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November 20, 2020

Biol 520C: Statistical modelling for biological data

#### Table of contents



- 1. Housekeeping
- 2. The Problem of Overfitting
- 3. Likelihood-Ratio Tests
- 4. Information Criteria
- 5. IC Considerations

# Housekeeping

#### Housekeeping



• Practical 04 is up on canvas, and due next Tuesday.





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Last lecture we covered linear mixed effects model that add additional structure to account for correlations within groups:

$$\mathbf{y_i} = X_i \boldsymbol{\beta} + Z_i \mathbf{b_i} + \boldsymbol{\varepsilon_i}$$





Lecture by lecture we've been increasing the complexity of our models



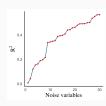
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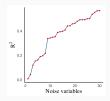
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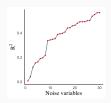


This puts us in a situation where we need to strike an optimal balance between having too many or too few features in our models.

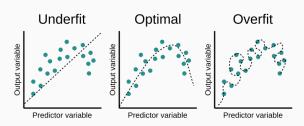


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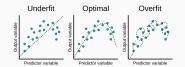


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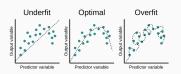
For Walters & Ludwig, spreading the information across age classes meant each age class' dynamics were included, but poorly estimated.







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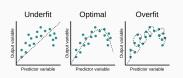






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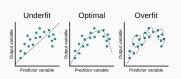


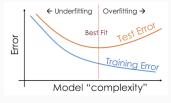


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This happens because you're fitting the noise not the signal.









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Note: Excluding a parameter does not mean an effect does not exist, it simply means we can't estimate it in a meaningful way from the information we have on hand





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- 2. Information criteria





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The likelihood-ratio test statistic is often expressed as a difference between the log-likelihoods

$$\lambda_{LR} = -2(\ln[\mathcal{L}(\text{Reduced})] - \ln[\mathcal{L}(\text{Full})])$$

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Both are simple linear models, and might even be based on the same data, but they are not nested.



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In other words, likelihood ratio tests can be used to identify both deterministic *and* stochastic components of your model (we'll cover non-gaussian models later, but keep this in mind).





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According to Wilks' theorem, as the sample size n approaches  $\infty$ , the test statistic  $\lambda_{LR}$  will be chi-squared distributed with degrees of freedom equal to difference in the number of parameters between the two models.



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According to Wilks' theorem, as the sample size n approaches  $\infty$ , the test statistic  $\lambda_{LR}$  will be chi-squared distributed with degrees of freedom equal to difference in the number of parameters between the two models.

This implies that we can compare  $\lambda_{LR}$  to the  $\chi^2$  value corresponding to a desired statistical significance threshold (usually  $\alpha=0.05$ ) as an approximate statistical test.





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Model df AIC BIC logLik Test L.Ratio p-value

FIT 1 4 16.11769 20.48186 -4.058844

FIT_Reduced 2 3 23.71490 26.98803 -8.857452 1 vs 2 9.597217 0.0019</pre>
```

This is telling us that the extra parameter is resulting in a significant improvement to the model, so the extra complexity is worth the cost.



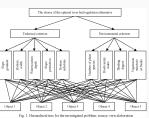


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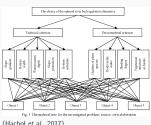


(Hachoł et al., 2017)



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If some of the models aren't nested in one another, there is no way to compare them using LRTs.





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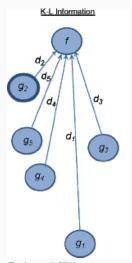
In practice, all IC methods reduce to finding the model that minimises some 'criterion' that is the sum of a term based on the likelihood and a penalty term

$$IC \approx \mathcal{L}(\text{model}) + \text{penalty term}$$





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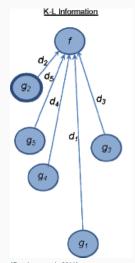


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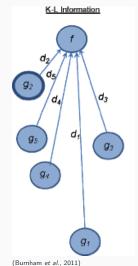


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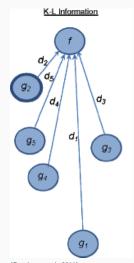




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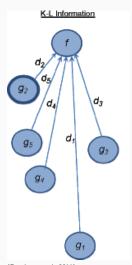


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The problem is that K-L information loss cannot be computed or estimated.



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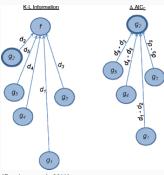
Akaike multiplied both terms by -2 to get his now famous:

$$AIC = -2\ln(\mathcal{L}) + 2K$$

Note: The term  $-2\ln(\mathcal{L})$  is well known among statisticians as the 'deviance', a goodness-of-fit statistic for a statistical model.



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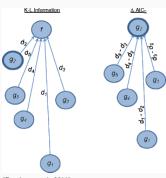


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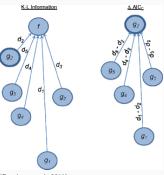
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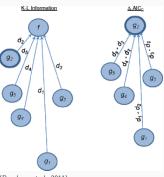
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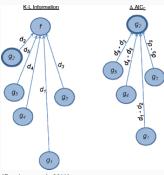
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We don't know how far the models are from the truth, but their relative positions should be the same, so we can now rank them amongst one another.



(Burnham et al., 2011)

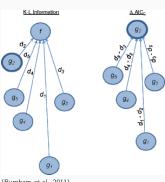


K-L information represents the distance between model  $g_i$  and reality.

Because we can't estimate 'reality', we instead rely on AIC (or other IC).

We don't know how far the models are from the truth, but their relative positions should be the same, so we can now rank them amongst one another.

Low K-L information means closer to reality, so with AIC, the lower the value the better.



(Burnham et al., 2011)





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A small sample size bias correction for AIC was derived that increases the penalty term and is more frequently used in practice. This criterion is denoted as AICc to make it distinct from AIC, and is given by:

$$AICc = AIC + \frac{2k^2 + 2k}{n - k - 1}$$

## Small sample size bias correction



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Question: What happens when  $n \to \infty$ ?





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$\triangle$ AICc	Evidence Ratio
2	2.7
4	7.4
6	20.1
8	54.6
9	90
10	148.4
11	244
12	403
13	665
14	1,097
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20	22,026
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For example: A model with a  $\triangle$ AICc of 2 is  $\sim$ 2.7 times less likely than the best fit model

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For example: A model with a  $\triangle$ AICc of 2 is  $\sim$ 2.7 times less likely than the best fit model, and a model with a  $\triangle$ AICc of 50 is 72 billion times less likely

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The  $\triangle$ AIC between a pair of models is

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If  $K_1 = K_2$ , then LRT =  $\Delta$ AIC.





