Bayesian model selection method and its application in modeling Covid-19 pandemic development

Truong-Vinh Hoang

MATH4UQ, RWTH Aachen July 23, 2020

- Presenting Bayesian approach for model selection reference: Chapter 5, Ando, Tomohiro. Bayesian model selection and statistical modeling. CRC Press, 2010.
- Apply for modeling the Covid-19 evolution

Outline

- Introduction
- Theoretical background
 - General framework
 - Evaluation of marginal likelihood
 - Analytical method: Exact calculation of marginal likelihood
 - Laplace's method for computing the marginal likelihood
 - Bayesian information criterion (BIC)
 - Expected predictive likelihood approach
- Examples with Covid19 data

General framework

Posterior, marginal likelihood

Setting: Select a model from a set of candidate models: M_1, \ldots, M_r

- Model M_k is characterized by probability density $f_k(\mathbf{x}|\theta_k)$ where θ_k is a p_k -dimensional vector of unknown parameter
- ullet $\pi_k(oldsymbol{ heta}_k)$ is the prior distribution for parameter vector $oldsymbol{ heta}_k$
- Posterior probability of the model M_k given data set $X_n = \{x_1, \dots, x_n\}$ of i.i.d samples

$$P(M_k|\mathbf{X}_n) = \frac{P(M_k) \int f_k(\mathbf{X}_n|\boldsymbol{\theta}_k) \pi_k(\boldsymbol{\theta}_k) d\boldsymbol{\theta}_k}{\sum_{\alpha=1}^r P(M_\alpha) \int f_\alpha(\mathbf{X}_n|\boldsymbol{\theta}_\alpha) \pi_\alpha(\boldsymbol{\theta}_\alpha) d\boldsymbol{\theta}_\alpha}$$

- $P(M_k)$ is the prior: e.g.
 - Uniform
 - Poisson prior: $P(M_k) \propto \lambda^{p_k} \exp(-\lambda)$, $\lambda > 0 \rightarrow$ higher probability on simpler models
 - $P(M_k) \propto \prod_{j=1}^p \pi_j^{\gamma_{k,j}} (1-\pi_j)^{1-\gamma_{k,j}}$, where π_j are the prior probability that the j-th predictor is included in the model
- $\int f_k(\mathbf{X}_n|\theta_k) \pi_k(\theta_k) d\theta_k$ is the marginal likelihood.

General framework

Bayes factor

Bayes factor (BF): comparing models, for testing hypotheses.

BF
$$(M_k, M_j) \equiv \frac{P(\boldsymbol{X}_n | M_k)}{P(\boldsymbol{X}_n | M_j)}$$

Measures the evidence for M_k vs. M_j based on the data information [posterior odds = Bayes factor \times the prior odds]

$$\frac{P(M_k|\mathbf{X}_n)}{P(M_j|\mathbf{X}_n)} = \frac{P(\mathbf{X}_n|M_k)}{P(\mathbf{X}_n|M_j)} \times \frac{P(M_k)}{P(M_j)}$$

Bayes factor can be reduced to classical likelihood ratio

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Methods to evaluate marginal likelihood $f(X_n|\theta_k, M_k)$

- Analytical method
 - E.g. Binomial model with conjugate prior
- Laplace's approximation
 - Bayesian information criterion (BIC)
 - Bayesian information criterion vs. Akaike's Information criterion
 - Generalized BIC
- Numerical method

Binomial model with conjugate prior

- Observations: n independent samples $\boldsymbol{X}_n = \{x_1, x_2, \dots, x_n\} \sim \text{Bin}(n, p)$ with unknown p,
- Conjugate prior: beta distribution with parameter α, β for p

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- Let $y_n = \sum_{i=1}^n x_i$, the marginal likelihood:

$$f(\boldsymbol{X}_{n}|\alpha,\beta) = \int_{0}^{1} \left[\binom{n}{y_{n}} p^{y_{n}} (1-p)^{n-y_{n}} \times \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} p^{\alpha-1} (1-p)^{\beta-1} \right] dp$$

$$= \binom{n}{y_{n}} \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \frac{\Gamma(y_{n}+\alpha)\Gamma(n+\beta-y_{n})}{\Gamma(n+\alpha+\beta)}$$

