MCMC implementation of rock fracture modelling

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Abstract

This paper deals with the problem of estimating fracture planes, given only the data at boreholes. We formulate an appropriate model for the problem, and give a solution to fitting the planes using a Markov chain Monte Carlo implementation. The basics of MCMC are given, with particular emphasis given to reversible jump, which is required for changing dimension. (A detailed worked example is given as an appendix). The methods are tested on both simulated and real data. The latter is a unique data set in the form of a granite block, which was sectioned into slices. All joints were located and recorded, and the joint planes obtained by stacking strike lines. This work is important in the risk assessment for the underground storage of hazardous waste. Problems and extensions are discussed.

KEY WORDS: Markov chain Monte Carlo; likelihood; reversible jump; fracture planes

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1 Introduction

In the work presented here we consider the problem of estimating fracture planes in 3 dimensions. The data is in the form of a number of vertical boreholes on a regular grid, and the depths at which fractures intersect these boreholes. The motivation here being in risk assessment for the safe storage of hazardous wastes in underground repositories. The unknowns are the number of fractures, and for each fracture its intercept, slope and extent. Having established a plausible model for the likelihood of such a data set, we estimate the parameters for the fractures using an implementation of Markov chain Monte Carlo. A statistical framework for 2 dimensions has been given in Mardia *et al.* (2005).

In this paper we shall present some details about the MCMC methodology, and how it was applied. We start in Section 2 with some notation and a description of the model. In Section 3 we introduce Markov chains, and then describe the idea behind Markov chain Monte Carlo. In particular we highlight the details underlying the reversible jump of the MCMC used. A major part of the problem of line fitting required that the dimension (the number of lines) was allowed to change, and this is where reversible jump was used. (In the Appendix we give in some detail a simple worked example of a reversible jump MCMC implementation, since this procedure is not well understood.) In section 4 we present a complete case study of a simulated 3D data set, its analysis, and results *and similarly in Section 5 for some real data*. We end with a discussion.

2 The Model

We first introduce some notation. We shall assume that the boreholes are on a regular grid.

Let us label the boreholes by i, l, where $i = 1, ..., I, l = 1, ..., L$ and the intersection points on each borehole by $j = 1, ..., n_{il}$, where n_{il} is the number of points on the i, l^{th} borehole. Let $(x_i, z_l$ be the location of the i, l^{th} borehole. Further, suppose that y_{ilj} denote the vertical position of the j^{th} intersection point on the i, l^{th} borehole, listed in increasing order in j, for each i, l, and let $Y = \{y_{ilj}\}$ denote this dataset. Also, let $k = 1, ..., K$ denote the (unknown) fracture planes. When planes are fitted to the data then the k^{th} plane will intersect a consecutive set of boreholes (in 2D) near $\alpha_k + \beta_{x_k} x_i + \beta_{z_k} z_l$.

A key parameter is a "matching function" $\pi(i, l, j) \in \{1, ..., K\}$ that associates each intersection point with one of the fracture planes. Denote the *shortest* orthogonal squared distances between the intersection points and the k^{th} fracture line by $d^2_{ilj;k}$. If d is normally distributed, with zero mean, then the likelihood for Y, π, K and the $\{\alpha_k, \beta_{x_k}, \beta_{z_k}\}$ is given

by

$$L(Y;\pi,K,\{\alpha_k,\beta_{x_k},\beta_{z_k}\}) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^n \prod_{i=1}^{I}\prod_{l=1}^{L}\prod_{j=1}^{n_{il}} \exp\left(-\frac{d^2_{ilj;\pi(i,l,j)}}{2\sigma^2}\right),$$

where $n = \sum\sum n_{il}$. Note that $d^2_{ilj;\pi(i,l,j)}$ can be written as

$$\frac{(\alpha_k + \beta_{x_k}x_i + \beta_{z_k}z_l - y_{ilj})^2}{1+\beta^2_{x_k}+\beta^2_{z_k}},$$

and we shall also write σ_k^2 for $\sigma^2(1+\beta^2_{x_k}+\beta^2_{z_k})$.

We introduce the following priors:

- For the intercept, α, we assume that the uniform distribution is a suitable prior, over the length of the borehole.
- For the slopes, we let $\beta = \tan\theta$, and have a prior for 2θ that it is distributed as von Mises.
- For the number of fractures K, we use the Poisson distribution.

Combining the likelihood above with prior densities for $K, \{\alpha_k, \beta_k\}$ gives us the posterior density $\pi(K, \{\alpha_k, \beta_k\}|Y)$. One way to calculate the posterior mean is by a simulation method which does not depend on the complicated normalising constant: a popular technique is Markov chain Monte Carlo. This procedure generates a Markov chain whose equilibrium distribution is the posterior density of $K, \{\alpha_k, \beta_k\}|Y$. For simplicity write $\mathbf{\Theta} = (K, \{\alpha_k, \beta_k\})$.

3 Basic Elements of Markov chain Monte Carlo

3.1 Markov Chains

A Markov chain is generated by sampling

$$X^{(t+1)} \sim p(x|x^{(t)}), t = 1, 2, ...,$$

where p is the transition kernel. Thus $X^{(t+1)}$ depends only on $X^{(t)}$, not on $X^{(0)}$, $X^{(1)}$, ..., $X^{(t-1)}$.

The chain has the following properties:

- As $t \to \infty$, the Markov chain converges (in distribution) to its *stationary* (or invariant) distribution.

- Assuming a stationary distribution exists, it is unique if the chain is *irreducible*. Irreducible means that any set of states can be reached from any other state in a finite number of moves.

- A Markov chain taking only a finite number of values is *aperiodic* if the greatest common divisor of return times to any particular state is 1.

- Assume the Markov chain has the stationary distribution $\pi(x)$, is aperiodic and irreducible, then we have an *ergodic* theorem:

$$\begin{aligned} \bar{h}_N &= \frac{1}{N}\sum_{t=1}^{N} h\left(X^{(t)}\right) \\ &\rightarrow E_\pi[h(X)] \text{ as } N \rightarrow \infty. \end{aligned}$$

  $\bar{h}_N$ is called an ergodic average.

3.2 Markov chain Monte Carlo

The question now is how do we construct a Markov chain whose stationary distribution is our target distribution $\pi(x)$? Metropolis et al (1953) showed how, with the method generalized by Hastings (1970).

At each iteration t

1. Sample candidate point Y from the proposal distribution $q(y|x^{(t)})$.

2. With probability
$$\alpha(x^{(t)}, y) = \min\{1, \frac{\pi(y)q(x^{(t)}|y)}{\pi(x^{(t)})q(y|x^{(t)})}\}$$
set $x^{(t+1)} = y$ (acceptance),
else set $x^{(t+1)} = x^{(t)}$ (rejection).

Note that:

- Any normalising constant in $\pi(x)$ is not required to run the algorithm, as it cancels in the ratio.

- If $q(y|x) = \pi(y)$, then we obtain independent samples.

- Usually q is chosen so that $q(y|x)$ is easy to sample from.

Typically, a burn in period is allowed in initial simulations and an average is taken of a subset of the remaining simulations.

3.3 Reversible jump MCMC

3.3.1 Reversibility

A Markov chain with transition kernel $p(y|x)$ and invariant distribution $\pi(x)$ is reversible if:

$$\pi(x)p(y|x) = \pi(y)p(x|y).$$

- This is a sufficient condition for $\pi(x)$ to be the invariant distribution of $p(.|.)$.
- Reversibility is *not* a necessary condition for MCMC to work.

3.3.2 Jump

Green (1995) extended the Metropolis-Hastings algorithm for varying dimensional state space.

Let $k \in Z$. Conditional on k, the state space is assumed to be m_k dimensional. Recall that the acceptance ratio is:

$$\alpha(x^{(t)}, y) = \min\{1, \frac{\pi(y)q(x|y)}{\pi(x)q(y|x)}\}.$$

We now require that the numerator and denominator have densities with respect to a common dominating measure ("dimension-balancing"). That is, a dominating measure for the joint distribution of the current state (in equilibrium) and the next one. We need to find a bijection

$$(x, u) \leftrightarrow (y, v)$$

where u and v are random numbers so that $\dim(x, u) = \dim(y, v)$ and $(y, v) = T(x, u)$, where the transformation is one-to-one.