```
library(nlme)

data <- read.csv("Ant_Richness.csv")

FIT <- gls(num_sp ~ latitude + elevation, data = data, method = "ML")</pre>
```



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library(nlme)
data <- read.csv("Ant_Richness.csv")

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Γ11 18.47063
library(MuMIn)
 AICc(FIT)
```



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#### Let's compare all possible models

FIT <- gls(num\_sp ~ latitude + elevation, data = data, method = "ML")



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```



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FIT <- gls(num_sp ~ latitude + elevation, data = data, method = "ML")
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FIT_lat <- gls(num_sp ~ latitude, data = data, method = "ML")
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## AICc model selection in R cont.



### Let's compare all possible models

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AICc(FIT); AICc(FIT_el); AICc(FIT_lat); AICc(INTERCEPT)
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[1] 18.47063
[1] 24.67657
[1] 25.04824
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This favours the full model.



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[1] 546.9268
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In a paper we would report that the next best model had a  $\triangle$ AICc of  $\sim$ 6.2, or was  $\sim$ 22 times less likely

## AICc model selection in R cont.



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In a paper we would report that the next best model had a  $\Delta AICc$  of  $\sim$ 6.2, or was  $\sim$ 22 times less likely, and the intercept only model had a  $\Delta AICc$  of  $\sim$ 12.6 and was >546 less likely than the full model.







```
FIT <- gls(num_sp \tilde{} latitude + elevation, data = data, method = "ML")
```



```
FIT <- gls(num_sp ~ latitude + elevation, data = data, method = "ML")
dredge(FIT)</pre>
```



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dredge(FIT)

Global model call: gls(model = num_sp ~ latitude + elevation, data = data, method = "ML")

---

Model selection table
(Intrc) elvtn lattd df logLik AICc delta weight
4 11.120 -0.001373 -0.2018 4 -4.059 18.5 0.00 0.922
2 2.489 -0.001613 3 -8.672 24.7 6.21 0.041
3 12.390 -0.2388 3 -8.857 25.0 6.58 0.034
1 2.114 2 -13.224 31.1 12.61 0.002

Models ranked by AICc(x)
```

# Other IC



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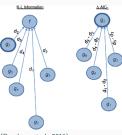
When  $\hat{c} = 1$  there is no overdispersion and QAIC = AIC.

# IC Considerations





Because we can't estimate 'reality', IC values only provide relative information (i.e., one model is always going to win out over other models).

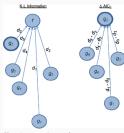


(Burnham et al., 2011)



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Just because a model is the best fit out of a pool of candidates doesn't mean it's any good.



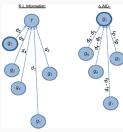
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After identifying a candidate model it's important to check all of the assumptions, and test the performance to make sure it's function reasonably well.



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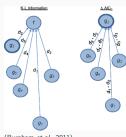


Because we can't estimate 'reality', IC values only provide relative information (i.e., one model is always going to win out over other models).

Just because a model is the best fit out of a pool of candidates doesn't mean it's any good.

After identifying a candidate model it's important to check all of the assumptions, and test the performance to make sure it's function reasonably well.

For example, comparing with the intercept only model tells us how much of an improvement our model is over simply looking at the mean.



(Burnham et al., 2011)





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$$\mathcal{L}(\theta|x)$$



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Models don't need to be nested, but if there are any differences in the datasets, the likelihoods, and therefore the IC, are not comparable (this can be a real problem in practice depending on if your data have NA values, and how they get handled in R).





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What would you do in this situation?



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What would you do in this situation?

This is where most of the controversy in model selection comes from, and we'll cover some options for handling that situation next lecture.

# References

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