problem set 3
cross-validation and kernel ridge regression

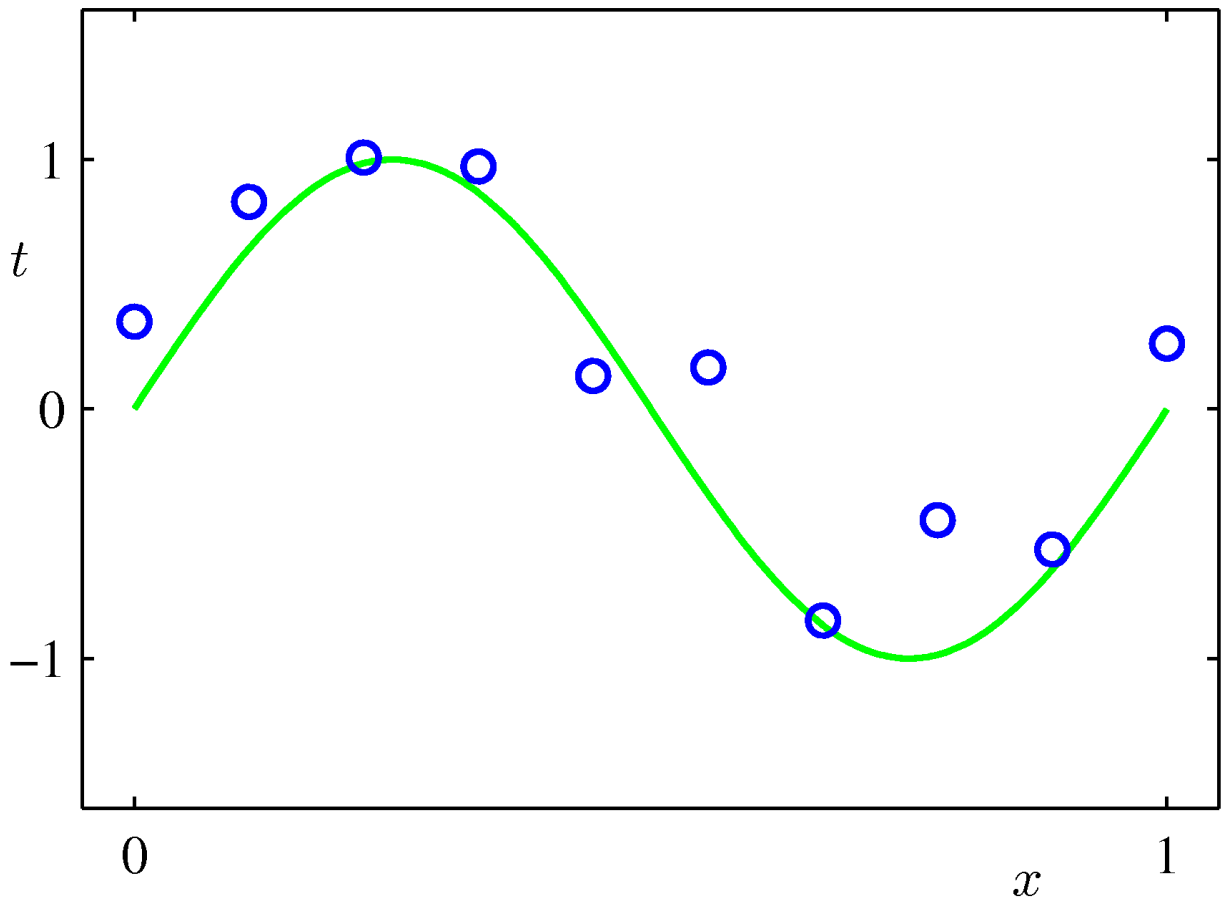
lab course machine learning
summer term 2013

