

Bayesian modelling using R + STAN = RSTSAN

https://github.com/clobos/Seminario_STAN_UNESP

Cristian Villegas, ESALQ/USP

UNESP Botucatu (29/08/2019)

Brief introduction to Stan

Stan is a state-of-the-art platform for statistical modeling and high-performance statistical computation. Thousands of users rely on Stan for statistical modeling, data analysis, and prediction in the social, biological, and physical sciences, engineering, and business.

Brief introduction to Stan

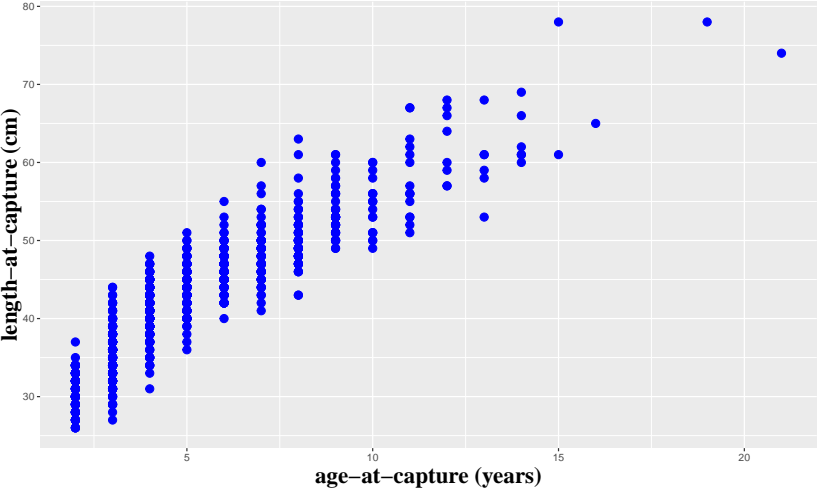
Users specify log density functions in Stan's probabilistic programming language and get:

- ▶ full Bayesian statistical inference with MCMC sampling (NUTS, HMC)
- ▶ approximate Bayesian inference with variational inference (ADVI)
- ▶ penalized maximum likelihood estimation with optimization (L-BFGS)

Brief introduction to Stan

Stan's math library provides differentiable probability functions & linear algebra (C++ autodiff). Additional R packages provide expression-based linear modeling, posterior visualization, and leave-one-out cross-validation.

Motivation Example



The Von Bertalanffy growth model (Classical approach)

The Von Bertalanffy growth model is given by

$$Y_i = \beta_1 (1 - \exp\{-\beta_2 (x_i - \beta_3)\}) + \varepsilon_i \quad \text{with} \quad \varepsilon_i \sim N(0, \sigma^2),$$

where Y_i is the length-at-capture and x_i is the age-at-capture for the i th fish, respectively. The parameter interpretation of the Von Bertalanffy growth model is given by

- ▶ β_1 is the asymptotic (average) length
- ▶ β_2 is the growth rate coefficient (units are years^{-1}), and
- ▶ β_3 represent the age when (average) length was zero.

The Von Bertalanffy growth model (Classical approach)

In R code the Von Bertalanffy growth model is given by

```
LVB<-function(x,beta1, beta2, beta3){  
  beta1*(1-exp(-beta2*(x-beta3)))  
}
```

The Von Bertalanffy nonlinear model (Classical approach)

```
ajuste_LVB <- nls(Length ~ LVB(Age, beta1, beta2, beta3),  
start = list(beta1 = max(dados.amostra$Length),  
              beta2 = 0.5,  
              beta3 = 0),  
data = dados.amostra)  
  
c(coef(ajuste_LVB), sigma=sigma(ajuste_LVB))
```

```
##          beta1          beta2          beta3          sigma  
## 73.8227693   0.1080882 -3.1551711   3.2475942
```


First Case: Bayesian Inference with Stan code

```
Von_Bertanlanffy_mcmc <- '  
data {  
  int<lower = 0> N ;  
  vector[N] x ;  
  vector[N] y ;  
}  
parameters {  
  real<lower = .0> beta1 ;  
  real<lower = .0> beta2 ;  
  real beta3 ;  
  real<lower = .0> sigma ;  
}  
model {  
  y ~ normal(beta1*(1-exp(-beta2*(x-beta3))), sigma) ;  
}  
'
```

Bayesian Inference: Stan code

```
ajuste_Von_Bertanlanffy <- stan(  
  model_code = Von_Bertanlanffy_mcmc,  
  data = list(N = nrow(dados.amostra),  
              x = dados.amostra$Age,  
              y = dados.amostra$Length),  
  chain = 3,  
  iter = 100,  
  warmup = 10,  
  thin = 1,  
  refresh=0)
```

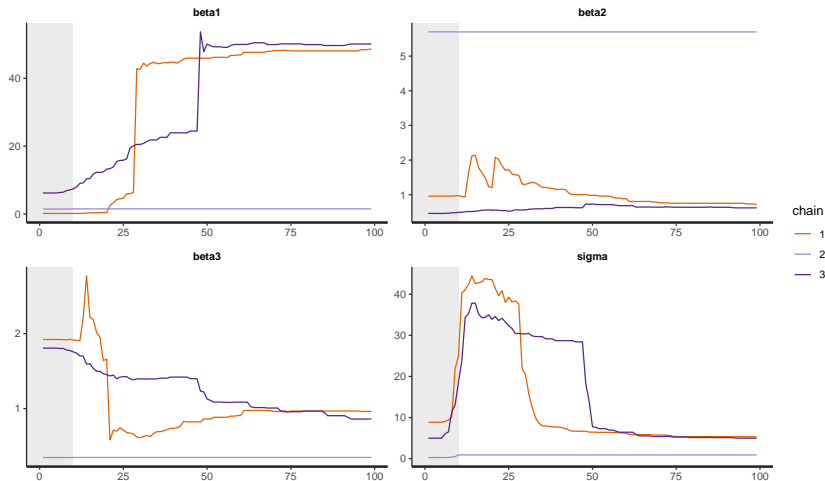
MCMC diagnostics using the bayesplot package

```
parametros<- c(paste('beta',1:3, sep=""), 'sigma')  
  
CI_theta <- summary(ajuste_Von_Bertanlanffy,  
                    pars = parametros,  
                    probs = c(0.025, 0.975))$summary  
print(round(CI_theta,2))
```

