

Kentaro Matsuura

Bayesian Statistical Modeling with Stan, R, and Python

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Kentaro Matsuura
HOXO-M Inc.
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Preface

About This Book

With the recent rise in popularity of Bayesian statistics, many books on this subject have been published. However, many of these books either only contain basic information, or contain too complicated formulas that are not easy to extend in practice. This book is, therefore, a departure from those books, and is intended to be a very practical book on Bayesian statistical modeling with real-world data analysis.

This book is about *Stan*, a software that conducts statistical modeling in the framework of Bayesian statistics. We also introduce how to use its R package *CmdStanR* and Python package *CmdStanPy*.

Statistical modeling is a process of fitting mathematical models with probabilistic distributions to the observed data, in order to understand phenomena and to further make predictions. In earlier days, such a method was not considered to be a practical method for the analysis of the real-world data, due to several reasons. For instance, it is not easy to collect a large amount of data and the computational time of the method was very long. In addition, fitting a complex model needs high mathematical skills, because the analytical solution is difficult and implementing its solution is even harder.

Yet nowadays, these are not the problems anymore. Today we can obtain a large amount of data relatively easily, and computers have become powerful and efficient compared to the earlier days. Also luckily, several programming languages that are specifically designed for statistical modeling have been developed. Therefore, statistical modeling has become one of the most efficient approaches for data analysis in the recent studies.

In this book, we use a new programming language, Stan, to conduct statistical modeling. Stan incorporates an excellent algorithm, and importantly, it is under active development by an awesome community. Its R and Python packages (*CmdStanR* and *CmdStanPy*) are released in parallel, which provide an easy starting point for the beginners. In Stan, many models can be written in about 30 lines of code. This

includes not only the basic models such as multivariate regression and logistic regression, but also more advanced modeling such as hierarchical models, state-space models, Gaussian processes, and many others. Moreover, it enables the problem-specific model extensions based on the problem that every user is trying to solve for. We believe that the skillsets and the way of thinking about the real-world problem using Stan in this book will be helpful for every reader, even if the syntax of the Stan changes in the future, or one day another statistical modeling framework comes out and replaces Stan.

Chapter Structure

This book is structured in a way so that by reading from the beginning to the end, readers can obtain a systematical knowledge and skillsets for statistical modeling using Stan. The chapter structure in this book is organized as follows (see Fig. 1).

Roughly, the chapters can be divided into four large sections. Chapters 1 and 2 are the introduction, and we mainly focus on the theoretical background on statistical modeling and Bayesian inference. Chapters 3–5 are the guide of how to use Stan, specifically for the beginners. We introduce how to use Stan itself, as well as `CmdStanR`, and `CmdStanPy` through the example of simple regression analysis such as multiple linear regression and logistic regression. Chapters 6–10 are for more advanced users, and the important components and techniques to master statistical modeling are introduced. Chapters 6, 8, and 10 are the main chapters, which increase your statistical modeling approach repertoire. Chapters 7 and 9 introduce approaches for model improvement. Chapters 11–14 focus on advanced topics, which are applied and discussed quite widely when conducting the real data analysis.

We listed a summary of contents in each chapter: In Chap. 1, we give a brief introduction to statistical modeling and its features, as well as the recommended statistical modeling workflow. In Chap. 2, we concisely summarize the terminologies used in Bayesian inference and MCMC. These terminologies will be necessary to understand the later chapters. In Chap. 3, we introduce how to install Stan and describe its basic syntax. In Chap. 4, we show how to use Stan with its interface `CmdStanR` or `CmdStanPy` through an example of simple linear regression. Specifically, we discuss how to generate an MCMC sample, and obtain Bayesian confidence intervals and Bayesian prediction intervals from the MCMC sample. We also show how to explain

