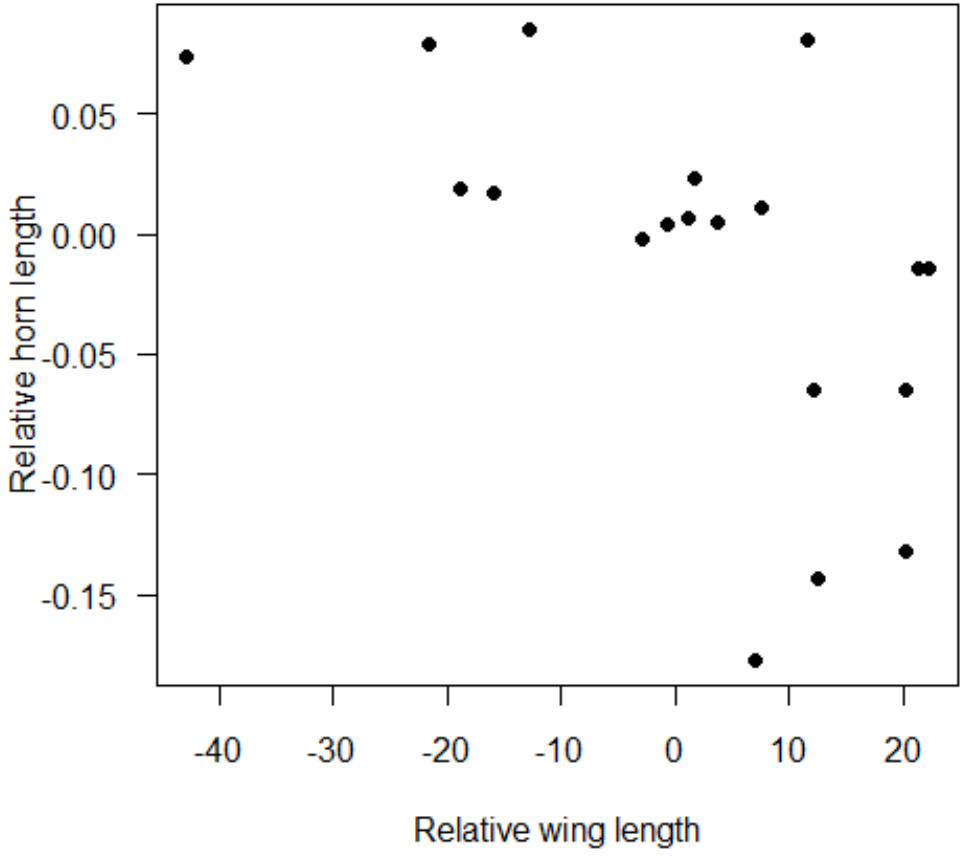
Outline for today

- The problem of model selection
- Choose among models by a criterion rather than significance testing
- Criteria: Mallow's C_p and AIC
- Search strategies: All subsets; stepAIC
- Several models may fit about equally well
- The science part: formulate a set of candidate models

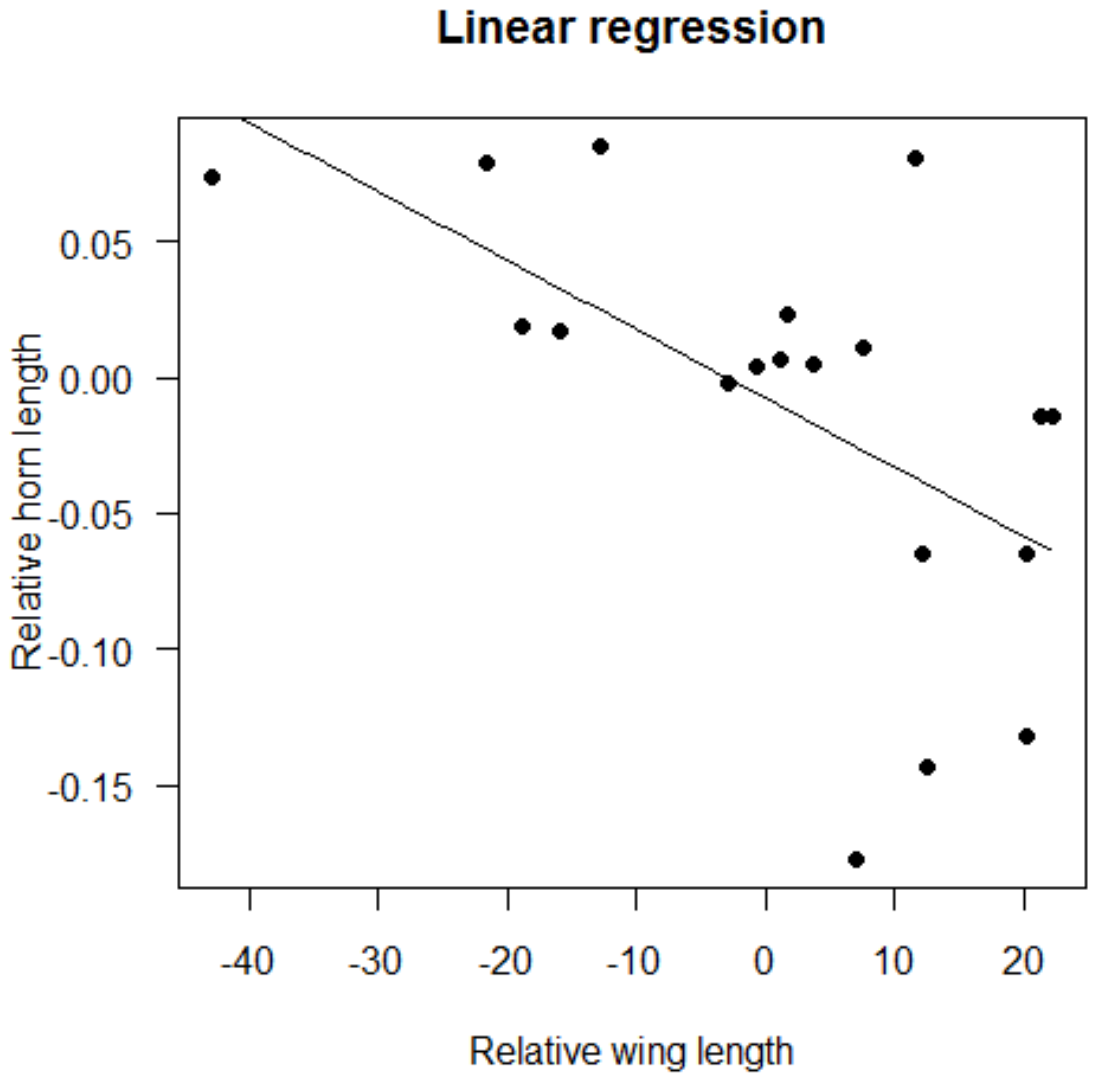
Example 1: Fit a polynomial regression model – when to stop?

Data: Trade-off between the sizes of wings and horns in 19 females of the beetle *Onthophagus sagittarius*. Both variables are size corrected.

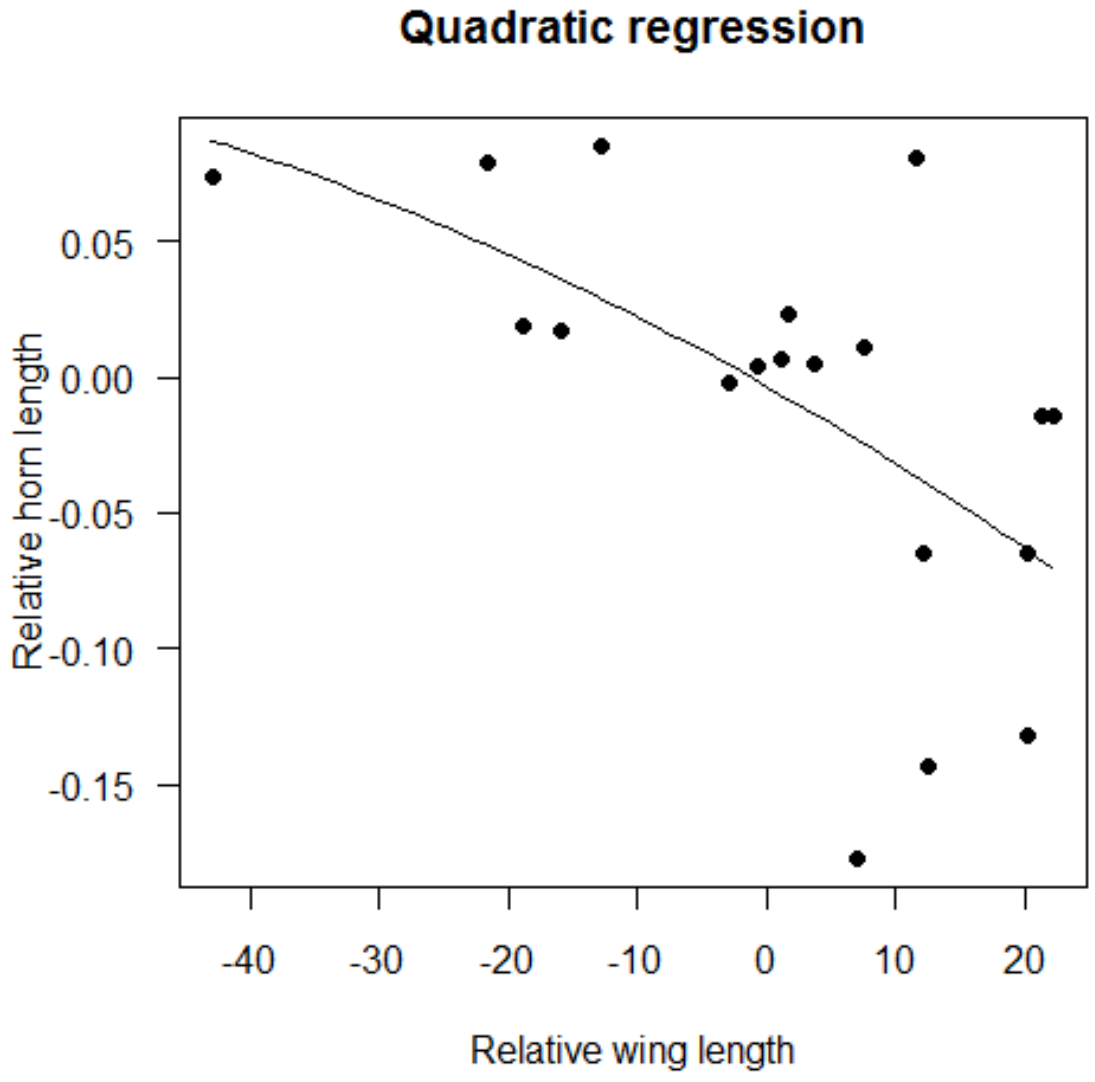
Emlen, D. J. 2001. Costs and the diversification of exaggerated animal structures. Science 291: 1534-1536.