Now the acceptance probability becomes:

$$\alpha((x, u), (y, v)) = \min\{1, \frac{\pi(y)g_2(v)}{\pi(x)g_1(u)}|\frac{\partial T(x, u)}{\partial(x, u)}|\},$$

where $g_1(u)$ and $g_2(v)$ are the densities of u and v.

The Appendix gives a simple worked example of a reversible jump MCMC implementation.

3.4 MCMC implementation

Recall that, for the MCMC implementation, at each iteration, we generate $\mathbf{\Theta}_{new}$ (usually from a proposal distribution g) and calculate the Hastings' ratio

$$p = \frac{\pi[\mathbf{\Theta}_{new}|Y]g(\mathbf{\Theta}_{old}|\mathbf{\Theta}_{new})}{\pi[\mathbf{\Theta}_{old}|Y]g(\mathbf{\Theta}_{new}|\mathbf{\Theta}_{old})}.$$

In some cases the proposal density is symmetric, $g(\boldsymbol{\Theta}_{old}|\boldsymbol{\Theta}_{new}) = g(\boldsymbol{\Theta}_{new}|\boldsymbol{\Theta}_{old})$, in which cases $p = \pi[\boldsymbol{\Theta}_{new}|Y]/\pi[\boldsymbol{\Theta}_{old}|Y]$. We accept $\boldsymbol{\Theta} = \boldsymbol{\Theta}_{new}$ with probability $\min(1, p)$, otherwise we keep $\boldsymbol{\Theta} = \boldsymbol{\Theta}_{old}$, *i.e.* if $p \geq 1$, we take $\boldsymbol{\Theta} = \boldsymbol{\Theta}_{new}$, whereas if $p < 1$, we perform a further randomisation by drawing a random sample from uniform (0,1), and accept $\boldsymbol{\Theta} = \boldsymbol{\Theta}_{new}$ with probability p. Typically, a burn in period would be allowed for the initial simulations and then an average is taken of a subset of the remaining simulations, although this is not quite appropriate here.

How to construct a Markov chain has been addressed above. At each iteration we first propose a type of change, chosen at random, from the following proposals:

- Slope - choose a plane at random, and vary the one of slopes as for 2D. The likelihood will only change for this single plane. Assume it is β_{x_k} on the k^{th} plane that has been moved, then we can write the Hastings' ratio p as

$$\frac{prior(\beta_{x_{new}})}{prior(\beta_{x_{old}})} \times \prod_{\pi(i,l,j)=k} \exp\left\{-\frac{1}{2}\left(\frac{(y_{ilj} - \alpha_{k(i,l,j)} - \beta_{x_{new},k(i,l,j)}x_i - \beta_{z_k}z_l)^2}{\sigma^2_{new,k}} - \frac{(y_{ilj} - \alpha_{k(i,l,j)} - \beta_{x_{old},k(i,l,j)}x_i - \beta_{z_k}z_l)^2}{\sigma^2_{old,k}}\right)\right\}$$

  The product is over the intersection points y_{ilj} lying on the k^{th} fracture.

- Intercept - similarly, choose a plane at random, and change the intercept, α. Allow a move up/down that is no more than 5 or 10% of the length of the borehole (proposed from a uniform distribution). The ratio p will be similar to as above, but the prior terms for α_{new} and α_{old} cancel out:

$$\prod_{\pi(i,l,j)=k} \exp\left\{-\frac{1}{2\sigma^2_k}\left((y_{ilj} - \alpha_{new,k(i,l,j)} - \beta_{x_{k(i,j)}}x_i - \beta z_{k(i,j)}z_l)^2 - (y_{ilj} - \alpha_{old,k(i,l,j)} - \beta_{k(i,l,j)}x_i - \beta_{z_{k(i,j)}}z_l)^2\right)\right\} \quad .$$

- Labels - choose a borehole at random, and from it choose two adjacent intersection points. Swap over the fracture labels associated with each intersection point, so each is now identified with a different fracture plane. The likelihood will only change at two points on borehole i, l, at j_1 and j_2 say. Assume these are originally associated

with planes k_1 and k_2 respectively. In this case the ratio can be written

$$\exp\left\{-\frac{1}{2}\left(\frac{\left(y_{ilj_1}-\alpha_{k_2}-\beta_{x_{k_2}}x_i-\beta_{z_{k_2}}z_l\right)^2}{\sigma_{k_2}^2}-\frac{\left(y_{ilj_1}-\alpha_{k_1}-\beta_{x_{k_1}}x_i-\beta_{z_{k_1}}z_l\right)^2}{\sigma_{k_1}^2}\right.\right.$$
$$\left.\left.-\frac{\left(y_{ilj_2}-\alpha_{k_2}-\beta_{x_{k_2}}x_i-\beta_{z_{k_2}}z_l\right)^2}{\sigma_{k_2}^2}+\frac{\left(y_{ilj_2}-\alpha_{k_1}-\beta_{x_{k_1}}x_i-\beta_{z_{k_1}}z_l\right)^2}{\sigma_{k_1}^2}\right)\right\}$$

- Endpoints - choose at random two planes which have edgepoints that are on adjacent boreholes; by this we mean they are *first/second order?* neighbours. This requires a list of all adjacent pairs of planes, the direction of the swap to be chosen at random. Assuming it has at least two points, move the adjacent edgepoint of the "left hand" plane to be an edgepoint of the "right hand" plane (or vice versa). The likelihood will only change at a single point, with two planes involved k_1 ("left hand" one) and k_2 ("right hand" one). The ratio becomes

$$\exp\left\{-\frac{1}{2}\left(\frac{\left(y_{ilj}-\alpha_{k_2}-\beta_{x_{k_2}}x_i-\beta_{z_{k_2}}z_l\right)^2}{\sigma_{k_2}^2}-\frac{\left(y_{ilj}-\alpha_{k_1}-\beta_{x_{k_1}}x_i-\beta_{z_{k_1}}z_l\right)^2}{\sigma_{k_1}^2}\right)\right\}$$

- Split - choose a plane at random, and split it into two. In this case the ratio can be written as follows (assume that it is the k^{th} plane that is being split into k_1 and k_2):

$$\frac{p(K+1)prior(\beta_{x_k})prior(\beta_{z_k})}{p(K)prior(\beta_{x_{k_1}})prior(\beta_{x_{k_2}})prior(\beta_{z_{k_1}})prior(\beta_{z_{k_2}})}$$
$$\times\prod_{\pi(i,l,j)=k_1}\exp\left\{-\frac{1}{2}\left(\frac{(y_{ilj}-\alpha_k-\beta_{x_k}x_i-\beta_{z_k}z_l)^2}{\sigma_k^2}-\frac{(y_{ilj}-\alpha_{k_1}-\beta_{x_{k_1}}x_i-\beta_{z_{k_1}}z_l)^2}{\sigma_{k_1}}\right)\right\}$$
$$\times\prod_{\pi(i,l,j)=k_2}\exp\left\{-\frac{1}{2}\left(\frac{(y_{ilj}-\alpha_k-\beta_{x_k}x_i-\beta_{z_k}z_l)^2}{\sigma_k^2}-\frac{(y_{ilj}-\alpha_{k_2}-\beta_{x_{k_2}}x_i-\beta_{z_{k_2}}z_l)^2}{\sigma_{k_2}}\right)\right\}$$
$$\times\frac{\phi(\alpha_{k_1})\phi(\beta_{x_{k_1}})\phi(\beta_{z_{k_1}})\phi(\alpha_{k_2})\phi(\beta_{x_{k_2}})\phi(\beta_{z_{k_2}})}{\phi(\alpha_k)\phi(\beta_{x_k})\phi(\beta_{z_k})}$$