Daniel Bartz

3. Juni 2014

Overfitting

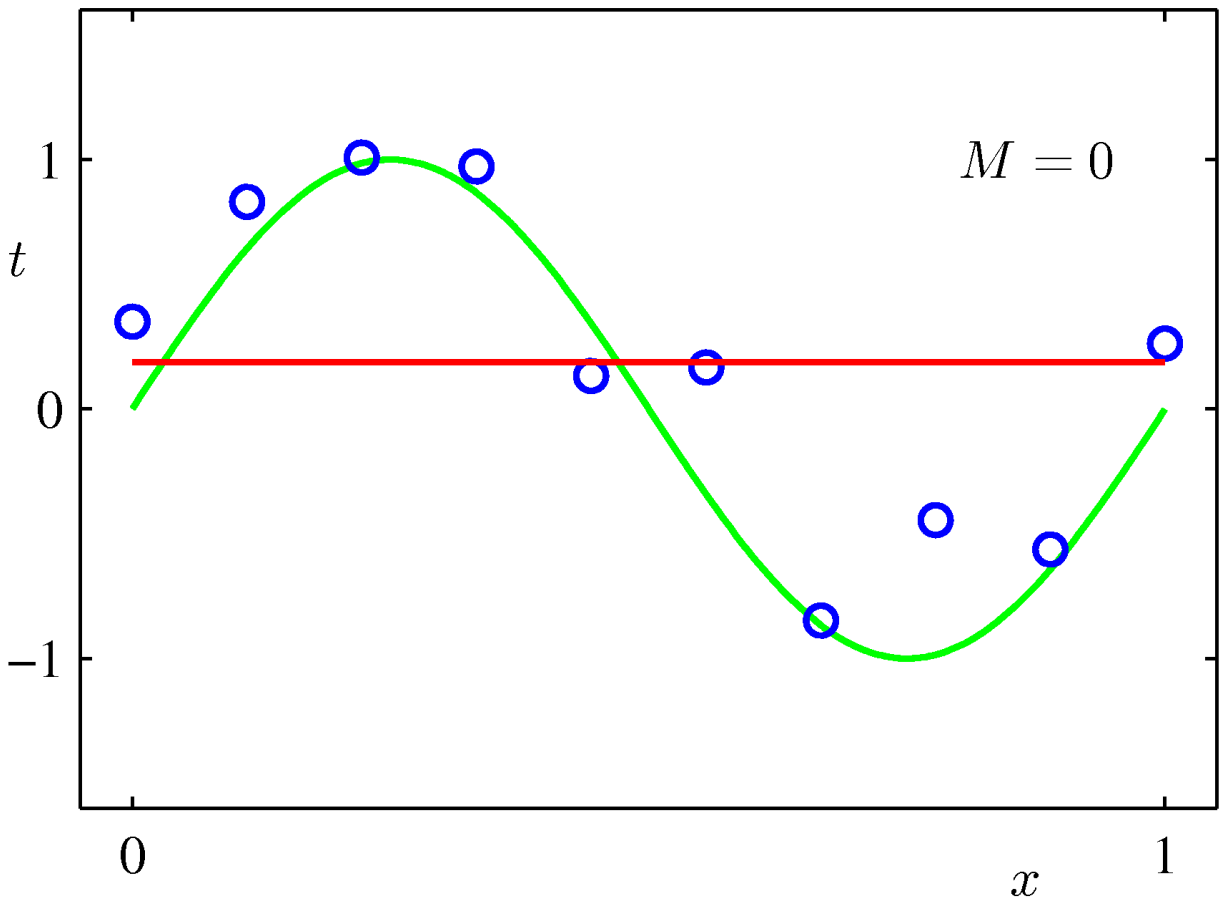
a simple regression problem



from Bishop: Pattern Recognition

Overfitting

ordinary least squares fit of a degree M polynomial



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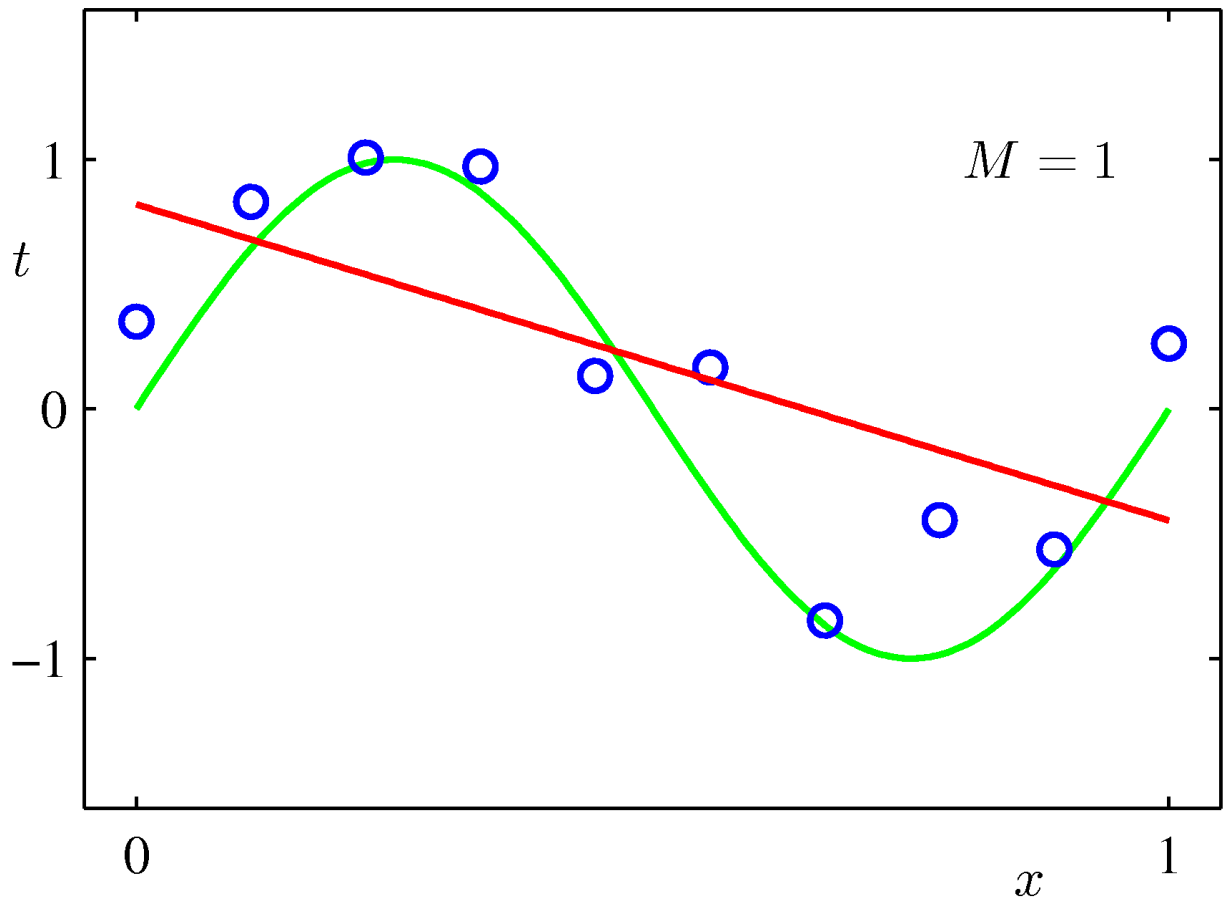

