CSCI567 Machine Learning (Spring 2018)

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Lecture on January 24, 2018

Outline

1. Review of Last Lecture
2. Nonlinear basis functions
3. Basic ideas of overcome overfitting
4. Bias/Variance Analysis
5. Maximum Likelihood Estimation

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Linear regression

Setup

- Input: $\boldsymbol{x} \in \mathbb{R}^{\mathsf{D}}$ (covariates, predictors, features, etc)
- Output: $y \in \mathbb{R}$ (responses, targets, outcomes, outputs, etc)
- Training data: $\mathcal{D} = \{(\boldsymbol{x}_n, y_n), n = 1, 2, \ldots, \mathsf{N}\}$
  We will use x_{nd} representing the dth dimension of the nth sample $\boldsymbol{x}_n$
- Model: $f : \boldsymbol{x} \to y$, with $f(\boldsymbol{x}) = w_0 + \sum_d w_d x_d = w_0 + \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}$, with ^{T} standing for vector transpose.

Finding the best model parameters by minimizing prediction errors

Design matrix and target vector

$$\boldsymbol{X} = \begin{pmatrix} \boldsymbol{x}_1^{\mathrm{T}} \\ \boldsymbol{x}_2^{\mathrm{T}} \\ \vdots \\ \boldsymbol{x}_{\mathsf{N}}^{\mathrm{T}} \end{pmatrix} \in \mathbb{R}^{\mathsf{N} \times D}, \quad \tilde{\boldsymbol{X}} = \begin{pmatrix} \mathbf{1} & \boldsymbol{X} \end{pmatrix} \in \mathbb{R}^{\mathsf{N} \times (D+1)}, \quad \boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{\mathsf{N}} \end{pmatrix}$$

Residual sum squares in matrix form

$$RSS(\tilde{\boldsymbol{w}}) = \left\{ \tilde{\boldsymbol{w}}^{\mathrm{T}} \tilde{\boldsymbol{X}}^{\mathrm{T}} \tilde{\boldsymbol{X}} \tilde{\boldsymbol{w}} - 2 \left(\tilde{\boldsymbol{X}}^{\mathrm{T}} \boldsymbol{y} \right)^{\mathrm{T}} \tilde{\boldsymbol{w}} \right\} + \text{const}$$

Optimal solution

Normal equation

$$\tilde{\boldsymbol{w}}^{LMS} = \left(\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}}\right)^{-1}\tilde{\boldsymbol{X}}^{\mathrm{T}}\boldsymbol{y}$$

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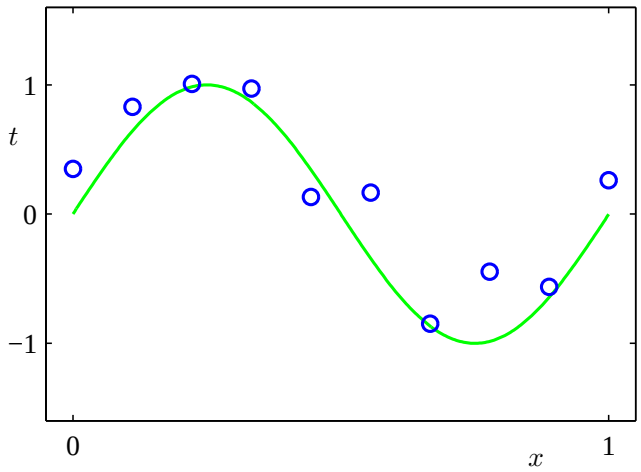
What if data does not fit to a line

Example of nonlinear regression



General nonlinear basis functions

We can use a nonlinear mapping

$$\boldsymbol{\phi}(\boldsymbol{x}) : \boldsymbol{x} \in \mathbb{R}^D \rightarrow \boldsymbol{z} \in \mathbb{R}^M$$

where M is the dimensionality of the new feature/input $\boldsymbol{z}$ (or $\boldsymbol{\phi}(\boldsymbol{x})$). Note that M could be either greater than D or less than or the same.

