METALLICITY

OCTOBER 30, 2010

1. Mixture model

Given n observed $(\frac{\alpha}{\mathrm{Fe}}, \frac{\mathrm{Fe}}{\mathrm{H}})$ metallicities as $\{(x_i, y_i)\}_{i=1}^{n}$, or as $(\mathbf{x}, \mathbf{y})$, each of which is drawn from one of m known model densities. We model the density of observations using the mixture model

$$f(x, y) = \sum_{j=1}^{m} \pi_j f_j(x, y) \tag{1}$$

where

$$\sum_{j=1}^{m} \pi_j = 1 \qquad \pi_j \geq 0, \quad j = 1, \ldots, m$$

From the summation constraint, $\boldsymbol{\pi}$ has $m-1$ free parameters:

$$\boldsymbol{\pi} = (\pi_1, \ldots, \pi_{m-1}, 1 - \pi_1 - \ldots - \pi_{m-1})$$

Thus the likelihood of (1) is

$$\begin{aligned} L(\boldsymbol{\pi}) &= \prod_{i=1}^{n} f(x_i, y_i) \\ &= \prod_{i=1}^{n} \Big\{ \sum_{j=1}^{m} \pi_j f_j(x_i, y_i) \Big\} \\ \log L(\boldsymbol{\pi}) &= \sum_{i=1}^{n} \log \Big(\sum_{j=1}^{m} \pi_j f_j(x_i, y_i) \Big) \end{aligned}$$

Maximizing $\log L(\boldsymbol{\pi})$ with respect to $\boldsymbol{\pi}$ will yield $\hat{\boldsymbol{\pi}}_{\mathrm{MLE}}$, but this arduous task can be avoided by adding a latent indicator, z, to the observed data $(\mathbf{x}, \mathbf{y})$, representing the model group from which that observation was generated. Let G_j be the j^{th} model group, and let

$$z_{ij} = \mathbf{1}\big\{(x_i, y_i) \mapsto G_j\big\}$$

The complete data likelihood is defined over the complete data $\big\{(x_i, y_i, \mathbf{z}_i)\big\}_{i=1}^{n}$ as

$$L(\boldsymbol{\pi}) = \prod_{i=1}^{n}\prod_{j=1}^{m}\Big\{f_j(x_i, y_i)\Big\}^{z_{ij}}\pi_j^{z_{ij}}$$

$$\ell(\boldsymbol{\pi}) = \sum_{i=1}^{n}\sum_{j=1}^{m} z_{ij}\log\big\{\pi_j f_j(x_i, y_i)\big\} \tag{2}$$

2. Expectation Maximization

One way to estimate $\boldsymbol{\pi}$ is to use a maximum likelihood estimate, $\hat{\boldsymbol{\pi}}$, computed using expectation maximization. Starting from an initial set of guesses, $\boldsymbol{\pi}^{(0)}$, we iteratively find the expected value of the likelihood, (2), conditional on the data, and then find the $\operatorname{argmax}_{\boldsymbol{\pi}}$ of this expectation. The maximizing value the t^{th} iteration, $\hat{\boldsymbol{\pi}}^{(t)}$, is then used as the starting value for the next run, and we continue until the likelihood changes by less than 10^{-3} over twenty five iterations.

2.1. Expectation step.

Expectation step. First we find the expected value of the log likelihood, (2), conditional on the data. Note that since z_{ij} is an indicator function, its expected value is equal to the probability that data point i comes from model j.

$$\mathrm{E}_{\boldsymbol{\pi}}\Big[\ell(\boldsymbol{\pi})\big|\mathbf{x}, \mathbf{y}\Big] = \sum_{i=1}^{n}\sum_{j=1}^{m}\mathrm{E}_{\boldsymbol{\pi}}\big[z_{ij}|x_i, y_i\big]\big\{\log f_j(x_i, y_i) + \log\pi_j\big\} \tag{3}$$