- Join - choose at random two planes where edgepoints are at adjacent boreholes, and join them together. Again the number of planes is changing, which makes for a slightly more complicated ratio (assume this time that it is planes k_1 and k_2 that are to be joined, denote the new, larger plane by k):

$$\frac{p(K-1)prior(\beta_{x_{k_1}})prior(\beta_{z_{k_1}})prior(\beta_{x_{k_2}})prior(\beta_{z_{k_2}})}{p(K)prior(\beta_{x_k})prior(\beta_{z_k})}$$
$$\times\prod_{\pi(i,l,j)=k_1}\exp\left\{-\frac{1}{2}\left(\frac{(y_{ilj}-\alpha_k-\beta_{x_k}x_i-\beta_{z_k}z_l)^2}{\sigma_k^2}-\frac{(y_{ilj}-\alpha_{k_1}-\beta_{x_{k_1}}x_i-\beta_{z_{k_1}}z_l)^2}{\sigma_{k_1}}\right)\right\}$$

$$\times \prod_{\pi(i,l,j)=k_2} \exp\left\{-\frac{1}{2}\left(\frac{(y_{ilj}-\alpha_k-\beta_{x_k}x_i-\beta_{z_k}z_l)^2}{\sigma_k^2}-\frac{(y_{ilj}-\alpha_{k_2}-\beta_{x_{k_2}}x_i-\beta_{z_{k_2}}z_l)^2}{\sigma_{k_2}}\right)\right\}$$
$$\times \frac{\phi(\alpha_k)\phi(\beta_{x_k})\phi(\beta_{z_k})}{\phi(\alpha_{k_1})\phi(\beta_{x_{k_1}})\phi(\beta_{z_{k_1}})\phi(\alpha_{k_2})\phi(\beta_{x_{k_2}})\phi(\beta_{z_{k_2}})}$$

- Standard variation

For more details about how these are implemented in practice, see Mardia *et al.*, (2005).

4 Simulated Data

We study an artificial dataset which was generated as follows. We take the size of the 3D box as having $1 \times 1 \times 1$ units. The centre points of the fractures were generated from a homogeneous Poisson process with an intensity value of 5. In this particular realisation, 5 points were generated and hence 5 fractures generated, in the following way.

The 3D fractures were defined by ellipses (centred on the points obtained above), which in turn were defined by the sizes of major and minor axis (a and b), the dip direction and dipping angles of the fracture plane (α and β), and the angle between the major axis and the dip direction (on the plane), γ. These five parameters were generated randomly from uniform distributions in the following ranges:

- $a \sim U(0.4, 0.8)$
- $b \sim U(0.2, 0.4)$
- $\alpha \sim U(0, 2\pi)$
- $\beta \sim U(-\pi/2, \pi/2)$
- $\gamma \sim U(-\pi, \pi)$

After the fractures were generated, 16 drill holes arranged in a regular 4×4 grid were used to sample the fractures. The locations of these drill holes used were:

- (0.2, 0.2) (0.2, 0.4) (0.2, 0.6) (0.2, 0.8)
- (0.4, 0.2) (0.4, 0.4) (0.4, 0.6) (0.4, 0.8)
- (0.6, 0.2) (0.6, 0.4) (0.6, 0.6) (0.6, 0.8)
- (0.8, 0.2) (0.8, 0.4) (0.8, 0.6) (0.8, 0.8)

There were 35 intersections between the 16 drillholes and the 5 fractures.

Currently only the (x, y, z) coordinates of the intersection are used, but potentially we could also use directional cosines of the normal vector of the intersection plane, if this information was shown to be available in real applications.

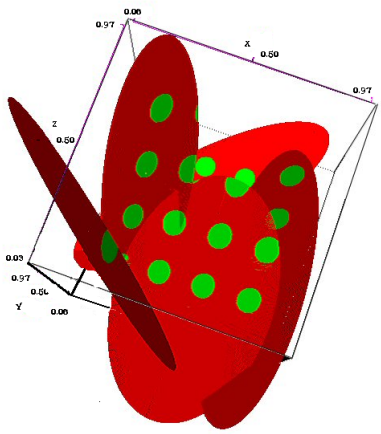


Figure 1: Actual fractures with borehole intersections

Figure 1 shows the intersection of the boreholes with actual fractures.

4.1 Parameters

We start with each intersection point having a plane assigned to it, with slopes having values 1.3, and 0.7, and the value of the intercept set so that the plane passes through the point. Thus we start with 35 planes.

Prior values:

- prior mean for θ, angle for first slope *i.e.* $\beta_x = 0.88$
- prior mean for ψ, angle for second slope *i.e.* $\beta_z = 0.88$
- concentration parameter κ for prior distribution for slope angles *i.e.* θ and $\psi = 5$
- proposal κ for θ and $\psi = 2$
- $\lambda = 3.5$ (for Poisson number of fractures)

- Normal proposal $\sigma = 0.05, 0.9, 1.0$ (for intercept and slopes proposals)

A Gibbs sampler was used to update σ. We take a gamma prior for σ^{-2} *i.e.* $\sigma^{-2} \sim \Gamma(\alpha_\sigma, \beta_\sigma)$. The posterior distribution for σ^{-2} is also a Gamma distribution:

$$\sigma^{-2} \sim \Gamma\left(\alpha_\sigma + K/2, \beta_\sigma + (1/4) \sum_{\pi(i,l,j)=k} \frac{(y_{ilj} - \alpha_{k(i,l,j)} - \beta_{x_{k(i,j)}} x_i - \beta_{z_{k(i,j)}} z_l)^2}{\sigma_k^2}\right)$$

We used $\alpha_\sigma = 1, \beta_\sigma = 2$.

4.2 Results

Figure 2 is a plot of fitted planes. There are 5 fitted fractures. This run took about 50000 iterations. Figure 3 shows a histogram for $\log \sigma$ and traces for σ, loglikelihood and number of planes. Number of planes steadily decrease and stabilises around 5 after 50000 iterations including 20000 for burn-in. Figure 4 shows histogram and traces of parameters for fitted planes. Figure 5 shows histogram of parameters for all fitted planes.

Tables 1 and 2 give summary statistics after burn-in period. Mean and variance for σ and number of planes are given in Table 1; the mean and variance for parameters for each plane are given in Table 2.

4.3 Goodness of fit

Still needs clarification, results (values!), and then conclusions as to the goodness of fit!!

Consider just one fitted plane at present. At each 10000^{th} iteration (after burn in), let $\mathbf{x}_m$ be the unit normal to the plane, $m = 1, \ldots, M$, where M will be in the region of about 10. Calculate

1. $\bar{\mathbf{x}} = \frac{1}{M} \sum_m \mathbf{x}_m$,
2. $\bar{R} = ||\bar{\mathbf{x}}||$,
3. $\bar{C} = \frac{1}{M} \sum_m \mathbf{x}_m' \mu_0$,

where μ_0 is the unit normal of the true plane (ellipse) (not normally available for real data).

Test $H_0 : \mu = \mu_0$ using

$$\frac{(\bar{R} - \bar{C})/(p-1)}{(1-\bar{R})/\{(n-1)(p-1)\}} \sim F_{p-1,(n-1)(p-1)}.$$

(See Mardia and Jupp, 1999, p 214). Here $p = 3, n = M$.

