CZECH TECHNICAL UNIVERSITY IN PRAGUE

Faculty of Electrical Engineering
Department of Cybernetics

Bias-variance trade-off. Crossvalidation. Regularization.

Petr Pošík

How to evaluate a predictive model?

Model evaluation

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

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  - For regression tasks: MSE, MAE, ...
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- Some of them can be regarded as finite approximations of the *Bayes risk*.
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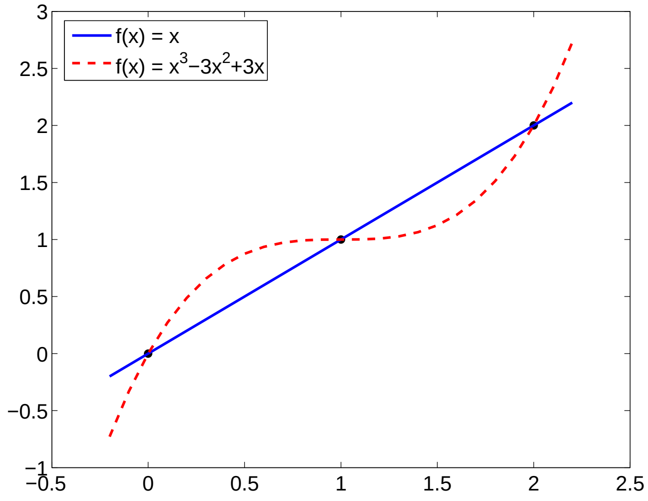

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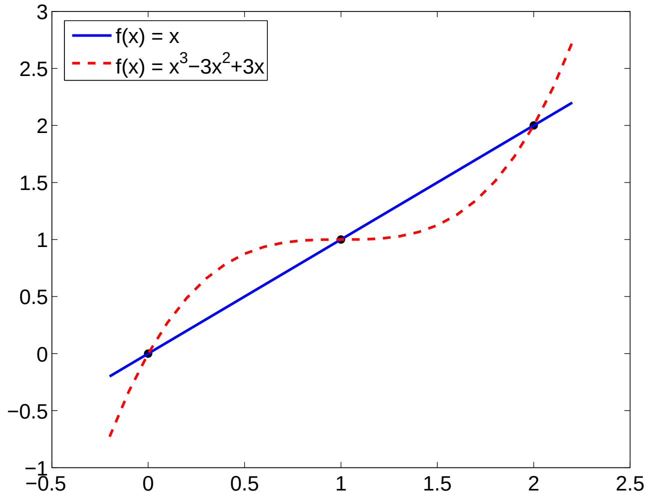

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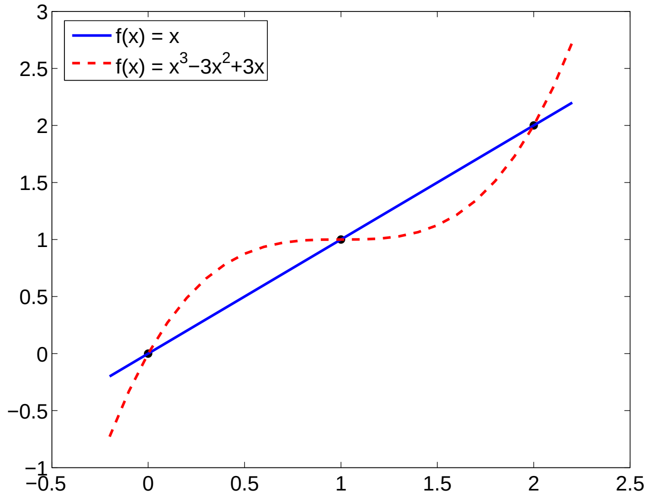