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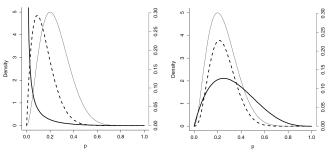
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- Example: Observation: n = 10, $y_n = 2$
- Model selection: $M_1: p \sim \text{Beta}(0.1, 4); M_2: p \sim \text{Beta}(2, 4); M_3: p \sim$ Beta(4, 4); M_4 : $p \sim \text{Beta}(8, 4)$

Binomial model with conjugate prior

Models: $M_1: p \sim \text{Beta}(0.1, 4); M_2: p \sim \text{Beta}(2, 4); M_3: p \sim \text{Beta}(4, 4); M_4: p \sim \text{Beta}(8, 4)$



left M_1 , right M_2

likelihood function (thin line), prior (thick line), posterior (dash line)

$$f(\mathbf{X}_{10}|M_1) = 0.0277, f(\mathbf{X}_{10}|M_2) = 0.1648, \rightarrow M_2 \text{ has the best BF}$$

 $f(\mathbf{X}_{10}|M_3) = 0.0848, f(\mathbf{X}_{10}|M_4) = 0.0168.$

Laplace's method

Asymptotic evaluation of the marginal likelihood

Assumption: the posterior density $\pi(\boldsymbol{\theta}|\boldsymbol{X}_n)$ is sufficiently well-behaved (highly peaked at the posterior mode $\widehat{\boldsymbol{\theta}}_n$). Let

$$s_n(\boldsymbol{\theta}) = \log \left\{ f\left(\boldsymbol{X}_n | \boldsymbol{\theta}\right) \pi(\boldsymbol{\theta}) \right\}$$

Taylor series expansion of s_n yields (first order derivative at $\widehat{\theta}_n=0$):

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$$s_n(\theta) \approx s_n(\widehat{\theta}_n) - \frac{n}{2}(\theta - \widehat{\theta}_n)^T S_n(\widehat{\theta}_n)(\theta - \widehat{\theta}_n)$$

where
$$S_n\left(\widehat{\boldsymbol{\theta}}_n\right) = -\left.\frac{1}{n}\frac{\partial^2 \log\{f(\boldsymbol{X}_n|\boldsymbol{\theta})\pi(\boldsymbol{\theta})\}}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^T}\right|_{\boldsymbol{\theta} = \widehat{\boldsymbol{\theta}}_n}$$

$$\begin{split} \exp\left\{s_n(\boldsymbol{\theta})\right\} &\approx \exp\left\{s_n\left(\widehat{\boldsymbol{\theta}}_n\right)\right\} \times \exp\left\{-\frac{n}{2}\left(\boldsymbol{\theta} - \widehat{\boldsymbol{\theta}}_n\right)^T S_n\left(\widehat{\boldsymbol{\theta}}_n\right)\left(\boldsymbol{\theta} - \widehat{\boldsymbol{\theta}}_n\right)\right\} \\ &\propto \mathcal{N}\left(\widehat{\boldsymbol{\theta}}_n, n^{-1} S_n\left(\widehat{\boldsymbol{\theta}}_n\right)^{-1}\right) \end{split}$$

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Laplace's method for computing the marginal likelihood

Marginal likelihood

Marginal likelihood

$$P(\boldsymbol{X}_{n}|M) = \int \exp\{s_{n}(\boldsymbol{\theta})\} d\boldsymbol{\theta}$$

$$\approx \exp\{s_{n}(\widehat{\boldsymbol{\theta}}_{n})\} \times \int \exp\{-\frac{n}{2}(\boldsymbol{\theta} - \widehat{\boldsymbol{\theta}}_{n})^{T} S_{n}(\widehat{\boldsymbol{\theta}}_{n})(\boldsymbol{\theta} - \widehat{\boldsymbol{\theta}}_{n})\} d\boldsymbol{\theta}$$

$$= f(\boldsymbol{X}_{n}|\widehat{\boldsymbol{\theta}}_{n}) \pi(\widehat{\boldsymbol{\theta}}_{n}) \times \frac{(2\pi)^{\frac{p}{2}}}{n^{\frac{p}{2}} |S_{n}(\widehat{\boldsymbol{\theta}}_{n})|^{\frac{1}{2}}}$$

