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Estimate the True Pass Probability for Near-Real-Time Monitor Challenge Data Using Bayesian Analysis

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Under the Direction of Yu-Sheng Hsu

ABSTRACT

The U.S. Army's Chemical Demilitarization are designed to store, treat and destroy the nation's aging chemical weapons. It operates Near-Real-Time Monitors and Deport Area Monitoring Systems to detect chemical agent at concentrations before they become dangerous to workers, public health and the environment. CDC recommends that the sampling and analytical methods measure within ±25% of the true concentration 95% of the time, and if this criterion is not met the alarm set point or reportable level should be adjusted. Two methods were provided by Army's Programmatic Laboratory and Monitoring Quality Assurance Plan to evaluate the monitoring systems based on CDC recommendations. This thesis addresses the potential problems associated with these two methods and proposes the Bayesian method in an effort to improve the assessment. Comparison of simulation results indicates that Bayesian method produces a relatively better estimate for verifying monitoring system performance as long as the prior given is correct.

INDEX WORDS: Bayesian Analysis, Quality Plan Challenge Data, Pass Rate

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List of Abbreviations

ACAMS	Automatic Continuous Air Monitoring System
ASC	Allowable Stack Concentration
CDC	Centers for Disease Control and Prevention
CDF	Chemical Demilitarization Facility
CDP	Chemical Demilitarization Program
CMA	Chemical Material Agency
CWC	Chemical Weapons Convention
DAAMS	Depot Area Monitoring System
DHHS	Department of Health and Human Services
ECL	Engineering Control Level/Emissions Control Level
EPA	Environmental Protection Agency
GB	Isopropyl Methylfluorophosphate
GSUDG	Georgia State University's Demilitarization Group
LMQAP	Laboratory and Monitoring Quality Assurance Plan
NTR	Near-Real-Time Monitor
QP	Quality Plant Samples
SARM	Standard Analytical Reference Material
SBCCOM	Soldier Biological and Chemical Command
STL/STEL	Short-term Exposure Limit

Chapter One: Background Introduction

In 1997, the United States along with 65 other countries signed the Chemical Weapons Convention (CWC) treaty, which prohibits the development, production, stockpiling and use of chemical weapons. Additionally, the stockpiles of chemical weapons are aging and, in some cases, leaking their chemical agent contents. The United States ratified the treaty in April 1997. According to the terms outlined, it provides the United States until April 2007 to destroy its declared stockpile of chemical weapons. And a one-time, five-year extension is allowed.

The U.S. Army has the responsibility to store, treat and dispose of chemical weapons safely and effectively. Originally the task was operated separately under the Army's Chemical Demilitarization Program (CDP) and the Soldier Biological and Chemical Command (SBCCOM). In year 2003, the U.S. Army created a new organization, the Chemical Materials Agency (CMA), which incorporates the CDP and portions of the SBCCOM to streamlines the operations and to allow for greater integration of these programs. The new agency, CMA, combines the demilitarization and storage functions under a single director and is responsible for safe storage and destruction the nation's aging chemical weapons, effective recovering of the nation's chemical warfare materiel and enhancing national security. It develops and uses technologies to safely store and eliminate chemical weapons while protecting the public, its workers and the environment.

CMA's Chemical Demilitarization Facilities (CDF) are designed to destroy the chemical agent in these munitions while minimizing risk to workers, the general public and

the environment. One type of demilitarization disposal facility uses high-temperature incineration technology to destroy weapons, a technology employed by the Army for more than a decade to safely and successfully dispose of more than a quarter of the nation's original chemical weapons. Multiple safety features are designed into the process, along with automated backup systems for each feature, to prevent agent or hazardous material release. In addition CDF Laboratories operate Near-Real-Time monitors (NRT), i.e. Automatic Continuous Air Monitoring System (ACAMS) or MINICAMS, to detect chemical agent at certain concentrations before they become dangerous to public health and the environment, and to provide real-time warning to the workers if these levels are approached or exceeded, so that evacuation and masking is accomplished. Depot Area Monitoring Systems (DAAMS) are also operated by the CDF Laboratories as chemical agent detection and confirmation systems.

NRT monitors are used for the detection of airborne concentrations of agents during disposal operations at CDF. NRT systems consist of an automatic gas chromatograph equipped with a detector, analytical column, and a pre-concentration tube. The system samples the environment every 3 to 15 minutes and provides a response to chemical agents. DAAMS consists of a field sampling tube filled with sorbent, a transfer tube filled with sorbent and a gas chromatograph equipped with a flame photometric or a mass selective detector. The DAAMS field tubes are either collocated with a NRT unit or used independently. When it is collocated with a NRT unit at a sampling station and an alarm occurs, the DAAMS tubes are retrieved and used to confirm or refute the presence of chemical agents by analyzing on a gas chromatograph. When only DAAMS tubes are located at a sampling station, the first tube is used to detect the presence of agent and a second tube

that is collocated is used to confirm or refute the presence of chemical agent by analyzing on a gas chromatograph configured with a dissimilar analytical column type and/or a different detector.

The Army's disposal activities are operated under congressional direction. Federal agencies and the independent National Academy of Sciences' National Research Council, together with equivalent agencies at the state and local level, are also involved in regulation of the type of oversight conducted by associated agencies, like Department of Defense, U.S. Environmental Protection Agency (EPA), Department of Health and Human Services (DHHS), Centers for Disease Control and Prevention (CDC), Congress, General Accounting Office and National Research Council.

The CMA's Programmatic Laboratory and Monitoring Quality Assurance Plan (LMQAP) has been developed to provide specific guidance to address requirements from the Department of the Army, environmental regulatory agencies, and DHHS. The CDC Public Health Service has responsibility to oversee the Demilitarization Program and make recommendations for protecting human health and safety. CDC recommendation "assumes that the sampling and analytical methods are measuring within ±25% of the true concentration 95% of the time. If this criterion is not met, an alarm level or action level below the exposure limit may be required." CDC also requires that a 95% confidence must be maintained at all conditions.

The CMA Programmatic LMQAP is required to be implemented at all CMA's CDF laboratories and monitoring teams to produce acceptable quality of monitoring and laboratory data. To ensure proper system operation and generation of technically defensible data, a precision and accuracy study is conducted through the use of quality plant (QP)

samples. QP sample is a sample media that has been spiked with a solution of dilute chemical standard analytical reference material (SARM) prior to being placed in the field or following aspiration of the blank tube in the field. The sample is spiked and then carried out to the sample collection point and exposed to the sample collection point atmosphere. The QP found concentration is recorded along with the exact amount of SARM. Information from the study is used to determine whether or not the method may reliably detect agent prior to its implementation in the field.

QP data were collected at CMA's Demilitarization sites. The system operations are verified through QP challenges at least daily and evaluated on a 28-day period. When NRT systems are being verified, they are injected with a known concentration of agent. All challenges are injected at the distal end of the sample line or directly into the instrument. For DAAMS methods, DAAMS tubes are either spiked with known concentrations of agent and placed in the field or spiked with a known concentration of agent after aspirating in the field. Those QP data are then evaluated by system, method, agent and/or station to determine whether certain agent may be detected with a 95% confidence at a specific alarm set point or reportable level.

Georgia State University's Demilitarization Group (GSUDG) is subcontracted with the Shaw Environment, Inc. Our team in Georgia State University Department of Mathematics and Statistics was given the task of assessing and verifying the statistical approach as defined by the LMQAP and currently used by CMA's CDF Laboratories.

In this thesis, the focus is on the evaluations of NRT systems and studies on several cases of NRT systems are presented. Two statistical approaches that are defined in LMQAP for evaluation of the system are introduced. A theoretically sound approach, Bayesian

method, is proposed and compared with the other two approaches in an effort to improve our assessment. Conclusions are drawn through Simulation studies. This thesis is organized in the following order. In Chapter 2, the two methods that are defined in the LMQAP and currently used by CMA's CDF are first introduced followed by the introduction of the concept and methodologies for Bayesian approach. In Chapter 3, the computational method for Bayesian estimation and construction of confidence intervals are detailed. Examples using CDF's ACAMS QP challenge data are illustrated in Chapter 4. In Chapter 5, simulation studies are conducted and results from different approaches are compared. Conclusion from the studies is presented in the last Chapter.

Chapter Two: Methodologies

To verify whether the monitoring systems are operated within CDC's criteria and to ensure that technical defensible data are generated, continuous baseline study is conducted for both NRT systems and DAAMS systems. In this chapter, data obtained from NRT systems are analyzed. The statistical evaluation of NRT system is divided into two main categories-- i.e. ASC (Allowable Stack Concentration) ACAMS station and non-ASC ACAMS station. These categories are further subdivided and evaluated by agent, station and monitoring level.

QP data are collected at least daily and evaluated every 28 days at each site to assess the system performance. The LMQAP requires that the performance of NRT QP challenges follow the following guidance-- Perform first challenge and if it meets the acceptance criteria, it is recorded as P_1. If the first challenge fails, F_1 is recorded and second challenge is performed. If the second challenge passed the acceptance criteria, it is recorded as P_2. Otherwise it is recorded as F_2 and corrective actions, like recalibration, changing pad etc., are performed until a passing QP is observed. Along with the pass/fail challenge, target concentration, found concentration, percentage recovery, instrument ID number, station location, ID number of the operator, date, time, corrective action performed etc., are also recorded.

Two statistical approaches (i.e., pass rate and normal) have been defined in LMQAP to verify whether CDC's requirements of ±25% of the true concentration 95% of the time are being met, or whether the system can meet CDC's requirements of maintaining a 95% confidence at a lower alarm set point.

2.1 Pass Rate Approach

Three types of pass rates are defined in LMQAP. However only the first-challenge pass rate is used to assess the "true" unit or system performance. The second-challenge pass rate is used to determine the performance after failure. The either-challenge pass rate is used to determine the performance in highly agent contaminated areas. A challenge passes if the concentration is ±25% of the true concentration.

The first-challenge pass rate (PR_1) is the percent of challenges that pass on the first attempt for each day or challenge cycle or event.

$$PR_1 = \frac{P_1}{P_1 + F_1}(100) \tag{2.1}$$

where

P_1 = number of challenges that passed on the first challenge

F_1 = number of challenges that failed on the first challenge

The second-challenge pass rate (PR_2) is the percent of challenges that pass on the second-challenge attempt for each day.

$$PR_2 = \frac{P_2}{P_2 + F_2}(100) \tag{2.2}$$

where

P_2 = number of challenges that passed on the second challenge

F_2 = number of challenges that failed on the second challenge

The either-challenge pass rate (PR_T) is the total percent of challenges that pass. It combines the first- and second-challenge passes and divides it by the total number of challenge events.

$$PR_T = \frac{P_1 + P_2}{P_1 + P_2 + F_2}(100) \tag{2.3}$$

where

P_1 = number of challenges that passed on the first challenge

F_2 = number of challenges that failed on the second challenge

P_2 = number of challenges that passed on the second challenge

Note, F_1 is not included in the denominator. This is because the pass rates are based on events and not the number of challenges. Events consist of two challenges. Therefore, the total number of events in this case is defined as the sum of first pass challenge and total second challenge, which is $P_1 + P_2 + F_2$.

2.2 Normal Approach

This approach assumes normal distribution for the challenge data grouped by method, agent and station.

The statistical response rate at the alarm level (SRR_{AL}) is the probability that a first challenge to the NRT monitor will generate a response greater than or equal to the alarm level.

$$SRR_{AL} = P(Y \geq AL) = P(Z \geq \frac{AL - \overline{X}}{SD}) \tag{2.4}$$

where

AL = alarm level

$\overline{X}$ = average response to the first QP challenges

SD = standard deviation of the response to the first QP challenges

These two approaches—pass rate and response rate, are currently used by CDF laboratories to evaluate the performance of NRT monitoring systems. However the reliability of these two approaches depends on the actual conditions. For example, pass rate is not reliable in case of small sample size; while response rate will not be valid when normality assumption is violated. Since QP data are collected daily and evaluated on a 28-day base, most of the ACAMS stations have only 28 observations for evaluation period. Thus pass rate may not be a reliable measurement for system evaluation purpose. And carefully examination of the ACAMS QP data revealed that most of the ACAMS station's QP first challenge response, i.e. found concentration, do not follow a normal distribution. Some are heavy tailed and some are slightly skewed. Furthermore, none of the above measurements take into account the relations among stations and sites.

Here, Bayesian method is proposed for modeling the probability that a ACAMS station will generate a response greater than or equal to the alarm level. In other words, the pass rate for each station is assumed to be a random variable from a certain prior distribution. The exchangeability of NRT which are configured the same (i.e., same column types and detectors) is also assumed. In this way, certain dependency among stations is considered. This is certainly a reasonable assumption because all monitors of the same kind were produced from either the same assembly line or using the same manufacture procedures.

2.3 Bayesian Method

Many statistical applications involve multiple parameters that are often related or connected in some way by the structures of the problem. A joint probability model for these parameters indicates the dependence among them. For this instance, the study object is the

response x_{ij} from station j having probability θ_j to be within a certain range. It is reasonable to expect that θ_j's of all stations are from a certain unknown prior distribution.

