Machine Learning in Precision Medicine

Linear Regression & Regularization

Prof. Dr. Christoph Lippert

Dr. Stefan Konigorski

Digital Health & Machine Learning

Formalities

All lecture and exercise materials are now available at
https://open.hpi.de/courses/MLPrecisionMedicineSoSe2019.

Further news and information through our mailing list, where you also submit your exercise solutions.

Further questions regarding formalities?

Contents of today: Linear Regression

- Introduction
- Maximum likelihood estimation
- Polynomial curve fitting
- Solutions to overfitting
- Regularizes least squares

Recap & Quiz

What is a linear (regression) model?

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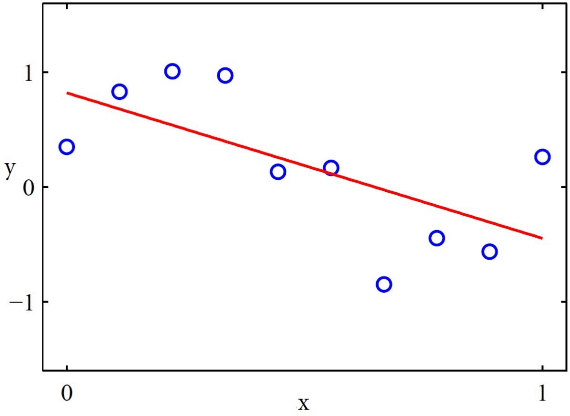

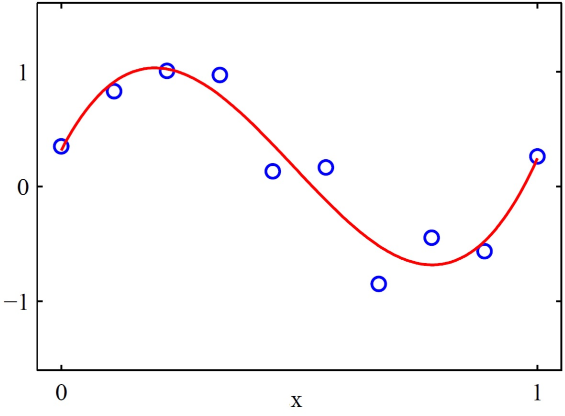

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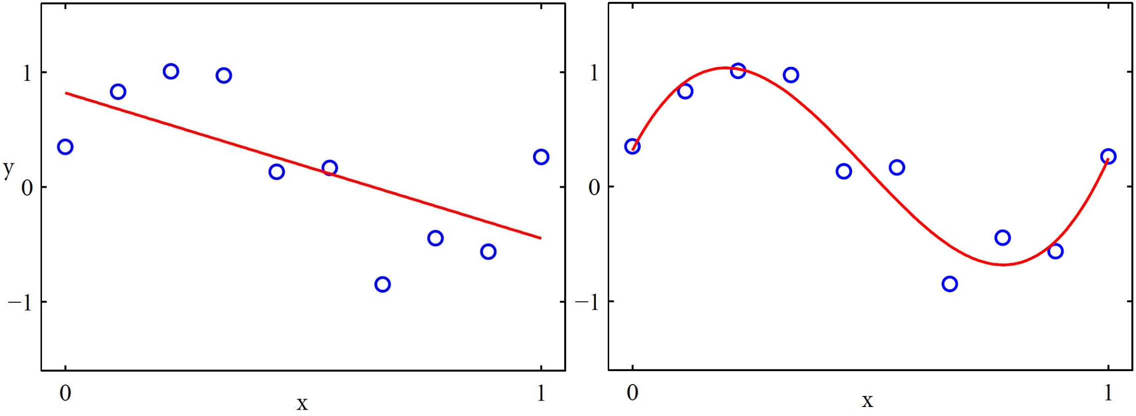

$\longrightarrow$ linear in parameters (e.g. x^3 could be redefined as z).

Recap & Quiz

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What is the rationale behind using maximum likelihood as a criterion for finding the best line fitting 2D data points?

How do you obtain the maximum likelihood values for your parameters ($=$ MLE, maximum likehood estimates)?
Set first derivative (w.r.t. each parameter of interest) of the log-likelihood to 0, solve.

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- Distribution (pdf) of model, whether points are iid (i.e. whether pdf of all points factorizes into product of single points)
- and ...
- that's all! Easy to get closed form, once you know (i.e. assume) a specific parametric distribution.