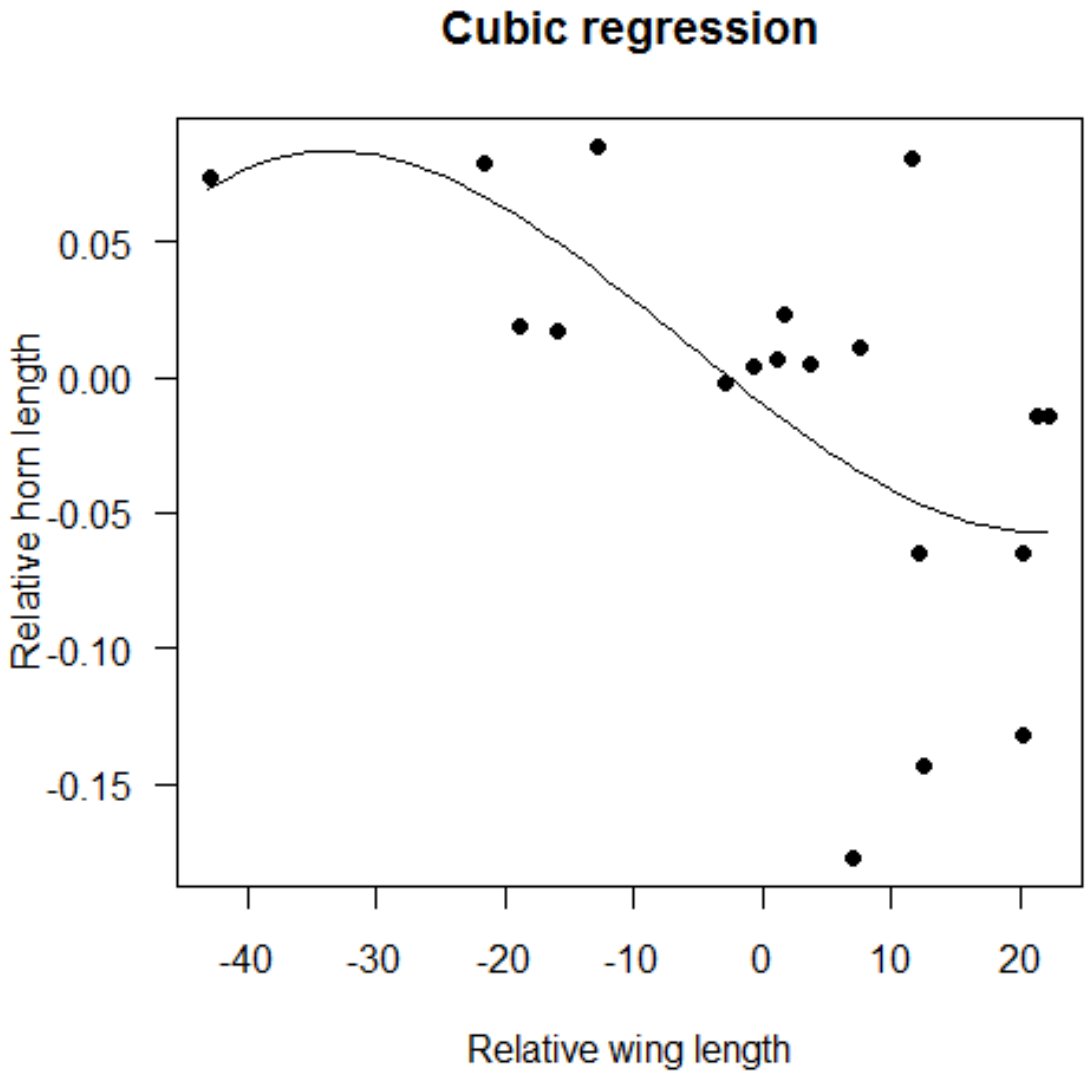
Start with a linear regression



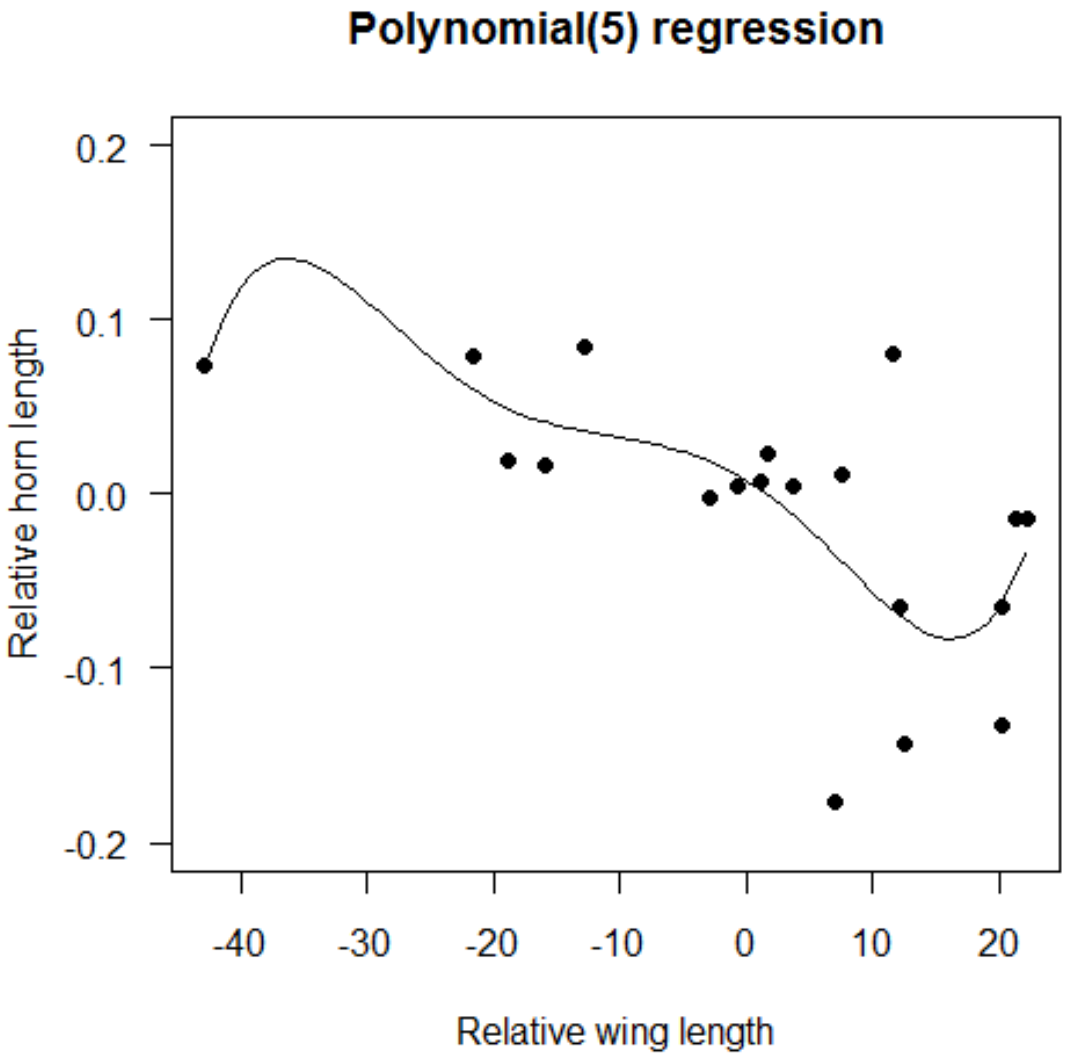
Why not a quadratic regression instead (polynomial degree 2)



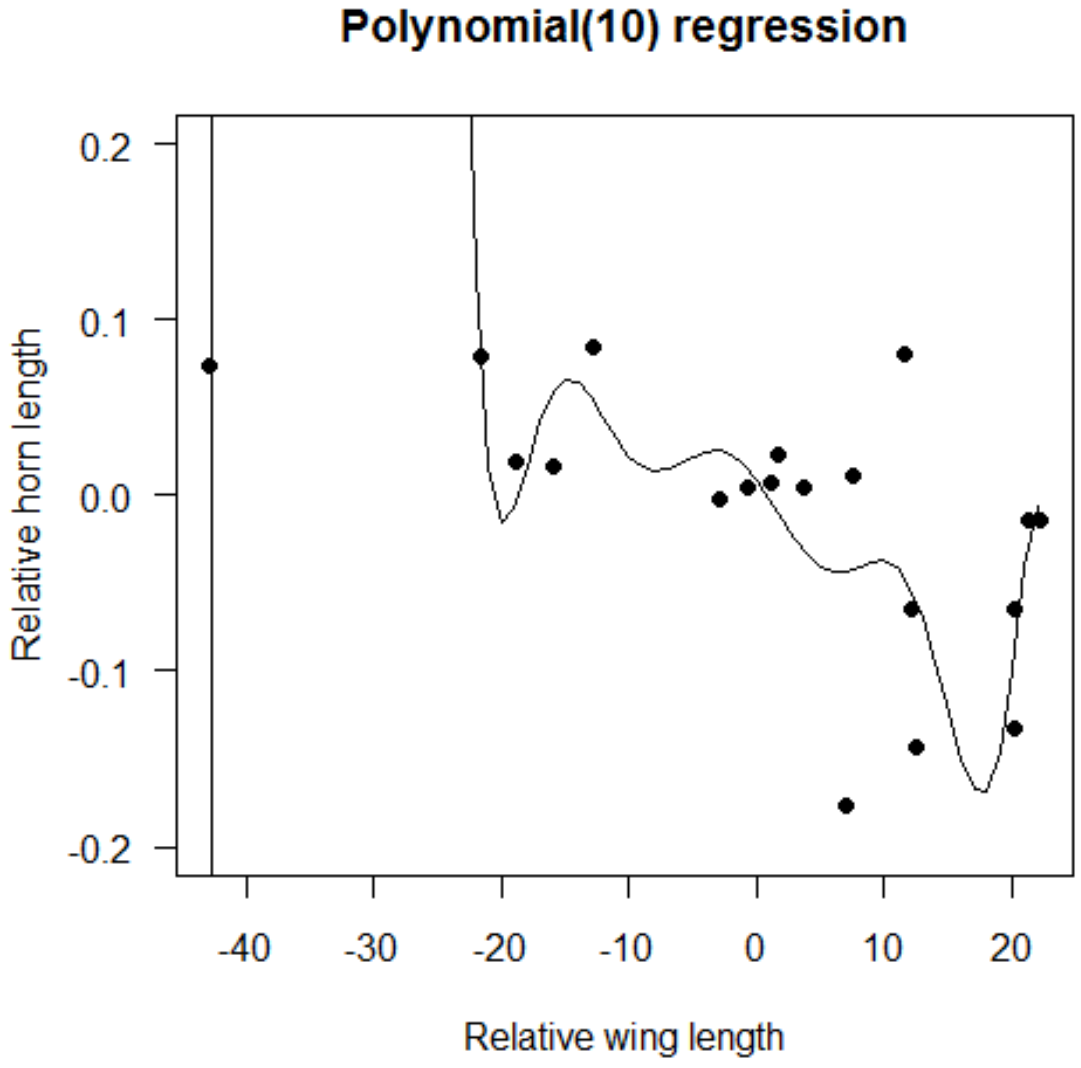
How about a cubic polynomial regression (degree 3)