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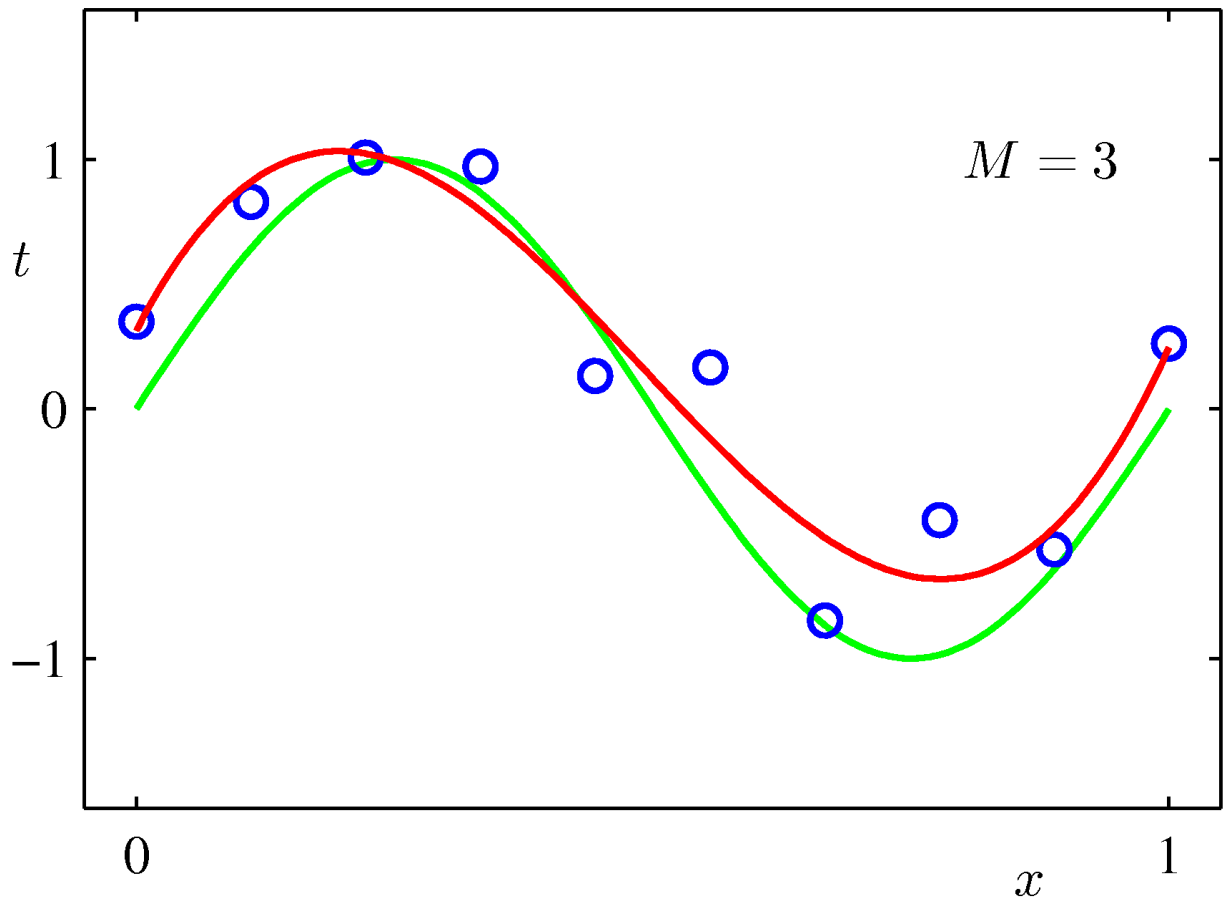

