Nonlinear Modeling: Model selection

Introduction to Statistical Modelling

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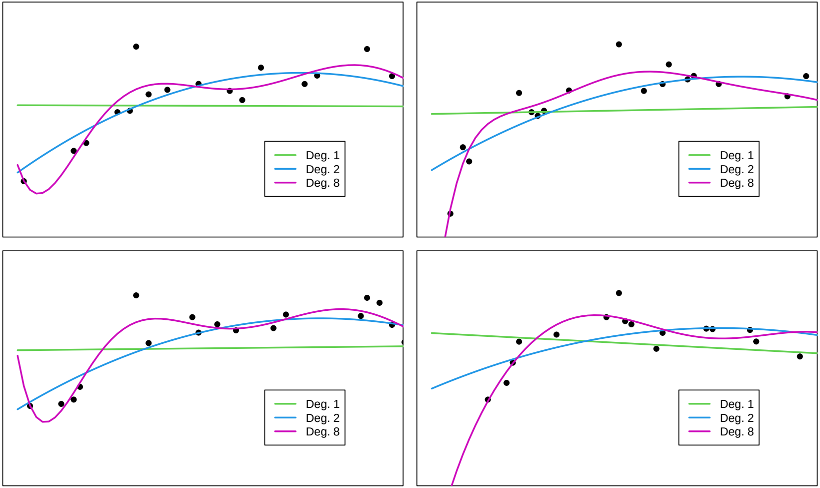
Model Selection

Model selection

- Also called *structure characterisation*
- Problem: “perfect” model and “true” parameters are unknown.
- Goal: **Select best model structure from set of candidate models, based on experimental data**

Which model fits the data the best?

- True model: $y = \sin(x) + \sqrt{x} + 0.3\epsilon$, where $\epsilon \sim N(0, 1)$
- Four datasets, fit polynomial of degree 1, 2, or 8



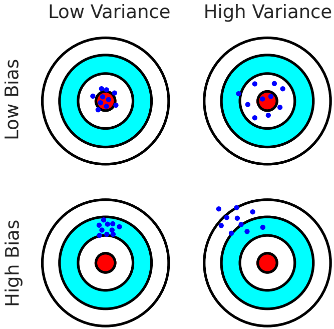
Two sources of error

Bias: *How well does the model fit the data?*

- Error due to non-modeled phenomena.
- Decreases as model gets more complex.

Variance: *How well does the model do on new, unseen data?*

- Decreases with more data.
- Increases as model gets more complex.

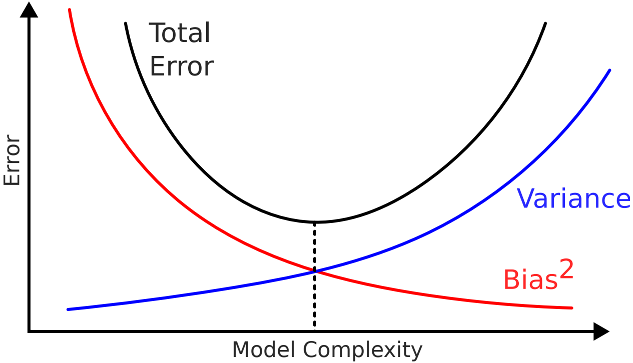


Bias and variance are complementary

For a model $M_D(x)$ on a dataset D, the error decomposes as

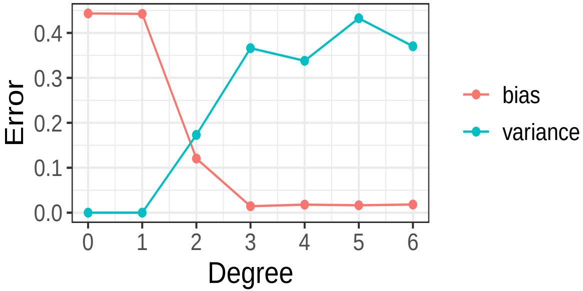
$$\mathrm{Error}[M_D(x)] = \mathrm{Bias}[M_D(x)]^2 + \mathrm{Var}[M_D(x)] + \mathrm{Noise}.$$

Goal model selection: select model with smallest total error = compromise between bias error and variance error



Model selection for linear models

- Same data as before (slide 1)
- Polynomial model $y \sim 1 + x + x^2 + \cdots + x^d$



- Model of degree 2 (quadratic curve) gives best fit (not too complex, not too simple)
- Bias and variance in general **difficult to calculate**

