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STOCK IDENTIFICATION BY MAXIMUM LIKELIHOOD METHOD: DERIVATION OF VARIANCE ESTIMATOR

Kazuhiko Hiramatsu
Far Seas Fisheries Research Laboratory

Hirohisa Kishino
The Institute of Statistical Mathematics

Fisheries Agency of Japan

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Abstract

Evaluating the precision of stock composition needs to consider two sources of sampling error, i.e., sampling of baseline data and that of mixed fishery data. Variance estimator including both sources is derived from the Fisher's information matrix.

1. Introduction

Maximum likelihood method has recently been used to resolve composition of a mixture of stock from genetic data and scale data (Fournier et al.1984; Pella and Milner 1987; Millar 1987; Wood et al. 1987; Millar 1988). The estimations are based on the differences in the distribution of the measured characteristics among stocks. The probability density function of characteristics for the j-th stock, g^j, is estimated by maximizing the likelihood function for the baseline samples of the j-th stock. Let π_j be the proportion of fish in the mixed samples that comes from the j-th stock. The maximum likelihood estimates for π_j's are found by maximizing the following likelihood function:

$$\prod_k \sum_j \pi_j g^j(y_k),$$

where y_k is the vector of characteristics of the k-th fish in the mixed samples. The precision of composition estimation has been evaluated by the following methods.

①Asymptotic covariance matrix derived by Fisher's information matrix (Pella and Milner 1987)
②Simulation(Fournier et al.1984; Wood et al.1987) or bootstrap resampling (Millar 1987)
③Infenitecimal jackknife (Millar 1987)

Althouh both the baseline and mixed samples variabirity should be considered for evaluating the presicion, method ① and ③ took into account only the mixed sample variability. On the other hand, method ② can take into account both sources of variability, but the amount of computing is considerable.

In this paper, we expand the method ① and derive the variance estimator taking account of both the baseline and mixed samples variability. The calculations are presented in a step by step manner.

2.Symbols and Definitions

m: The number of stock groups,

n_j: the number of the baseline samples in the j-th stock,

y_k^j: characterisrics of the kth fish in the j-th stock (vector),

$g^j(y|\theta^j)$: the probability density function of characteristics for the j-th stock,

θ^j: parameters which specify the distribution of characteristics of j-th stock.

$\theta^j \equiv (\theta_1^j, \ldots .\theta_p^j)^t$,

where t means transposed.

n: The number of the mixed samples,

y_k: characteristics of the k-th fish in the mixed samples (vector),

π_j: the proportion of the mixed fishery that are of the j-th stock (estimated parameter), where $\Sigma \pi_j=1$.

$\pi \equiv (\pi_1, \ldots . \pi_{m-1})^t$.

The log-likelihood function for baseline data is:

$$L^j(\theta^j|y_1^j, \ldots y_{nj}^j) \equiv \sum_{k=1}^{nj} \log\{g^j(y_k^j|\theta^j)\}, \quad j=1,..,m . \tag{1}$$

The log-likelihood function for mixed data is:

$$L(\pi, \theta|y_1, \ldots y_n) \equiv \sum_{k=1}^{n} \log\{f(y_k|\pi, \theta)\}, \tag{2}$$

where

$$f(y|\pi, \theta) = \sum_{j=1}^{m} \pi_j g^j(y|\theta^j)$$

is the probability density function of characteristics for the mixed samples.

$$\nabla_{\theta^j} \equiv \left(\frac{\partial}{\partial \theta_1{}^j}, \frac{\partial}{\partial \theta_2{}^j}, \ldots \frac{\partial}{\partial \theta_p{}^j} \right)^t,$$

$$\nabla_\theta \equiv (\nabla_{\theta^1}^t, \ldots \nabla_{\theta^m}^t)^t,$$

$$\nabla_\pi \equiv \left(\frac{\partial}{\partial \pi_1}, \ldots \frac{\partial}{\partial \pi_{m-1}} \right)^t.$$

$$i_{\pi\pi} \equiv E\,[\nabla_\pi \log(f) \cdot \nabla_\pi^t \log(f)] = -E\,[\nabla_\pi \nabla_\pi^t \log(f)],$$

