Lecture 4 Model Fitting

Mathematical Modeling

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1. Preliminaries
2. About confidence intervals
3. Back to visual model fitting
4. Analytic Model Fitting

Data and Modeling: Three Situations in Data Modeling

Given a data set we may take three approaches:

1. **Fit an already selected model type to the data**
   - The model type is already fixed
   - For example: a linear, or a quadratic model; mass-action model
2. **Choose the most appropriate model from several alternative models that have been fitted to the data**
   - Decide whether the best-fitting exponential model is better than the best-fitting polynomial model
3. **Make predictions based solely on the data**
   - No hypothesis regarding the type of model
   - Predict intermediate and/or future behavior based just on the data set

Model Fitting vs. Interpolation

Model fitting

- The modeler has a **hypothesis** regarding the mathematical form of the model.
- It is just a matter of finding the numercial parameters that make the chosen model explain (fit) the experimental data set.
- Some deviations from the data are going to be willingly accepted.
- **Emphasis on the model.**

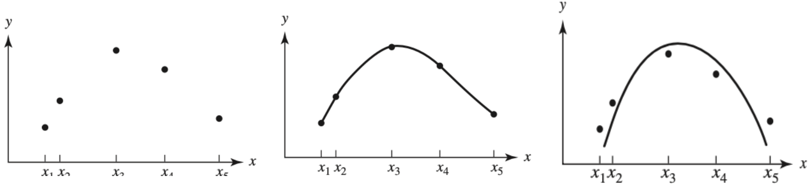
Interpolation

- **No a-priori hypothesis** regarding the model form.
- The modeler is strongly guided by the data.
- Aims to capture the data trend to predict in-between (or sometimes outside) the given points.
- **Emphasis on the data.**

Fitting and interpolating at the same time

- A fitted model may need to be replaced with an interpolating curve.
- The interpolating curve may have better mathematical properties for model analysis.
- Sometimes called **model approximation**.

- We are given a set of data
- Two approaches
  - Model fitting: we look for a **quadratic polynomial** to explain the data
  - Interpolation: look for a curve going exactly through the data points



Sources of error in modeling

Formulation errors

- Result from errors in the **model** formulation
- Significant variables were ignored
- Interrelationships between variables were ignored or simplified
- Relating the data to the model in the wrong way

Truncation errors

- Come from the math techniques used in building the model
- For example, an infinite series expansion may be truncated to a polynomial

Round-off errors

- Numerical errors coming from representing real numbers with finite precision

Measurement errors

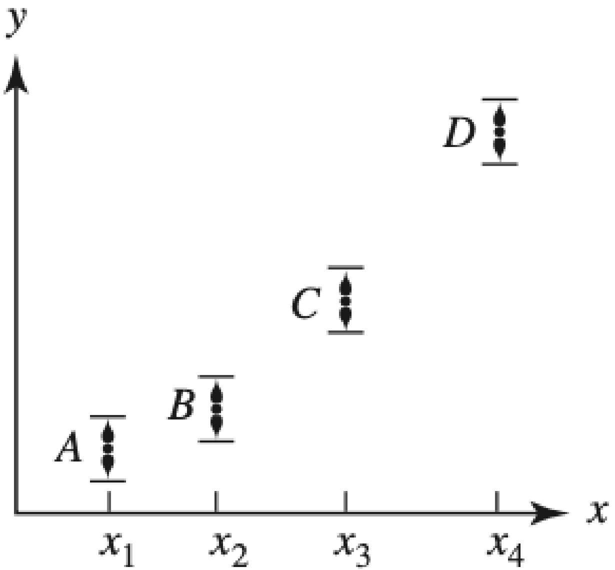
- Imprecision in the collection of data
- Physical limitations of the instruments
- Human errors

Content of this lecture

- **Model fitting**
  - Visual model fitting
  - (Confidence intervals)
  - Analytic model fitting
  - Choosing the best model

Visual model fitting

- The modeler has a hypothesis regarding the type of model to be fitted
- The numerical value of parameters needs to be fixed so that the model explains the available data
  - The range of the parameters is known
- Data set
  - The size of the data set is a trade-off between the cost of obtaining the data and the accuracy to be obtained for the model
  - **Minimum** at least as many data points as the number of parameters to fix
  - Spacing of the data points important
    - More data points on those intervals where the model should be fitted particularly well,
    - or where the maximum use of the model is expected,
    - or where abrupt changes in the model behavior are expected
  - Use the data together with its **confidence intervals**


y
A
B
C
D
x
x_1
x_2
x_3
x_4

Confidence intervals

Setup: a population and a parameter taking different values for different members of the population.