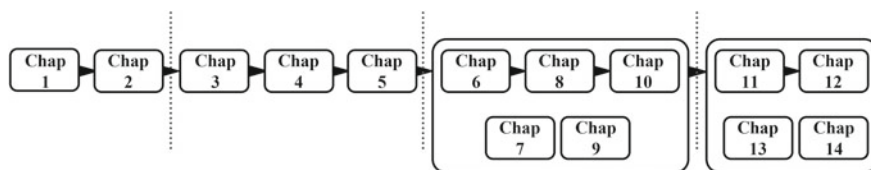


Fig. 1 A flow diagram showing the connections between chapters

the obtained inference results. In Chap. 5, we follow the statistical modeling workflow introduced in Chap. 1. The examples of multiple linear regression, logistic regression, and Poisson regression are also given. We also show examples of how to use plots to check the used models. In Chap. 6, we deviate slightly from the Stan itself and introduce basic probabilistic distributions. We mainly focus on the distributions that are used frequently in analytical practice. In Chap. 7, we summarize some potential issues and troubles when applying regression models to realistic problems. This chapter also includes the introductions on non-linear models, censored data, and data with outliers. In Chap. 8, we introduce hierarchical models (multilevel models). This type of model is used to account for group differences and individual differences. It will be one of the most widely used model types in the future. In Chap. 9, we introduce the troubleshooting approach when the MCMC does not converge, with the focus on setting the weakly informative priors. In Chap. 10, we introduce how to address discrete parameters. The current version of Stan has the limitation that is not able to use the discrete parameters, and we introduce how to solve such issues. In Chap. 11, we use state-space models for time series data. In Chap. 12, we use Markov Random Field models and Gaussian Processes for spatial data. In Chap. 13, we introduce how to efficiently use the MCMC sample from a posterior distribution (or a predictive distribution). In Chap. 14, we discuss some advanced topics, specifically we choose some examples from survival time analysis, matrix factorization, and model selection using information criteria.

Prerequisite Background Knowledge

We do not require the readers to have the previous experience on statistical modeling. However, since building models and checking the models are time-consuming and labor-intensive processes, we hope the readers have the mindset and enthusiasm to enjoy such processes.

To conduct statistical modeling, it requires a wide range of knowledge and skills such as the statistics knowledge (especially probability distributions), skill to imagine the mechanisms of the observed phenomenon and to express them using mathematical formulas as well as programming languages. One of the aims of this book is to extend and improve these types of skillsets. That being said, in this book, we assume that the readers have the following basic knowledge and skillsets already as the requirement.

- The fundamental knowledge of probability and statistics: probability, probability distributions, probability density functions, conditional probability, joint probability, marginal probability, correlation coefficients. The knowledge of statistical tests is not required. The next section introduces each of these terminologies briefly, but it would also be helpful to look up some web resources including Wikipedia for those who are less familiar.
- Programming skills: You should be familiar with either R or Python. Specifically, we require the readers to be able to conduct fundamental data processing and data visualizations.

The Terminologies and Symbols Used in This Book

Sum and Products

Σ represents the summation:

$$\sum_{k=1}^K a_k = a_1 + a_2 + \dots + a_K,$$

and Π represents the product:

$$\prod_{k=1}^K a_k = a_1 \times a_2 \times \dots \times a_K.$$

Probability Distribution

Probability distribution is the expression of how likely a random variable takes each of the possible values. It also can be simply called as distributions. The probability distribution of random variable a is written as $p(a)$.

Probability Mass Function (PMF)

When the random variable is a discrete variable, the probability distribution is called a *probability mass function*.

Probability Density Function (PDF)

When the random variable is a continuous variable, the probability distribution is called a *probability density function*. It is also called a *density*. Note that if the probability density function is denoted as $p(x)$, the value at $p(x)$ (for instance, $p(x = 0)$) is not a probability. Rather, the integral of $p(x)$ is a probability. For instance, the probability that $0 \leq x \leq 0.2$ can be expressed as follows:

$$\int_0^{0.2} p(x) dx$$

Joint Distribution

When there are multiple random variables, a *joint distribution* expresses the probability that how likely each of these random variables takes the possible values for them. It is a type of probability distribution. When there are two random variables a and b , we write their joint distribution as $p(a, b)$, and when we have total of K random variables $\theta_1, \theta_2, \dots, \theta_K$, we write their joint distribution as $p(\theta_1, \theta_2, \dots, \theta_K)$.