A key feature of such applications is that the observed data x_{ij} with each observations indexed by i, within groups indexed by j, j=1,…, J, can be used to estimate aspects of the distribution of the θ_js even though the values of θ_js are not themselves observed. It is natural to model such a problem with observable outcomes modeled conditionally on certain parameters, which themselves are given a probabilistic specification in terms of further parameters of some hyperprior distribution. The advantage of using this model is to use a prior distribution to structure some dependency into the parameters.

Considering the problem of estimating θ_j-- the probability of a response to be within the assigned range for station j, observed found concentration x_{ij} and a prior distribution constructed from stations in the same analytical group are used for the estimation. θ_js shall be treated as random samples from a common population. Since in the same analytical group, there is no ordering or special characteristic available to distinguish any of the station from any of the others, the exchangeability among θ_js is assumed in their prior distribution. That is $p(\theta_1,\ldots, \theta_J)$ is invariant to permutations of the indexes (1,…, J) and parameters $(\theta_1,\ldots, \theta_J)$ are exchangeable in their joint distribution. Using a simple exchangeable model for θ_js, which treat each θ_j as an independent sample from a prior distribution governed by some unknown parameter vector, the conditional probability of θ under ϕ is:

$$p(\theta \mid \phi) = \prod_{j=1}^{J} p(\theta_j \mid \phi) \tag{2.5}$$

Since ϕ is unknown, it has its own prior distribution, $p(\phi)$. The joint prior distribution is:

$$p(\phi, \theta) = p(\phi)p(\theta \mid \phi) \tag{2.6}$$

, and the appropriate Bayesian joint posterior distribution is:

$$p(\phi,\theta \mid y) \propto p(\phi,\theta)p(y \mid \phi,\theta) \Rightarrow$$

$$p(\phi,\theta \mid y) \propto p(\phi,\theta)p(y \mid \theta) \text{, substitute in (2.6)} \Rightarrow$$

$$p(\phi,\theta \mid y) \propto p(\phi)p(\theta \mid \phi)p(y \mid \theta) \tag{2.7}$$

Where y denotes the number of passes for each station. p(y| ϕ, θ) is simplified by p(y| θ) since data distribution p(y| ϕ, θ) depends only on θ and ϕ affect y only through θ.

ϕ is estimated by obtaining its marginal posterior distribution, p(ϕ|y). For many standard models, this marginal posterior distribution can be computed algebraically using the conditional probability formula,

$$p(\phi \mid y) = \frac{p(\phi,\theta \mid y)}{p(\theta \mid \phi, y)} \tag{2.8}$$

For this study, y_j, the number of passes for station j, is assumed to follow independent binomial distribution, denoted by $y_j \sim \text{Bin}(n_j, \theta_j)$, where n_j is the sample size for station j, j=1, 2, …, J. And parameters θ_js are assumed to be independent samples from a beta distribution, denoted by $\theta_j \sim \text{Beta}(\alpha, \beta)$. Beta distribution is chosen for θ_js because Beta distribution has a bell-shaped probability density and takes values only on the interval 0 to 1, which are probability values. Now the analytic form of the joint posterior distribution, p(α, β, θ| y), can be determined by substituting appropriate joint density functions into the formula (2.7). It is not hard to see the resulting posterior distribution is:

$$p(\alpha,\beta,\theta \mid y) \propto p(\alpha,\beta)p(\theta \mid \alpha,\beta)p(y \mid \theta) \Rightarrow$$

$$p(\alpha,\beta,\theta \mid y) \propto p(\alpha,\beta)\prod_{j=1}^{J}\frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}\theta_j^{\alpha-1}(1-\theta_j)^{\beta-1}\prod_{j=1}^{J}\theta_j^{y_j}(1-\theta_j)^{n_j-y_j} \tag{2.9}$$

Next, to obtain the marginal posterior density of (α, β), first the conditional joint density, p(θ| α, β, y), need to be find out. Since given (α, β), θ_js have independent posterior density and follow beta distribution, the joint density for θ_js is:

$$p(\theta \mid \alpha, \beta, y) = \prod_{j=1}^{J} \frac{\Gamma(\alpha + \beta + n_j)}{\Gamma(\alpha + y_j)\Gamma(\beta + n_j - y_j)} \theta_j^{\alpha + y_j - 1} (1 - \theta_j)^{\beta + n_j - y_j - 1} \tag{2.10}$$

Then the marginal posterior distribution of (α, β) can be determined by substituting (2.9), (2.10) into the conditional probability formula (2.8), and the result is:

$$p(\alpha, \beta \mid y) \propto p(\alpha, \beta) \prod_{j=1}^{J} \frac{\Gamma(\alpha + \beta)\Gamma(\alpha + y_j)\Gamma(\beta + n_j - y_j)}{\Gamma(\alpha)\Gamma(\beta)\Gamma(\alpha + \beta + n_j)} \tag{2.11}$$

Now a hyperprior distribution must be assigned to (α, β). Since little is known about (α, β), one would seek a relatively diffuse hyperprior distribution for (α, β). It would seem reasonable to assign independent hyperprior distribution to the prior mean and 'sample size'. (α, β) is reparameterized in terms of $\log it(\frac{\alpha}{\alpha + \beta}) = \log(\frac{\alpha}{\beta})$ and log(α + β), which are the logit of the mean and logarithm of the 'sample size' in the beta distribution for θ_js. Logistic and logarithm transformation are used to put each on a (-∞, ∞) scale. Since a uniform prior density on these transformed parameters yields an improper posterior density, a diffuse hyperprior density of uniform on $(\frac{\alpha}{\alpha + \beta}, (\alpha + \beta)^{-1/2})$ is chosen. The appropriate Jacobians are computed to obtain the density p(α, β) and p[log(α/ β), log(α+β)]. Steps are shown below:

Let $\alpha_0 = \frac{\alpha}{\alpha + \beta}$ and $\beta_0 = (\alpha + \beta)^{-1/2}$, then

$$|J(\alpha,\beta)| = \begin{vmatrix} \frac{\partial \alpha_0}{\partial \alpha} & \frac{\partial \beta_0}{\partial \alpha} \\ \frac{\partial \alpha_0}{\partial \beta} & \frac{\partial \beta_0}{\partial \beta} \end{vmatrix} = \begin{vmatrix} \frac{\beta}{(\alpha+\beta)^2} & -\frac{1}{2}(\alpha+\beta)^{-2/3} \\ \frac{-\alpha}{(\alpha+\beta)^2} & -\frac{1}{2}(\alpha+\beta)^{-2/3} \end{vmatrix} = -\frac{1}{2}(\alpha+\beta)^{-5/2}$$

and $\quad p(\alpha,\beta) = p(\alpha_0,\beta_0)|J(\alpha,\beta)| \Rightarrow$

$$p(\alpha,\beta) \propto (\alpha+\beta)^{-5/2} \tag{2.12}$$

Let $\alpha_1 = \log\frac{\alpha}{\beta}$ and $\beta_1 = \log(\alpha+\beta)$, then

$$\begin{cases} \frac{\alpha}{\beta} = e^{\alpha_1} \\ \alpha+\beta = e^{\beta_1} \end{cases} \Rightarrow \begin{cases} \frac{\alpha}{\alpha+\beta} = \frac{e^{\alpha_1}}{1+e^{\alpha_1}} \\ (\alpha+\beta)^{-1/2} = e^{-\frac{1}{2}\beta_1} \end{cases} \Rightarrow \begin{cases} \alpha_0 = \frac{e^{\alpha_1}}{1+e^{\alpha_1}} \\ \beta_0 = e^{-\frac{1}{2}\beta_1} \end{cases} \quad \text{then}$$

$$|J(\alpha_1,\beta_1)| = \begin{vmatrix} \frac{\partial \alpha_0}{\partial \alpha_1} & \frac{\partial \beta_0}{\partial \alpha_1} \\ \frac{\partial \alpha_0}{\partial \beta_1} & \frac{\partial \beta_0}{\partial \beta_1} \end{vmatrix} = \begin{vmatrix} \frac{e^{\alpha_1}}{(1+e^{\alpha_1})^2} & 0 \\ 0 & -\frac{1}{2}e^{-\frac{1}{2}\beta_1} \end{vmatrix} = -\frac{e^{\alpha_1}e^{-\frac{1}{2}\beta_1}}{2(1+e^{\alpha_1})^2} = -\frac{1}{2}\alpha\beta(\alpha+\beta)^{-5/2}$$

and $\quad p[\log\frac{\alpha}{\beta}, \log(\alpha+\beta)] = p(\alpha_0,\beta_0)|J(\alpha_1,\beta_1)| \Rightarrow$

$$p[\log\frac{\alpha}{\beta}, \log(\alpha+\beta)] \propto \alpha\beta(\alpha+\beta)^{-5/2} \tag{2.13}$$

By now the full probability model for data and parameters has been established, the marginal posterior distribution of the hyperparameters, p(α, β| y), can be calculated easily for any specified value of (α, β). The Bayesian estimate for (α, β) and θ_js can then be obtained and confidence interval for estimate of θ_js can be computed through simulation process.

Chapter Three: Computational Method

Since simple algebraic expression of the Bayesian estimate seems to be unobtainable, the actual calculation of the Bayesian estimate for (α, β) is obtained by computation on grid. To set up the grid, the first step is to choose the center of the grid. The mean and standard deviation of the population distribution are set to the sample mean and standard deviation and (α, β) is solved using simple algebra (see appendix A). This is a crude point estimate of (α, β) and denotes by $(\hat{\alpha}, \hat{\beta})$. To get the grid center, it is transformed to $[\log(\hat{\alpha} / \hat{\beta}), \log(\hat{\alpha} + \hat{\beta})]$. And the effective range of the grid is obtained by plus/minus certain factors to this grid center. In the second step, the marginal posterior densities of the hyperparameters, p(α, β| y), for each point on the grid are computed using function (2.11) with prior density (2.12). Multiplied them by the appropriate Jacobian, the log densities p[log(α/β), log(α + β)|y] are obtained. These are the relative posterior densities. They are finally normalized by approximating the distribution as a step function over the grid and setting the total probability to 1. Then the posterior moments can be computed using the following formula,

E(α| y) is estimated by $$\tilde{\alpha} = \sum_{\log(\frac{\alpha}{\beta}),\log(\alpha+\beta)} \alpha . p\left(\log(\frac{\alpha}{\beta}), \log(\alpha+\beta) \middle| y \right) \quad (3.1)$$

E(β| y) is estimated by $$\tilde{\beta} = \sum_{\log(\frac{\alpha}{\beta}),\log(\alpha+\beta)} \beta . p\left(\log(\frac{\alpha}{\beta}), \log(\alpha+\beta) \middle| y \right) \quad (3.2)$$

Since for each j = 1,…, J, θ_j| α, β, y follow Beta(α + y_j, β + n_j - y_j), then

E(θ_j|α, β, y) is estimated by $$\tilde{\theta}_j = \frac{\tilde{\alpha} + y_j}{\tilde{\alpha} + \tilde{\beta} + n_j} \quad (3.3)$$

Now, the Bayesian estimates for (α, β) and θ_js are obtained, the confidence intervals for $\tilde{\theta}_j$ s can be computed through simulation.

First, find the marginal posterior distribution of log(α/β) using,

$$p[\log(\alpha/\beta) \mid y] = \sum p[\log(\alpha/\beta), \log(\alpha+\beta) \mid y] \tag{3.4}$$

where sum is over values of log(α+β). Using this marginal posterior distribution, a conditional cumulative distribution of log(α/β) given by y can be obtained. With this cumulative distribution and using the inverse distribution function technique, random samples from this conditional distribution of log(α/β) can be drawn.

Secondly, obtain the conditional distribution of log(α+β) given log(α/β) by,

$$p[\log(\alpha+\beta) \mid \log(\alpha/\beta), y] = \frac{p[\log(\alpha/\beta), \log(\alpha+\beta) \mid y]}{p[\log(\alpha/\beta) \mid y]} \tag{3.5}$$

Again the conditional cumulative distribution can be found. The inverse distribution function technique is applied with already sampled log(α/β). Therefore pairs of draws of [log(α/β), log(α+β)] are obtained from their marginal posterior distribution and then can be transformed to (α, β).

Finally, for each j = 1, …, J, sample θ_j from its conditional posterior distribution, $p(\theta_j|$ α, β, y), by drawing random samples from Beta($\alpha + y_j$, $\beta + n_j - y_j$) using a standard random sample generating procedure for Beta distribution.

Repeat this procedure to generate k random samples of (α, β) and θ_js, and compute the 100α th and 100(1- α)th percentile to obtain 100(1-2 α) percent confidence intervals for θjs. An example from this study is provided in the next chapter to illustrate the idea.