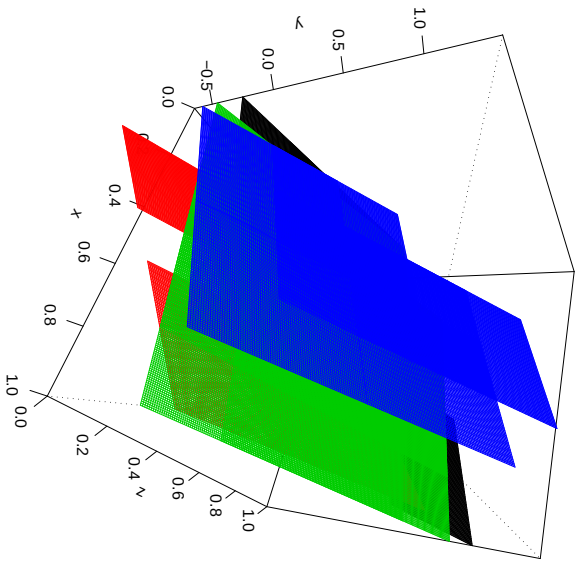


Figure 2: Fitted planes

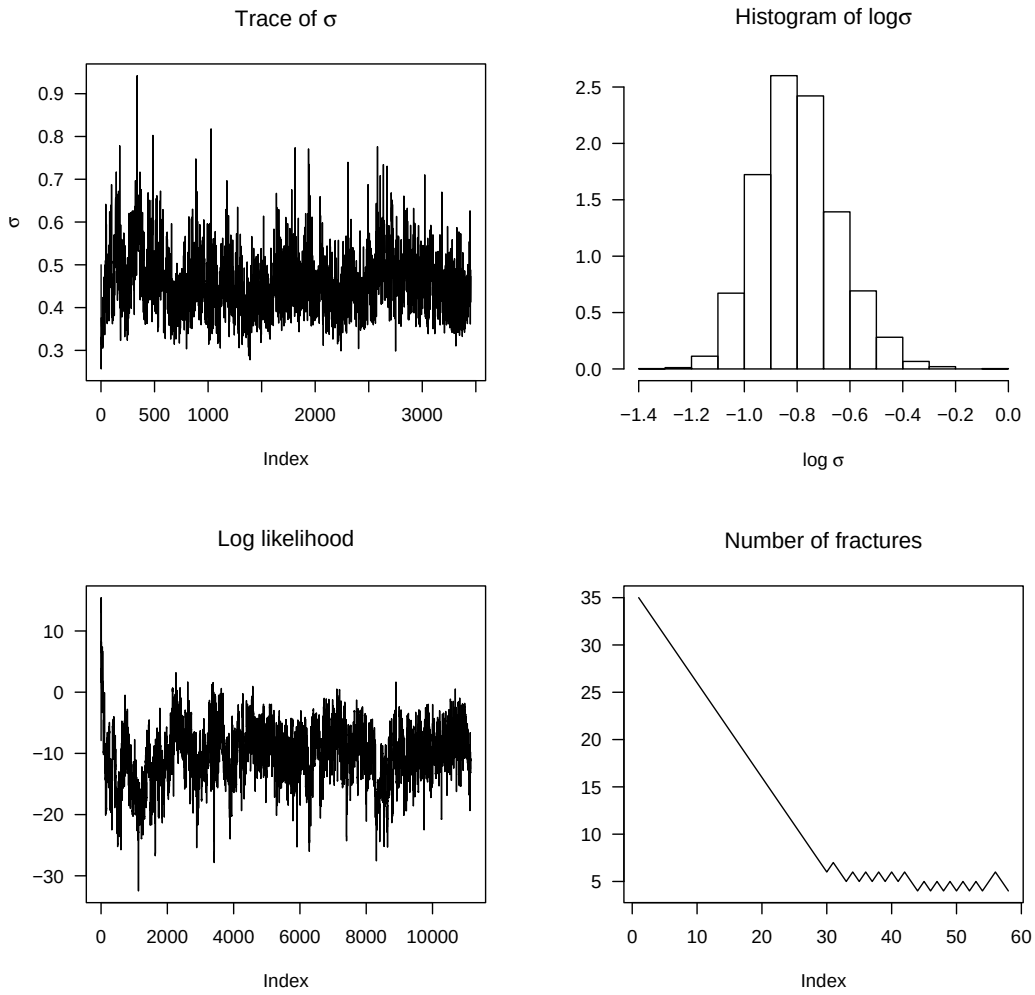
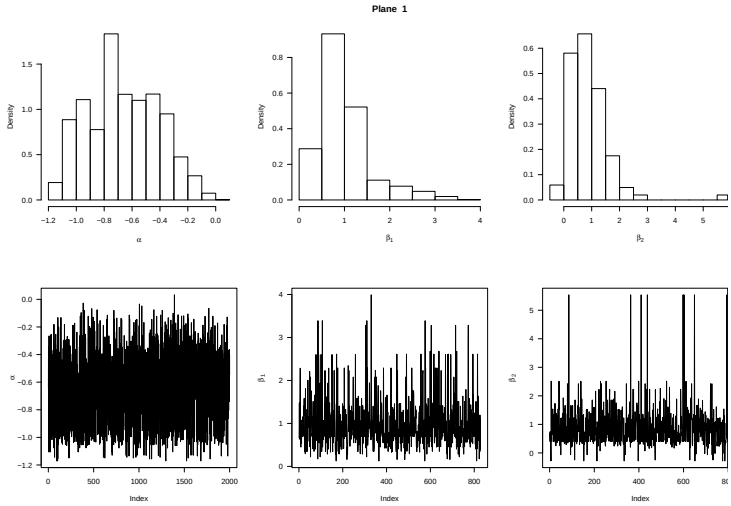
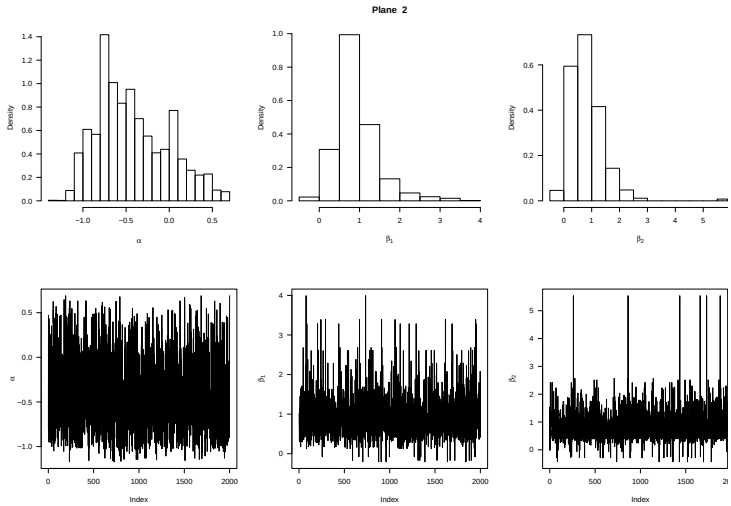
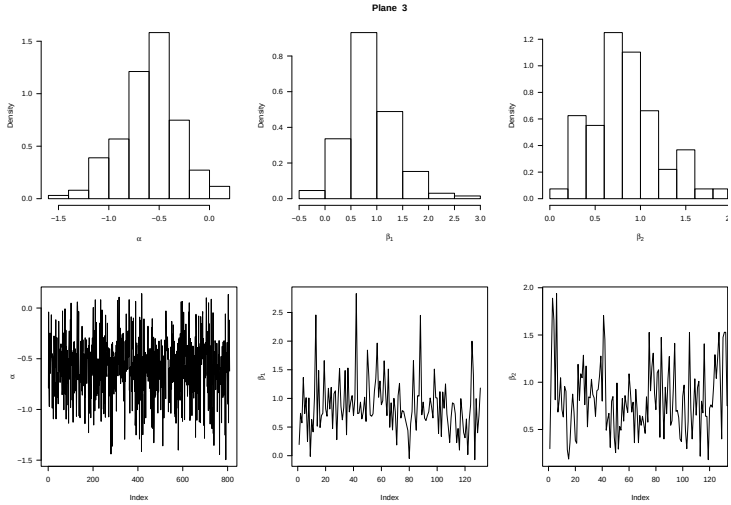
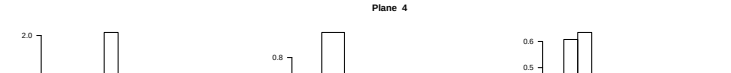


Figure 3: Plot of $\log \sigma$ histogram and traces for σ, loglikelihood and number of planes.


