METALLICITY

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1. Mixture model

Given n observed $(\frac{\alpha}{\text{Fe}}, \frac{\text{Fe}}{\text{H}})$ metallicities as $\big\{(x_i, y_i)\big\}_{i=1}^{n}$, 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 $\hat{\boldsymbol{\pi}}_{\text{MLE}}$, 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 $\text{argmax}_{\boldsymbol{\pi}}$ 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.

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

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

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

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

$$\mathrm{E}_{\boldsymbol{\pi}}\left[z_{ij}|x_i, y_i\right] = \frac{\pi_j f_j(x_i, y_i)}{\sum_{j=1}^{m} \pi_j f_j(x_i, y_i)} \tag{3}$$

To iteratively evaluate this expectation, we let $w_{ij}^{(t)}$ be (3) 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. Maximizing with respect to $\boldsymbol{\pi}$.

$$\begin{aligned} 0 &= \frac{\partial}{\partial \pi_k} \mathrm{E}_{\boldsymbol{\pi}}\left[\ell(\boldsymbol{\pi})\middle|\mathbf{x}, \mathbf{y}\right] \\ &= \sum_{i=1}^{n} \left\{ w_{ij}^{(0)} \frac{1}{\pi_k} - w_{im}^{(0)} \frac{1}{1 - \pi_1 - \ldots - \pi_{m-1}} \right\}, k = 1, \ldots, m-1 \end{aligned}$$

as $\pi_m = 1 - \pi_1 - \ldots - \pi_{m-1}$.

$$\frac{1}{\pi_1} \sum_{i=1}^{n} w_{i1}^{(0)} = \ldots = \frac{1}{\pi_{m-1}} \sum_{i=1}^{n} w_{i,m-1}^{(0)} = c$$

$$\hat{\pi}_k = \frac{\sum_{i=1}^{n} w_{ik}^{(0)}}{c}$$

$$\pi_j^{(1)} = \frac{\sum_{i=1}^{n} w_{ij}^{(0)}}{n}$$

And in general,

$$\pi_j^{(t+1)} = \frac{\sum_{i=1}^{n} w_{ij}^{(t)}}{n}$$

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 $\boldsymbol{\pi}_\times = (\pi_1, \ldots, \pi_{m-1})$. Using $f_{ij} = f_j(x_i, y_i)$ for brevity, the likelihood can then be expressed as:

$$\ell(\boldsymbol{\pi}_\times) = \sum_{i=1}^{n} \log \left\{ \left(\sum_{j=1}^{m-1} \pi_j f_{ij} \right) + (1 - \pi_1, \ldots, \pi_{m-1}) f_{im} \right\} \tag{4}$$

The observed information matrix, I, is the $m-1 \times m-1$ negative hessian of (4), evaluated at the observed data points:

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

where

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

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

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

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

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

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

FIGURE 1. Left: correlation where size of sphere represents correlation value, and opacity of sphere represents $\pi_q + \pi_p$. Right: correlation where size of sphere represents $\pi_q + \pi_p$ and opacity represents correlation. Top plots ignore sign of correlation; bottom ones color negative correlation orange.