Chapter Four: A Study of ACAMS Challenge Data

To ensure proper system operation, QP data were generated at CMA's CDF on a daily bases. It is reported and evaluated every 28 days. The data of 3 time periods—from May 3, 2005 to July 25, 2005, was recorded for analysis. The data consist of both ACAMS stations and DAAMS stations. ACAMS stations are further divided into GB-ASC, GB-STEL and GB-ECL stations. There are 6, 86 and 4 stations for each type of the ACAMS stations. Alarm level ±25% is chosen for this analysis. It is corresponding to CDC's recommendation of "measurement within ±25% of the true concentration 95% of the time".

Although many analyses have been done to this project, in this thesis the focus is on the Bayesian analysis for GB-STEL stations. The analysis is done for each of the stations for three 28-day time periods and for the whole time period.

4.1 Compute Bayesian Estimates of (α, β) and θjs

First, stations were grouped into four groups according to their time period. Then, the first-challenge pass rate (PR_1), the proportion of first pass, were calculated at ±25% alarm level for each station in each group (see Table 4.2-4.5). y_j denotes the total number of first pass for station j at alarm level, where j = 1, …, J, and J is the total number of stations in analytical group. n_j denotes the total number of first challenges for the j^{th} station. Then pass rate is $PR_{1j} = \frac{y_j}{n_j}$ for the j^{th} station.

θ_j, the pass probability of the j^{th} station, varies from station to station because of differences in each individual monitor and operation conditions among systems. Beta

distribution with parameters α, β, denoted by Beta(α, β), were chosen as the prior distribution for θ, and its mean and variance are $\mu = \frac{\alpha}{\alpha+\beta}$ and $\sigma^2 = \frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}$. Next, the estimates $(\hat{\alpha}, \hat{\beta})$ were obtained using method of moments, i.e. equating sample mean and variance of PR_{1j}s with $\frac{\alpha}{\alpha+\beta}$ and $\frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}$, respectively, and solving for α and β. The solutions yield the point estimates of (α, β) for each group (see Table 4.1). Independent hyperprior distributions were assigned to the prior mean and 'sample size', i.e. $\frac{\alpha}{\alpha+\beta}$ and $\alpha+\beta$, and they were transformed to $\log it(\frac{\alpha}{\alpha+\beta}) = \log(\frac{\alpha}{\beta})$ and log(α+β). Using previous point estimates $(\hat{\alpha}, \hat{\beta})$ as starting point, the grid center was set up to $[\log(\hat{\alpha}/\hat{\beta}), \log(\hat{\alpha}+\hat{\beta})]$ and a factor of log2 was added to the grid center to obtain an effective range of the grid. Then it was divide evenly into an n*n grid. For each point on the grid, the value of the point was converted to its corresponding (α, β) for the next step.

Next, the posterior densities p(α, β| y) for each point on the grid were calculated using function (2.11) with prior density (2.12). The results were further multiplied by the appropriate Jacobian, i.e. α*β, to obtain the densities p[log(α/β), log(α+β)| y]. Contour plots of these unnormalized marginal posterior densities showed whether the effective range of the grid included all the important parts of the marginal posterior distribution. If not, the grid range would need to be adjusted and p[log(α/β), log(α+β)| y] need to be recomputed until all the contour lines fall in the grid range. The resulting graphs are shown in Figure 4.1-4.4.

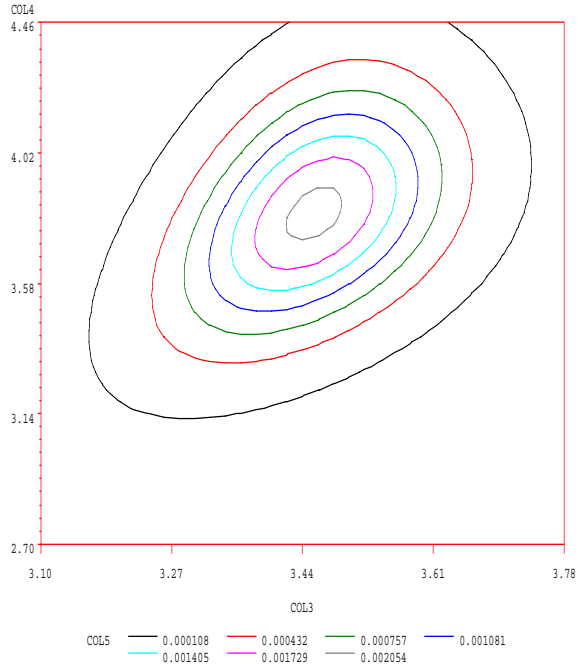

Figure 4.1. Contour plot for GB_STEL Total

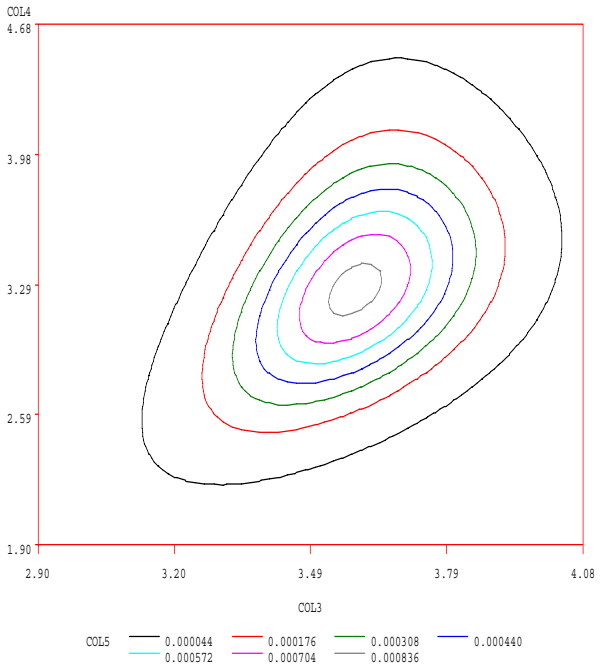

Figure4.2. Contour plot for GB_STEL Time 1

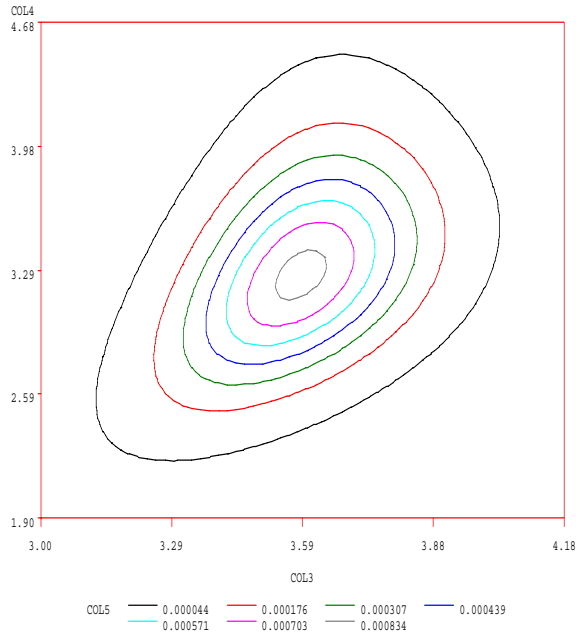

Figure 4.3. Contour plot for GB_STEL Time 2

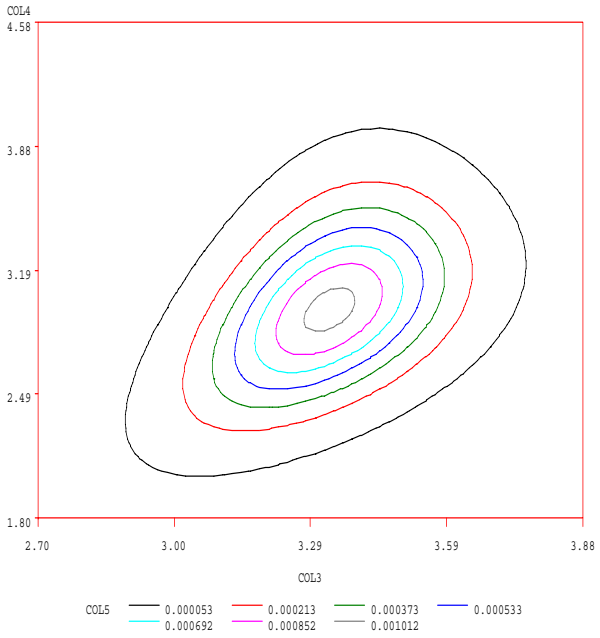

Figure4.4. Contour plot for GB_STEL Time 3

The obvious feature of the contour plots is that the mode lay not far from the point estimate as expected.

These relative posterior densities were then normalized by dividing each value of p[log(α/β), log(α+β)| y] the sum of p[log(α/β), log(α+β)| y] from all grid points. Thus the total posterior density is set to 1.

Finally, Bayesian expected value of (α, β), denoted by $(\widetilde{\alpha}, \widetilde{\beta})$, were computed using formula (3.1) and (3.2). The expected value of θjs, denoted by $\widetilde{\theta}_j$, j=1, …, J, were computed using formula (3.3). The resulting Bayesian estimates of $(\widetilde{\alpha}, \widetilde{\beta})$ and $\widetilde{\theta}_j$ are presented in Table 4.1-4.5. Response rate SRR_{AL} at alarm set point 0.5 for each station and time period were also computed using formula (2.4) and presented in Table 4.2-4.5 for comparison. A graph was drawn and shown in Figure 4.5 to compare the three different approaches for assessing the pass probability.

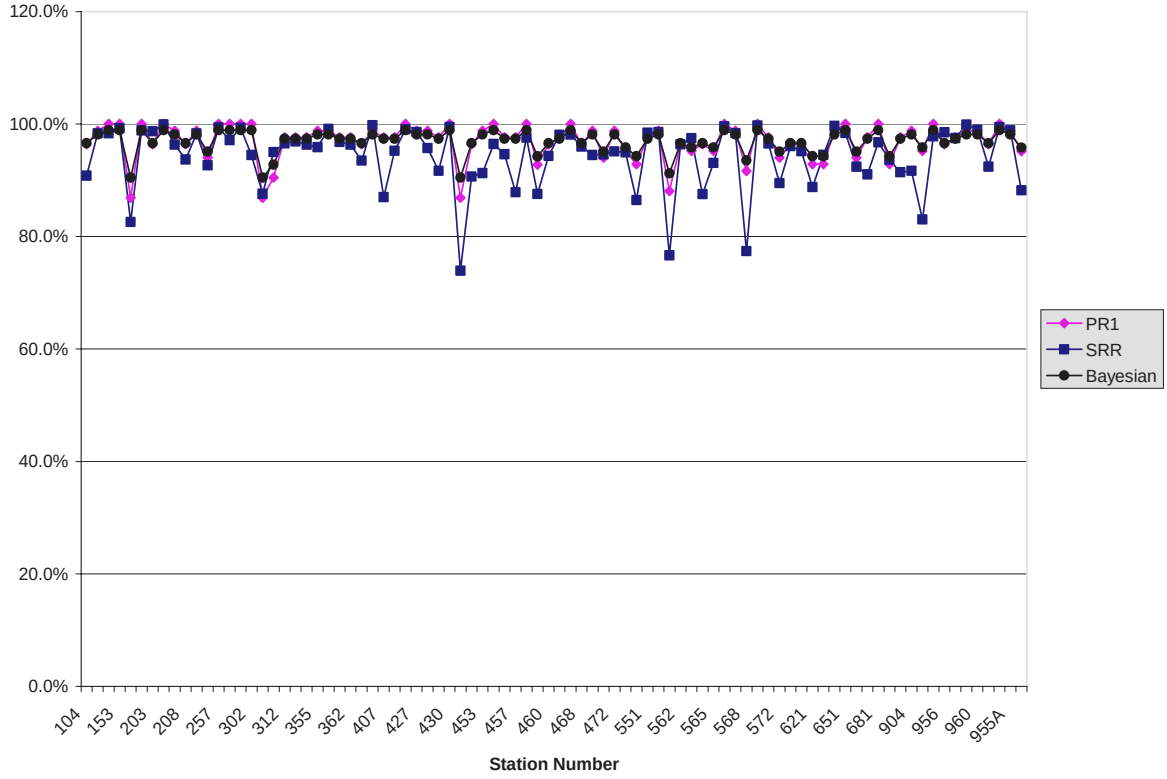

Figure 4.5. First challenge pass rate, response rate vs. Bayesian probability estimation for GB_STEL stations from May 3, 2005 to July 25, 2005.

The figure above shows that the response rates have the biggest station variations among the three methods while Bayesian estimates are the smoothest one. It is clear that Bayesian probability estimates are shrunk from their sample point estimates toward the population distribution. Results from Table 4.2-4.5 also show that the three estimates are close to each other when found concentration follows normal distribution, while response rates lay far from the other two when data distribution failed the normality tests.

