Bayesian Two-Stage method for estimating ODE parameters

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ODE model

- Suppose that we have a regression model

$$Y = f_\theta(t) + \epsilon,\ \theta \in \Theta \subseteq \mathbb{R}^p$$

- The functional form of f_θ is not known.
- But the function is assumed to satisfy ODE given by

$$\begin{aligned} \frac{df_\theta(t)}{dt} &= F(t, f_\theta(t), \theta) \\ \text{or} \quad F\left(t, f_\theta(t), \frac{df_\theta(t)}{dt}, \ldots, \frac{d^q f_\theta(t)}{dt^q}, \theta\right) &= 0 \end{aligned}$$

- F is a known real-valued function.

Example

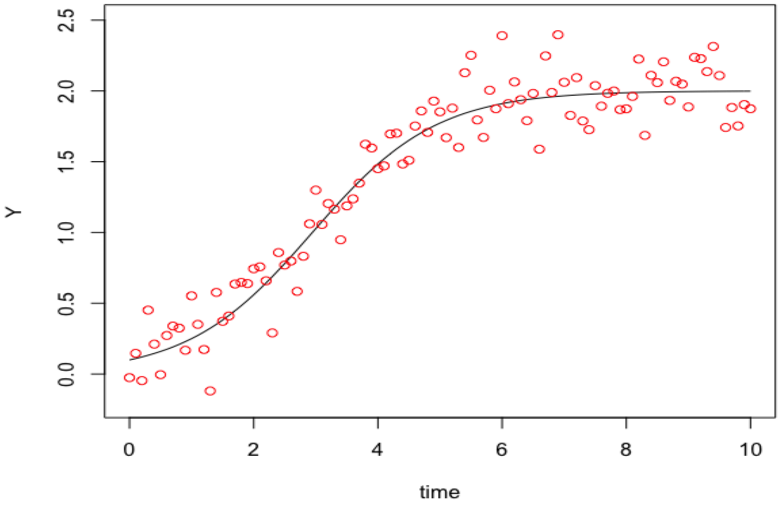
- Consider the following model

$$Y = f_\theta(t) + \epsilon,\ \theta \in \Theta \subseteq \mathbb{R}^2$$

- $f_\theta(t)$ satisfies ODE given by

$$\begin{aligned} \frac{df_\theta(t)}{dt} &= F(t, f_\theta(t), \theta) \\ &= f_\theta(t)(\theta_2 + \theta_1 f_\theta(t)) \end{aligned}$$

Example



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Two-Stage method

- 다음과 같은 모형을 생각한다.

$$Y = f_\theta(t) + \epsilon,$$
$$\frac{df_\theta(t)}{dt} = F(t, f_\theta(t), \theta)$$

- 1단계 : cubic spline 를 이용하여 Y 적합. ($\hat{Y}(t)$)
- 2단계 : $\left|\left|\frac{d\hat{Y}(t)}{dt} - F(t, \hat{Y}(t), \theta)\right|\right|^2$ 를 최소화하는 θ 찾기.

한계점

- 복잡한 모형에 대해서 정확성이 떨어진다.
- 구간 추정을 할 수 없다.

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Bayesian Two-Stage method

- 2단계 방법를 약간 변형
- 구간 추정 가능

1단계

- Penalized B-spline 으로 데이터 적합.
- B : B-spline 기저 행렬 (n by p)
- $\Omega = \ddot{B}^T \ddot{B}$

$$
\begin{aligned}
[\beta|Y] &\propto [Y|\beta][\beta] \\
&\propto \exp\Big[-\frac{1}{2}(Y - B\beta)^T \Sigma^{-1}(Y - B\beta)\Big] \exp\Big[-\frac{1}{2\lambda^2}\beta^T \Omega \beta\Big]
\end{aligned}
$$

$$
\Rightarrow \quad f^{(i)}(t) = B\beta^{(i)} \quad \text{where} \quad \beta^{(i)} \sim [\beta|Y]
$$

- $[\beta|Y] \sim N(\mu_\beta, \Sigma_\beta)$

$$
\text{where} \quad \mu_\beta = (\frac{B^T B}{\sigma^2} + \lambda\Omega)^{-1} B^T Y\,, \quad \Sigma_\beta = (\frac{B^T B}{\sigma^2} + \lambda\Omega)^{-1},
$$

2단계

$$
\begin{aligned}
[\theta|Y] &= \int [\theta, \dot{f}|u]\, d\dot{f} \\
&= \int [\theta|\dot{f}][\dot{f}|Y]\, d\dot{f} \\
&\approx \frac{1}{m}\sum_{i=1}^{m}[\theta|\dot{f}^{(i)}] \\
&\propto \sum_{i=1}^{m}[\dot{f}^{(i)}|\theta][\theta]
\end{aligned}
$$

- 위의 사후분포 계산을 위해서는 $[\dot{f}^{(i)}|\theta]$ 를 알아야 한다.

