Bayes estimates as an approximation to maximum likelihood estimates

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ESM S3: Comparison of estimates of σ between empirical Jeffreys prior method and data cloning method

S3-1: Comparison of $\hat{\sigma}$ between empirical Jeffreys prior method and data cloning method

The state-space model for estimating the sika deer population in Sorachi subprefecture has two parameters: the number of sika deer in 2007 (N_{2007}) and the standard deviation of observation error (σ). The estimates \hat{N}_{2007} were almost the same between two methods, but the estimates $\hat{\sigma}$ were slightly different. Figure S1, which was yielded by the R-code listed in ESM S3-2, indicates the comparison between estimates. The logarithmic marginal likelihood is plotted against σ which was transformed by Box-Cox transformation with $\lambda_{\sigma} = -0.5$. The transformation does not influence the logarithmic marginal likelihood but it influences the shape of curve. λ_{σ} was determined so that the skewness of marginal likelihood surface is nearly zero, and hence the marginal likelihood surface is close to a normal distribution; that is, the surface of logarithmic marginal likelihood is close to a quadratic equation. The solid curve was calculated by the quadratic regression. The estimated curve was $y = 0.256 - 3.411x - 0.369x^2$. The highest point of curve is the marginal ML estimate obtained by the quadratic regression seems close to the correct marginal ML estimate. The marginal ML estimate obtained by using empirical Jeffreys prior was 0.0915, which also seems close to the correct marginal ML estimate. In contrast, the ML estimate obtained by using data cloning via dclone package was $\hat{\sigma} = 0.0812$, which seems somewhat different from the marginal ML estimate as shown in Fig. S1, although such a difference is practically trivial.

The standard deviation of observation error (σ) estimated by the data cloning method was slightly different from the corresponding marginal ML estimate. This may be related to the fact that a clone is not a true random sample but it is a copy of the same data set. We have 5 observations in the current dataset. Therefore, the elements of the non-marginalized ML estimate of variance- covariance matrix will be 4/5 times those of the marginalized ML estimate of variance- covariance matrix. The effect of marginalization in the estimation of variance disappears when we add many clones. If we want to obtain the marginal ML estimate, therefore, the estimated variance should be adjusted by the original number of observations. The adjusted marginal ML estimate of σ will be $\hat{\sigma} = 0.0812 \times$ $\sqrt{(5/4)} = 0.0908.$



Fig. S1 Comparison between estimates of σ . Logarithmic marginal likelihood was plotted against the transformed quantity of σ . The curve was calculated by the quadratic regression. DC and EJP indicate the estimates that were obtained by using data cloning and empirical Jeffreys prior, respectively.

S3-2: R-code for obtaining ML estimates of σ by using quadratic regression from the output of ESM S1

```
# R-code for obtaining ML estimate of sigma by using quadratic regression
# Output from ESM S1-1 is used.
# Create the data frame of histogram
Strans <- out$sims.list$Strans</pre>
freq <- hist(Strans, breaks=70, plot=FALSE)</pre>
histlength <- length(freq$breaks)</pre>
x <- (freq$breaks[1:(histlength-1)] + freq$breaks[2:histlength])/2</pre>
histStrans <- data.frame(x, y=freq$counts)</pre>
# Extract the central part of histogram
histStrans <- subset(histStrans, y > mean(y))
histStrans$logy <- log(histStrans$y)</pre>
# Quadratic regression
histStrans.glm <- glm(logy ~ x + I(x^2), data=histStrans)</pre>
# Estimation of mode
estimate <- coef(histStrans.glm)</pre>
a <- estimate["(Intercept)"]</pre>
b <- estimate["x"]</pre>
c <- estimate["I(x^2)"]</pre>
StransMode <- -b/(2*c)</pre>
# back-transformaion of sigma
lambdaS <- -0.5
sigma <- (lambdaS*StransMode+1)^(1/lambdaS)</pre>
cat("ML estimate by quadratic regression =", sigma, "¥n")
# Plot the log-likelihood and the quadratic curve
plot(logy~x, data=histStrans, xlab="Transformed sigma", ylab="Logarithmic likelihood",
cex.lab=1.2, cex.axis=1)
quad <- function(x) a + b*x + c*x^2
plot(quad, -6.5, -2.5, add=TRUE)
# Emprical Jeffreys prior estimate (EJP)
abline(v=-4.61100, lty=1)
text(-4.48, 7.2, "EJP")
# dclone estimate (DC)
dclone.sigma <- (0.08122681^lambdaS-1)/lambdaS</pre>
abline(v=dclone.sigma, lty=2)
text(-5.12, 7.2, "DC")
```