Note that $\boldsymbol{z}$ is a vector

$$z_1 = \phi_1(\boldsymbol{x}), z_2 = \phi_2(\boldsymbol{x}), \cdots, z_M = \phi_M(\boldsymbol{x})$$

Nonlinear regression thru nonlinearly transformed features

With the new features – we call them nonlinear basis functions – we can apply our learning techniques:

- linear methods: prediction is based on $\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x})$
- more broadly, other methods: nearest neighbors, decision trees, etc

to minimize our errors on the transformed training data

Regression with nonlinear basis

Residual sum squares

$$\sum_n [\boldsymbol{w}^{\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x}_n) - y_n]^2$$

where $\boldsymbol{w} \in \mathbb{R}^M$, the same dimensionality as the transformed features $\boldsymbol{\phi}(\boldsymbol{x})$.

Regression with nonlinear basis

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$$\sum_n [\boldsymbol{w}^{\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x}_n) - y_n]^2$$

where $\boldsymbol{w} \in \mathbb{R}^M$, the same dimensionality as the transformed features $\boldsymbol{\phi}(\boldsymbol{x})$.

The LMS solution can be formulated with the new design matrix

$$\boldsymbol{\Phi} = \begin{pmatrix} \boldsymbol{\phi}(\boldsymbol{x}_1)^{\mathrm{T}} \\ \boldsymbol{\phi}(\boldsymbol{x}_2)^{\mathrm{T}} \\ \vdots \\ \boldsymbol{\phi}(\boldsymbol{x}_N)^{\mathrm{T}} \end{pmatrix} \in \mathbb{R}^{N \times M}, \quad \boldsymbol{w}^{\mathrm{LMS}} = \left(\boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{\Phi}\right)^{-1} \boldsymbol{\Phi}^{\mathrm{T}} \boldsymbol{y}$$

Example with regression

Polynomial basis functions

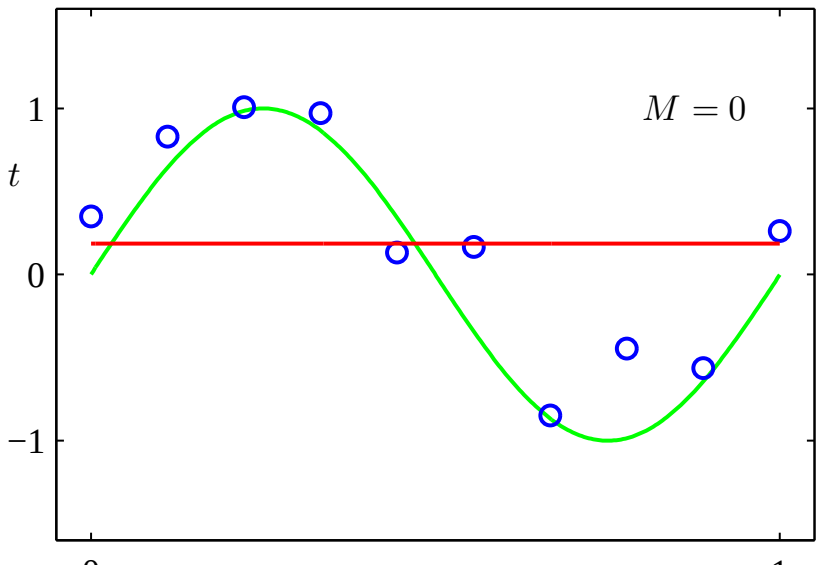
$$\boldsymbol{\phi}(x) = \begin{bmatrix} 1 \\ x \\ x^2 \\ \vdots \\ x^M \end{bmatrix} \Rightarrow f(x) = w_0 + \sum_{m=1}^{M} w_m x^m$$