##		mean	se_mean	sd	2.5%	97.5%	n_eff	Rhat
##	beta1	25.45	13.46	21.95	0.37	50.18	2.66	2.30
##	beta2	2.46	1.88	2.31	0.54	5.70	1.52	17.00
##	beta3	0.84	0.30	0.45	0.35	1.91	2.28	1.97
##	sigma	10.32	5.17	12.87	0.90	42.48	6.20	1.78

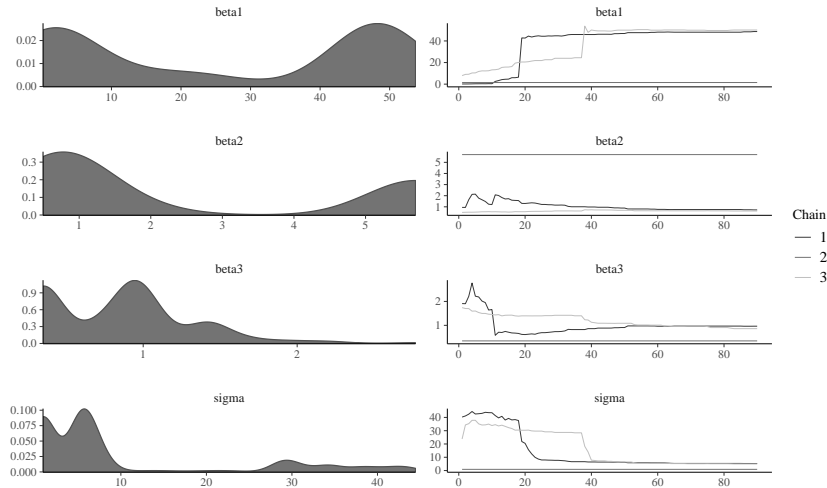
MCMC diagnostics using the bayesplot package

```
traceplot(ajuste_Von_Bertanlanffy, pars = parametros,  
          inc_warmup = TRUE)
```



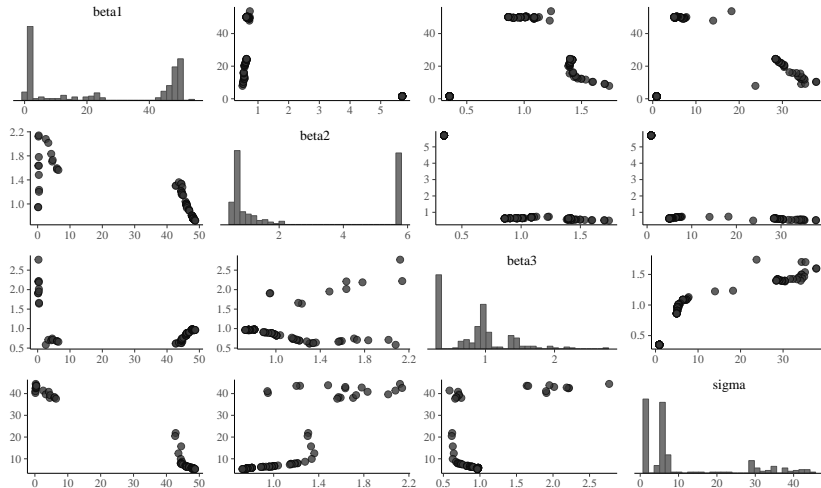
MCMC diagnostics using the bayesplot package

```
mcmc_combo(mcmc_cadeia, pars = parametros, n_warmup=0)
```



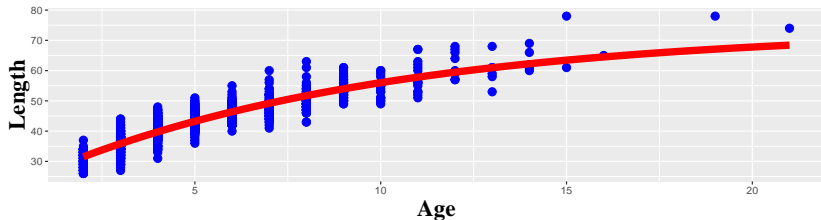
MCMC diagnostics using the bayesplot package

```
mcmc_pairs(mcmc_cadeia, pars = parametros)
```

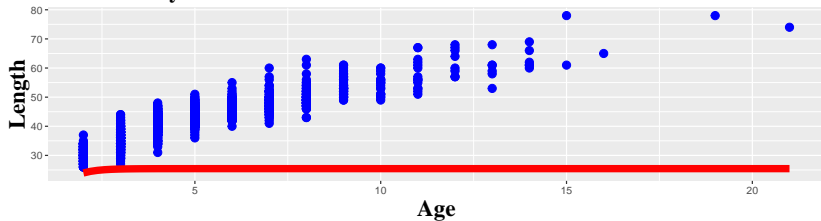


Comparing fitted curves based on Classical and Bayesian Inference

Based on Classical Inference



Based on Bayesian Inference



Comparing the parameter estimation based on Classical and Bayesian Inference

```
c(coef(ajuste_LVB),sigma=sigma(ajuste_LVB))
```

```
##          beta1          beta2          beta3          sigma
## 73.8227693   0.1080882  -3.1551711   3.2475942
```

```
print(CI_theta[,1])
```

```
##          beta1          beta2          beta3          sigma
## 25.4525584   2.4567863   0.8429762  10.3197269
```