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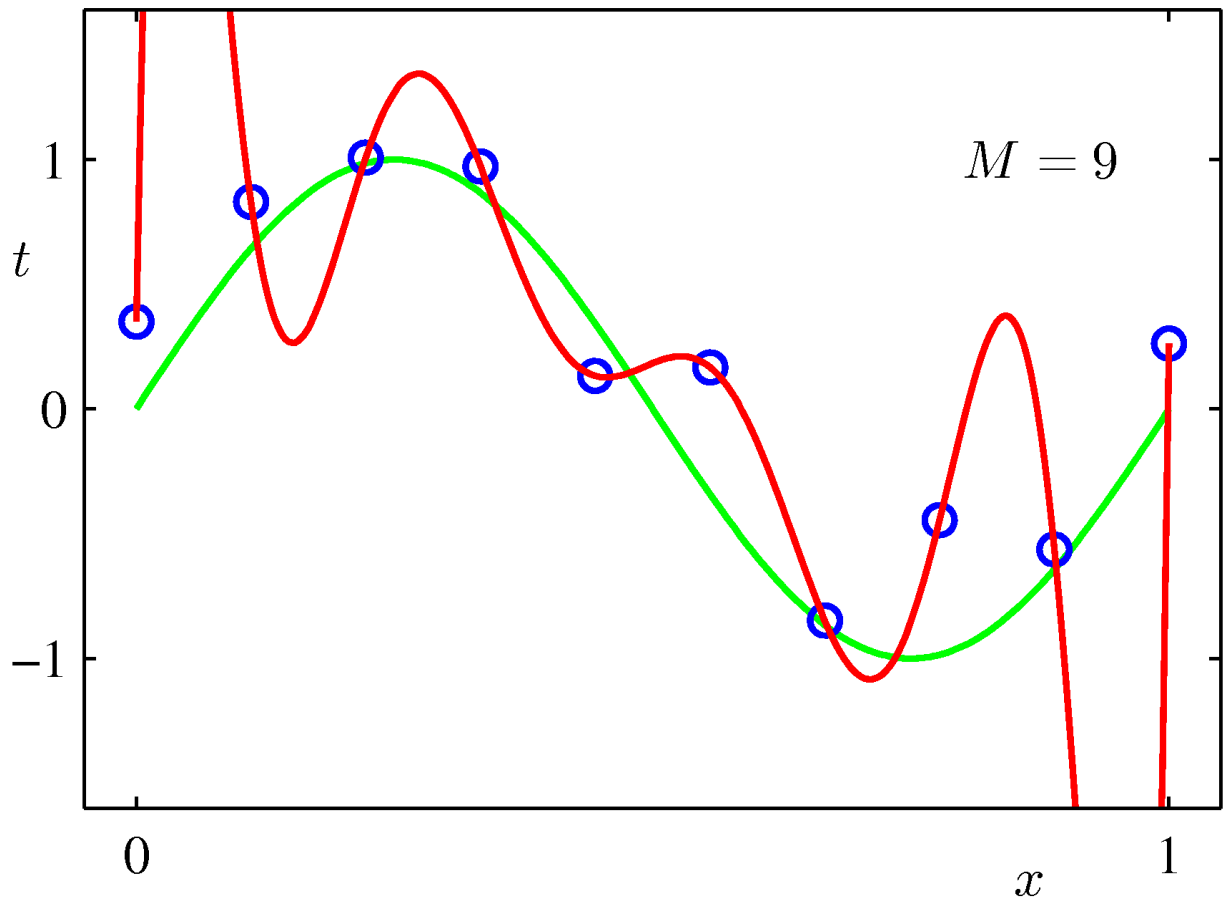

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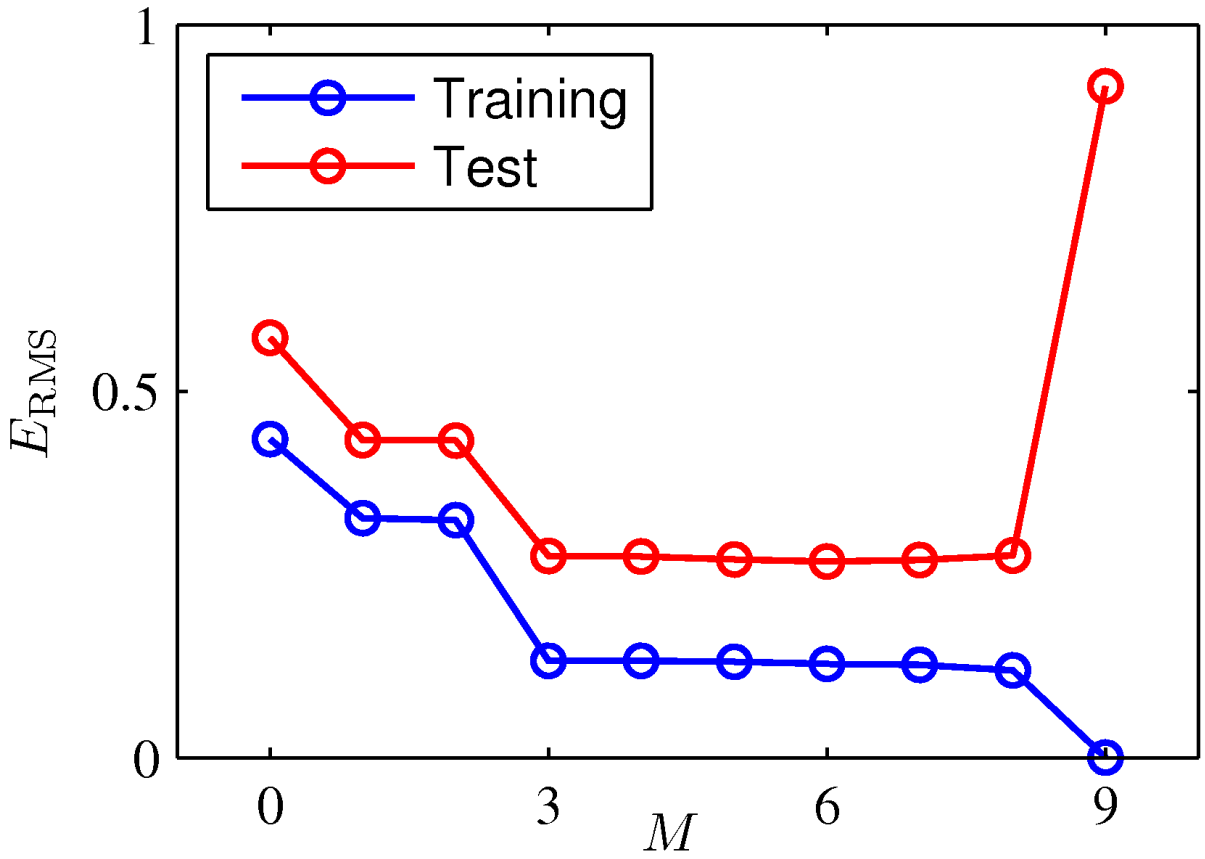
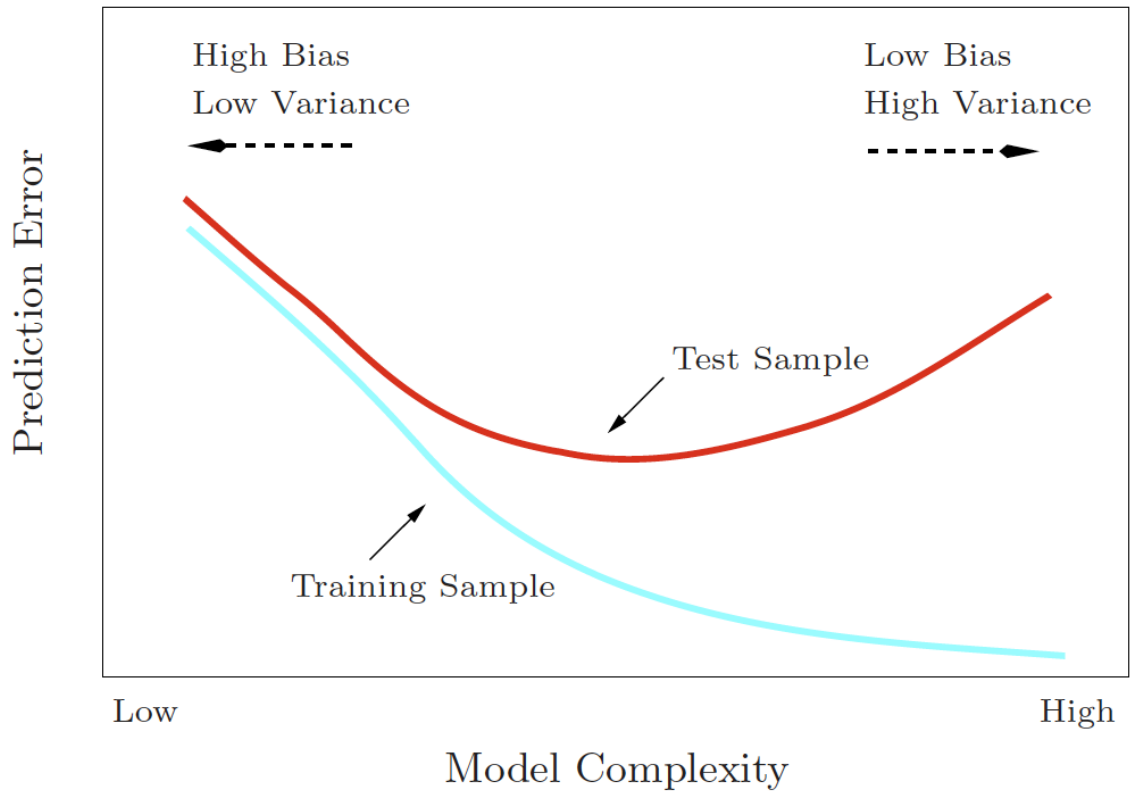


