440.17
Coke ~ Ectasy + Amphet

             Df Deviance    AIC
+ Heroin      1   219.57 1328.8
+ Crack       1   219.62 1329.2
+ Benzos      1   226.76 1389.6
+ Ketamine    1   228.76 1406.1
+ Amyl        1   229.62 1413.1
+ Nicotine    1   229.92 1415.6
+ Cannabis    1   230.48 1420.2
+ Meth        1   230.48 1420.2
+ Ascore      1   230.99 1424.3
+ Mushrooms   1   231.14 1425.6
+ Impulsive   1   232.35 1435.4
+ VSA         1   232.53 1436.9
+ Nscore      1   232.74 1438.6
+ SS          1   232.90 1439.9
<none>           233.87 1440.2
+ legath      1   233.11 1441.6
+ Alchol      1   233.13 1441.8
+ Age         1   233.19 1442.2
+ Semer       1   233.30 1443.1
+ Ethnicity   1   233.49 1444.7
+ LSD         1   233.54 1445.1
+ Cscore      1   233.55 1445.1
+ Education   1   233.66 1446.0
+ Caff        1   233.72 1446.5
+ Choc        1   233.76 1446.8
+ Gender      1   233.76 1446.8
+ Escore      1   233.82 1447.3
+ Oscore      1   233.85 1447.5
+ Country     1   233.85 1447.5
```

```
Step:  AIC=1255.54
Coke ~ Ectasy + Amphet + Heroin + Crack + Amyl

             Df Deviance    AIC
+ Nicotine    1   206.87 1239.1
+ Cannabis    1   207.18 1242.0
+ Benzos      1   207.46 1244.5
+ Ketamine    1   207.67 1246.4
+ Ascore      1   207.98 1249.2
+ Mushrooms   1   208.48 1253.8
<none>           209.52 1255.5
+ Alchol      1   208.87 1257.2
+ Impulsive   1   208.98 1258.2
+ legath      1   208.99 1258.3
+ Education   1   209.03 1258.7
+ Age         1   209.08 1259.2
+ Gender      1   209.10 1259.3
+ Nscore      1   209.12 1259.5
+ SS          1   209.12 1259.5
+ Semer       1   209.22 1260.4
+ Ethnicity   1   209.24 1260.5
+ Caff        1   209.34 1261.5
+ Escore      1   209.35 1261.5
+ Meth        1   209.40 1262.0
+ Cscore      1   209.43 1262.3
+ VSA         1   209.48 1262.8
+ Oscore      1   209.50 1262.9
+ Choc        1   209.50 1262.9
+ LSD         1   209.52 1263.1
+ Country     1   209.52 1263.1
```

5. R 실습


```
            Df Deviance    AIC
<none>           199.40 1215.0
+ Education  1   198.85 1217.3
+ Escore     1   198.86 1217.5
+ Mushrooms  1   198.96 1218.4
+ Alchol     1   199.06 1219.3
+ legath     1   199.12 1220.0
+ Semer      1   199.19 1220.6
+ Oscore     1   199.22 1220.8
+ Country    1   199.22 1220.8
+ SS         1   199.29 1221.5
+ Impulsive  1   199.30 1221.6
+ Ethnicity  1   199.31 1221.8
+ Caff       1   199.32 1221.8
+ Choc       1   199.35 1222.1
+ LSD        1   199.35 1222.1
+ Cscore     1   199.38 1222.3
+ VSA        1   199.38 1222.3
+ Nscore     1   199.40 1222.5
+ Meth       1   199.40 1222.5

Call:  glm(formula = Coke ~ Ectasy + Amphet + Heroin + Crack + Amyl +
    Nicotine + Benzos + Ketamine + Ascore + Gender + Age + Cannabis,
    data = overdose)

Coefficients:
(Intercept)       Ectasy       Amphet       Heroin        Crack         Amyl     Nicotine       Benzos     Ketamine       Ascore       Gender
   -0.02665      0.32438      0.18340      0.17659      0.18134      0.11249      0.06601      0.05523      0.09318     -0.02729      0.05605
        Age     Cannabis
    0.03529      0.07477