Second Case: Bayesian Inference with Stan code

```
Von_Bertanlanffy_mcmc <- '  
data {  
  int<lower = 0> N ;  
  vector[N] x ;  
  vector[N] y ;  
}  
parameters {  
  real<lower = .0> beta1 ;  
  real<lower = .0> beta2 ;  
  real beta3 ;  
  real<lower = .0> sigma ;  
}  
model {  
  y ~ normal(beta1*(1-exp(-beta2*(x-beta3))), sigma) ;  
}  
'
```

Bayesian Inference: Stan code

```
ajuste_Von_Bertanlanffy <- stan(  
  model_code = Von_Bertanlanffy_mcmc,  
  data = list(N = nrow(dados.amostra),  
              x = dados.amostra$Age,  
              y = dados.amostra$Length),  
  chain = 3,  
  iter = 11000,  
  warmup = 1000,  
  thin = 10,  
  refresh=0)
```

MCMC diagnostics using the bayesplot package

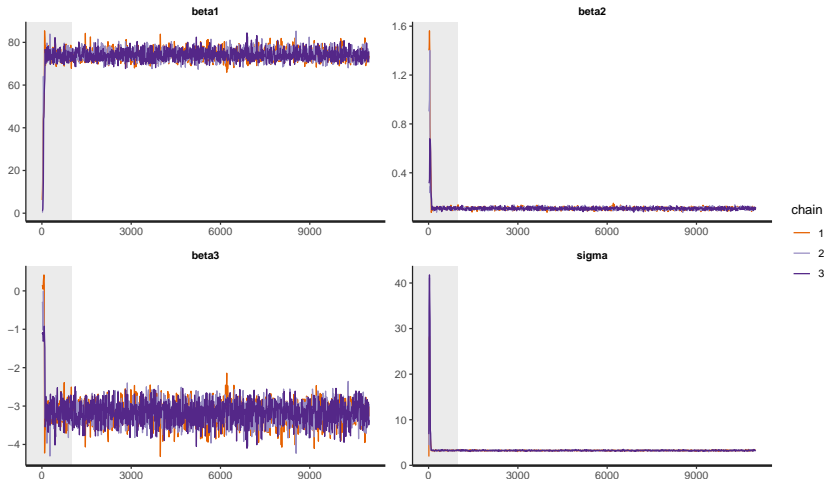
```
parametros<- c(paste('beta',1:3, sep=""), 'sigma')

CI_theta <- summary(ajuste_Von_Bertanlanffy,
                    pars = parametros,
                    probs = c(0.025, 0.975))$summary
print(round(CI_theta,2))
```

##		mean	se_mean	sd	2.5%	97.5%	n_eff	Rhat
##	beta1	74.09	0.05	2.54	69.63	79.49	2847.90	1
##	beta2	0.11	0.00	0.01	0.09	0.13	2885.81	1
##	beta3	-3.18	0.01	0.28	-3.76	-2.66	2932.61	1
##	sigma	3.25	0.00	0.07	3.11	3.40	3051.84	1

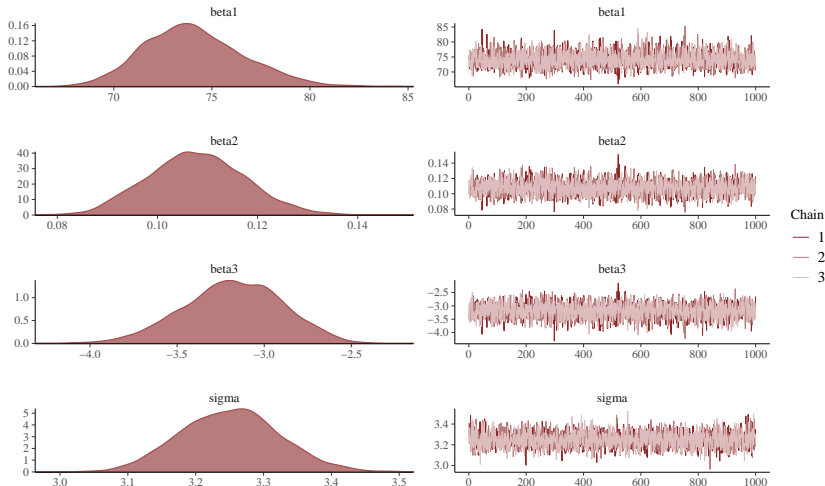
MCMC diagnostics using the bayesplot package

```
traceplot(ajuste_Von_Bertanlanffy, pars = parametros,  
          inc_warmup = TRUE)
```