from Bishop: Pattern Recognition

This is more general!

bias variance trade-off in model complexity



from Hastie: Elements of statistical learning

in-sample vs out-of-sample testing

Never ever test your algorithm on the same data on which you fit!

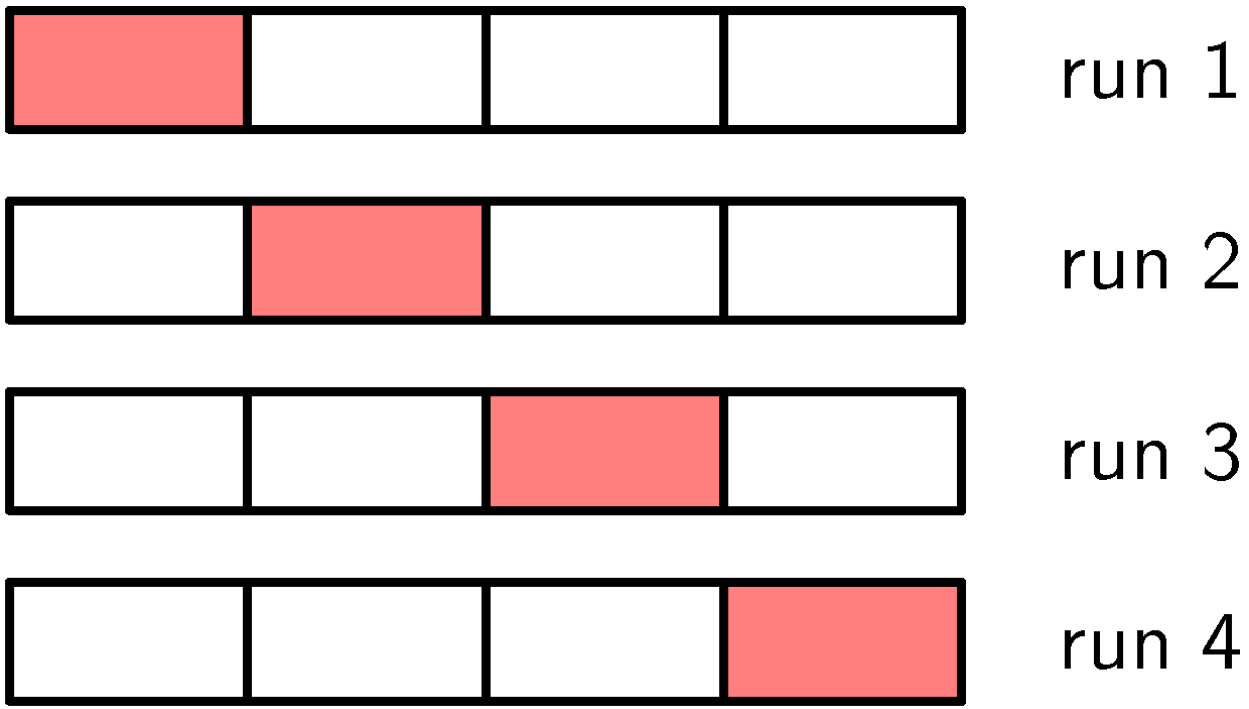
- you will obtain to optimistic error estimates!
- in-sample tests favor complex models