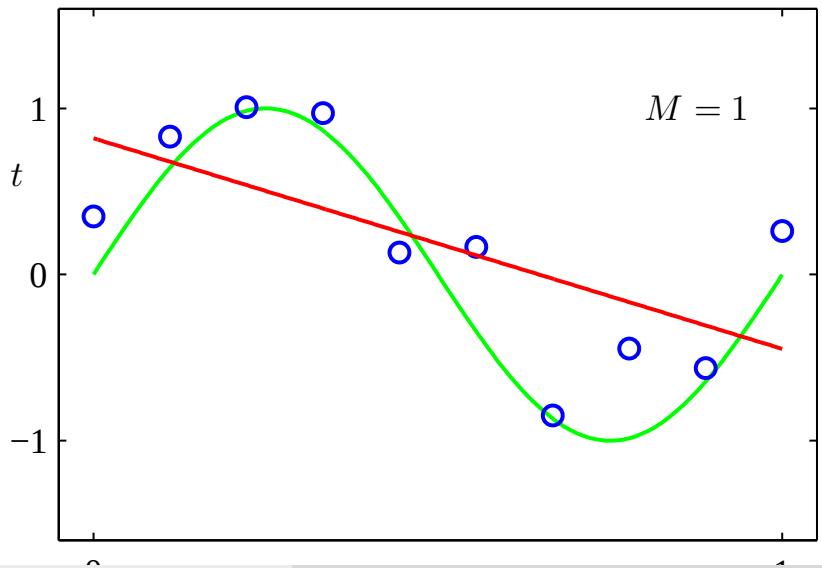
Example with regression

Polynomial basis functions

$$\boldsymbol{\phi}(x) = \begin{bmatrix} 1 \\ x \\ x^2 \\ \vdots \\ x^M \end{bmatrix} \Rightarrow f(x) = w_0 + \sum_{m=1}^{M} w_m x^m$$

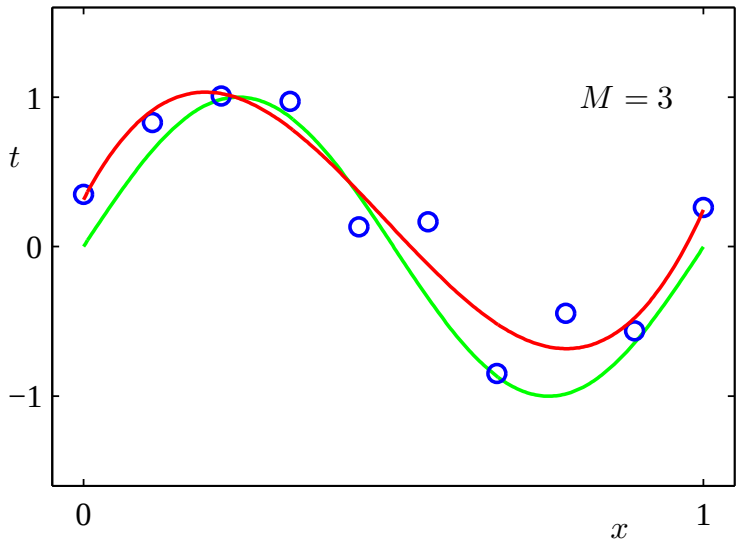
Fitting samples from a sine function: *underrfitting* as $f(x)$ is too simple





