Maximum Likelihood and an Approximate Expectation and Maximization Procedures to Estimate Dispersion Parameters in a Data Set of Combination of Censored and Uncensored Traits

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Abstract

A method for estimating variance and covariance components for both uncensored and censored traits is described. The paper considers two cases: An uncensored trait and a right-censored trait; and two uncensored traits. A multivariate normal distribution is assumed for these traits and Bayesian arguments are employed to derive estimation procedures for dispersion parameters such as genetic variance and environmental variance. Observations are transformed by a Cholesky decomposition of the residual variance-covariance matrix so that residual covariance becomes zero. The residual variance for a right-censored trait and the residual covariance of a right-censored trait and an uncensored trait are estimated by two methods: maximum likelihood (ML) approach and an approximate expectation and maximization (EM) algorithm which is equivalent to restricted maximum likelihood (REML). A numerical example is used to illustrate the steps involved in applying the proposed methods. Comparison of the size of dispersion parameters in both between ML and an approximate EM procedures and between ignoring and accounting for censoring is tested in a numerical example.

Additional key words: censored data, (co)variance estimation, herd-life

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Introduction

The importance of herd-life as an adaptation trait in low-input, high stress environments has been pointed out by Togashi and Rege[16]. The same study also stressed the need to include herd-life in genetic evaluations and developed an iterative procedure for solving mixed linear model equations involving herd-life, a right-censored trait and for estimating location parameters such as fixed and random effects, assuming dispersion parameters are known in data sets consisting of a mixture of one continuous (uncensored) trait and another continuous trait treated either as uncensored or as censored. The term "censored" is explained in an appendix. The present paper presents an iterative procedure for estimating dispersion parameters. Expectation maximization (EM) algorithm (Dempster et al.[1]), involving two steps, the expectation step (E-step) and the maximization step (M-step), has been applied to the estimation of genetic (co)variances of an uncensored or a discrete trait and residual variances of uncensored traits by Foulley et al.[3] and Simianer and Schaeffer[11]. These procedures are equivalent to REML by Patterson and Thompson[8]. Maximum likelihood (ML) procedure has been applied to the estimation of the residual correlation between one uncensored and one binary trait by Simianer and Schaeffer[11]. Wolynetz[17] presented maximum likelihood estimation procedure for variance component for a censored normally distributed trait. However, because the degrees of freedom needed to estimate fixed effects are not accounted for in ML procedures, ML estimates of residual variance are biased. Togashi et al.[15] presented an approximate EM type algorithm for a combination of uncensored and binary traits. Taking the general approach of Togashi et al.[15], the present study applies the EM algorithm to the estimation of genetic (co)variances and residual (co)variances in a data set with combinations of measurements on one uncensored and one right-censored trait. The study also develops an estimation procedure for residual variance of a right-censored trait and residual covariance of one uncensored and one right-censored trait applying a variation of the ML procedure of Wolynetz[17]. Major purpose of this paper is to illustrate the developed ML and an approximate EM procedures by using a numerical example. In addition, in a numerical example, this paper also tries a simple comparison of the size of dispersion parameters in both between ML and an approximate EM and between ignoring and accounting for censoring.

Materials and Methods

1. Models and data structure

It is assumed that each animal has records on the two continuous traits whether they are censored or not. Two models are considered. Model 1 consists of an uncensored trait and a right-censored trait. Model 2 consists of two uncensored traits. Let $Y1_i$ be an uncensored datum for trait 1 measured on the i-th animal and $Y2_i$ be a datum for trait 2 which is right-censored at point L_i under model 1 and uncensored under model 2. The distribution of $Y1_i$ and $Y2_i$ is assumed to follow a multivariate normal. In model 1 data set, i.e. Y1 uncensored and Y2 right-censored, observations in trait 1 form an $s1 \times 1$ vector Y1 and observations in trait 2 which are right-censored form an $s1 \times 1$ vector $Y2' = (L_1, L_2, ..., L_{s1})$, where s1 is the number of observations in model 1. In model 2 data set, i.e. both Y1 and Y2 uncensored, observations for trait 1 and trait 2 form $s2 \times 1$ vectors Y*1 and Y*2, respectively, where s2 is the number of observations in model 2.

The resulting linear bivariate model in matrix notation is:

Model 1:

$$\begin{vmatrix} Y1 \\ Y2 \end{vmatrix} = \begin{vmatrix} X & 0 \\ 0 & X \end{vmatrix} \begin{vmatrix} b1 \\ b2 \end{vmatrix} + \begin{vmatrix} Z & 0 \\ 0 & Z \end{vmatrix} \begin{vmatrix} u1 \\ u2 \end{vmatrix} + \begin{vmatrix} e1 \\ e2 \end{vmatrix}$$

Model 2:

$$\begin{vmatrix} Y^*1 \\ Y^*2 \end{vmatrix} = \begin{vmatrix} X^* & 0 \\ 0 & X^* \end{vmatrix} \begin{vmatrix} b1 \\ b2 \end{vmatrix} + \begin{vmatrix} Z^* & 0 \\ 0 & Z^* \end{vmatrix} \begin{vmatrix} u1 \\ u2 \end{vmatrix} + \begin{vmatrix} e^*1 \\ e^*2 \end{vmatrix}$$

where: bj = p × 1 vector of fixed effects for trait j,
uj = q × 1 vector of additive genetic effects for trait j,
ej = s1 × 1 vector of residuals for trait j,
e*j =s2 × 1 vector of residuals for trait j,
X = s1 × p incidence matrix corresponding to bj,
X*=s2 × p incidence matrix corresponding to bj,
Z = s1 × q incidence matrix corresponding to uj,
Z* = s2 × q incidence matrix corresponding to uj,
p = the total number of levels of all fixed effects for model 1 and model 2,
q = the number of additive genetic effects,≧s1 + s2.