$$i_{\pi\theta} \equiv E\,[\nabla_\pi \log(f) \cdot \nabla_\theta^t \log(f)] = -E\,[\nabla_\pi \nabla_\theta^t \log(f)],$$

$$i_{\theta^j\theta^j} \equiv E\,[\nabla_{\theta^j} \log(g^j) \cdot \nabla_{\theta^j}^t \log(g^j)] = -E\,[\nabla_{\theta^j} \nabla_{\theta^j}^t \log(g^j)],$$

$$I_{\pi\pi} = n \cdot i_{\pi\pi}, \qquad I_{\pi\theta} = n \cdot i_{\pi\theta}, \qquad I_{\theta^j\theta^j} = n_j \cdot i_{\theta^j\theta^j},$$

where E [ ] is an expectation and i is Fisher's information matrix.

Maximum likelihood estimates $\hat{\theta}$ and $\hat{\pi}$ are the value of θ and π which satisfy the equations

$$\nabla_{\theta^j} L^j(\theta^j) = 0 \qquad j=1, \ldots, m, \tag{3}$$

$$\nabla_\pi L(\pi, \hat{\theta}) = 0, \text{ and } \pi_m = 1 - \sum_j^{m-1} \pi_j. \tag{4}$$

3.Derivation of Variance Estimator of θ

For brevity, we omit the superscript j in this section. By the Taylor series expansion of $\nabla_\theta L(\hat{\theta})$ about θ,

$$\nabla_\theta L(\hat{\theta}) \fallingdotseq \nabla_\theta L(\theta) + \nabla_\theta \nabla_\theta^t L(\theta) \cdot (\hat{\theta} - \theta), \tag{5}$$

where $\hat{\theta}$ is maximum likelihood estimate and θ is the true value. Scince $\nabla_\theta L(\hat{\theta})=0$,

$$\hat{\theta}-\theta \fallingdotseq -(\nabla_\theta \nabla_\theta^t L(\theta))^{-1}\cdot\nabla_\theta L(\theta),$$

$$\sqrt{n}(\hat{\theta}-\theta) \fallingdotseq -(\frac{1}{n}\nabla_\theta \nabla_\theta^t L(\theta))^{-1}\cdot\frac{1}{\sqrt{n}}\nabla_\theta L(\theta)$$

$$=-(\frac{1}{n}\sum_{k=1}^{n}\nabla_\theta\nabla_\theta^t \log\{g(y_k|\theta)\})^{-1}\cdot\frac{1}{\sqrt{n}}\sum_{k=1}^{n}\nabla_\theta\log\{g(y_k|\theta)\}.$$

Taking the limit of $n\to\infty$,

$$\frac{1}{n}\sum_{k=1}^{n}\nabla_\theta\nabla_\theta^t\log\{g(y_k|\theta)\}\to E[\nabla_\theta\nabla_\theta^t\log\{g(Y|\theta)\}],$$

(law of large numbers)

where Y represents the random variable following the distribution $g(\cdot|\theta)$, and

$$\frac{1}{\sqrt{n}}\sum_{k=1}^{n}\nabla_\theta\log\{g(y_k|\theta)\}\to N(0,U),$$

(central limit theorem)

where $N(0,U)$ is the normal distribution with mean 0 and variance U.

Here,

$$U=V[\nabla_\theta\log(g)]$$

$$=E[\nabla_\theta\log(g)\cdot\nabla_\theta^t\log(g)]$$

$$=i_{\theta\theta}.$$

Hence,

$$\sqrt{n}\,(\hat{\theta}-\theta) \sim i_{\theta\theta}^{-1}\cdot N(0,\, i_{\theta\theta})$$

$$\sim N(0,\, i_{\theta\theta}^{-1}), \qquad \text{asymptotically .}$$

Finally, the asymptotic variance-covariance matrix of $\hat{\theta}$ is obtained.

$$V\,[\hat{\theta}] = (n\, i_{\theta\theta})^{-1}$$

$$= I_{\theta\theta}^{-1}\ . \tag{6}$$

It can be estimated by $\{-\nabla_\theta \nabla_\theta^t L(\hat{\theta})\}^{-1}$.