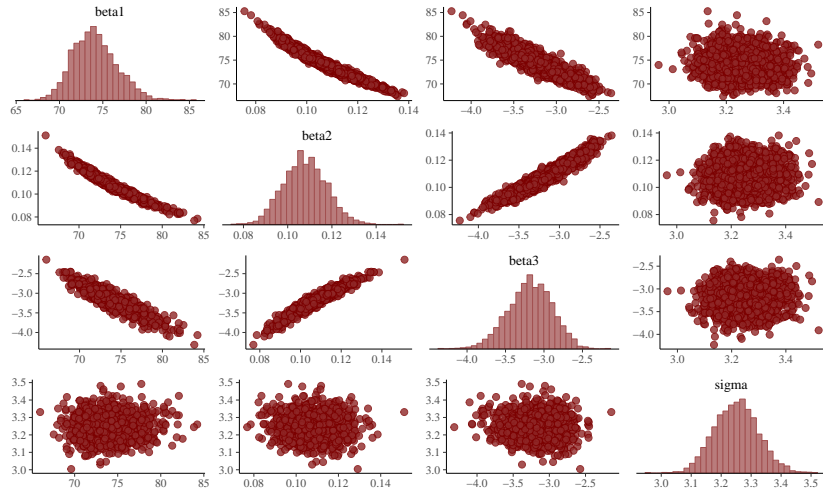
MCMC diagnostics using the bayesplot package

```
mcmc_combo(mcmc_cadeia, pars = parametros, n_warmup=0)
```



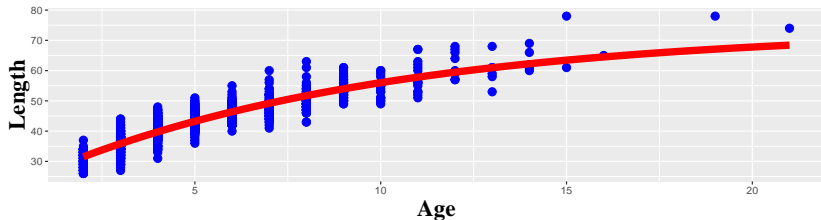
MCMC diagnostics using the bayesplot package

```
mcmc_pairs(mcmc_cadeia, pars = parametros)
```

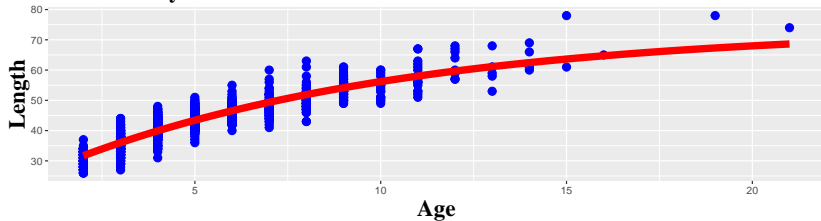


Comparing fitted curves based on Classical and Bayesian Inference

Based on Classical Inference



Based on Bayesian Inference



Comparing the parameter estimation based on Classical and Bayesian Inference

```
c(coef(ajuste_LVB),sigma=sigma(ajuste_LVB))
```

```
##          beta1          beta2          beta3          sigma
## 73.8227693  0.1080882 -3.1551711  3.2475942
```

```
print(CI_theta[,1])
```

```
##          beta1          beta2          beta3          sigma
## 74.0883836  0.1077937 -3.1803626  3.2509435
```


Normal distribution without covariates in Stan

$Y \sim N(\mu, \sigma^2)$. Therefore, $\theta = (\mu, \sigma^2)^\top$. Here, we specify the prior distribution for each parameter.

Bayesian Inference: Stan code (specific prior)

```
normal_dist_example<- '  
data {  
  int<lower=0> N;  
  vector[N] y;  
}  
parameters {  
  real mu;  
  real<lower=0> sigma;  
}  
model {  
  y ~ normal(mu, sigma);  
  mu~ normal(0,1e6);  
  sigma ~ student_t(3,0,1);  
}  
,
```

Bayesian Inference: Stan code (specific prior)

```
normal_dist_fit <- stan(model_code = normal_dist_example,  
  data = list(N = dim(stackloss)[1],  
    y = stackloss$stack.loss),  
  chain = 3,  
  iter = 11000,  
  warmup = 1000,  
  thin = 10,  
  refresh = 0)
```

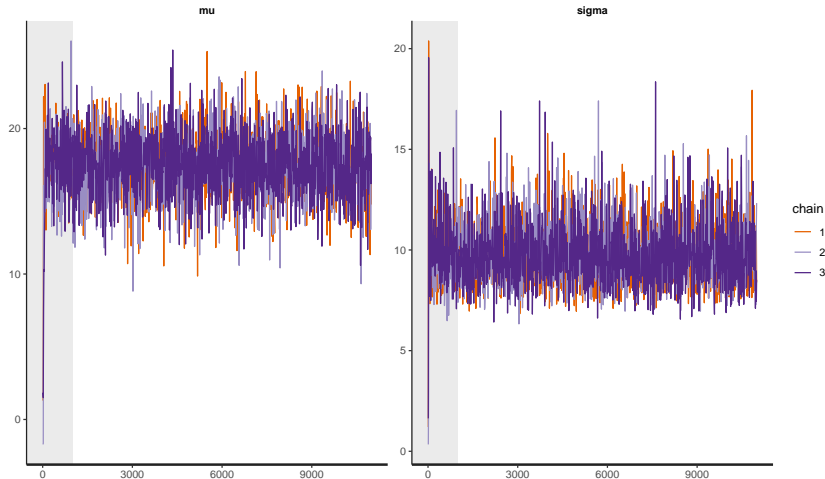
MCMC diagnostics using the bayesplot package

```
parametros<- c("mu", "sigma")  
  
CI_theta <- summary(normal_dist_fit,  
                    pars = parametros,  
                    probs = c(0.025, 0.975))$summary  
print(round(CI_theta,2))
```