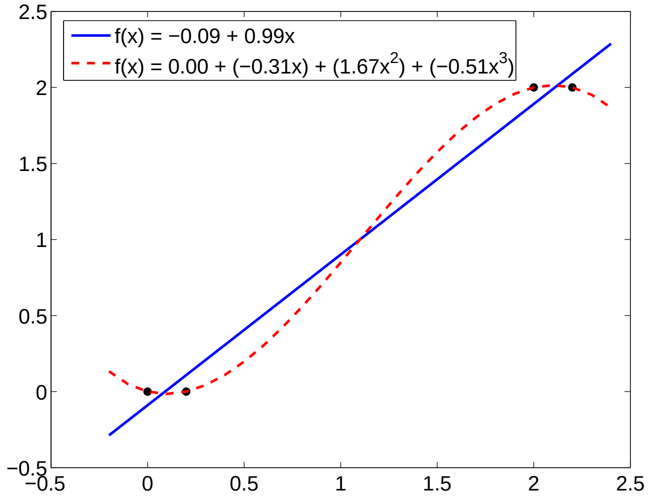

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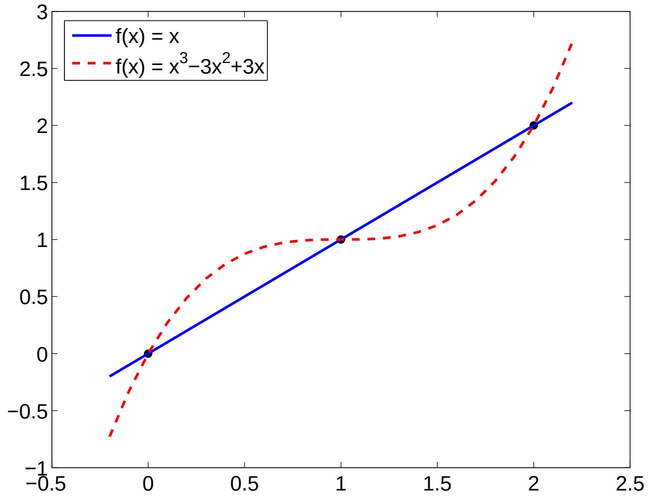

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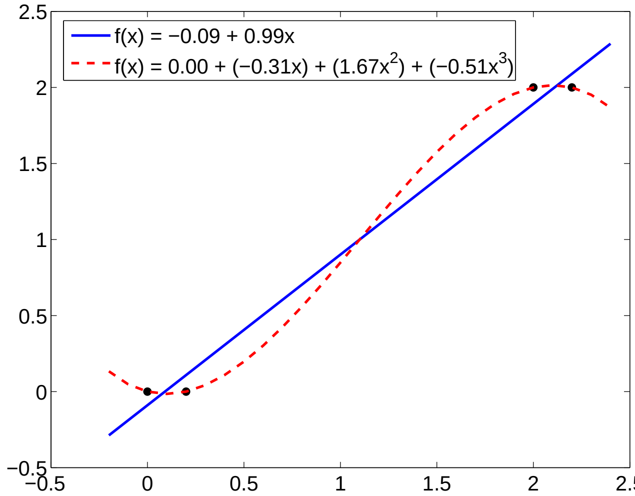

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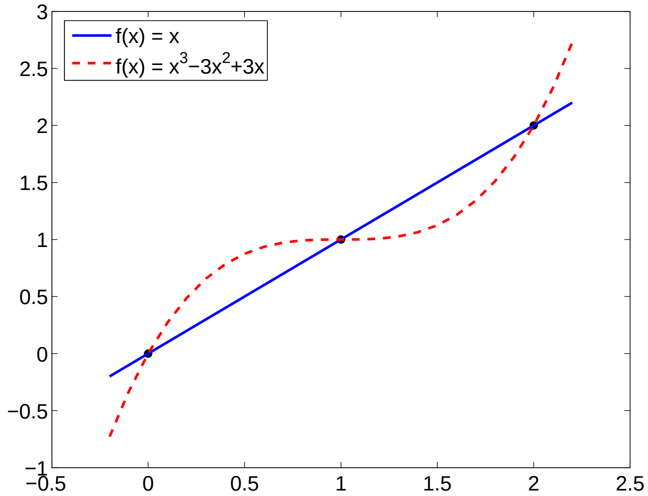