where p is the dimension of vector $\boldsymbol{\theta}$

• BF(
$$M_k, M_j$$
) $\approx \frac{f_k(\mathbf{X}_n | \widehat{\boldsymbol{\theta}}_{kn})}{f_j(\mathbf{X}_n | \widehat{\boldsymbol{\theta}}_{jn})} \times \frac{\pi_k(\widehat{\boldsymbol{\theta}}_{kn})}{\pi_j(\widehat{\boldsymbol{\theta}}_{jn})} \times \frac{|S_{jn}(\widehat{\boldsymbol{\theta}}_{jn})|^{\frac{1}{2}}}{|S_{kn}(\widehat{\boldsymbol{\theta}}_{kn})|^{\frac{1}{2}}} \times \left(\frac{2\pi}{n}\right)^{\frac{\rho_k - \rho_j}{2}}$

Laplace's method for computing the marginal likelihood

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- Deterministic approaches: first two terms
- Third term: prefer model with less sensitivity
- Last term: complexity of the model (p_k)

Laplace's method for computing the marginal likelihood

Bayesian information criterion

We will consider two cases:

- $\log \pi(\theta) = O_p(1)$, $n \gg 1 \rightarrow$ prior information is ignored
- $\log \pi(\theta) = O_p(n)$

 O_p : stochastic boundedness:

if $X_n = O_p(a_n)$ For any $\epsilon > 0$, there exists a finite m > 0 and a finite N > 0 such that, $P(|X_n/a_n| > m) < \varepsilon$, $\forall n > N$.

Bayesian information criterion

Assumption: $\log \pi(\theta) = O_p(1)$, $n \gg 1 \rightarrow$ prior information is ignored. The marginal likelihood is approximated as:

$$P\left(\boldsymbol{X}_{n}|M\right) \approx f\left(\boldsymbol{X}_{n}|\widehat{\boldsymbol{\theta}}_{\mathsf{MLE}}\right) \pi\left(\widehat{\boldsymbol{\theta}}_{\mathsf{MLE}}\right) imes \frac{\left(2\pi\right)^{\frac{p}{2}}}{n^{\frac{p}{2}}\left|J_{n}\left(\widehat{\boldsymbol{\theta}}_{\mathsf{MLE}}\right)\right|^{\frac{1}{2}}}$$

 J_n is minus the Hessian matrix of function $\frac{1}{n}\log f(\boldsymbol{X}_n|\widehat{\boldsymbol{\theta}})$ at $\widehat{\boldsymbol{\theta}}_{\mathsf{MLE}}$

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$$BIC = -2\log f\left(\boldsymbol{X}_{n}|\widehat{\boldsymbol{\theta}}_{MLE}\right) + p\log n$$

BIC gives a rough approximation to log(BF)

$$\log(\mathsf{BF}(M_k, M_j)) = \log\left[P\left(\boldsymbol{X}_n | M_k\right)\right] - \left[P\left(\boldsymbol{X}_n | M_j\right)\right] \approx (\mathsf{BIC}_j - \mathsf{BIC}_k)/2$$

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$$\lim_{n \to \infty} \frac{(\mathsf{BIC}_j - \mathsf{BIC}_k)/2 - \log(\mathsf{BF}(M_k, M_j)}{\log(\mathsf{BF}(M_k, M_j))} = 0$$

BIC does not involve J_n



Model selection by minimizing ICs: $IC_k = -2 \log f_k(\boldsymbol{X}_n | \hat{\boldsymbol{\theta}}_{\text{MLE }k}) + c_{n,p_k}$ $c_{n,p}$: penalty to encourage the selection of a parsimonious model (fewer parameter dimension)

• BIC: $c_{n,p} = p \log(n)$, AIC: $c_{n,p} = 2p$

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The best model $f_0(z|\theta_0)$ that has the lowest Kullback-Leibler divergence ¹ from true model G(z), or equivalently maximum expected log-likelihood:

$$\int \log f_0(z|\theta_0)dG(z) = \max_k \left\{ \sup_{\theta_k} \int \log f_k(z|\theta_k)dG(z) \right\}$$