##	mean	se_mean	sd	2.5%	97.5%	n_eff	Rhat
## mu	17.50	0.04	2.15	13.18	21.80	2970.46	1
## sigma	9.82	0.03	1.53	7.40	13.27	2973.68	1

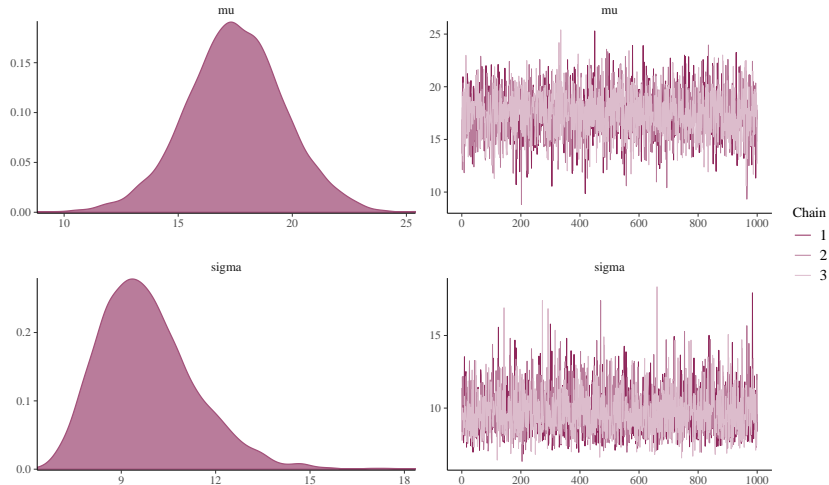
MCMC diagnostics using the bayesplot package

```
traceplot(normal_dist_fit, pars = parametros,  
          inc_warmup = TRUE)
```



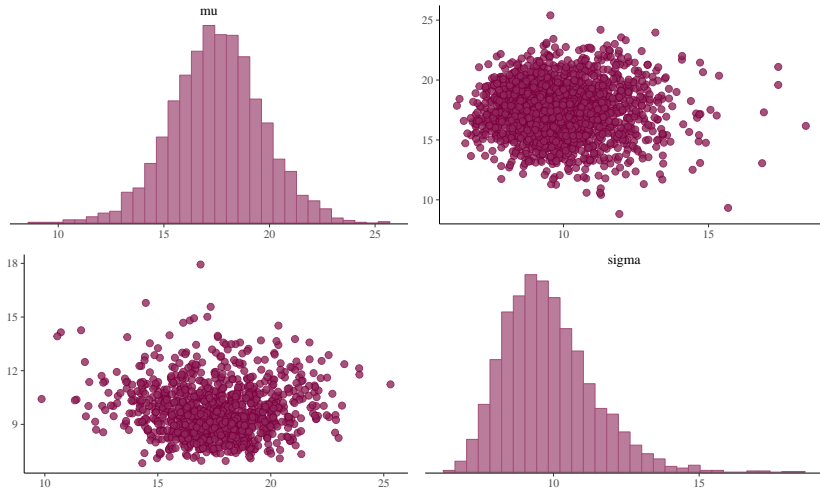
MCMC diagnostics using the bayesplot package

```
mcmc_combo(mcmc_cadeia, pars = parametros, n_warmup=0)
```



MCMC diagnostics using the bayesplot package

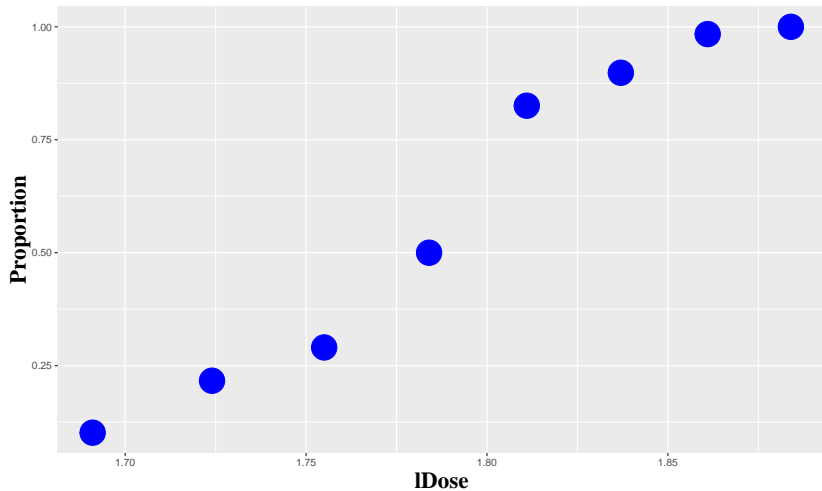
```
mcmc_pairs(mcmc_cadeia, pars = parametros)
```



Logistic Regression

Binomial response with logit link function. Here, we do not specify the prior distribution for each parameter.

Motivation Example



Bayesian Inference: Stan code

```
logistic_example<- 'data {  
  int<lower=0> N;vector[N] x;  
  int<lower=0> y[N]; int<lower=0> n[N];  
}  
parameters {real beta1;real beta2;  
}  
transformed parameters {  
  real exp_eta[N]; real<lower=0, upper=1> prob[N];  
  for (i in 1:N) {exp_eta[i] = exp(beta1 + beta2*x[i]);  
  prob[i]= exp_eta[i]/(exp_eta[i] + 1);  
}  
}  
model {  
  y ~ binomial_logit(n, beta1 + beta2 * x);  
}  
,
```

Bayesian Inference: Stan code

```
logistic_fit <- stan(model_code = logistic_example,  
data = list(N = dim(beetleDat)[1],  
             n = beetleDat$n,  
             x = beetleDat$lDose,  
             y = beetleDat$x),  
             chain = 3,  
             iter = 11000,  
             warmup = 1000,  
             thin = 10,  
             refresh=0)
```