4.Derivation of Variance Estimator of π

By the Toylor series expansion of $\nabla_\pi L(\hat{\pi},\hat{\theta})$ about π and θ,

$$\nabla_\pi L(\hat{\pi},\hat{\theta}) \fallingdotseq \nabla_\pi L(\pi,\theta) + \nabla_\pi\nabla_\pi^t L(\pi,\theta)\cdot(\hat{\pi}-\pi)$$

$$+\nabla_\pi\nabla_\theta^t L(\pi,\theta)\cdot(\hat{\theta}-\theta)\ . \tag{7}$$

Since $\nabla_\pi L(\hat{\pi},\hat{\theta})=0$,

$$\sqrt{n}\,(\hat{\pi}-\pi) \fallingdotseq -\left(\frac{1}{n}\nabla_\pi\nabla_\pi^t L(\pi,\theta)\right)^{-1}$$

$$\times \left\{\frac{1}{\sqrt{n}}\nabla_\pi L(\pi,\theta) + \frac{1}{\sqrt{n}}\nabla_\pi\nabla_\theta^t L(\pi,\theta)\cdot(\hat{\theta}-\theta)\right\}\ . \tag{8}$$

Taking the limit of $n\to\infty$,

$$\frac{1}{n}\nabla_\pi\nabla_\pi^t L(\pi,\theta) \to -\, i_{\pi\pi}\ .$$

$$\frac{1}{\sqrt{n}}\nabla_\pi L(\pi,\theta)\rightarrow N(0,\ i_{\pi\pi}).$$

As for the baseline samples, we take the limit $n_j\rightarrow\infty$ in the way $n_j/n \rightarrow a_j>0$. First, we decompose as follows:

$$\frac{1}{\sqrt{n}}\nabla_\pi\nabla_\theta^t L(\pi,\theta)\cdot(\hat{\theta}-\theta)$$

$$=\frac{1}{\sqrt{n}}\sum_{j=1}^{m}\nabla_\pi\nabla_{\theta^j}^t\ L(\pi,\theta)\cdot(\hat{\theta}^j-\theta^j)$$

$$=\sum_{j=1}^{m}\frac{1}{\sqrt{a_j\cdot n}}\nabla_\pi\nabla_{\theta^j}^t\ L(\pi,\theta)\cdot\sqrt{n_j}\,(\hat{\theta}^j-\theta^j)\ .$$

In this equation,

$$\frac{1}{n}\nabla_\pi\nabla_{\theta^j}^t\ L(\pi,\theta)\ \rightarrow\ -i_{\pi\theta^j}\,.$$

$$\sqrt{n_j}\,(\hat{\theta}^j-\theta^j)\ \rightarrow\ N(0,\ i_{\theta^j\theta^j}^{-1}\ ).$$

Hence,

$$\sqrt{n}\,(\hat{\pi}-\pi)\ \rightarrow\ i_{\pi\pi}^{-1}\cdot\ (w-\sum_{j=1}^{m}\frac{1}{\sqrt{a_j}}\,i_{\pi\theta^j}u^j)\ ,$$

where w and u^j's follow the normal distributions with means 0 and variances $i_{\pi\pi}$ and $-\ i_{\theta^j\theta^j}^{-1}$'s, respectively. Scince the surveys of the mixed populations and the baseline populations are independent, w and u^j's are independent among others. Therefore,

$\sqrt{n}\,(\hat{\pi}-\pi)$

$$\to N\left[0,\ (i_{\pi\pi})^{-1}\cdot\left\{i_{\pi\pi}+\sum_{j=1}^{m}\frac{1}{a_j}\,i_{\pi\theta^j}\cdot(i_{\theta^j\theta^j})^{-1}\cdot i_{\theta^j\pi}\right\}\cdot(i_{\pi\pi})^{-1}\right].$$

In particular, the asymptotic variance-covariance matrix of π is given by

$$V[\hat{\pi}]=(n\,i_{\pi\pi})^{-1}\cdot\left\{n\,i_{\pi\pi}+\sum_{j=1}^{m}(n\,i_{\pi\theta^j})\cdot(n_j\,i_{\theta^j\theta^j})^{-1}\cdot(n\,i_{\theta^j\pi})\right\}\cdot(n\,i_{\pi\pi})^{-1}$$

$$=(I_{\pi\pi})^{-1}\cdot\left\{I_{\pi\pi}+I_{\pi\theta}\begin{bmatrix}I_{\theta^1\theta^1} & & \\ & \ddots & \\ & & I_{\theta^m\theta^m}\end{bmatrix}^{-1}I_{\theta\pi}\right\}\cdot(I_{\pi\pi})^{-1}. \qquad (9)$$