4.2 Compute Confidence Interval for $\widetilde{\theta}_j$ s

Confidence intervals for $\widetilde{\theta}_j$ s can be computed through simulation. First, find the marginal posterior distribution of log(α/β) using formula (3.4) and obtain the conditional cumulative distribution. Then draw 1000 random samples of log(α/β) from its conditional distribution using inverse distribution function technique. Second, obtain the conditional distribution of log(α+β) given log(α/β) using formula (3.5) and find the conditional cumulative distribution. Using the same technique, draw random sample of log(α+β) given already sampled log(α/β). This procedure is illustrated in Table 4.6.

Next, transform these1000 pairs of [log(α/β), log(α+β)] to (α, β) using simple algebra to yield 1000 pairs of random draws of the hyperparameters. Then use written functions in any computer software package, like SAS, to generate random sample from Beta ($\alpha + y_j$, $\beta + n_j - y_j$) for each θj, j=1, …, J, and for each draw of (α, β). Therefore obtain 1000 random samples for each θj.

Finally, sort these 1000 random samples for each θj in ascending order and compute the (5^{th}, 95^{th}) and (2.5^{th}, 97.5^{th}) percentile to get 90% and 95% confidence intervals for θjs. Confidence intervals for this study were computed using the above method and are presented in Table 4.2-4.5.

Table 4.1. Point estimate vs. Bayesian estimate of (α, β) and grid centers for GB_STEL challenge data.

Time Period	$\hat{\alpha}$	$\hat{\beta}$	$\log(\frac{\hat{\alpha}}{\hat{\beta}})$	$\log(\hat{\alpha}+\hat{\beta})$	$\tilde{\alpha}$	$\tilde{\beta}$	$\log(\frac{\tilde{\alpha}}{\tilde{\beta}})$	$\log(\tilde{\alpha}+\tilde{\beta})$
Total Time Period	27.866	0.863	3.474	3.358	45.113	1.420	3.458	3.840
Time Period 1	13.148	0.348	3.631	2.602	29.060	0.793	3.601	3.396
Time Period 2	12.413	0.399	3.437	2.550	29.098	0.793	3.603	3.398
Time Period 3	11.683	0.401	3.371	2.492	20.576	0.726	3.345	3.059

Note: $[\log(\frac{\hat{\alpha}}{\hat{\beta}}),\ \log(\hat{\alpha}+\hat{\beta})]$ is the original grid center; $[\log(\frac{\tilde{\alpha}}{\tilde{\beta}}),\ \log(\tilde{\alpha}+\tilde{\beta})]$ is the center for the contour plot.

Table 4.2. First challenge pass rate, response rate and Bayesian estimate of θ_js for GB_STEL challenge data (Total).

Station	PR_1	$SRR_{0.75}$	$\tilde{\theta}$	Lb_95	Ub_95	Lb_90	Ub_90	Normal Test
104	96.4%	90.8%	96.6%	92.3%	99.0%	93.2%	98.8%	N
107	98.8%	98.4%	98.1%	95.2%	99.7%	95.8%	99.6%	Y
152	100.0%	98.3%	98.9%	96.7%	100.0%	97.2%	99.9%	Y
153	100.0%	99.2%	98.9%	96.4%	100.0%	96.9%	99.9%	Y
155	86.9%	82.6%	90.5%	83.9%	95.0%	85.0%	94.3%	N
156	100.0%	98.9%	98.9%	96.5%	100.0%	97.1%	99.9%	Y
203	96.4%	98.7%	96.6%	92.8%	98.9%	93.7%	98.7%	N
204	100.0%	99.9%	98.9%	96.6%	99.9%	97.2%	99.9%	Y

Station	PR_1	$SRR_{0.75}$	$\widetilde{\theta}$	Lb_95	Ub_95	Lb_90	Ub_90	Normal Test
205	98.8%	96.3%	98.1%	95.6%	99.7%	96.1%	99.6%	Y
208	96.4%	93.7%	96.6%	93.1%	98.9%	93.7%	98.7%	N
221	98.8%	98.3%	98.1%	95.1%	99.7%	95.8%	99.6%	Y
222	94.0%	92.7%	95.1%	90.9%	98.2%	91.6%	97.9%	N
257	100.0%	99.4%	98.9%	96.1%	99.9%	97.0%	99.9%	Y
258	100.0%	97.1%	98.9%	96.7%	100.0%	97.2%	99.9%	Y
262	100.0%	99.3%	98.9%	96.6%	100.0%	97.3%	99.9%	Y
302	100.0%	94.5%	98.9%	96.3%	99.9%	97.0%	99.9%	N
303	86.9%	87.6%	90.5%	84.7%	94.7%	85.6%	94.3%	Y
311	90.5%	95.0%	92.8%	87.9%	96.6%	88.7%	96.0%	N
312	97.6%	96.6%	97.4%	93.8%	99.3%	94.6%	99.0%	Y
352	97.6%	96.9%	97.4%	94.1%	99.4%	94.6%	99.2%	Y
354	97.6%	96.3%	97.4%	94.0%	99.3%	94.6%	99.2%	Y
355	98.8%	95.9%	98.1%	95.3%	99.7%	96.0%	99.6%	N
356	98.8%	99.1%	98.1%	95.3%	99.8%	95.9%	99.6%	Y
359	97.6%	96.8%	97.4%	94.3%	99.4%	94.8%	99.2%	N
362	97.6%	96.3%	97.4%	94.1%	99.4%	94.8%	99.2%	Y
403	96.4%	93.5%	96.6%	92.8%	99.0%	93.5%	98.8%	Y
404	98.8%	99.8%	98.1%	95.2%	99.7%	95.9%	99.6%	N
407	97.6%	87.0%	97.4%	93.9%	99.4%	94.8%	99.2%	N

Station	PR_1	$SRR_{0.75}$	$\widetilde{\theta}$	Lb_95	Ub_95	Lb_90	Ub_90	Normal Test
408	97.6%	95.3%	97.4%	93.8%	99.4%	94.5%	99.2%	N
416	100.0%	99.1%	98.9%	96.4%	99.9%	97.1%	99.9%	Y
427	98.8%	98.6%	98.1%	95.2%	99.7%	95.7%	99.6%	N
428	98.8%	95.7%	98.1%	95.6%	99.7%	96.1%	99.6%	Y
429	97.6%	91.7%	97.4%	93.8%	99.4%	94.6%	99.2%	N
430	100.0%	99.5%	98.9%	96.5%	100.0%	97.1%	99.9%	Y
450	86.9%	73.9%	90.5%	84.2%	95.1%	85.4%	94.3%	N
451	96.4%	90.7%	96.6%	93.0%	99.0%	93.7%	98.7%	N
453	98.8%	91.3%	98.1%	95.2%	99.7%	96.0%	99.6%	N
454	100.0%	96.5%	98.9%	96.7%	100.0%	97.1%	99.9%	N
456	97.6%	94.6%	97.4%	94.0%	99.4%	94.7%	99.2%	Y
457	97.6%	87.9%	97.4%	93.8%	99.4%	94.9%	99.2%	N
458	100.0%	97.6%	98.9%	96.6%	100.0%	97.2%	99.9%	N
459	92.8%	87.6%	94.3%	89.2%	97.8%	90.4%	97.3%	Y
460	96.4%	94.3%	96.6%	93.0%	99.0%	93.7%	98.7%	N
463	97.6%	98.1%	97.4%	94.1%	99.3%	94.8%	99.1%	N
465	100.0%	98.1%	98.9%	96.6%	99.9%	97.2%	99.9%	N
468	96.4%	96.0%	96.6%	92.7%	98.9%	93.5%	98.7%	N
469	98.8%	94.5%	98.1%	95.1%	99.7%	95.9%	99.6%	N
471	94.0%	94.6%	95.1%	90.6%	98.0%	91.6%	97.7%	Y

Station	PR_1	$SRR_{0.75}$	$\widetilde{\theta}$	Lb_95	Ub_95	Lb_90	Ub_90	Normal Test
472	98.8%	95.1%	98.1%	95.2%	99.7%	96.1%	99.6%	N
473	95.2%	95.0%	95.8%	91.6%	98.5%	92.5%	98.2%	Y
474	92.9%	86.5%	94.3%	89.6%	97.6%	90.6%	97.1%	N
551	97.6%	98.5%	97.4%	94.0%	99.4%	94.6%	99.2%	Y
552	98.8%	98.6%	98.1%	94.9%	99.7%	95.4%	99.6%	Y
560	88.1%	76.7%	91.3%	85.7%	95.2%	86.4%	94.9%	N
562	96.4%	96.4%	96.6%	93.0%	99.0%	93.7%	98.8%	Y
563	95.2%	97.5%	95.8%	91.8%	98.5%	92.6%	98.3%	Y
564	96.4%	87.5%	96.6%	93.0%	99.0%	93.8%	98.8%	N
565	95.2%	93.1%	95.8%	91.6%	98.5%	92.6%	98.3%	N
566	100.0%	99.6%	98.9%	96.4%	99.9%	97.0%	99.9%	Y
567	98.8%	98.4%	98.1%	95.3%	99.7%	96.0%	99.6%	N
568	91.7%	77.4%	93.5%	88.8%	97.3%	89.7%	96.7%	N
569	100.0%	99.8%	98.9%	96.6%	99.9%	97.2%	99.9%	N
570	97.6%	96.5%	97.4%	93.9%	99.4%	94.7%	99.2%	Y
572	94.0%	89.5%	95.1%	90.5%	98.1%	91.3%	97.7%	N
601	96.4%	96.1%	96.6%	93.3%	98.9%	93.8%	98.7%	N
611	96.4%	95.2%	96.6%	92.8%	99.0%	93.5%	98.7%	Y
621	92.9%	88.8%	94.3%	89.6%	97.7%	90.4%	97.2%	Y
631	92.9%	94.5%	94.3%	89.4%	97.7%	90.7%	97.2%	Y

Station	PR_1	$SRR_{0.75}$	$\widetilde{\theta}$	Lb_95	Ub_95	Lb_90	Ub_90	Normal Test
641	98.8%	99.7%	98.1%	95.4%	99.7%	95.9%	99.7%	Y
651	100.0%	98.4%	98.9%	96.7%	99.9%	97.1%	99.9%	Y
661	94.0%	92.4%	95.1%	90.5%	98.1%	91.4%	97.8%	Y
671	97.6%	91.0%	97.4%	93.5%	99.5%	94.5%	99.3%	N
681	100.0%	96.7%	98.9%	96.6%	100.0%	97.3%	99.9%	Y
691	92.9%	93.7%	94.3%	89.1%	97.5%	90.2%	97.1%	N
901	97.6%	91.4%	97.4%	93.9%	99.4%	94.5%	99.2%	N
904	98.8%	91.7%	98.1%	95.1%	99.8%	96.1%	99.7%	N
953	95.2%	83.0%	95.8%	91.9%	98.6%	92.6%	98.3%	N
954	100.0%	97.8%	98.9%	96.4%	99.9%	97.1%	99.9%	Y
956	96.4%	98.5%	96.6%	92.6%	98.9%	93.4%	98.8%	N
957	97.6%	97.5%	97.4%	93.9%	99.4%	94.8%	99.2%	Y
959	98.8%	99.9%	98.1%	95.3%	99.7%	96.0%	99.6%	N
960	98.8%	99.0%	98.1%	95.2%	99.8%	95.7%	99.6%	Y
961	96.4%	92.4%	96.6%	92.9%	98.9%	93.5%	98.7%	Y
962	100.0%	99.4%	98.9%	96.4%	100.0%	97.2%	99.9%	N
955A	98.8%	98.9%	98.1%	95.3%	99.8%	96.1%	99.6%	Y
955B	95.2%	88.2%	95.8%	91.5%	98.6%	92.0%	98.3%	N

PR_1: First challenge pass rate; $SRR_{0.75}$: Responds rate; $\hat{\theta}$: Bayesian's pass probability; Lb_95: Lower bound of 95% C.I. for $\hat{\theta}$; Ub_95: Upper bound of 95% C.I. for $\hat{\theta}$; Lb_90: Lower bound of 90% C.I. for $\hat{\theta}$; Ub_90: Upper bound of 90% C.I. for $\hat{\theta}$;

Table 4.3-4.5 with results for time period 1 to 3 can be found in Appendix E.

Time 1: May 3, 2005 to May 30, 2005; Time 2: May 31, 2005 to Jun. 20, 2005; Time 3: Jun. 21, 2005 to Jul. 25, 2005.

Table 4.6. Illustration for computing marginal posterior distribution.

α	β	log(α/ β)	log(α+ β)	p[log(α/ β), log(α+ β)| y]	p[log(α/ β)| y]	∑p[log(α/ β)| y]	p[log(α+ β)| log(α/ β), y]	∑p[log(α+ β)| log(α/ β), y]
14.24	0.64	3.1	2.7	8.05148E-05	0.00087	0.00087	0.092493	0.092493
19.22	0.87	3.1	3	0.000610026			0.700779	0.793272
31.69	1.43	3.1	3.5	0.000177423			0.203818	0.997091
52.25	2.35	3.1	4	2.5327E-06			0.002909	1
14.25	0.63	3.12	2.7	9.51621E-05	0.001355	0.002226	0.070205	0.070205
19.24	0.85	3.12	3	0.000915058			0.675075	0.74528
31.72	1.40	3.12	3.5	0.000338813			0.249956	0.995237
52.29	2.31	3.12	4	6.45681E-06			0.004763	1
14.26	0.62	3.14	2.7	0.0001808983	0.002073	0.004299	0.052572	0.052572
19.25	0.83	3.14	3	0.001327445			0.640348	0.692921
31.74	1.37	3.14	3.5	0.000621037			0.299583	0.992504
		3.14	4	1.55397E-05			0.007496	1
.	.	3.16	2.7	0.000120992	0.003109	0.007408	0.038915	0.038915
.	.	.	.	.	.	.	.	.
		.	.	.	.	.	.	.