If you have enough data, use a split into training and test data

- for synthetic data, you can generate enough data points
- for real data, you will want to make more efficient use of your data

cross-validation: efficient data usage

use different splits in training and test data set:



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cross-validation: parameters

number of folds and repetitions:

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cv results:

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- cross-validated error estimate (can be optimistic!)
- standard deviation of the error estimate

Ordinary Least Squares (OLS) Regression

recap:

$$E_{ols} = \| \underbrace{Y}_{n \times 1} - \underbrace{X^{\mathsf{T}}}_{n \times p} \underbrace{\beta}_{p \times 1} \|^2$$

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Ridge Regression

- OLS: $\beta_{ols} = (XX^{\mathsf{T}})^{-1}XY$

penalizing large coefficients:

$$E_{rr} = \| \underbrace{Y}_{n\times 1} - \underbrace{X^{\mathsf{T}}}_{n\times p} \cdot \underbrace{\beta}_{p\times 1} \|^2 + \lambda \| \underbrace{\beta}_{p\times 1} \|^2$$

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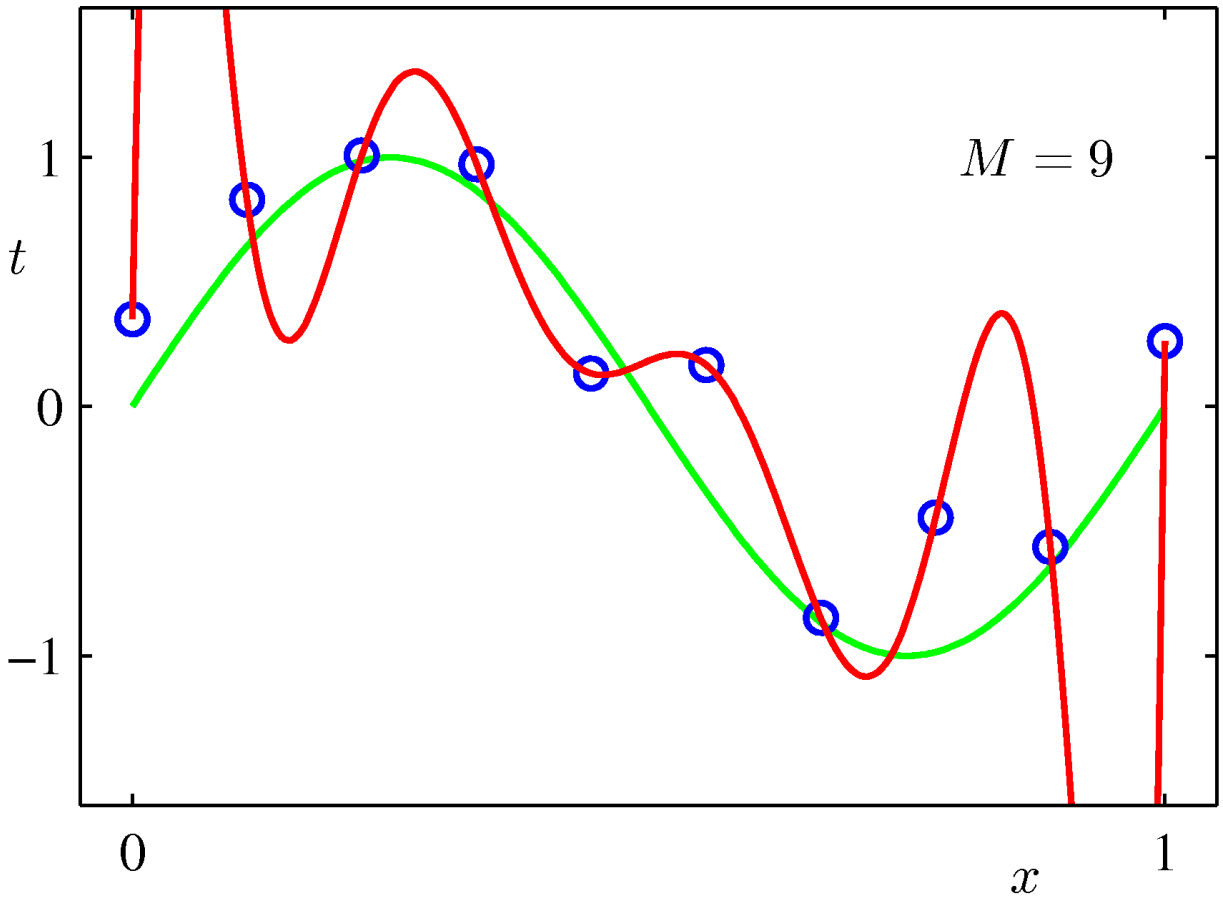
Ridge Regression application

