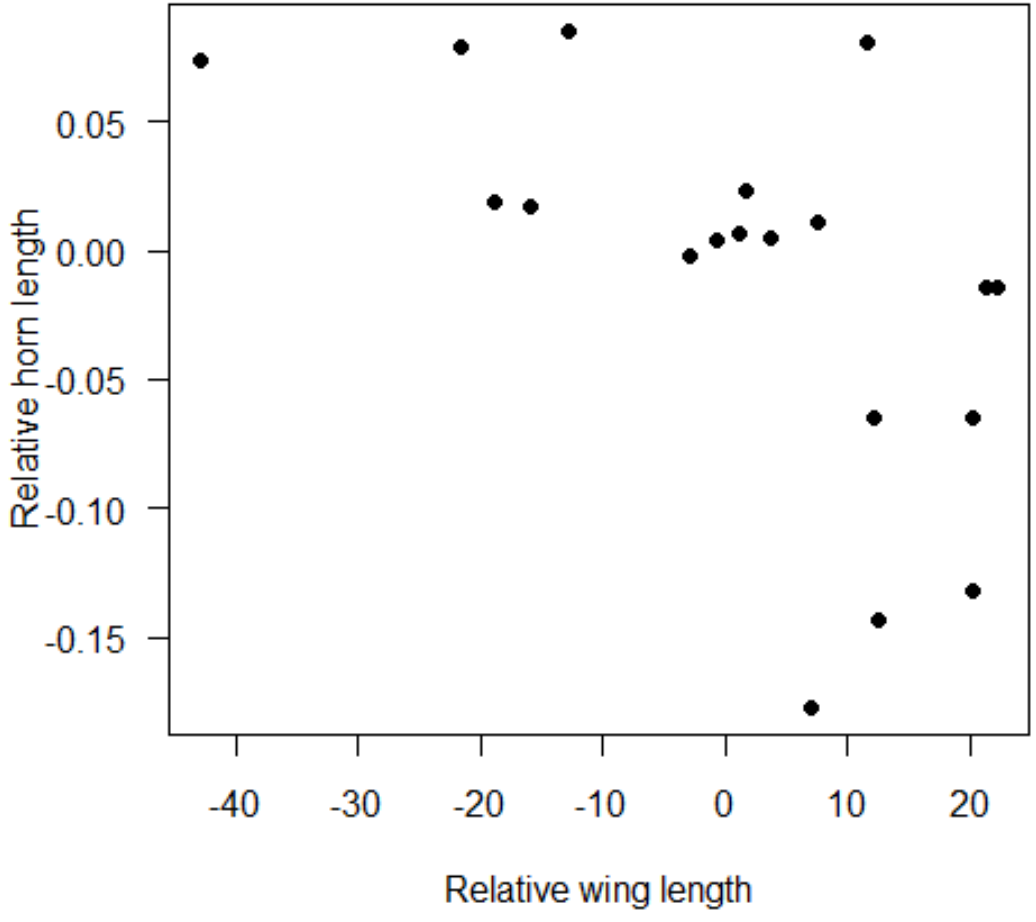
Outline for today

- Example 1: polynomial regression – which degree is best?
- The problem of model selection
- Choose among models using an explicit criterion
- Goals of model selection
- Criteria: Mallow's Cp and AIC
- Search strategies: All subsets; stepAIC
- Example 2: Predicting ant species richness
- Several models may fit about equally well
- The science part: formulate a set of candidate models
- Example 3: Adaptive evolution in the fossil record

Example 1: Fit a polynomial regression model – which degree is best?

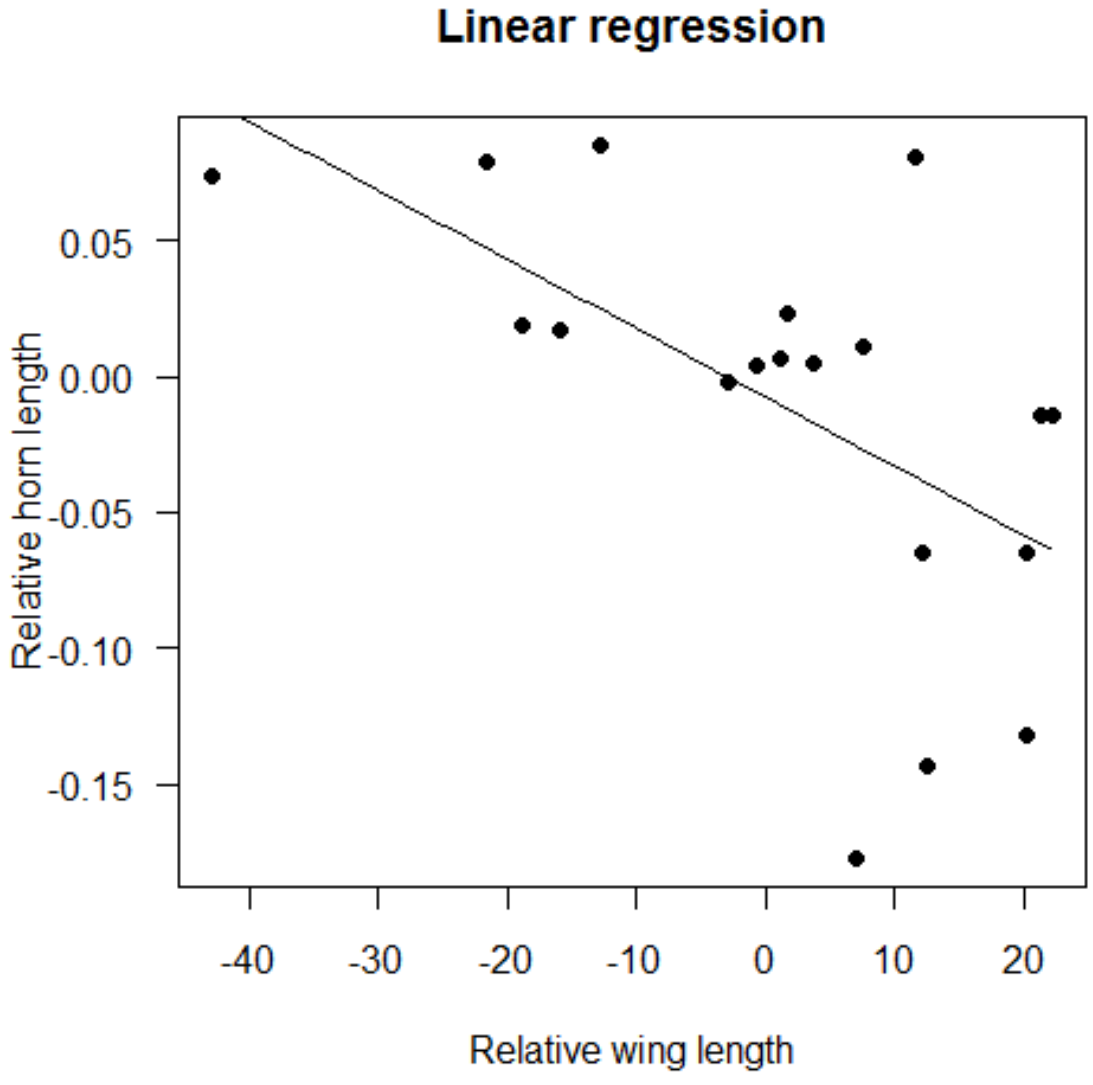
Data: Trade-off between the sizes of wings and horns in 19 females of the beetle *Onthophagus sagittarius*. Both variables are size corrected.

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



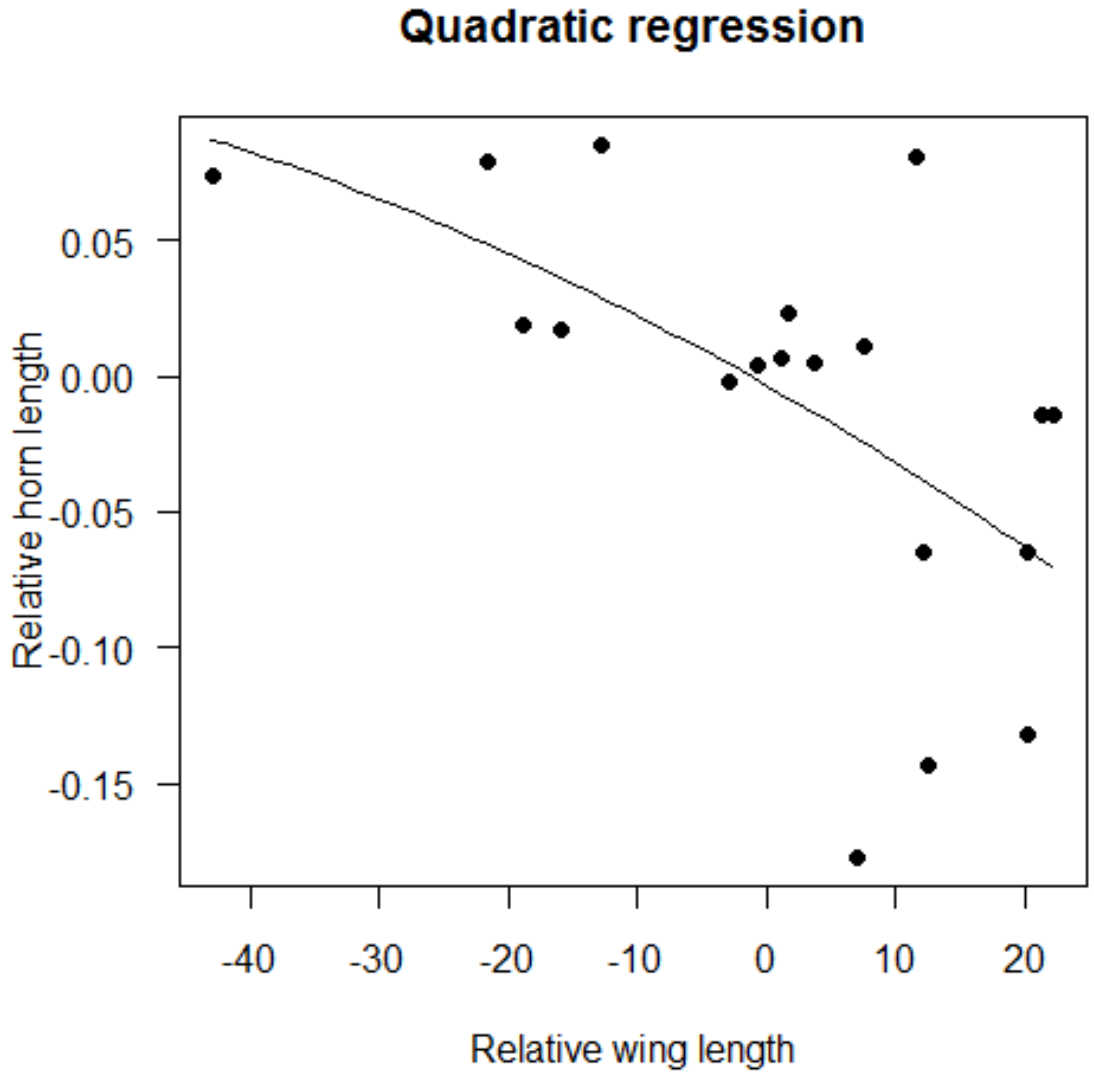
Example 1: Fit a polynomial regression model – which degree is best?