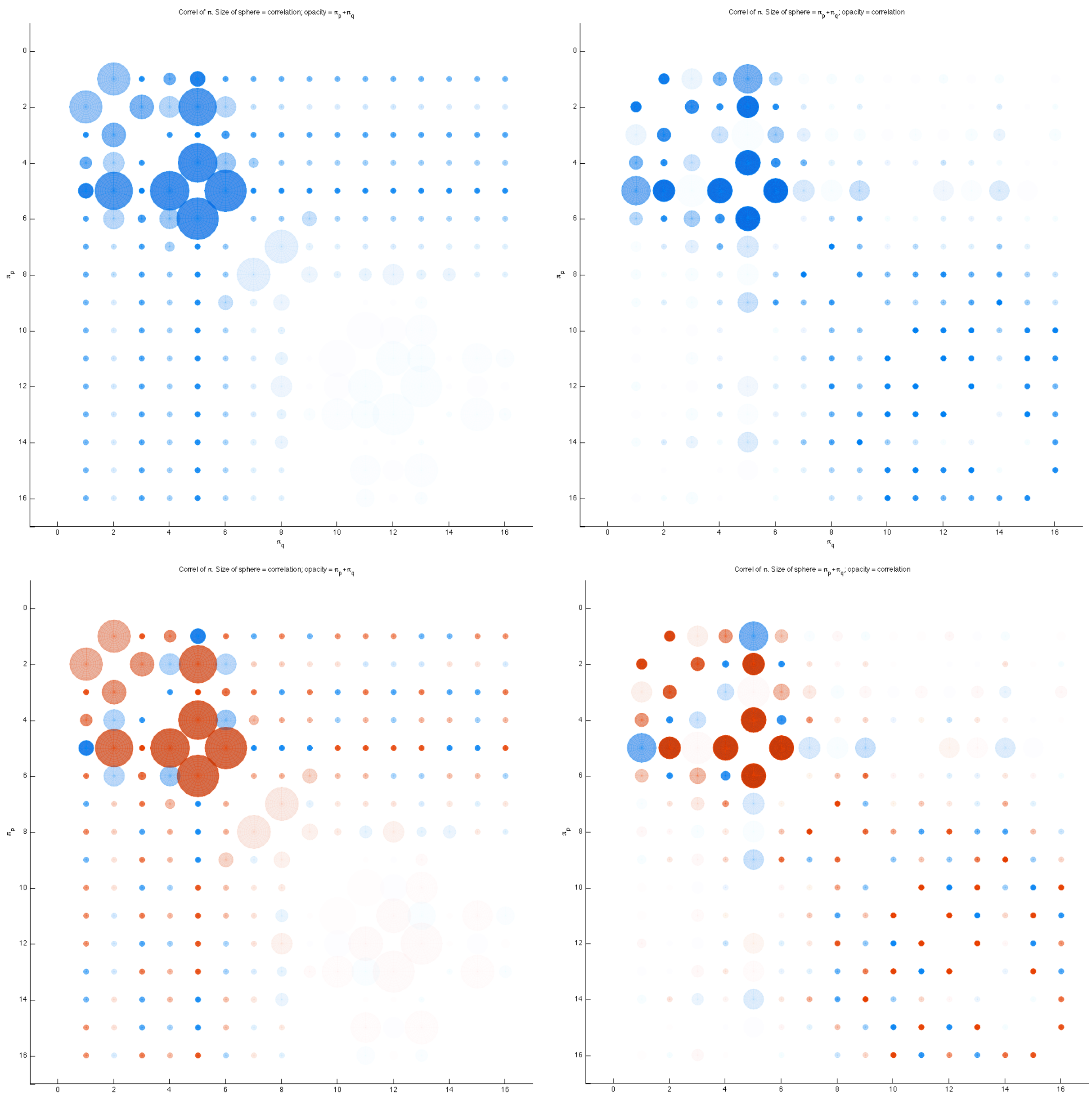

FIGURE 2. Left: standard deviation of each π_j. Right: Z-score, with 1 and 2 standard deviations marked as dotted lines. Colors are same as EM diagnostic plots. Size represents the value of π_j.

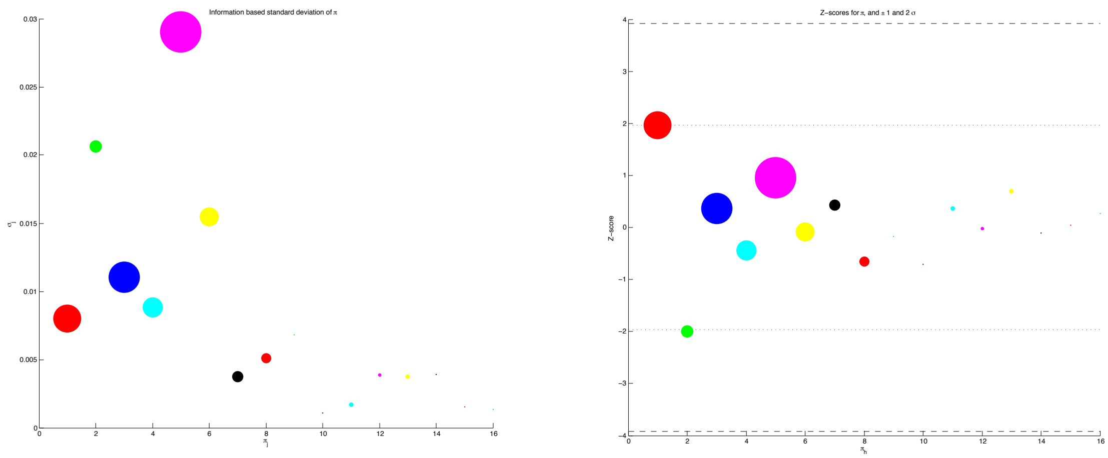

FIGURE 3. Model 3 EM results

	$\hat{\pi}_j$	π_j	$\sigma_{\hat{\pi}_j}$	Z-score
1	16.04	14.47	16.04	1.965
2	3.32	7.44	3.32	-1.995
3	21.39	20.99	21.39	0.363
4	8.85	9.23	8.85	-0.439
5	36.44	33.66	36.44	0.96
6	7.88	8.02	7.88	-0.088
7	2.56	2.4	2.56	0.428
8	2.24	2.57	2.24	-0.655
9	0	0.12	0	-0.174
10	0	0.08	0	-0.706
11	0.42	0.36	0.42	0.367
12	0.25	0.25	0.25	-0.016
13	0.49	0.23	0.49	0.694
14	0.01	0.05	0.01	-0.103
15	0.03	0.02	0.03	0.044
16	0.08	0.05	0.08	0.27

Table 1. Correlation matrix

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
-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
-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
-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
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
-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
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
-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
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
-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
-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
-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
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
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
-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
-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

4. Likelihood ratio test

Given certain conditions

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

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

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

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.

Model 2 Realization 2

log L(θ estimate) = 9234.5
log L(θ true) = 9222.0