The expectations and variance-covariance matrices of the random variables are:

$$E\begin{vmatrix} Y1 \\ Y2 \end{vmatrix} = \begin{vmatrix} Xb1 \\ Xb2 \end{vmatrix}, \quad E\begin{vmatrix} Y^*1 \\ Y^*2 \end{vmatrix} = \begin{vmatrix} X^*b1 \\ X^*b2 \end{vmatrix},$$

$$E\begin{vmatrix} u1 \\ u2 \end{vmatrix} = \begin{vmatrix} 0 \\ 0 \end{vmatrix}, \quad E\begin{vmatrix} e1 \\ e2 \end{vmatrix} = \begin{vmatrix} 0 \\ 0 \end{vmatrix}$$

$$E\begin{vmatrix} e^*1 \\ e^*2 \end{vmatrix} = \begin{vmatrix} 0 \\ 0 \end{vmatrix}, \quad V\begin{vmatrix} u1 \\ u2 \end{vmatrix} = G0\#A, \; G0 = \begin{vmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{vmatrix}$$

$$V\begin{vmatrix} e1 \\ e2 \end{vmatrix} = R\#I_{s1}, \; V\begin{vmatrix} e1^* \\ e2^* \end{vmatrix} = R\#I_{s2}, \; R = \begin{vmatrix} r_{11} & r_{12} \\ r_{21} & r_{22} \end{vmatrix}$$

where: G_0 = 2 × 2 additive genetic variance-covariance matrix,
A = q × q additive genetic relationship matrix,
R = 2 × 2 residual variance-covariance matrix,
# = direct (Kronecker-) product (Searle[10]),
g_{jj} = additive genetic variance of trait j,
r_{jj} = residual variance of trait j,
g_{12} = additive genetic covariance between traits 1 and 2,
r_{12} = residual covariance between traits 1 and 2.

The unknown parameters are the location parameters,
θ' = {b′, u′}; b′ = {b1′, b2′}; u′ = {u1′, u2′} and the dispersion parameters,
γ' = {g′, r′}′; g′ = {g_{11}, g_{12}, g_{22}}; r′={σ^2e1, σe12, σ^2e2}.

It is assumed that the same model applies to each trait.

2. Method of inference

Likelihood function given dispersion parameters

R is decomposed as R = T T′, where T is a lower triangular matrix which exists for any positive definite or positive semi-definite matrix. T is written as

$$\begin{vmatrix} t_{11} & 0 \\ t_{21} & t_{22} \end{vmatrix}.$$

T^{-1} is used to perform a Cholesky transformation (Stoer and Bulirsch[14]) to remove the residual covariance between transformed variables. T^{-1} can be written as

$$\begin{vmatrix} t^{11} & 0 \\ t^{21} & t^{22} \end{vmatrix}.$$

Let the tilde symbol, (the underline), under a variable indicate that same variable on the transformed scale. Then:

$$\begin{vmatrix} \underline{y1_i} \\ \underline{y2_i} \end{vmatrix} = T^{-1}\begin{vmatrix} y1_i \\ y2_i \end{vmatrix} \text{ and } \begin{vmatrix} \underline{y^*1_i} \\ \underline{y^*2_i} \end{vmatrix} = T^{-1}\begin{vmatrix} y^*1_i \\ y^*2_i \end{vmatrix}$$

and similarly for elements of b,u,e and e*. On the transformed scale, variances and covariances are:

$$\underline{G0} = T^{-1}G0T^{-1'} = \begin{vmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{vmatrix}, \text{and}$$

$\underline{R} = T^{-1}RT^{-1'} = I$.

Given location and dispersion parameters, likelihood function of transformed variables can be represented as

$$f(Y \mid \theta, \gamma)$$
$$\propto \{\exp[-0.5(\underline{Y^*1} - X^*\underline{b1} - Z^*\underline{u1})'(\underline{Y^*1} - X^*\underline{b1} - Z^*\underline{u1})]/|I_{s2}|^{0.5}$$
$$\cdot \exp[-0.5(\underline{Y^*2} - X^*\underline{b2} - Z^*\underline{u2})'(\underline{Y^*2} - X^*\underline{b2} - Z^*\underline{u2})]/|I_{s2}|^{0.5}$$
$$\cdot \exp[-0.5(\underline{Y1} - X\underline{b1} - Z\underline{u1})'(\underline{Y1} - X\underline{b1} - Z\underline{u1})]/|I_{s1}|^{0.5}\} \prod_{i=1}^{s1} Q(m_i) \quad \ldots\ldots\ldots(1)$$

where $Q(m_i)$ is the probability of $y2_i$ being larger than or equal to L_i.

The original $y2_i$ can thus, be represented as ;

$y2_i = (\underline{y2}_i - t^{21} y1_i)/t^{22}$

$= [(x'_i \underline{b2} + z'_i \underline{u2})/t^{22} - y1_i t^{21}/t^{22}] + \underline{e2}_i/t^{22}$

$= L\mu_i + e_N$,

where $L\mu_i = (x'_i \underline{b2} + z'_i \underline{u2})/t^{22} - y1_i t^{21}/t^{22}$, $e_N = \underline{e2}_i/t^{22}$, x'_i and z'_i are rows of X and Z pertaining to animal i.

$V(e_N) = V[(t^{21} e1_i + t^{22} e2_i)/t^{22}] = \sigma^2 e2\ (1 - r^2_{e12}) = (t^{22})^{-2}$,

where r_{e12}=residual correlation of trait 1 and trait 2.

Then,

$Q(m_i) = \int_{mi} Z(t)\,dt$,

where $m_i = (L_i - L\mu_i)/\sigma e_N$ and $Z(\cdot)$ is a standard normal distribution function.

Transformed additive genetic effect vector ($U' = (u1', u2')$) is assumed to follow a priori a multivariate normal distribution, i.e., $U \sim N(0, G)$ which is independent of the distribution of fixed effects. Assuming flat priors for fixed effects, the prior distribution is taken to be uniform over the whole space.