Better still, a polynomial degree 5

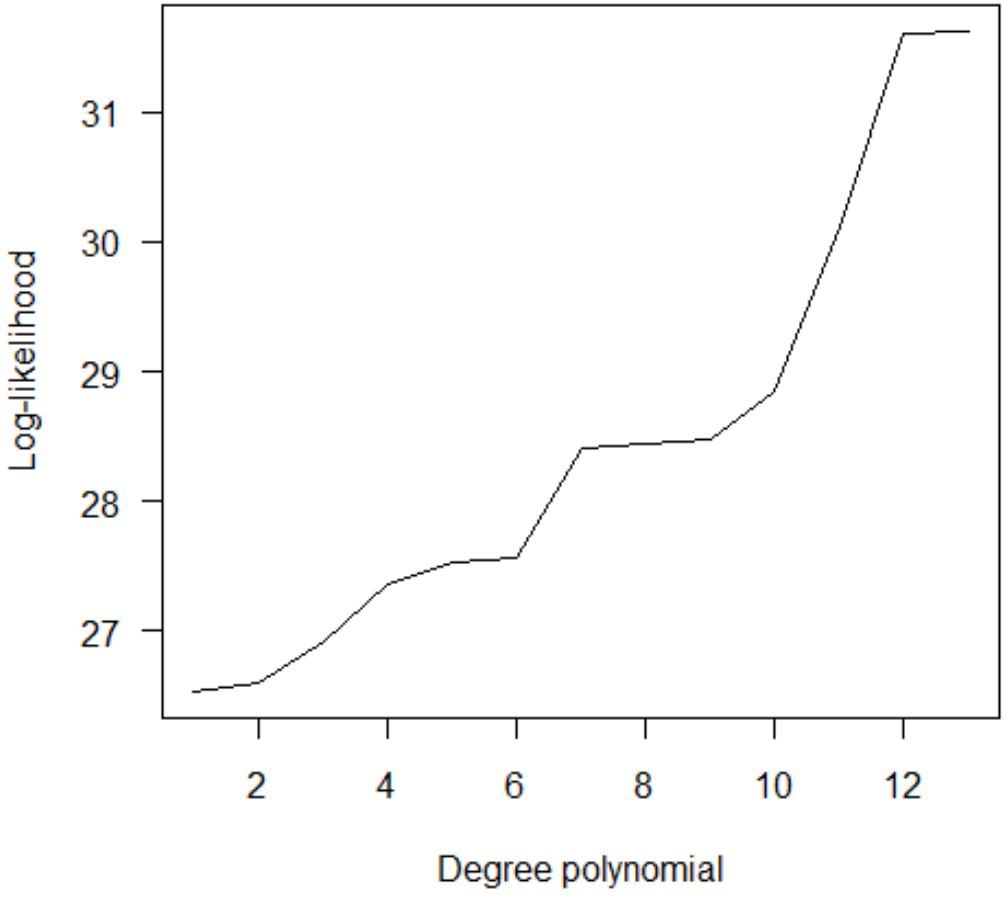


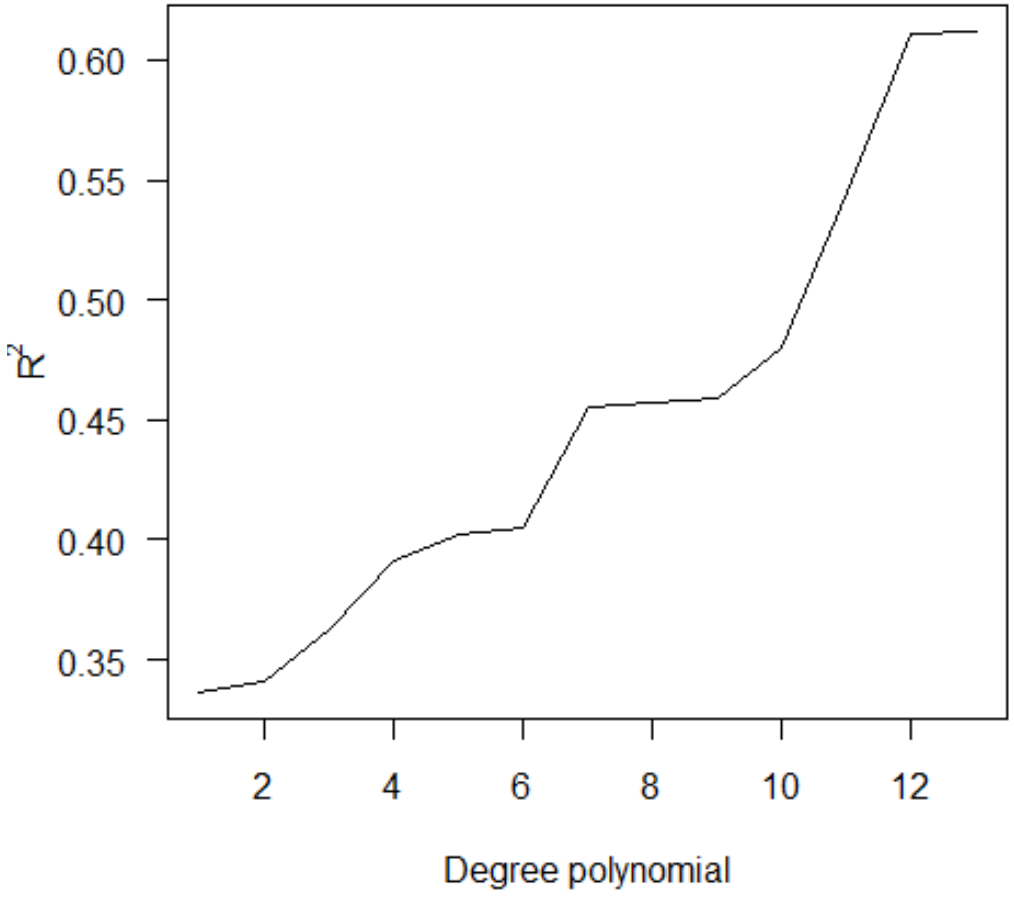
A polynomial, degree 10



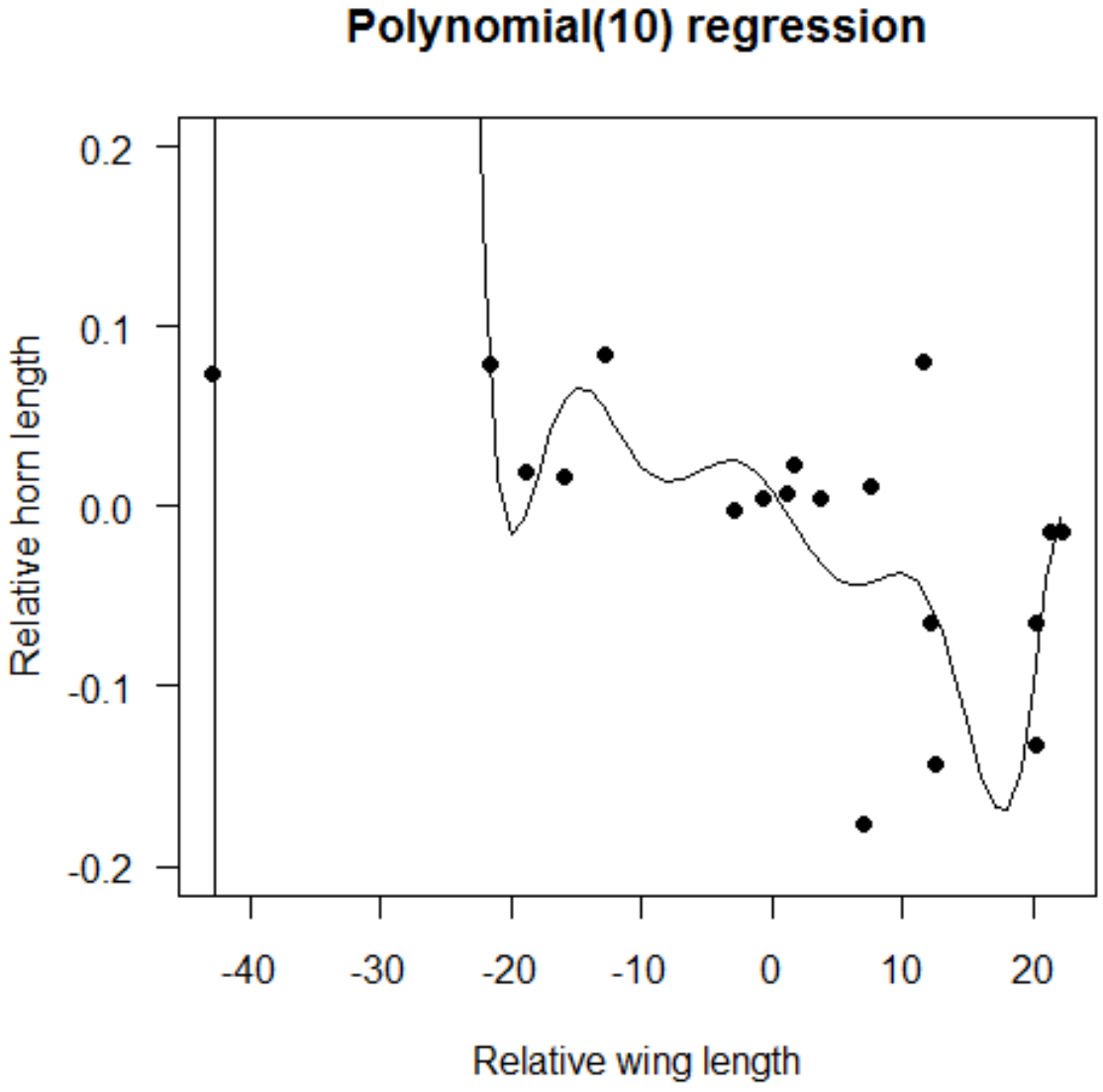
R^2 and log-likelihood increase with number of parameters in model

Isn't this good? Isn't this what we want – the best fit possible to data?





