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Model of Potassium Ion's Dynamics in KcsA Ion Channel

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Model of Potassium ion's dynamics in KcsA ion channel

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ABSTRACT. Consider the speed of the ions at different temperatures. The ions speed was taken in 6 temperature groups of 5, 10, 100, 150, 250 and 300 at 50000 seconds. In fact, for each temperature, there are up to 50,000 speed data. The goal of this model is to predict other temperatures. After graphing the data, a linear model for six groups will be proposed.
Keywords: Ions speed, Predict, Bayesian, Linear model.
AMS Mathematical Subject Classification [2010]: 13D45, 39B42.

1. Introduction

Consider the speed of the ions at different temperatures. The ions speed was taken in 6 temperature groups of 5, 10, 100, 150, 250 and 300 at 50000 seconds. In fact, for each temperature, there are up to 50,000 speed data. The goal of this model is to predict other temperatures. After graphing the data, a linear model for six groups will be proposed.

2. Linear model of ions speed

We consider the linear mixed model as follows:

$$y_{ij} = \beta_1 + \beta_2 * t_i + \beta_3 * temp_i + b_{1i} + b2jt_j + \varepsilon_{ij}. \quad i = 1, ..., N \;\; \& \;\; j = 1, ..., m \tag{1}$$

where y_{ij} is the ion speed at temperature i and occation t_j, t_j is the j-th occation, β_1, β_2 and β_3 are fixed effects, b_{1i} and b_i are random effects and ε_{ij} is the error therm. The random intercept b_{1i} represent the deviation of tempeture i th intercept from the mean β_1 and random slope b_{2j} represents the deviation of j-th pccation from the mean slope β_2.
It's common to assume that random effects b_{1i} and b_{2j} are independent and ε_{ij} is uncorrelated with both $b_1 i$ and b_{2j}. It's also usual to consider the normal distribution for all random variables in this model as follows:

$$\varepsilon_{ij} \sim N(0, \sigma^2_\varepsilon), \quad b_{1i} \sim N(0, \sigma^2_{b_{1i}}), \quad b_{2j} \sim N(0, \sigma^2_{b_{2j}}).$$

To estimate of the parameters we use the Bayesian in ference, espicially the Gibbs sampling method that is based on the Morkov chain Monte Carlo approach. For using this method we should specify the prior distribation for parameters. Gibbs sampling is a iteratve algorithm that compute the Beyesian posterior of parameters by using the prior distribations and initial values. [1]
We used the openBUGS software and considered the N(0,1000) for fixed effects and Inverse-Gamma(1,0.1) for variance components. By considering 5000 iterations with burn in and also after cheching the diagnostics of convergence the resolts are obtained.
Tabel 1 presents the posterior estimates of parameters.

The posterior means and cofidence intervals of 95% Highest posterior Density (HDP) of fixed effects show that and the estimates of variance components of random effects show that this model

TABLE 1. Posterior Analysis from Speeds

	mean	sd	MC$_{error}$	val2.5pc	median	val97.5pc	start	sample
β_1	0.05742	0.03465	0.004109	-0.01923	0.06263	0.1081	1001	5000
β_2	1.08E-07	5.15E-08	1.81E-09	9.12E-09	1.07E-07	2.15E-07	1001	5000
β_3	-3.93E-04	1.20E-04	1.42E-05	-6.20E-04	-3.96E-04	-1.51E-04	1001	5000
σ_1^2	0.09713	0.1093	0.002195	0.02243	0.06827	0.3471	1001	5000
σ_2^2	0.001524	1.12E-04	1.24E-05	0.001303	0.001518	0.001725	1001	5000
σ_e^2	0.1321	3.91E-04	1.10E-05	0.1314	0.1321	0.1329	1001	5000

is a suitable model and it can be obtained from different velocities. For example, for temperature 2 Kelvin, speed is equal to:

$$y_{ij} = \beta_1 + \beta_2 * t_i + \beta_3 * 2 + b2jt_j + \varepsilon_{ij}. \quad j = 1, ..., 5000 \tag{2}$$

Speed predictions are written in program R version i386 3.5.0 alpha. Also, for this model, the amount of priori and posterior descriptions has been investigated and the best is estimate as the appropriate model. Than, no other priores and posteriors has been said.
Figure 1 shows the linear average of the temperature from 0 to 310.

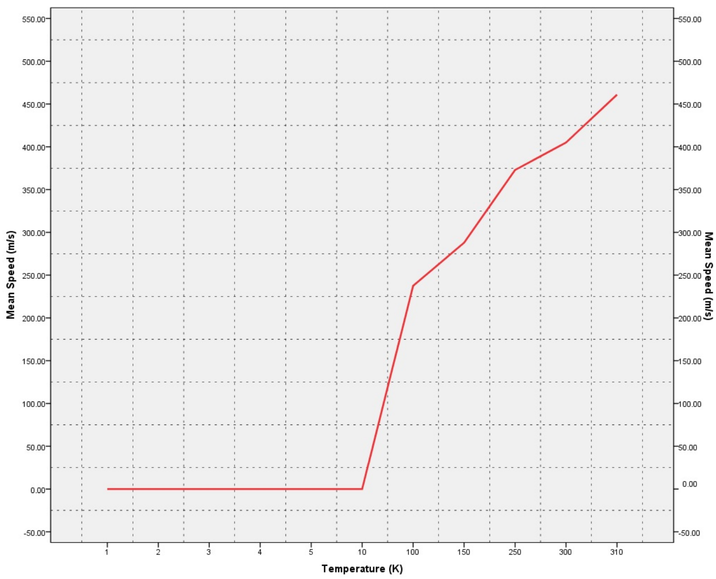

FIGURE 1. Speed in $\frac{m}{s}$ of six groups of temperatures

The extended abstract should have 2–4 pages. Papers prepared in less than 2 pages, more than 4 pages or out of the style of the meeting, will be returned.

Here you should state the introduction, preliminaries and your notations. Authors are required to state clearly the contribution of the extended abstract and its significance in the introduction. There could be some short survey of relevant literature.

openBUGS code

```
model{
for(i in 1:N){ y[i] dnorm(mu[i], tau.e)
mu[i]¡-beta[1]+beta[2]*t[i]+beta[3]*temperature[i]+alpha1[id[i]]+alpha2[t[i]] }
```

```
for(i in 1:N){ypred[i] dnorm(mu[i],tau.e)}
for(i in 1:M){alpha1[i] dnorm(0,tau.a1)}
for(i in 1:T){alpha2[i] dnorm(0,tau.a2)}
for(i in 1:N){r[i]¡-y[i]-ypred[i]}
sigma2.e¡-1/tau.e
sigma2.a1¡-1/tau.a1
sigma2.a2¡-1/tau.a2
for(i in 1:3){beta[i] dnorm(0,.00001)}
tau.e dgamma(.1,.1)
tau.a1 dgamma(.1,.1)
tau.a2 dgamma(.1,.1)

#initial values
list(beta=c(0,0,0),tau.e=1,tau.a1=1,tau.a2=1)
#data
list(N=300000,M=6,T=50000)
y[] temperature[] t[] id[]
```

References

1. Congdon, Peter. Bayesian statistical modelling. *John Wiley & Sons*, **704** (2007) 109-132.

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