Therefore, log-posterior likelihood function for location parameters, given data and dispersion parameters, is expressed as:

$$\begin{aligned}\mathrm{Log}\ \{f(\theta \mid Y, \gamma)\} \propto & -0.5(\underline{Y*1} - X*\underline{b1} - Z*\underline{u1})'(\underline{Y*1} - X*\underline{b1} - Z*u1) \\ & -0.5(\underline{Y*2} - X*\underline{b2} - Z*\underline{u2})'(\underline{Y*2} - X*\underline{b2} - Z*\underline{u2}) \\ & -0.5(\underline{Y1} - X\underline{b1} - Z\underline{u1})'(\underline{Y1} - X\underline{b1} - Z\underline{u1}) \\ & + \Sigma_i \log(Q(m_i)) - 0.5 \begin{vmatrix} \underline{u1} \\ \underline{u2} \end{vmatrix}' G^{-1} \begin{vmatrix} \underline{u1} \\ \underline{u2} \end{vmatrix}. \quad \text{.....(2)}\end{aligned}$$

The model of this posterior equation can be estimated using the Newton-Raphson algorithm, which leads to the nonlinear system of equations for the t-th round of iteration. The equations are:

$$\begin{vmatrix} X*'X*+X'X & 0 & X*'Z*+X'Z & 0 \\ 0 & X*'*+X'DX & 0 & X*'Z*+X'DZ \\ & & Z*'Z*+Z'Z & g^{12}A^{-1} \\ & & +g^{11}A^{-1} & \\ \text{symmetry} & & & Z*'Z*+Z'DZ \\ & & & +g^{22}A^{-1} \end{vmatrix} \begin{matrix} (t-1) \\ \\ \\ \\ \end{matrix} \begin{vmatrix} \underline{b1} \\ \underline{b2} \\ \underline{u1} \\ \underline{u2} \end{vmatrix} (t)$$

$$= RHS^{(t-1)}. \quad \text{.....(3)}$$

where the $RHS^{(t-1)}$ corresponding to the parameter sub-vectors are as follows:

$\underline{b1}$: $X*'\underline{Y*1} + X'\underline{Y1}$

$\underline{b2}$: $X*'\underline{Y*2} + X'DX\underline{b2} + X'DZ\underline{u2} + X'h$

$\underline{u1}$: $Z*'\underline{Y*1} + Z'\underline{Y1}$

$\underline{u2}$: $Z*'\underline{Y2} + Z'DX\underline{b2} + Z'DZ\underline{u2} + Z'h$.

D is a q × q diagonal matrix with i-th diagonal denoted as d_i given by $d_i = h_i(h_i - m_i)$ and h_i is the i-th element of a vector h of order s1, the i-th value of which is: $h_i = Z(m_i)/Q(m_i)$.

Genetic variance and covariance matrix for all denoted ($\underline{G}$) is represented as : $\underline{G} = \underline{G0}\#A$,

so $\underline{G}^{-1} = \underline{G0}^{-1}\#A^{-1}$, where $\underline{G0}^{-1} = \begin{vmatrix} g^{11} & g^{12} \\ g^{21} & g^{22} \end{vmatrix}$

3. Estimation of residual variance of a right-censored trait and residual covariance

Maximum likelihood algorithm

Likelihood function (La) for residual variance of the second trait on the transformed scale ($\sigma^2\underline{e2}$) in equation 1 can be written as:

$$La = [\exp[-0.5(\underline{Y*2} - X*\underline{b2} - Z*\underline{u2})'\, I_{s2}\sigma^2\, \underline{e2}^{-1}(\underline{Y*2} - X*\underline{b2} - Z*\underline{u2})]/|I_{s2}\sigma^2\underline{e2}|] \prod_{i=1}^{s1} Q(m_i). \quad \text{..... (4)}$$

The normal equation evaluated at the maximum likelihood of $\sigma^2\underline{e2}$, given Y*2, b2, u2 and $L\mu$, where $L\mu$ is an s1 × 1 vector with $L\mu_i$ as i-th element can be written as:

$$\delta \log La/\delta\sigma^2\underline{e2} = (1/\sigma^2\underline{e2})(\underline{Y*2} - X*\underline{b2} - Z*\underline{u2})'(\underline{Y*2} - X*\underline{b2} - Z*\underline{u2}) - s2 + \Sigma_i(h^2_i - d_i) = 0 \quad \text{.....(5)}$$

We define w_i as:

$w_i = L\mu_i + \sigma e_N h_i$.

Then $h_i = (w_i - L\mu_i)/\sigma e_N$.

So $h^2_i = t^2_{22}(w_i - L\mu_i)^2/\sigma^2\underline{e2}$, since $\sigma\underline{e2} = t^{22}\sigma e_N$.

From (5), $\sigma^2\underline{e2} = [(\underline{Y^*2} - X^*\underline{b2} - Z^*\underline{u2})'(\underline{Y^*2} - X^*\underline{b2} - Z^*\underline{u2}) + \Sigma_i\{t^{22}(w_i - L\mu_i)\}^2]/(s2 + \Sigma_i d_i)$

$= [(\underline{Y^*2} - X^*\underline{b2} - Z^*\underline{u2})'(\underline{Y^*2} - X^*\underline{b2} - Z^*\underline{u2}) + \Sigma_i\{t^{22}\sigma e_N h_i\}^2](s2 + \Sigma_i d_i)$.

But, because $t^{22} = 1/\sigma e_N$, $\sigma^2\underline{e2}$ can be written as:

$$\sigma^2\underline{e2} = [(\underline{Y^*2} - X^*\underline{b2} - Z^*\underline{u2})'(\underline{Y^*2} - X^*\underline{b2} - Z^*\underline{u2}) + \Sigma_i h^2_i]/(s2 + \Sigma_i d_i). \quad \text{..... (6)}$$

Approximate EM type algorithm

We divide the residual effect of the second trait (on the transformed scale) in model 1 into two parts, that is:

$\underline{Y2} = X\underline{b2} + Z\underline{u2} + e2^{**} + (\underline{e2} - e2^{**})$,

where $e2^{**}$ is an $s1 \times 1$ vector with expectation of $E(\underline{e2} \mid \underline{e2} \geqq m)$ and m is an $s1 \times 1$ vector with m_i as i-th element and $\underline{e2}$ is an $s1 \times 1$ vector of residuals in model 1 on transformed scale. Additionally, $E(\underline{e2}_i \mid \underline{e2}_i \geqq m_i) = h_i$.

As h_i is a function of location parameter ($\underline{b2}$, $\underline{u2}$), $e2^{**}$ can be transformed by a Taylor's series about $\hat{\zeta}$,

$$e2^{**}(\zeta) \fallingdotseq e2^{**}(\hat{\zeta}) + \frac{\delta e2^{**}}{\delta\zeta'}(\zeta - \hat{\zeta}),$$

where $\zeta' = (\underline{b2}', \underline{u2}')$.

Thus, $\delta e2^{**}/\delta\zeta' = \delta h/\delta\zeta' = (-DX, -DZ)$.

Therefore, $e2^{**}(\zeta) \fallingdotseq e2^{**}(\hat{\zeta}) + (-DX, -DZ)(\zeta - \hat{\zeta})$.

