Nonlinear Modeling: Model selection
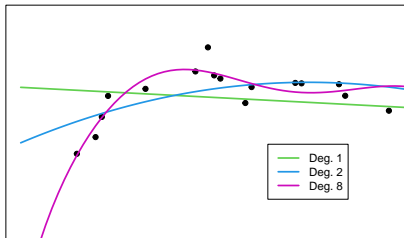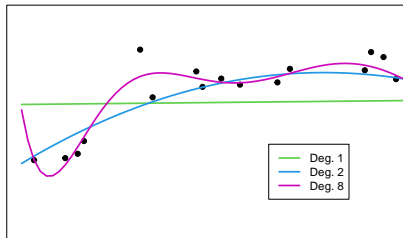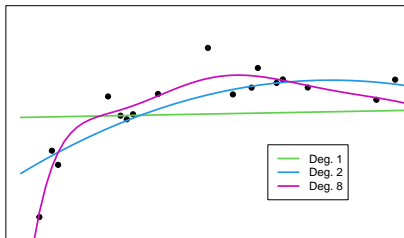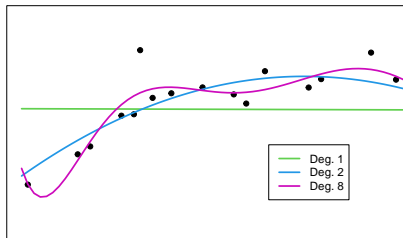## Introduction to Statistical Modelling

Prof. Joris Vankerschaver

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?

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.
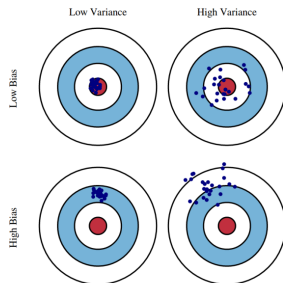- Increases as model gets more complex.

Figure adapted from http://scott.fortmann-roe.com/docs/BiasVariance.html

Bias and variance are complementary

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

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

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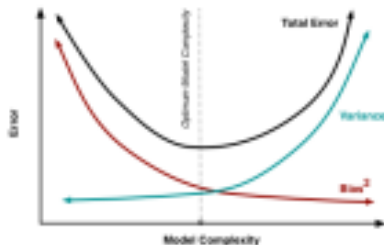

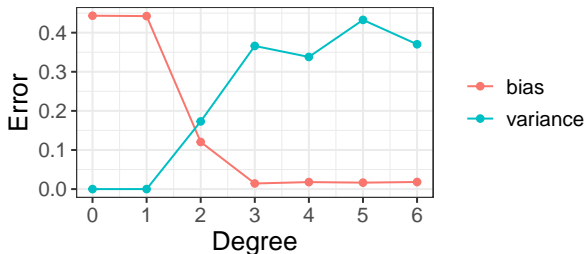Figure adapted from http://scott.fortmann-roe.com/docs/BiasVariance.html

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**, need easier criteria.

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 $\rightarrow$ measure and test several models

Case study: biodegradation data

1.5 data points per minute, acquired using dissolved oxygen (DO) sensor.
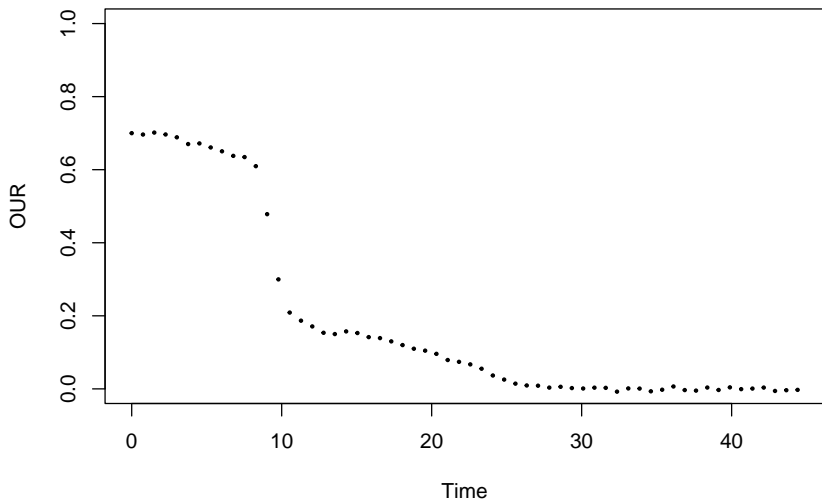
Case study: general model

- k pollutants $S_1, ..., S_k$.

- 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*.

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

Case study: candidate models

Model 3: simultaneous degradation of two pollutants according to Monod kinetics (*double Monod*) without interaction.
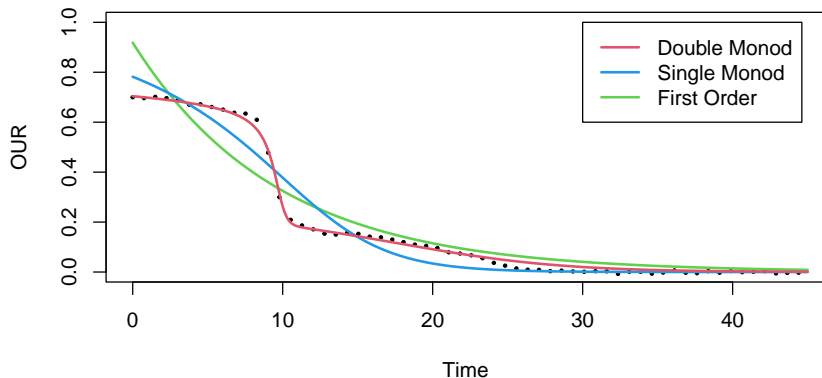
$$r_{S_1} = \frac{\mu_{max1}X}{Y_1} \frac{S_1}{K_{S_1} + S_1}$$