Degrees of Freedom: 1884 Total (i.e. Null);  1872 Residual
Null Deviance:      436.6
Residual Deviance: 199.4        AIC: 1143
```

CHAPTER 02

EDA와 데이터 전처리

STEP 01

BIC

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rstanarm

STEP 04

Result

1. Semer

Step1 Step2 Step3 Step4

In [11]:
```
a=overdose[overdose['Semer']!='CL0'].index
overdose.drop(a)
```

Out[11]:

	ID	Age	Gender	Education	Country	Ethnicity	Nscore	Escore	Oscore	Ascore	...	Ectasy	Heroin	Ketamine	legath	LSD	Meth	Mushroo
0	1	0.49788	0	-0.05921	0.96082	0.12600	0.31287	-0.57545	-0.58331	-0.91699	...	CL0	CL0	CL0	CL0	CL0	CL0	
1	2	-0.07854	1	1.98437	0.96082	-0.31685	-0.67825	1.93886	1.43533	0.76096	...	CL4	CL0	CL2	CL0	CL2	CL3	
2	3	0.49788	1	-0.05921	0.96082	-0.31685	-0.46725	0.80523	-0.84732	-1.62090	...	CL0	CL0	CL0	CL0	CL0	CL0	
3	4	-0.95197	0	1.16365	0.96082	-0.31685	-0.14882	-0.80615	-0.01928	0.59042	...	CL0	CL0	CL2	CL0	CL0	CL0	
4	5	0.49788	0	1.98437	0.96082	-0.31685	0.73545	-1.63340	-0.45174	-0.30172	...	CL1	CL0	CL0	CL1	CL0	CL0	
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	
1880	1884	-0.95197	0	-0.61113	-0.57009	-0.31685	-1.19430	1.74091	1.88511	0.76096	...	CL0	CL0	CL0	CL3	CL3	CL0	
1881	1885	-0.95197	1	-0.61113	-0.57009	-0.31685	-0.24649	1.74091	0.58331	0.76096	...	CL2	CL0	CL0	CL3	CL5	CL4	
1882	1886	-0.07854	0	0.45468	-0.57009	-0.31685	1.13281	-1.37639	-1.27553	-1.77200	...	CL4	CL0	CL2	CL0	CL2	CL0	
1883	1887	-0.95197	0	-0.61113	-0.57009	-0.31685	0.91093	-1.92173	0.29338	-1.62090	...	CL3	CL0	CL0	CL3	CL3	CL0	
1884	1888	-0.95197	1	-0.61113	0.21128	-0.31685	-0.46725	2.12700	1.65653	1.11406	...	CL3	CL0	CL0	CL3	CL3	CL0	

2. 변수 변환

(1) 약물 레벨

In [12]:
```
addict_range={'CL0':0,'CL1':0,'CL2':1,'CL3':1,'CL4':1,'CL5':1,'CL6':1}
```

In [13]:
```
for i in range(13,32):
    overdose.iloc[:,i]=overdose.iloc[:,i].apply(lambda x : addict_range[x])
```

(2) 정규화된 변수 ⇒ nominal

In [16]:
```
education_range={'Education':{-2.43591:'Left school before 16yrs',
                              -1.73790:'Left school at 16yrs',
                              -1.43719:'Left school at 17yrs',
                              -1.22751:'Left school at 18yrs',
                              -0.61113:'Some college or university, no certificate/diploma',
                              -0.05921:'Professional certificate/diploma',
                               0.45468:'University degree',
                               1.16365:'Masters degree',
                               1.98437:'Doctorate degree'}}
```

3. Categorical Coding