The first term represents the contribution of the mixed samples variability and the second term is that of the baseline samples variability. This result is similer with the covariance matrix of the classification approach (equation (11) in Pella and Robertson 1978). $I_{\pi\pi}$ and $I_{\pi\theta}$ are estimated by $\nabla_\pi\nabla_\pi^t L(\hat{\pi},\hat{\theta})$ and $\nabla_\pi\nabla_\theta^t L(\hat{\pi},\hat{\theta})$, respectively.

According to the definition of L,

$$\frac{\partial L}{\partial \pi_j}=\sum_{k=1}^{n}\frac{g^j(y_k|\theta^j)-g^m(y_k|\theta^m)}{f(y_k|\pi,\theta)} \qquad j=1,\ldots,m-1,,$$

$$\because f(y|\pi,\theta)=\sum_{j=1}^{m}\pi_j g^j(y|\theta^j)$$

$$=\sum_{j=1}^{m-1}\pi_j g^j(y|\theta^j)+\left(1-\sum_{j=1}^{m-1}\pi_j\right)g^m(y|\theta^m).$$

$$\frac{\partial^2 L}{\partial \pi_j\partial \pi_{j'}}=\frac{\partial}{\partial \pi_j}\sum_{k=1}^{n}\frac{g^{j'}(y_k|\theta^{j'})-g^m(y_k|\theta^m)}{f(y_k|\pi,\theta)}$$

$$= -\sum_{k=1}^{n} \frac{1}{f^2(y_k|\pi,\theta)} (g^j(y_k|\theta^j) - g^m(y_k|\theta^m))$$

$$\times (g^{j'}(y_k|\theta^{j'}) - g^m(y_k|\theta^m)) .$$

$$\frac{\partial^2 L}{\partial\theta_s \partial\pi_j} = \frac{\partial}{\partial\theta_s} \sum_{k=1}^{n} \frac{g^j(y_k|\theta^j) - g^m(y_k|\theta^m)}{f(y_k|\pi,\theta)}$$

$$= \sum_{k=1}^{n} \frac{1}{f^2(y_k|\pi,\theta)} \{ f (\frac{\partial g^j}{\partial\theta_s} - \frac{\partial g^m}{\partial\theta_s}) - (g^j - g^m) \frac{\partial f}{\partial\theta_s} \}$$

$$= \sum_{k=1}^{n} \frac{1}{f^2} \{ f (\frac{\partial g^j}{\partial\theta_s} - \frac{\partial g^m}{\partial\theta_s})$$

$$- (g^j - g^m) \cdot (\sum_{j=1}^{m-1} \pi_j \frac{\partial g^j}{\partial\theta_s} + (1 - \sum_{j=1}^{m-1} \pi_j) \frac{\partial g^m}{\partial\theta_s}) \} ,$$

where θ_s is an element of vector θ.

For the evaluation of $V[\hat{\pi}]$, we need further to calculate $\frac{\partial g^j}{\partial\theta}$ and $\nabla_\theta\nabla_\theta^t L^j(\hat{\theta})$ for the baseline likelihoods. Although they are usually obtained numerically, we will obtain the explicit formula for the multivariate normal distribution in Appendix. Explicit expression is also possible for the multinomial distributions.

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Appendix:Multivariate Normal Distribution

The INPFC is now using the multivariate normal distribution model for the distribution of baseline data characteristics (Millar 1988). In this model, we can obtain an explicit expression of the variance of θ and π.