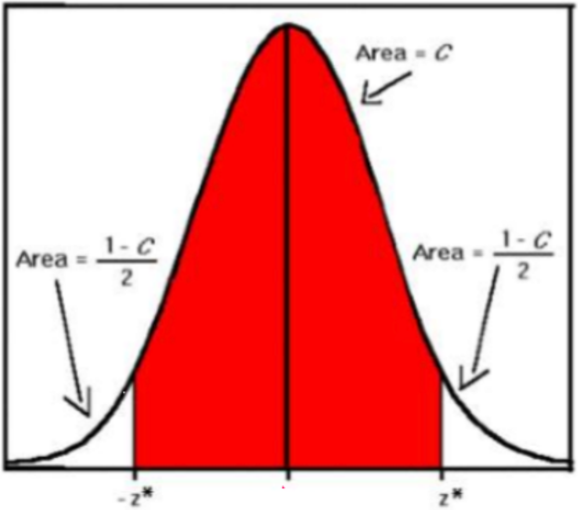
- Goal: We need to estimate the population mean value of that parameter only through a population sample
- Outcome: an interval where (the true value of) the population mean lies with large probability
- The interval is called confidence interval
- The probability is called confidence level

Example

- Measure the voting intentions for a certain party in an election
  - The answer may be presented as **40%**
  - It should be interpreted as an interval centered at 40% that is smaller or larger depending on the confidence level
  - The 90% confidence interval that could be calculated from the data might be for example 38% to 42%, while the 95% interval might be for example 36% to 44%

Confidence intervals (cont.): mathematical setup

- For a given sample, its mean is a stochastic variable
- If the measurements follow a normal distribution, the sample mean will have the distribution $N(\mu, \sigma/\sqrt{n})$
- From the calculated sample mean we need to report an interval where the real population mean μ lies with large probability
- The interval is related to the percentages of the area of the normal density curve
  - For example a 95% confidence interval should cover 95% of the area under the normal curve
- The value z^* of the point on the standard normal density curve $N(0, 1)$ such that the probability of observing a value greater than z^* is equal to p is known as the upper p-critical value of the standard normal distribution


Area = C
Area = $\frac{1-C}{2}$
Area = $\frac{1-C}{2}$
- z*
z*

Confidence intervals: unknown mean, known standard deviation

- Confidence intervals for unknown mean μ and known standard deviation σ
  - Given a sample of size n with mean m, a C-confidence interval for the population mean is:

$$(m - z^{*}\sigma/\sqrt{n}, \quad m + z^{*}\sigma/\sqrt{n})$$

    where z^{*} is the upper $(1 - C)/2$ critical value for the standard normal distribution
  - The error margin is $z^{*}\sigma/\sqrt{n}$

Note: the interval above is exact only for populations that are normally distributed. For other populations, the interval is approximately correct for large samples by the central limit theorem.

Confidence intervals: unknown mean, unknown standard deviation

- Confidence intervals for unknown mean μ and unknown standard deviation σ
  - The unknown standard deviation is replaced by the estimated standard deviation:

$$s^2 = \frac{1}{n-1} \sum (x_i - m)^2$$

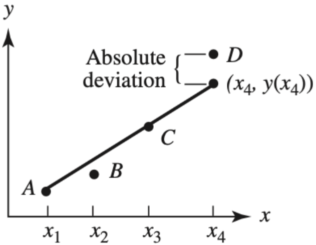
  - Given a sample of size n, its mean follows the t distribution $t(n-1)$ with mean μ and standard deviation $s/\sqrt{n}$
  - As the sample size n increases, the t distribution approaches the normal distribution
  - A C-confidence interval for the population mean is:

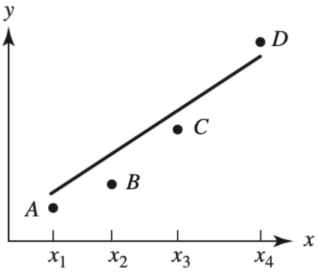
$$(m - t^* s/\sqrt{n}, \quad m + t^* s/\sqrt{n})$$

    where t^* is the upper $(1-C)/2$ critical value for the $t(n-1)$ distribution
  - The error margin is $t^* s/\sqrt{n}$

Visual model fitting

- Using the original data
  - Look at the deviations between the model prediction and the available data set
  - Aim to minimize the deviations
    - The largest deviation
    - Sum of all deviations
    - The sum of squares of deviations
    - ...
  - Example: fit a linear model $y = ax + b$ to the data on the previous slide
- **Note:** Although these methods of visually fitting the data may seem imprecise, they might be quite compatible with the accuracy of the modeling process
  - Grossness of the assumptions and the imprecision in the data collection may not warrantee a more sophisticated analysis


y
Absolute deviation
D
$(x_4, y(x_4))$
C
B
A
x
x_1 x_2 x_3 x_4


y
D
C
B
A
x
x_1 x_2 x_3 x_4

Visual model fitting

- Transforming the data
  - Much easier to fit visually to linear data
  - Problem: How about if the data is not linear?
  - Solution: transform the data!
- Examples:
  - Fit a model $y = Ce^x$ is the same as fitting a model $\ln(y) = \ln(C) + x$
    - Replace the (x, y) data with the (x, ln(y)) data (log-transform) and do a linear fit
  - Fit a model $y = Cx^a$ is the same as fitting a model $\ln(y) = \ln(C) + a\ln(x)$
    - Replace the (x, y) data with the (ln(x), ln(y)) data (log-log-transform) and do a linear fit

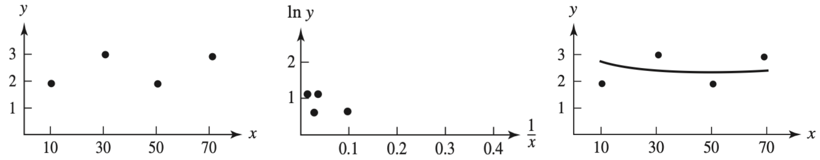
Data transformations

- When doing data transformations the concept of distance is also transformed
    - Fitting a transformed model to minimize the deviations may not yield a final model with minimum deviation to the original data
    - Always verify the final model against the original data!

Data transformations

Example

- Fit a model $y = Ce^{1/x}$
- Log-transform of the data: $\ln(y) = \ln(C) + \frac{1}{x}$
  - Data gets squeezed together
  - Absolute deviations appear small
  - Not all good fits on the log-scale will be good fits on the original scale



Data transformations

- Data may get squeezed
  - Modeler may be tricked in selecting a poor model based on the transformed data
  - Very important to remember when comparing alternative models
- Always compare using the original data
- Note: computer-based environments may use (hidden) implicit data transformations
  - Check how the indicators of model fit are computed

Analytic model fitting

- Methods for judging the fitness of a model
  - Chebyshev approximation criterion
  - Sum of absolute deviations
  - Least-squares criterion
  - ...

First criterion for goodness of a fit: Chebyshev approximation

- **Chebyshev criterion:**
  - Given a data set (x_i, y_i), $1 \le i \le m$, and a model $y = f(k, x)$, with k the vector of parameters to be fit, select those parameter values which minimize:

$$\max |y_i - f(x_i)|, \ 1 \le i \le m$$

- In other words: minimize the largest absolute deviation

Example: Chebyshev approximation

- We are given a segment AC and three measurements: of AC itself, of AB and of BC, where B is a point on the segment AC
  - **Example:** AC $= 19$, AB $= 13$, BC $= 7$
- Problem: find the values for the length of each segment that give the best fit using the **Chebyshev criterion**
- Notation: let x_1, x_2, $x_1 + x_2$ be the lengths of the segments AB, BC, and AC, respectively
- The deviations are:

$$x_1 - 13 = r_1, \quad x_2 - 7 = r_2, \quad x_1 + x_2 - 19 = r_3$$

Chebyshev approximation (cont.)