Chapter Five: Simulation Study

Simulation studies were conducted to compare the performance between Bayesian estimates and pass rate. Different values of (α, β) were studied, including (2, 0.5), (0.4, 0.1), (0.2, 0.05); (4.5, 0.5), (0.9, 0.1), (0.45, 0.05); (9.5, 0.5), (1.9, 0.1), and (0.95, 0.05), which represent mean values of 80%, 90%, and 95%, and relatively small to large standard deviations for beta distributions. Beta mean of 80%, 90%, and 95% was chosen to reflect the majority first challenge pass rate values in this project. Two sets of sample size chosen are 30x30 and 100x100 for small and large samples. The simulation results are presented through Table 5.1-5.2. Each entry of the Table is based on 100 simulated data sets.

To begin the simulation process, first random samples of size k were drawn from Beta distribution for each selected values of the parameter (α, β), where k=30 or 100. The k proportions, denoted by θ_j, j = 1, …, k, are the k probability values. In the second step, for each θ_j, proportion of success was simulated out of n trails, where n = 30 or 100. Next, point estimate of $\hat{\theta}_j$ was computed by $\hat{\theta}_j = \frac{y_j}{n}$. Point estimate of (α, β), denoted by $(\hat{\alpha}, \hat{\beta})$, was estimated by setting its mean and variance to the sample mean and variance of $\hat{\theta}_j$ s. Then use the computational method described in chapter 3, Bayesian estimate of $(\tilde{\alpha}, \tilde{\beta})$ and $\tilde{\theta}_j$ s were obtained. This procedure was repeated 100 times and sum of squared errors (SSE) were computed using the following formulae,

$$SSE(\hat{\theta}_j) = \sum_{i=1}^{100} (\hat{\theta}_j - \theta_j)^2 \qquad (5.1)$$

$$SSE(\tilde{\theta}_j) = \sum_{i=1}^{100} (\tilde{\theta}_j - \theta_j)^2 \tag{5.2}$$

SSE of $\hat{\theta}_j$ s and $\tilde{\theta}_j$ s for each choice of (α, β) are compared in Table 5.1-5.2.

Table 5.1. Compare the sum of squared errors of $\hat{\theta}$ vs. $\tilde{\theta}$ (I). n=30*30

E(θ)	σ^2	(α, β)	$SSE(\hat{\theta})$	$SSE(\tilde{\theta})$
0.8	0.0457	(2, 0.5)	17.8835	16.7437
	0.1067	(0.4, 0.1)	8.5194	8.4961
	0.128	(0.2, 0.05)	5.0518	5.0476
0.9	0.015	(4.5, 0.5)	11.9084	9.7708
	0.045	(0.9, 0.1)	7.8706	7.5145
	0.06	(0.45, 0.05)	4.5315	4.4686
0.95	0.0043	(9.5, 0.5)	6.9413	5.0749
	0.0158	(1.9, 0.1)	5.1954	4.7591
	0.0238	(0.95, 0.05)	4.3073	4.1809

Table 5.2. Compare the sum of squared errors of $\hat{\theta}$ vs. $\tilde{\theta}$ (II). n=100*100

E(θ)	σ^2	(α, β)	$SSE(\hat{\theta})$	$SSE(\tilde{\theta})$
0.8	0.0457	(2, 0.5)	13.2286	12.9257
	0.1067	(0.4, 0.1)	5.8213	5.7952
	0.128	(0.2, 0.05)	3.8157	3.8176
0.9	0.015	(4.5, 0.5)	8.7964	8.3283
	0.045	(0.9, 0.1)	5.4189	5.3889
	0.06	(0.45, 0.05)	3.6556	3.6290
0.95	0.0043	(9.5, 0.5)	4.8955	4.3985
	0.0158	(1.9, 0.1)	3.5955	3.4761
	0.0238	(0.95, 0.05)	2.8954	2.8760

This simulation results showed that Bayesian estimate of pass probability has relatively small sum of squares than pass rate method. This result is much clear with small sample size and sample variance.

Chapter Six: Conclusion

The use of Bayesian analysis is a theoretical sound estimation. It reflects the dependence among parameters. Hence, it may furnish a more reasonable estimate of the true underlying parameters. And the simulation studies show that Bayesian estimates have relative better estimates in terms of sum of squared errors and especially in case of small sample size, where pass rate may not be reliable.

Although our study shows that Bayesian method performs better, the biggest disadvantage of Bayesian method is that we have to assume the prior distribution is correct. Besides the computation of Bayesian estimate is much more complicate than that of the other two approaches—pass rate and response rate. And there are two major difficulties associated with the computation of Bayesian estimates using the computational method illustrated in this thesis. One is computational overflow, and the other is computation limitation for Gamma function. The computational overflow occurs when computing the marginal posterior density of (α, β). It is relatively easy to overcome by multiplying a constant to the density function. The other difficulty is the computation of Gamma function. In SAS, Gamma function can only take values less than 172. For problems with large observed number of x_{ij} or large value of estimated $(\hat{\alpha}, \hat{\beta})$, it can post a problem for getting the desired range of computable grid, thus affect the estimation of the parameters.

Other computational methods for calculating Bayesian posterior densities, like Gibbs sampler, importance sampling, Monte Carlo sampling etc., have been discussed in many papers and may be potentially more efficient. They may assist in future studies and make some improvements.

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Appendix A: Binomial and Beta distribution

A.1 Binomial Distribution

$$b(x;n,\theta)=\binom{n}{x}\theta^{x}(1-\theta)^{1-x} \quad \text{for } x = 0, 1, 2, \ldots, n$$

Parameters: n is a positive integer and $0 < \theta < 1$

Mean and variance: $\mu = n\theta$ and $\sigma^2 = n\theta(1-\theta)$

A.2 Beta Distribution

$$f(x;\alpha,\beta)=\begin{cases}\dfrac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\cdot\Gamma(\beta)}x^{\alpha-1}(1-x)^{\beta-1} & \text{for} \quad 0<x<1\\ 0 & \text{elsewhere}\end{cases}$$

Parameters: $\alpha > 0$ and $\beta > 0$

Mean and variance: $\mu=\dfrac{\alpha}{\alpha+\beta}$ and $\sigma^2=\dfrac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}$

A.3 Point Estimate for (α , β)

First, the population mean and variance are estimated by sample mean and variance, i.e.

$$\hat{\mu}=\bar{\theta} \quad \text{and} \quad \hat{\sigma}^2=S_\theta$$

Then,
$$\begin{cases}\hat{\mu}=\dfrac{\alpha}{\alpha+\beta}\\ \hat{\sigma}^2=\dfrac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}\end{cases}\Rightarrow\begin{cases}\hat{\beta}=\dfrac{(1-\hat{\mu})^2}{\hat{\sigma}^2}\hat{\mu}+\hat{\mu}-1\\ \hat{\alpha}=\dfrac{1-\hat{\mu}}{\hat{\sigma}^2}\hat{\mu}^2-\hat{\mu}\end{cases}$$

Appendix B: Main SAS Code for Parameter Estimation of Challenge Data

```
libname datlib 'C:\Documents and Settings\Administrater\My Documents\qq\paper\acams';
%inc "C:\Documents and Settings\Administrater\My Documents\qq\paper\macro\center.sas";
%inc "C:\Documents and Settings\Administrater\My Documents\qq\paper\macro\grid.sas";
%inc "C:\Documents and Settings\Administrater\My Documents\qq\paper\macro
        \contour.sas";
%inc "C:\Documents and Settings\Administrater\My Documents\qq\paper\macro\ctable.sas";
%inc "C:\Documents and Settings\Administrater\My Documents\qq\paper\macro
        \search.sas";
%inc "C:\Documents and Settings\Administrater\My Documents\qq\paper\macro\CI.sas";
/*************************************************************************
*                        Macro for preparing data for estimation        *
*************************************************************************/
%macro get_data;
data study1;
        set datlib.&dat;
        if station=. then delete;
        if found_concentration>=0.75 & found_concentration<=1.25 then p25=1; else p25=0;
        if found_concentration>=0.5 & found_concentration<=1.5 then p50=1; else p50=0;
run;
proc sql;
        create table study2
        as select station, count(station) as total, sum(p25) as succ25, sum(p50) as succ50,
        calculated succ25/calculated total as th25, calculated succ50/calculated total as th50
        from study1 group by station;
quit;
%center(study2, th25, center); *compute the grid center;
proc sort data=study1; by station; run;
proc means data=study1 noprint;
        var found_concentration;
```

```
        by station;
        output out=study3 mean=mn std=sd;
run;
data response (keep=station mn sd SRR);
        set study3;
        z=(0.75-mn)/sd;
        SRR=1-probnorm(z);
run;
%mend get_data;
/*************************************************************************
*                          Macro to compute confidence interval                          *
*************************************************************************/
%macro comp_ci;
%ctable(contour, table1, table2);
data sample(drop=i seed_1 seed_2 x);
        retain seed_1 435256 seed_2 527490;
        do i=1 to 1000;
                call ranuni(seed_1, x); p1=round(x,0.0001);
                call ranuni(seed_2, x); p2=round(x,0.0001);
                output sample;
        end;
run;
%search(table1, table2, sample, draws);  *search table, draw 1000 alph, beta;
%CI(draws, study2, succ25, total, th25, CI); *simulate 1000 draws of theta, compute CI;
%mend comp_ci;
/*************************************************************************
*                          Macro to export computation results                          *
*************************************************************************/
%macro out_result;
data estimate1a;
```

```
        merge center(keep=alph_head beta_head) est_a;
data estimate1b;
        merge study2(keep=station th25) est_b(keep=col1 rename=(col1=th_dhead)) CI;
run;
proc export data=estimate1a
        outfile='C:\Documents and Settings\Administrater\My Documents\qq\paper\ann
                \&out._a.xls'; run;
proc export data=estimate1b
        outfile='C:\Documents and Settings\Administrater\My Documents\qq\paper\ann
                \&out._b.xls'; run;
proc export data=response
        outfile='C:\Documents and Settings\Administrater\My Documents\qq\paper\ann
                \&out._c.xls'; run;
%mend out_result;
/*************************************************************************
*                          Computation for GB_STEL total                  *
*************************************************************************/
%let dat= GB_stel;
%get_data;  *prepare data;
%grid(center, 1.5, 2, 35, 89, grid);  *set grid;
%contour(study1, succ25, total, grid, 6, contour, est_a, est_b);  *parameter estimation;
proc gcontour data=contour; plot col4*col3=col5; run;
%comp_ci;  *compute CI;
%let out= est1;
%out_result;  *export result;
/*************************************************************************
*                          Computation for GB_STEL time 1                 *
*************************************************************************/
%let dat= GB_stel1;
%get_data;  *prepare data;
```

```
%grid(center, 2, 2, 60, 140, grid);  *set grid;
%contour(study1, succ25, total, grid, 4, contour, est_a, est_b);  *parameter estimation;
proc gcontour data=contour; plot col4*col3=col5; run;
%comp_ci;  *compute CI;
%let out= est2;
%out_result;  *export result;
/*************************************************************************
*                          Computation for GB_STEL time 2                 *
*************************************************************************/
%let dat= GB_stel2;
%get_data;  *prepare data;
%grid(center, 1.5, 2, 60, 140, grid);  *set grid;
%contour(study1, succ25, total, grid, 4, contour, est_a, est_b);  *parameter estimation;
proc gcontour data=contour; plot col4*col3=col5; run;
%comp_ci;  *compute CI;
%let out= est3;
%out_result;  *export result;
/*************************************************************************
*                          Computation for GB_STEL time 3                 *
*************************************************************************/
%let dat= GB_stel3;
%get_data;  *prepare data;
%grid(center, 2, 2, 60, 140, grid);  *set grid;
%contour(study1, succ25, total, grid, 4, contour, est_a, est_b);  *parameter estimation;
proc gcontour data=contour; plot col4*col3=col5; run;
%comp_ci;  *compute CI;
%let out= est4;
%out_result;  *export result;
```