Plane 1
Density
α
β1
β2
Index


Plane 2
Density
α
β1
β2
Index


Plane 3
Density
α
β1
β2
Index


Plane 4
Density
Index

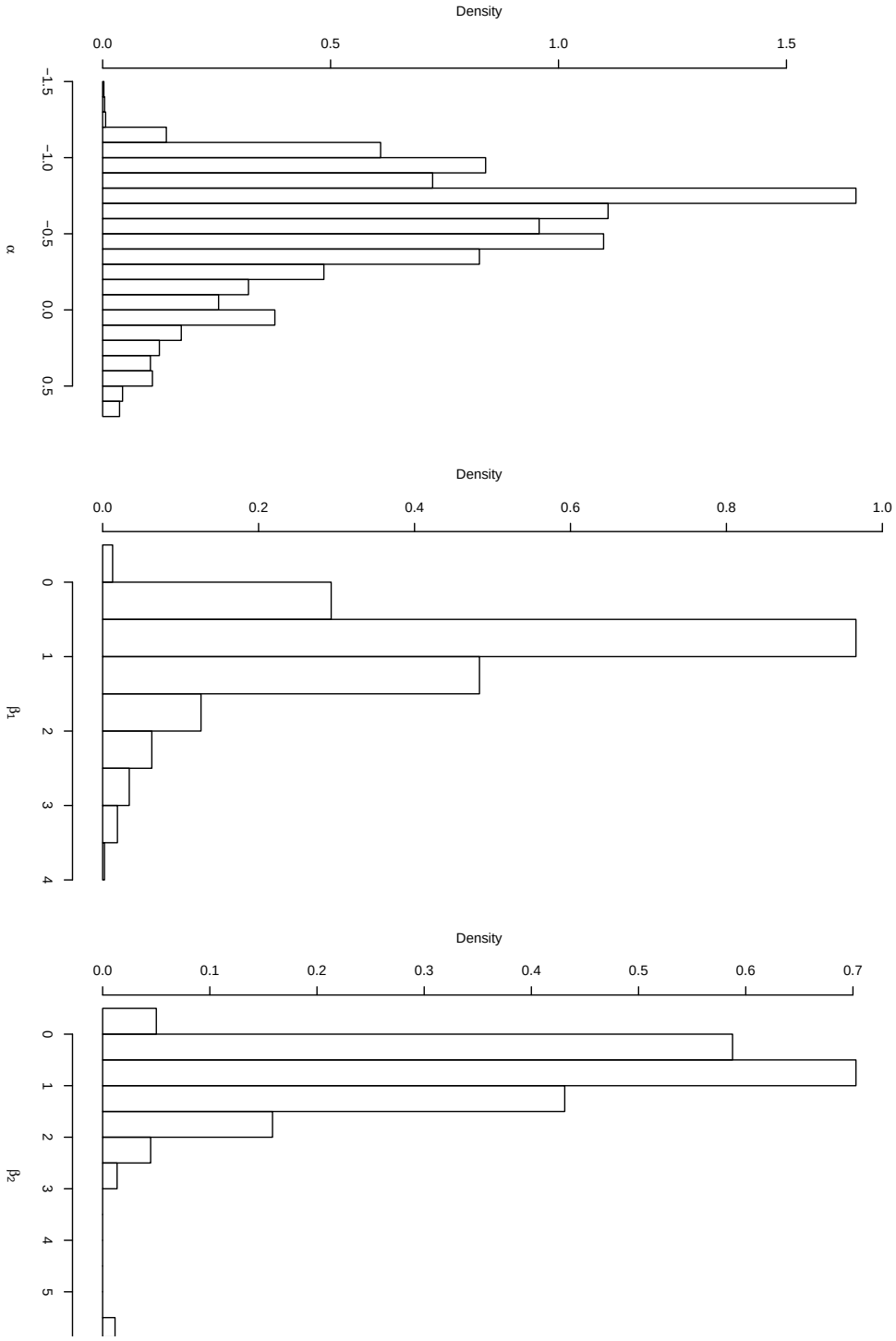


Figure 5: Histogram of parameters for all fitted planes

5 Real Data

We study a real dataset, which was in the form of a metre cubed granite block, sectioned into seven slices. All joints were located and recorded, and the joint planes obtained by stacking strike lines, see Martin *et al.* (2005) for details. This data was then discretised: using the grid size of 20x10 we created a regular drillhole grid of 11x12. These drillholes had 161 intersections with the 392 fractures. Of these fractures, over 200 are small (not extending outside of the block), and they are just 10-20 which are dominant.

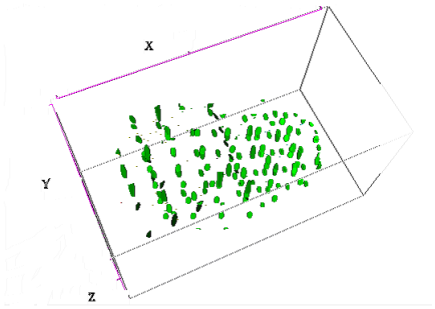


Figure 6: Actual fractures with borehole intersections

Figure 6 shows the intersection of the boreholes with actual fractures, and 7 shows the actual planes.

5.1 Parameters

We start with each intersection point having a plane assigned to it, with slopes having values 1.0, and 0.5, and the value of the intercept set so that the plane passes through the point. Thus we start with 35 planes.

Prior values:

- prior mean for θ, angle for first slope *i.e.* $\beta_x = 0.5$
- prior mean for ψ, angle for second slope *i.e.* $\beta_z = 0.9$

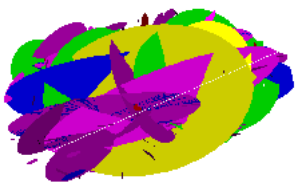


Figure 7: Actual planes

- concentration parameter κ for prior distribution for slope angles *i.e.* θ and $\psi = 2$
- proposal κ for θ and $\psi = 1$
- $\lambda = 0.001$ (for Poisson number of fractures)
- Normal proposal $\sigma = 3.5, 2.9, 0.5$ (for intercept and slopes proposals)

We used $\alpha_\sigma = 1, \beta_\sigma = 2$.

5.2 Results

Figure 8 is a plot of fitted planes. There are 74 fitted fractures. This solution is after 20000 iterations. Figure 9 shows a histogram for $\log \sigma$ and traces for σ, loglikelihood and number of planes for a thinned sample. The number of planes steadily decrease and stabilises around 74. Figure 10 shows histogram and traces of parameters $\alpha_k, \beta_{x_k}, \beta_{z_k}$ for some, typical selected fitted planes. One can see that the chain has reached equilibrium. Figure 11 shows histogram of parameters for all fitted planes. The distribution for the intercept is clearly bimodal, since there are two 'sets', one approximately perpendicular to the other; while those for the slopes are unimodal.

The mean and variance for parameters for each plane are given in Table 3.

5.3 Goodness of fit

Still needs clarification, results (values!), and then conclusions as to the goodness of fit!!

6 Discussion

In Mardia *et al* (2005) we presented a method of fitting lines to fractures for borehole data in two dimensions. This has now been successfully implemented in three dimensions. As we noted then, with the form of the data available, we can only measure the extent of a fracture over the boreholes it intersects, so we be estimating its smallest size. The true fracture is almost certainly of greater extent, which needs to be addressed.

Currently the implementation is such that the fractures themselves have no width (or aperture), an issue which is being addressed.

In both the 2D and 3D work, the spacing between boreholes is obviously very important. If the spacing could be narrowed, we would expect the fit of our fractures to be better, and the distributions for the parameters to be less variable. Conversely, wider spacing will be used to test the robustness of our methods.

