Non-linear models. Basis expansion. Overfitting. Regularization.

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When a linear model is not enough. . .

Quiz

When a linear model is not enough, . . .

A we are doomed. There are no other methods than linear ones.

B we can easily use non-linear models. They are as easy to train as the linear methods.

C we must use non-linear models, but their training is much more demanding.

D we can use a special type of non-linear models which can be trained in the same way as the linear methods.

Basis expansion

a.k.a. **feature space straightening**.

Why?

- Linear decision boundary (or linear regression model) may not be flexible enough to perform accurate classification (regression).
- The algorithms for fitting linear models can be used to fit (certain type of) *non-linear models*!

How?

- Let's define a new multidimensional image space F.
- Feature vectors $\boldsymbol{x}$ are transformed into this image space F (new features are derived) using mapping Φ:

$$\begin{aligned} \boldsymbol{x} &\rightarrow \boldsymbol{z} = \Phi(\boldsymbol{x}), \\ \boldsymbol{x} = (x_1, x_2, \ldots, x_D) &\rightarrow \boldsymbol{z} = (\Phi_1(\boldsymbol{x}), \Phi_2(\boldsymbol{x}), \ldots, \Phi_G(\boldsymbol{x})), \end{aligned}$$

  while usually $D \ll G$.
- In the image space, a linear model is trained. However, this is equivalent to training a non-linear model in the original space.

$$\begin{aligned} f_G(\boldsymbol{z}) &= w_1 z_1 + w_2 z_2 + \ldots + w_G z_G + w_0 \\ f(\boldsymbol{x}) = f_G(\Phi(\boldsymbol{x})) &= w_1 \Phi_1(\boldsymbol{x}) + w_2 \Phi_2(\boldsymbol{x}) + \ldots + w_G \Phi_G(\boldsymbol{x}) + w_0 \end{aligned}$$

Two coordinate systems

Transformation into a high-dimensional image space

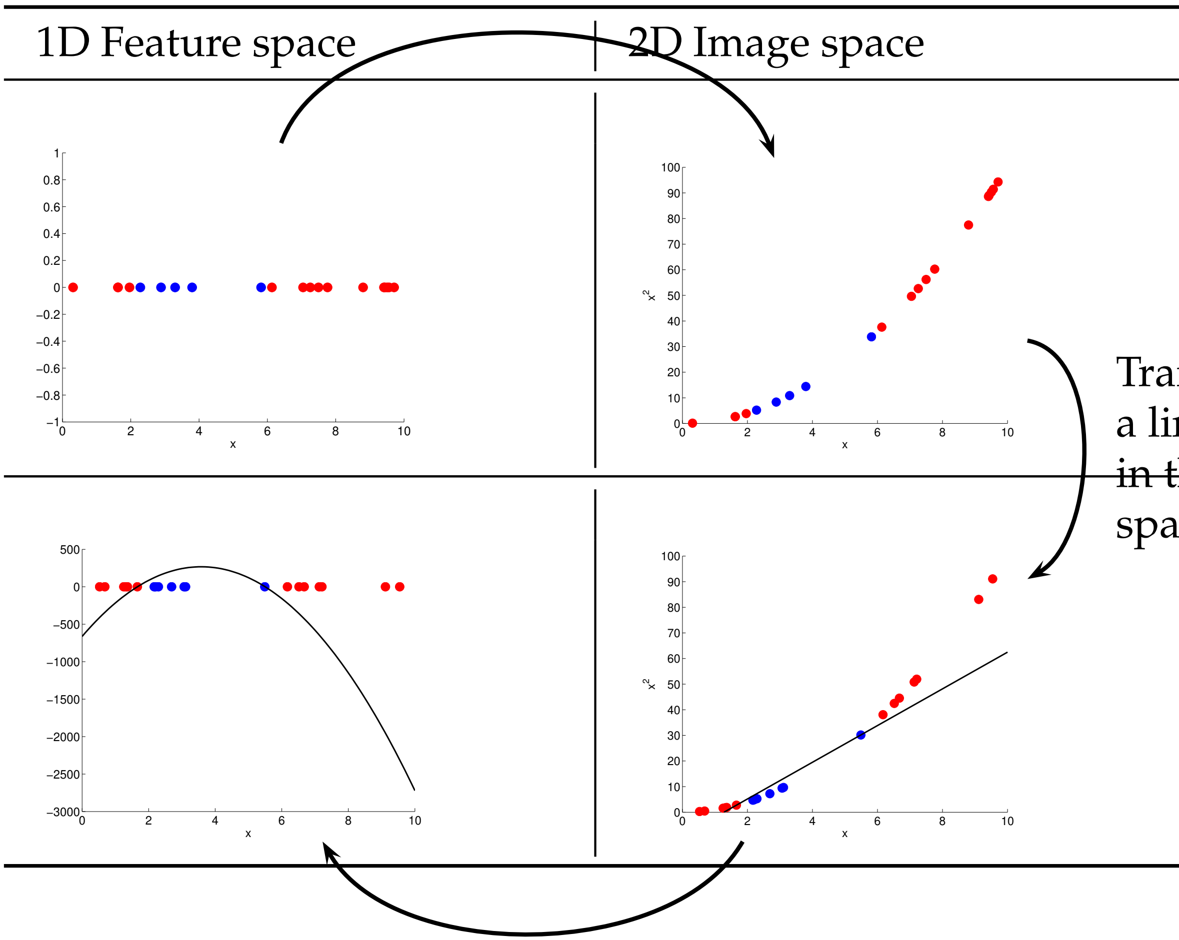
Feature space	Image space
$\boldsymbol{x} = (x_1, x_2, \ldots, x_D)$	$\boldsymbol{z} = (z_1, z_2, \ldots, z_G)$ $z_1 = \log x_1$ $z_2 = x_1^2 x_3$ $z_3 = e^{x_2}$ $\ldots$
$f(\boldsymbol{x}) = w_1 \log x_1 + w_2 x_1^2 x_3 + w_3 e^{x_2} + \ldots + w_0$	$f_G(\boldsymbol{z}) = w_1 z_1 + w_2 z_2 + w_3 z_3 + \ldots + w_0$