Start with a linear regression



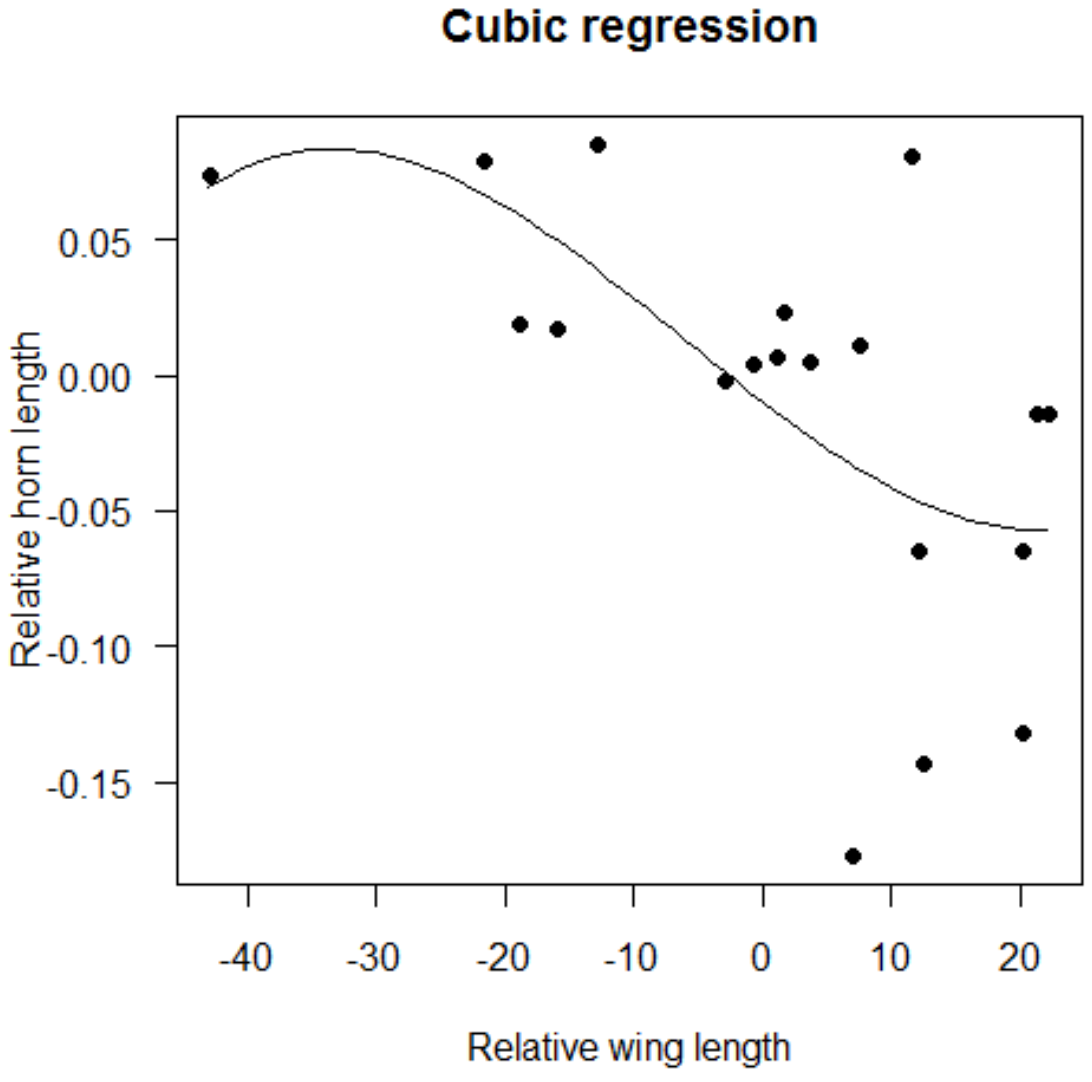
Example 1: Fit a polynomial regression model – which degree is best?

Why not a quadratic regression instead (polynomial degree 2)



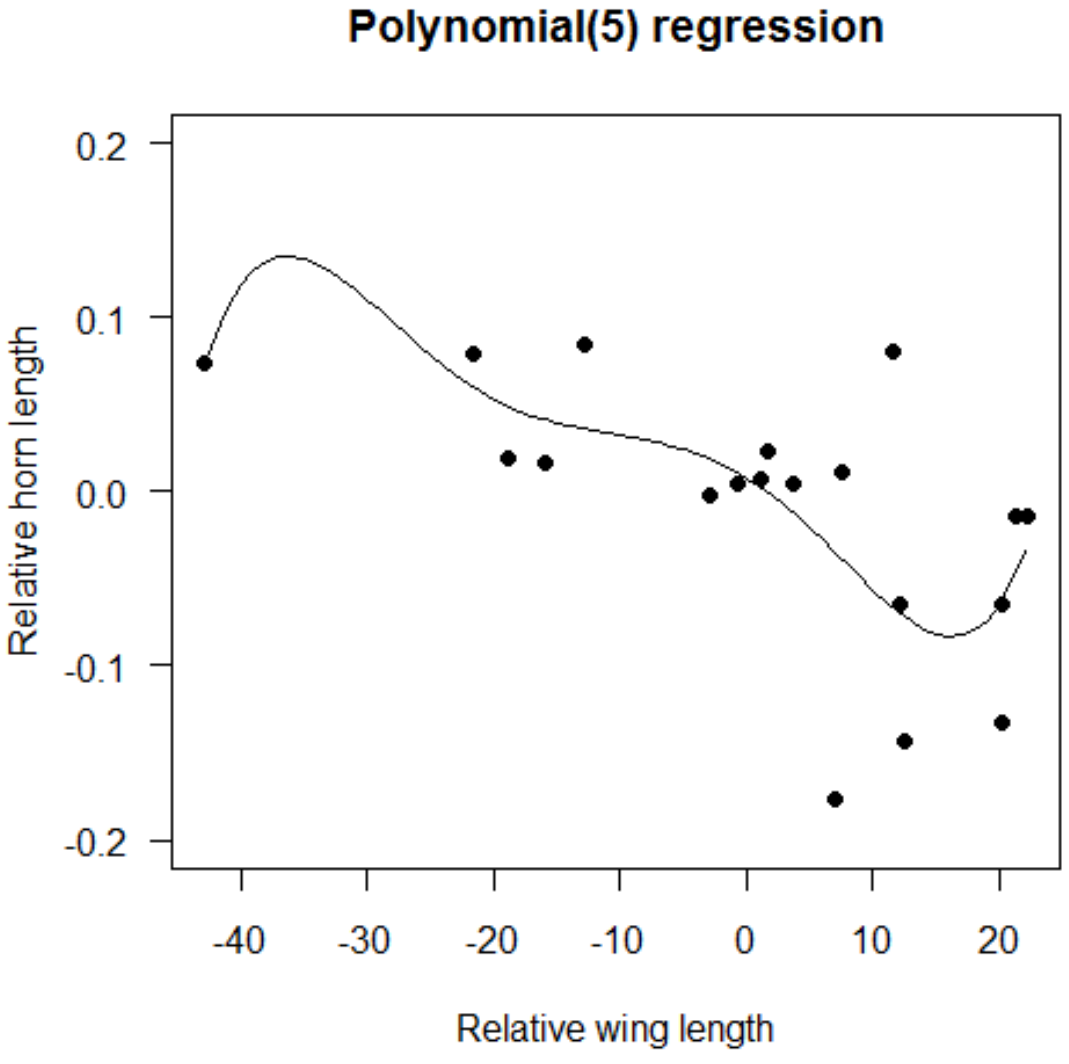
Example 1: Fit a polynomial regression model – which degree is best?