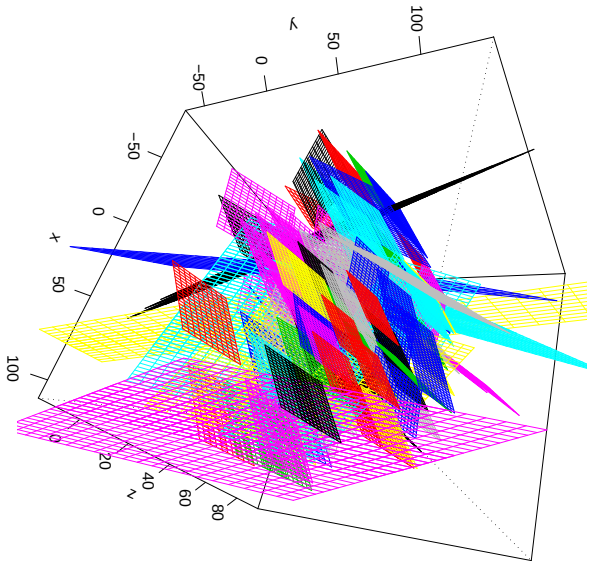


Figure 8: Fitted planes

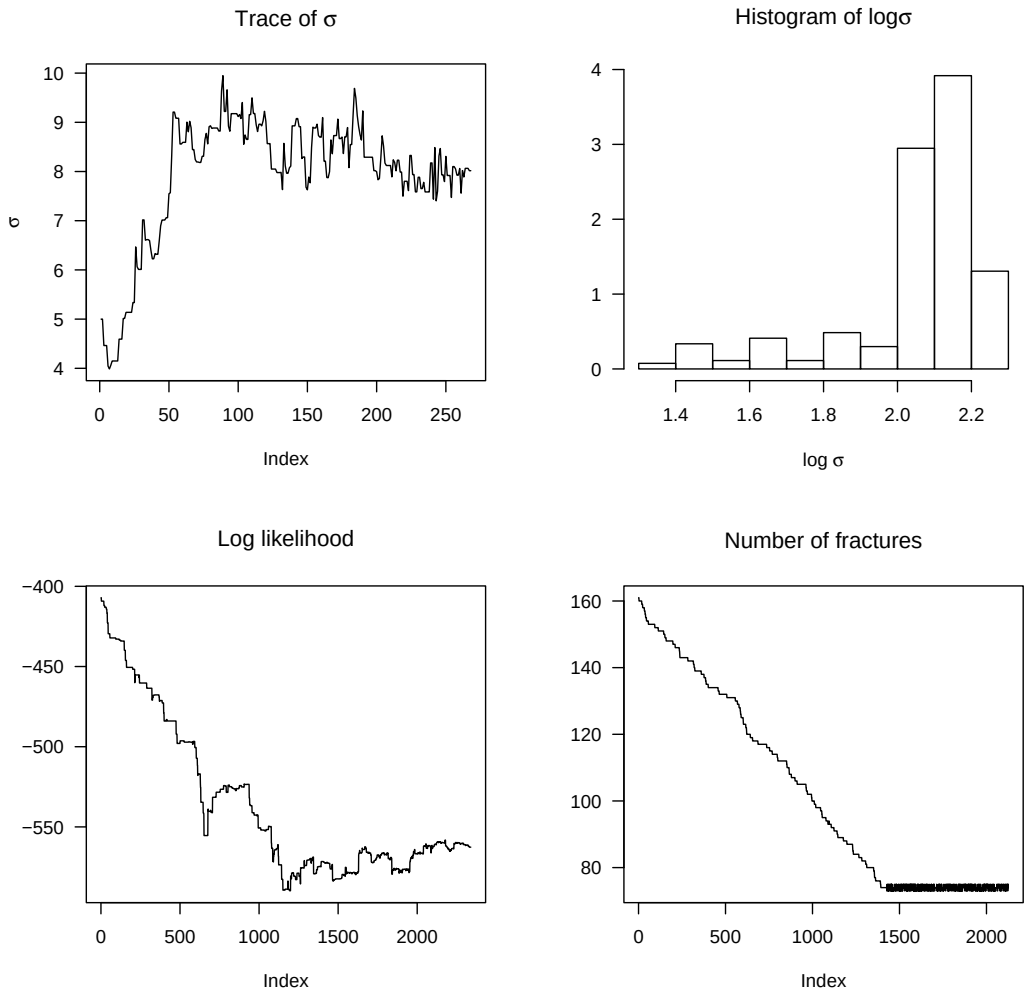
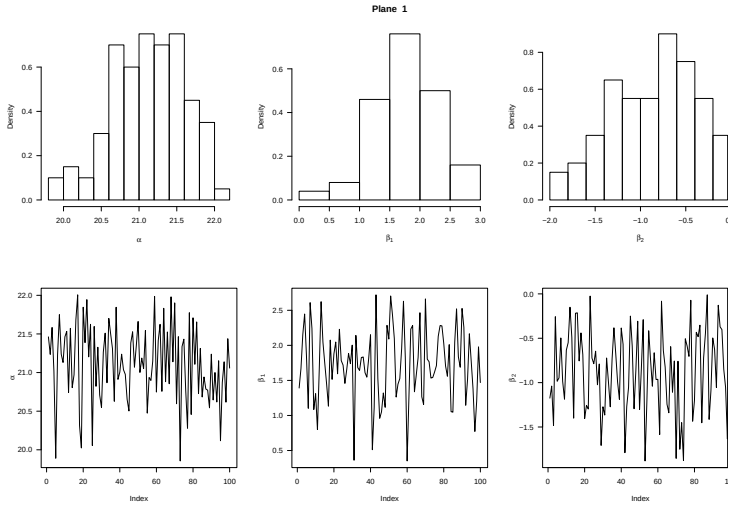
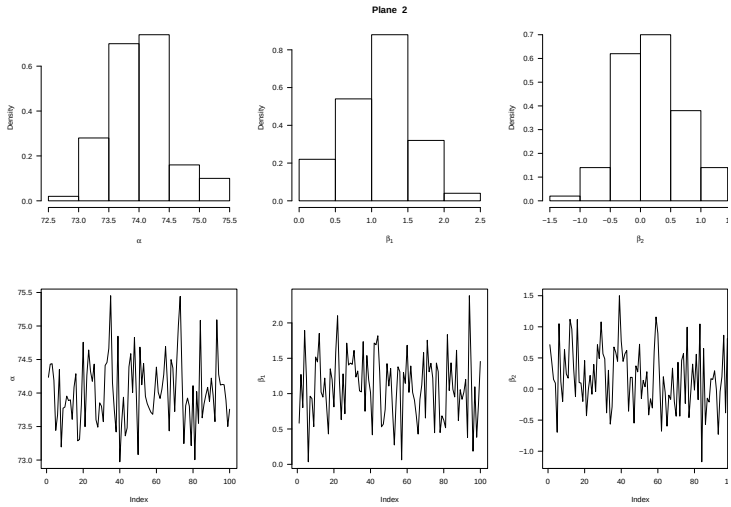
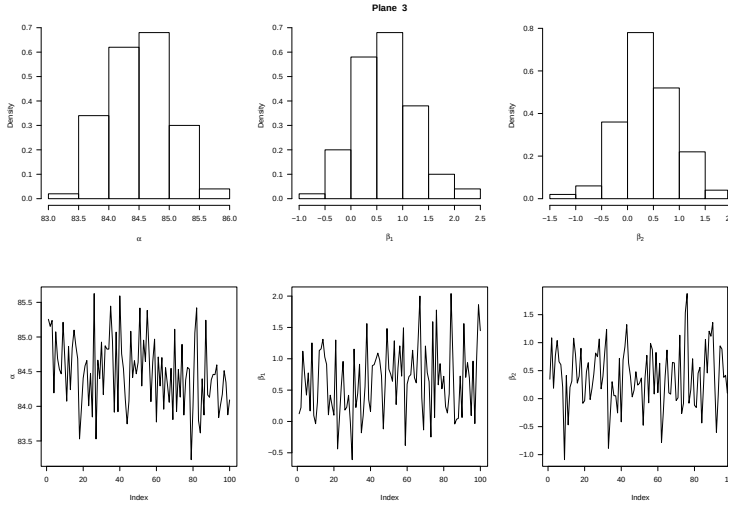
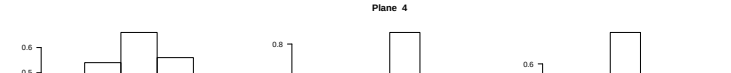


Figure 9: Plot of $\log \sigma$ histogram and traces for σ, loglikelihood and number of planes.