Since we're ultimately maximizing, the non-constant component is of primary interest, and can be analytically specified by applying Bayes' rule:

$$\begin{aligned}
\mathrm{E}_{\boldsymbol{\pi}}\Big[z_{ij}|x_i, y_i\Big] &= \text{Probability}\Big((x_i, y_i) \mapsto G_j\big|x_i, y_i\Big) \\
&= \Pr_{\boldsymbol{\pi}}(z_{ij}|x_i, y_i) \\
&= \frac{p(x_i, y_i|z_{ij} = 1)p(z_{ij} = 1)}{p(x_i, y_i)}
\end{aligned}$$

Thus the expected value of the indicator variable, z_{ij}, given the data and the parameters, $\boldsymbol{\pi}$, of the data's distribution defined by (1) is

$$\mathrm{E}_{\boldsymbol{\pi}}\Big[z_{ij}|x_i, y_i\Big] = \frac{\pi_j f_j(x_i, y_i)}{\sum_{j=1}^{m} \pi_j f_j(x_i, y_i)} \tag{4}$$

To iteratively evaluate this expectation, we let $w_{ij}^{(t)}$ be (4) at the t^{th} step:

$$w_{ij}^{(t+1)} = \begin{cases} \dfrac{\pi_j^{(t)} f_j(x_i, y_i)}{\displaystyle\sum_{k=1}^{m} \pi_k^{(t)} f_k(x_i, y_i)} & j = 1, \ldots, m-1 \\ \\ 1 - w_{i1} - \ldots - w_{i,m-1} & j = m \end{cases}$$

Since $\boldsymbol{\pi}$ is not defined for the first evaluation, we use a random initialization to generate $\mathbf{w}_j^{(0)}$. Convergence is not sensitive to the choice of values in this case, but may be if the likelihood is riddled with local maxima.

2.2. **Maximization step.** We now have an explicit formulation for the expected log likelihood (4) given a single parameter $\boldsymbol{\pi}$, plus the data. The argument of the maximum of (4) at each iteration t provides an estimate that approaches the MLE of $\boldsymbol{\pi}$, and is given by:

$$\hat{\boldsymbol{\pi}}^{(t)} = \underset{\boldsymbol{\pi}}{\operatorname{argmax}} \, \mathrm{E}\Big[\ell(\boldsymbol{\pi})\Big|\mathbf{x}, \mathbf{y}, \hat{\boldsymbol{\pi}}^{(t-1)}\Big] \tag{5}$$

Accounting for the $m-1$ free parameters of $\boldsymbol{\pi}$, differentiation of (4) proceeds, for $k = 1, \ldots, m-1$, as:

$$\frac{\partial}{\partial \pi_k} \mathrm{E}\Big[\ell(\boldsymbol{\pi})\Big|\mathbf{x}, \mathbf{y}\Big] = \sum_{i=1}^{n} \left\{ w_{ik}^{(t-1)} \frac{1}{\pi_k} - w_{im}^{(t-1)} \frac{1}{1 - \pi_1 - \ldots - \pi_{m-1}} \right\}$$

$$\frac{1}{\pi_k} \sum_{i=1}^{n} w_{ik}^{(t-1)} = \frac{1}{1 - \pi_1 - \ldots - \pi_{m-1}} \sum_{i=1}^{n} w_{im}^{(t-1)}$$

Consequently, using some constant, c, we must have

$$\frac{1}{\pi_k} \sum_{i=1}^{n} w_{ik}^{(t-1)} = \ldots = \frac{1}{\pi_{m-1}} \sum_{i=1}^{n} w_{i,m-1}^{(t-1)} = c$$

$$\hat{\pi}_k^{(t)} = \frac{\sum_{i=1}^{n} w_{ik}^{(t-1)}}{c}$$

The unknown constant c appears problematic, but, because $\sum_{j=1}^{m} \pi_j = 1$, algebraic manipulation reveals that $c = n$, yielding a final solution that can be numerically evaluated:

$$\hat{\pi}_k^{(t)} = \frac{\sum_{i=1}^{n} w_{ij}^{(t-1)}}{n}$$
$$\hat{\pi}_m^{(t)} = 1 - \pi_1 - \ldots - \pi_{m-1}$$