Training a linear model in the image space

Non-linear model in the feature space

Two coordinate systems: simple graphical example

Transformation into
a high-dimensional
image space



Training
a linear model
in the image
space

Non-linear model in the
feature space

Basis expansion: remarks

Advantages:

- Universal, generally usable method.

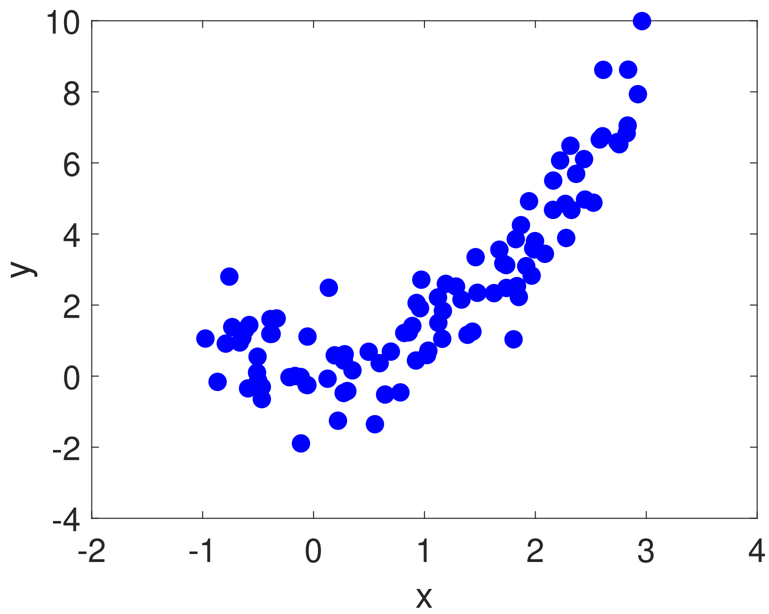
Disadvantages:

- We must define what new features shall form the high-dimensional space F.
- The examples must be really transformed into the high-dimensional space F.
- When too many derived features are used, the resulting models are prone to overfitting (see next slides).

For certain type of algorithms, there is a method how to perform the basis expansion without actually carrying out the mapping! (See the next lecture.)

How to evaluate a predictive model?

Quiz



Which of the following models will have *the smallest training error* if fitted to the above data?

A $\hat{y} = w_0 + w_1 x$

B $\hat{y} = w_0 + w_1 x + w_2 x^2$

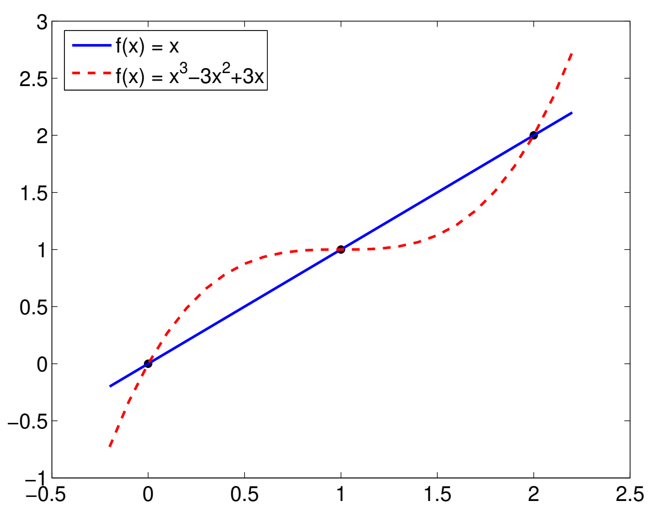
C $\hat{y} = w_0 + w_1 x + w_2 x^2 + w_3 x^3$