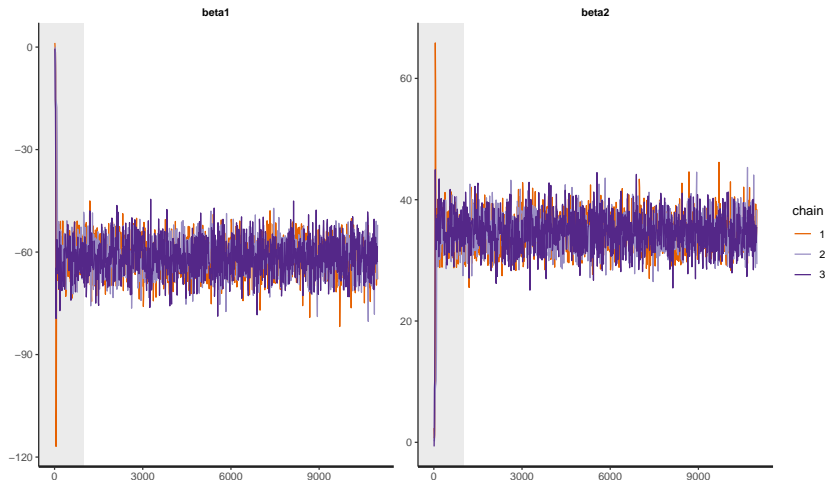
MCMC diagnostics using the bayesplot package

```
parametros<- c(paste('beta',1:2, sep=""))  
  
CI_theta <- summary(logistic_fit,  
                    pars = parametros,  
                    probs = c(0.025, 0.975))$summary  
print(round(CI_theta,2))
```

##		mean	se_mean	sd	2.5%	97.5%	n_eff	Rhat
##	beta1	-61.37	0.11	5.25	-72.01	-51.43	2420.70	1
##	beta2	34.64	0.06	2.95	29.07	40.58	2422.88	1

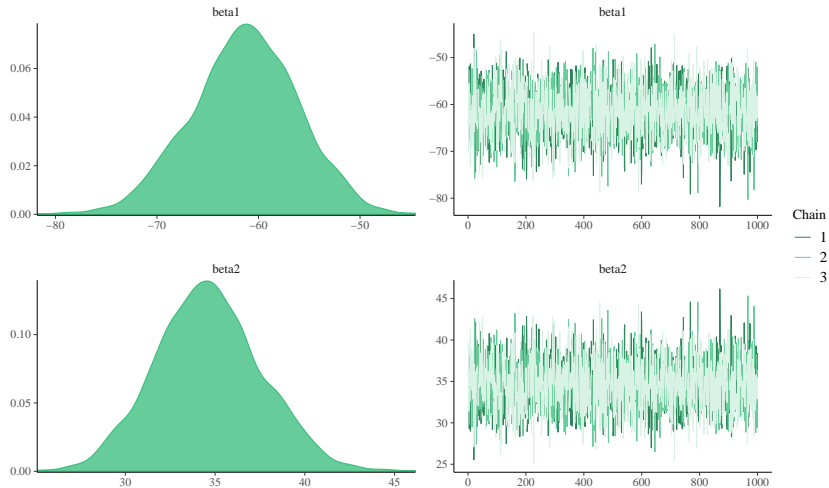
MCMC diagnostics using the bayesplot package

```
traceplot(logistic_fit, pars = parametros,  
          inc_warmup = TRUE)
```



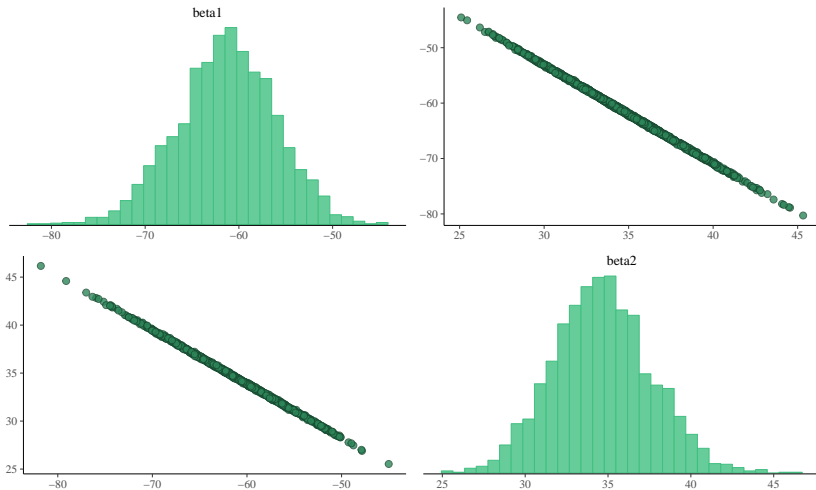
MCMC diagnostics using the bayesplot package

```
mcmc_combo(mcmc_cadeia, pars = parametros, n_warmup=0)
```