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Consistency in picking model $\log f_0(z|\theta_0)$ requires for all non-optimal f_k :

$$\lim \inf_{n \to \infty} \left[\frac{1}{n} \int \log f_0(\boldsymbol{X}_n | \boldsymbol{\theta}_0) dG(\boldsymbol{X}_n) - \frac{1}{n} \int \log f_k(\boldsymbol{X}_n | \boldsymbol{\theta}_{k0}) dG(\boldsymbol{X}_n) \right] > 0$$

¹discussed later in Expec<mark>t</mark>ed predicitve likelihood approach* () () () () () () ()

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if $f_0(z|\theta_0)$ is unique, the consistency of selection holds; if $f_0(z|\theta_0)$ is not-unique (e.g f_k, f_j), only BIC satisfies the consistency in picking the simplest model: $\log\left(\frac{f_k(\boldsymbol{X}_n|\theta_{k0})}{f_i(\boldsymbol{X}_n|\theta_{i0})}\right) = O_p(1)$, and $c_{n,p} \to \infty$

¹discussed later in Expected predicitve likelihood approach

Generalized Bayesian information criterion

Consider $\log \pi(\theta) = O_p(n)$. The marginal likelihood is approximated as:

$$P(\boldsymbol{X}_n|M) \approx f(\boldsymbol{X}_n|\widehat{\boldsymbol{\theta}}_n) \pi(\widehat{\boldsymbol{\theta}}_n) \times \frac{(2\pi)^{\frac{p}{2}}}{n^{\frac{p}{2}} |S_n(\widehat{\boldsymbol{\theta}}_n)|^{\frac{1}{2}}}$$

 $S_n(\widehat{\boldsymbol{\theta}})$ is minus the Hessian matrix of function $\frac{1}{n}\log f(\boldsymbol{X}_n|\boldsymbol{\theta})\pi(\boldsymbol{\theta})$ at the mode of posterior distribution $\widehat{\boldsymbol{\theta}}_n$ Generalized Bayesian information criterion:

$$\mathsf{GBIC} = -2\log f\left(\boldsymbol{X}_n|\widehat{\boldsymbol{\theta}}\right) - 2\log \pi(\widehat{\boldsymbol{\theta}}) + p\log n + \log|S_n(\widehat{\boldsymbol{\theta}})| - p\log(2\pi)$$

Choosing model with the largest posterior \equiv the model that minimizes the criterion.

Difficulty: require to compute the Hessian matrix



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Expected predictive likelihood approach

Motivation: the main weakness of BF is its sensitivity to the prior Let g be the true density of observations, $\boldsymbol{Z}_n = \{z_1, \ldots, z_n\}$ is a set of i.i.d. unseen future observations $f(\boldsymbol{Z}_n|\boldsymbol{X}_n, M)$: Bayesian predictive distribution

$$f(\boldsymbol{Z}_n|\boldsymbol{X}_n,M) = \int f(\boldsymbol{Z}_n|\boldsymbol{X}_n,\theta)\pi(\theta|\boldsymbol{X}_n)d\theta$$

Predictive ability of a given model M using Kullback-Leibler divergence

$$KL(g||f) = \int \left[\log \frac{g(\mathbf{Z}_n)}{f(\mathbf{Z}_n|\mathbf{X}_n, M)}\right] g(\mathbf{Z}_n) d\mathbf{Z}_n$$
$$= \int \log g(\mathbf{Z}_n) g(\mathbf{Z}_n) d\mathbf{Z}_n - \int \log \left(f(\mathbf{Z}_n|\mathbf{X}_n, M)\right) g(\mathbf{Z}_n) d\mathbf{Z}_n$$

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Expected log-predictive likelihood \to a general approach for evaluating the goodness of fit (validation step)

$$\eta(M) = \int \log f(\boldsymbol{Z}_n | \boldsymbol{X}_n, M) g(\boldsymbol{Z}_n) d\boldsymbol{Z}_n$$

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Problem setting

We will compare SIR models with different setting in modeling of Covid-19 pandemic evolution in Germany, Italy, Uruguay, and Saudi Arabia. Model selection is performed in three steps

- Introduction of SIR models
- Parameter identification using Bayesian approach
- Evaluation of model marginal likelihood and Bayes factor