D $\hat{y} = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + w_4 x^4$

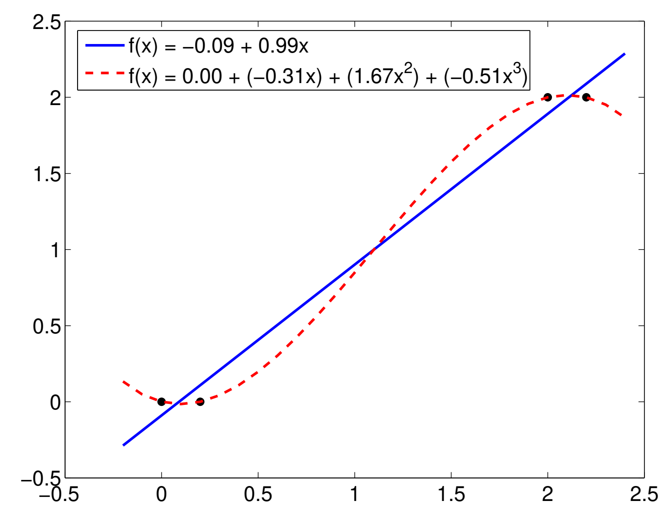
Model evaluation

Fundamental question: What is a good measure of "model quality" from the machine-learning standpoint?

- We have various measures of model error:
  - For regression tasks: MSE, MAE, ...
  - For classification tasks: misclassification rate, measures based on confusion matrix, ...
- Some of them can be regarded as finite approximations of the *Bayes risk*.
- Are these functions *good approximations* when measured on the same data that were used for training?



Using MSE only, both models are equivalent!!!



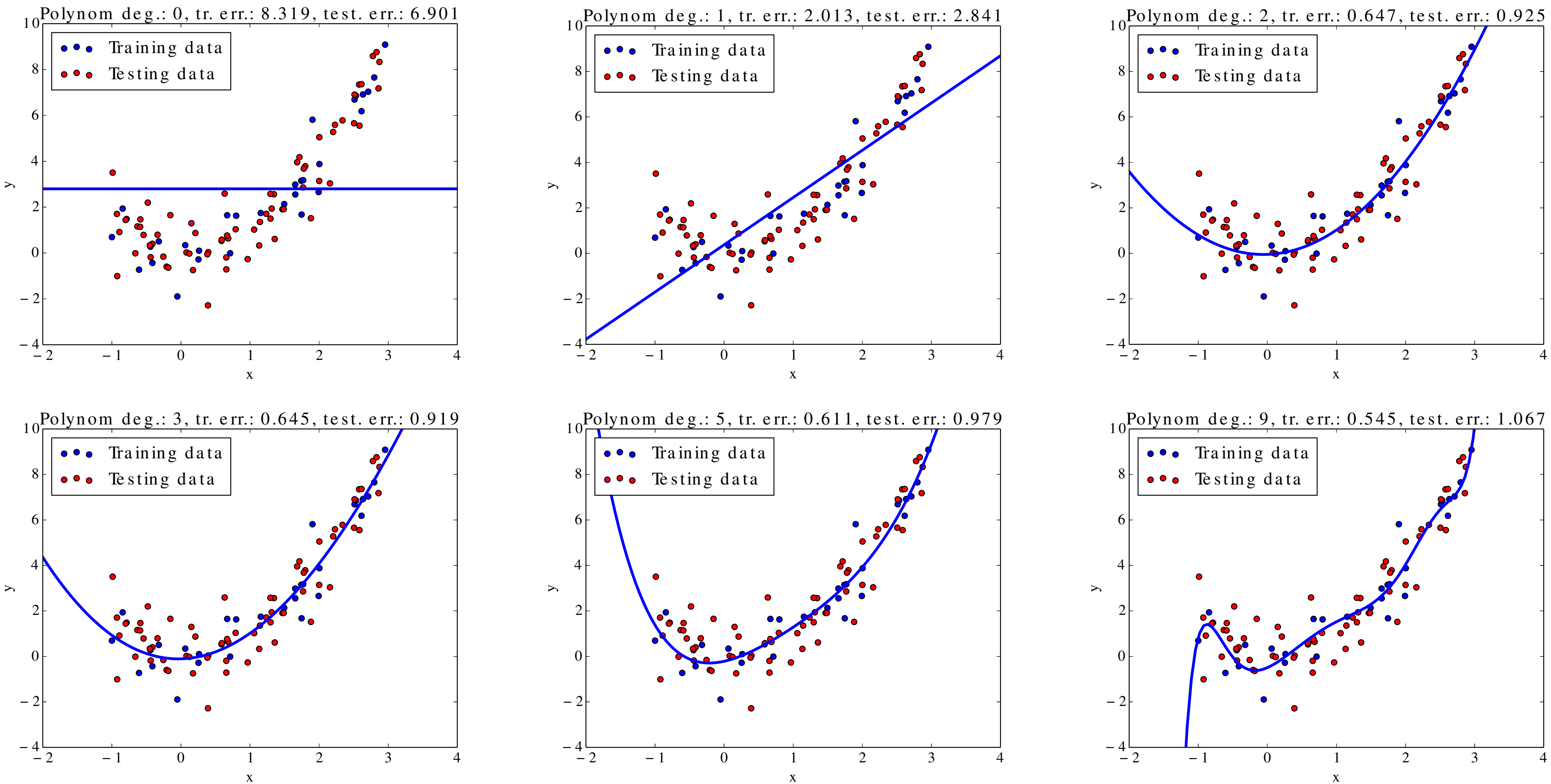
Using MSE only, the cubic model is better than linear!!!