2단계

- 다음을 가정하자.

$$\dot{f}(t) \sim GP(F(t, f(t), \theta), C)$$

- 다음과 같은 Stochastic diffusion model로 볼 수 있다.

$$df(t) = F(t, f(t), \theta))dt + \sigma dW_t$$

- W_t : Brownian motion process
    - $W_0 = 0$
    - W is a process with stationary independent increments
    - $W_{t+s} - W_s \sim N(0, t)$
    - With probability 1, the function $t \mapsto W_t$ is continuous in t.

2단계

- 다음과 같은 간단한 SDE 를 생각해보자.

$$dX(t) = a(X(t), t)dt + dW_t$$

- Q 측도 : $dX_t = dW_t$
- P 측도 : $dX_t = a(X_t, t)dt + dW_t$
- $L(X) = \frac{dP(X)}{dQ(X)}$

가능도

- $t_k = k\Delta t$, $X_k = X(t_k)$, $\Delta W_k = W_{t_{k+1}} - W_{t_k}$
- $\vec{X} = (X_1, \ldots, X_n)$
- 앞의 SDE 를 다음과 같이 근사할 수 있다.

$$X_{k+1} = X_k + a(X_k, t_k)\Delta t + \Delta W_k$$

가능도

- $V(\vec{X})$: Joint density of $\vec{X}$ for Q

$$V(\vec{X}) = \Pi_k \frac{1}{\sqrt{2\pi\Delta t}} exp(-\frac{1}{2\Delta t}(X_{k+1} - X_k)^2)$$

- $G(\vec{X})$: Joint density of $\vec{X}$ for P

$$G(\vec{X}) = \Pi_k \frac{1}{\sqrt{2\pi\Delta t}} exp(-\frac{1}{2\Delta t}(X_{k+1} - X_k - a(X_k, t_k)\Delta t)^2)$$

$$\begin{aligned} \Rightarrow L(X) &= \lim_{\Delta t \to 0} \frac{G(\vec{X})}{V(\vec{X})} \\ &= \exp\left(\int_0^T a(X(t), t)dX(t) - \frac{1}{2}\int_0^T a^2(X(t), t)dt\right) \end{aligned}$$

가능도

$$
\begin{aligned}
&df(t) = F(t, f(t), \theta)dt + \sigma dW_t \\
\Rightarrow\ &L(\theta|f) = \exp\left(\frac{1}{\sigma^2}\int F(t, f(t), \theta)df(t) - \frac{1}{2\sigma^2}\int F^2(t, f(t), \theta)dt\right)
\end{aligned}
$$

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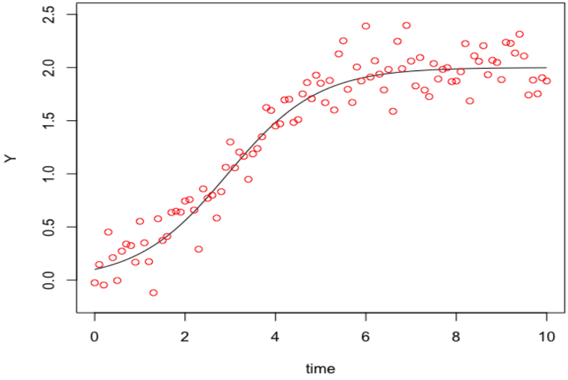
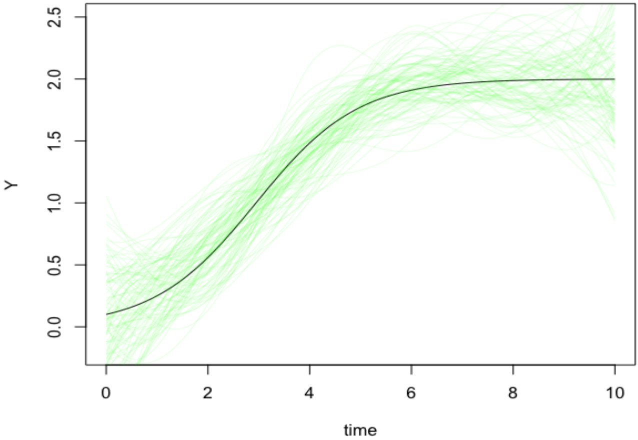
Lotka-Volterra equations