Adding more high-order basis

M=3



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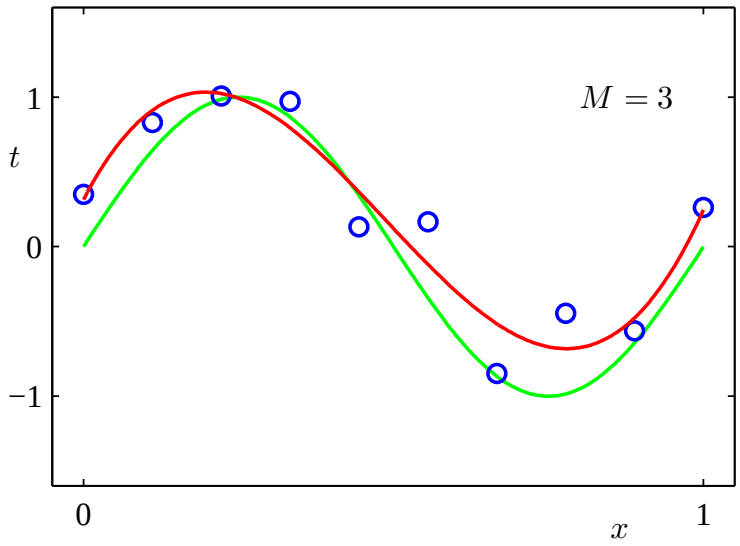
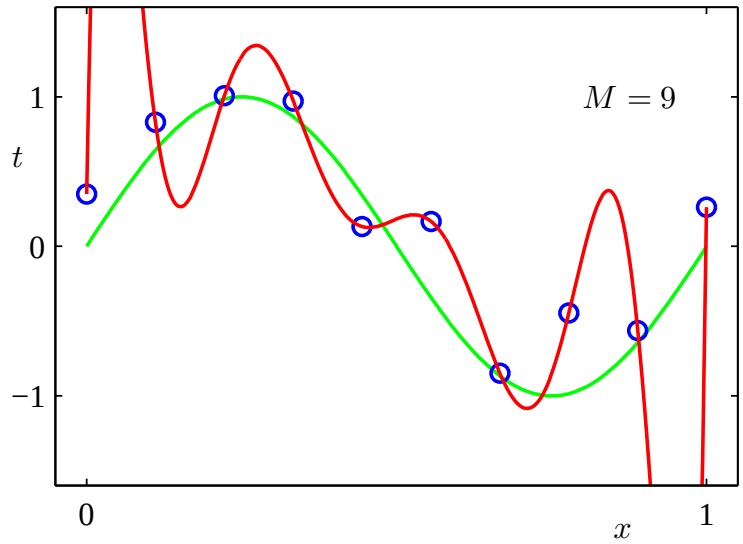


M=9: *overfitting*



Being too adaptive leads *better* results on the training data, but *not so great* on data that has not been seen!

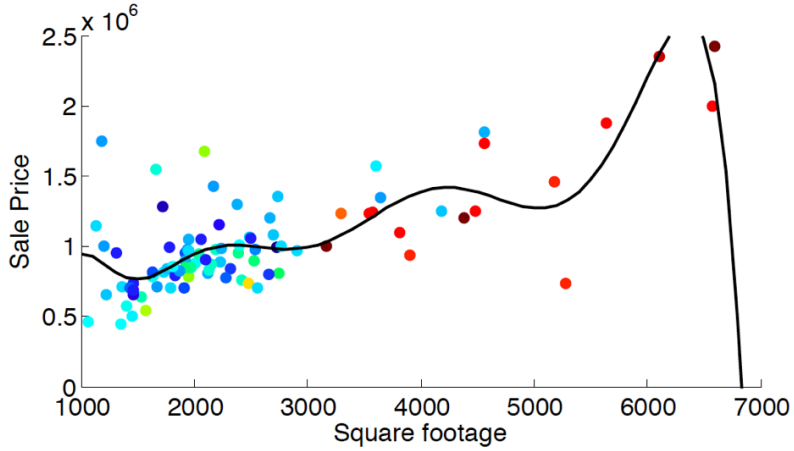
Overfiting

Parameters for higher-order polynomials are very large

	$M=0$	$M=1$	$M=3$	$M=9$
w_0	0.19	0.82	0.31	0.35
w_1		-1.27	7.99	232.37
w_2			-25.43	-5321.83
w_3			17.37	48568.31
w_4				-231639.30
w_5				640042.26
w_6				-1061800.52
w_7				1042400.18
w_8				-557682.99
w_9				125201.43