What is wrong with this picture



may explain this data well, but doesn't do a good job of explaining new data points

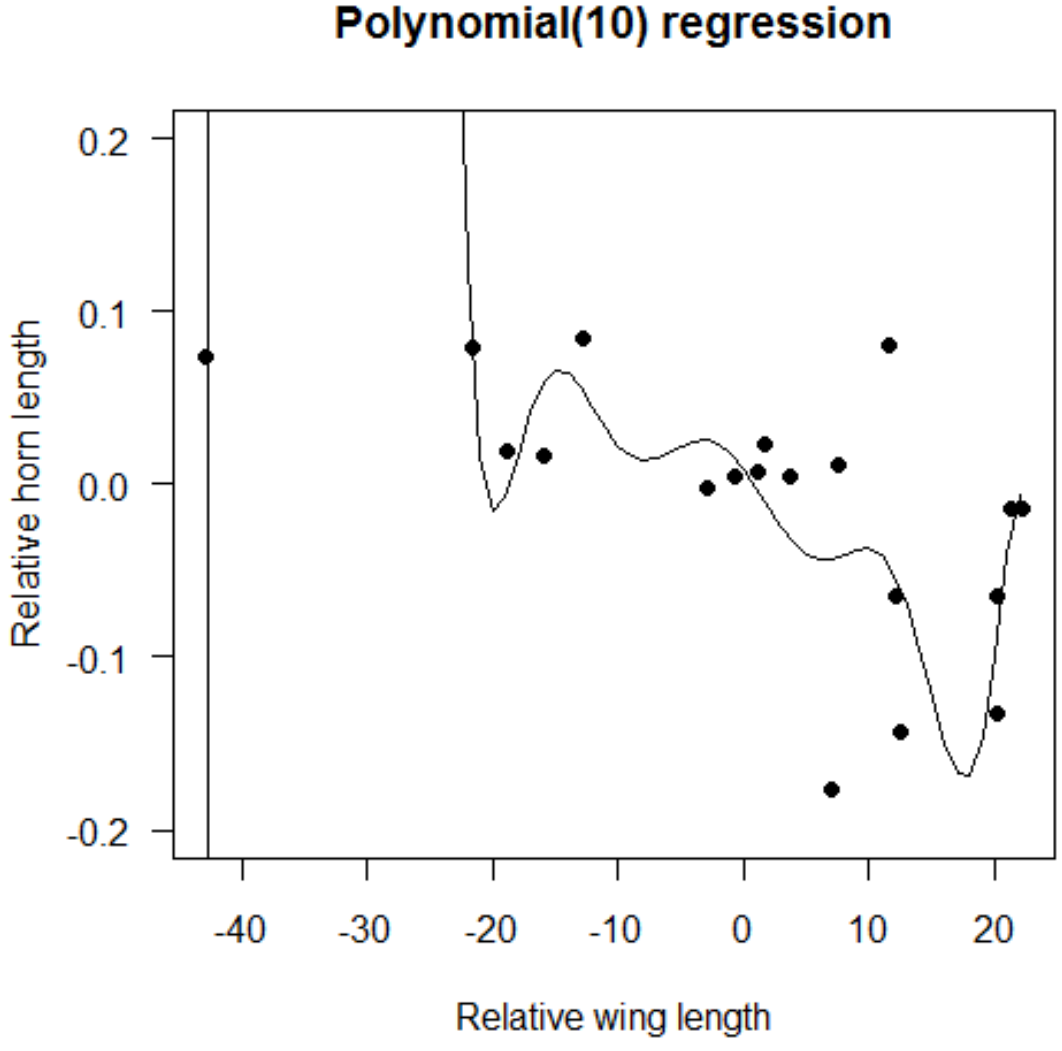
Maybe it violates some principle

Parsimony principle: Fit no more parameters than is necessary. If two or more models fit the data almost equally well, prefer the simpler model.

"models should be pared down until they are minimal adequate"

-- Crawley 2007, p325

But how is "minimal adequate" decided? What criterion is used?



Stepwise elimination of terms is a common practice

This approach involves fitting a multiple regression with many variables, followed by a cycle of deleting model terms that are not statistically significant and then refitting. Continue until only statistically significant terms remain. The procedure ends us up with a single, final model, the “minimum adequate model.”

By what criterion does this approach actually yield the “best” model?

Each cycle in which a variable is dropped from the model involves “accepting” a null hypothesis. Might this not lead to the wrong model by committing a sequence of Type 2 errors?

How repeatable is this process? With a different sample, would we arrive at the same model every time? Might there be other combinations of variables that fit the data nearly as well?

One criterion: choose the model that predicts best

The *bias-variance tradeoff*: both influence prediction errors of a model.

Training error: how well the model fits the actual data

Test error: how well the model fits a new sample of data

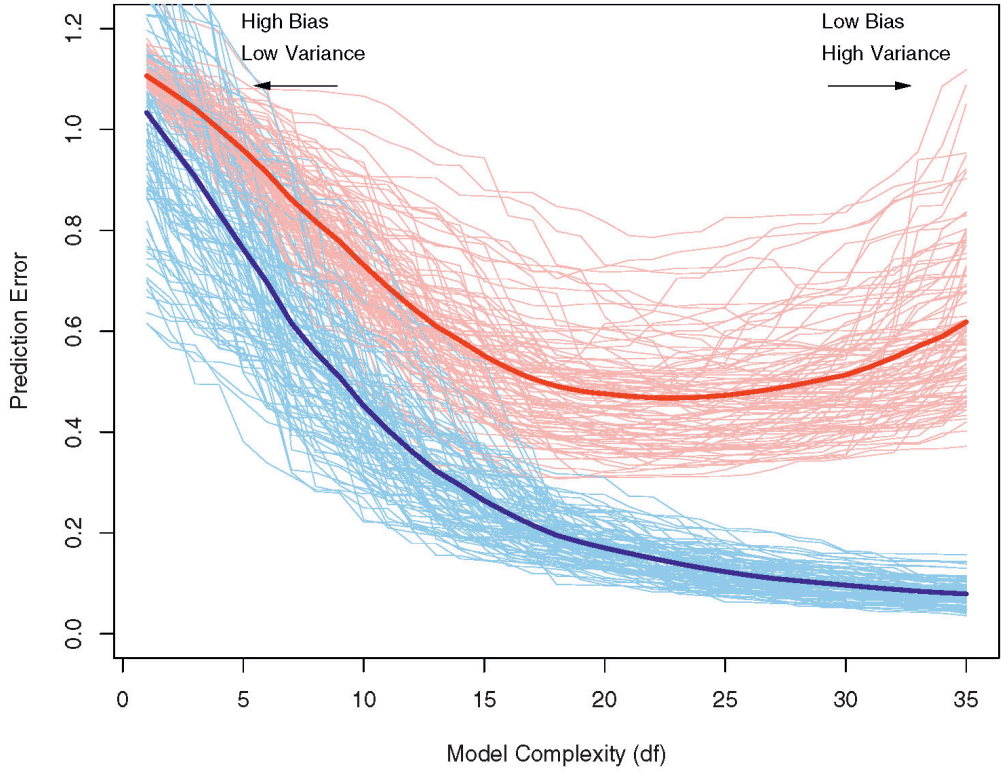


FIGURE 7.1. *Behavior of test sample and training sample error as the model complexity is varied. The light blue curves show the training error* $\overline{\text{err}}$*, while the light red curves show the conditional test error* $\text{Err}_{\mathcal{T}}$ *for 100 training sets of size 50 each, as the model complexity is increased. The solid curves show the expected test error* Err *and the expected training error* $\text{E}[\overline{\text{err}}]$*.*

Hastie et al. (2009)

red line: better prediction using an intermediate complexity
even though the best model (blue line) is the one of the highest complexity

There are only two sources of prediction error: bias - prediction that we make will be offset consistently
fitting fewer models than 35 will result in a high degree of bias

If you fit a model with greater and greater complexity your bias goes down

noise goes up with increasing complexity, decreasing ability to predict

"Cross-validation score" is one way to estimate prediction error:

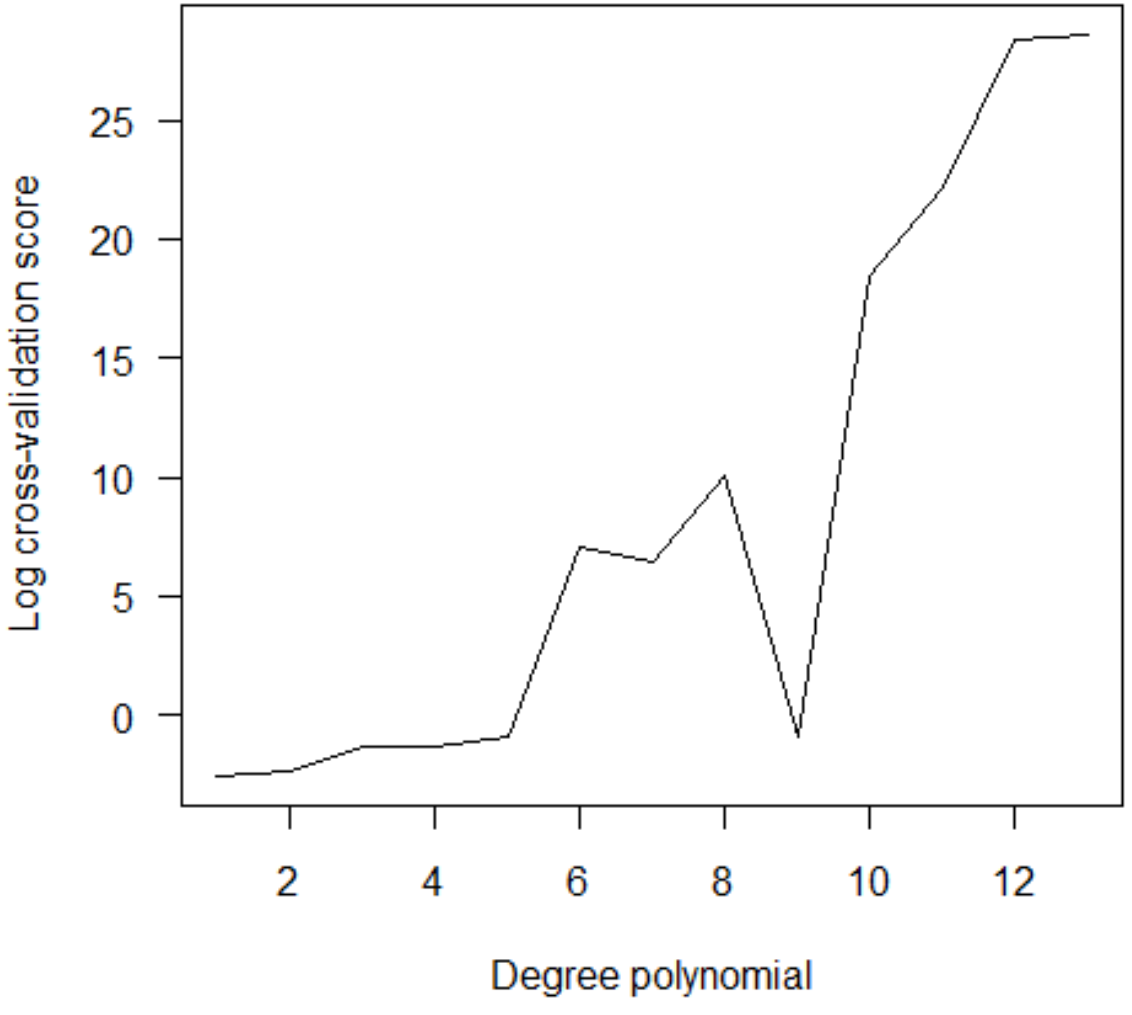
$$\text{CVscore} = \sum e_{(i)}^2$$

(larger CV score is worse), where

$$e_{(i)}^2 = \left(y_i - \hat{y}_{(i)}\right)^2$$

$\hat{y}_{(i)}$ is the predicted value for y_i when the model is fitted to the data leaving out y_i.