- $\theta_1 = -0.5,\ \theta_2 = 1,\ t \in [0, 10],\ f(0) = 0.1$

$$\frac{df_\theta(t)}{dt} = f_\theta(t)(\theta_2 + \theta_1 f_\theta(t))$$



Lotka-Volterra equations



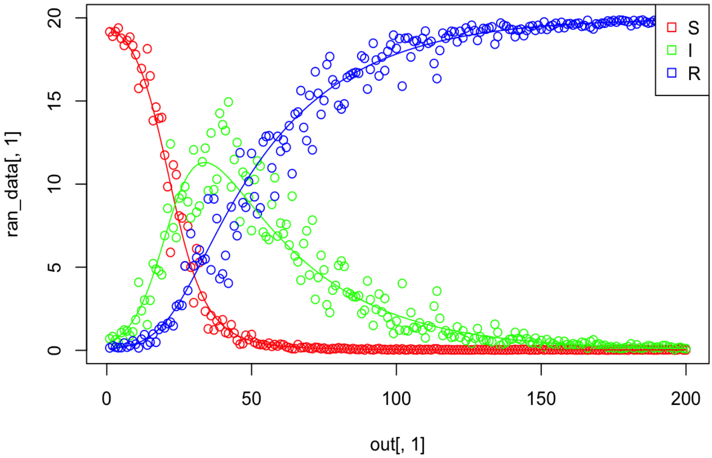
- $\hat{\theta}_1 = -0.487, \ \hat{\theta}_2 = 0.971$

SIR model

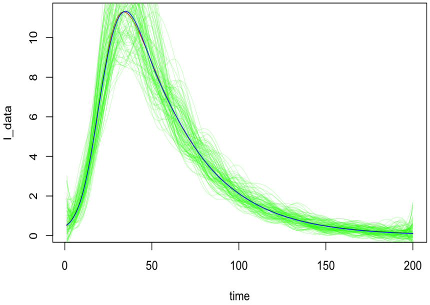
- $\beta = 0.2, \ \gamma = 0.03$
- $S(1) = 19.4, \ I(1) = 0.5, \ R(1) = 0.1$

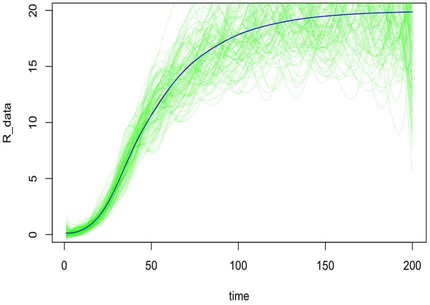
$$\begin{aligned}\frac{dS(t)}{dt} &= -\beta\frac{I(t)}{N}S(t)\\ \frac{dI(t)}{dt} &= \beta\frac{I(t)}{N}S(t) - \gamma I(t)\\ \frac{dR(t)}{dt} &= \gamma I(t)\end{aligned}$$

SIR model



SIR model





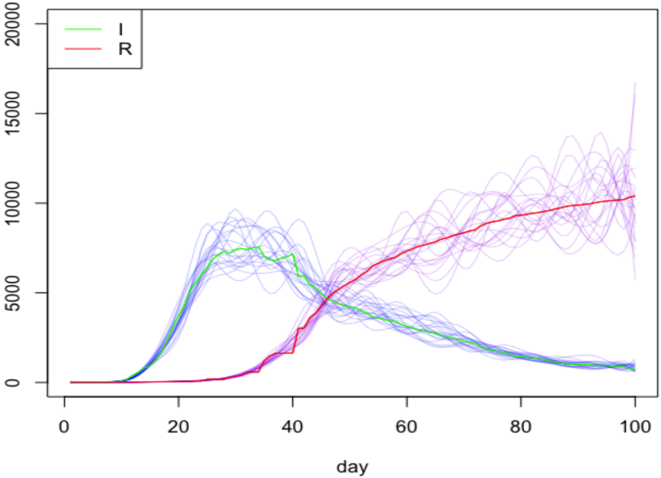
- $\hat{\beta} = 0.1887,\ \hat{\gamma} = 0.0326$