Ignoring $(\underline{e2} - e2^{**})$, the variance of $\sigma^2\underline{e2}$ becomes $\sigma^2 e2^{**}$.

Thus:

$$V(\underline{e2}) = [DX, DZ]V(\zeta - \hat{\zeta}) \begin{vmatrix} X'D \\ Z'D \end{vmatrix}$$

$$= [DX, DZ] \begin{vmatrix} C_{b2b2} & C_{b2u2} \\ C_{u2b2} & C_{u2u2} \end{vmatrix} \begin{vmatrix} X'D \\ Z'D \end{vmatrix}$$

$$= D(XC_{b2b2} + ZC_{u2b2})X'D + D(XC_{b2u2} + ZC_{u2u2})Z'D.$$

Therefore,

$$tr(V(\underline{e2})) = trXC_{b2b2}X'D^2 + 2\,trXC_{b2u2}Z'D^2 + tr\,ZC_{u2u2}Z'D^2. \quad \text{..... (7)}$$

The $s2 \times 1$ residual effect vector ($\underline{e^*2}$) of the second trait in model 2 on transformed scale can be written as:

$$\underline{e^*2} = \hat{\underline{e}}^*2 - (X^*:Z^*) \begin{vmatrix} \underline{b2} - \hat{\underline{b2}} \\ \underline{u2} - \hat{\underline{u2}} \end{vmatrix}.$$

Therefore,

$$V(\underline{e^*2}) = X^*C_{b2b2}X^{*\prime} + X^*C_{b2u2}Z^{*\prime} + Z^*C_{u2b2}X^{*\prime} + Z^*C_{u2u2}Z^{*\prime}.$$

Then,

$$tr[V(\underline{e^*2})] = trC_{b2b2}X^{*\prime}X^* + 2\,trC_{b2u2}Z^{*\prime}X^* + trC_{u2u2}Z^{*\prime}Z^*. \quad \text{..... (8)}$$

By combining the residuals of transformed trait 2 in model 1 and model 2 and applying EM algorithm (Dempster et al,[1, 2]), we get:

$$\sigma^2\underline{e2} = [h'h + \hat{\underline{e}}^*2'\hat{\underline{e}}^*2 + tr(V(\underline{e2})) + tr(V(\underline{e^*2}))]/(s1 + s2). \quad \text{.....(9)}$$

Approximation

Posterior mean of location parameters and C_{ij} cannot be derived explicitly (e.g. Harville and Mee[5], Stiratelli et al.[13]). However approximation can be done using posterior mode and the inverse of coefficient matrix in the iterative step (Simianer and Schaeffer[11]). Accordingly, equation (6) derived by maximum likelihood and (9) derived by approximate EM type algorithm are represented as (10) and (11), respectively. This representation facilitates the iteration process.

$$\sigma^2\underline{e2}^{(t+1)} = \{(\underline{Y^*2} - X^*\underline{b2}^{(t)} - Z^*\underline{u2}^{(t)})'(\underline{Y^*2} - X^*\underline{b2}^{(t)} - Z^*\underline{u2}^{(t)}) + \Sigma_i(h_i^{(t)} \times h_i^{(t)})\}(s2 + \Sigma_i d_i^{(t)}) \quad \text{.....(10)}$$

$$\sigma^2\underline{e2}^{(t+1)} = [h'^{(t)}h^{(t)} + \hat{\underline{e}}^*2'^{(t)}\hat{\underline{e}}^*2^{(t)} + tr(V(\underline{e2}))^{(t)} + tr(V(\underline{e^*2}))^{(t)}]/(s1 + s2), \quad \text{.....(11)}$$

where, in t-th trace element, C_{ij} is replaced by the inverse of the coefficient matrix of t-th round of equation (3). For example, $C_{b2u2}^{(t)}$ is the inverse of t-th round of equation (3) corresponding to b2 and u2.

Trace elements of equation (11) are shown in equation (7) and (8). These elements are obtained by adding the element for each individual. For example, the elements of $tr(X\,C_{b2b2}X'D^2)$ are obtained by adding the elements of the inverted left hand side of (3) corresponding to the level of fixed effect in each individual multiplied by d^2_i.

The new estimates about $\sigma^2\underline{e1}^{(t+1)}$ and $\sigma^2\underline{e2}^{(t+1)}$ need to be transformed back. This is done as follows:

$$\begin{vmatrix} \sigma^2 e1 & \sigma e12 \\ \sigma e12 & \sigma^2 e2 \end{vmatrix}^{(t+1)} = T \begin{vmatrix} \sigma^2 \underline{e1} & 0 \\ 0 & \sigma^2 \underline{e2} \end{vmatrix}^{(t+1)} T'.$$

Numerical Example

Herd-life and milk yield were taken as a right-censored trait and a uncensored trait, respectively. The subset of data set by Rege[9] was used in the present study. The numerical example applied a simple sire model with only one fixed effect. The data structure is given in Table 1. The linear model used to describe both traits was:

$Y_{ijk}=b_i+s_j+e_{ijk}$,

where

b_i= fixed effect of herd-calving year (i=1,...,12),

s_j= random effect of j-th sire (j=1,2,..., 20).

All the relationships among sires were ignored, i. e. A=I to illustrate the procedure simply and to reflect the realistic situation of difficulty in implementing cow registration in Africa. Residual covariance and residual variance for herd-life were estimated by both ML and an approximate EM type algorithm as described in the previous section. Additionally, dispersion parameters were estimated treating right-censored points as uncensored data which results in a data set of two continuous uncensored traits.

1. Iterative estimation procedure in numerical example

The data were normal-standardized. Mean and standard deviations for milk yield were taken as 3637 and 644.5 while the corresponding values for herd-life were 2856.2 and 761.6, respectively, these values having been obtained from the entire data set of Rege[9]. Initial dispersion parameters $\sigma^2 e1$, $\sigma e12$, $\sigma^2 e2$, $\sigma^2 s1$, $\sigma s12$ and $\sigma^2 s2$ were 0.9375, 0.09506, 0.9750, 0.0625, 0.009882, and 0.025, respectively, corresponding to heritability for milk yield, heritability for herd-life, genetic correlations and residual correlations of 0.25, 0.1, 0.25 and 0.1, respectively. The term $\sigma^2 s1$ represents sire variance and so do $\sigma^2 s2$ and $\sigma s12$. Starting values (priors) for fixed and random effects were zero.