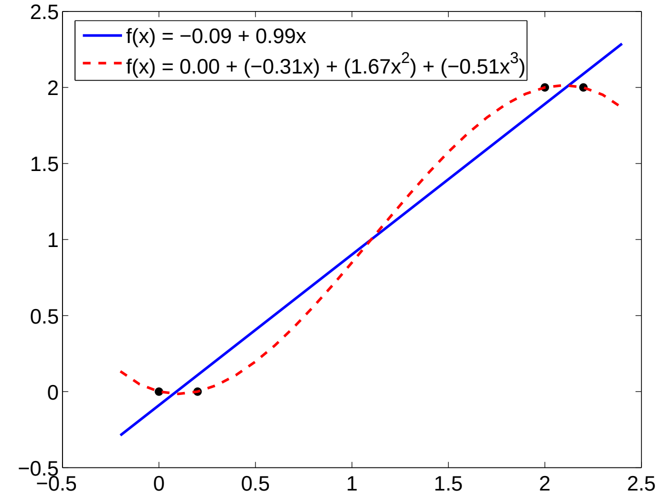

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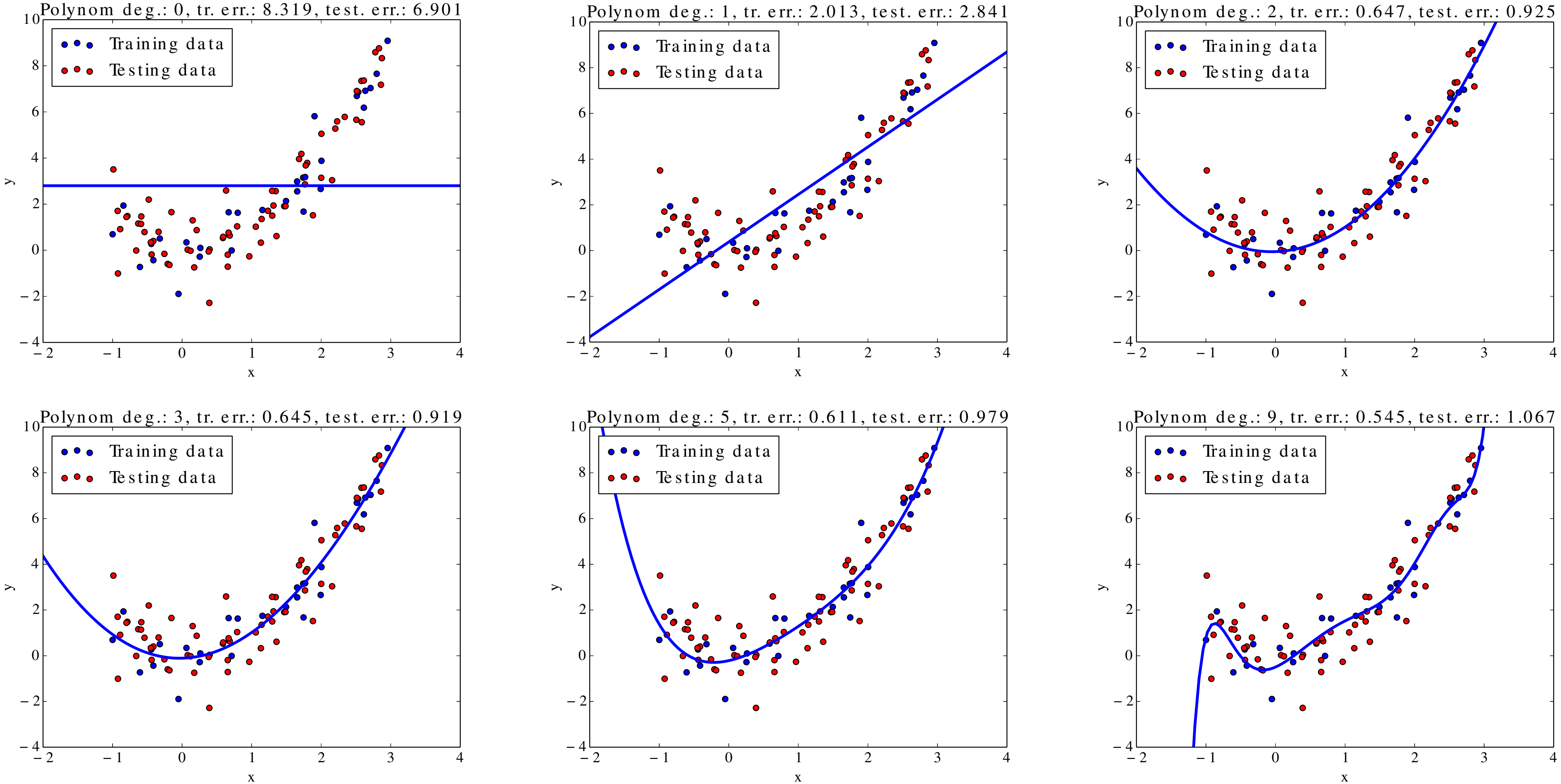
A basic method of evaluation is *model validation on a different, independent data set* from the same source, i.e. on **testing data**.