Plane 1
Density
α
β1
β2
Index


Plane 2
Density
α
β1
β2
Index


Plane 3
Density
α
β1
β2
Index


Plane 4
Density

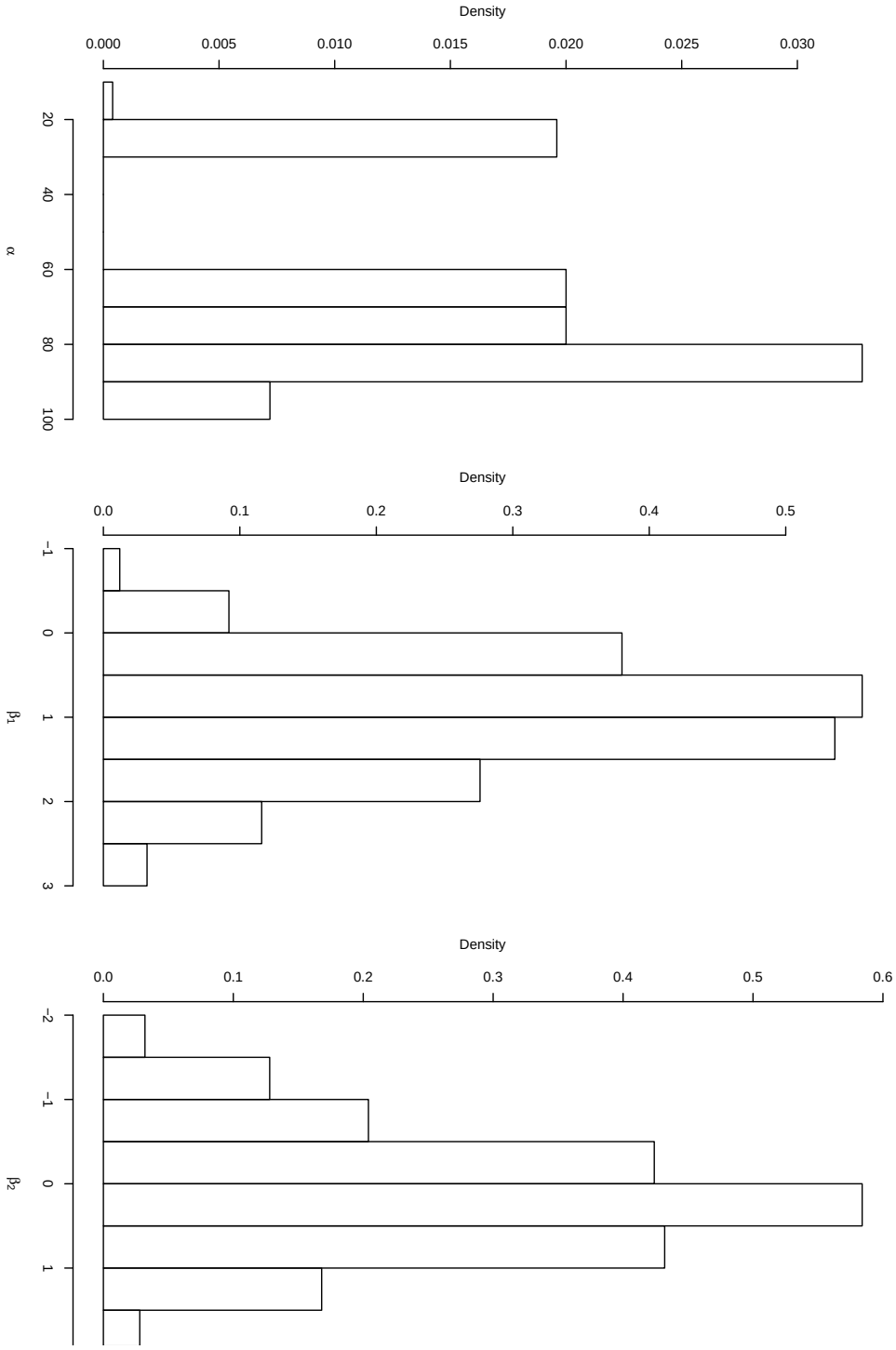


Figure 11: Histogram of parameters for all fitted planes

Whilst the above work was done using regular spacing between boreholes in both directions, that is highly unlikely to be available in practice. Fortunately this is not a pre-requisite of the work. When boreholes are not regular (but still vertical) in 3D, then a Dirichlet tessellation would first be required, to obtain some kind of neighbourhood structure. Everything would then follow through as before.

Need to mention the 'Leeds Rock Fracture Data Set', and if it's available the proper url of where to find it, Martin et al, (2005). Currently, http://www.leeds.ac.uk/leeds/newpages/srfwww
.

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parameter	Mean	Variance
σ	0.452	0.004
K	5	0.538

Table 1: Summary statistics for variance and number of planes (K)

	Mean			Variance		
Plane	α	β_1	β_2	α	β_1	β_2
1	-0.6606222	0.9888447	0.8921117	0.06315236	0.3221692	0.5064716
2	-0.4232051	0.9144914	0.8347839	0.16872656	0.2756030	0.3374168
3	-0.5874654	0.8730266	0.8347474	0.08249880	0.2310765	0.1329101
4	-0.6692581	1.0076696	0.8674655	0.05821510	0.3531499	0.4335066

Table 2: Summary statistics for intercept and slopes for each plane

	Mean			Variance		
Plane	α	β_1	β_2	α	β_1	β_2
1	21.11648	1.7286239	-0.8579004	0.2415271	0.2651661	0.2215859
2	74.02104	1.1009483	0.1884384	0.2506027	0.2130126	0.2530745
3	84.49335	0.6528070	0.3913499	0.2565937	0.3142909	0.2886932
4	89.78068	0.7286372	0.3970051	0.2719496	0.2516330	0.2632971
5	65.31833	0.6756642	0.5274866	0.2985271	0.2588637	0.2436438

Table 3: Summary statistics for intercept and slopes for each plane

Appendix: an illustrative example of reversible jump

Recall that the problem is to construct a Markov chain whose stationary distribution is $\pi(x)$. Suppose here that we have just two states (or dimensions). State 1 has one variable, $X = \theta$, while state 2 has two, $X' = (\theta_1, \theta_2)$. (At each step, the chain produced will have either one or two values). Let us take

$$\pi(X) = q_1 N_1(\frac{y_1 + y_2}{2}, \sigma^2) \tag{1}$$

and

$$\pi(X') = q_2 N_2 \left(\begin{pmatrix} y_1 \\ y_2 \end{pmatrix}, \sigma_\pi^2 I_2 \right) \tag{2}$$

where $q_1 + q_2 = 1$. Here π is the target (posterior) distribution, as in Sections 2 and 3. y_1 and y_2 are simply data values, and there is nothing special about our use of the normal distribution. (We will assume here that the pdf is too difficult to simulate from directly!) We shall proceed by proposing new values for the chain, and allowing transitions between the two states. Let p_{ij} be the probability of choosing state j given you are in state i. To transform between different dimensions, $X \to X'$, say, propose X', from $g(X, X')$. There will be four proposals needed in all (we either stay in the state we are in, or swap to the other one):

1. $g(X, X')$:
$$\begin{pmatrix} \theta_1^{new} \\ \theta_2^{new} \end{pmatrix} \sim N_2 \left(\begin{pmatrix} \theta \\ \theta \end{pmatrix}, \sigma_g^2 I_2 \right)$$

2. $g(X', X)$:
$$\theta^{new} \sim N_1(\frac{\theta_1 + \theta_2}{2}, \tau^2)$$

3. $g(X, X)$:
$$\theta^{new} \sim N(\theta^{old}, \tau^2)$$

4. $g(X', X')$:
$$\begin{pmatrix} \theta_1^{new} \\ \theta_2^{new} \end{pmatrix} \sim N_2 \left(\begin{pmatrix} \theta_1^{old} \\ \theta_2^{old} \end{pmatrix}, \sigma_g^2 I_2 \right)$$

From Green, (1995), p715, Hastings' ratio for acceptance (for state 1 to state 2) is:

$$\frac{\pi(dX')g(X', dX)}{\pi(dX)g(X, dX')}$$

If we were in state 1, with some $X = \theta$ given, we then simulate a new state - assume this to be 2. We would then propose new values for θ_1, θ_2, simulated from $g(X, X')$. The acceptance probability for this transition from state 1 $\rightarrow$ state 2 is

$$\alpha = \min\{1, \frac{q_2\ \phi(\theta_1^N; y_1, \sigma_\pi^2)\ \phi(\theta_2^N; y_2, \sigma_\pi^2)\ p_{21}\ \phi(\theta; (\theta_1^N + \theta_2^N)/2, \tau^2)}{q_1\ \phi(\theta; (y_1 + y_2)/2, \sigma^2)\ p_{12}\ \phi(\theta_1^N; \theta, \sigma_g^2)\ \phi(\theta_2^N; \theta, \sigma_g^2)}\}.$$

The superscript N differentiates between the proposed, new values, and the previous (current) values. The acceptance prob for state 2 $\rightarrow$ state 1 is as above, with the final term inverted.