Appendix C: Main SAS Code for Simulation Study

```
libname datalib 'C:\Documents and Settings\Administrater\My Documents\qq\paper\data30a';
%inc "C:\Documents and Settings\Administrater\My Documents\qq\paper\macro\center.sas";
%inc "C:\Documents and Settings\Administrater\My Documents\qq\paper\macro\grid.sas";
%inc "C:\Documents and Settings\Administrater\My Documents\qq\paper\macro
      \contour.sas";
%inc "C:\Documents and Settings\Administrater\My Documents\qq\paper\macro
      \g_sample.sas";
%inc "C:\Documents and Settings\Administrater\My Documents\qq\paper\macro\main.sas";
*-------------------------------------------------------------------------------------------------------------;
%main(2, 0.5, 2.5, 4, 50, 75, 9, mg_a, mg_b, sse);
data datalib.mg1a;  set mg_a;
data datalib.mg1b;  set mg_b;
data datalib.sse1;  set sse;  run;
*-------------------------------------------------------------------------------------------------------------;
%main(4.5, 0.5, 3, 5, 50, 75, 9, mg_a, mg_b, sse);
data datalib.mg2a;  set mg_a;
data datalib.mg2b;  set mg_b;
data datalib.sse2;  set sse;  run;
*-------------------------------------------------------------------------------------------------------------;
%main(9.5, 0.5, 3.5, 5.5, 40, 75, 8, mg_a, mg_b, sse);
data datalib.mg3a;  set mg_a;
data datalib.mg3b;  set mg_b;
data datalib.sse3;  set sse;  run;
*-------------------------------------------------------------------------------------------------------------;
%main(0.4, 0.1, 3.5, 5.5, 50, 75, 6, mg_a, mg_b, sse);
data datalib.mg4a;  set mg_a;
data datalib.mg4b;  set mg_b;
data datalib.sse4;  set sse;  run;
*-------------------------------------------------------------------------------------------------------------;
```

```
%main(0.9, 0.1, 4.5, 6.5, 75, 85, 6, mg_a, mg_b, sse);
data datalib.mg5a;  set mg_a;
data datalib.mg5b;  set mg_b;
data datalib.sse5;  set sse; run;
*-------------------------------------------------------------------------------------------------------;
%main(1.9, 0.1, 10, 18, 75, 90, 6, mg_a, mg_b, sse);
data datalib.mg6a; set mg_a;
data datalib.mg6b; set mg_b;
data datalib.sse6; set sse; run;
*-------------------------------------------------------------------------------------------------------;
%main(0.2, 0.05, 5, 6.5, 65, 75, 5, mg_a, mg_b, sse);
data datalib.mg7a; set mg_a;
data datalib.mg7b; set mg_b;
data datalib.sse7; set sse; run;
*-------------------------------------------------------------------------------------------------------;
%main(0.45, 0.05, 7.5, 8.5, 70, 80, 5, mg_a, mg_b, sse);
data datalib.mg8a; set mg_a;
data datalib.mg8b; set mg_b;
data datalib.sse8; set sse; run;
*-------------------------------------------------------------------------------------------------------;
%main(0.95, 0.05, 12, 19.5, 75, 95, 5, mg_a, mg_b, sse);
data datalib.mg9a; set mg_a;
data datalib.mg9b; set mg_b;
data datalib.sse9; set sse; run;
```

Appendix D: SAS Macros Called by both Programs

```
/*****************************************************************************
*                          MAIN – computation for simulation study                          *
*****************************************************************************/
%macro main(alph, beta,  * selected alph, beta values;
            fact1, fact2,  * grid start point;
            range1, range2,   *grid range;
            factor,   * constant to avoid computation overflow;
            merge1, merge2, SSE  * output dataset;
            );
%do i=1 %to 100;
    %g_sample(&alph, &beta, dat);
    %center(dat, th_head, cent);
    %grid(cent, &fact1, &fact2, &range1, &range2, grid);
    %let voild=F;
    %contour(dat, y, n, grid, &factor, contour, est1, est2);
    %if &voild=T %then %do; %let i=%eval(&i-1); %end;
    %else %do;
        data temp1;
            merge cent est1;
        data temp2;
            merge dat est2(rename=(col1=th_dhead));
        run;
        %if &i=1 %then %do;
            data &merge1;
                set temp1;
            data &merge2;
                set temp2;
            run;
        %end;
```

```
                %else %do;
                        data &merge1;
                                set &merge1 temp1;
                        data &merge2;
                                set &merge2 temp2;
                        run;
                %end;
        %end;
%end;

proc iml;
use &merge1;
read all var{alph_head beta_head alph_dhead beta_dhead} into X;
close &merge1;
SSE_alph_head=sum((X[,1]-&alph)##2);
SSE_beta_head=sum((X[,2]-&beta)##2);
SSE_alph_dhead=sum((X[,3]-&alph)##2);
SSE_beta_dhead=sum((X[,4]-&beta)##2);

use &merge2;
read all var{th th_head th_dhead} into Y;
close &merge2;
SSE_th_head=sum((Y[,2]-Y[,1])##2);
SSE_th_dhead=sum((Y[,3]-Y[,1])##2);

create &SSE var{SSE_alph_head SSE_beta_head SSE_alph_dhead SSE_beta_dhead
SSE_th_head SSE_th_dhead};
append;
close &SSE;
quit;
```

```
%mend main;
/*************************************************************************
*                          CENTER --- calculate grid center             *
*************************************************************************/
%macro center(in_dat, *input dataset;
              th_head, *variable name for theta head;
              g_center *output grid center;
             );
proc means data=&in_dat noprint;
        var &th_head;
        output out=tmp mean=mu std=sigma;
run;
data &g_center;
        set tmp;
        alph_head=(mu**2-mu**3)/sigma**2-mu;
        beta_head=(1/mu-1)*alph_head;
        center1=log(alph_head/beta_head);
        center2=log(alph_head+beta_head);
run;
%mend center;
/*************************************************************************
*                          GRID --- set up grid                         *
*************************************************************************/
%macro grid (g_center, *input dataset for grid center;
             fact1, fact2, *input factor for lower left corner of the grid;
             range1, range2, *set the grid range;
             grid *output dataset for the grid;
             );
data &grid(keep=g_alph g_beta par1 par2);
        set &g_center;
```

```
        par1=round((center1-log(&fact1)),0.1);
        star2=round((center2-log(&fact2)),0.1);
        do i=1 to &range1;
                par2=star2;
                do j=1 to &range2;
                        x=exp(par1); y=exp(par2);
                        g_alph=x*y/(1+x); g_beta=y/(1+x);
                        drop x y i j; output;
                        par2=par2+0.02;
                end;
                par1=par1+0.02;
        end;
run;
%mend grid;
/*************************************************************************
*                                  CONTOUR                                *
*   --- calculate the posterior density for points on the grid, E(alph), E(beta) and E(theta).    *
*************************************************************************/
%macro contour (in_dat, *input dataset;
                succ, *variable name for # of pass challenges;
                total, *variable name for total # of challenges;
                grid, *dataset for grid center;
                factor, *Constance to avoid computation overflow;
                contour, *output dataset of posterior density;
                estimate1, *output Bayesian estimates of E(alph) and E(beta).
                estimate2 *output Bayesian estimate of E(theta).
                );
proc iml;
start mod1(a, b, X, n);
        ans=1; const=gamma(a+b)/(gamma(a)*gamma(b));
```

```
        do i=1 to n;
                tmp=gamma(a+X[i,1])*gamma(b+X[i,2]-
X[i,1])/gamma(a+b+X[i,2])*10**&factor;
                ans=ans*const*tmp;
        end;
        return (ans);
finish mod1;

use &in_dat;
read all var{&succ &total} into X;
n=nrow(X);
close &in_dat;

use &grid;
setin &grid point 0;
do data;
        read next var{g_alph g_beta par1 par2};
        prob1=(g_alph+g_beta)**(-5/2)*mod1(g_alph, g_beta, X, n);
        prob2=g_alph*g_beta*prob1;
        tmp=g_alph||g_beta||par1||par2||prob2;
        Z=Z//tmp;
end;
close &grid;

summ=Z[+,5];
if summ^=0 then do;
        Z[,5]=Z[,5]/summ;
        alph_dhead=t(Z[,1])*Z[,5]; beta_dhead=t(Z[,2])*Z[,5];
        th_dhead=(X[,1]+alph_dhead)/(X[,2]+alph_dhead+beta_dhead);
```

```
        create &estimate1 var{alph_dhead beta_dhead};
        append;
        close &estimate1;

        create &estimate2 from th_dhead;
        append from th_dhead;
        close &estimate2;

        create &contour from Z;
        append from Z;
        close &contour;
        end;
else call symput('voild','T');
quit;
%mend contour;
/*************************************************************************
*                    CTABLE --- create tables of joint densities for drawing samples          *
*************************************************************************/
%macro ctable(contour, * dataset of computed posterior density;
                table1, table2 * joint density tables for drawing samples;
                );
proc sql;
        create table out1 as select col3 as par1, sum(col5) as pp from &contour
        group by col3;
        create table out2 as select a.col3 as par1, a.col4 as par2, a.col5/b.pp as pp
        from &contour a, out1 b where a.col3=b.par1;
quit;
data tmp1(drop=F);
        set out1;
        F+pp; FF1=round(F, 0.0001);
```

```
        if FF1>0 & FF1<1 then output;
run;
data tmp2(drop=F);
        set out2;
        F+pp; FF2=mod(round(F,0.0001),1);
        if FF2^=0 then output;
run;
proc sql;
        create table &table1 as select round(mean(par1),0.01) as parr1, FF1 from tmp1 group
by FF1;
        create table &table2 as select par1 as parr1, mean(par2) as parr2, FF2 from tmp2
group by par1, FF2;
quit;
%mend ctable;
/*************************************************************************
*                          SEARCH --- search tables and draw samples                          *
*************************************************************************/
%macro search(table1, table2, sample, draws);
proc iml;
use &table1;
read all var{parr1 FF1} into X;
n1=nrow(X);
close &table1;

use &table2;
read all var{parr1 parr2 FF2} into Y;
n2=nrow(Y);
close &table2;

use &sample;
```

```
setin &sample point 0;
do data;
        read next var{p1 p2};
        stop=0; i=1;
        do until (stop=1);
                i=i+1;
                if p1<=X[i,2] then do;
                        a=abs(p1-X[i-1,2]); b=abs(p1-X[i,2]); stop=1;
                        if a<b then tmp1=X[i-1,1]; else tmp1=X[i,1];
                end;
                if i=n1 then do; tmp1=X[i,1]; stop=1; end;
        end;
        stop=0; i=1;
        do until (stop=1);
                i=i+1;
                if abs(tmp1-Y[i,1])<0.01 & p2<=Y[i,3] then do;
                        a=abs(p2-Y[i-1,3]); b=abs(p2-Y[i,3]); stop=1;
                        FF2a=Y[i-1,3]; FF2b=Y[i,3];
                        if a<b then tmp2=Y[i-1,2]; else tmp2=Y[i,2];
                end;
                if i=n2 then do; stop=1; tmp2=.; end;
        end;
        a=exp(tmp1); b=exp(tmp2);
        alph=round(a*b/(1+a),0.001); beta=round(b/(1+a),0.001);
        tmp=alph||beta;
        Z=Z//tmp;
end;
close &sample;

create &draws from Z;
```

```
append from Z;
close &draws;

quit;
%mend search;
/*************************************************************************
*                  CI --- compute confidence intervals for Bayesian estimate of theta                *
*************************************************************************/
%macro CI(draws, *input sample dataset of alph, beta;
                in_dat, *input dataset;
                succ, *input variable name for # of pass challenges;
                total, *input variable name for total # of challenges;
                th_draws, *output theta sample drawn;
                CI *output confidence intervals;
                 );
proc iml;
use &draws;
read all var{col1 col2} into X;
close &draws;
n=nrow(X);

use &in_dat;
setin &in_dat point 0;
do data;
        read next var{&succ &total};
        th=j(1,n,.);
        do i=1 to n;
                th[i]=round(rand('beta', X[i,1]+&succ, X[i,2]+&total-&succ),0.001);
        end;
        Y=Y//th;
```

```
end;
close &in_dat;

create &th_draws from Y;
append from Y;
close &th_draws;
quit;

data &CI(keep=Lb_95 Ub_95 Lb_90 Ub_90 means median);
        set &th_draws;
        Lb_95=ordinal(25, of col1-col1000);
        Ub_95=ordinal(975, of col1-col1000);
        Lb_90=ordinal(50, of col1-col1000);
        Ub_90=ordinal(950, of col1-col1000);
        median=ordinal(500, of col1-col1000);
        means=mean(of col1-col1000);
run;
%mend CI;
/*************************************************************************
*                          G_SAMPLE --- generate simulation dataset      *
*************************************************************************/
%macro g_sample(alph, beta,  *input designed alph, beta value;
                    sample_dat  *output drawn samples;
                     );
data tmp(drop=i);
        do i=1 to 30;
                th=round(rand('beta', &alph, &beta),0.001);
                if th=1 then th=0.999;
                if th=0 then th=0.001;
                output;
```

```
        end;
run;
data &sample_dat(drop=seed);
        set tmp;
        retain seed 45; n=30;
        call ranbin(seed, n, th, y);
        th_head=y/n;
run;
%mend g_sample;
```

Appendix E: Table 4.3-4.5

Table 4.3. First challenge pass rate, response rate and Bayesian estimate of θ_js for GB_STEL challenge data (Time 1).