```
overdose <- data
overdose$Country<-as.factor(overdose$Country)
overdose$Country
overdose$Country<-relevel(overdose$Country,ref='USA')
overdose$Ethnicity<-as.factor(overdose$Ethnicity)
overdose$Ethnicity<-relevel(overdose$Ethnicity,ref='Black')
overdose$Education<-as.factor(overdose$Education)
overdose$Eduation<-relevel(overdose$Education,ref='Doctorate degree')
overdose$Age<-as.factor(overdose$Age)
overdose$Age<-relevel(overdose$Age,ref='65+')
data <-overdose
data <- subset(data, select = -Semer)
```

3. Categorical Coding

Age, Gender, Education, Country, Ethinicity
: 숫자형으로 코딩된 각 변수의 value 값을 다시 매칭해서 범주형 변수로 변환

as.factor( )
: 특정 column을 vector를 기준으로 factorizing

Country
0.96082
0.96082
0.96082
0.96082
0.96082
0.24923
-0.57009
0.96082
0.24923
0.96082
0.96082
-0.28519
0.96082

Country
UK
UK
UK
UK
UK
Canada
USA
UK
Canada
UK
UK
Other
UK

4. Logistic Regression

로지스틱 회귀에서 범주형 변수의 의미

Example

(가정) country 변수에서 USA 를 기준으로 factorize

이후 특정 마약을 종속변수로 한 logistic regression 결과, Canada 변수의 기울기가 2라면
⇒ USA 에 비해서 Canada 국적을 가진 사람이 e^2배 더 해당 마약을 사용할 가능성이 있다
⇒ 해당 사건의 odd ratio가 e^2

Reference 설정 - relevel( )

Country	USA
Ethnicity	Black
Education	Doctorate degree
Age	65+

Ordinal

CHAPTER 03

rstanarm

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Result

1. Why rstanarm?

glm function

: 일반화된 선형 모델의 최대 우도 추정 수행

rstanarm package

: stan_glm 함수를 사용해 binomial GLM
MCMC를 통한 완전한 bayesian 추정 수행

2. Distribution

prior 설정하기

R Code