How about a cubic polynomial regression (degree 3)



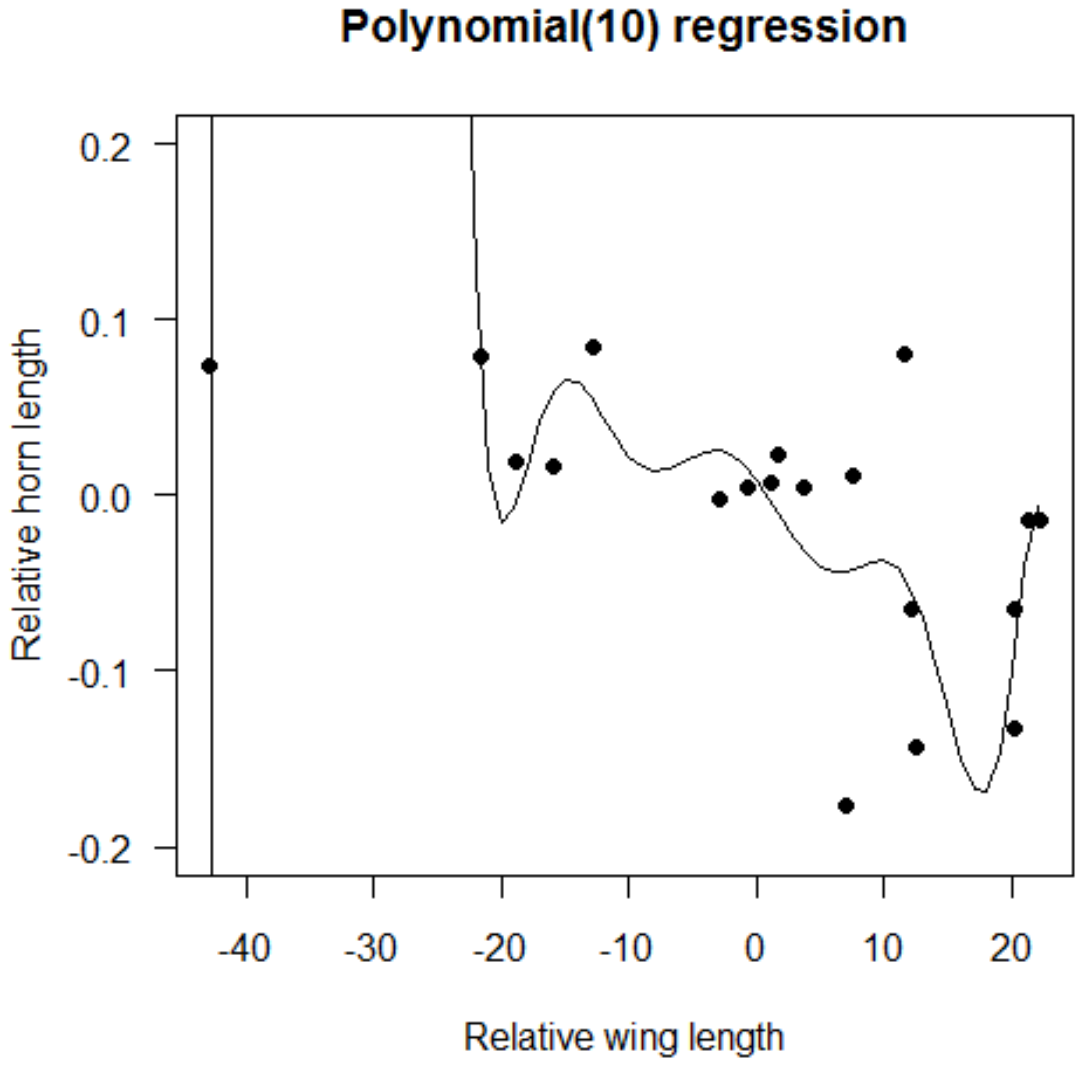
Example 1: Fit a polynomial regression model – which degree is best?

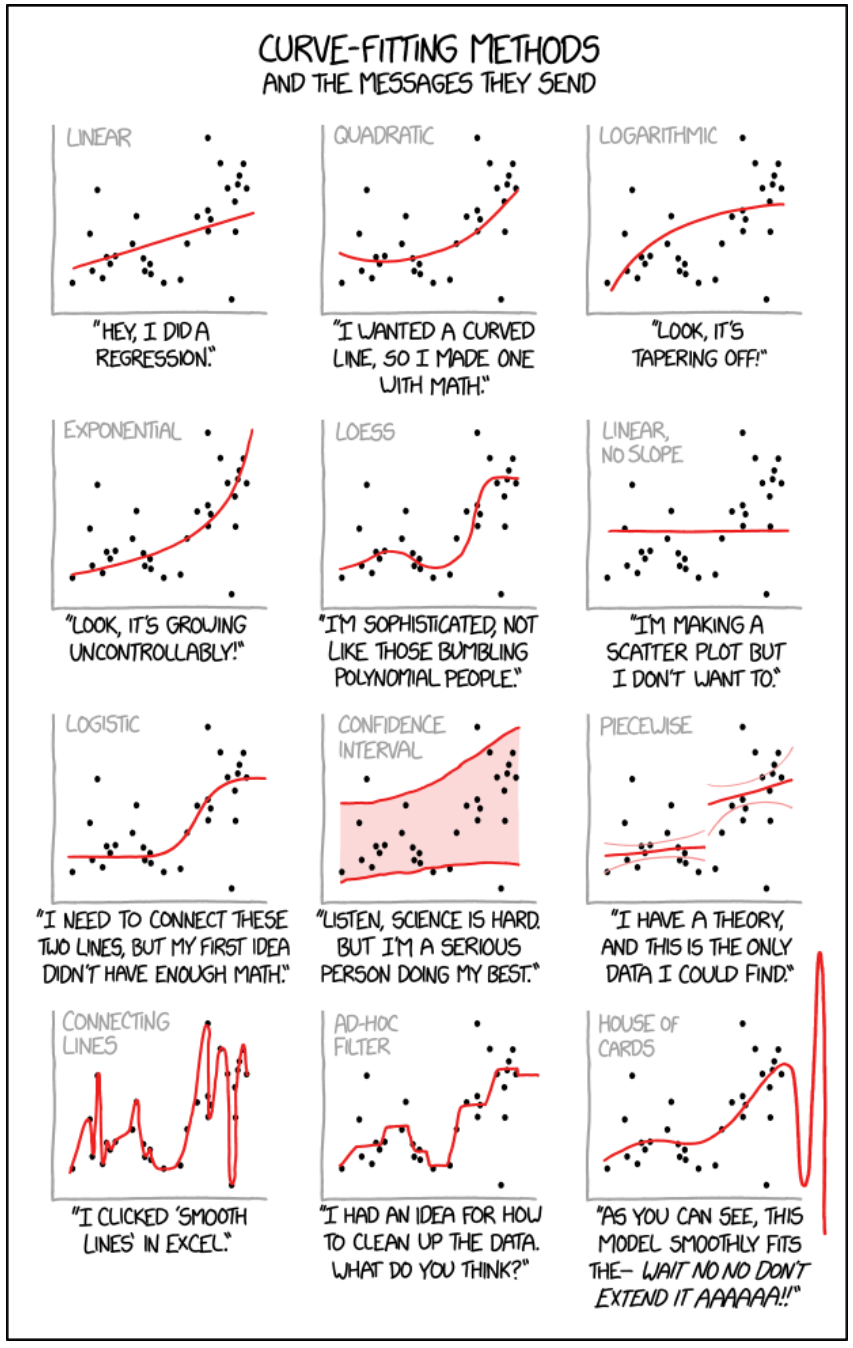
Better still, a polynomial degree 5



Example 1: Fit a polynomial regression model – which degree is best?