A basic method of evaluation is *model validation on a different, independent data set* from the same source, i.e. on **testing data**.

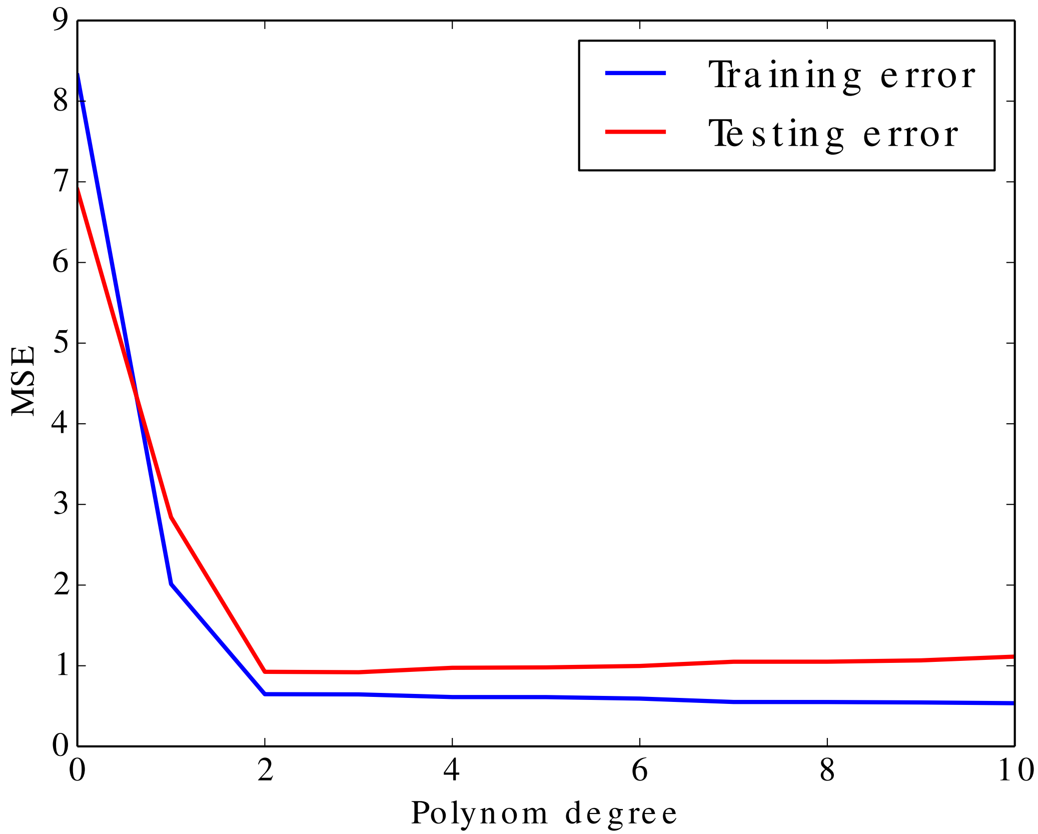
Validation on testing data

Example: Polynomial regression with varrying degree:

$$X \sim U(-1, 3)$$
$$Y \sim X^2 + N(0, 1)$$



Training and testing error



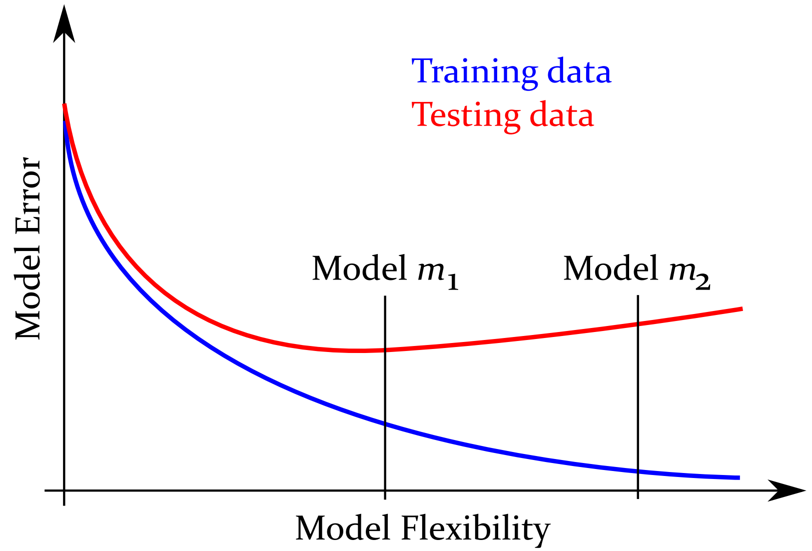
- The *training error* decreases with increasing model flexibility.
- The *testing error* is minimal for certain degree of model flexibility.

Overfitting

Definition of overfitting:

- Let M be the space of candidate models.
- Let $m_1 \in M$ and $m_2 \in M$ be 2 different models from this space.
- Let $\mathrm{Err}_{\mathrm{Tr}}(m)$ be an error of the model m measured on the training dataset (training error).
- Let $\mathrm{Err}_{\mathrm{Tst}}(m)$ be an error of the model m measured on the testing dataset (testing error).
- We say that m_2 is overfitted if there is another m_1 for which

$$\mathrm{Err}_{\mathrm{Tr}}(m_2) < \mathrm{Err}_{\mathrm{Tr}}(m_1) \wedge \mathrm{Err}_{\mathrm{Tst}}(m_2) > \mathrm{Err}_{\mathrm{Tst}}(m_1)$$



- "When overfitted, the model works well for the training data, but fails for new (testing) data."
- Overfitting is a general phenomenon *affecting all kinds of inductive learning* of models with tunable flexibility.

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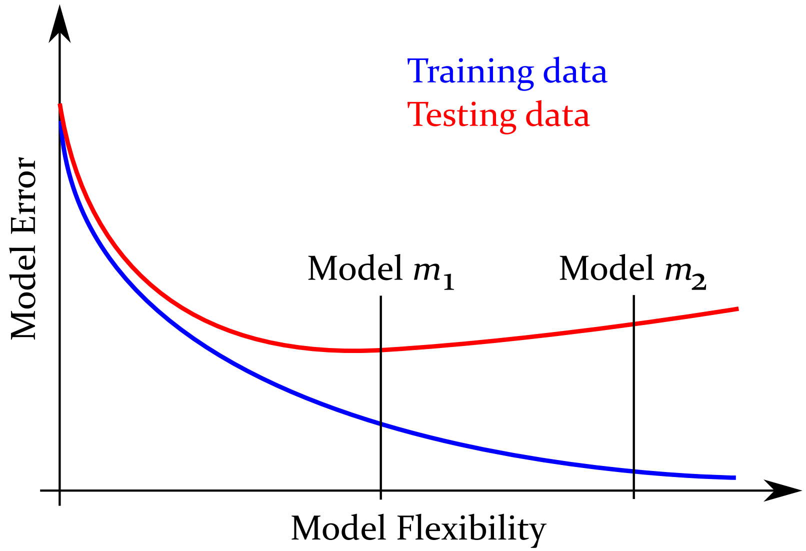