Station	PR_1	$SRR_{0.75}$	$\widetilde{\theta}$	Lb_95	Ub_95	Lb_90	Ub_90
104	96.4%	96.5%	96.9%	92.7%	99.1%	93.5%	98.9%
107	98.8%	97.6%	98.6%	95.2%	99.9%	96.0%	99.8%
152	100.0%	99.5%	98.6%	97.2%	100.0%	97.8%	100.0%
153	100.0%	98.1%	98.6%	97.1%	100.0%	97.7%	100.0%
155	86.9%	91.5%	91.7%	82.8%	94.4%	84.0%	93.8%
156	100.0%	99.5%	98.6%	97.2%	100.0%	97.7%	100.0%
203	96.4%	98.4%	95.2%	92.7%	99.1%	93.9%	98.8%
204	100.0%	99.5%	98.6%	97.1%	100.0%	97.7%	100.0%
205	98.8%	98.0%	96.9%	95.2%	99.9%	95.9%	99.8%
208	96.4%	97.3%	96.9%	92.9%	99.1%	93.6%	98.8%
221	98.8%	99.7%	98.6%	95.4%	99.8%	96.2%	99.8%
222	94.0%	90.7%	98.6%	89.7%	97.9%	90.7%	97.6%
257	100.0%	99.6%	98.6%	97.1%	100.0%	97.8%	100.0%
258	100.0%	98.5%	98.6%	97.3%	100.0%	97.7%	100.0%
262	100.0%	98.2%	98.6%	97.0%	100.0%	97.6%	100.0%
302	100.0%	95.7%	98.6%	97.3%	100.0%	97.8%	100.0%
303	86.9%	90.6%	88.3%	82.8%	94.7%	84.1%	93.9%

311	90.5%	97.7%	96.9%	86.9%	96.5%	87.8%	96.0%
312	97.6%	98.6%	96.9%	94.1%	99.6%	94.7%	99.4%
352	97.6%	98.9%	96.9%	93.9%	99.5%	94.8%	99.3%
354	97.6%	97.1%	95.2%	94.2%	99.5%	94.9%	99.4%
355	98.8%	98.7%	96.9%	95.6%	99.8%	96.3%	99.8%
356	98.8%	98.4%	96.9%	95.6%	99.9%	96.1%	99.8%
359	97.6%	94.7%	98.6%	94.2%	99.5%	94.8%	99.4%
362	97.6%	97.3%	98.6%	93.9%	99.6%	95.0%	99.4%
403	96.4%	93.4%	98.6%	92.1%	99.2%	93.1%	98.9%
404	98.8%	100.0%	96.9%	95.1%	99.8%	95.8%	99.8%
407	97.6%	95.9%	95.2%	93.9%	99.5%	94.7%	99.4%
408	97.6%	97.4%	98.6%	94.1%	99.5%	94.8%	99.4%
416	100.0%	98.6%	98.6%	97.1%	100.0%	97.7%	100.0%
427	98.8%	99.3%	96.9%	95.5%	99.9%	96.1%	99.8%
428	98.8%	96.1%	98.6%	95.8%	99.9%	96.3%	99.8%
429	97.6%	75.5%	98.6%	94.2%	99.6%	94.8%	99.4%
430	100.0%	99.7%	98.6%	97.1%	100.0%	97.8%	100.0%
450	86.9%	68.4%	98.6%	83.2%	94.6%	84.2%	94.0%
451	96.4%	94.7%	95.2%	92.5%	99.1%	93.4%	98.9%
453	98.8%	85.4%	98.6%	95.2%	99.9%	95.8%	99.8%
454	100.0%	95.1%	98.6%	97.3%	100.0%	97.8%	100.0%

456	97.6%	95.0%	98.6%	94.1%	99.6%	94.9%	99.4%
457	97.6%	71.5%	98.6%	94.0%	99.6%	94.7%	99.4%
458	100.0%	97.5%	98.6%	97.0%	100.0%	97.7%	100.0%
459	92.8%	90.2%	95.1%	88.8%	97.7%	89.5%	97.2%
460	96.4%	94.2%	98.6%	92.6%	99.2%	93.3%	99.0%
463	97.6%	98.4%	98.6%	93.9%	99.5%	94.6%	99.4%
465	100.0%	98.6%	98.6%	97.0%	100.0%	97.6%	100.0%
468	96.4%	99.3%	95.2%	92.5%	99.3%	93.3%	98.9%
469	98.8%	97.7%	96.9%	95.1%	99.9%	96.1%	99.7%
471	94.0%	96.5%	93.4%	90.5%	97.9%	91.1%	97.7%
472	98.8%	95.3%	96.9%	95.3%	99.8%	96.3%	99.8%
473	95.2%	96.3%	96.9%	91.4%	98.7%	92.3%	98.4%
474	92.9%	94.3%	90.0%	88.8%	97.7%	89.7%	97.4%
551	97.6%	97.9%	98.6%	94.5%	99.5%	95.0%	99.3%
552	98.8%	96.6%	98.6%	95.4%	99.8%	96.2%	99.7%
560	88.1%	66.0%	96.9%	84.1%	95.3%	85.1%	94.6%
562	96.4%	92.7%	98.6%	92.3%	99.1%	93.1%	98.9%
563	95.2%	95.1%	98.6%	91.5%	98.6%	92.3%	98.3%
564	96.4%	97.5%	95.2%	92.3%	99.1%	93.1%	98.8%
565	95.2%	99.2%	95.2%	91.2%	98.6%	92.2%	98.3%
566	100.0%	99.0%	98.6%	97.3%	100.0%	97.9%	100.0%

567	98.8%	97.6%	98.6%	95.4%	99.8%	96.3%	99.7%
568	91.7%	82.0%	98.6%	87.4%	97.0%	88.3%	96.7%
569	100.0%	99.9%	98.6%	96.8%	100.0%	97.7%	100.0%
570	97.6%	96.9%	98.6%	94.0%	99.5%	94.7%	99.4%
572	94.0%	97.9%	93.4%	90.0%	98.1%	90.9%	97.6%
601	96.4%	88.6%	98.6%	91.9%	99.1%	92.8%	98.8%
611	96.4%	89.8%	98.6%	92.7%	99.2%	93.5%	99.0%
621	92.9%	89.4%	98.6%	88.5%	97.7%	89.9%	97.2%
631	92.9%	96.0%	93.4%	88.6%	97.3%	89.9%	97.0%
641	98.8%	99.6%	98.6%	95.5%	99.9%	96.0%	99.8%
651	100.0%	99.0%	98.6%	96.9%	100.0%	97.5%	100.0%
661	94.0%	92.9%	98.6%	90.4%	98.1%	91.0%	97.8%
671	97.6%	85.9%	96.9%	94.2%	99.5%	94.9%	99.3%
681	100.0%	96.4%	98.6%	97.2%	100.0%	97.7%	100.0%
691	92.9%	85.0%	95.2%	88.9%	97.5%	90.0%	97.1%
901	97.6%	94.6%	96.9%	94.0%	99.6%	94.7%	99.4%
904	98.8%	99.6%	96.9%	95.4%	99.8%	96.3%	99.7%
953	95.2%	74.7%	98.6%	91.3%	98.6%	92.1%	98.3%
954	100.0%	98.7%	98.6%	96.9%	100.0%	97.5%	100.0%
956	96.4%	99.2%	98.6%	92.4%	99.0%	93.3%	98.8%
957	97.6%	92.4%	98.6%	94.1%	99.6%	94.8%	99.4%

959	98.8%	99.7%	98.6%	95.7%	99.8%	96.2%	99.7%
960	98.8%	99.4%	96.9%	95.5%	99.9%	96.3%	99.8%
961	96.4%	92.7%	98.6%	92.7%	99.1%	93.6%	98.9%
962	100.0%	100.0%	98.6%	97.0%	100.0%	97.5%	100.0%
955A	98.8%	99.1%	96.9%	95.2%	99.8%	95.9%	99.8%
955B	95.2%	84.4%	96.8%	91.5%	98.5%	92.1%	98.2%

Table 4.4. First challenge pass rate, response rate and Bayesian estimate of θ_js for GB_STEL challenge data (Time 2).

Station	PR_1	$SRR_{0.75}$	$\widetilde{\theta}$	Lb_95	Ub_95	Lb_90	Ub_90
104	96.4%	96.5%	96.9%	92.7%	99.1%	93.5%	98.9%
107	98.8%	97.6%	98.6%	95.2%	99.9%	96.0%	99.8%
152	100.0%	99.5%	98.6%	97.2%	100.0%	97.8%	100.0%
153	100.0%	98.1%	98.6%	97.1%	100.0%	97.7%	100.0%
155	86.9%	91.5%	91.7%	82.8%	94.4%	84.0%	93.8%
156	100.0%	99.5%	98.6%	97.2%	100.0%	97.7%	100.0%
203	96.4%	98.4%	95.2%	92.7%	99.1%	93.9%	98.8%
204	100.0%	99.5%	98.6%	97.1%	100.0%	97.7%	100.0%
205	98.8%	98.0%	96.9%	95.2%	99.9%	95.9%	99.8%
208	96.4%	97.3%	96.9%	92.9%	99.1%	93.6%	98.8%
221	98.8%	99.7%	98.6%	95.4%	99.8%	96.2%	99.8%

Station	PR_1	$SRR_{0.75}$	$\widetilde{\theta}$	Lb_95	Ub_95	Lb_90	Ub_90
222	94.0%	90.7%	98.6%	89.7%	97.9%	90.7%	97.6%
257	100.0%	99.6%	98.6%	97.1%	100.0%	97.8%	100.0%
258	100.0%	98.5%	98.6%	97.3%	100.0%	97.7%	100.0%
262	100.0%	98.2%	98.6%	97.0%	100.0%	97.6%	100.0%
302	100.0%	95.7%	98.6%	97.3%	100.0%	97.8%	100.0%
303	86.9%	90.6%	88.3%	82.8%	94.7%	84.1%	93.9%
311	90.5%	97.7%	96.9%	86.9%	96.5%	87.8%	96.0%
312	97.6%	98.6%	96.9%	94.1%	99.6%	94.7%	99.4%
352	97.6%	98.9%	96.9%	93.9%	99.5%	94.8%	99.3%
354	97.6%	97.1%	95.2%	94.2%	99.5%	94.9%	99.4%
355	98.8%	98.7%	96.9%	95.6%	99.8%	96.3%	99.8%
356	98.8%	98.4%	96.9%	95.6%	99.9%	96.1%	99.8%
359	97.6%	94.7%	98.6%	94.2%	99.5%	94.8%	99.4%
362	97.6%	97.3%	98.6%	93.9%	99.6%	95.0%	99.4%
403	96.4%	93.4%	98.6%	92.1%	99.2%	93.1%	98.9%
404	98.8%	100.0%	96.9%	95.1%	99.8%	95.8%	99.8%
407	97.6%	95.9%	95.2%	93.9%	99.5%	94.7%	99.4%
408	97.6%	97.4%	98.6%	94.1%	99.5%	94.8%	99.4%
416	100.0%	98.6%	98.6%	97.1%	100.0%	97.7%	100.0%
427	98.8%	99.3%	96.9%	95.5%	99.9%	96.1%	99.8%

Station	PR_1	$SRR_{0.75}$	$\widetilde{\theta}$	Lb_95	Ub_95	Lb_90	Ub_90
428	98.8%	96.1%	98.6%	95.8%	99.9%	96.3%	99.8%
429	97.6%	75.5%	98.6%	94.2%	99.6%	94.8%	99.4%
430	100.0%	99.7%	98.6%	97.1%	100.0%	97.8%	100.0%
450	86.9%	68.4%	98.6%	83.2%	94.6%	84.2%	94.0%
451	96.4%	94.7%	95.2%	92.5%	99.1%	93.4%	98.9%
453	98.8%	85.4%	98.6%	95.2%	99.9%	95.8%	99.8%
454	100.0%	95.1%	98.6%	97.3%	100.0%	97.8%	100.0%
456	97.6%	95.0%	98.6%	94.1%	99.6%	94.9%	99.4%
457	97.6%	71.5%	98.6%	94.0%	99.6%	94.7%	99.4%
458	100.0%	97.5%	98.6%	97.0%	100.0%	97.7%	100.0%
459	92.8%	90.2%	95.1%	88.8%	97.7%	89.5%	97.2%
460	96.4%	94.2%	98.6%	92.6%	99.2%	93.3%	99.0%
463	97.6%	98.4%	98.6%	93.9%	99.5%	94.6%	99.4%
465	100.0%	98.6%	98.6%	97.0%	100.0%	97.6%	100.0%
468	96.4%	99.3%	95.2%	92.5%	99.3%	93.3%	98.9%
469	98.8%	97.7%	96.9%	95.1%	99.9%	96.1%	99.7%
471	94.0%	96.5%	93.4%	90.5%	97.9%	91.1%	97.7%
472	98.8%	95.3%	96.9%	95.3%	99.8%	96.3%	99.8%
473	95.2%	96.3%	96.9%	91.4%	98.7%	92.3%	98.4%
474	92.9%	94.3%	90.0%	88.8%	97.7%	89.7%	97.4%