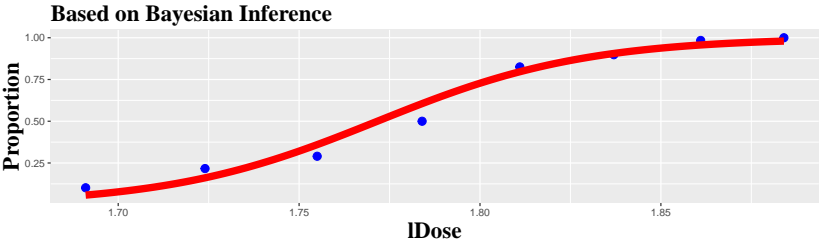
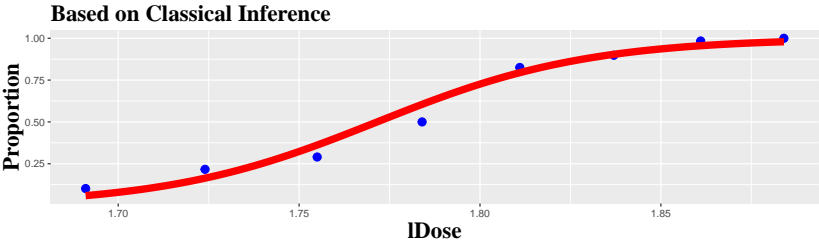
MCMC diagnostics using the bayesplot package

```
mcmc_pairs(mcmc_cadeia, pars = parametros)
```



<https://www.youtube.com/watch?v=uSjsJg8fcwY>

Fitted curve based on Bayesian Inference



Comparing the parameter estimation based on Classical and Bayesian Inference

```
c(beta1=coef(fitLogistic)[1], beta2=coef(fitLogistic)[2])
```

```
## beta1.(Intercept)      beta2.lDose  
##           -60.74013           34.28593
```

```
print(CI_theta[,1])
```

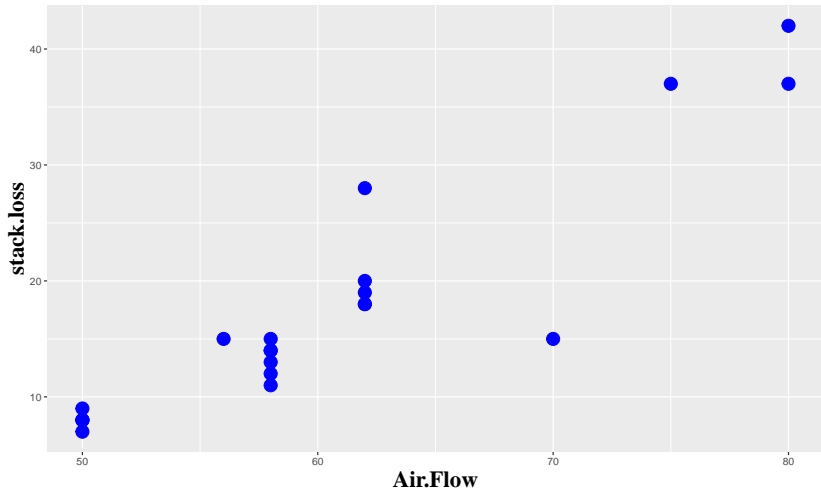
```
##      beta1      beta2  
## -61.37130  34.64121
```

Normal Linear Model

$$Y_i = \beta_1 + \beta_2 x_i + \varepsilon_i \quad \text{with} \quad \varepsilon_i \sim N(0, \sigma^2),$$

where Y_i is stack loss and x_i is flow of cooling air, respectively. Therefore $\theta = (\beta_1, \beta_2, \sigma^2)^\top$. Here, we do not specify the prior distribution for each parameter.

Motivation Example



Bayesian Inference: Stan code

```
lm_example<- '  
data {  
  int<lower=0> N;  
  vector[N] x;  
  vector[N] y;  
}  
parameters {  
  real beta1;  
  real beta2;  
  real<lower=0> sigma;  
}  
model {  
  y ~ normal(beta1+beta2*x, sigma);  
}  
'
```

Bayesian Inference: Stan code

```
lm_fit <- stan(model_code = lm_example,  
data = list(N = dim(stackloss)[1],  
            x = stackloss$Air.Flow,  
y = stackloss$stack.loss),  
            chain = 3,  
            iter = 11000,  
            warmup = 1000,  
            thin = 10,  
            refresh=0)
```

MCMC diagnostics using the bayesplot package

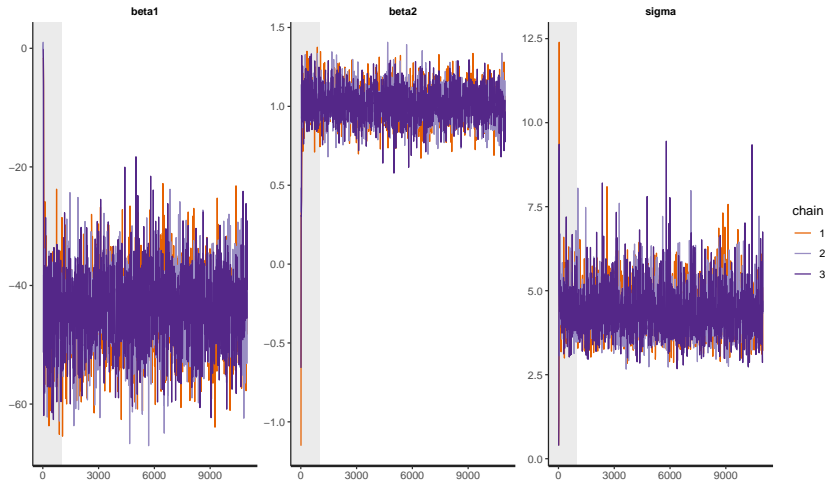
```
parametros<- c(paste('beta',1:2, sep=""), 'sigma')

CI_theta <- summary(lm_fit,
                    pars = parametros,
                    probs = c(0.025, 0.975))$summary
print(round(CI_theta,2))
```