Marginalization and Marginal Distribution

Marginalization is the elimination of variables by summing up or integrating a joint distribution with respect to random variables in the joint distribution over their possible values. The probability distribution obtained by marginalization is called a *marginal distribution*. For instance, by summing up the joint probability with respect to a discrete random variable a , we can obtain the marginal distribution $p(b)$ from $p(a, b)$:

$$p(b) = \sum_a p(a, b)$$

Similarly, when a is a continuous random variable, by integrating the joint distribution with respect to a , we can obtain the marginal distribution $p(b)$ from $p(a, b)$:

$$p(b) = \int p(a, b) da$$

Figure 2 shows the relationship between joint distribution and marginal distribution. The example where both a and b are discrete variables is shown in the left table of Fig. 2. The table shows the distribution of the species and sexes of animals in a pet store. The region surrounded by the solid gray line is the joint distribution $p(\text{Animal}, \text{Sex})$. The region surrounded by the dotted gray line on the right side is the marginal distribution $p(\text{Sex})$, which is obtained by summing up the probability with respect to *Animal*. Similarly, the region surrounded by the dashed gray line on the bottom side is the marginal probability $p(\text{Animal})$, which is obtained by summing up the probability with respect to *Sex*. It is called a marginal distribution because we commonly show the summed probability on the margins of a table as shown here. The right plot on Fig. 2 shows when both a and b are continuous variables. The contour lines represent the joint distribution $p(a, b)$. The density plot on the right side of the plot is $p(b)$ which is obtained by integrating $p(a, b)$ with respect to a . The density distribution on the top is $p(a)$, which is obtained by integrating $p(a, b)$ with respect to b .

Conditional Probability Distribution

We consider a joint distribution $p(a, b)$. The distribution of the random variable a , when a value b_0 is given to the random variable b , is called the *conditional probability distribution*, and is written as $p(a|b_0)$. The following equation holds true:

$$p(a|b_0) = \frac{p(a, b_0)}{p(b_0)}$$

Figure 3 shows the conditional probability distribution using the data from Fig. 2. The region surrounded by the solid gray line on the left table on Fig. 3 is the conditional probability distribution $p(a|b_0)$ when the sex $b_0 = \text{Female}$ is given. The density

$b \backslash a$	Cats	Dogs	Birds	Total
Male	0.19	0.23	0.12	0.54
Female	0.22	0.16	0.08	0.46
Total	0.41	0.39	0.20	1.00

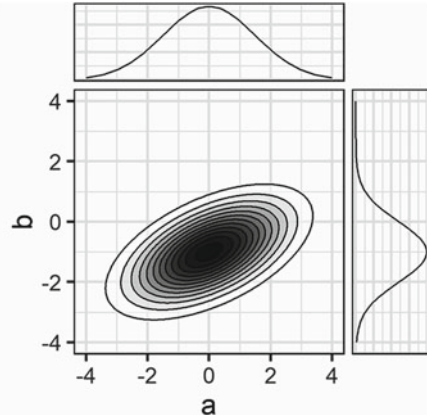


Fig. 2 Examples of joint distribution and marginal distribution

$b \backslash a$	Cats	Dogs	Birds	Total
Male				
Female	$\frac{0.22}{0.46}$	$\frac{0.16}{0.46}$	$\frac{0.08}{0.46}$	$\frac{0.46}{0.46}$

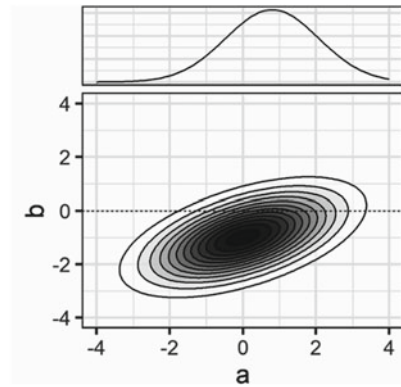


Fig. 3 Examples of conditional probability distribution

function on the top right of Fig. 3 is the conditional probability distribution $p(a|b_0)$ when $b_0 = 0$ is given.

In addition, when the location and the shape of the probability distribution of a random variable y is determined by parameter θ , we write it as $p(y|\theta)$.

Notation of $y \sim p(y)$

The expression of $y \sim p(y)$ represents that the values of a random variable y is generated probabilistically from a probability distribution $p(y)$. In other words, a random variable y follows a probability distribution $p(y)$. For instance, if we write a Poisson distribution with parameter λ as $\text{Poisson}(y|\lambda)$, then $y \sim \text{Poisson}(y|\lambda)$ represents that the values of y is probabilistically generated from $\text{Poisson}(y|\lambda)$, or y follows $\text{Poisson}(y|\lambda)$. We can also write it by omitting y , like $y \sim \text{Poisson}(\lambda)$.