A polynomial, degree 10



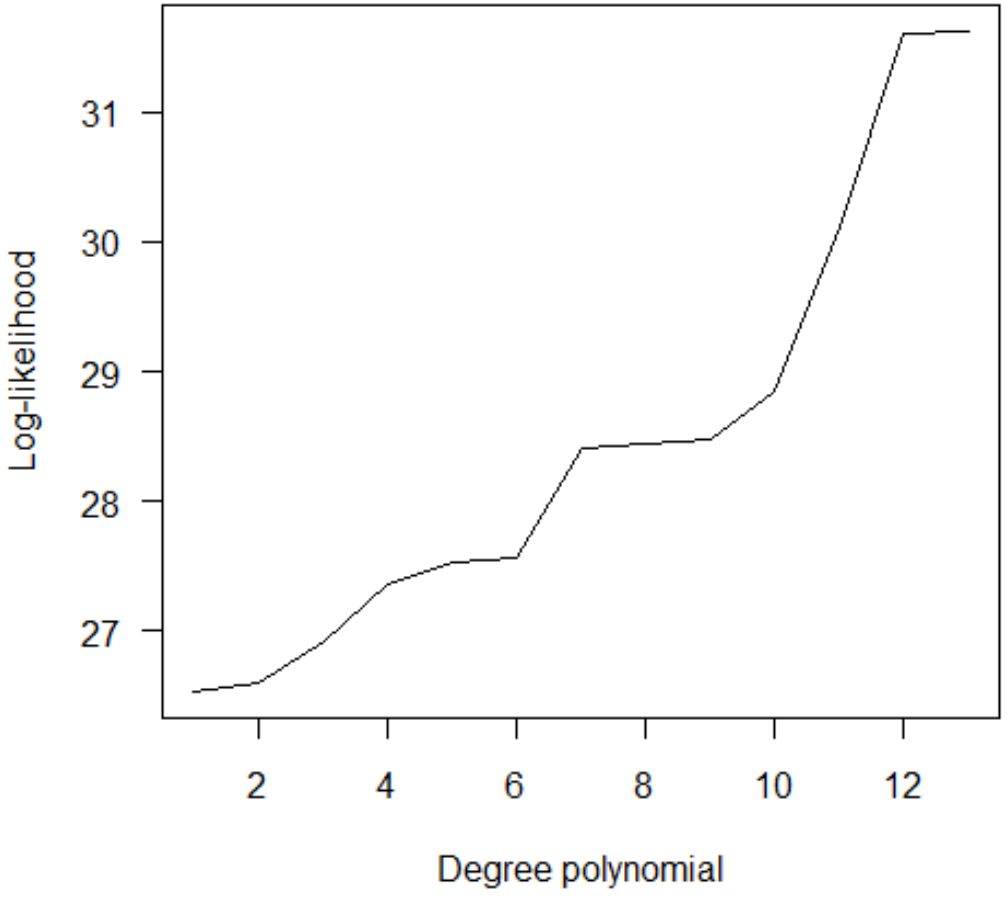


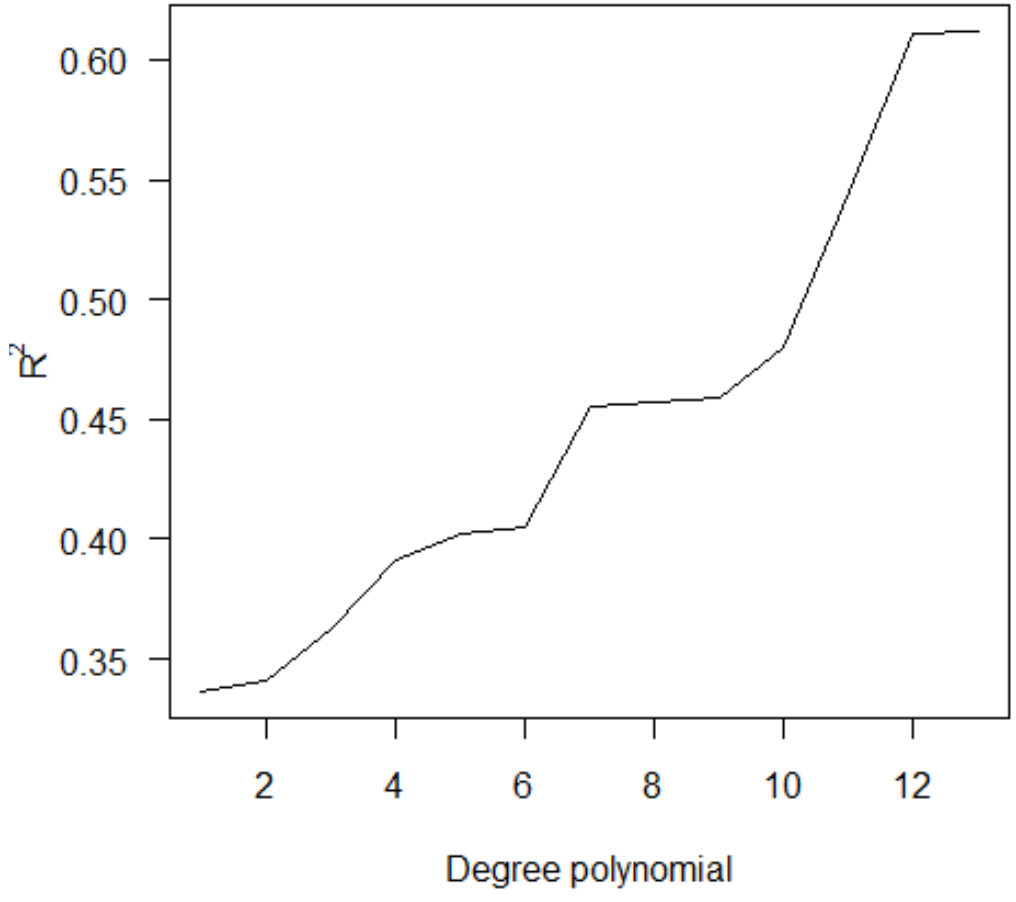
xkcd.com/2048

The problem of model selection

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

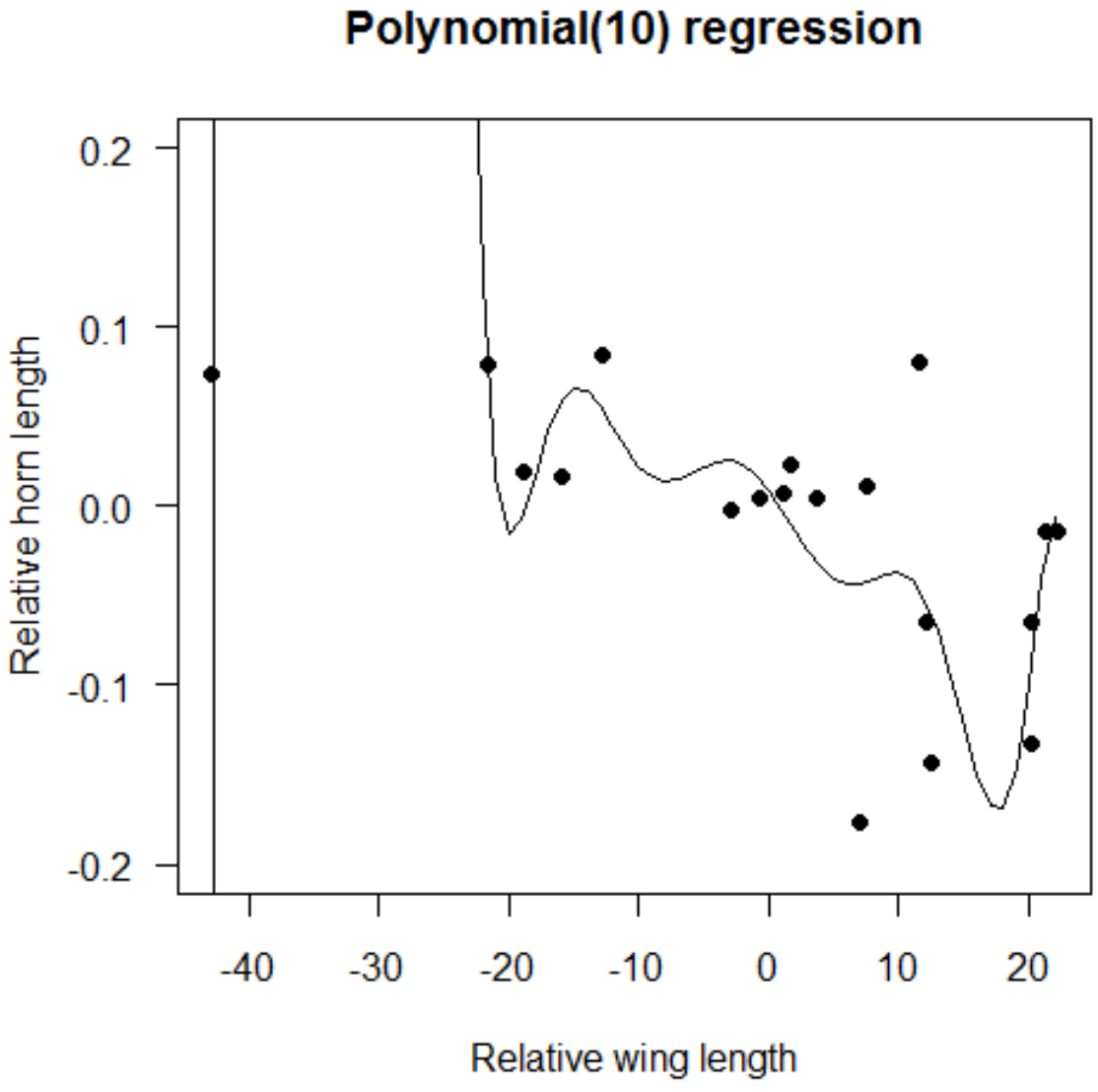
Isn't this good? Isn't this what we want – the best fit possible to data?





The problem of model selection

What is wrong with this picture?



The problem of model selection

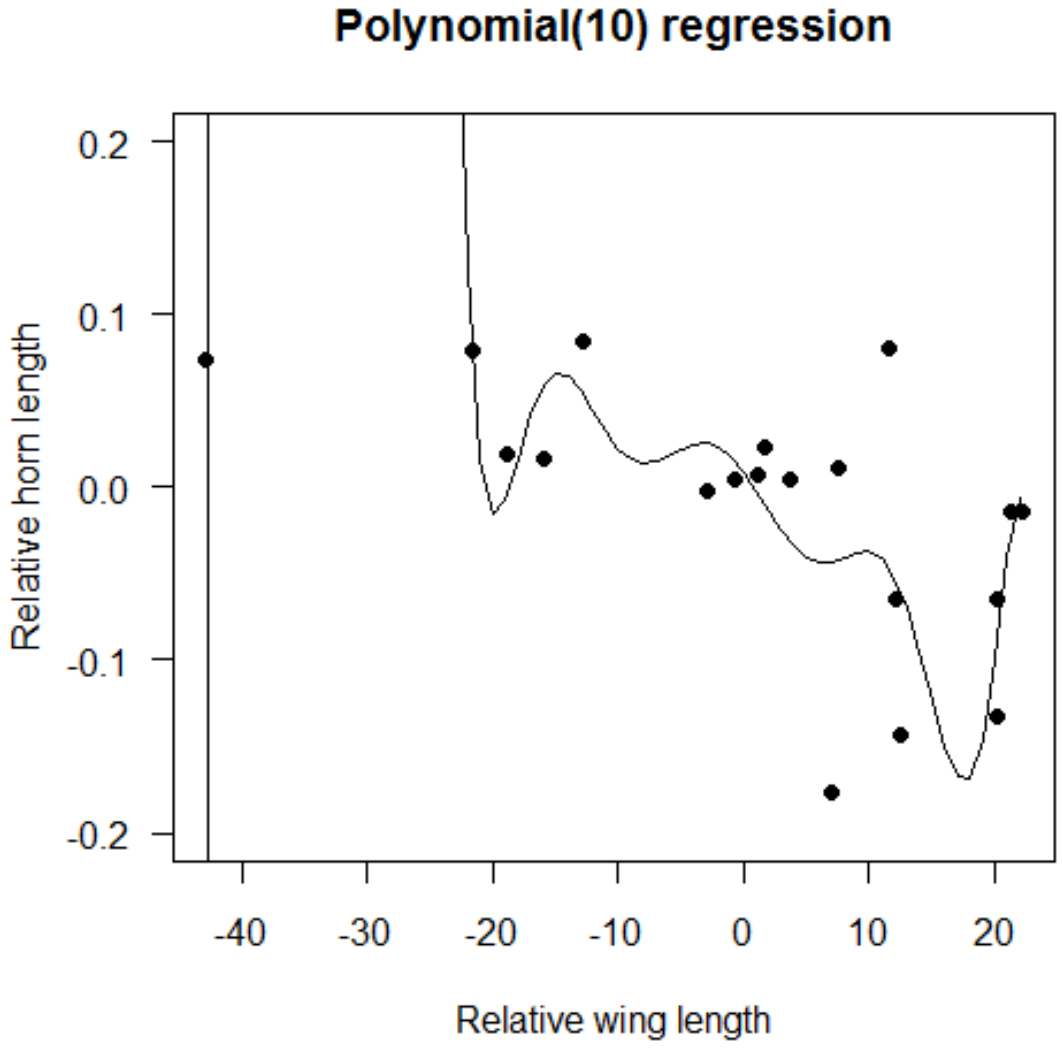
Does it violate some principle?

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?



The problem of model selection

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.”

Does stepwise elimination of terms actually yield the "best" model?

1. What criterion are we actually using to decide which model is "best"?

2. Each step in which a variable is dropped from the model involves "accepting" a null hypothesis. What happens if we drop a false null hypothesis? How can a sequence of Type 2 errors lead us to the "best" model?

3. How repeatable is the outcome of stepwise regression? With a different sample, would stepwise elimination bring us to the same model again?