Maximum likelihood

- Setting: data $\mathcal{D}$ consisting of N data points $\{\mathbf{x}_n, y_n\}_{n=1}^N$, where $\mathbf{x}_n$ contains D features $\mathbf{x}_n = (x_{n1}, \dots, x_{nD})$.

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- Just to make sure: what are the parameters to be learned?

Maximum likelihood

- Taking the logarithm, we obtain

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\ln p(\mathbf{y}|\boldsymbol{\theta}, \sigma^2) &= \sum_{n=1}^{N} \ln \mathcal{N}\left(y_n \,\middle|\, \mathbf{x}_n \cdot \boldsymbol{\beta}, \sigma^2\right) \\
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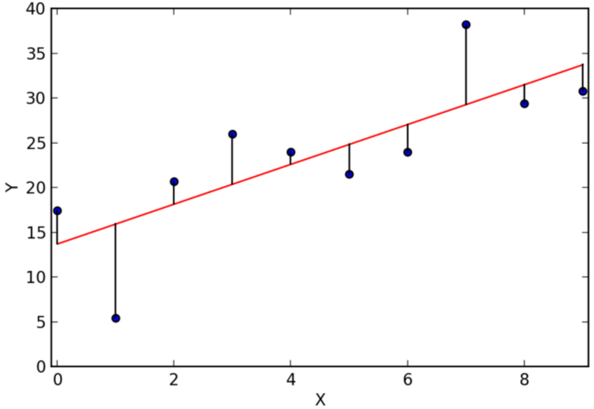
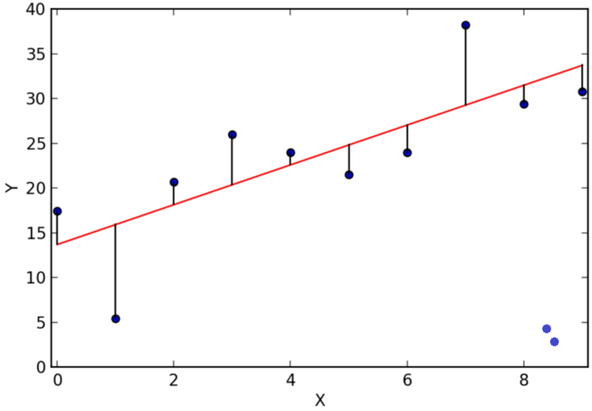
- i.e. MLEs under linear model are (relatively) robust against wrong distribution assumption!

Maximum Likelihood and Least Squares



$$\underset{\boldsymbol{\beta}}{\operatorname{argmin}} \frac{1}{2} \sum_{n=1}^{N} (y_n - \mathbf{x}_n \cdot \boldsymbol{\beta})^2$$

Maximum Likelihood and Least Squares



How would the estimated regression line change?

Derive parameter values

- Derivative w.r.t. a single weight entry β_i

$$\frac{d}{\mathrm{d}\beta_d} \ln p(\mathbf{y}|\boldsymbol{\beta}, \sigma^2) = \frac{d}{\mathrm{d}\beta_d} \left[-\frac{N}{2} \ln 2\pi\sigma^2 - \frac{1}{2\sigma^2} \sum_{n=1}^{N} (y_n - \mathbf{x}_n \cdot \boldsymbol{\beta})^2 \right]$$

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- Learn parameter values for σ^2 similarly.

Polynomial curve fitting

- The above can be extended to more general functions of $\mathbf{x}_n$ that are linear in $\boldsymbol{\beta}$. For simplicity, focus here on $\mathbf{x}_n = x$ (i.e. one feature).

  For example:

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- Use the polynomials up to degree M to construct new features

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  with $\boldsymbol{\phi}(x) = (1, x, x^2, \ldots, x^M), \quad \phi_m(x) = x^m, \quad \boldsymbol{\beta} = (\beta_0, \beta_1, \ldots, \beta_M)^T \in \mathbb{R}^M$.

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- Similarly, $\boldsymbol{\phi}$ can be any feature mapping ($\rightarrow$ call ϕ_m basis functions, see next lecture).