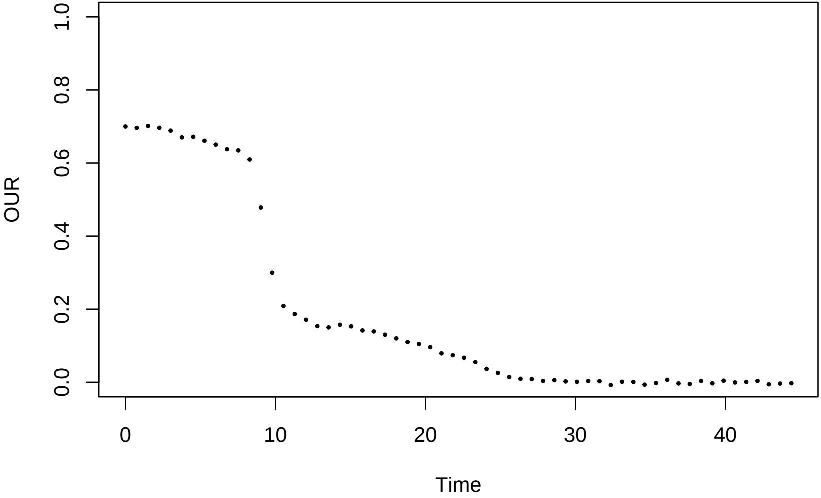
Case study: biodegradation test

Waste treatment: Measure the oxygen uptake rate (OUR) during oxidation of biodegradable waste products by activated sludge.

- Shape respirogram depends on degradation kinetics and quantity added products
- Not known a priori → measure and test several models

Case study: biodegradation data

1.5 data points per minute, acquired using dissolved oxygen (DO) sensor.



Case study: general model

- k pollutants $S_1, \ldots, S_k$.
- Oxygen uptake rate

$$OUR = \sum_{i=1}^{k} (1 - Y_i) r_{S_i}$$

where Y_i is the yield, (fraction of substrate S_i that is not oxidated but transformed in biomass X), and r_{S_i} the degradation rate of S_i.

- Candidate models differ in number of pollutants k and choice of degradation rates r_{S_i}.

Case study: candidate models

Model 1: degradation of one pollutant according to first-order kinetics. Gives *exponentially* decreasing OUR-curve.

$$r_{S_1} = \frac{k_{max1} X}{Y_1} S_1$$
$$OUR = (1 - Y_1) r_{S_1}$$

Case study: candidate models

Model 2: degradation of one pollutant according to *Monod kinetics*.

$$
\begin{aligned}
r_{S_1} &= \frac{\mu_{max1} X}{Y_1} \frac{S_1}{K_{S_1} + S_1} \\
OUR &= (1 - Y_1) r_{S_1}
\end{aligned}
$$

Case study: candidate models

Model 3: simultaneous degradation of two pollutants according to Monod kinetics (*double Monod*) without interaction.

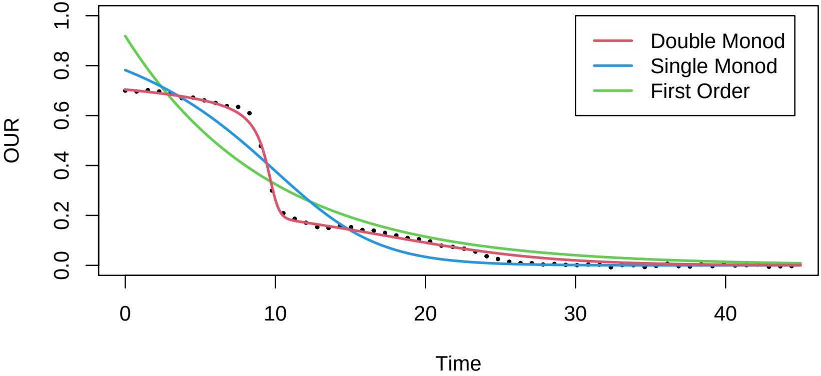
$$r_{S_1} = \frac{\mu_{max1} X}{Y_1} \frac{S_1}{K_{S_1} + S_1}$$

$$r_{S_2} = \frac{\mu_{max2} X}{Y_1} \frac{S_2}{K_{S_2} + S_2}$$

$$OUR = (1 - Y_1) r_{S_1} + (1 - Y_2) r_{S_2}$$

Case study: parameter estimation

Dataset (dots) and best fits (calibrated candidate models based on an SSE-based objective function) of the different models