Problem formulation: find the minimal r such that:

$$|r_1| \leq r, \quad |r_2| \leq r, \quad |r_3| \leq r$$

Equivalently:

$$-r \leq r_i \leq r \Rightarrow r - r_i \geq 0, \quad r + r_i \geq 0$$

In our example:

$$\begin{aligned} r - x_1 + 13 &\geq 0 \\ r + x_1 - 13 &\geq 0 \\ r - x_2 + 7 &\geq 0 \\ r + x_2 - 7 &\geq 0 \\ r - x_1 - x_2 + 19 &\geq 0 \\ r + x_1 + x_2 - 19 &\geq 0 \end{aligned}$$

Linear programming! Solved through the simplex method

Chebyshev approximation

Note: in general, the resulting optimization problem may not be linear!

- Example: $f(x) = \sin(kx)$
- For this reason, the criterion is not much used in practice

Second criterion for goodness of a fit: sum of absolute deviations

Criterion:

- Given a data set (x_i, y_i), $1 \leq i \leq m$, and a model $y = f(k, x)$, with k the vector of parameters to be fit, select those parameter values which minimize:

$$\sum_{1 \leq i \leq m} |y_i - f(x_i)|$$

- In other words: minimize the sum of absolute deviations
- General approach: differentiate the sum with respect to each parameter, solve the 0-equations to find the critical points
- Problem: because of the modules, the derivatives may not be continuous

Example on the previous slide:

- Find $x_1, x_2 \geq 0$ such that $|x_1 - 13| + |x_2 - 7| + |x_1 + x_2 - 19|$ is minimal

Third criterion for goodness of a fit: least-squares

Criterion:

- Given a data set (x_i, y_i), $1 \leq i \leq m$, and a model $y = f(k, x)$, with k the vector of parameters to be fit, select those parameter values which minimize:

$$\sum_{1 \leq i \leq m} |y_i - f(x_i)|^2$$

- In other words: minimize the sum of squares of absolute deviations

Third criterion for goodness of a fit: least-squares

- Widely used criterion because the resulting problem can be easily solved using calculus: if f is mathematically "well-behaved" function (say, analytical), then so is the sum of squares

Example on the previous slide:

- Find $x_1, x_2 \geq 0$ such that

$$(x_1 - 13)^2 + (x_2 - 7)^2 + (x_1 + x_2 - 19)^2$$

  is minimal
- **Solution:** differentiate (partial derivative) with respect to the two parameters:
  - $2(x_1 - 13) + 2(x_1 + x_2 - 19) = 0$
  - $2(x_2 - 7) + 2(x_1 + x_2 - 19) = 0$
  - Equivalently: $2x_1 + x_2 = 32$, $x_1 + 2x_2 = 26$
  - Solution: $x_1 = 12 + \frac{2}{3}$, $x_2 = 6 + \frac{2}{3}$, $x_1 + x_2 = 19 + \frac{1}{3}$

Example: fitting a straight line

- Fitting a straight line with the least squares criterion
  - look for a model $y = Ax + B$
  - data set: (x_i, y_i), $1 \leq i \leq m$
  - Denote the least-squares solution by $y = ax + b$

- the minimization of $\sum_{1\leq i\leq m}(y_i - ax_i - b)^2$
- Necessary conditions: the partial derivatives of the sum with respect to a and b are zero:

$$\begin{cases} \dfrac{\partial S}{\partial a}(a,b) = -2\displaystyle\sum_{i=1}^{m}(y_i - ax_i - b)x_i = 0 \\ \dfrac{\partial S}{\partial b}(a,b) = -2\displaystyle\sum_{i=1}^{m}(y_i - ax_i - b) = 0 \end{cases}$$

$$\begin{cases} a = \dfrac{m\sum_{i=1}^{m} x_i y_i - \sum_{i=1}^{m} x_i \sum_{i=1}^{m} y_i}{m\sum_{i=1}^{m} x_i^2 - \left(\sum_{i=1}^{m} x_i\right)^2} \\ \\ b = \dfrac{\sum_{i=1}^{m} x_i^2 \sum_{i=1}^{m} y_i - \sum_{i=1}^{m} x_i y_i \sum_{i=1}^{m} x_i}{m\sum_{i=1}^{m} x_i^2 - \left(\sum_{i=1}^{m} x_i\right)^2} \end{cases}$$