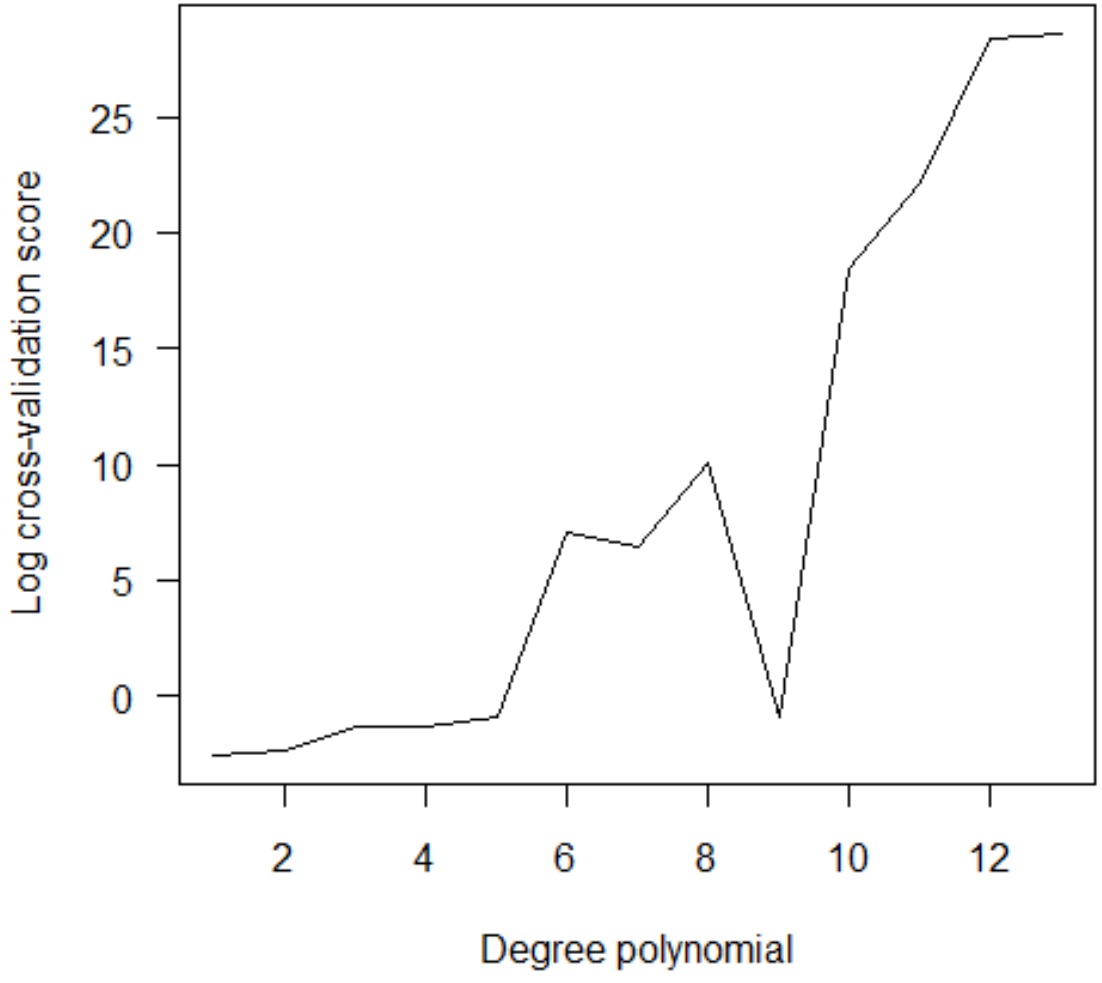
In our beetle example, the CV score worsens with increasing numbers of parameters in the model. Here, linear is "best". But other models do nearly equally well.



What else is worrying about my polynomial regression analysis

I'm data dredging. I didn't have any hypotheses to help guide my search. This can lead to dubious results.

E.g., my 9th degree polynomial is surprisingly good at prediction. But is there any good a priori reason to include it among the set of models to evaluate?



Some reasonable objectives

- We want a model that approximates the true relationship between the variables.
- We want a model that predicts well.
- We would like to know what other models also fit the data nearly as well as the "best".
- We would like to be able to compare models, not just nested models, those for which one model, the "reduced," is a subset of the other, the "full" model.

Reminder: Reduced vs. full models are referred to as "nested models", because the one contains a subset of the terms occurring in the other. Models in which the terms contained in one are not a subset of the terms in the other are called "non-nested" models. (Don't confuse with nested experimental designs or nested sampling designs.)

How to accomplish these goals

To answer this, we need a model selection approach to give us:

- A **criterion** to compare models:
  - Mallow's C_p
  - AIC (Akaike's Information Criterion)
  - BIC (Bayesian Information Criterion)

  and
- A **strategy** for searching the candidate models

Mallow's C_p is frequently used in multiple regression

Criterion: Mallow's C_p. Proposed in 1973.

$$C_p = \frac{\mathrm{SS}_{\text{error}}}{\hat{\sigma}^2} - n + 2p$$

$\mathrm{SS}_{\text{error}}$ is the error sum of squares for the model with p predictors
$\hat{\sigma}^2$ is the estimated error mean square of the true model (e.g., all predictors).
n is the sample size.
p is the number of predictors (explanatory variables) in model (including intercept).

C_p estimates the mean square prediction error. It is equivalent to AIC for linear regression if the assumptions of normality and independence of errors is met.

The p behaves like a penalty for including too many predictors (explanatory variables). This feature is shared with all other model selection criteria.

Mallow's C_p is frequently used in multiple regression

It is implemented in R with "all subsets regression" in the `leaps` package

Strategy: Test all possible models and select the one with smallest C_p

`leaps` uses an efficient algorithm to choose among a potentially huge number of models.

Typically we are modeling **observational** data. We are not dealing with data from an experiment, where we can make intelligent choices based on the experimental design.

By investigating all possible subsets of variables, we are admitting that the only intelligent decision we've made is the choice of variables to try. No other scientific insight was used to decide an *a priori* set of models.

Example 2a: Ant species richness

Data: Effects of latitude, elevation, and habitat on ant species richness.

Gotelli, N.J. & Ellison, A.M. (2002b). Biogeography at a regional scale: determinants of ant species density in bogs and forests of New England. Ecology, 83, 1604–1609.

	site	nspecies	habitat	latitude	elevation
1	TPB	6	forest	41.97	389
2	HBC	16	forest	42.00	8
3	CKB	18	forest	42.03	152
4	SKP	17	forest	42.05	1
...					
23	TPB	5	bog	41.97	389
24	HBC	6	bog	42.00	8
25	CKB	14	bog	42.03	152
26	SKP	7	bog	42.05	1
...					

n = 44 sites

(Bog and forest sites were technically paired by latitude and elevation, but residuals were uncorrelated, so we'll follow authors' lead in treating data as independent for the purposes of this exercise)

Example 2a: Ant species richness

Regression model with all possible terms:

```
z <- lm(log(nspecies) ~ habitat * latitude * elevation)
```

This evaluates all subsets of Habitat, Latitude, Elevation and their 2- and 3-way interactions.

`leaps` requires that all variables be numeric (I disguised habitat as a numeric variable by scoring: 0=bog, 1=forest)

Not all the evaluated models are necessarily sensible (dubious to fit a model with a 3-way interaction and no main effects).

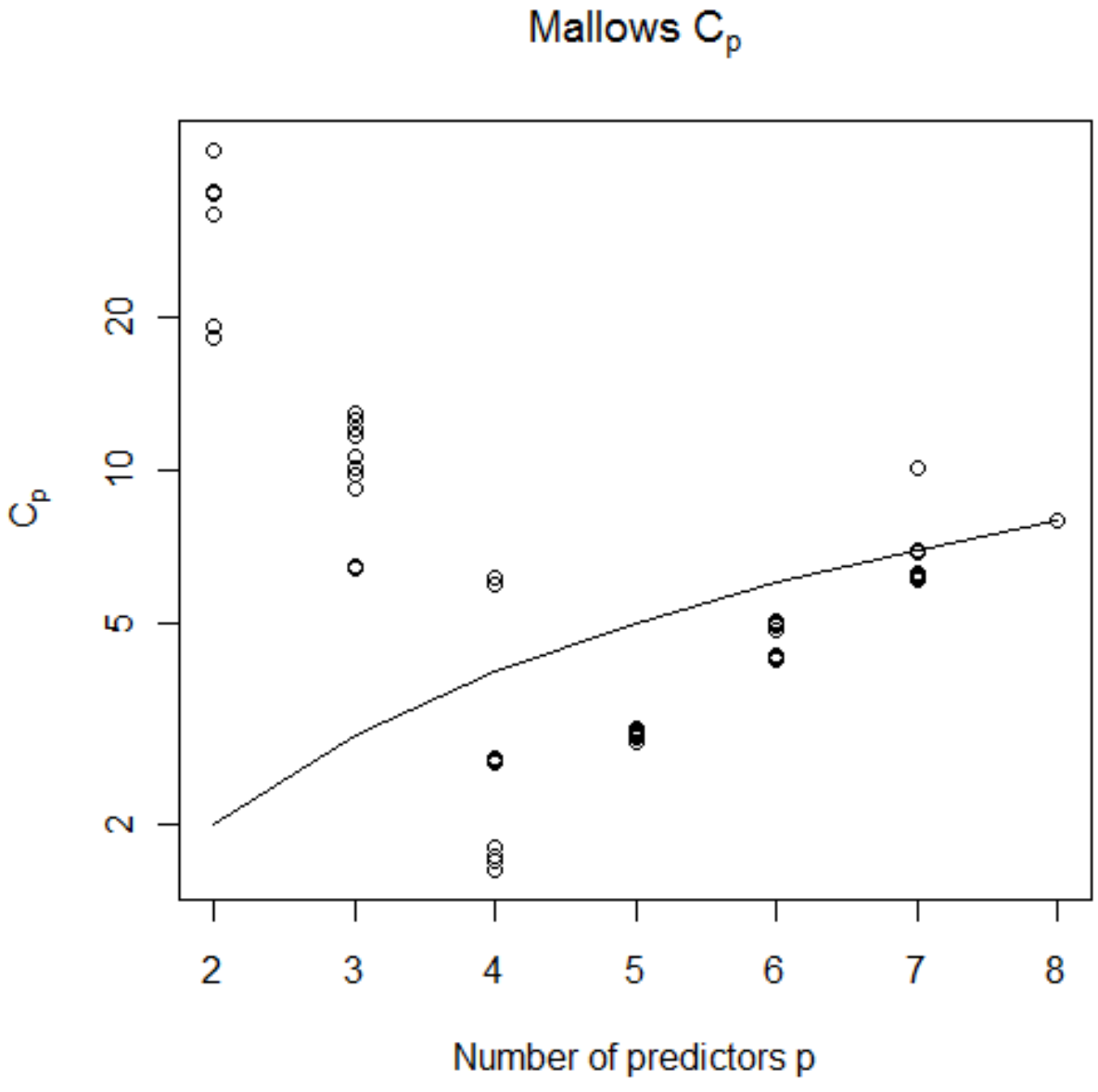
Example 2a: Ant species richness

By default, `leaps` saves the top 10 models for each value of p.