In our case, computation of $\hat{\boldsymbol{\pi}}$ converges relatively quickly for all starting values: on the order of 600 iterations, or half a minute, for our stopping criteria. Large π_k values typically emerge after two or three iterations, and most change, absolutely speaking, occurs in the first fifty to one hundred iterations.

3. Covariance and correlation of $\hat{\boldsymbol{\pi}}$

The asymptotic covariance matrix of $\hat{\boldsymbol{\pi}}$ can be approximated by the inverse of the observed Fisher information matrix, I.

As $\pi_m = 1 - \sum_{j=1}^{m-1} \pi_j$, there are only $m-1$ free parameters. Thus let $\boldsymbol{\pi}' = (\pi_1, \ldots, \pi_{m-1})$. Using $f_{ij} = f_j(x_i, y_i)$ for brevity, the likelihood can then be expressed as:

$$\ell(\boldsymbol{\pi}') = \sum_{i=1}^{n} \log \left\{ \left(\sum_{j=1}^{m-1} \pi_j f_{ij} \right) + (1 - \pi_1, \ldots, \pi_{m-1}) f_{im} \right\} \tag{6}$$

The observed information matrix, I, is the $m-1 \times m-1$ negative hessian of (6), evaluated at the observed data points:

$$I(\boldsymbol{\pi}'|\mathbf{x}, \mathbf{y}) = -\frac{\partial^2 \ell(\boldsymbol{\pi}')}{\partial \boldsymbol{\pi}' \partial \boldsymbol{\pi}'^T} = - \begin{bmatrix} \frac{\partial^2 \ell(\boldsymbol{\pi}')}{\partial^2 \pi_1} & \frac{\partial^2 \ell(\boldsymbol{\pi}')}{\partial \pi_1 \partial \pi_2} & \cdots & \frac{\partial^2 \ell(\boldsymbol{\pi}')}{\partial \pi_1 \partial \pi_{m-1}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial^2 \ell(\boldsymbol{\pi}')}{\partial \pi_{m-1} \partial \pi_1} & \frac{\partial^2 \ell(\boldsymbol{\pi}')}{\partial \pi_{m-1} \partial \pi_2} & \cdots & \frac{\partial^2 \ell(\boldsymbol{\pi}')}{\partial^2 \pi_{m-1}} \end{bmatrix}$$

where

$$\frac{\partial \ell(\boldsymbol{\pi}')}{\partial \pi_k} = \sum_{i=1}^{n} \frac{f_{ik} - f_{im}}{\sum_{j=1}^{m} \pi_j f_{ij}} \qquad \text{and} \qquad \frac{\partial^2 \ell(\boldsymbol{\pi}')}{\partial \pi_k \partial \pi_r} = -\sum_{i=1}^{n} \frac{(f_{ik} - f_{im})(f_{ir} - f_{im})}{(\sum_{j=1}^{g} \pi_j f_{ij})^2}$$

The observed information derived covariance matrix of $\boldsymbol{\pi}'$ yields the following estimates for covariance and correlation for all m estimated weights in $\hat{\boldsymbol{\pi}}$:

$$\mathrm{Cov}(\hat{\pi}_p, \hat{\pi}_q) = \begin{cases} \left[I^{-1}(\hat{\boldsymbol{\pi}}') \right]_{pq} & p, q < m \\ -\sum_{j=1}^{m-1} \mathrm{Cov}(\hat{\pi}_j, \hat{\pi}_q) & p = m, q < m \\ \sum_{j=1}^{m-1} \sum_{k=1}^{m-1} \mathrm{Cov}(\hat{\pi}_j, \hat{\pi}_q) & p, q = m \end{cases}$$