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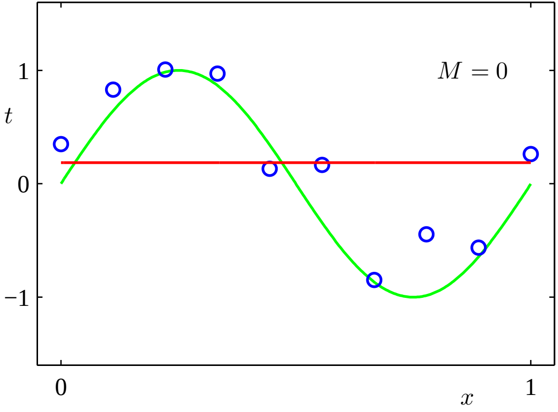
The degree M of the polynomial is crucial.



(C.M. Bishop, Pattern Recognition and Machine Learning)

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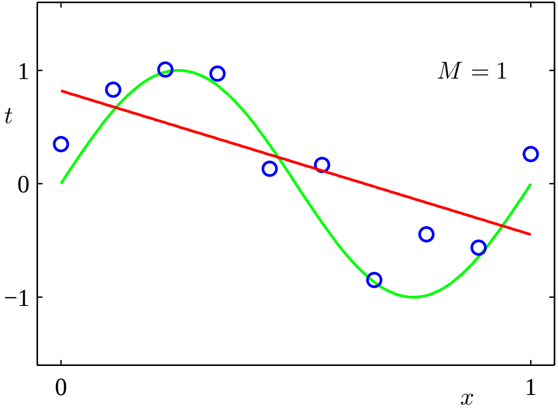

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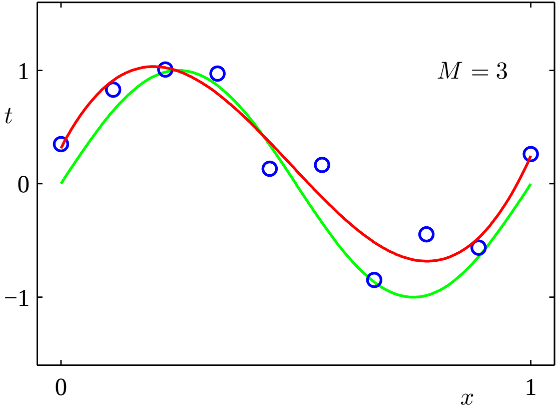

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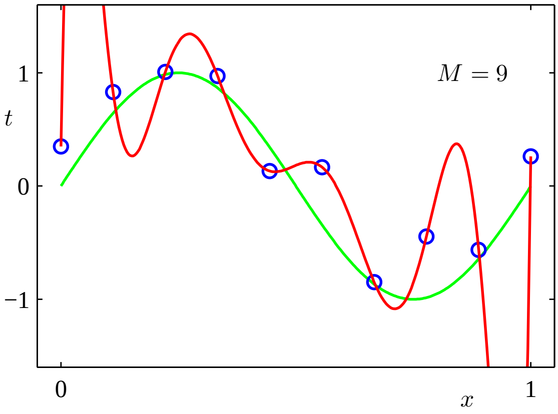

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Problems?

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Problems? Overfitting!

Train vs. Test error

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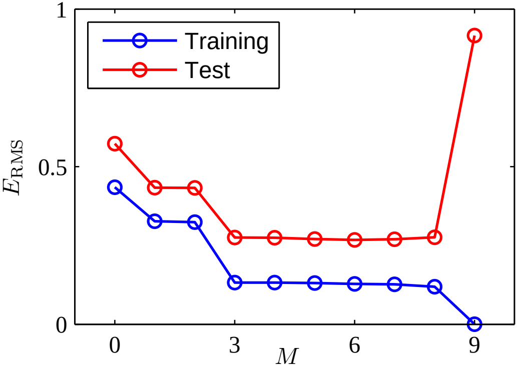

(C.M. Bishop, Pattern Recognition and Machine Learning)

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Train vs. Test error

How do you compute the test error?