4. Might models with different subsets of variables fit the data nearly as well?

Alternative: choose among models using an explicit criterion

A reasonable criterion: choose the model that predicts best.

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

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

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

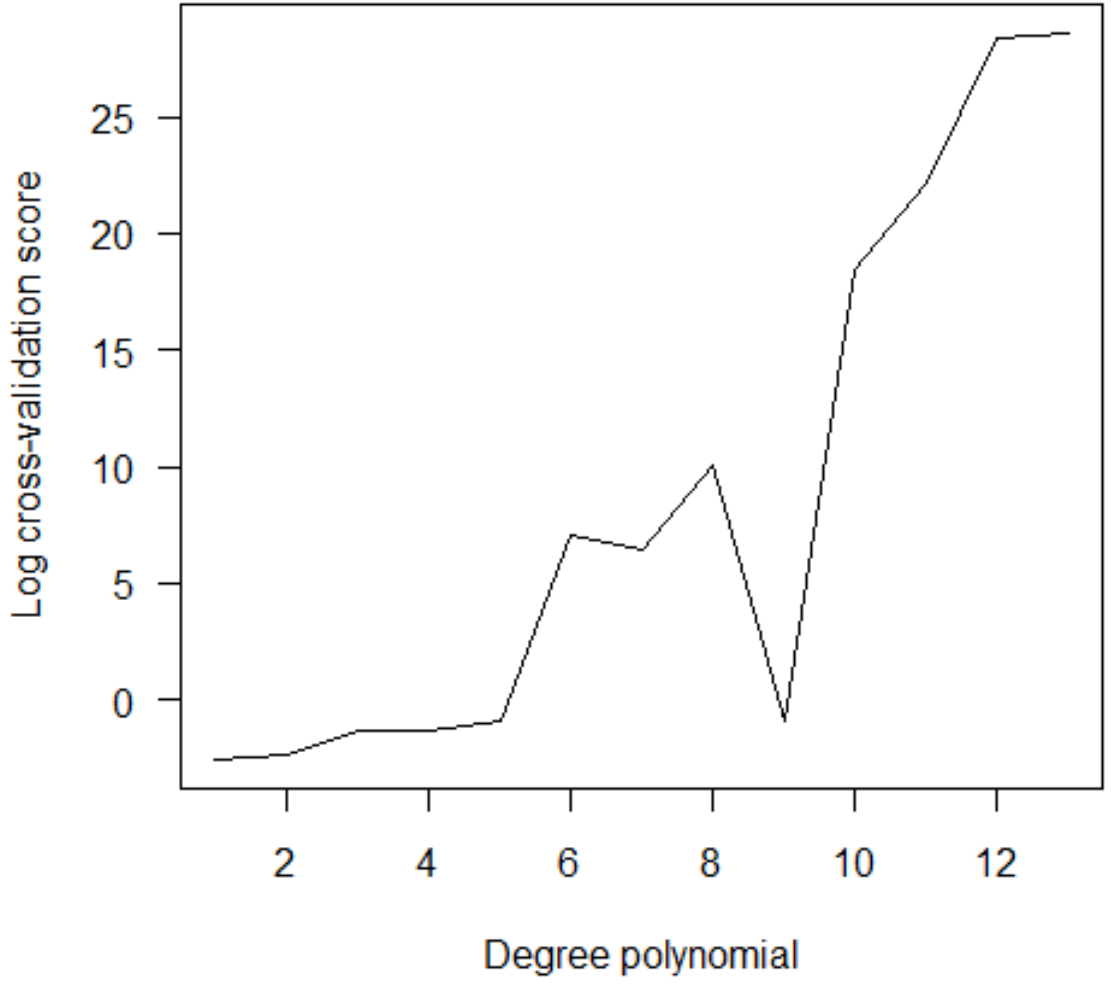
y_i are the observations for the response variable.

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

A larger CVscore corresponds to a worse prediction (more prediction error).

Choose among models using an explicit criterion

In our beetle example, the CVscore increases (prediction error worsens) with increasing numbers of parameters in the model. Here, the simple linear regression was “best”. But some *other polynomials do nearly equally well*.



Why does prediction error tend to increase with model complexity?

Prediction worsens as models become complex because of *bias-variance tradeoff*.

The simplest models have low variance but high bias resulting from missing terms.

The most complex models have low bias but high variance resulting from estimating too many parameters ("overfitting") with limited data.

Training error: how well a model fits the data used to fit the model.

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

Hastie et al. (2009)

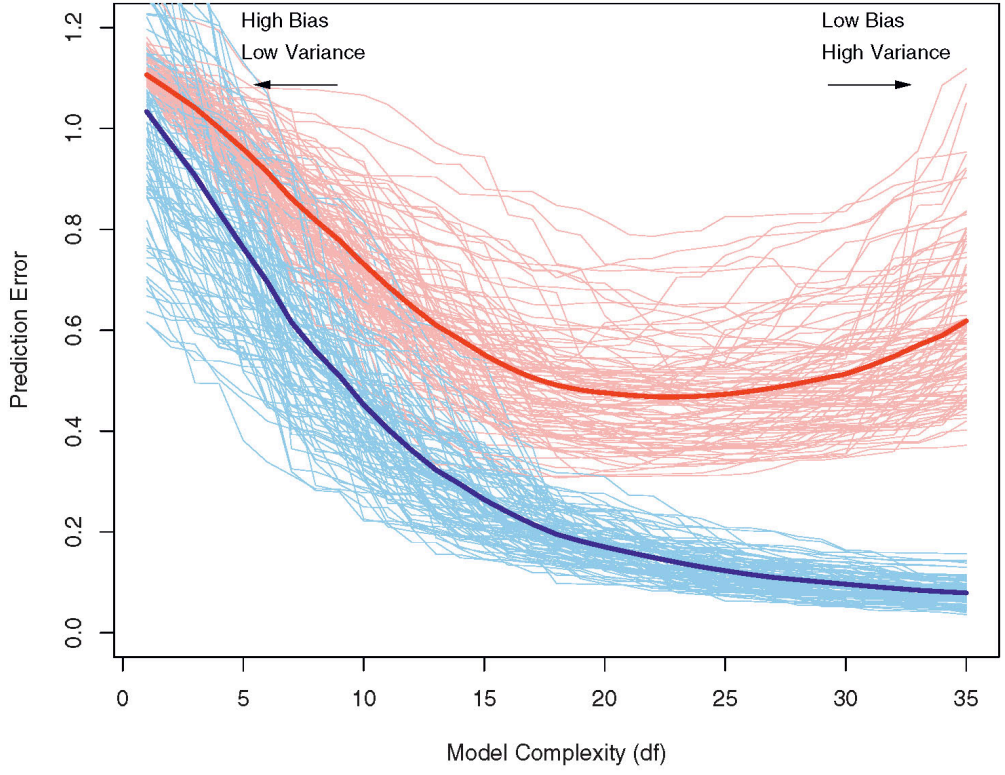


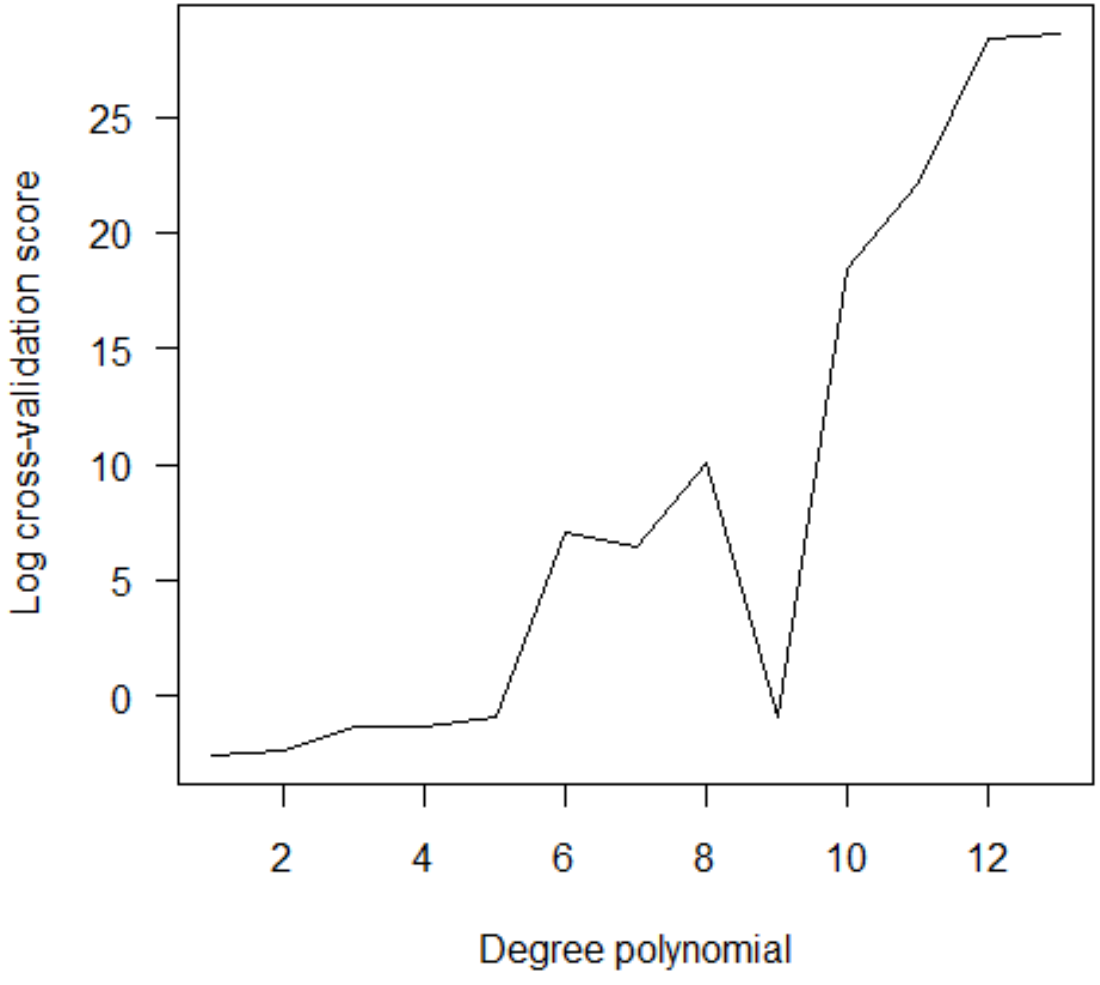
FIGURE 7.1. *Behavior of test sample and training sample error as the model complexity is varied. The light blue curves show the training error* $\overline{\text{err}}$*, while the light red curves show the conditional test error* $\text{Err}_{\mathcal{T}}$ *for* 100 *training sets of size* 50 *each,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

The problem of model selection

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 too can lead to non-reproducible 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 candidate models to evaluate?