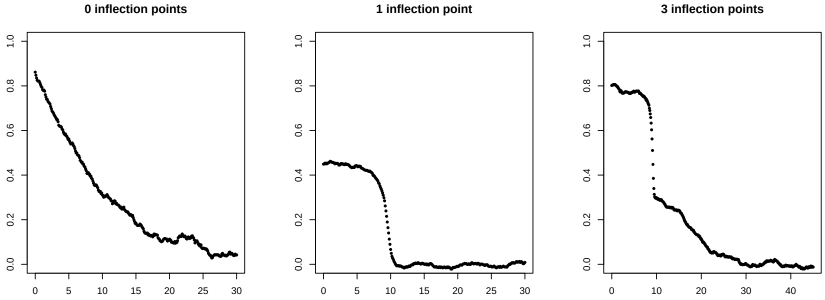
Methods for model selection

Methods for model selection

- *A priori* model selection: before parameter estimation
  - Reduces number of parameter estimations necessary = time gain
  - Techniques not easy to determine: ad hoc methods
- *A posteriori* model selection: after parameter estimation
  - General methods available
  - Need parameter estimation for all candidate models = increase in calculation times

A priori model selection

- Restrict set of model candidates based on properties of data that are independent of parameters.
- Biodegradation example: inflection points.



0 inflection points

1 inflection point

3 inflection points

A posteriori model selection

- Compose set of candidate models
- Collect experimental dataset(s)
- Perform parameter estimation for all models
- Rank candidate models and select best
- Methods
    - Goodness-of-fit and complexity penalization
    - Evaluation of undermodelling
    - Statistical hypothesis test
    - Residual analysis

Goodness-of-fit and complexity penalization

Select least complex model that describes data (sufficiently) well.

Balance two terms:

1. **Goodness of fit**, measured by sum-squared of residuals (SSR)
2. **Complexity of the model**, as a function of number of parameters.

Many different criteria to make this concrete.

Akaike Information Criterion (AIC)

Model complexity penality: $2p$, with p number of parameters:

$$AIC = N \ln\left(\frac{SSR}{N}\right) + 2p.$$

Properties:

- Sometimes preferred when prediction accuracy is important and sample size is small
- Not necessarily consistent (will not select true model even if sample size is large)

Bayes Information Criterion (BIC)

Model complexity penalty: $p \ln N$

$$BIC = N \ln \left(\frac{SSR}{N} \right) + p \ln N.$$

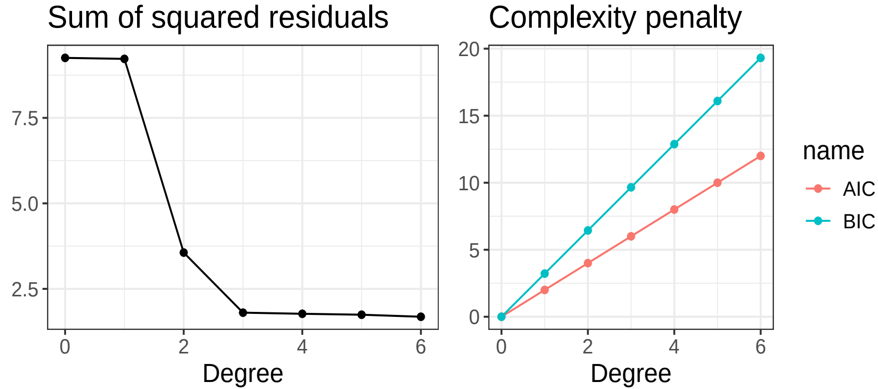
Properties:

- Will select a simpler model than AIC.
- Consistent (under some conditions)

AIC/BIC: Polynomial example

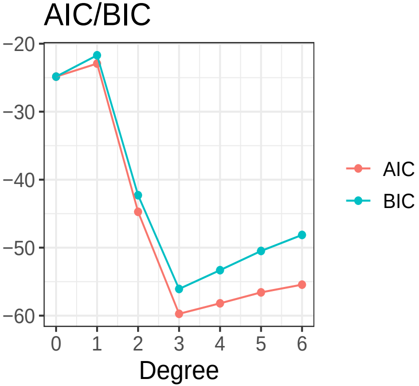
- SSR always decreases when number of parameters increases
- Penalty terms cause goodness-of-fit to increase at a certain point

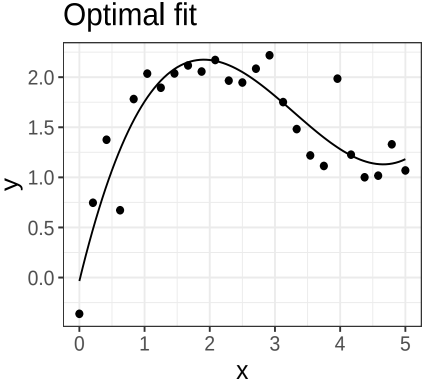
Example: Select best linear model $y \sim 1 + x + \cdots + x^d$ according to AIC/BIC/... for given data.



AIC/BIC: Polynomial example

Optimal model provides a **good fit** (SSR low) and is **not too complex** (penalty low).