The line in the figure indicates $C_p = p$ (vertical axis is in log units)

The best model has 4 predictors (3 variables plus intercept)

But other models fit the data nearly as well, i.e., all those for which $C_p < p$

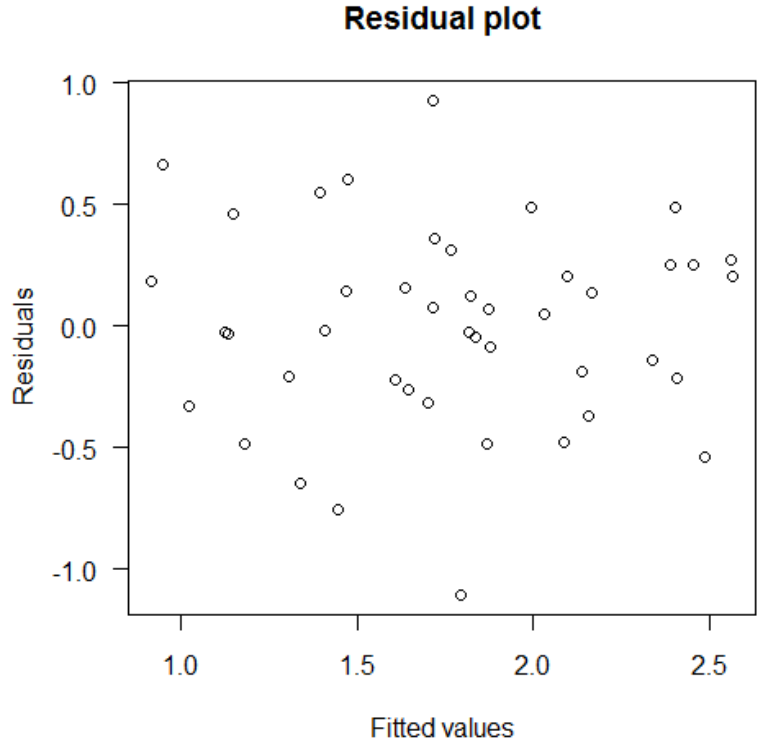


Example 2a: Ant species richness

Best model (smallest C_p):

```
z <- lm(log(nspecies) ~ habitat + latitude + elevation)
```

```
              Estimate Std. Error t value Pr(>|t|)
(Intercept) 10.3180285  2.6101963   3.953 0.000306 ***
habitat      0.6898845  0.1269432   5.435 2.94e-06 ***
latitude    -0.2007838  0.0609920  -3.292 0.002085 **
elevation   -0.0010856  0.0004049  -2.681 0.010610 *
```



Example 2a: Ant species richness

A total of 34 models had $C_p < p$

Habitat	Latitude	Elevation	Habitat:Latitude	Habitat:Elevation	Latitude: Elevation	H:L:E
TRUE	TRUE	TRUE	FALSE	FALSE	FALSE	FALSE
FALSE	TRUE	TRUE	TRUE	FALSE	FALSE	FALSE
TRUE	TRUE	FALSE	FALSE	FALSE	TRUE	FALSE
FALSE	TRUE	FALSE	TRUE	FALSE	TRUE	FALSE
FALSE	TRUE	FALSE	TRUE	TRUE	FALSE	FALSE
TRUE	TRUE	FALSE	FALSE	TRUE	FALSE	FALSE
FALSE	TRUE	FALSE	TRUE	FALSE	FALSE	TRUE
TRUE	TRUE	FALSE	FALSE	FALSE	FALSE	TRUE
TRUE	TRUE	TRUE	FALSE	FALSE	TRUE	FALSE
FALSE	TRUE	TRUE	TRUE	FALSE	TRUE	FALSE
TRUE	TRUE	TRUE	FALSE	TRUE	FALSE	FALSE
TRUE	TRUE	TRUE	FALSE	FALSE	FALSE	TRUE
FALSE	TRUE	TRUE	TRUE	TRUE	FALSE	FALSE
FALSE	TRUE	TRUE	TRUE	FALSE	FALSE	TRUE
TRUE	TRUE	FALSE	FALSE	TRUE	TRUE	FALSE
TRUE	TRUE	FALSE	FALSE	FALSE	TRUE	TRUE
FALSE	TRUE	FALSE	TRUE	TRUE	TRUE	FALSE
FALSE	TRUE	FALSE	TRUE	FALSE	TRUE	TRUE
TRUE	TRUE	TRUE	FALSE	FALSE	TRUE	TRUE
TRUE	TRUE	TRUE	FALSE	TRUE	TRUE	FALSE
FALSE	TRUE	TRUE	TRUE	FALSE	TRUE	TRUE
FALSE	TRUE	TRUE	TRUE	TRUE	TRUE	FALSE
TRUE	TRUE	TRUE	TRUE	FALSE	TRUE	FALSE
TRUE	TRUE	TRUE	FALSE	TRUE	FALSE	TRUE
TRUE	TRUE	TRUE	TRUE	TRUE	FALSE	FALSE
TRUE	TRUE	TRUE	TRUE	FALSE	FALSE	TRUE
FALSE	TRUE	TRUE	TRUE	TRUE	FALSE	TRUE
TRUE	TRUE	FALSE	FALSE	TRUE	TRUE	TRUE

Example 2a: Conclusions

If regression is purely for prediction, all of the models with $C_p < p$ predict about equally well. In which case there's no reason to get carried away about your "best" model.

Interpretation is more complex if regression is used for explanation. If numerous models are nearly equally good at fitting the data, it is difficult to claim to have found the predictors that "best explain" the response.

Keep in mind that, like correlation, "regression is not causation". It is not possible to find the true causes of variation in the explanatory variable without experimentation anyway.

AIC (Akaike's Information Criterion)

Criterion: minimize AIC.

$$\text{AIC} = -2 \ln L(\text{model} \mid \text{data}) + 2k$$

k is the number of parameters estimated in the model (including intercept and σ^2)

higher the likelihood the better your AIC score

First part of AIC is the log-likelihood of the model given the data.

Second part is 2*k*, which acts like a penalty for the number of variables in the model (this is an interpretation, not why the 2*k* is part of the formula).

Just as with the log-likelihood, what matters is not AIC itself but the difference in AIC between models.

AIC (Akaike's Information Criterion)

$$\mathrm{AIC} = -2 \ln L(\mathrm{model} \mid \mathrm{data}) + 2k$$

AIC is an estimate of the expected distance ("information lost") between the fitted model and the "true" model.

There are two reasons why a model fitted to data might depart from the truth.

1. Bias: The fitted model may contain too few parameters, underestimating the complexity of reality.
2. Variance: There is not enough data to yield good estimates of many parameters, leading to high sampling error (low precision).

AIC yields a balance between these two sources of information loss.

AIC (Akaike's Information Criterion)

Search strategy: One method is the stepwise procedure for selection of variables implemented in the `stepAIC` command in the `MASS` library in R.

Can use for categorical and numerical variables.

`stepAIC` obeys "marginality restrictions". Not all terms are on equal footing. For example

- Squared term x^2 is not fitted unless x is also present in the model
- the interaction a:b is not fitted unless both a and b are also present
- a:b:c not fitted unless all two-way interactions of a, b, c, are present

The search algorithm is therefore intelligent and economical.

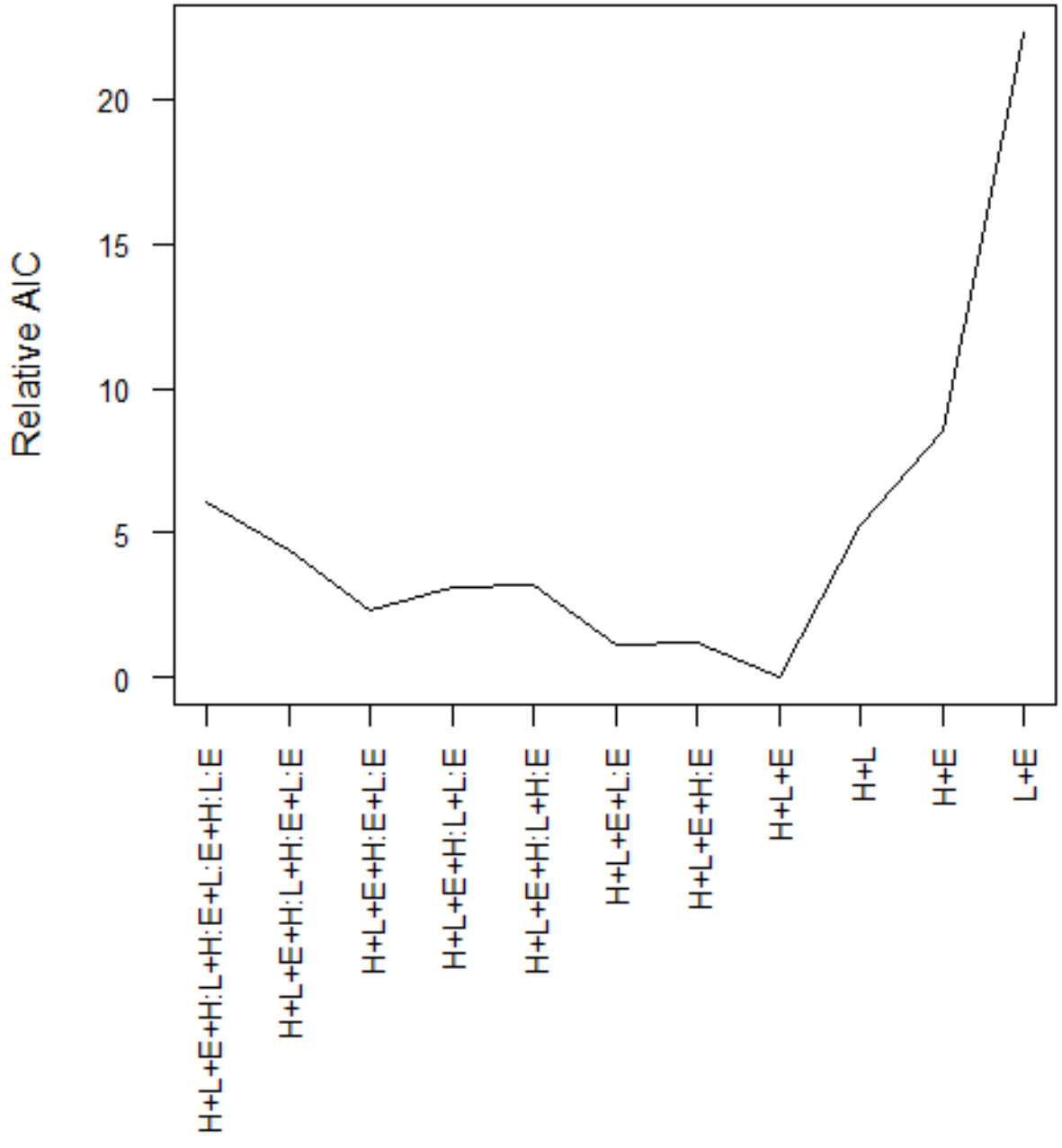
(However, we are still data dredging.)

Example 2b: Ant species richness

Same data as that analyzed earlier.

AIC difference (Δ) is the difference between a model's AIC score and that of the "best" model.