Time-Varying SIR model

$$
\begin{aligned}
\frac{dS(t)}{dt} &= -\beta(t)\frac{I(t)}{N}S(t) \\
\frac{dI(t)}{dt} &= \beta(t)\frac{I(t)}{N}S(t) - \gamma(t)I(t) \\
\frac{dR(t)}{dt} &= \gamma(t)I(t)
\end{aligned}
$$

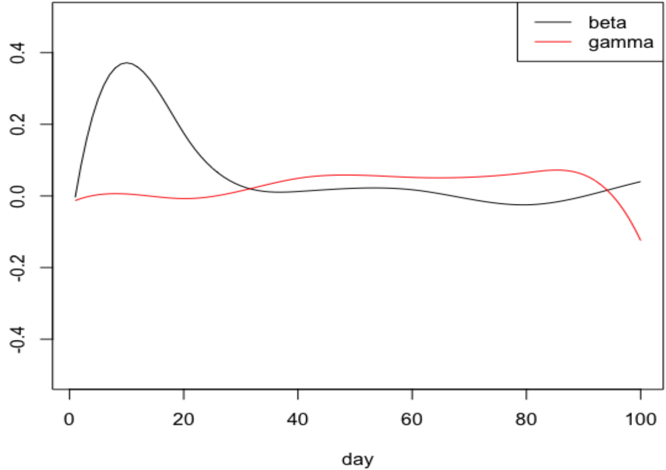
- 2/11 부터 5/20까지의 국내 데이터 이용.
- I, R 의 식을 이용.
- $\beta(t) = B_1(t)\theta_\beta, \quad \gamma(t) = B_1(t)\theta_\gamma$