Independence

When we say that two random variables a and b are mutually *independent*, we mean that this equation holds true: $p(a, b) = p(a)p(b)$. Further, from the definition of conditional probability distribution, this is equivalent to $p(a|b) = p(a)$.

Normalization

In this book, we use the term *normalization* to refer multiplying a constant to a function (or dividing by a constant), for the function to satisfy the condition of the probability density function. The constant that is used for normalization is called the normalization constant.

Partial Derivative

Consider a function of two variables $f(\theta_1, \theta_2)$. We consider the derivative by fixing θ_2 as a constant and changing θ_1

$$\lim_{\Delta\theta_1 \rightarrow 0} \frac{f(\theta_1 + \Delta\theta_1, \theta_2) - f(\theta_1, \theta_2)}{\Delta\theta_1}$$

and this is called *partial derivative* of $f(\theta_1, \theta_2)$ with respect to θ_1 . The same would apply for multivariate function $f(\theta_1, \theta_2, \dots, \theta_K)$, and when taking its derivative, we only need to consider all variables as constants, except for θ_1 .

Uppercase Letters

In this book, all the uppercase letters such as Y and *Age* refer to the given data, unless otherwise specified.

Vectors and Matrices

In this book, vectors are denoted with arrows on top of each letter (\vec{x}), whereas matrices are denoted with uppercase letters with bold font (\mathbf{X}). When it is only said to be a vector, its default is a column vector. Sometimes we use transpose sign T with a row vector to express a column vector. The main reason of doing this is simply to save the paper space.

$$\vec{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = (x_1 \ x_2 \ x_3)^T$$

Subscripts and “[]”

There are two types of subscripts. One is to represent the contents of the variable like σ_y (which represents σ , the standard deviation, of y). The other type is to represent the elements in a vector or a matrix. For instance, when we want to specify the k -th element in a vector $\vec{\theta}$, we write it as θ_k . In the latter case, sometimes we use “[]” to represent θ_k as of $\theta[k]$. Similarly, we write $\theta[n, k]$ to represent $\theta_{n,k}$ as well. Additoinally, $\vec{Y}[3]$ represents that the third element of Y is a vector.

Others

In the field of statistical modeling, terms such as mixed models, mixed effect models, fixed effects, and random effects are frequently used. This book also deals with the models that are related to these terms but does not use these. This is because we consider it important to understand model formulas rather than the terms themselves. In addition, since multilevel models and hierarchical models have the same mathematical formula, they are both called hierarchical models in this book.

The Source Code Used in the Book

All the source code and data in each chapter, including the visualization part, are freely available on this book's GitHub repository: https://github.com/MatsuuraKentaro/Bayesian_Statistical_Modeling_with_Stan_R_and_Python.

Also, in some of the chapters, we added some practice examples where the readers can code by themselves and deepen the understanding. The answers to those practical examples are also released on the same GitHub repository. Please use it as a reference. Lastly, in this book, we kept the following formats consistent:

- The set of equations to represent a model (Model Formula X.Y)
- Stan code (`modelX-Y.stan`)
- R and Python code (`run-modelX-Y.R`, `run-modelX-Y.py`)

The computing environment under which this book was written was Windows 11 (64bit), R 4.1.3, Stan 2.29.2, CmdStanR 0.5.0, CmdStanPy 1.0.1.

Tokyo, Japan

Kentaro Matsuura

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Contents

Part I Background of Modeling and Bayesian Inference

1	Overview of Statistical Modeling	3
1.1	What is Statistical Modeling?	3
1.2	Purposes of Statistical Modeling	5
1.3	Preparation for Data Analysis	6
1.3.1	Before Data Collection	6
1.3.2	After Collecting Data	6
1.4	Recommended Statistical Modeling Workflow	7
1.5	Role of Domain Knowledge	9
1.6	How to Represent Model	11
1.7	Model Selection Using Information Criteria	12
	Reference	12
2	Overview of Bayesian Inference	13
2.1	Problems of Traditional Statistics	13
2.2	Likelihood and Maximum Likelihood Estimation (MLE)	14
2.3	Bayesian Inference and MCMC	17
2.4	Bayesian Confidence Interval, Bayesian Predictive Distribution, and Bayesian Prediction Interval	20
2.5	Relationship Between MLE and Bayesian Inference	26
2.6	Selection of Prior Distributions in This Book	27
	References	28