##		mean	se_mean	sd	2.5%	97.5%	n_eff	Rhat
##	beta1	-43.85	0.12	6.57	-56.83	-30.91	2816.31	1
##	beta2	1.02	0.00	0.11	0.80	1.23	2831.99	1
##	sigma	4.39	0.01	0.77	3.20	6.14	2976.60	1

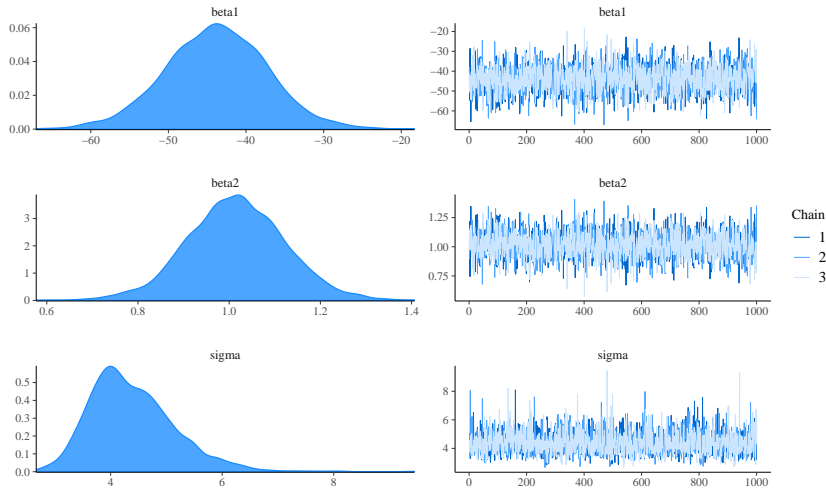
MCMC diagnostics using the bayesplot package

```
traceplot(lm_fit, pars = parametros, inc_warmup = TRUE)
```



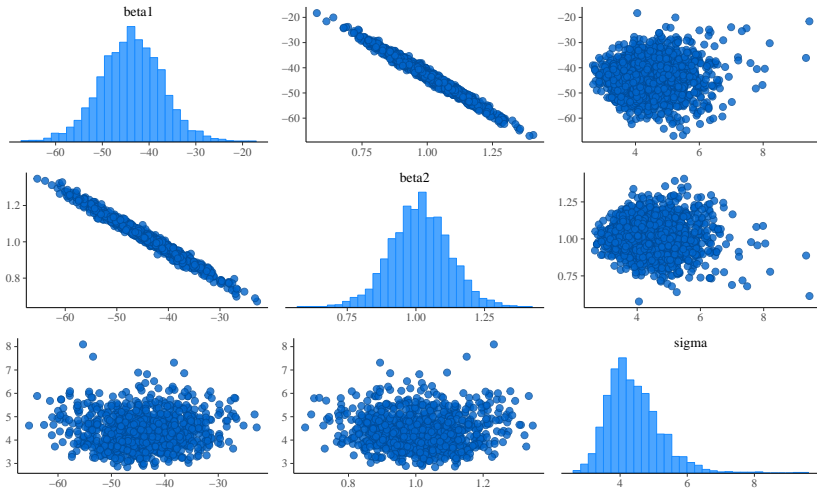
MCMC diagnostics using the bayesplot package

```
mcmc_combo(mcmc_cadeia, pars = parametros, n_warmup=0)
```



MCMC diagnostics using the bayesplot package

```
mcmc_pairs(mcmc_cadeia, pars = parametros)
```



Comparing the parameter estimation based on Classical and Bayesian Inference

```
c(beta1=coef(ajuste)[1],beta2=coef(ajuste)[2],  
  sigma=sigma(ajuste))
```

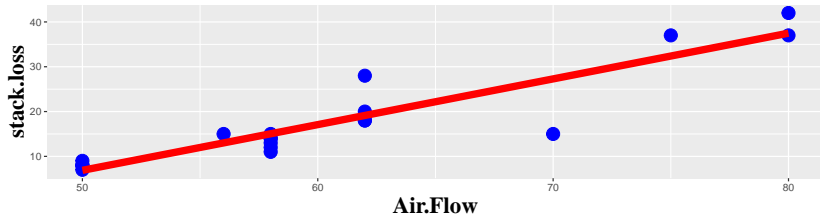
```
## beta1.(Intercept)      beta2.Air.Flow          sigma  
##          -44.132025           1.020309         4.098242
```

```
print(CI_theta[,1])
```

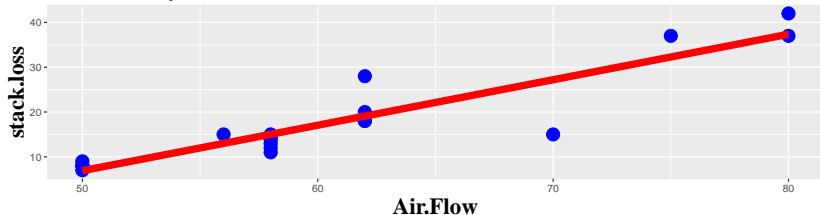
```
##          beta1          beta2          sigma  
## -43.847882    1.015100    4.393619
```

Comparing fitted curves based on Classical and Bayesian Inference

Based on Classical Inference



Based on Bayesian Inference



More Details about other R packages

- ▶ `rstanarm`
- ▶ `shinystan`

References

- ▶ https://mc-stan.org/docs/2_20/stan-users-guide/index.html
- ▶ https://mc-stan.org/docs/2_20/reference-manual/index.html
- ▶ https://mc-stan.org/docs/2_20/functions-reference/index.html