Validation on testing data

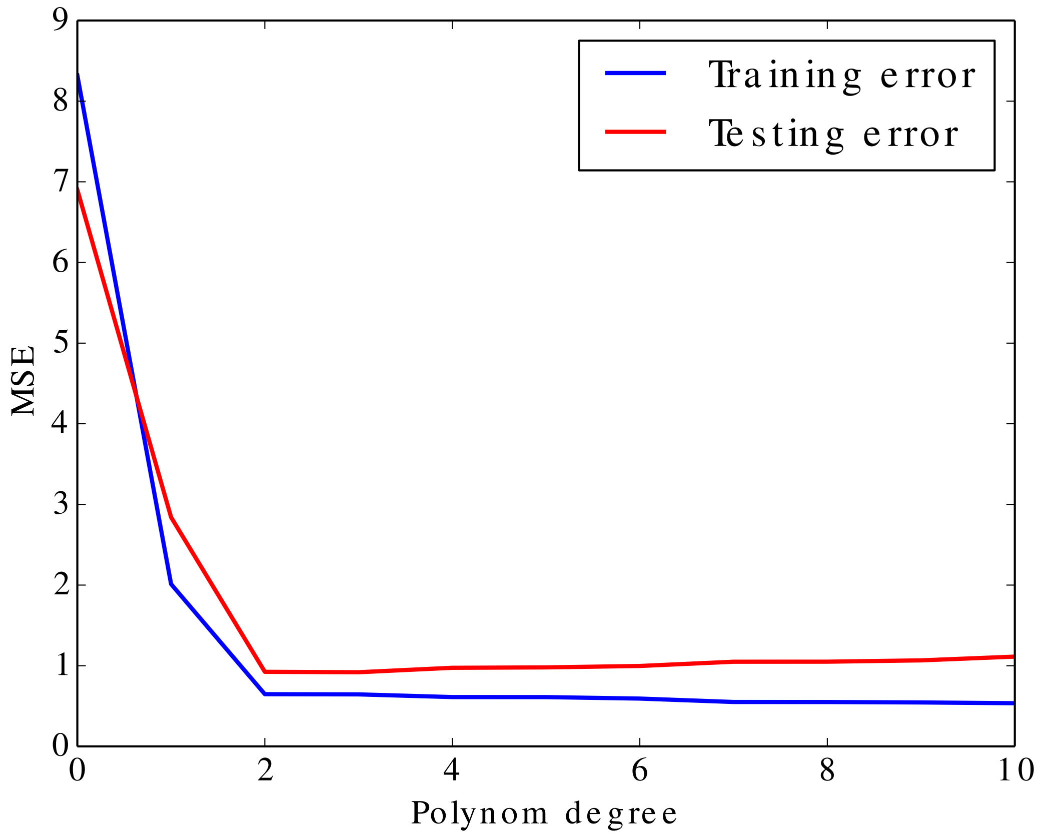
Example: Polynomial regression with varrying degree:

$$X \sim U(-1, 3)$$

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



Training and testing error



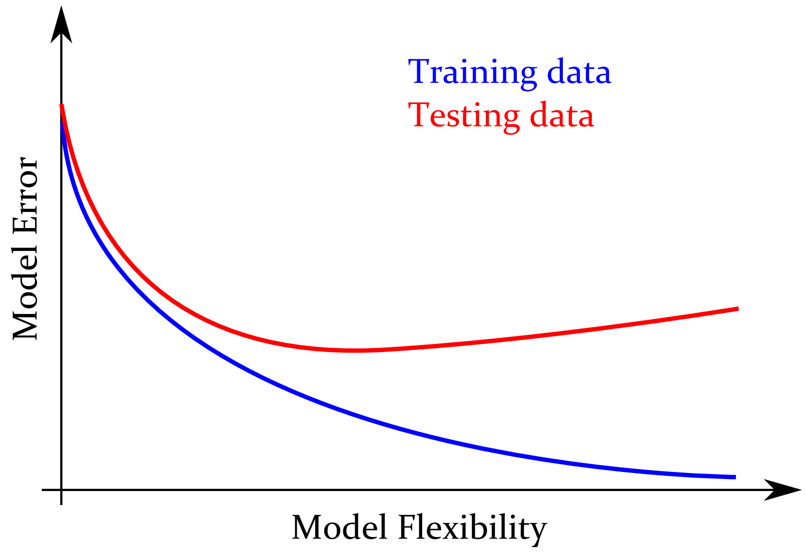
- The *training error* decreases with increasing model flexibility.
- The *testing error* is minimal for certain degree of model flexibility.

Overfitting

Definition of overfitting:

- Let H be a hypothesis space.
- Let $h \in H$ and $h' \in H$ be 2 different hypotheses from this space.
- Let $\mathrm{Err}_{\mathrm{Tr}}(h)$ be an error of the hypothesis h measured on the training dataset (training error).
- Let $\mathrm{Err}_{\mathrm{Tst}}(h)$ be an error of the hypothesis h measured on the testing dataset (testing error).
- We say that h is overfitted if there is another h' for which

$$\mathrm{Err}_{\mathrm{Tr}}(h) < \mathrm{Err}_{\mathrm{Tr}}(h') \wedge \mathrm{Err}_{\mathrm{Tst}}(h) > \mathrm{Err}_{\mathrm{Tst}}(h')$$



- "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*.

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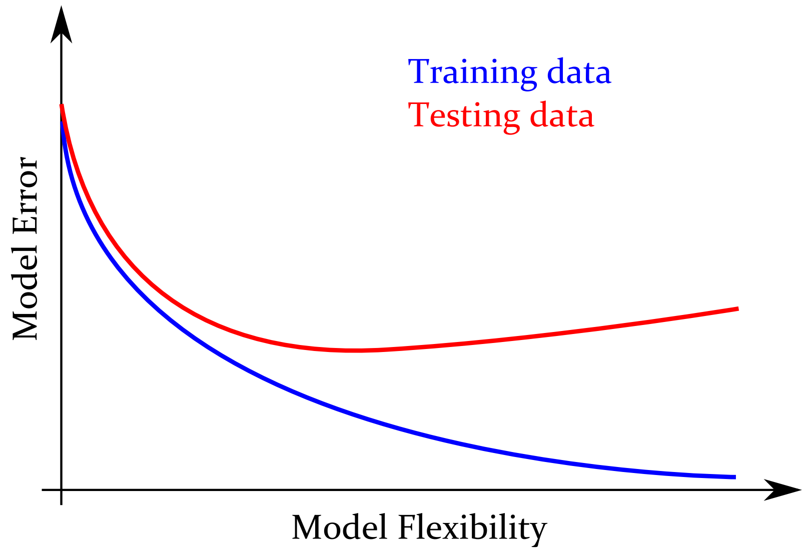