Step 1. Cholesky transformation on variances

$$R=\begin{vmatrix} .9375 & .09561 \\ .09561 & .9750 \end{vmatrix} = TT', \quad T=\begin{vmatrix} .96825 & 0 \\ 0.09874 & .98247 \end{vmatrix},$$

$$T^{-1}=\begin{vmatrix} 1.03279 & 0 \\ -.10380 & 1.01784 \end{vmatrix}.$$

On the transformed scale, sire variance and covariances were:

$$\underline{G0}=T^{-1}G0T^{-1'}=\begin{vmatrix} 1.03279 & 0 \\ -.10380 & 1.01784 \end{vmatrix}\begin{vmatrix} .0625 & .009882 \\ .009882 & .025 \end{vmatrix}\begin{vmatrix} 1.03279 & -.10380 \\ 0 & 1.01784 \end{vmatrix}$$

$$=\begin{vmatrix} .06667 & .00369 \\ .00369 & .02449 \end{vmatrix}.$$

Table 1. Data structure of numerical example

	First lactation milk yield	Herd-life
Total(N)	139	139
No.of sires	20	20
No.of uncensored data	139	125
No. of censored data	0	14
mean	3492.5kg	2858.2 days
σ x	963.5	423.4
range	1451-5824	2228-4230
Phenotypic correlation	-0.1855	

$$\underline{G0}^{-1} = \begin{vmatrix} g^{11} & g^{12} \\ g^{21} & g^{22} \end{vmatrix} = \begin{vmatrix} 15.12618 & -2.27833 \\ -2.27833 & 41.18393 \end{vmatrix}.$$

Step 2. Cholesky decomposition on a variate of model 1, i.e. milk yield is uncensored but herd-life is right-censored

In the first datum of model 1, the normal standardized milk yield and normal standardized right-censored points are –2.32118 and –0.01471, respectively. Thus:

$L\mu_1 = (x'_1\underline{b2} + z'_1\underline{u2})/t^{22} - y1_1 \cdot t^{21}/t^{22}$

$=(x'_1 0 + z'_1 0)/1.01784 - (-2.32118) \cdot (-0.10380)/1.01784$

$=-0.23672$

$\sigma e_N = \sigma e2(1-r^2_{e12})^{0.5} = 0.98247$

$m_1 = (L_1 - L\mu_1)/\sigma e_N = (-0.01471 + 0.23672)/.98247$

$=.22597$

$Q(m_1) = \int_{m1} z(t)\,dt = 0.41061$

$Z(m_1) = 0.38889$

$h_1 = Z(m_1)/Q(m_1) = 0.9471$ and

$d_1 = h_1(h_1 - m_1) = 0.68298$.

Values of the other variable for model 1, that is, h_i and d_i are calculated in the same way. The variates of milk yield in model 1 are transformed as:

$\underline{y1}_1 = t^{11} \cdot y1_1 = 1.03279 \times (-2.32118) = -2.39729.$

The remaining $\underline{y1}_i$ values (for milk yield in model 1) are obtained in the same way.

Step 3. Cholesky decomposition on a variate of model 2, i.e. both milk yield and herd-life are uncensored

In the first datum of model 2, normal standardized milk yield and normal standardized herd-life are –1.82777 and 0.50657, respectively. Thus:

$$\begin{vmatrix} \underline{y*1}_1 \\ \underline{y*2}_1 \end{vmatrix} = T^{-1} \begin{vmatrix} -1.82777 \\ 0.50657 \end{vmatrix}$$

$$= \begin{vmatrix} 1.03279 & 0 \\ -.10380 & 1.01784 \end{vmatrix} \begin{vmatrix} -1.82777 \\ 0.50657 \end{vmatrix}$$

$$= \begin{vmatrix} -1.88770 \\ 0.70533 \end{vmatrix}.$$

The rest of model 2 values, $\underline{y*1}_i$ and $\underline{y*2}_i$ are calculated in the same way.

Step 4. Initial step of constructing and solving the mixed model equations of (3)

Using the elements of h and D obtained in step 2 and transformed variates of $\underline{y*1}$ and $\underline{y*2}$ obtained in step 3, mixed model equation (3) are constructed and solved. Inbreeding and all the relationship among sires are ignored so that, A = I.

Step 5. Iterative step of constructing and solving the mixed model equations

The elements of h and D are replaced by new estimates for location parameters and the elements of RHS for $\underline{b2}$ and $\underline{u2}$ are obtained from the previous estimates of $\underline{b2}^{(t-1)}$ and $\underline{u2}^{(t-1)}$. This procedure for solving $\underline{b1}$, $\underline{b2}$, $\underline{u1}$ and $\underline{u2}$ is iterated and the stopping criterion on original scale (not standardized scale) is met. The criterion used was:

$$\sum_i^{2(p+q)} [(\theta_i^t - \theta_i^{t-1})/\theta_i^t]^2 < 1.0^{-7}$$

where θ_i is the location parameter of b1, b2, u1 and u2.

Step 6. Estimation of sire variances and covariance

The final solutions for sire effects in step 5 were as follows:

$\underline{u1}'$ = (0.04145, 0.01949, 0.02673, ..., 0.15775) and

$\underline{u2}'$ = (–0.00193, 0.08066, 0.01909, ..., 0.06814).