Overfitting can be quite disastrous

Fitting the housing price data with $M = 3$

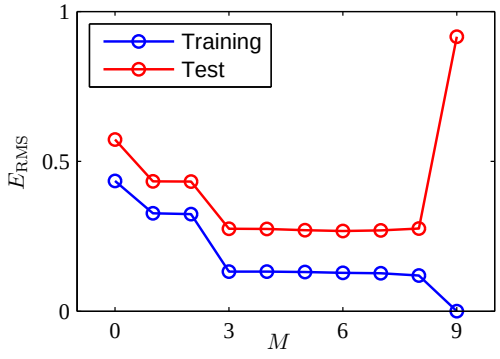


Note that the price would goes to zero (or negative) if you buy bigger ones!
This is called poor generalization/overfitting.

Detecting overfitting

Plot model complexity versus objective function

As model becomes more complex, performance on training keeps improving while on test data improve first and deteriorate later.



- Horizontal axis: *measure of model complexity*
  In this example, we use the maximum order of the polynomial basis functions.

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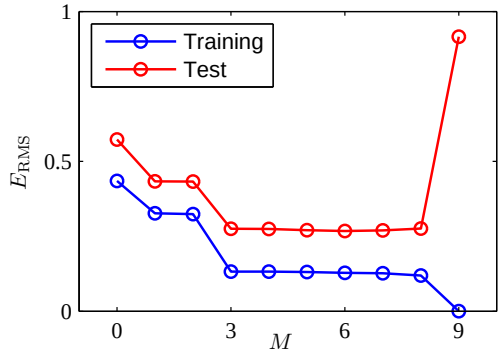

- Horizontal axis: *measure of model complexity*
  In this example, we use the maximum order of the polynomial basis functions.
- Vertical axis:
  1. For regression, the vertical axis would be RSS or RMS (squared root of RSS)
  2. For classification, the vertical axis would be classification error rate or cross-entropy error function (more on the latter later)

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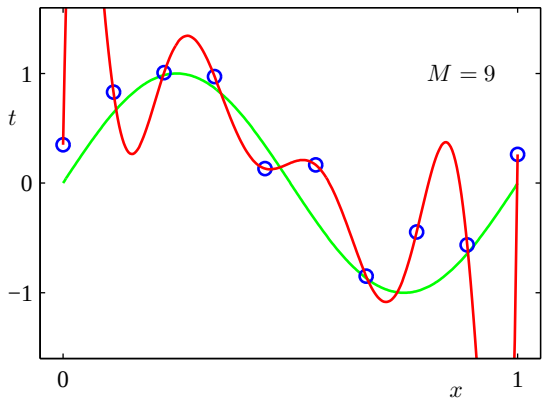
3 Basic ideas of overcome overfitting
- Use more training data
- Regularization methods
- Cross-validation

4 Bias/Variance Analysis

5 Maximum Likelihood Estimation

Use more training data to prevent over fitting

The more, the merrier



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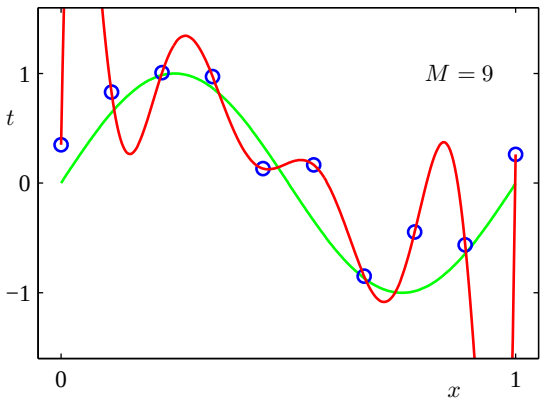