$$\mathrm{Var}(\hat{\pi}_j) = \sigma_j^2 = \left\{ \mathrm{Cov}(\hat{\boldsymbol{\pi}}) \right\}_{jj}$$

$$\mathrm{Corr}(\hat{\pi}_p, \hat{\pi}_q) = \frac{\mathrm{Cov}(\hat{\pi}_p, \hat{\pi}_q)}{\sqrt{\sigma_p^2 \sigma_q^2}}$$

$$\text{Z-score} = \frac{\hat{\pi}_j - \pi}{\sigma_{\hat{\pi}_j}}$$

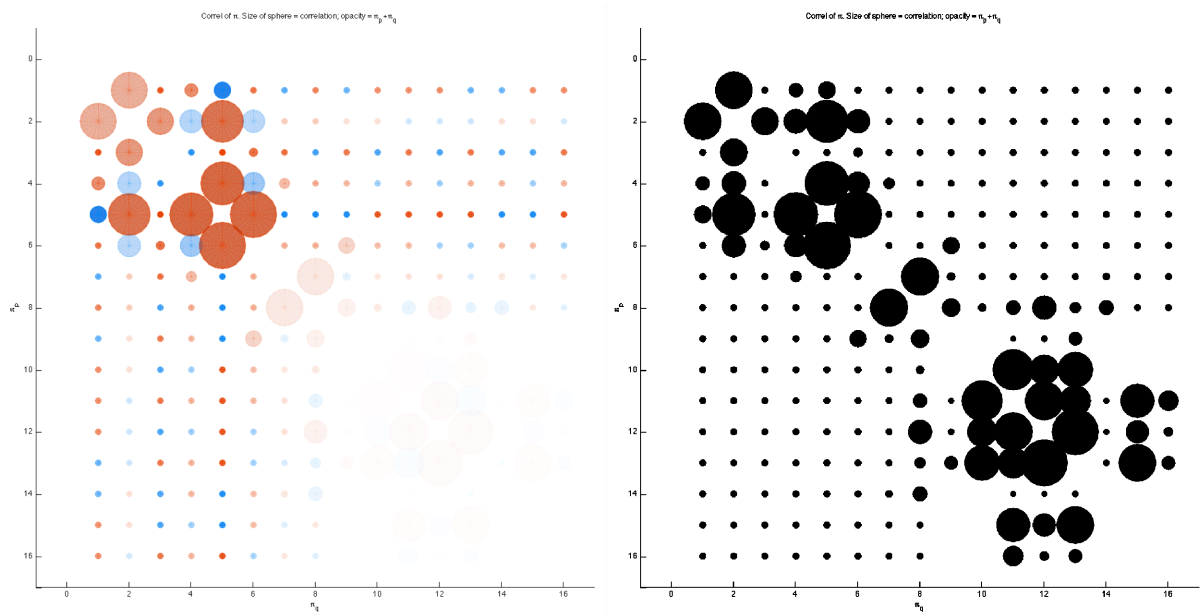
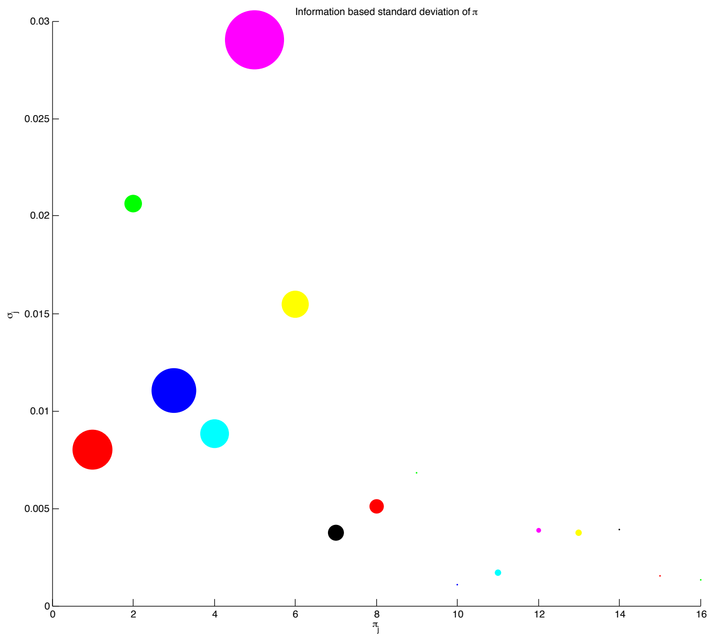