And, C_{ij}, the inverted left hand side of (3) corresponding to $\underline{bi}$ and $\underline{bj}$ was given and the trace C_{ij} was as follows:

$tr\,(C_{11}) = 0.04229 + 0.04441 + 0.04107 + ... + 0.05329$

$= 1.02539$

$tr\,(C_{12}) = 0.00195 + 0.00209 + 0.00187 + ... + 0.00271$

$= 0.05167$

$tr\,(C_{22}) = 0.01999 + 0.02049 + 0.01968 + ... + 0.02225$

$= 0.43935.$

And

$\underline{u1}'\underline{u1} = 0.31233$

$\underline{u1}'\underline{u2} = 0.00661$

$\underline{u2}'\underline{u2} = 0.02074.$

Then:

$\sigma^2 s1 = (\underline{u1}' \underline{u1} + \text{tr } C_{11})/20 = 0.06689$
$\sigma s12 = (\underline{u1}' \underline{u2} + \text{tr} C_{12})/20 = 0.00291$
$\sigma^2 s2 = (\underline{u2}' \underline{u2} + \text{tr } C_{22})/20 = 0.02301.$
The new estimates need to be transformed back:

$$G0^{(2)} = T \begin{vmatrix} 0.06689 & 0.00291 \\ 0.00291 & 0.02301 \end{vmatrix} T'$$

$$= \begin{vmatrix} 0.06271 & 0.00917 \\ 0.00917 & 0.02343 \end{vmatrix}.$$

Step 7. Estimation of residual variance of transformed milk yield

Transformed varieties of milk yield in model 1 ($\underline{Y1}$) were:
$\underline{Y1}' = (-2.39729, -3.22577, -0.83008, ..., -1.32204).$
Transformed varieties of milk yield in model 2 ($\underline{Y1}^*$) were:
$\underline{Y1}^{*\prime} = (-1.88771, -2.37325, -2.56875, ..., 0.55766).$
Transformed fixed effects for milk yield ($\underline{b1}$) given in step 5 were:
$\underline{b1}' = (-2.29821, -1.46951, 2.21465, ..., -0.45381).$
Transformed sire effects on milk yield ($\underline{u1}$) obtained in step 5 were:
$\underline{u1}' = (0.04145, 0.01949, 0.02673, ..., 0.15775).$
The elements of RHS corresponding to $\underline{b1}$, i.e. $(X^{*\prime}\underline{Y^*1} + X'\underline{Y1})$ given in step 5 were:
$(X^{*\prime}\underline{Y^*1} + X'\underline{Y1})' = (-2.37358, -1.51770, -2.28728, ..., -0.46870).$
The elements of RHS corresponding to $\underline{u1}$, i.e. $(Z^{*\prime}\underline{Y^*1} + Z'\underline{Y1})$ given in step 5 were:
$(Z^{*\prime}\underline{Y^*1} + Z'\underline{Y1})' = (0.04281, 0.02012, 0.02760, ..., 0.16293).$
Thus:
$\sigma^2 \underline{e1} = [(\underline{Y^*1}:Y1)'(\underline{Y^*1}:\underline{Y1}) - \underline{b1}'(X^{*\prime}\underline{Y^*1} + X'\underline{Y1}) - \underline{u1}'(Z^{*\prime}\underline{Y^*1} + Z'\underline{Y1})]/(900+100-12) = 1.09952.$

Step 8.1 Estimation of residual variance of transformed trait 2 by maximum likelihood

The elements of h obtained after convergence of location parameters in step 5 were:
$h' = (0.63151, 0.78862, 0.87758, ..., 0.74961).$
The diagonal elements of D, that is $d' = (d_1, d_2, ..., d_{s1})$ from step 5 were:
$d' = (0.57242, 0.63344, 0.66252, ..., 0.61954).$
Transformed variates of trait 2 ($\underline{Y^*2}$) in model 2 were:
$\underline{Y^*2}' = (0.70532, 0.27701, 0.36348, ..., -0.32494).$
Fixed effects given in step 5 for transformed trait 2 were:
$\underline{b2}' = (-0.02356, -0.38969, 0.25933, ..., 0.45146).$
Therefore:
$\sigma^2 \underline{e2} = \{(\underline{Y^*2} - X^*\underline{b2} - Z^*\underline{u2})'(\underline{Y^*2} - X^*\underline{b2} - Z^*\underline{u2}) + h'h\}/(125 + \sum_i d_i)$
$= 0.31538$, where 125 is the value for s1, i.e. number of records in model 1.

Step 8.2 Estimation of residual variance of transformed traits 2 by an approximate EM type algorithm

The varieties of residual effects of transformed trait 2 in model 2 ($\underline{e2}^*$) were:
$(\underline{e2}^*)' = (0.73081, 0.30250, 0.38897, ..., -0.82612).$
And
$\text{tr } C_{b2b2} X^{*\prime} X^* = 11.54769$
$\text{tr } C_{u2u2} Z^{*\prime} Z^* = 2.65767$
$\text{tr } X C_{b2u2} Z' D^2 = -0.02073$
$\text{tr } C_{b2u2} Z^{*\prime} X^* = -0.77990$
$\text{tr } X C_{b2b2} X' D^2 = 0.38981$
$\text{tr } Z C_{u2u2} Z' D^2 = 0.10904.$
Therefore:
$\sigma^2 \underline{e2} = [h'h + \underline{e^*2}'\underline{e^*2} + \text{tr } C_{b2b2} X^{*\prime} X^* + 2\text{tr } C_{b2u2} Z^{*\prime} X^* + \text{tr} C_{u2u2} Z^{*\prime} Z^* + \text{tr } X C_{b2b2} X' D^2 + \text{tr} X C_{b2u2} Z' D^2 + \text{tr} Z C_{u2u2} Z' D^2]/(14 + 125)$
$= 0.39056$, where 14 is the value for s2, i.e. number of data in model 2.

Step 9.1 Back-transformation and Cholesky transformation based on new residual (co)variances obtained by maximum likelihood

$$R^{(2)} = T\underline{R}T' = \begin{vmatrix} .96825 & 0 \\ .09874 & .98247 \end{vmatrix} \begin{vmatrix} 1.09952 & 0 \\ 0 & 0.31538 \end{vmatrix} \begin{vmatrix} .96825 & .09874 \\ 0 & .98247 \end{vmatrix}$$

$$= \begin{vmatrix} 1.03081 & .10512 \\ .10512 & .31514 \end{vmatrix}.$$

$$R^{(2)} = TT' = \begin{vmatrix} 1.01529 & 0 \\ .10354 & .55174 \end{vmatrix} \begin{vmatrix} 1.01529 & 0.10354 \\ 0 & 0.55174 \end{vmatrix}.$$

Same steps (1 to 9.1) are repeated when maximum likelihood procedure is applied to residual variance for transformed trait 2.