Time-Varying SIR model

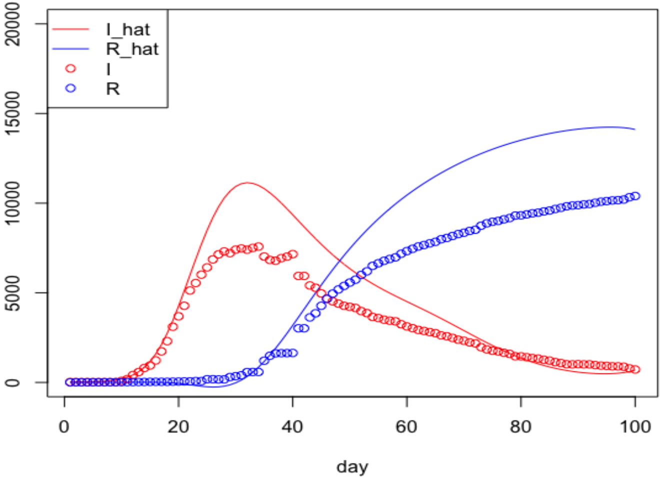


Result

- B1 자유도 : 8

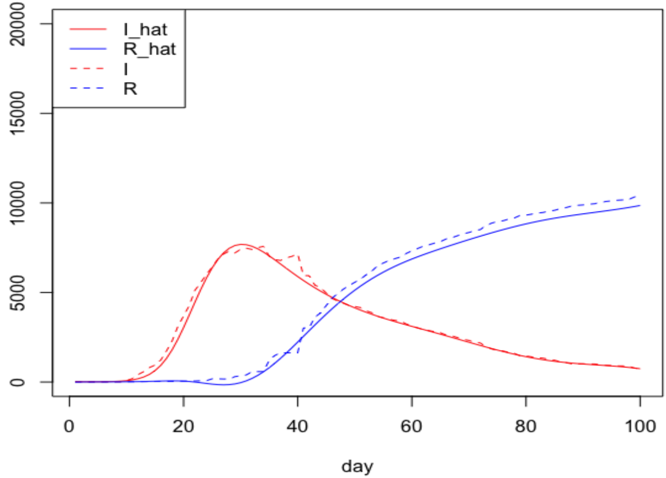


Result



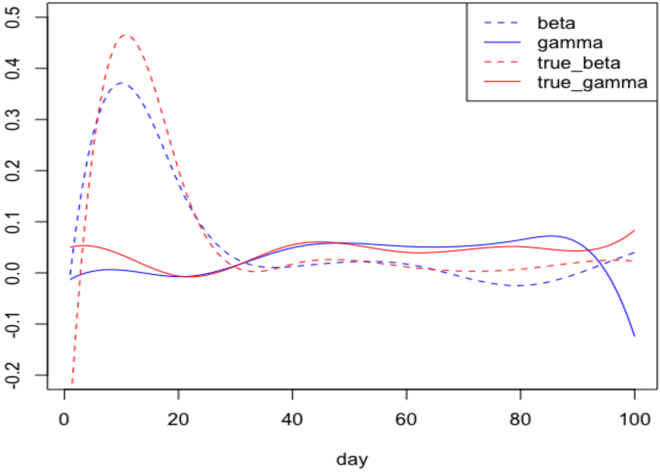
Result

- 실제로는 거의 완벽하게 fitting 이 된다.



Result

- 초기값(day=0) 에 의해서 차이가 발생하는 것으로 보인다.



Remind

$$
\begin{aligned}
[\theta | Y] &= \int [\theta, I, R | Y] \, dI \, dR \\
&= \int [\theta | I, R][I, R | Y] \, dI \, dR \\
&\approx \frac{1}{m} \sum_{i=1}^{m} [\theta | I^{(i)}, R^{(i)}] \\
&\approx \frac{1}{m} \sum_{i=1}^{m} [I^{(i)} | \theta][R^{(i)} | \theta][\theta]
\end{aligned}
$$

Remind

$$[I^{(i)}|\theta] \propto \frac{\exp(-\frac{1}{2\sigma^2}\sum_t (I^{(i)}(t+1) - I^{(i)}(t) - v_I(t))^2)}{\exp(-\frac{1}{2\sigma^2}\sum_t (I^{(i)}(t+1) - I^{(i)}(t))^2)}$$

$$[R^{(i)}|\theta] \propto \frac{\exp(-\frac{1}{2\sigma^2}\sum_t (R^{(i)}(t+1) - R^{(i)}(t) - v_R(t))^2)}{\exp(-\frac{1}{2\sigma^2}\sum_t (R^{(i)}(t+1) - R^{(i)}(t))^2)}$$

where $\quad v_I(t) = \beta(t)\dfrac{I(t)}{N}S(t) - \gamma(t)I(t), \quad v_R(t) = \gamma(t)I(t),$

$$\beta(t) = B_1(t)\theta_\beta, \quad \gamma(t) = B_1(t)\theta_\gamma$$

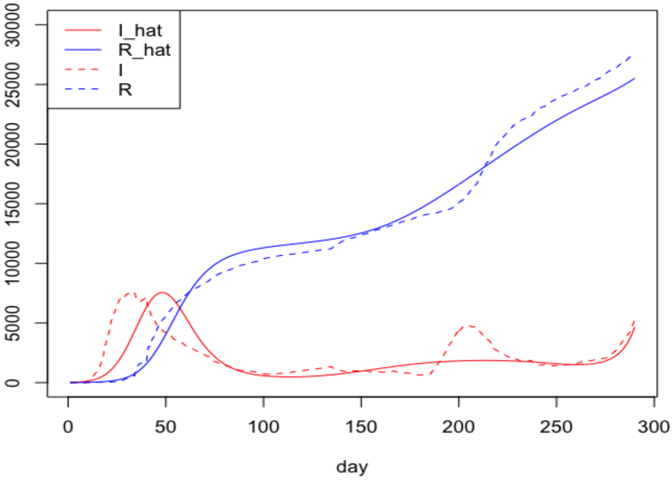
Discussion

- t가 작을 때 모수 추정값이 약간 차이가 발생하면, 이 차이가 t=T 까지 누적된다.
- $\beta(\hat{1})$이 실제보다 크게 추정되어서 integration 한 $\hat{I}(2)$가 실제 $I(2)$보다 커지면 그 뒤의 모수가 정확히 추정되어도 integration 결과가 왜곡될 수 있다.

- 적은 수의 기저를 사용해서 데이터를 근사하는 것에 어려움이 있다.
- 1단계에서의 샘플 추출과 $v(t)$에서 $I(t), S(t)$ 의 선택을 수정해야 한다.

Approximation

- 기저 10개를 이용하여 실제 데이터를 근사하였다.



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