```
t_prior <- student_t(df = 7, location = 0, scale = 2.5)
Caff_post <- stan_glm(formula, data = overdose,
                      family = binomial(link = "logit"),
                      prior = t_prior, prior_intercept = t_prior,
                      QR=TRUE, seed = 2001, refresh=0)
```

MCMC를 이용한 posterior distribution 도출

: posterior median estimates와 90% intervals을 구할 수 있다

CHAPTER 04

Result

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Result

1. 경향성

Age	환각버섯, 니코틴, vsa, 케타민, 코카인, 리갈하이, lsd, 엑스터시 , 암페타민, 아밀, 대마 회귀계수의 신뢰구간이 0을 포함하거나 신뢰구간의 크기가 너무 커 결론을 내리기 어려움
Gender	리갈하이, lsd, meth, 엑스터시, 암페타민, 아밀, 크랙, 대마, 환각버섯, 니코틴, 케타민, 히로인 유의미한 확률로 남자일 때 해당 마약을 할 가능성 높음
Country	뉴질랜드: 리갈하이, 대마 | 오스트레일리아: 암페타민 | 영국: 아밀 회귀계수의 신뢰구간이 0을 포함하는 경우가 다수 있어 신뢰하기 어려움
Ethnicity	환각버섯 흑인보다 백인, 백인-아시아인 혼혈이 해당 마약을 할 가능성 높음

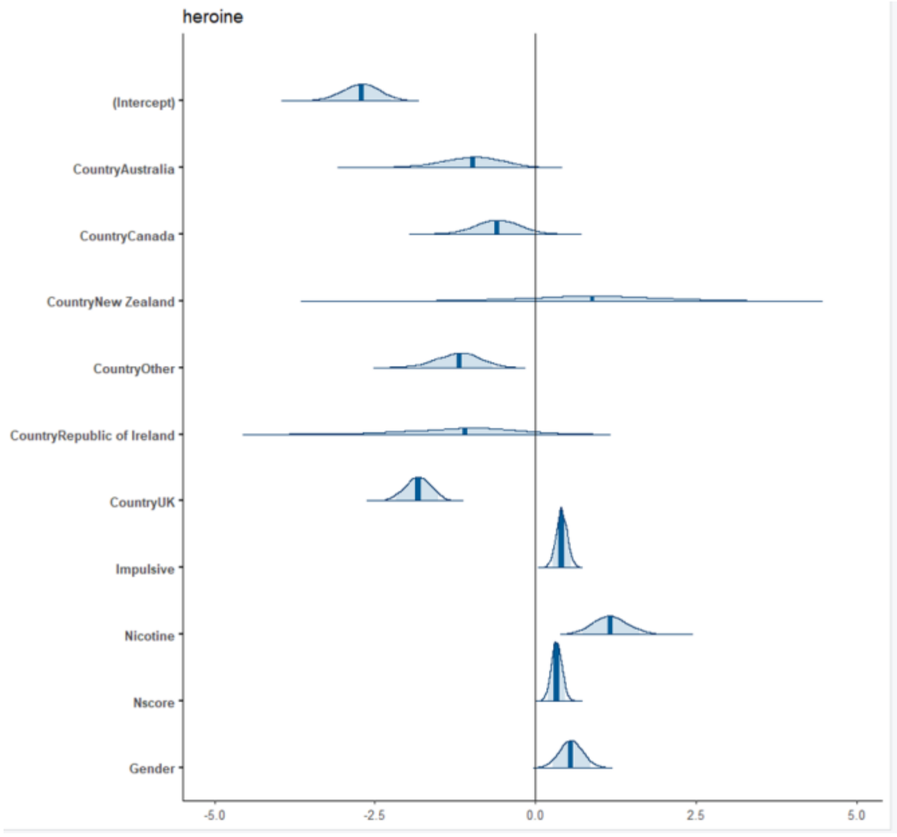
1. 경향성

Step1 Step2 Step3 Step4

Nscore	meth, 헤로인 신경증 점수가 높을수록 해당 마약을 할 가능성 높음
Oscore	리갈하이, LSD, 엑스터시, 벤조디아제핀, 대마, 환각버섯, 니코틴, 케타민 개방성 점수가 높을수록 해당 마약을 할 가능성 높음
Cscore	리갈하이, 엑스터시, 암페타민, 카나비스, 니코틴, VSA, 케타민, 코카인 모든 약물에 대해 성실성 점수가 낮을수록 해당 약물을 할 가능성 높음
Impulsize	크랙, 히로인 충동성 점수가 높을수록 해당 약물을 할 가능성 높음
SS	리갈하이, LSD, 액스터시 등 모든 약물에 대해서 감각추구 점수가 높을수록 마약을 할 가능성 높음

2. Bayesian Analysis

(1) 헤로인



	5%	95%
(Intercept)	-3.21	-2.25
CountryAustralia	-1.85	-0.28
CountryCanada	-1.18	-0.02
CountryNew Zealand	-0.85	2.63
CountryOther	-1.79	-0.67
CountryRepublic of Ireland	-2.66	0.10
CountryUK	-2.17	-1.50