Step 9.2 Back transformation and Cholesky transformation based on new residual (co)variances obtained by an approximate EM type algorithm

$$R^{(2)} = T\underline{R}T' = \begin{vmatrix} .96825 & 0 \\ .09874 & .98247 \end{vmatrix} \begin{vmatrix} 1.09952 & 0 \\ 0 & .39656 \end{vmatrix} \begin{vmatrix} .96825 & .09874 \\ 0 & .98247 \end{vmatrix}$$

$$= \begin{vmatrix} 1.03081 & .10512 \\ .10512 & .39350 \end{vmatrix}.$$

$$R^{(2)} = TT' = \begin{vmatrix} 1.01529 & 0 \\ .10354 & .61869 \end{vmatrix} \begin{vmatrix} 1.01529 & .10354 \\ 0 & .61869 \end{vmatrix}.$$

Same steps (1 to 9.2) are repeated when an approximate EM type algorithm is applied to residual variance for transformed trait 2.

Step 10. Criterion for terminating iteration of dispersion parameters

Iteration stops when the following criterion on original scale (not standardized scale) is met:

$$\sum_{i=1}^{6} [(\gamma_i^t - \gamma_i^{t-1})/\gamma_i^t]^2 < 1.0^{-7}$$

where the term γ_i represents dispersion parameter of residual variance or sire variance.

2. Result of Numerical Example

Values of parameters during selected rounds of iteration are summarized in Tables 2 and 3 for maximum likelihood and EM procedures, respectively. Convergence occurred at the 37th round in both cases. The residual variance for herd-life by maximum likelihood was smaller than that by an approximate EM type algorithm.

Table 2. Summary of ML parameter estimates at selected rounds of iteration

	Round of iteration				
Parameters	1	10	20	30	37
σ^2s1	25961.4	22780.5	22017.0	21340.0	20694.7
σ s12	4850.7	−1090.2	−6357.1	−8953.5	−9818.3
σ^2s2	14500.9	16117.9	20114.4	21541.5	21701.6
σ^2e1	389418.9	460156.4	460634.2	461213.0	461681.7
σ e12	46928.6	55453.1	55510.7	55580.5	55637.0
σ^2e2	565533.7	141909.9	139018.5	138152.1	138035.5

σ^2s1 :sire variance for milk yield
σ s12 :sire covariance between milk yield and herd-life
σ^2s2 :sire variance for herd-life
σ^2e1 :residual variance for milk yield
σ e12 :residual covariance between milk yield and herd-life
σ^2e2 :residual variance for herd-life

Estimates of heritability for milk yield and for herd-life and of genetic and residual correlation by maximum likelihood were 0.1716, 0.5434, −0.4633 and 0.2204, respectively. Corresponding estimates by an approximate EM type algorithm were 0.1718, 0.4239, −.4516 and 0.2099, respectively. Values of parameters during selected rounds of iteration treating right-censored points as continuous measurements are summarized in Tables 4 and 5 for ML and EM procedures, respectively. Convergence occurred at 34th and 38th rounds for ML and EM procedures, respectively. Estimates of heritability for milk yield and for herd-life and of genetic and residual correlations by ML treating right-censored points as continuous measurements were 0.1545, 0.3994, −0.3653 and 0.2273. Corresponding estimates by EM were 0.1580, 0.2577, −0.3108 and 0.2120. This seems to be that ignoring censoring results in lower heritability and genetic correlation.

Discussion

Maximum likelihood estimate for residual variance of transformed trait 2 (σ^2e2) was obtained by maximizing f(σ^2e2, ml Y*2, b2, u2, Lμ) with respect to σ^2e2. That is, prior values of location parameters were required. Posterior expectation taken with respect to the conditional distribution f(θ | Y, γ) plays a basic role in the expectation step in an approximate EM type algorithm. As Dempster et al.[2] illustrated, the maximum likelihood estimates for residual variances which are obtained by using posterior expectations

Table 3. Summary of approximate EM parameter estimates at selected rounds of iteration

	Round of iteration				
Parameters	1	10	20	30	37
σ^2s1	25961.4	22653.2	21657.5	21182.2	20718.0
σs12	4850.7	−457.7	−4998.5	−7688.4	−8731.4
σ^2s2	14500.9	13967.1	16349.4	17704.8	18043.1
σ^2e1	389418.9	460258.0	460793.9	461208.9	461569.3
σe12	46928.6	55465.4	55530.0	55580.0	55623.3
σ^2e2	535533.7	155331.8	153384.0	152454.8	152205.4

σ^2s1 :sire variance for milk yield
σs12 :sire covariance between milk yield and herd-life
σ^2s2 :sire variance for herd-life
σ^2e1 :residual variance for milk yield
σe12 :residual covariance between milk yield and herd-life
σ^2e2 :residual variance for herd-life

Table 4. Summary of ML parameter estimates at selected rounds of iteration treating right-censored points as continuous measurements

	Round of iteration				
Parameters	1	10	20	30	37
σ^2s1	25961.4	22551.5	20751.1	19487.4	18596.6
σs12	4850.7	−183.5	−3525.8	−5226.3	−5984.1
σ^2s2	14500.9	13691.5	14386.2	14518.6	14429.0
σ^2e1	389418.9	460345.2	461375.5	462206.6	462798.7
σe12	46928.6	55475.9	55600.1	55700.2	55771.6
σ^2e2	565533.7	131103.9	130285.3	130062.4	130062.8

σ^2s1 :sire variance for milk yield
σs12 :sire covariance between milk yield and herd-life
σ^2s2 :sire variance for herd-life
σ^2e1 :residual variance for milk yield
σe12 :residual covariance between milk yield and herd-life
σ^2e2 :residual variance for herd-life

Table 5. Summary of approximate EM parameter estimates at selected rounds of iteration treating right-censored points as continuous measurements

	Round of iteration				
Parameters	1	10	20	30	37
σ^2s1	25961.4	22465.9	20536.7	19389.1	19011.8
σ s12	4850.7	394.5	−2357.9	−3915.3	−4346.8
σ^2s2	14500.9	11269.8	10680.5	10385.2	10289.5
σ^2e1	389418.9	460418.1	461467.1	462174.0	462416.5
σ e12	46928.6	55484.7	55611.1	55696.3	55725.5
σ^2e2	565533.7	149435.9	149405.5	149398.4	149409.7