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

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

Case study: parameter estimation

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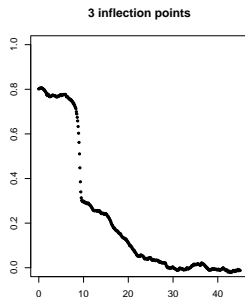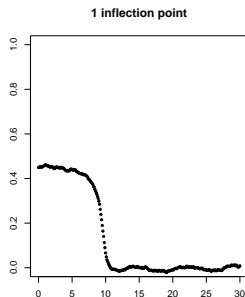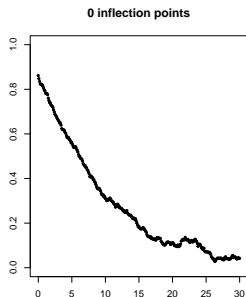
Methods for model selection

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.

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 penalty: $2p$, 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: $p \ln N$

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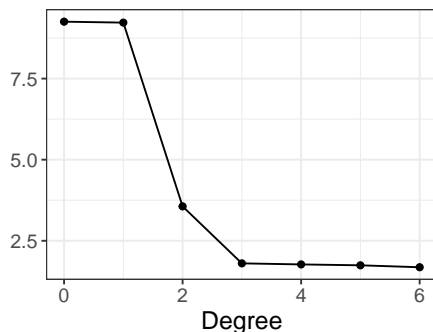
Properties:

- Will select a simpler model than AIC.
- Consistent (under some conditions)
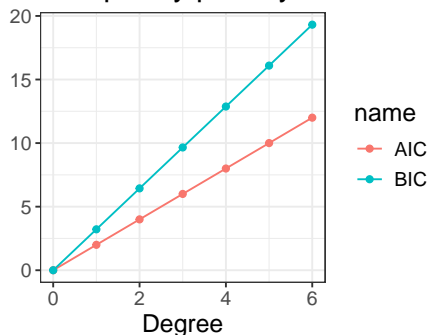
AIC/BIC: Polynomial example

- 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/$\cdots$ for given data.
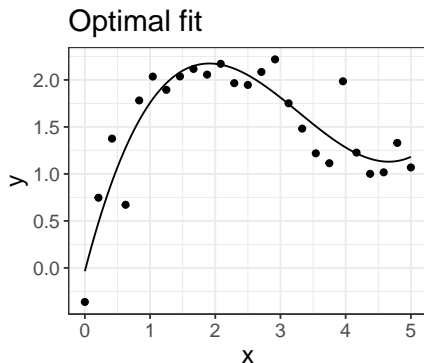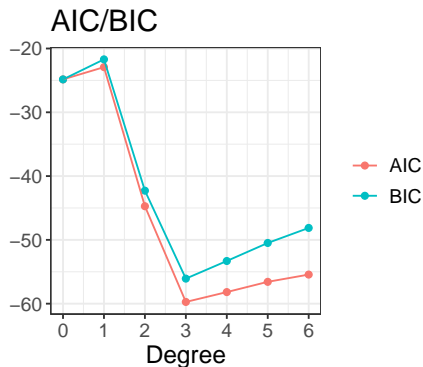

Sum of squared residuals

Complexity penalty

AIC/BIC: Polynomial example

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

- 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
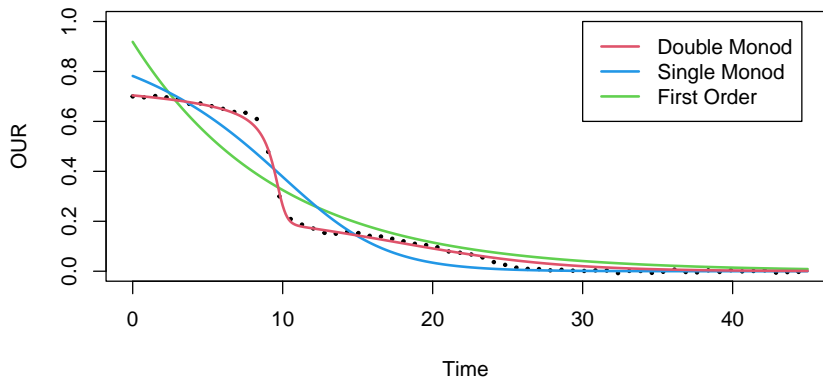
Autocorrelation test: Residuals as a function of time
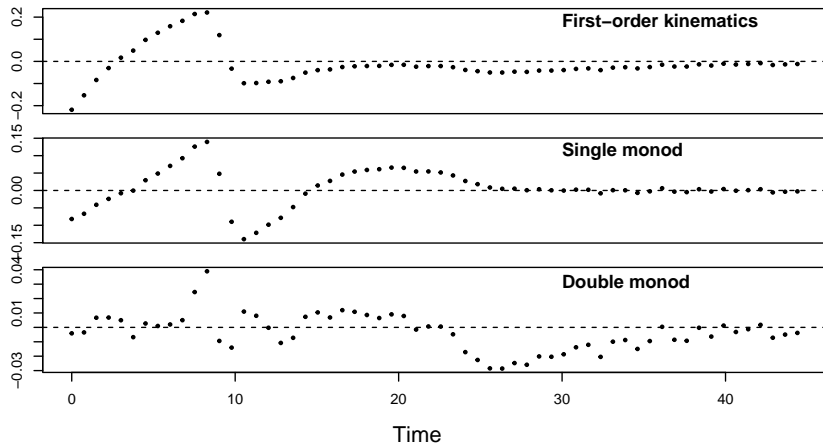
Autocorrelation test

- 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.