Now, g^j is given by

$$g^j(y|\mu^j,\Omega)\sim\frac{1}{|\Omega|^{1/2}}\exp\{-\frac{1}{2}(y-\mu^j)^t\Omega^{-1}(y-\mu^j)\},$$

where $\mu^j=(\mu_1{}^j,\ldots\mu_p{}^j)^t$ and Ω are means and variance-covariance matrix of the distributions, respectively. We assume that variance matrix is common for all baseline populations. $|\Omega|$ represents determinant of matrix Ω. In this case,

$$\theta=(\mu_1{}^1,\ldots\mu_p{}^1,\ \mu_1{}^2,\ldots\mu_p{}^m,\ \Omega_{11},\ \Omega_{12},\ldots\Omega_{pp})^t,$$

where Ω_{st} is an element of matrix Ω. Since Ω is symmetric matrix, the number of free parameters specifying Ω is $p(p+1)/2$. For simplicity, however, we deal here all elements of Ω as the free parameters. The results are the same. The log-likelihood function for baseline data is given by

$$L'(\mu,\Omega|y)\equiv\sum_{j=1}^{m}\sum_{k=1}^{n_j}\log\{g^j(y_k{}^j|\mu^j,\Omega)\}$$

$$=-\frac{1}{2}\sum_{j=1}^{m}n_j\log|\Omega|-\frac{1}{2}\sum_{j=1}^{m}\sum_{k=1}^{n_j}(y_k{}^j-\mu^j)^t\Omega^{-1}(y_k{}^j-\mu^j).$$

The maximum likelihood estimate of μ and Ω are as follows:

$$\hat{\mu}_s{}^j=\frac{1}{n_j}\sum_{k=1}^{n_j}y_k{}^j{}_s,$$

$$\hat{\Omega}_{st}=\frac{1}{\sum_j n_j}\sum_{j=1}^{m}\sum_{k=1}^{n_j}(y_k{}^j-\hat{\mu}^j)_s\cdot(y_k{}^j-\hat{\mu}^j)_t.$$

In order to estimate the variance of θ and π, we should calculate

$$\frac{\partial g^j}{\partial \mu_q{}^j},\quad \frac{\partial g^j}{\partial \Omega_{st}},\quad \frac{\partial^2 L'}{\partial \mu_r{}^j \partial \mu_q{}^j},\quad \frac{\partial^2 L'}{\partial \mu_q{}^j \partial \Omega_{st}},\ \text{and}\ \frac{\partial^2 L'}{\partial \Omega_{qr} \partial \Omega_{st}}.$$

To begin with,

$$\frac{\partial g^j}{\partial \mu_q{}^j}=\{e_q{}^t\Omega^{-1}(y-\mu^j)\}\,g^j,$$

where $e_q=(0,\ldots0,1,0,\ldots0)^t$.

$$\uparrow$$

the q-th element

$$\frac{\partial g^j}{\partial \Omega_{st}}=-\frac{1}{2}\exp\{-\frac{1}{2}(y-\mu^j)^t\Omega^{-1}(y-\mu^j)\}\cdot\{\frac{1}{|\Omega|^{3/2}}\frac{\partial|\Omega|}{\partial \Omega_{st}}$$

$$+\frac{1}{|\Omega|^{1/2}}(y-\mu^j)^t\frac{\partial \Omega^{-1}}{\partial \Omega_{st}}(y-\mu^j)\}$$

$$=-\frac{1}{2}g^j\{\frac{\Delta_{st}}{|\Omega|}-(y-\mu^j)^t\Omega^{-1}E_{st}\Omega^{-1}(y-\mu^j)\}.$$

Here, Δ_{st} is the st-th cofactor of the matrix Ω and E_{st} is defined as

$E_{st}=1$ in (s,t) element,
$\quad =0$ elsewhere.

$$= -\frac{1}{2} g^{j} \{(\Omega^{-1})_{st} - \sum_{u=1}^{p} (y-\mu^{j})_{u} (\Omega^{-1})_{su}$$

$$\times \sum_{u=1}^{p} (\Omega^{-1})_{tu} (y-\mu^{j})_{u}\} \ .$$

$$\frac{\partial L'}{\partial \mu_{q}^{j}} = \frac{1}{2} \sum_{k=1}^{nj} \sum_{u=1}^{p} \{(\Omega^{-1})_{qu} + (\Omega^{-1})_{uq}\} \ (y_{k}^{j} - \mu^{j})_{u}$$

$$= \sum_{k=1}^{nj} \sum_{u=1}^{p} (\Omega^{-1})_{qu} (y_{k}^{j} - \mu^{j})_{u} .$$

$$\frac{\partial^{2} L'}{\partial \mu_{r}^{j} \partial \mu_{q}^{j}} = -n_{j} (\Omega^{-1})_{rq} .$$