Part II Introduction to Stan

3	Overview of Stan	31
3.1	Probabilistic Programming Language	31
3.2	Why Stan?	32
3.3	Why R and Python?	34

- 3.4 Preparation of Stan, CmdStanR, and CmdStanPy 35
- 3.5 Basic Grammar and Syntax of Stan 36
 - 3.5.1 Block Structure 36
 - 3.5.2 Basic Grammar and Syntax 36
 - 3.5.3 Coding Style Guide 38
- 3.6 lp__ and target in Stan 40
- References 42
- 4 Simple Linear Regression 43**
 - 4.1 Statistical Modeling Workflow Before Parameter Inference 43
 - 4.1.1 Set Up Purposes 44
 - 4.1.2 Check Data Distribution 44
 - 4.1.3 Describe Model Formula 45
 - 4.1.4 Maximum Likelihood Estimation Using R 46
 - 4.1.5 Implement the Model with Stan 47
 - 4.2 Bayesian Inference Using NUTS (MCMC) 49
 - 4.2.1 Estimate Parameters from R or Python 49
 - 4.2.2 Summarize the Estimation Result 51
 - 4.2.3 Save the Estimation Result 52
 - 4.2.4 Adjust the Settings of MCMC 54
 - 4.2.5 Draw the MCMC Sample 57
 - 4.2.6 Joint Posterior Distributions and Marginalized Posterior Distributions 59
 - 4.2.7 Bayesian Confidence Intervals and Bayesian Prediction Intervals 60
 - 4.3 transformed parameters Block and generated quantities Block 61
 - 4.4 Other Inference Methods Besides NUTS 64
 - 4.4.1 Bayesian Inference with ADVI 64
 - 4.4.2 MAP Estimation with L-BFGS 64
 - 4.5 Supplementary Information and Exercises 65
 - 4.5.1 Exercises 66
 - Reference 66
- 5 Basic Regressions and Model Checking 67**
 - 5.1 Multiple Linear Regression 67
 - 5.1.1 Set Up Purposes 68
 - 5.1.2 Check Data Distribution 68
 - 5.1.3 Imagine Data Generating Mechanisms 69
 - 5.1.4 Describe Model Formula 70
 - 5.1.5 Implement the Model 71
 - 5.1.6 Estimate Parameters 72
 - 5.1.7 Interpret Results 74

- 5.2 Check Models 75
 - 5.2.1 Posterior Predictive Check (PPC) 76
 - 5.2.2 Posterior Residual Check (PRC) 77
 - 5.2.3 Scatterplot Matrix of MCMC Sample 78
- 5.3 Binomial Logistic Regression 79
 - 5.3.1 Set Up Purposes 80
 - 5.3.2 Check Data Distribution 80
 - 5.3.3 Imagine Data Generating Mechanisms 80
 - 5.3.4 Describe Model Formula 82
 - 5.3.5 Implement the Model 83
 - 5.3.6 Interpret Results 84
- 5.4 Logistic Regression 85
 - 5.4.1 Set Up Purposes 86
 - 5.4.2 Check Data Distribution 86
 - 5.4.3 Imagine Data Generating Mechanisms 86
 - 5.4.4 Describe Model Formula 87
 - 5.4.5 Implement Models 87
 - 5.4.6 PPC 88
- 5.5 Poisson Regression 89
 - 5.5.1 Imagine Data Generating Mechanisms 90
 - 5.5.2 Describe Model Formula 90
 - 5.5.3 Implement the Model 91
 - 5.5.4 Interpret Results 92
- 5.6 Expression Using Matrix Operation 93
- 5.7 Supplemental Information and Exercises 94
 - 5.7.1 Exercises 95