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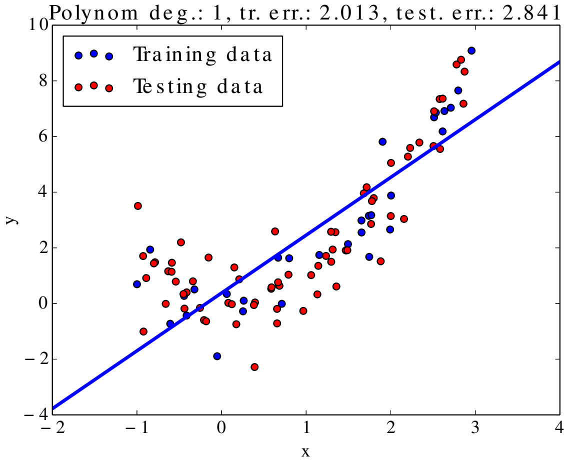
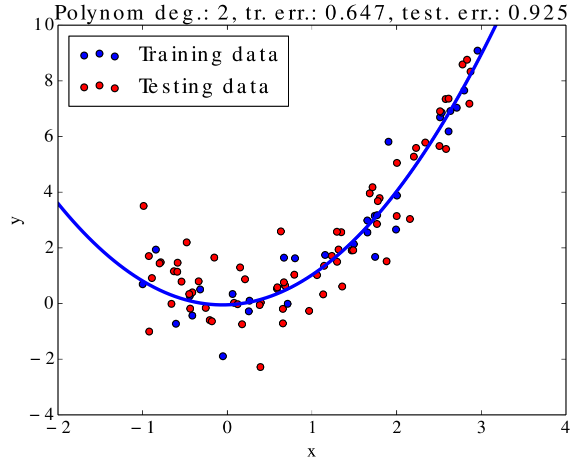
We want models and learning algorithms with a good **generalization ability**, i.e.

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

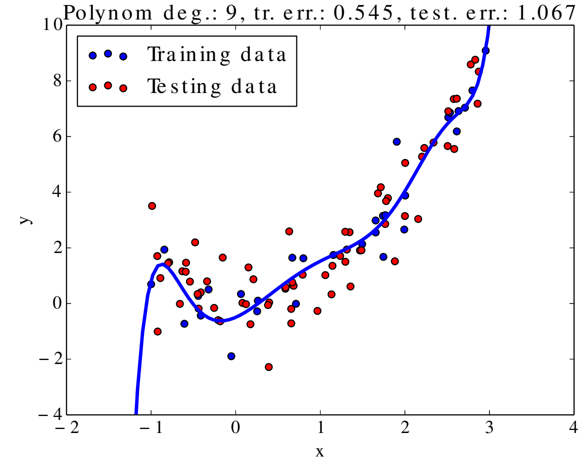
Bias vs Variance



High bias:
model not flexible enough
(Underfit)



"Just right"
(Good fit)



High variance:
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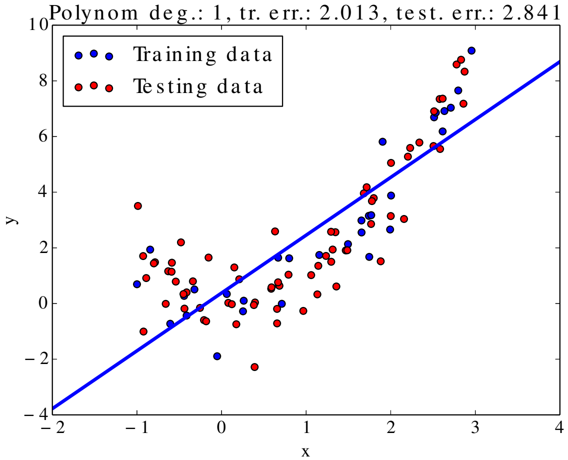