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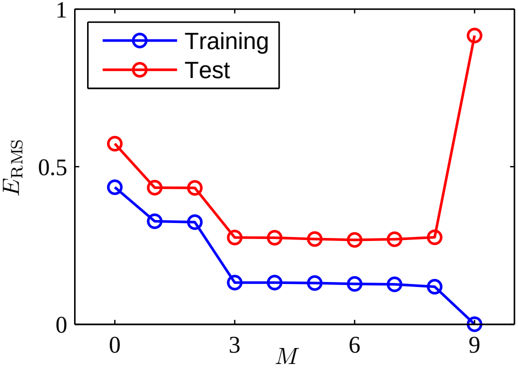

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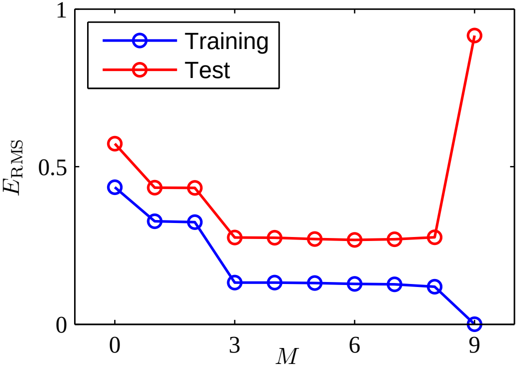

(C.M. Bishop, Pattern Recognition and Machine Learning)

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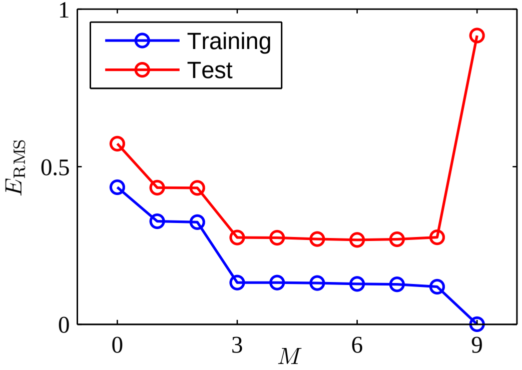


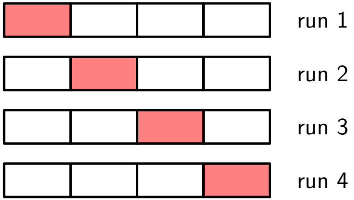
(C.M. Bishop, Pattern Recognition and Machine Learning)

- Intuition? Interpretation?

How do you compute the test error?

Cross validation:

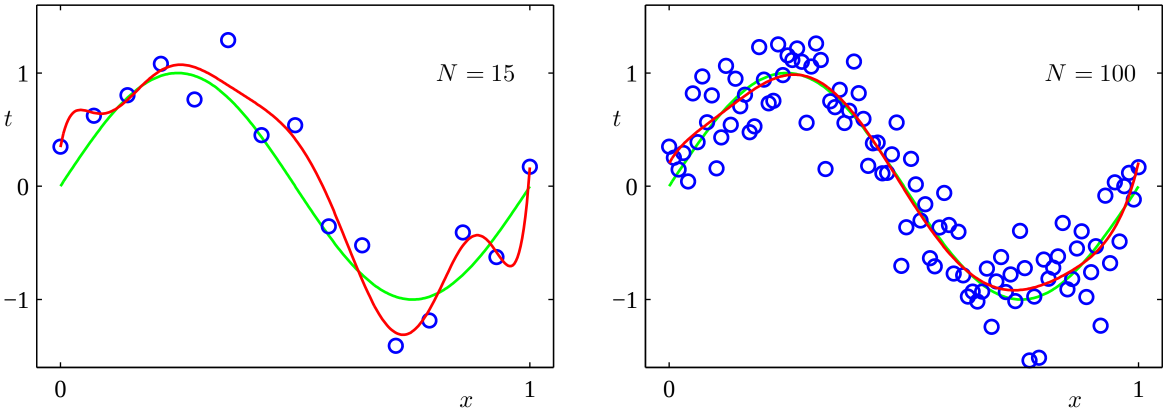
- randomly assign samples $(\mathbf{x}_n, y_n)$ to S sets of equal size
- for each set $s \in S$ (e.g. $S = 4$) and $m \in [1, \ldots, M]$:
  - train model on $S - 1$ remaining sets
  - predict on s and compute MSE or root MSE E_{RMS}.
- compute average MSE for degree m.
- pick m with lowest MSE.



(C.M. Bishop, Pattern Recognition and Machine Learning)

What else can you do to improve model, i.e. learn better weights, find better curve fit, and be less prone to overfitting?