"Best" model is again the model with the three additive terms Habitat, Latitude, and Elevation



How AIC differs from classical statistical approaches

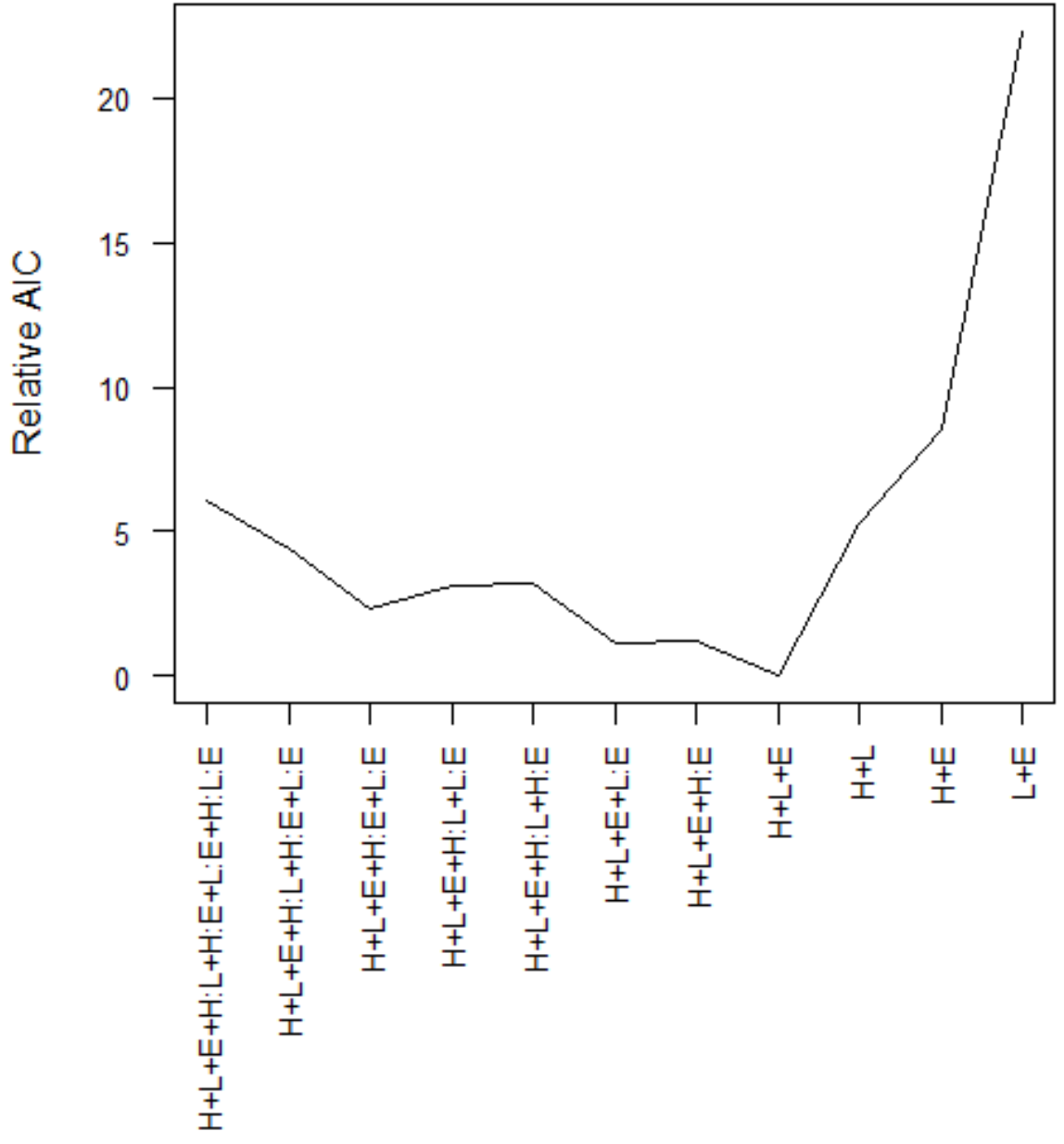
~~significance~~

No hypothesis testing.

No null model.

No *P*-value.

No model is formally “rejected”.



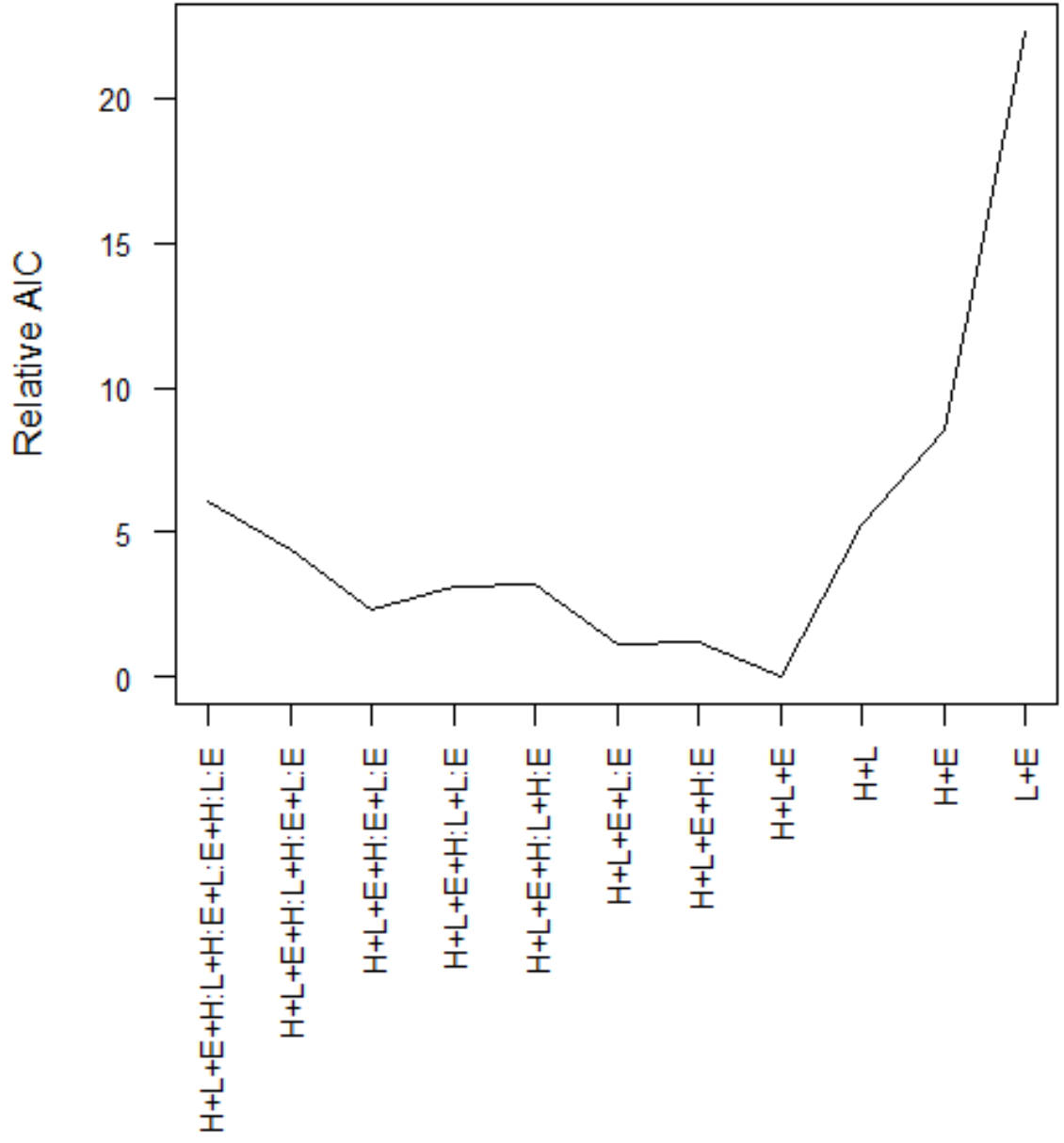
How AIC differs from classical statistical approaches

Several models may be about equally good.

<u>AIC difference (Δ) support</u>
0 – 2 Substantial support
4 – 7 Considerably less support
> 10 Essentially no support

Your “best” model isn’t necessarily the true model.

Remember: AIC balances the bias-variance trade-off. It does a good job to minimize information loss, on average.



Model uncertainty

AIC difference (Δ) support
0 – 2 Substantial support
4 – 7 Considerably less support
> 10 Essentially no support

The reason for model uncertainty is sampling error. Keep in mind that the data being used to select the “best” model is sampled from a population, and would be different if we returned to that same population for another sample.

Think of all the models that have some support as constituting a “confidence set” of models, analogous to a confidence interval when estimating a parameter.

Going further: Multimodel Inference

Avoids the need to base inference solely conditional upon the single “best” model.

Multimodel Inference allows inferences to be made about a parameter based on a set of models that are ranked and weighted according to level of support from the data.

“Model averaging” is an example: a model-average estimate takes a weighted estimate of the parameter estimates from each model deemed to have sufficient support.

The best source for further information is

Burnham, K. P., and D. R. Anderson. 2002. Model selection and multimodel inference: a practical information-theoretic approach. 2nd. New York, Springer

Selecting among candidate models

The information-theoretic approach shows it true advantage when comparing alternative conceptual or mathematical models to data

This is where data dredging ends and science begins:

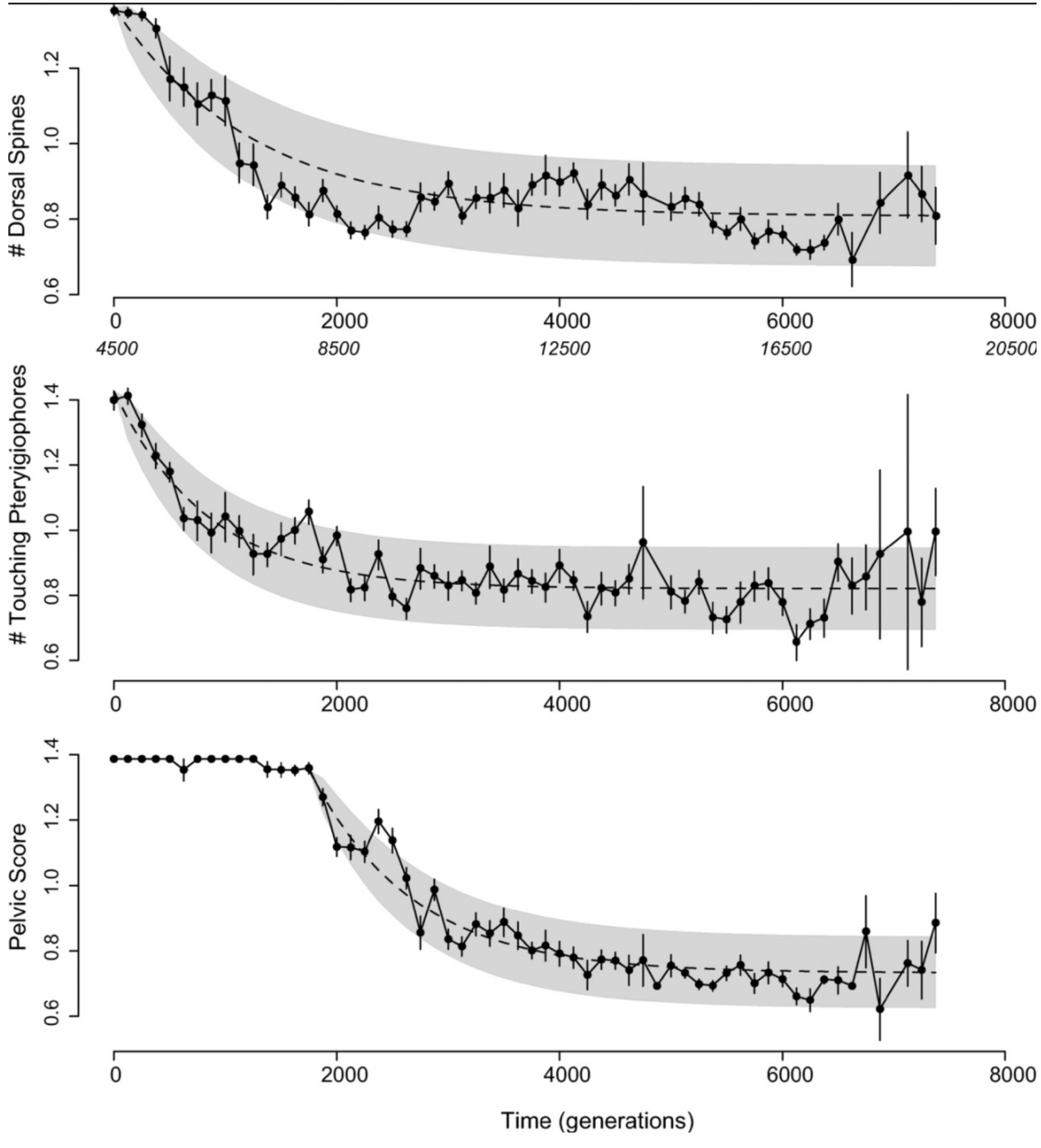
Formulating a set of candidate models

No model is considered the “null” model. Rather, all models are evaluated on the same footing.