FIGURE 1. Left: correlation where size of sphere represents correlation value, and opacity of sphere represents $\pi_q + \pi_p$. Orange bubbles represent negative correlation, and blue positive. Right: Same graph, but without transparency.

TABLE 1. Correlation matrix

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	1	-0.592	-0.026	-0.219	0.274	-0.101	0.005	-0.008	0.007	-0.004	-0.003	-0.006	0.003	0.008	-0.001	-0.002
2	-0.592	1	-0.436	0.385	-0.685	0.378	-0.03	-0.006	-0.026	-0.003	0.002	0.002	0.003	-0.029	-0.004	0.006
3	-0.026	-0.436	1	0.074	-0.008	-0.141	-0.036	0.008	-0.006	0.004	-0.006	0.004	-0.008	0.025	0.002	-0.009
4	-0.219	0.385	0.074	1	-0.706	0.368	-0.173	-0.021	-0.045	0.013	-0.012	0.051	-0.022	-0.01	0.002	-0.003
5	0.274	-0.685	-0.008	-0.706	1	-0.757	0.057	0.008	0.083	-0.002	0	-0.018	-0.006	0.051	0.002	-0.001
6	-0.101	0.378	-0.141	0.368	-0.757	1	-0.012	-0.07	-0.264	-0.007	-0.01	0.027	0.02	-0.028	-0.009	0.01
7	0.005	-0.03	-0.036	-0.173	0.057	-0.012	1	-0.602	0.129	-0.013	-0.065	-0.023	0.025	-0.109	0.021	-0.002
8	-0.008	-0.006	0.008	-0.021	0.008	-0.07	-0.602	1	-0.29	-0.125	0.226	-0.381	0.173	0.232	-0.082	0.049
9	0.007	-0.026	-0.006	-0.045	0.083	-0.264	0.129	-0.29	1	0.112	-0.072	0.111	-0.211	-0.751	0.095	-0.048
10	-0.004	-0.003	0.004	0.013	-0.002	-0.007	-0.013	-0.125	0.112	1	-0.665	0.488	-0.567	0.091	0.439	-0.54
11	-0.003	0.002	-0.006	-0.012	0	-0.01	-0.065	0.226	-0.072	-0.665	1	-0.62	0.502	-0.044	-0.542	0.326
12	-0.006	0.002	0.004	0.051	-0.018	0.027	-0.023	-0.381	0.111	0.488	-0.62	1	-0.748	-0.006	0.376	-0.156
13	0.003	0.003	-0.008	-0.022	-0.006	0.02	0.025	0.173	-0.211	-0.567	0.502	-0.748	1	0.015	-0.599	0.218
14	0.008	-0.029	0.025	-0.01	0.051	-0.028	-0.109	0.232	-0.751	0.091	-0.044	-0.006	0.015	1	0.008	-0.248
15	-0.001	-0.004	0.002	0.002	0.002	-0.009	0.021	-0.082	0.095	0.439	-0.542	0.376	-0.599	0.008	1	-0.382
16	-0.002	0.006	-0.009	-0.003	-0.001	0.01	-0.002	0.049	-0.048	-0.54	0.326	-0.156	0.218	-0.248	-0.382	1