$$\frac{\partial L'}{\partial \Omega_{st}} = -\frac{1}{2} \sum_{j=1}^{m} n_{j} (\Omega^{-1})_{st} + \frac{1}{2} \sum_{j=1}^{m} \sum_{k=1}^{nj} [\ \{\sum_{u=1}^{p} (\Omega^{-1})_{us} (y_{k}^{j} - \mu^{j})_{u}\}$$

$$\times \ \{\sum_{u=1}^{p} (\Omega^{-1})_{tu} (y_{k}^{j} - \mu^{j})_{u}\}\ ] \ .$$

$$\frac{\partial^{2} L'}{\partial \mu_{q}^{j} \partial \Omega_{st}} = -\frac{1}{2} \sum_{k=1}^{nj} (\Omega^{-1})_{qs} \ \{\sum_{u=1}^{p} (\Omega^{-1})_{tu} (y_{k}^{j} - \mu^{j})_{u}\}$$

$$-\frac{1}{2} \sum_{k=1}^{nj} (\Omega^{-1})_{tq} \ \{\sum_{u=1}^{p} (\Omega^{-1})_{us} (y_{k}^{j} - \mu^{j})_{u}\} \ .$$

$$\frac{\partial^{2} L'}{\partial \Omega_{qr} \partial \Omega_{st}} = -\frac{1}{2} \sum_{j=1}^{m} n_{j} \frac{\partial (\Omega^{-1})_{st}}{\partial \Omega_{qr}} + \frac{1}{2} \sum_{j=1}^{m} \sum_{k=1}^{nj} [\ \{\sum_{u=1}^{p} \frac{\partial (\Omega^{-1})_{us}}{\partial \Omega_{qr}}$$

$$\times (y_{k}^{j} - \mu^{j})_{u}\} \ \cdot \ \{\sum_{v=1}^{p} (\Omega^{-1})_{tv} (y_{k}^{j} - \mu^{j})_{v}\}$$

$$+\ \left\{\sum_{u=1}^{p}(\Omega^{-1})_{us}(y_k{}^{j}-\mu^{j})_u\right\}\cdot\left\{\sum_{v=1}^{p}\frac{\partial(\Omega^{-1})_{tv}}{\partial\Omega_{qr}}(y_k{}^{j}-\mu^{j})_v\right\}\Bigg]$$

$$=\frac{1}{2}\sum_{j=1}^{m}n_j(\Omega^{-1})_{sq}(\Omega^{-1})_{rt}$$

$$-\frac{1}{2}\sum_{j=1}^{m}\sum_{k=1}^{nj}\Bigg[\left\{\sum_{u=1}^{p}(\Omega^{-1})_{uq}(\Omega^{-1})_{rs}(y_k{}^{j}-\mu^{j})_u\right\}\left\{\sum_{v=1}^{p}(\Omega^{-1})_{tv}(y_k{}^{j}-\mu^{j})_v\right\}$$

$$+\left\{\sum_{u=1}^{p}(\Omega^{-1})_{us}(y_k{}^{j}-\mu^{j})_u\right\}\left\{\sum_{v=1}^{p}(\Omega^{-1})_{tq}(\Omega^{-1})_{rv}(y_k{}^{j}-\mu^{j})_v\right\}\Bigg]$$

$$=\frac{1}{2}\sum_{j=1}^{m}n_j(\Omega^{-1})_{sq}(\Omega^{-1})_{rt}$$

$$-\frac{1}{2}\sum_{j=1}^{m}\sum_{k=1}^{nj}\Bigg[(\Omega^{-1})_{rs}\left\{\sum_{u=1}^{p}(\Omega^{-1})_{uq}(y_k{}^{j}-\mu^{j})_u\right\}\left\{\sum_{v=1}^{p}(\Omega^{-1})_{tv}(y_k{}^{j}-\mu^{j})_v\right\}$$

$$+(\Omega^{-1})_{tq}\left\{\sum_{u=1}^{p}(\Omega^{-1})_{us}(y_k{}^{j}-\mu^{j})_u\right\}\left\{\sum_{v=1}^{p}(\Omega^{-1})_{rv}(y_k{}^{j}-\mu^{j})_v\right\}\Bigg]\ .$$