Example 3: Adaptive evolution in the fossil record

Data: Armor measurements of 5000 fossil *Gasterosteus doryssus* (threespine stickleback) from an open pit diatomite mine in Nevada. Time=0 corresponds to the first appearance of a highly-armored form in the fossil record.

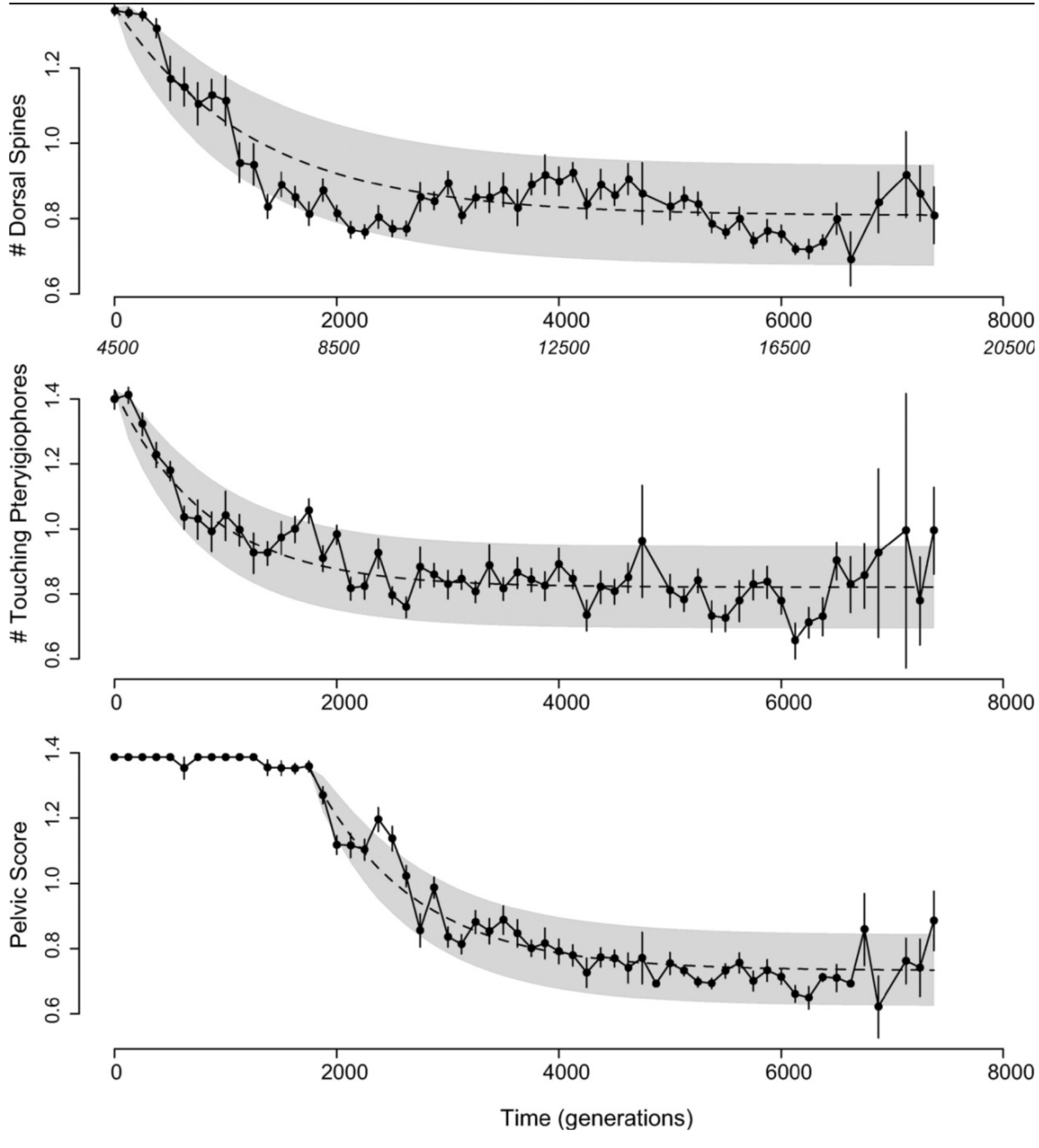
G. Hunt, M. A. Bell & M. P Travis 2008, *Evolution* 62: 700–710.



Example 3: Adaptive evolution in the fossil record

A previous analysis was not able to reject a null hypothesis of random drift in the trait means.

1 generation = 2 years



Example 3: Adaptive evolution in the fossil record

Hunt et al used AIC to compare the fits of two evolutionary models fitted to the data.

1. Neutral random walk (like Brownian motion)
Two parameters need to be estimated from the data: 1) initial trait mean; 2) variance of the random step size each generation.

2. Adaptive peak shift (Orstein–Uhlenbeck process)
Four parameters to be estimated: 1) initial trait mean; 2) variance of the random step size each generation; 3) phenotypic position of the optimum; 4) strength of the "pull" toward the optimum.

Example 3: Adaptive evolution in the fossil record

Results: AIC difference (Δ) of neutral model is large (no support)

Trait	Model	logL	K	AIC_C	Akaike weight	LRT
No. of dorsal spines	Neutral	86.48	2	−168.73	0.002	
	Adaptive	94.94	4	−181.11	**0.998**	16.92, $P = 0.0003$
Pterygiophores	Neutral	65.91	2	−127.59	0.001	
	Adaptive	74.80	4	−140.84	**0.999**	17.78, $P = 0.0002$
Pelvic score	Neutral	58.38	2	−112.46	0.001	
	Adaptive	68.33	4	−127.65	**0.999**	19.89, $P = 0.00005$

The adaptive model beats neutral drift for all three traits.

Akaike weight is the weight of evidence in favor of a model being the actual best model for the situation at hand, assuming that one of the models in the set really is the best. A 95% confidence set of models is obtained by ranking the models and summing the weights until that sum is ≥ 0.95.

Example 3: Adaptive evolution in the fossil record

Trait	Model	logL	K	AIC_C	Akaike weight	LRT
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	Adaptive	68.33	4	−127.65	**0.999**	19.89, $P = 0.00005$

Stepping back from the model selection approach, the authors showed that the adaptive model rejects neutrality in a likelihood ratio test (here the models are *not* on equal footing – one of them, the simpler, is set as the null hypothesis).

This suggests that even under the conventional hypothesis testing framework, specifying 2 specific candidate models is already superior to an approach in which the alternative hypothesis is merely “everything but the null hypothesis.”

Conclusion: Model Selection

It is not clear that stepwise elimination and null hypothesis significance testing is the ideal approach for model selection. Information-theoretic approaches have explicit criteria and better properties.

These approaches work best when thoughtful science is used to specify the candidate models under consideration (minimizing data dredging).

Working with a set of models that fit the data about equally well rather than with the one single best model recognizes that there is model uncertainty.

If you want even more certainty about which variables are the ones that really matter, then you will need to do an experiment.

Digression: Exploring your data is not all bad

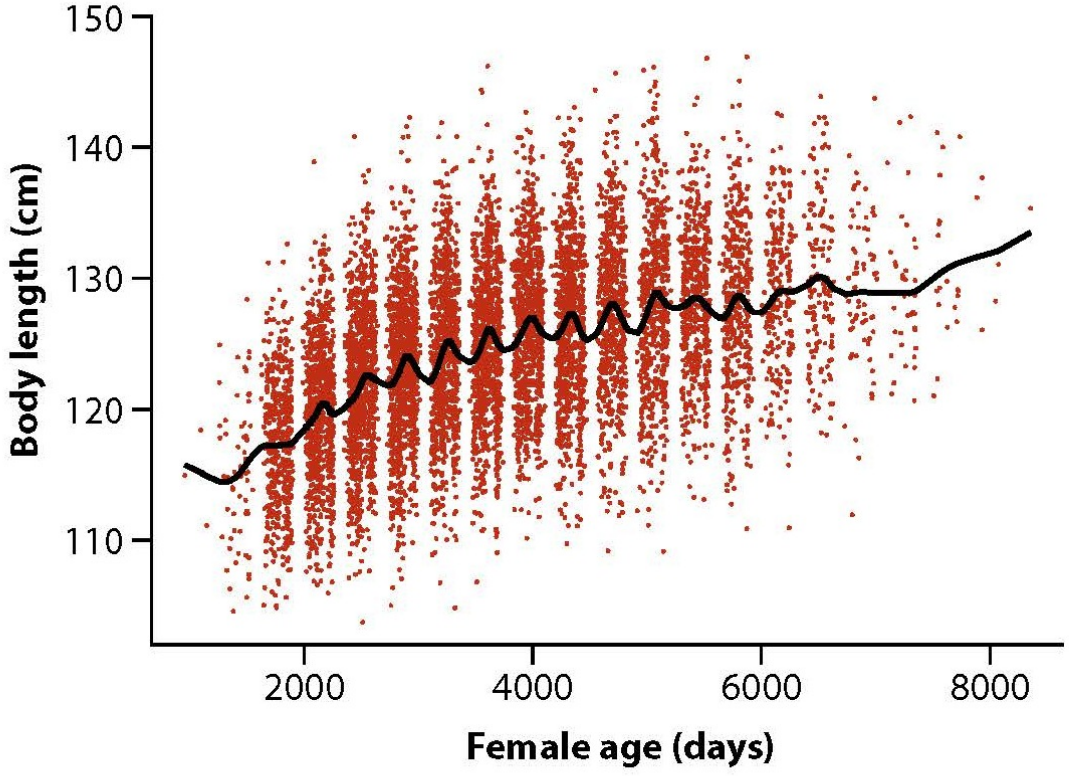

Figure 17.8-3 Measurements of body length as a function of age for female fur seals, with the "spline" fit in black.

Discussion paper for next week:

Cohen. J. 1994. The earth is round ($p < 0.05$). Am. Psych. 49: 997-1003.

Download from "**handouts**" tab on course web site.

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