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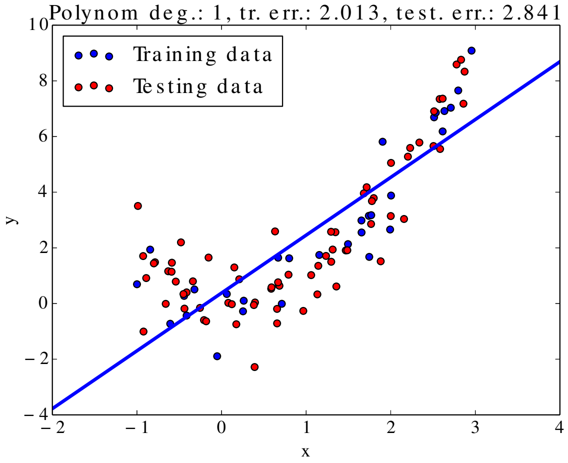
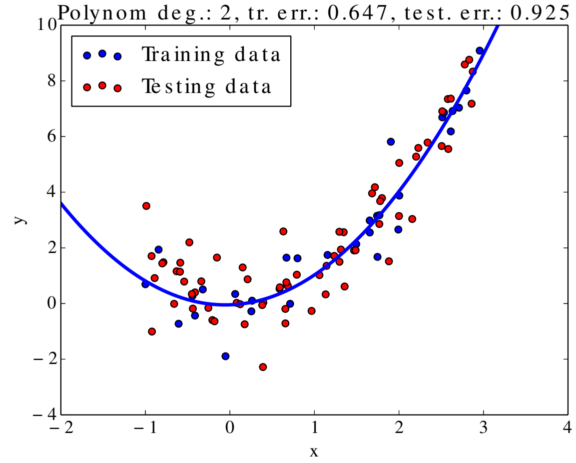
- Overfitting is a general phenomenon *affecting all kinds of inductive learning* of models with tunable flexibility.

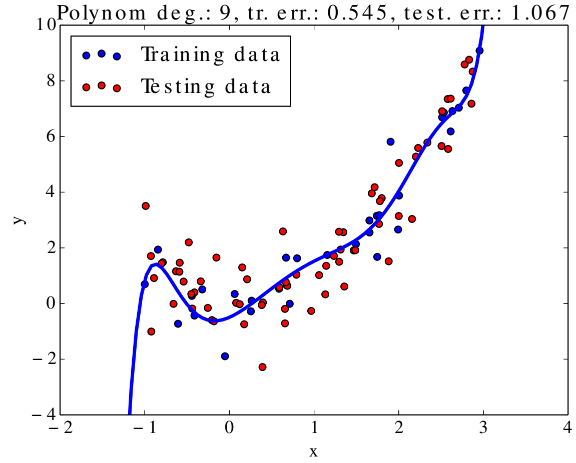
We want models and learning algorithms with a good **generalization ability**, i.e.

- we want models that encode *only the relationships valid in the whole domain*, not those that encode the specifics of the training data, i.e.
- we want algorithms able to find *only the relationships valid in the whole domain* and ignore specifics of the training data.

Bias vs Variance







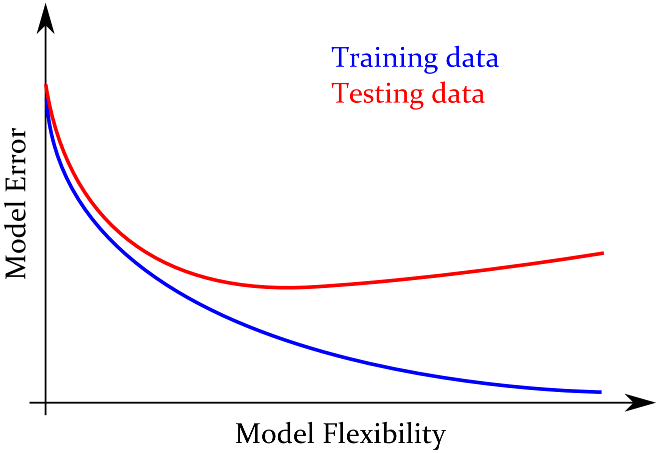
High bias:
model not flexible enough
(Underfit)

"Just right"
(Good fit)

High variance:
model flexibility too high
(Overfit)

High bias problem:

- $\text{Err}_{\text{Tr}}(h)$ is high
- $\text{Err}_{\text{Tst}}(h) \approx \text{Err}_{\text{Tr}}(h)$



High variance problem:

- $\text{Err}_{\text{Tr}}(h)$ is low
- $\text{Err}_{\text{Tst}}(h) >> \text{Err}_{\text{Tr}}(h)$

Crossvalidation

How to estimate the true error of a model on new, unseen data?

Simple crossvalidation:

- Split the data into training and testing subsets.
- Train the model on training data.
- Evaluate the model error on testing data.