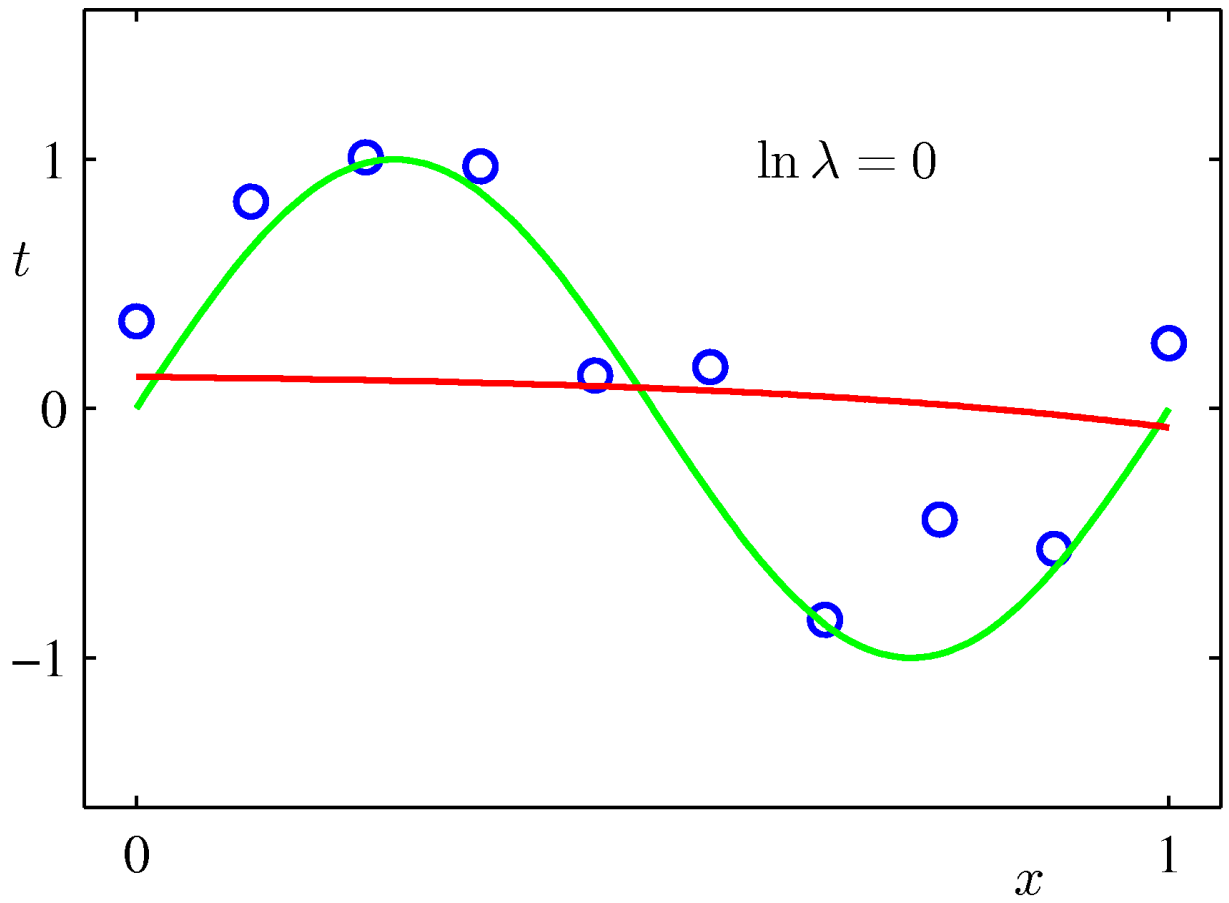
no regularization $\lambda = 0$:



from Bishop: Pattern Recognition

Ridge Regression application

too high regularization λ:



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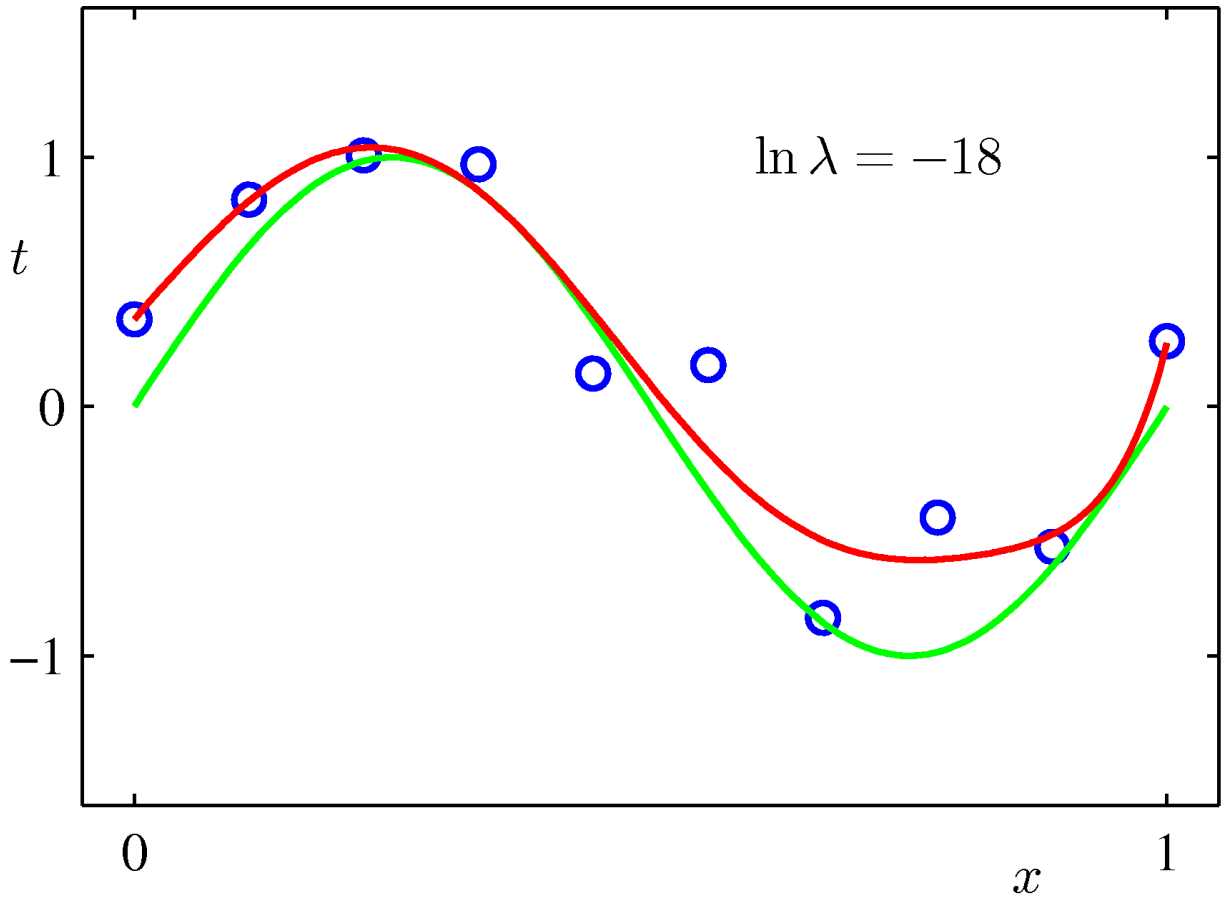
Ridge Regression application