Get more data



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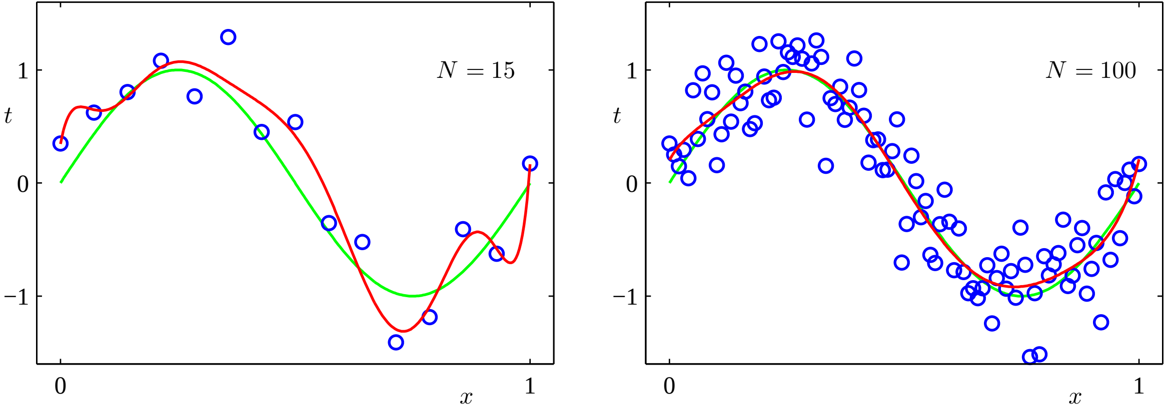
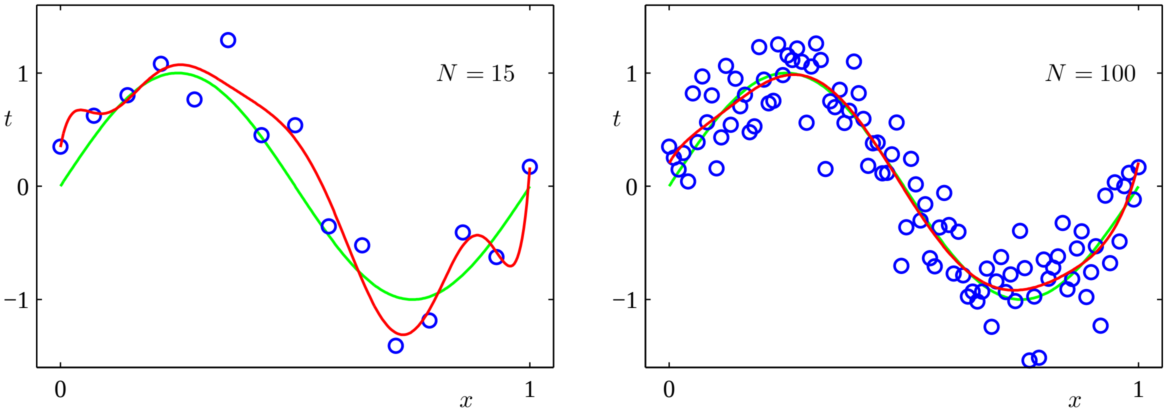


Others ways to avoid overfitting and fit complex model for limited number of observations?

Get more data



Others ways to avoid overfitting and fit complex model for limited number of observations?

Regularization of weights

Regularization

Regularize the regression weights $\boldsymbol{\beta}$.

Loss function: $$\mathrm{E}_2(\boldsymbol{\beta}) = \underbrace{\frac{1}{2}\sum_{n=1}^{N}(y_n - \mathbf{x}_n \cdot \boldsymbol{\beta})^2}_{\text{squared error}} + \underbrace{\frac{\lambda}{2}\sum_{d=1}^{D}\beta_d^2}_{l_2\text{-norm regularizer}}$$

where $||\boldsymbol{\beta}||^2 = \sqrt{\sum_{d=1}^{D}\beta_d^2}$ is the l_2-norm of $\boldsymbol{\beta}$.

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What effect does this have? How will the learned weights be different?

- Penalizes large weights.
- Reduces the complexity of the function that associates $\mathbf{x}$ with $\mathbf{y}$, i.e. learn parsimonious model.
- Also known as shrinkage methods.