Station	PR_1	$SRR_{0.75}$	$\widetilde{\theta}$	Lb_95	Ub_95	Lb_90	Ub_90
551	97.6%	97.9%	98.6%	94.5%	99.5%	95.0%	99.3%
552	98.8%	96.6%	98.6%	95.4%	99.8%	96.2%	99.7%
560	88.1%	66.0%	96.9%	84.1%	95.3%	85.1%	94.6%
562	96.4%	92.7%	98.6%	92.3%	99.1%	93.1%	98.9%
563	95.2%	95.1%	98.6%	91.5%	98.6%	92.3%	98.3%
564	96.4%	97.5%	95.2%	92.3%	99.1%	93.1%	98.8%
565	95.2%	99.2%	95.2%	91.2%	98.6%	92.2%	98.3%
566	100.0%	99.0%	98.6%	97.3%	100.0%	97.9%	100.0%
567	98.8%	97.6%	98.6%	95.4%	99.8%	96.3%	99.7%
568	91.7%	82.0%	98.6%	87.4%	97.0%	88.3%	96.7%
569	100.0%	99.9%	98.6%	96.8%	100.0%	97.7%	100.0%
570	97.6%	96.9%	98.6%	94.0%	99.5%	94.7%	99.4%
572	94.0%	97.9%	93.4%	90.0%	98.1%	90.9%	97.6%
601	96.4%	88.6%	98.6%	91.9%	99.1%	92.8%	98.8%
611	96.4%	89.8%	98.6%	92.7%	99.2%	93.5%	99.0%
621	92.9%	89.4%	98.6%	88.5%	97.7%	89.9%	97.2%
631	92.9%	96.0%	93.4%	88.6%	97.3%	89.9%	97.0%
641	98.8%	99.6%	98.6%	95.5%	99.9%	96.0%	99.8%
651	100.0%	99.0%	98.6%	96.9%	100.0%	97.5%	100.0%
661	94.0%	92.9%	98.6%	90.4%	98.1%	91.0%	97.8%

Station	PR_1	$SRR_{0.75}$	$\widetilde{\theta}$	Lb_95	Ub_95	Lb_90	Ub_90
671	97.6%	85.9%	96.9%	94.2%	99.5%	94.9%	99.3%
681	100.0%	96.4%	98.6%	97.2%	100.0%	97.7%	100.0%
691	92.9%	85.0%	95.2%	88.9%	97.5%	90.0%	97.1%
901	97.6%	94.6%	96.9%	94.0%	99.6%	94.7%	99.4%
904	98.8%	99.6%	96.9%	95.4%	99.8%	96.3%	99.7%
953	95.2%	74.7%	98.6%	91.3%	98.6%	92.1%	98.3%
954	100.0%	98.7%	98.6%	96.9%	100.0%	97.5%	100.0%
956	96.4%	99.2%	98.6%	92.4%	99.0%	93.3%	98.8%
957	97.6%	92.4%	98.6%	94.1%	99.6%	94.8%	99.4%
959	98.8%	99.7%	98.6%	95.7%	99.8%	96.2%	99.7%
960	98.8%	99.4%	96.9%	95.5%	99.9%	96.3%	99.8%
961	96.4%	92.7%	98.6%	92.7%	99.1%	93.6%	98.9%
962	100.0%	100.0%	98.6%	97.0%	100.0%	97.5%	100.0%
955A	98.8%	99.1%	96.9%	95.2%	99.8%	95.9%	99.8%
955B	95.2%	84.4%	96.8%	91.5%	98.5%	92.1%	98.2%

Table 4.5. First challenge pass rate, response rate and Bayesian estimate of θ_js for GB_STEL challenge data (Time 3).

Station	PR_1	$SRR_{0.75}$	$\hat{\theta}$	Lb_95	Ub_95	Lb_90	Ub_90
104	96.4%	97.0%	96.5%	88.9%	99.6%	90.8%	99.3%
107	98.8%	99.5%	96.5%	89.6%	99.7%	91.2%	99.5%
152	100.0%	96.3%	98.5%	94.0%	100.0%	95.4%	100.0%
153	100.0%	99.9%	98.5%	94.2%	100.0%	95.5%	100.0%
155	86.9%	69.5%	90.4%	80.7%	96.9%	82.1%	96.1%
156	100.0%	98.7%	98.5%	93.8%	100.0%	94.8%	100.0%
203	96.4%	99.3%	98.5%	93.1%	100.0%	94.8%	100.0%
204	100.0%	100.0%	98.5%	93.6%	100.0%	94.9%	100.0%
205	98.8%	97.6%	98.5%	93.0%	100.0%	94.6%	100.0%
208	96.4%	90.3%	94.5%	86.0%	98.9%	87.7%	98.6%
221	98.8%	95.9%	96.5%	89.3%	99.7%	91.3%	99.5%
222	94.0%	89.7%	94.5%	86.2%	99.1%	88.0%	98.6%
257	100.0%	98.1%	98.5%	93.3%	100.0%	95.1%	100.0%
258	100.0%	93.8%	98.5%	93.5%	100.0%	95.2%	100.0%
262	100.0%	99.8%	98.5%	93.9%	100.0%	95.1%	100.0%
302	100.0%	98.0%	98.5%	93.0%	100.0%	94.7%	100.0%
303	86.9%	92.6%	92.4%	82.0%	97.8%	84.3%	97.3%
311	90.5%	94.6%	86.4%	73.5%	94.3%	75.3%	93.6%
312	97.6%	94.2%	96.5%	89.5%	99.7%	91.3%	99.5%

Station	PR_1	$SRR_{0.75}$	$\hat{\theta}$	Lb_95	Ub_95	Lb_90	Ub_90
352	97.6%	96.8%	96.5%	89.4%	99.6%	91.1%	99.4%
354	97.6%	99.4%	98.5%	93.8%	100.0%	94.9%	100.0%
355	98.8%	98.6%	98.5%	93.5%	100.0%	94.8%	100.0%
356	98.8%	99.5%	98.5%	93.9%	100.0%	95.4%	100.0%
359	97.6%	97.8%	96.5%	89.4%	99.6%	91.1%	99.4%
362	97.6%	91.8%	94.5%	86.9%	99.0%	88.2%	98.7%
403	96.4%	96.0%	96.5%	89.3%	99.6%	91.2%	99.4%
404	98.8%	99.3%	98.5%	94.1%	100.0%	95.0%	100.0%
407	97.6%	98.1%	98.5%	93.8%	100.0%	95.2%	100.0%
408	97.6%	85.9%	94.5%	86.3%	99.0%	88.5%	98.7%
416	100.0%	99.9%	98.5%	94.1%	100.0%	95.1%	100.0%
427	98.8%	98.0%	98.5%	93.8%	100.0%	95.0%	100.0%
428	98.8%	96.4%	98.5%	93.3%	100.0%	94.8%	100.0%
429	97.6%	99.9%	98.5%	93.8%	100.0%	94.7%	100.0%
430	100.0%	99.9%	98.5%	93.5%	100.0%	95.0%	100.0%
450	86.9%	67.2%	92.4%	82.2%	97.9%	84.6%	97.5%
451	96.4%	99.2%	98.5%	93.7%	100.0%	95.2%	100.0%
453	98.8%	94.7%	98.5%	93.8%	100.0%	94.8%	100.0%
454	100.0%	97.9%	98.5%	94.2%	100.0%	95.2%	100.0%
456	97.6%	96.6%	96.5%	89.4%	99.6%	91.1%	99.5%

Station	PR_1	$SRR_{0.75}$	$\hat{\theta}$	Lb_95	Ub_95	Lb_90	Ub_90
457	97.6%	97.8%	98.5%	93.8%	100.0%	94.9%	100.0%
458	100.0%	97.7%	98.5%	93.5%	100.0%	94.7%	100.0%
459	92.8%	85.7%	94.5%	86.8%	98.9%	88.3%	98.6%
460	96.4%	91.4%	96.5%	90.0%	99.7%	91.3%	99.5%
463	97.6%	95.5%	94.5%	86.2%	98.8%	88.4%	98.5%
465	100.0%	98.4%	98.5%	93.3%	100.0%	95.0%	100.0%
468	96.4%	88.5%	96.5%	90.6%	99.7%	91.8%	99.6%
469	98.8%	99.3%	98.5%	94.1%	100.0%	95.5%	100.0%
471	94.0%	98.3%	96.5%	89.3%	99.6%	90.6%	99.5%
472	98.8%	96.1%	98.5%	94.0%	100.0%	95.1%	100.0%
473	95.2%	94.2%	94.5%	85.7%	99.0%	88.1%	98.6%
474	92.9%	85.7%	96.5%	89.7%	99.6%	91.3%	99.5%
551	97.6%	99.7%	96.5%	89.6%	99.7%	91.2%	99.5%
552	98.8%	99.9%	98.5%	93.7%	100.0%	94.8%	100.0%
560	88.1%	73.6%	90.4%	80.3%	96.8%	82.7%	96.3%
562	96.4%	98.1%	98.5%	94.0%	100.0%	95.2%	100.0%
563	95.2%	97.0%	92.4%	83.6%	97.9%	85.7%	97.4%
564	96.4%	99.5%	98.5%	93.7%	100.0%	95.0%	100.0%
565	95.2%	97.7%	94.5%	86.5%	99.0%	88.0%	98.5%
566	100.0%	99.7%	98.5%	93.7%	100.0%	95.0%	100.0%

Station	PR_1	$SRR_{0.75}$	$\hat{\theta}$	Lb_95	Ub_95	Lb_90	Ub_90
567	98.8%	98.7%	98.5%	93.6%	100.0%	94.9%	100.0%
568	91.7%	64.0%	86.4%	74.8%	94.5%	76.7%	93.6%
569	100.0%	99.2%	98.5%	93.4%	100.0%	94.7%	100.0%
570	97.6%	95.8%	94.5%	85.6%	98.9%	87.6%	98.5%
572	94.0%	80.8%	96.5%	89.3%	99.6%	91.6%	99.5%
601	96.4%	99.5%	98.5%	93.7%	100.0%	94.9%	100.0%
611	96.4%	96.1%	98.5%	94.2%	100.0%	95.2%	100.0%
621	92.9%	77.5%	88.4%	76.2%	95.7%	78.7%	94.8%
631	92.9%	97.3%	98.5%	93.5%	100.0%	94.9%	100.0%
641	98.8%	99.8%	96.5%	90.5%	99.6%	91.7%	99.4%
651	100.0%	99.6%	98.5%	93.3%	100.0%	95.0%	100.0%
661	94.0%	86.3%	90.4%	79.6%	96.8%	81.7%	96.1%
671	97.6%	97.1%	98.5%	92.9%	100.0%	95.0%	100.0%
681	100.0%	98.1%	98.5%	93.9%	100.0%	94.9%	100.0%
691	92.9%	99.8%	96.5%	89.6%	99.7%	91.5%	99.6%
901	97.6%	81.5%	96.5%	89.7%	99.7%	91.2%	99.5%
904	98.8%	99.3%	98.5%	93.6%	100.0%	94.8%	100.0%
953	95.2%	80.6%	94.5%	86.3%	98.9%	88.0%	98.6%
954	100.0%	98.7%	98.5%	94.0%	100.0%	95.0%	100.0%
956	96.4%	95.5%	94.5%	86.2%	98.9%	88.1%	98.4%

Station	PR_1	$SRR_{0.75}$	$\hat{\theta}$	Lb_95	Ub_95	Lb_90	Ub_90
957	97.6%	99.0%	98.5%	93.7%	100.0%	95.1%	100.0%
959	98.8%	100.0%	98.5%	94.2%	100.0%	94.9%	100.0%
960	98.8%	99.7%	98.5%	94.1%	100.0%	95.3%	100.0%
961	96.4%	85.7%	96.5%	89.1%	99.6%	90.4%	99.4%
962	100.0%	99.9%	98.5%	94.2%	100.0%	95.4%	100.0%
955A	98.8%	99.0%	98.5%	93.4%	100.0%	94.9%	100.0%
955B	95.2%	97.1%	94.5%	85.4%	98.9%	87.6%	98.5%

PR_1: First challenge pass rate; $SRR_{0.75}$: Responds rate; $\hat{\theta}$: Bayesian's pass probability; Lb_95: Lower bound of 95% C.I. for $\hat{\theta}$; Ub_95: Upper bound of 95% C.I. for $\hat{\theta}$; Lb_90: Lower bound of 90% C.I. for $\hat{\theta}$; Ub_90: Upper bound of 90% C.I. for $\hat{\theta}$;

Time 1: May 3, 2005 to May 30, 2005; Time 2: May 31, 2005 to Jun. 20, 2005; Time 3: Jun. 21, 2005 to Jul. 25, 2005.