K-fold crossvalidation:

- Split the data into k folds (k is usually 5 or 10).
- In each iteration:
  - Use $k-1$ folds to train the model.
  - Use 1 fold to test the model, i.e. measure error.

Iter. 1	Training	Training	Testing
Iter. 2	Training	Testing	Training
Iter. k	Testing	Training	Training

- Aggregate (average) the k error measurements to get the final error estimate.
- Train the model on the whole data set.

Leave-one-out (LOO) crossvalidation:

- $k = |T|$, i.e. the number of folds is equal to the training set size.
- Time consuming for large $|T|$.

How to determine a suitable model flexibility

Simply test models of varying complexities and choose the one with the best testing error, right?

- The testing data are used here to *tune a meta-parameter* of the model.
- *The testing data* are used to train (a part of) the model, thus essentially *become part of training data*.
- The error on testing data is *no longer an unbiased estimate* of model error; it underestimates it.
- A new, separate data set is needed to estimate the model error.

Using simple crossvalidation:

1. *Training data:* use cca 50 % of data for model building.
2. *Validation data:* use cca 25 % of data to search for the suitable model flexibility.
3. Train the suitable model on training + validation data.
4. *Testing data:* use cca 25 % of data for the final estimate of the model error.

Using k-fold crossvalidation

1. *Training data:* use cca 75 % of data to find and train a suitable model using crossvalidation.
2. *Testing data:* use cca 25 % of data for the final estimate of the model error.

The ratios are not set in stone, there are other possibilities, e.g. 60:20:20, etc.

Non-linear models

How to evaluate a predictive model?
- Quiz
- Model evaluation
- Traning and testing
- Overfitting
- Bias vs Variance
- Crossvalidation
- Model complexity
- Preventing overfitting

Regularization

Summary

How to prevent overfitting?

1. **Feature selection:** Reduce the number of features.
   - Select manually, which features to keep.
   - Try to identify a suitable subset of features during learning phase (many feature selection methods exist; none is perfect).

2. **Regularization:**
   - Keep all the features, but reduce the magnitude of their weights w.
   - Works well, if we have a lot of features each of which contributes a bit to predicting y.

Regularization

Quiz

Which of the following methods will NOT help with overfitting:

A Choosing only a subset of input variables.

B Increasing the number of training data.

C Penalizing the size of model parameters.

D Basis expansion, i.e., deriving new features from the old ones.

Ridge regularization (a.k.a. Tikhonov regularization)

Ridge regularization penalizes the size of the model coefficients:

- Modification of the optimization criterion:

$$J(\boldsymbol{w}) = \frac{1}{|T|} \sum_{i=1}^{|T|} \left(y^{(i)} - h_{\boldsymbol{w}}(\boldsymbol{x}^{(i)}) \right)^2 + \alpha \sum_{d=1}^{D} w_d^2.$$

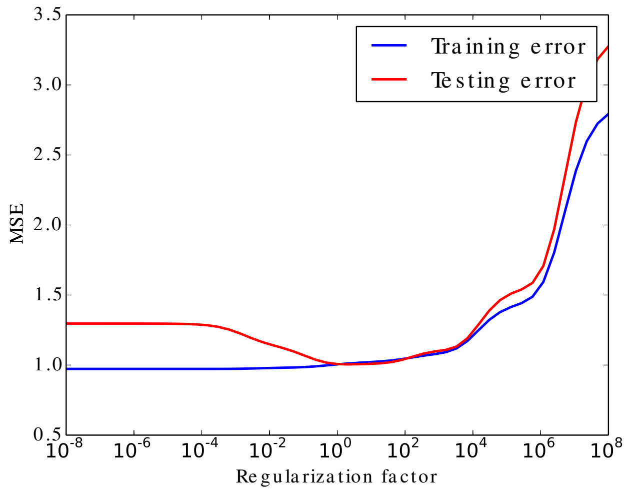
- The solution is given by a modified **Normal equation**

$$\boldsymbol{w}^* = (\boldsymbol{X}^T \boldsymbol{X} + \alpha \mathbf{I})^{-1} \boldsymbol{X}^T \boldsymbol{y}$$