Example: fitting a power curve

- Fitting a power curve with the least squares criterion
  - Goal: fit a curve of the form $y = ax^n$ where n is fixed, to a given data set
  - Minimize the following sum:

$$S = \sum_{i=1}^{m}(y_i - f(x_i))^2 = \sum_{i=1}^{m}(y_i - ax_i^n)^2$$

  - The only parameter here is a
  - Necessary condition: the derivative $\frac{dS}{da}(a) = 0$

$$\frac{dS}{da}(a) = -2\sum_{i=1}^{m} x_i^n(y_i - ax_i^n) = 0$$

$$a = \frac{\sum_{i=1}^{m} x_i^n y_i}{\sum_{i=1}^{m} x_i^{2n}}$$

Relating the 3 criteria

Geometric intuition

- Chebyshev criterion: minimize the largest absolute deviation
  - more weight given to the worst point
- Minimize the sum of absolute deviations
  - tends to treat each data point equally and to average the deviations
- Least-squares
  - somewhat in-between

Relating the 3 criteria

Analytical relationship between Chebyshev and least-squares

- Let $f_1(x)$ be the solution given by the Chebyshev criterion
  - Let $c_i = |y_i - f_1(x_i)|$
  - Let $c_{\max}$ be the largest c_i: the largest absolute deviation
  - f_1 is calculated so that $c_{\max}$ is minimal
- Let $f_2(x)$ be the solution given by the least-squares criterion
  - Let $d_i = |y_i - f_2(x_i)|$
  - f_2 is calculated so that $d_1^2 + d_2^2 + \cdots + d_m^2$ is minimal
  - Let $d_{\max}$ be the largest d_i

- Optimality of the Chebyshev solution: $c_{\max} \leq d_{\max}$
- Optimality of the least-squares solution: $d_1^2 + \cdots + d_m^2 \leq c_1^2 + \cdots + c_m^2$
- $c_m^2 \leq mc_{\max}^2$
- Define $D = \sqrt{(d_1^2 + \cdots + d_m^2)/m}$
- **Conclusion:** $D \leq c_{\max} \leq d_{\max}$

Note: least-squares is more widely used; if the difference between D and $d_{\max}$ is however considerable, consider using Chebyshev instead

Choosing a best model

- For the same data set and the same type of model different results may be obtained depending on the type of fit
  - other methods for model fitting also exist, potentially giving different results for the same data set (nondeterministic methods)
- **Question:** which model to choose as being "best"?
  - if one were allowed to change the type of math model (e.g., look for a cubic, rather than a quadratic polynomial) even better fits may be found
  - The answer should be given depending on the purpose of the model, the required precision, accuracy of the data, etc.
    - a preset sum of squares may be enough to judge a model "good"
  - Careful about applying the numerical criteria blindly
  - Example: for the following 4 data sets, the model $y = x$ yields the same sum of squared deviations

Fit quality

- Various methods for defining a quantitative measure for the quality of a model fit
  - Here present just one, from Kuhnel et al, BMC Systems Biology (2008)
  - Only one data set at a time
  - Gives a measure of the average deviation of the model prediction from the experimental data, normalized by (the average of) the absolute values of the model prediction
  - This measure of fit quality does not discriminate against models aiming to explain experimental data with large absolute values

- Let exp be the experimental data; m the number of experimental points

$$\texttt{qual(exp)} = \sqrt{\frac{\texttt{sum\_of\_squared\_deviations}}{m \cdot \texttt{mean\_of\_predicted\_values}}} \cdot 100\%$$

- Rule of thumb (Kuhnel et al): lower than 20% value for qual(exp) can be considered as a good fit

Learning objectives

- Understand the concepts of **model fitting** and **data interpolation**
- Indicate several possible sources of errors in modeling
- Understand the concept of confidence interval
- Ability to formulate the following **3 fitting criteria** for a given model:
    - Chebyshev approximation
    - Sum of absolute deviation
    - Least squares