Modeling of Covid-19 pandemic evolution SIR models

SIR model

$$\begin{cases} \frac{dS}{dt} = -\beta \frac{IS}{N} \\ \frac{dI}{dt} = \beta \frac{IS}{N} - \gamma I \\ \frac{dR}{dt} = \gamma I \end{cases}$$

- *S*, *I*, *R* and *N* refer to the susceptible, infected, recovered and total populations, respectively
- $\theta = \{\beta, \gamma, S_0, I_0\}$ are parameter to be identified

Modeling of Covid-19 pandemic evolution SIR models

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We consider two models $P(M_1) = P(M_2) = 0.5$:

- M_1 : β is varying with time while γ is constant $(p_1 = 7)$
- M_2 : both β and γ are time-dependent ($p_2 = 12$)

 β in M_1 , M_2 , and γ in M_2 are represented as piecewise linear functions with a time interval of 20 days (except for Uruguay with 10 days interval).

Bayesian approach for parameter identification and model selection

- ullet Let π_k be the prior densities of the parameters $oldsymbol{ heta}_k$ of model M_k
- X: observations of new infected and recovered cases during time intervals of 14 days
 - reduce the sensitivity due to data errors
- $oldsymbol{\bullet}$ Using Bayesian approach, the posterior of the parameters $oldsymbol{ heta}_i$ is obtained as

$$\pi_i(\boldsymbol{\theta}_i|\boldsymbol{X}) \propto f(\boldsymbol{X}|\boldsymbol{\theta}_i, M_i)\pi_i(\boldsymbol{\theta}_i)$$

where f is the likelihood function

- Computational method: MH-MCMC
- Marginal predictive likelihood of model M (estimated using MCMC samples)

$$f(\mathbf{Z}|\mathbf{X}, M) = \int f(\mathbf{Z}|\boldsymbol{\theta}_i, M_i) \pi_i(\boldsymbol{\theta}_i|\mathbf{X}) d\boldsymbol{\theta}_i$$

 Z: observations of new infected and recovered cases during time intervals of 20 days

Bayesian parameter identification

Likelihood function

Construct likelihood function is a difficult task

Motivation: the number of infected cases > that confirmed

- using the conventional Gaussian likelihood function \to Probability of (predicted cases are smaller than confirmed case) ~ 0.5
- Seroprevalence studies of anti-SARS-CoV-2 IgG antibodies suggest 200% in Spain and 1100% in Switzerland (estimate from small population samples)
- **Assumption**: number of infections/recovers is up to 120% of that confirmed (belief based likelihood)
- (not ideal assumption)

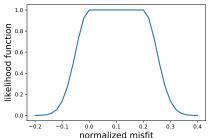
Bayesian parameter identification

Likelihood function

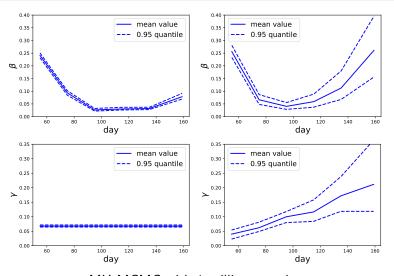
Assumption: number of infections/recovers is up to 120% of that confirmed

Let $\overline{\text{err}}$ be the normalized misfit of the model prediction: $\overline{\text{err}} = \frac{x_i - y_i(\boldsymbol{\theta}_k)}{x_i}$ where x_i is an observation, and y_i is the corresponding model prediction

$$f(x_i|\boldsymbol{\theta}_k) = \begin{cases} 1 & \text{if } 0 \leq \overline{\text{err}} \leq 0.2\\ \mathcal{N}(0, 0.05^2) * \sqrt{2\pi}0.05 & \text{if } \overline{\text{err}} < 0\\ \mathcal{N}(0.2, 0.05^2) * \sqrt{2\pi}0.05 & \text{if } \overline{\text{err}} > 0.2 \end{cases}$$