Linear Regression
Regularization

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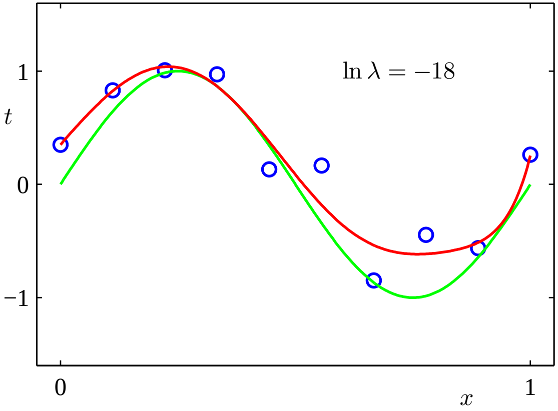

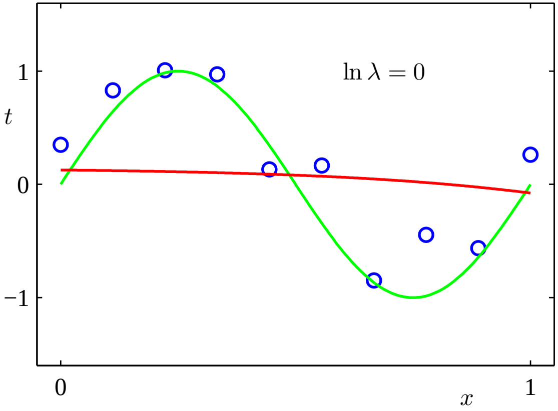

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Quiz: How to chose an optimal λ?

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Answer: Look at the test error!

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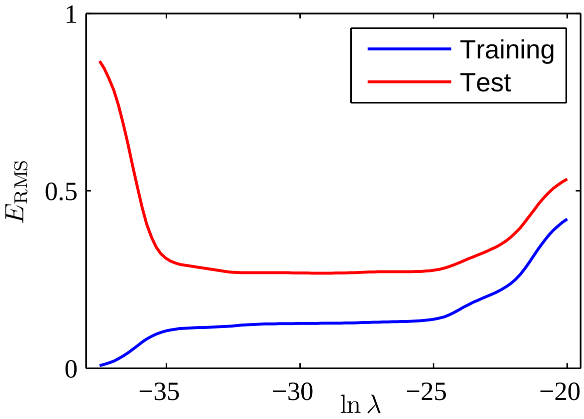

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Solving ridge regression

Minimize the loss function $\mathrm{E}_2(\boldsymbol{\beta}) = \underbrace{\frac{1}{2}\sum_{n=1}^{N}(y_n - \mathbf{x}_n \cdot \boldsymbol{\beta})^2}_{\text{squared error}} \quad + \quad \underbrace{\frac{\lambda}{2}\sum_{d=1}^{D}\beta_d^2}_{l_2\text{-norm regularizer}}$

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- Derivative w.r.t. a single weight entry β_i

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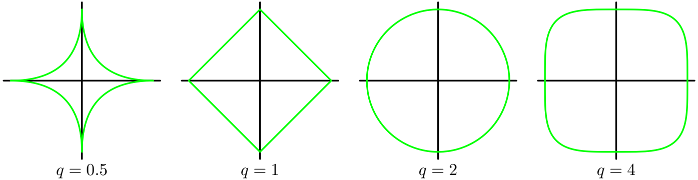
$$\Longrightarrow \boldsymbol{\beta}_{Ridge} = \left(\mathbf{X}^{\mathrm{T}}\mathbf{X} + \lambda\mathbf{I}\right)^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{y}$$

Regularization

A more general regularization:

$$\mathrm{E}_q(\boldsymbol{\beta}) = \underbrace{\frac{1}{2}\sum_{n=1}^{N}(y_n - \mathbf{x}_n \cdot \boldsymbol{\beta})^2}_{\text{squared error}} + \underbrace{\frac{\lambda}{2}\sum_{d=1}^{D}|\beta_d|^q}_{l_q\text{-norm regularizer}}$$



(C.M. Bishop, Pattern Recognition and Machine Learning)

Regularization

A more general regularization:

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- l_1: Lasso $\rightarrow$ feature selection, sparse solution
- l_2: Ridge $\rightarrow$ shrinks weights to 0
- Linear combination of l_1 and l_2: Elastic net

Summary

- Maximum likelihood in linear regression
- Polynomial linear regression
- Cross-classification
- Regularized regression with l_2-norm (ridge regression)

Questions?