Goals of model selection

Some reasonable objectives:

- A model that predicts well.
- A model that approximates the true relationship between the variables.
- Information on which models fit the data nearly as well as the “best” model.
- To compare non-nested* models, not just compare each “full” model to “reduced” models having a subset of its terms.

*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.)

Goals of model selection

To accomplish these goals, we need a model selection approach that includes:

- 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. It is equivalent to AIC in the case of multiple regression with independent normal errors. I start with C_p here because it is implemented in all-subsets regression in R.

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

$\mathrm{SS}_{\mathrm{error}}$ 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. 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 in the `leaps` package. `leaps` uses an efficient algorithm to choose among a potentially huge number of models.

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

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. We are data dredging.

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 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).

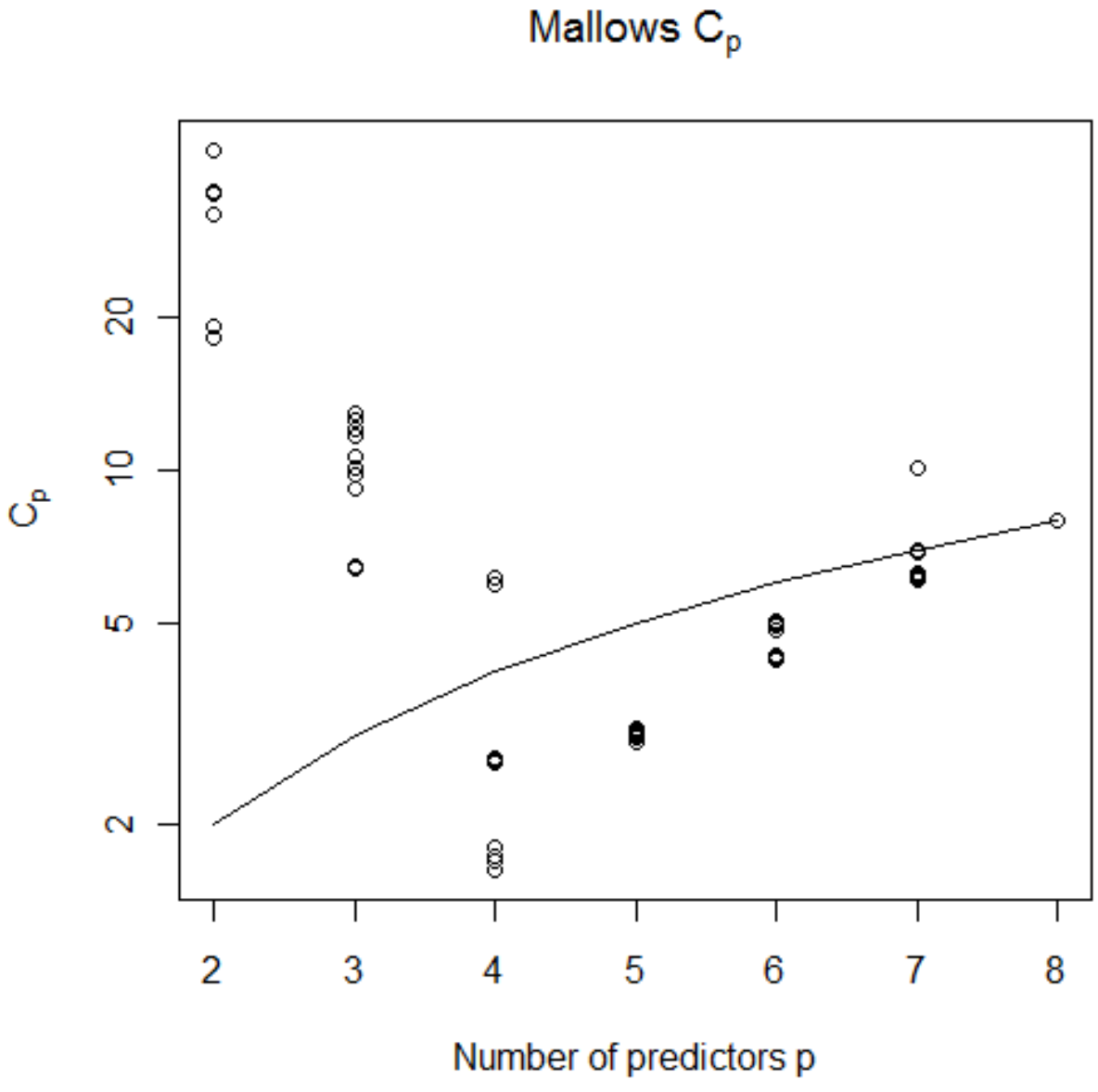
Example 2a: Ant species richness

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 $C_p < p$

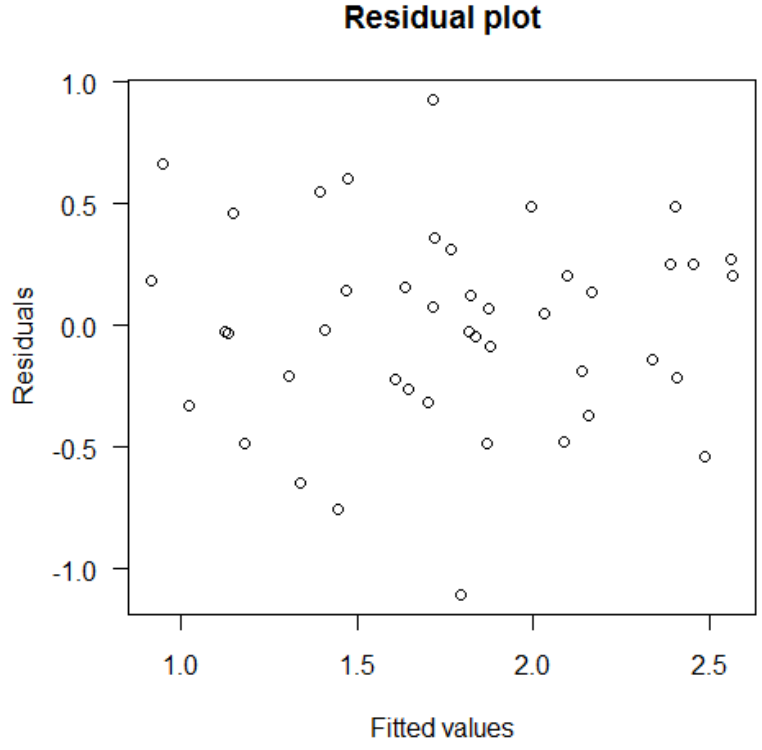


Example 2a: Ant species richness

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 with excitement over your single "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)

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

Second part is 2*k*, which acts like a penalty – the price paid for including *k* 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 <u>difference</u> between models in their AIC.

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 a stepwise procedure for selection of variables implemented by `stepAIC` 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.

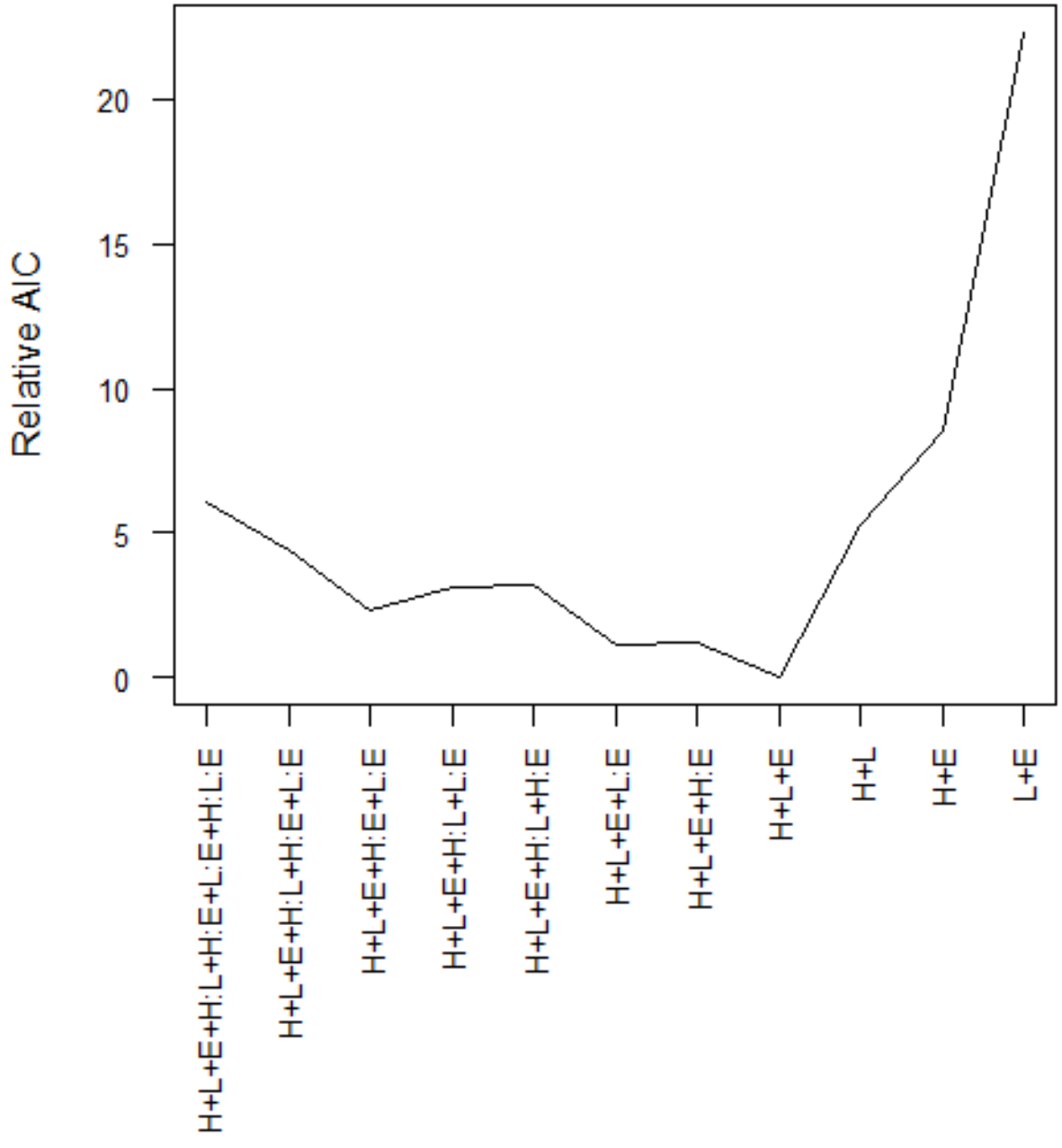
(However, we are still data dredging.)