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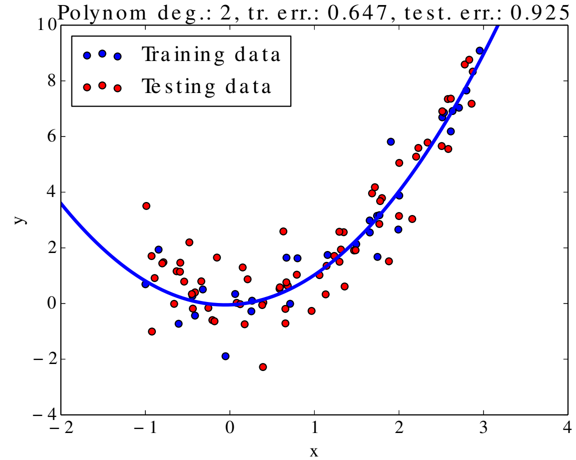

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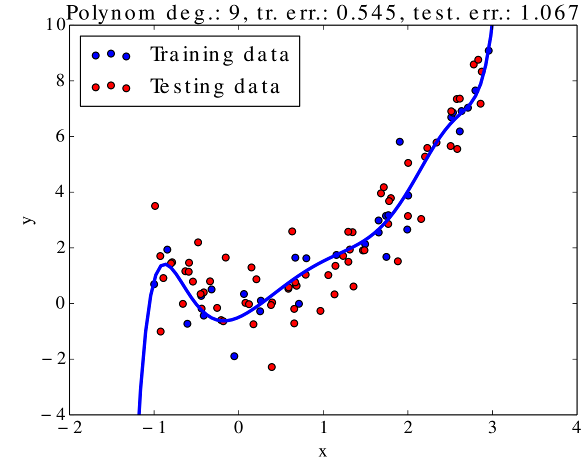

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High bias problem:

- $\mathrm{Err}_{\mathrm{Tr}}(h)$ is high
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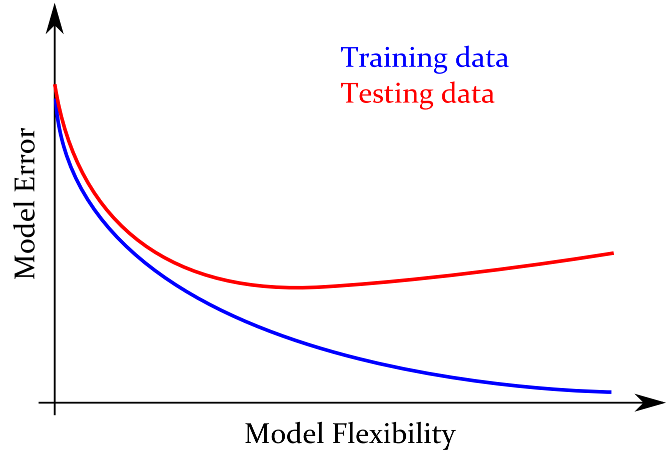

High variance problem:

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

Crossvalidation

Simple crossvalidation:

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

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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.

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Leave-one-out (LOO) crossvalidation:

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

How to determine a suitable model flexibility

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.

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Using *k*-fold crossvalidation

1. *Training data:* use cca 75 % of data to find and train a suitable model using crossvalidation.
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The ratios are not set in stone, there are other possibilities, e.g. 60:20:20, etc.

How to prevent overfitting?

1. Reduce number of features.
   - Select manually, which features to keep.
   - Try to identify a suitable subset of features during learning phase.
2. Regularization
   - Keep all features, but reduce the magnitude of parameters $\boldsymbol{w}$.
   - Works well, if we have a lot of features each of which contributes a bit to predicting y.