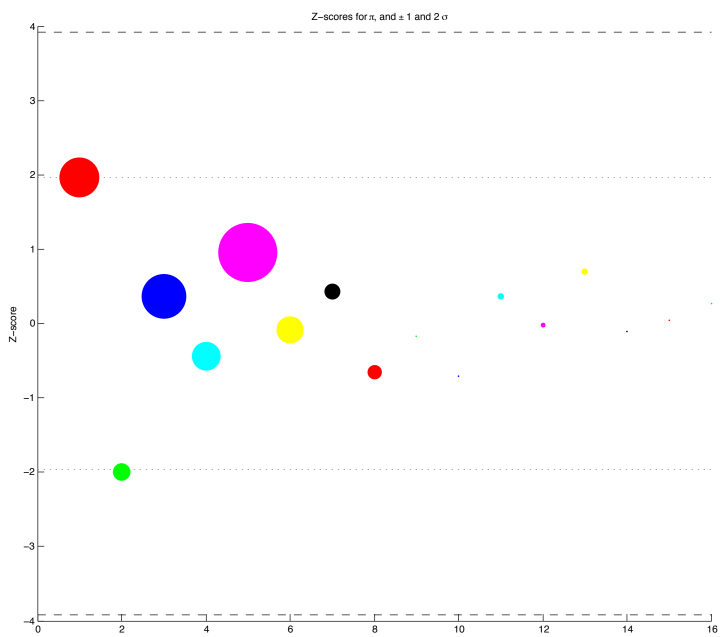


FIGURE 2. Left: standard deviation of each π_j. Right: Z-score, with 1 and 2 standard deviations marked as dotted lines. Colors are same as EM diagnostic plots. Size represents the value of π_j.