σ^2s1 :sire variance for milk yield
σ s12 :sire covariance between milk yield and herd-life
σ^2s2 :sire variance for herd-life
σ^2e1 :residual variance for milk yield
σ e12 :residual covariance between milk yield and herd-life
σ^2e2 :residual variance for herd-life

coincide with the estimates by restricted maximum likelihood under normality. It is not possible to evaluate the posterior expectations for location parameters in posterior likelihood function (equation 2) to obtain the residual effects of e1 and e2, since integration of nuisance parameters is complex. As suggested by Foulley et al.[4], to obtain residual variances the mode of the posterior function for location parameters is replaced by restricted maximum likelihood estimates. Under non-linearity, the inverse of equation (3) yields only an approximation to the (co)variance matrix of estimators for location parameters. This approximation may be a reasonable one when sample size is large. For the right-censored trait (herd-life), only the expectation of residual effect greater than standardized right-censored point (m_i) is considered. The part of the difference of residual effect and this expectation, i. e. ($\underline{e2}$ - e2**), is ignored. This assumption may seem unrealistic, but it is adequate. Because e2** is a conditional expectation given data of a continuous trait and right-censored point, most of the residual variance can be considered to be explained by V(e2**). In this procedure to estimate V(e2**), expectation is taken with respect to f(location parameters | dispersion parameters, Y). Thus, there is no need to make any assumption on location parameters in an approximate EM type algorithm. In this regard, an approximate EM type algorithm is an improvement over ML. The procedure presented should be of practical use in analyzing animal breeding field data. The main disadvantage of approximate EM type algorithm is the need to have the inverse elements of the mixed model equations at every iteration. This is not a problem in a sire model even for large data sets but could present a drawback in an animal model, especially if the data set is large. Thus, there is need to develop computing strategies to overcome this problem if the procedure is to gain wider application in animal model.

The procedure of Togashi and Rege[16] for estimating location parameters does not need the formation of the coefficient matrix in-core but assumes that dispersion parameters are known. The procedure presented in the present paper is specifically designed for estimation of dispersion parameters but location parameters are also estimated in the process. However, because the present procedure requires formation and inversion of the coefficient matrix at each iteration, it is not a procedure of choice for location parameters, especially for large data sets. It may, however, be done from subsets of large data sets by applying the present procedure. Additionally, and as has been pointed out, the present procedure can be applied in relatively large data sets with the

sire model or maternal grandsire model.

Conditional expectation of residual, given data and current (co)variance components in the iterative step, was used instead of real residual. The residual (co)variance matrix was derived based on the residual: $e = \hat{e} - (X:Z)\ ((b - \hat{b}), (u - \hat{u}))'$ where X and Z are the design matrices for fixed effect (b) and random effect (u), respectively. In an approximate EM type algorithm, residual (co)variance matrix is derived based on the conditional expectation of residual. That is, $e2^{**}(\delta) \fallingdotseq e2^{**}(\hat{\delta}) + [-DX, -DZ]\ (\delta - \hat{\delta})$. In the process of equating $e2^{**}{}'e2^{**}$ to its posterior expectation given data and current (co)variance components in the iterative step, residual (co)variance matrix based on conditional expectation, i.e. $V(e2^{**})$ would be more reasonable.

In general, convergence is not guaranteed with REML or ML algorithm. Even if the procedure does converge, the final estimate may not be the one that maximize the likelihood function over the entire range of parameter values. That is, there is no guarantee that a global maximum will be reached. However, convergence normally occurs if the number of observations is large and this would likely be the maximum of the likelihood function.

In the present study, a Cholesky transformation was applied so that residual covariance becomes zero. The approach outlined in this paper assumes that every individual animal has a complete set of record on both traits of interest. In general, the Cholesky transformation can be applied to any data set in which traits 1 to (j-1) are present and traits j to t are missing, where t is the total number of traits.

This study assumed zero non-additive genetic variance. However, specific gene combinations and the way in which they are assembled might have an important effect on such traits as herd-life. Hence, there would be some room for this procedure to be improved by including non-additive genetic variance, possibly by applying such approaches as those by Henderson[6], Smith and Maki-Tanila[12] and Hoeschele[7].

Residual variance for right-censored trait was smaller in ML than in an approximate EM type algorithm in the numerical example. This was probably due to the difference in the degrees of freedom associated with fixed effects. Heritability for herd-life and genetic correlation treating right-censored points as continuous measurements were lower than those of treating them as right-censored measurements. This could be due to ignoring potential genetic ability to be able to stay more days in the herd. Thus, treating right-censored points in herd-life as continuous traits could lead to bias for estimation of dispersion parameters. However it could also be influenced by the size of heritability and right-censored position of the data set. For instance, the possible range of residual ($\underline{e2}$) is determined by the position of right-censored point. Thus, when the possible range of $\underline{e2}$ in standard normal distribution is small, $V(\underline{e2} - e2^{**})$ would become small as well. In this case $V(e2^{**})$ may be a preferred estimator. Further research is needed to understand how both ML and approximate EM type algorithm are influenced by degrees of freedom of fixed effects, the size of heritability and position of right-censored point. In a numerical example, only one set of starting values was conducted to illustrate the procedure, another set of values may, however, be necessary for detailed analysis. In addition, simulation to grasp how the size of dispersion parameters is affected by the above issues may be necessary.

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Appendix

Let y_i be an observation and $L_i \leqq y_i \leqq U_i$ where L_i and U_i are known. Several different situations can be distinguished. First, when $L_i = U_i$, the ith observation is exactly specified, i.e. uncensored. Second, when $L_i = -\infty$, the ith observation is said to be censored on the left at U_i. Third, when $U_i = \infty$, the ith observation is said to be censored on the right at L_i.

打ち切りおよび非打ち切り型形質の最尤法と概略化した制限最尤法による分散成分の推定

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摘　要

非打ち切り型データと打ち切り型データとを含む混合モデル式において分散ならびに共分散成分の推定を最尤法とDempsterら（1977，1984）のＥＭアルゴリズムを拡大しておこなう推定式（概略制限最尤法）を開発した。分散ならびに共分散成分は非打ち切り型データと打ち切り型データにおいて，２次元正規分布を仮定した上でベイジアン手法により求めた。２つの開発手法の適用例が手法の段階毎に具体的な数値例をもって示された。数値例の中で打ち切り型データを用いた最尤法と概略制限最尤法とによる遺伝分散や遺伝共分散の比較，さらに打ち切り型データの打ち切り点を非打ち切り型データととらえた時の遺伝分散や遺伝共分散の比較も試みた。

キーワード：打ち切り型データ，（共）分散成分，牛群滞在期間

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