AIC/BIC


Optimal fit

- Both AIC and BIC select fit of degree 3
- In general AIC and BIC don't have to agree

AIC/BIC: Biodegradation example

Model	p	SSR	AIC	BIC
Exponential	2	0.36	-303.67	-299.48
Single Monod	3	0.16	-348.74	-342.45
Double Monod	6	0.01	-508.87	-496.30

Statistical hypothesis test

- Choice between 2 models: simple and more complex
- Is complex model statistically speaking better?
- Verify using F-test:

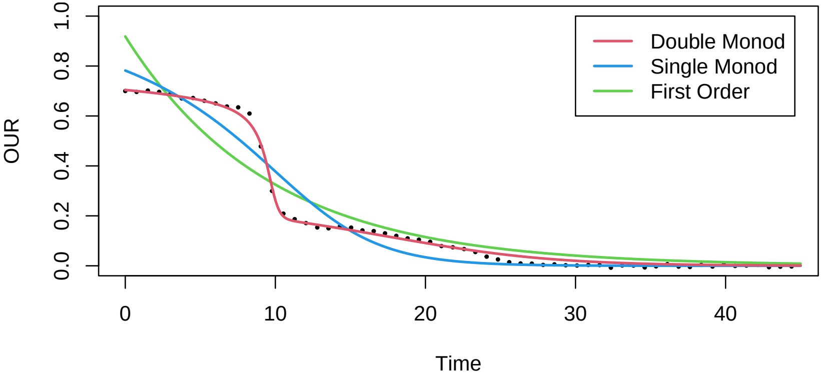
$$F = \frac{\left(\dfrac{SSR_{simple} - SSR_{complex}}{p_{complex} - p_{simple}}\right)}{\left(\dfrac{SSR_{complex}}{N - p_{complex}}\right)}$$

- Compare test criterion with tabulated $F_{1-\alpha, p_{complex} - p_{simple}, N - p_{complex}}$ for significance level α
- If value larger, complex model better (and vice versa)

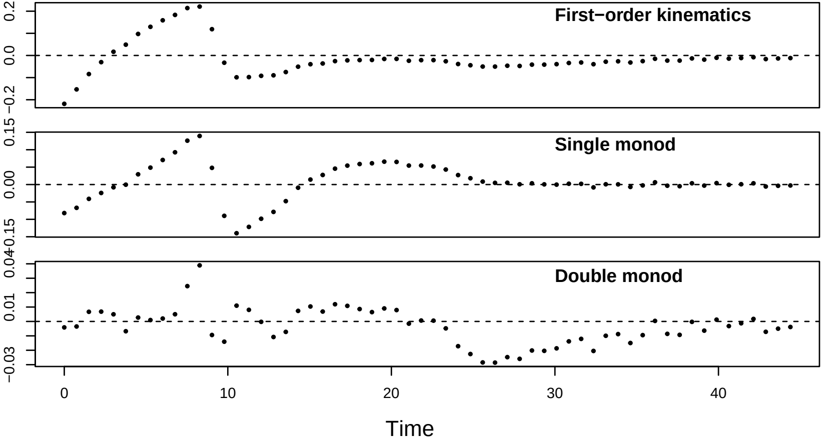
Residual analysis

- Hypothesis: model is appropriate if properties of residuals are same as properties of measurement errors
- Two popular techniques for evaluation independence of residuals
  - Autocorrelation test (see Parameter Estimation)
  - Runs test (nonparametric test)

Autocorrelation test: Biodegradation example

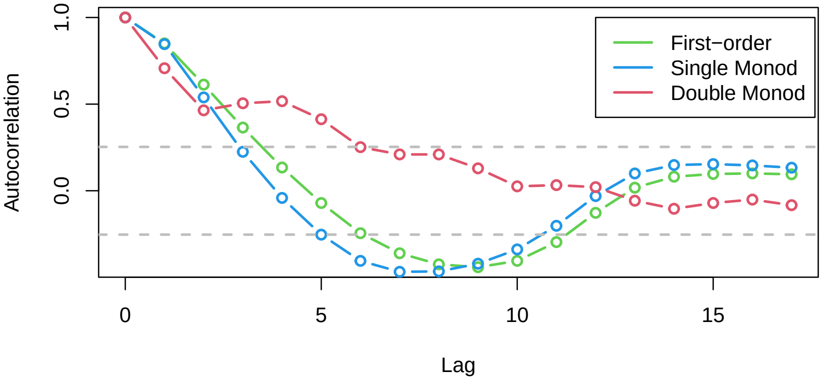


Autocorrelation test: Residuals as a function of time



Autocorrelation test

- Residuals show some correlation for all three models, indicating that there is some unresolved structure in the data.
- Correlations for double Monod decay much quicker than the other two models.


Autocorrelation
Lag
First−order
Single Monod
Double Monod