Regularization

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

Ridge regularization penalizes the size of the model coefficients:

- Modification of the optimization criterion:

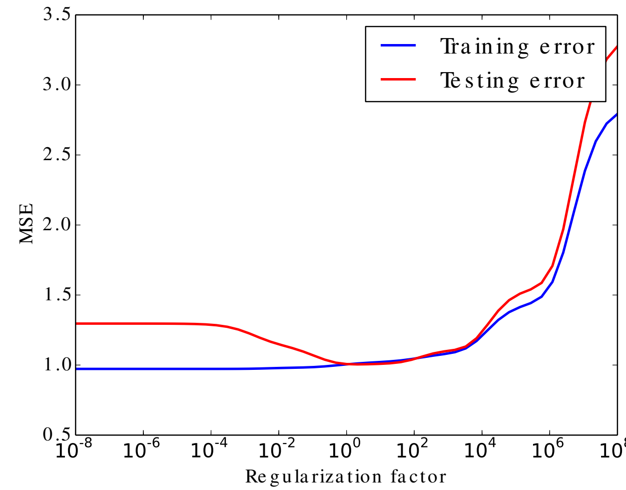
$$J(\boldsymbol{w}) = \frac{1}{|T|}\sum_{i=1}^{|T|}\left(y^{(i)} - h_{\boldsymbol{w}}(\boldsymbol{x}^{(i)})\right)^2 + \alpha \sum_{d=1}^{D} w_d^2.$$

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

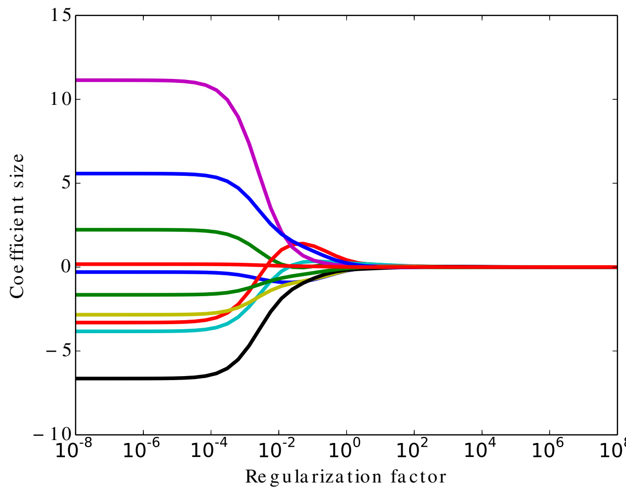
$$\boldsymbol{w}^* = (\boldsymbol{X}^T\boldsymbol{X} + \alpha\mathbf{I})^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

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

Training and testing errors as functions of regularization parameter:



The values of coefficients as functions of regularization parameter:



Lasso regularization

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- Solution is usually found by quadratic programming.
- As $\alpha \to \infty$, Lasso regularization *decreases the number of non-zero coefficients*.

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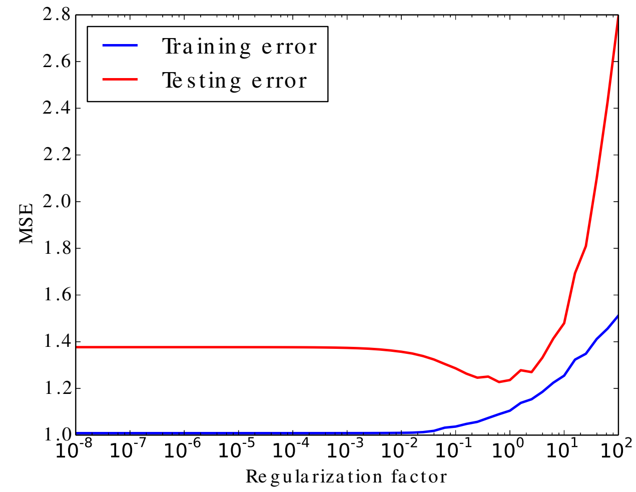

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