appropriate regularization λ:



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Kernel Ridge Regression

reformulation of Ridge regression based on scalar products

- define: $\beta = \underbrace{X}_{p \times n} \underbrace{\alpha}_{n \times 1}$

$$E_{krr} = \|Y - X^{\mathsf{T}} \cdot \beta\|^2 + \lambda \|\beta\|^2$$

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Kernel Ridge Regression

some properties of KRR

- for the linear kernel, regularization is essential: for n $>$ p, $\underbrace{K}_{n\times n} = \underbrace{X^{\mathsf{T}}}_{n\times p}\underbrace{X}_{p\times n}$ is not invertible!

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- for the linear kernel, regularization is essential:
  for n $>$ p, $\underbrace{K}_{n\times n} = \underbrace{X^{\mathsf{T}}}_{n\times p}\underbrace{X}_{p\times n}$ is not invertible!
- nonlinear regression can be performed by replacing the scalar product with a kernel function:

Name	Kernel	Parameter
polynomial	$k(x,z) = (\langle x,z\rangle + 1)^p$	degree $p \in \{1,2,3,\ldots\}$
gaussian	$k(x,z) = \exp(-\|x-z\|^2/2w^2)$	kernel width w

Efficient LOOCV

For regression, leave-one-out-cross validation does not have to be performed explicitely

- the LOOCV-error: $E_{cv} = \sum_{i=1}^{n} (y_i - x_i \hat{\beta}_{-i})^2$
  Here, $\hat{\beta}_{-i}$ denotes the estimate on all datapoints but i:
  $\hat{\beta}_{-i} = (X_{-i} X_{-i}^{\mathsf{T}} + \lambda I)^{-1} X_{-1} y_{-1}$

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$$
\begin{aligned}
(X_{-i} X_{-i}^{\mathsf{T}} + \lambda I)^{-1} &= (X X^{\mathsf{T}} + \lambda I - x_i x_i^{\mathsf{T}})^{-1} \\
&= \frac{(X X^{\mathsf{T}} + \lambda I)^{-1} x_i x_i^{\mathsf{T}} (X X^{\mathsf{T}} + \lambda I)^{-1}}{1 - x_i^{\mathsf{T}} (X X^{\mathsf{T}} + \lambda I)^{-1} x_i}
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- Here, the Sherman-Morrison-Woodbury identity has been used

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- for the different regularization parameters, a single matrix inversion is sufficient as well: XX^{T} is symmetric, therefore we have

$$XX^{\mathsf{T}} = U^{\mathsf{T}} D U$$

  where D is a diagonal matrix.

- Therefore the inverse is easy to calculate:

$$(XX^{\mathsf{T}} + \lambda I)^{-1} = U(D + \lambda I)^{-1} U^{\mathsf{T}}$$

  with

$$(D + \lambda I)^{-1}_{ii} = (D_{ii} + \lambda)^{-1}$$

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- some –less interesting– algebra later we have

$$E_{cv} = \sum_{i=1}^{n} \frac{(y_i - x_i\beta)^2}{1 - (X^\mathsf{T} U(D + \lambda I)^{-1} U^\mathsf{T} X)_{ii}}$$

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- For kernel ridge regression, a similar formlula holds (see handbook)

classes

object oriented programming

- cross-validation:

```
method = cv(X, y, method,
        { param_name, value_range, ... }, nfolds,
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    def predict():
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itertools and splash

a package for iterations

- easy generation of the parameter combination

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import itertools as it
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- splash operator converts a list argument into single arguments:

```
a = [[0,1],[2,3,4]]
combs1 = it.product(a)
combs2 = it.product(*a)
```

We want your class mates to enjoy the presentations

you should

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take advantage of being a group:

- compare your results

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  - it does not take too long

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- compare your interpretations

We want your class mates to enjoy the presentations

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. . . any volunteers for next week?

Have fun coding!

Questions?