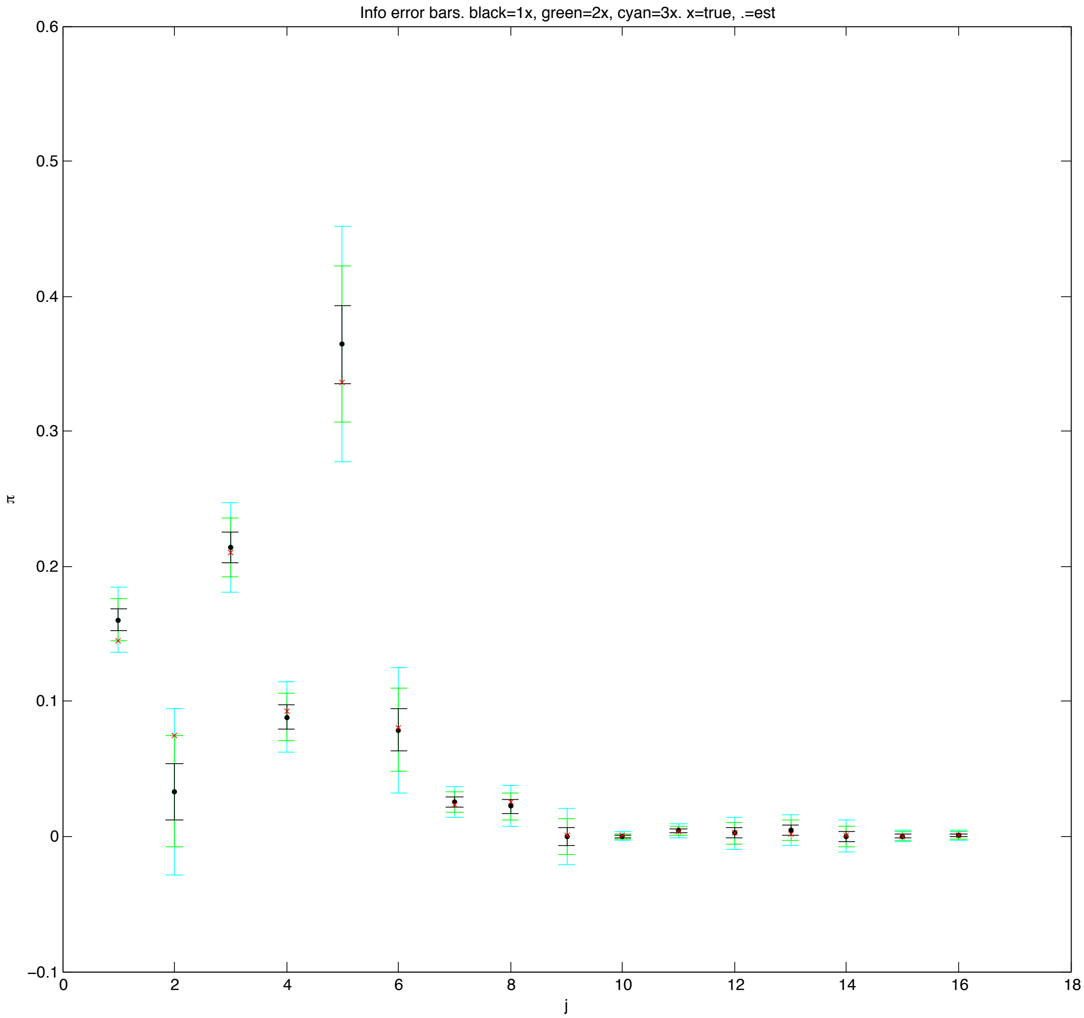


FIGURE 3. $\boldsymbol{\pi}$ plus information based error bars for $\pm\sigma$ (black), $\pm 2\sigma$ (green), and $\pm 3\sigma$ (cyan). A red $\times$ represents the true value, and a black dot represents the estimated values, $\hat{\boldsymbol{\pi}}$.

	$\hat{\pi}_j$	π_j	Std. dev.	Z-score
1	16.04	14.47	0.0080	1.965
2	3.32	7.44	0.0206	-1.995
3	21.39	20.99	0.0110	0.363
4	8.85	9.23	0.0088	-0.439
5	36.44	33.66	0.0290	0.96
6	7.88	8.02	0.0154	-0.088
7	2.56	2.4	0.0037	0.428
8	2.24	2.57	0.0051	-0.655
9	0	0.12	0.0068	-0.174
10	0	0.08	0.0010	-0.706
11	0.42	0.36	0.0017	0.367
12	0.25	0.25	0.0038	-0.016
13	0.49	0.23	0.0037	0.694
14	0.01	0.05	0.0039	-0.103
15	0.03	0.02	0.0015	0.044
16	0.08	0.05	0.0013	0.27

FIGURE 4. Model 3 EM results

4. Likelihood ratio test

Given certain regularity conditions, let

$$H_0 : \boldsymbol{\pi} = \boldsymbol{\pi}_{\text{true}}$$
$$H_1 : \boldsymbol{\pi} \neq \boldsymbol{\pi}_{\text{true}}$$

The likelihood ratio test is then

$$\Lambda = -2 \log \frac{\sup_{\boldsymbol{\pi}=\boldsymbol{\pi}_{\text{true}}} \ell(\boldsymbol{\pi})}{\sup_{\boldsymbol{\pi}} \ell(\boldsymbol{\pi})} = -2\big\{ l(\boldsymbol{\pi}_{\text{true}}) - l(\hat{\boldsymbol{\pi}}) \big\} \sim \chi^2_{m-1}$$

For halo 3,

$$\Lambda_{\text{Halo 3}} = 25.025 \sim \chi^2_{15}$$
$$\text{p-value 10k} = 4.961\%$$
$$\text{p-value 30k} = 1.3 \times 10^{-5}\%$$
$$\text{p-value 50k} = 1.4 \times 10^{-12}\%$$

Thus we accept H_0 when requiring 95% or less confidence; there is only a 4.961% chance we would see a value this extreme or more given H_0 is true. This holds for 400 to 1600 EM iterations.