Part III Essential Technics for Mastering Statistical Modeling

- 6 Introduction of Probability Distributions 99**
 - 6.1 Notations 100
 - 6.2 Uniform Distribution 101
 - 6.3 Bernoulli Distribution 102
 - 6.4 Binomial Distribution 103
 - 6.5 Beta Distribution 104
 - 6.6 Categorical Distribution 106
 - 6.7 Multinomial Distribution 108
 - 6.8 Dirichlet Distribution 109
 - 6.9 Exponential Distribution 111
 - 6.10 Poisson Distribution 112
 - 6.11 Gamma Distribution 114
 - 6.12 Normal Distribution 116
 - 6.13 Lognormal Distribution 118
 - 6.14 Multivariate Normal Distribution 119
 - 6.15 Cauchy Distribution 123

- 6.16 Student-t Distribution 125
- 6.17 Double Exponential Distribution (Laplace Distribution) 126
- 6.18 Exercise 128
- References 128
- 7 Issues of Regression 129**
 - 7.1 Log Transformation 129
 - 7.2 Nonlinear Model 133
 - 7.2.1 Exponential Function 134
 - 7.2.2 Emax Function 137
 - 7.2.3 Sigmoid Emax Function 137
 - 7.2.4 Other Functions 139
 - 7.3 Interaction 141
 - 7.4 Multicollinearity 142
 - 7.5 Model Misspecification 143
 - 7.6 Variable Selection 145
 - 7.7 Censoring 146
 - 7.8 Outlier 148
 - References 150
- 8 Hierarchical Model 151**
 - 8.1 Introduction of Hierarchical Models 152
 - 8.1.1 Set Up Purposes and Check Data Distribution 152
 - 8.1.2 Without Considering Group Difference 153
 - 8.1.3 Groups Have Varying Intercepts and Slopes 154
 - 8.1.4 Hierarchical Model 156
 - 8.1.5 Model Comparison 161
 - 8.1.6 Equivalent Representation of Hierarchical Models 163
 - 8.2 Hierarchical Model with Multiple Layers 164
 - 8.2.1 Set Up Purposes and Check Data Distribution 165
 - 8.2.2 Imagine Data Generating Mechanisms and Describe Model Formula 167
 - 8.2.3 Implement the Model 168
 - 8.3 Hierarchical Model for Nonlinear Model 169
 - 8.3.1 Set Up Purposes and Check Data Distribution 169
 - 8.3.2 Imagine Data Generating Mechanisms and Describe Model Formula 170
 - 8.3.3 Implement Models 171
 - 8.3.4 Interpret Results 172
 - 8.4 Missing Data 173
 - 8.5 Hierarchical Model for Logistic Regression Model 177
 - 8.5.1 Set Up Purposes 177
 - 8.5.2 Imagine Data Generating Mechanisms 178
 - 8.5.3 Describe Model Formula 178

- 8.5.4 Implement Models 179
- 8.5.5 Interpreting Results 180
- 8.6 Exercises 180
- References 181
- 9 How to Improve MCMC Convergence 183**
 - 9.1 Removing Nonidentifiable Parameters 183
 - 9.1.1 Parameter Identifiability 184
 - 9.1.2 Individual Difference 185
 - 9.1.3 Label Switching 185
 - 9.1.4 Multinomial Logistic Regression 187
 - 9.1.5 The Tortoise and the Hare 189
 - 9.2 Use Weakly-Informative Priors to Restrict the Posterior Distributions 192
 - 9.2.1 Weakly Informative Prior for Parameters in $(-\infty, \infty)$ 193
 - 9.2.2 Weakly Informative Prior for Parameters with Positive Values 194
 - 9.2.3 Weakly Informative Prior for Parameters in Range $[0, 1]$ 200
 - 9.2.4 Weakly Informative Prior for Covariance Matrix 200
 - 9.3 Loosen Posterior Distribution by Reparameterization 206
 - 9.3.1 Neal’s Funnel 207
 - 9.3.2 Reparameterization of Hierarchical Models 209
 - 9.3.3 Reparameterization of Multivariate Normal Distribution 210
 - 9.4 Other Cases 211
 - 9.5 Supplementary Information 211
 - References 212
- 10 Discrete Parameters 213**
 - 10.1 Techniques to Handle Discrete Parameters 213
 - 10.1.1 `log_sum_exp` Function 214
 - 10.1.2 Marginalizing Out Discrete Parameters 214
 - 10.1.3 Using Mathematical Relationships 220
 - 10.2 Mixture of Normal Distributions 221
 - 10.3 Zero-Inflated Distribution 227
 - 10.3.1 Set Up Purposes and Check Data Distribution 228
 - 10.3.2 Imagine Data Generating Mechanisms 228
 - 10.3.3 Describe Model Formula 230
 - 10.3.4 Implement Models 230
 - 10.3.5 Interpret Results 232
 - 10.4 Supplementary Information and Exercises 232
 - 10.4.1 Exercises 233
 - Reference 233