The acceptance prob. for state 1 $\rightarrow$ state 1 simplifies to

$$\alpha = \min\{1, \frac{\phi(\theta^N; (y_1 + y_2)/2, \sigma^2)}{\phi(\theta; (y_1 + y_2)/2, \sigma^2)}\},$$

whilst the acceptance prob. for state 2 $\rightarrow$ state 2 simplifies to

$$\alpha = \min\{1, \frac{\phi(\theta_1^N; y_1, \sigma_\pi^2)\ \phi(\theta_2^N; y_2, \sigma_\pi^2)}{\phi(\theta_1; y_1, \sigma_\pi^2)\ \phi(\theta_2; y_2, \sigma_\pi^2)}\}.$$

We now try to illustrate how this works in practice. In all three sets of results that follow, we let $\sigma = 1, \sigma_\pi = 2, \tau = 3, \sigma_g = 2, y_1 = -2, y_2 = 5$ in (1) and (2), and the program was run for 100,000 iterations. The summary statistics for the chain can be viewed for each of the two states. For the values above, the approximate results we should expect to see are as follows:

- θ: mean = 1.5, sd = 1.0
- θ_1: mean = -2.0, sd = 2.0
- θ_2: mean = 5.0, sd = 2.0

At every step (iteration) whichever state we are in, one of the proposals is chosen at random, and there is then a probability of transition to the other state or staying put. Whichever happens, a new value or values is/are generated, and accepted or not with the probabilities above. The next value(s) in the chain is either the new value(s) obtained, or the old value(s) repeated. It is important to note that if we are state 1, say, then we stay in state 1 in one of two ways; either a transition is rejected (and so the next value in the chain is the same as the previous), or else we accept a transition from state 1 to state 2 (in which case we get a new value in the chain).

6.1 $p_{21} = p_{12} = 0.5$

With these values of p, for whichever state you are in, there is an equal chance of attempting a transition, as there is of generating new value(s) from the same state.

6.1.1 $q_1 = q_2 = 0.5$

With these values of q we would expect the chain to spend approximately equal amounts of time in each of the two states. The following table gives the number of proposed and accepted transitions from and to each state, and summary statistics for each of the two states. n denotes how long the chain spent in each state:

- State 1 → State 1: 8940/23974
- State 1 → State 2: 3347/23654
- State 2 → State 1: 3346/26195
- State 2 → State 2: 14491/26177
- θ: mean = 1.484, sd = 1.025, n = 47627
- θ_1: mean = -1.988, sd = 2.021, n = 52373
- θ_2: mean = 4.990, sd = 2.033, n = 52373

6.1.2 $q_1 = 0.4, q_2 = 0.6$

Here we expect the chain to spend more time in state 2. Transitions from and to each state, and summary statistics:

- State 1 → State 1: 7343/19333
- State 1 → State 2: 3281/19361
- State 2 → State 1: 3281/30646
- State 2 → State 2: 16989/30660
- θ: mean = 1.466, sd = 1.048, n = 38694
- θ_1: mean = -2.056, sd = 2.038, n = 61306
- θ_2: mean = 4.989, sd = 1.995, n = 61306

6.1.3 $q_1 = 0.2, q_2 = 0.8$

Here we expect the chain to spend most of its time in state 2. Transitions from and to each state, and summary statistics:

- State 1 → State 1: 3586/9733
- State 1 → State 2: 2664/9722
- State 2 → State 1: 2663/40141
- State 2 → State 2: 22140/40404
- θ: mean = 1.488, sd = 1.030, n = 19454
- θ_1: mean = -1.994, sd = 2.005, n = 80546
- θ_2: mean = 4.990, sd = 2.007, n = 80546

6.2 $p_{21} = p_{12} = 0.7$

With these values of p, for whichever state you are in, an attempt to switch to the other state is about twice as likely as an attempt to generate a new value(s) from the same state.

6.2.1 $q_1 = q_2 = 0.5$

With these values of q we would expect the chain to spend approximately equal amounts of time in each of the two states. The following table gives the number of proposed and accepted transitions from and to each state, and the summary statistics:

- State 1 → State 1: 5506/14563
- State 1 → State 2: 4698/33789
- State 2 → State 1: 4697/35942
- State 2 → State 2: 8642/15706
- θ: mean = 1.491, sd = 1.038, n = 48351
- θ_1: mean = -1.995, sd = 2.030, n = 51649
- θ_2: mean = 5.029, sd = 2.028, n = 51649

6.2.2 $q_1 = 0.4, q_2 = 0.6$

Here we expect the chain to spend more time in state 2. Transitions from and to each state, and summary statistics:

- State 1 → State 1: 4289/11316
- State 1 → State 2: 4751/26868
- State 2 → State 1: 4750/43124
- State 2 → State 2: 10460/18692
- θ: mean = 1.495, sd = 1.045, n = 38183
- θ_1: mean = -2.030, sd = 1.988, n = 61817
- θ_2: mean = 4.988, sd = 2.050, n = 61817

6.2.3 $q_1 = 0.2, q_2 = 0.8$

Here we expect the chain to spend most of its time in state 2. Transitions from and to each state, and summary statistics:

- State 1 → State 1: 2225/5790
- State 1 → State 2: 3757/13564
- State 2 → State 1: 3756/56422
- State 2 → State 2: 13327/24204
- θ: mean = 1.552, sd = 1.027, n = 19353
- θ_1: mean = -1.988, sd = 2.004, n = 80647
- θ_2: mean = 5.005, sd = 2.031, n = 80647

6.3 $p_{12} = 0.2, p_{21} = 0.7$

With these values of p, when in state 1, the chain is very likely to generate a new value from state 1. However, when in state 2, a transition back to state 1 is most likely to be attempted.

6.3.1 $q_1 = q_2 = 0.5$

With these values of q we would expect the chain to spend approximately equal amounts of time in each of the two states. The following table gives the number of proposed and accepted transitions from and to each state, and the summary statistics:

- State 1 → State 1: 14565/38619
- State 1 → State 2: 2387/9650
- State 2 → State 1: 2387/36071
- State 2 → State 2: 8749/15660
- θ: mean = 1.508, sd = 1.011, n = 48269
- θ_1: mean = -2.057, sd = 1.996, n = 51731
- θ_2: mean = 5.020, sd = 1.951, n = 51731

6.3.2 $q_1 = 0.4, q_2 = 0.6$

Here we expect the chain to spend more time in state 2. Transitions from and to each state, and summary statistics:

- State 1 → State 1: 12051/32499
- State 1 → State 2: 2465/7874
- State 2 → State 1: 2464/41796
- State 2 → State 2: 9895/17831
- θ: mean = 1.493, sd = 1.011, n = 40372
- θ_1: mean = -1.976, sd = 2.017, n = 59628
- θ_2: mean = 5.052, sd = 2.001, n = 59628

6.3.3 $q_1 = 0.2, q_2 = 0.8$

Here we expect the chain to spend most of its time in state 2.

Transitions from and to each state, and summary statistics:

- State 1 → State 1: 5925/16104

- State 1 → State 2: 1849/4086
- State 2 → State 1: 1848/55973
- State 2 → State 2: 13132/23837
- θ: mean = 1.507, sd = 1.031, n = 20189
- θ_1: mean = -1.957, sd = 2.052, n = 79811
- θ_2: mean = 4.962, sd = 2.026, n = 79811

In all of the above examples we are getting summary statistics very much in line with what we expected, with the chain spending time in each of the two states in line with the two q values.