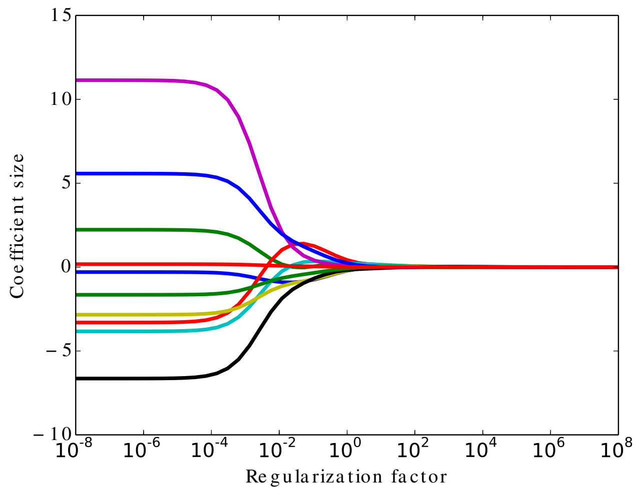
- As $\alpha \to 0$, $\boldsymbol{w}^{\text{ridge}} \to \boldsymbol{w}^{\text{OLS}}$.
- As $\alpha \to \infty$, $\boldsymbol{w}^{\text{ridge}} \to 0$.

OLS - ordinary least squares. Just a simple multiple linear regression.

Training and testing errors as functions of regularization parameter:



The values of coefficients (weights $\boldsymbol{w}$) as functions of regularization parameter:



Lasso regularization

Lasso regularization penalizes the size of the model coefficients:

- Modification of the optimization criterion:

$$J(\boldsymbol{w}) = \frac{1}{|T|}\sum_{i=1}^{|T|}\left(y^{(i)} - h_{\boldsymbol{w}}(\boldsymbol{x}^{(i)})\right)^2 + \alpha \sum_{d=1}^{D} |w_d|.$$

- As $\alpha \to \infty$, Lasso regularization *decreases the number of non-zero coefficients*, effectively also performing *feature selection* and creating *sparse models*.

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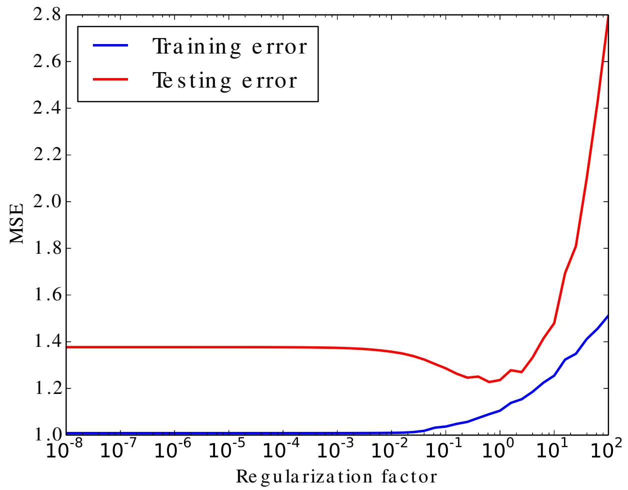

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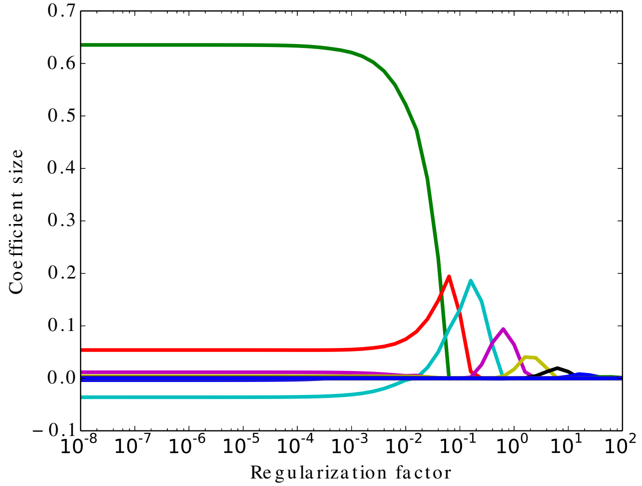

Summary

Competencies

After this lecture, a student shall be able to ...

1. explain the reason for doing basis expansion (feature space straightening), and describe its principle;
2. show the effect of basis expansion with a linear model on a simple example for both classification and regression settings;
3. implement user-defined basis expansions in certain programming language;
4. list advantages and disadvantages of basis expansion;
5. explain why the error measured on the training data is not a good estimate of the expected error of the model for new data, and whether it under- or overestimates the true error;
6. explain basic methods to get unbiased estimate of the true model error (testing data, k-fold crossvalidation, LOO crossvalidation);
7. describe the general form of the dependency of training and testing errors on the model complexity/flexibility/capacity;
8. define overfitting;
9. discuss high bias and high variance problems of models;
10. explain how to proceed if a suitable model complexity must be chosen as part of the training process;
11. list 2 basic methods for overfitting prevention;
12. describe the principles of ridge (Tikhonov) and lasso regularizations and their effects on the model parameters.