Part IV Advanced Topics for Real-World Data Analysis

11 Time Series Data Analysis with State Space Model 237

11.1 Introduction to Space State Models 237

11.1.1 Set Up Purposes 239

11.1.2 Check Data Distribution 239

11.1.3 Imagine the Mechanisms of Data Generation
Process 240

11.1.4 Describe Model Formula 241

11.1.5 Implement the Model 242

11.1.6 Interpret the Results 243

11.2 Extending System Model 244

11.2.1 Trend Component 244

11.2.2 Regression Component 246

11.2.3 Seasonal Component 247

11.2.4 Switch Component 252

11.2.5 Pulse Component 255

11.2.6 Stationary AR Component 258

11.2.7 Reparameterization of Component 259

11.3 Extending the Observation Model 261

11.3.1 Outliers 261

11.3.2 Binary Values 262

11.3.3 Count Data 262

11.3.4 Vector 263

11.4 State Space Model with Missing Data 263

11.4.1 Observations at Certain Time Points are Missing 263

11.4.2 Time Intervals are not the Same (Unequal
Intervals) 263

11.4.3 Vector 264

11.5 (Example 1) Difference Between Two Time Series 264

11.6 (Example 2) Changes in Body Weight and Body Fat 267

11.7 (Example 3) The Transition of Tennis Players’ Capabilities 269

11.8 (Example 4) Decomposition of Sales Data 274

11.9 Supplementary Materials and Exercises 283

11.9.1 Exercises 284

References 284

**12 Spatial Data Analysis Using Gaussian Markov Random Fields
and Gaussian Processes** 285

12.1 Equivalence Between State Space Model
and One-Dimensional GMRF 286

12.1.1 Posterior Probability of the State Space Model 286

12.1.2 The Equivalence Between the Temporal
and Spatial Structures 287

- 12.2 (Example 1) Data on One-Dimensional Location 289
- 12.3 (Example 2) Fix the “Age Heaping” 291
- 12.4 Two-Dimensional GMRF 296
- 12.5 (Example 3) Geospatial Data on the Map 300
- 12.6 (Example 4) Data on Two-Dimensional Grid 302
- 12.7 Introduction to GP 307
 - 12.7.1 Implementation of GP (1) 310
 - 12.7.2 Implementation of GP (2) 313
 - 12.7.3 Prediction with GP 314
 - 12.7.4 Other Kernel Functions 319
- 12.8 (Example 5) Data on One-Dimensional Location 320
- 12.9 (Example 6) Data on Two-Dimensional Grid 321
- 12.10 Inducing Variable Method 324
- 12.11 Supplementary Information and Exercises 327
 - 12.11.1 Exercises 328
- References 328
- 13 Usages of MCMC Samples from Posterior and Predictive Distributions** 331
 - 13.1 Simulation Based Sample Size Calculation 331
 - 13.2 Bayesian Decision Theory 335
 - 13.3 Thompson Sampling and Bayesian Optimization 338
 - 13.3.1 Thompson Sampling 338
 - 13.3.2 Bayesian Optimization 341
- References 344
- 14 Other Advanced Topics** 345
 - 14.1 Survival Analysis 345
 - 14.2 Matrix Decomposition and Dimensionality Reduction 352
 - 14.2.1 Matrix Decomposition 352
 - 14.2.2 Dimensionality Reduction 359
 - 14.3 Model Selection Based on Information Criteria 367
 - 14.3.1 Introduction of Generalization Error and WAIC 367
 - 14.3.2 Simulation Study to Evaluate Information Criteria 370
 - 14.3.3 WAIC in a Hierarchical Model 375
 - 14.4 Supplementary Information and Exercises 382
 - 14.4.1 Exercises 383
- References 383
- Appendix: Differences from BUGS Language** 385