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



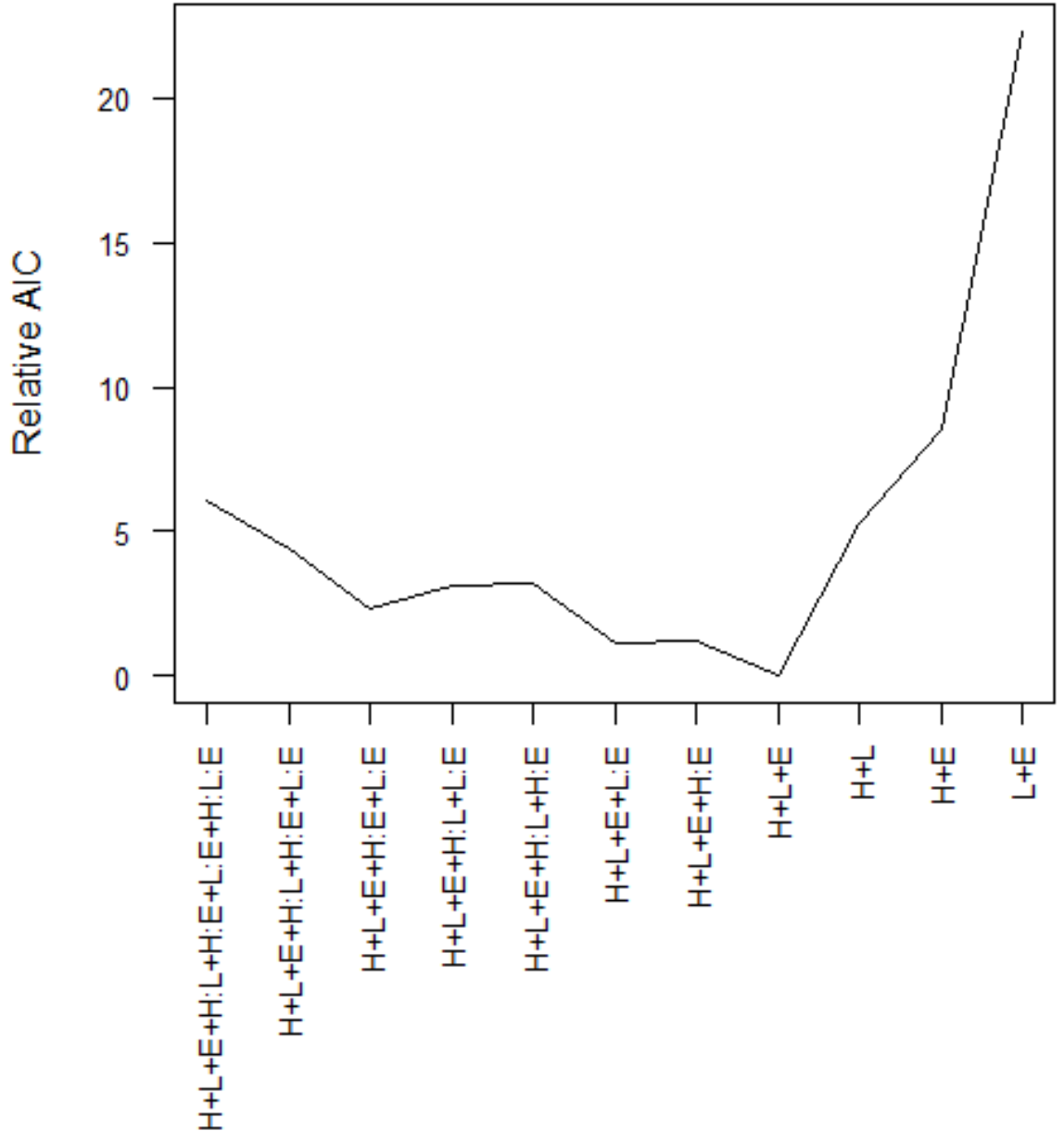
How AIC differs from classical statistical approaches

No hypothesis testing.

No null model.

No *P*-value.

No model is formally “rejected”.



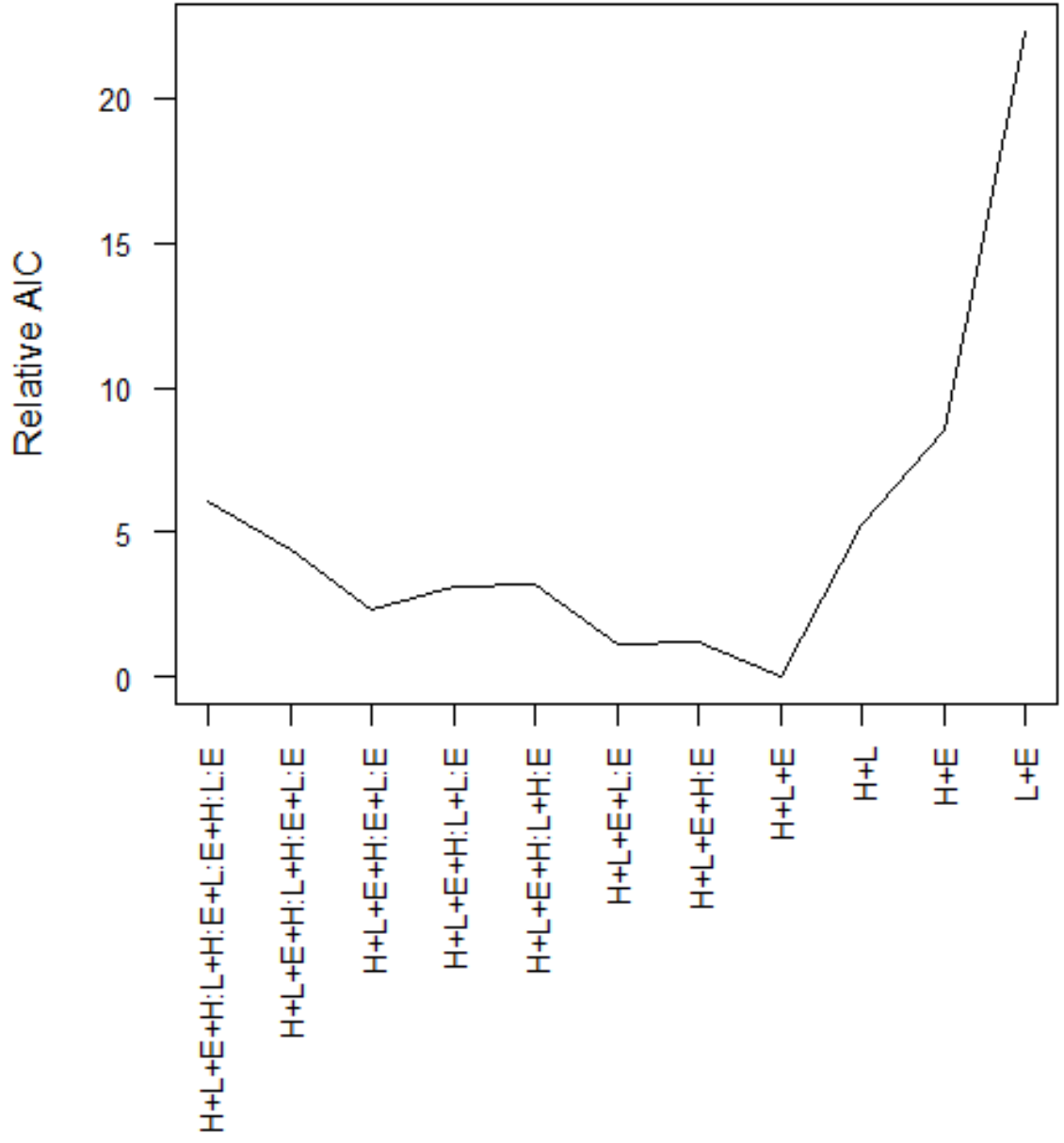
How AIC differs from classical statistical approaches

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.



How AIC differs from classical statistical approaches

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.

How AIC differs from classical statistical approaches

Going further: Multimodel Inference

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. It avoids the need to base inference solely conditional upon the single "best" model.

"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.

Implemented in `MuMIn` package in R.