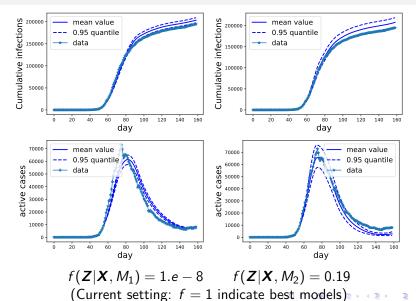


Germany (day 60: 22.03.2020, day 160: 28.06.2020)

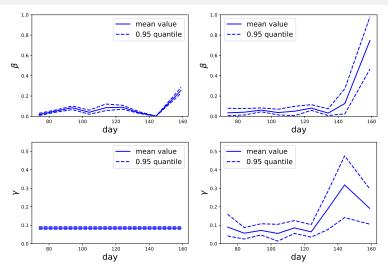


MH-MCMC with 1 million samples

Germany, day 60: 22.03.2020, day 159: 28.06.2020

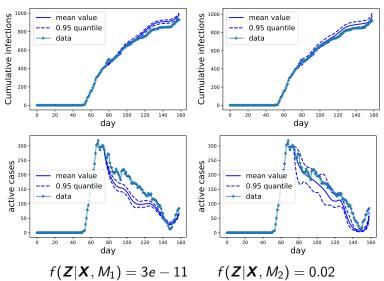


Uruguay, day 70: 01.04.2020, day 159: 28.06.2020

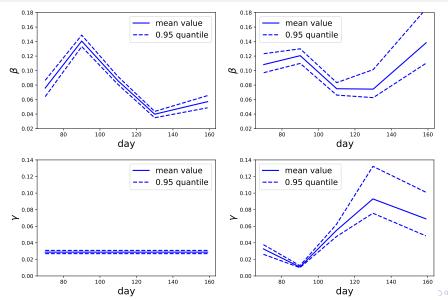


 β and γ in Model 2 are represented as piecewise linear functions with time interval 10 days.

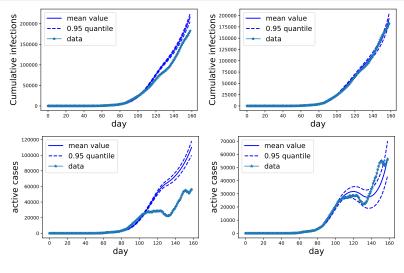
Uruguay, day 70: 01.04.2020, day 159: 28.06.2020



Saudi Arabia, day 70: 01.04.2020, day 159: 28.06.2020

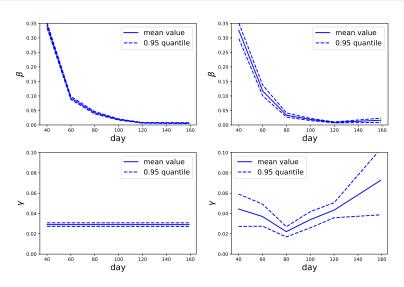


Saudi Arabia, day 70: 01.04.2020, day 159: 28.06.2020

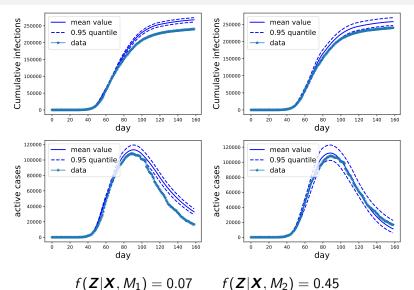


 $f(\mathbf{Z}|\mathbf{X}, M_1) = 3e - 4$ $f(\mathbf{Z}|\mathbf{X}, M_2) = 0.05$

Italy, day 40: 02.03.2020, day 159: 28.06.2020



Italy, day 40: 02.03.2020, day 159: 28.06.2020



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Summary

	$f(\boldsymbol{Z} \boldsymbol{X},M_1)$	$f(\boldsymbol{Z} \boldsymbol{X},M_2)$
Germany	1e-8	0.19
Uruguay	3e-11	0.02
Saudi Arabia	3e-4	0.05
Italy	0.07	0.45

There is strong evidence supporting Model 2

Conclusion

- An overview of Bayesian approach for model selection
- Different information criterions (BIC, GBIC, AIC)
- Predictive Bayesian distribution
- Apply for modeling the evolution of Covid-19 pandemic

Open problems:

- How to construct likelihood function
- Compare with SEIR, (E: exposed)
- Efficient method for identification