Impulsive	0.26	0.55
Nicotine	0.74	1.63
Nscore	0.20	0.46
Gender	0.27	0.86

β 의 의미

- Logistic regression: $log(\frac{p(x)}{1-p(x)}) = \beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p$
- Odds: $odds(x) = \frac{p(x)}{1-p(x)} = e^{\beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p}$
- Odds ratio between x_k=1 and x_k=0 (fix others): $e^{p_k} = \frac{p(Y=1|x_k)}{p(Y=1|x_0)}$

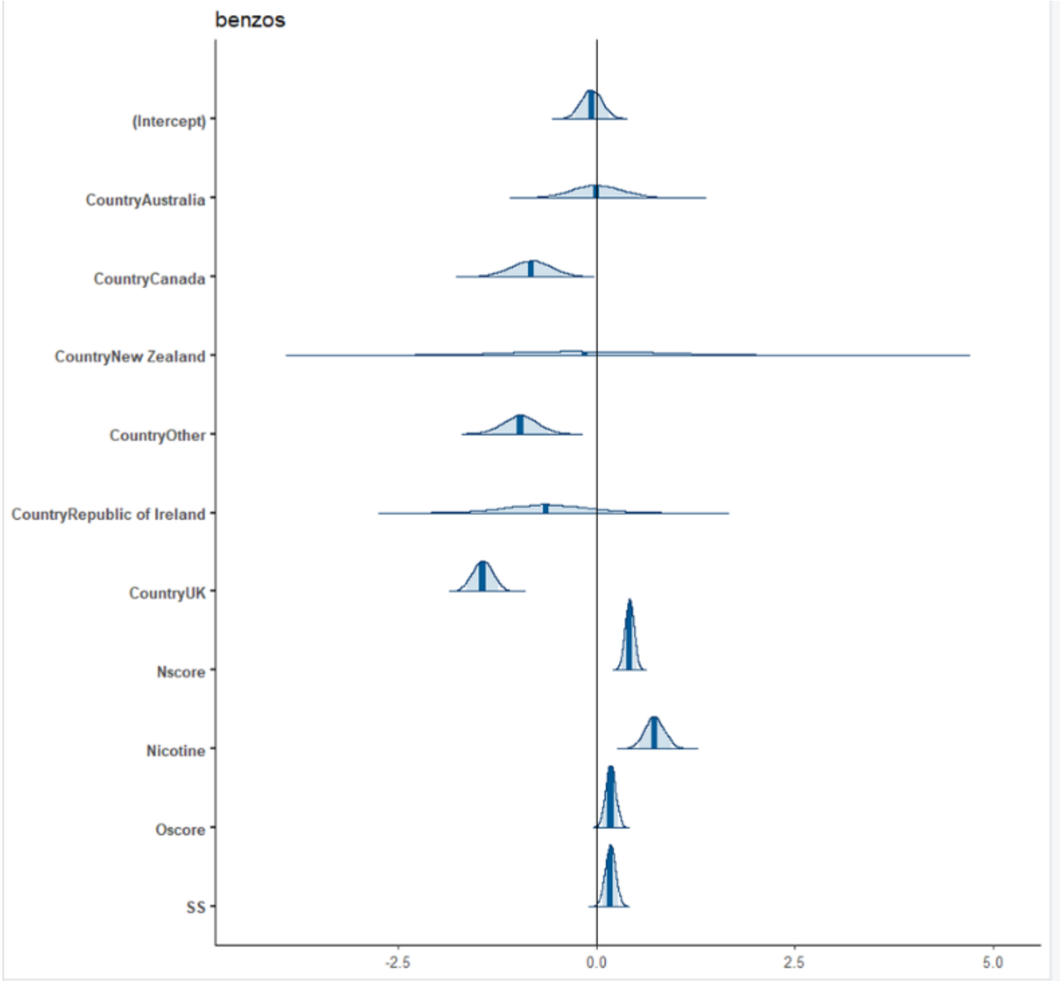
$$\frac{odds(x_{k=1})}{odds(x_{k=0})} = \frac{e^{\beta_0 + \beta_1 x_1 + \ldots + \beta_k x_k + \ldots + \beta_p x_p}}{e^{\beta_0 + \beta_1 x_1 + \ldots + \beta_k 0 + \ldots + \beta_p x_p}} = e^{\beta_k x_k} = e^{\beta_k}$$

- Interpretation of β_k:

  If we increase x_k 1, odds is increased by $e^{\beta k}$

  - β_k>0: p(Y=1 | xk) becomes increased as x_k large
  - β_k<0: p(Y=1 | xk) becomes decreased as x_k large

(2) 벤조디아제핀




```
> round(posterior_interval(benzos, prob = 0.9), 2)
                                5%   95%
(Intercept)                  -0.27  0.17
CountryAustralia             -0.50  0.52
CountryCanada                -1.24 -0.42
CountryNew Zealand           -1.75  1.63
CountryOther                 -1.32 -0.60
CountryRepublic of Ireland   -1.44  0.21
CountryUK                    -1.64 -1.23
Nscore                        0.33  0.51
Nicotine                      0.53  0.94
Oscore                        0.08  0.28
SS                            0.07  0.28
>
```


THANK
YOU