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

Avoid data-dredging by formulating a set of candidate models

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

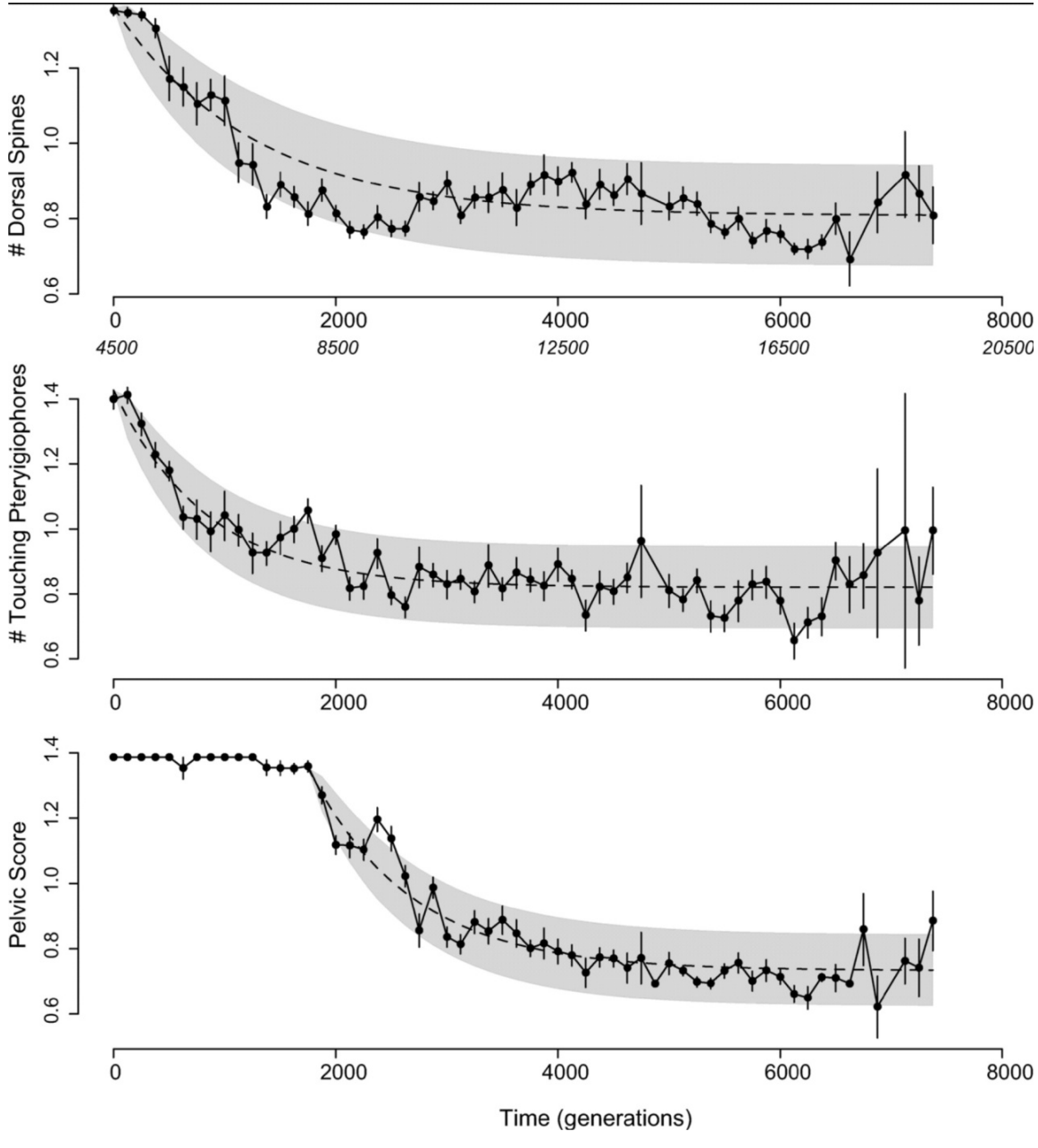
This is where data dredging ends and science begins.

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.

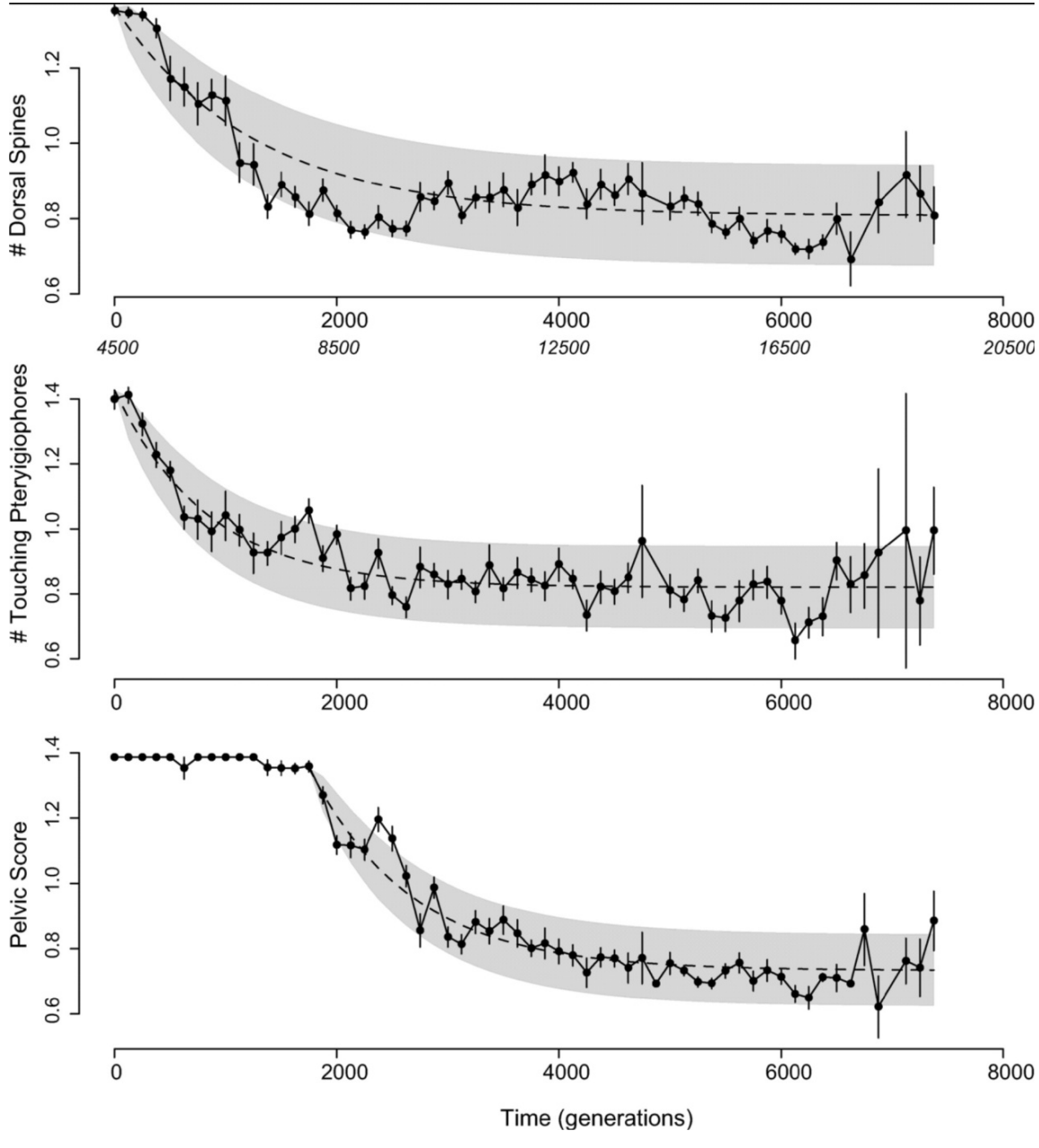
G. Hunt, M. A. Bell & M. P Travis 2008, *Evolution* 62: 700–710.



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 the AIC criterion 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 a single “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 best model among the set being considered, and 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
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, $P = 0.00005$

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.”

Conclusions

Stepwise elimination of terms and null hypothesis significance testing is not the ideal approach for model selection. Information-theoretic approaches have explicit criteria and better properties.

Using this approach involves giving up on *P*-values.

These IT approaches work best when thoughtful science is used to specify the candidate models under consideration before testing (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 more certainty about which variables cause variation in the response variable, then you will need to do an experiment.

Digression: Exploring your data can be good

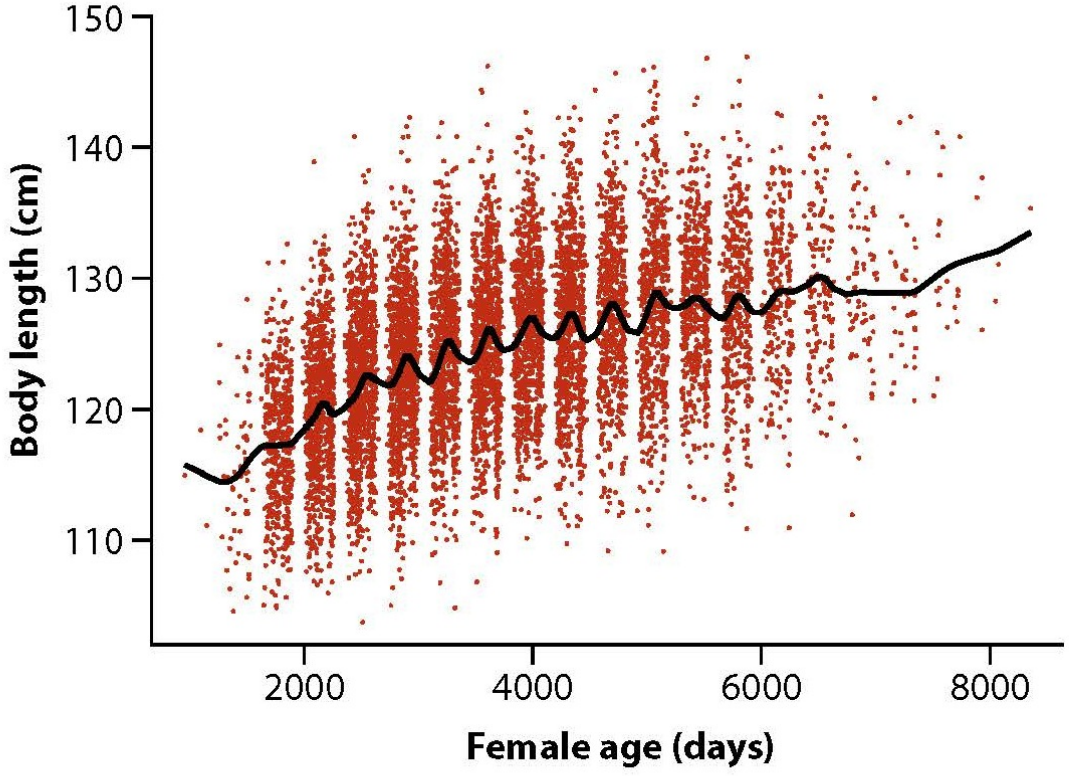


Figure 17.8-3 Measurements of body length as a function of age for female fur seals, with the "spline" fit in black.

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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