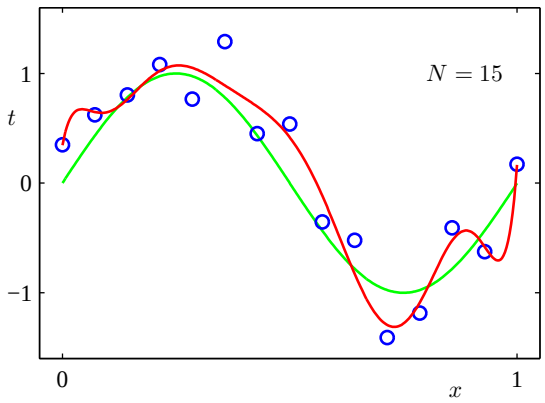

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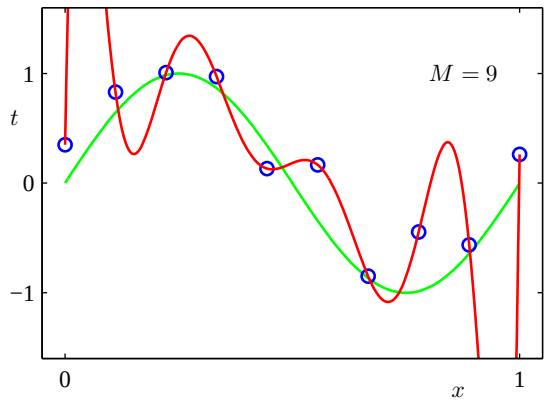

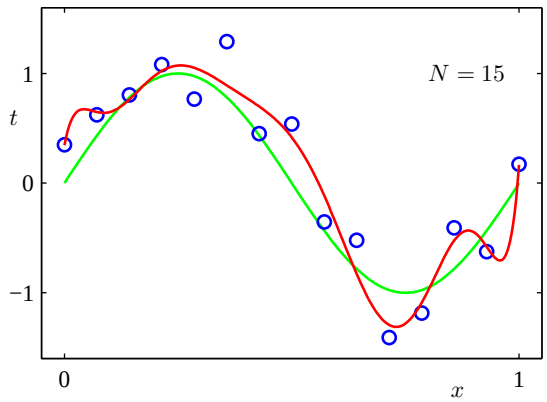

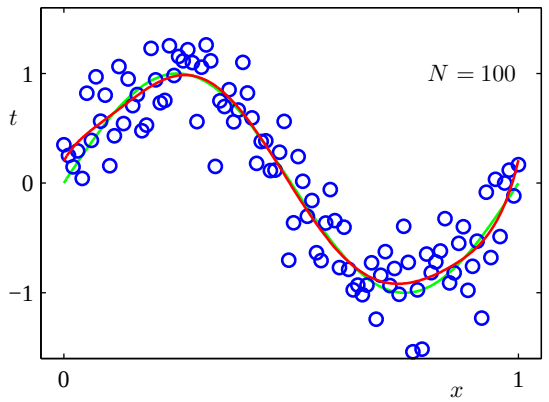

What if we do not have a lot of data?

What is a simple model?

For a linear model for regression

$$\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$$

what do we mean by *being simple*?

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For a linear model for regression

$$\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$$

what do we mean by *being simple*?

Intuition

- $w_1x_1 + w_2x_2$ is more complex than either w_1x_1 or w_2x_2.
- The smaller the w_i, the simpler the model is
- The simplest model probably has a lot of $w_i = 0$ or w_i is being small.

Example: fitting data with polynomials

Our regression model

$$y = \sum_{m=1}^{M} w_m x^m$$

Thus, smaller w_m will likely lead to a smaller order of polynomial, thus potentially preventing overfitting.

How to make $\boldsymbol{w}$ small?

Regularized linear regression: a new error to minimize

$$\min \mathcal{E}(\boldsymbol{w}) = \min \sum_n (\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n - y_n)^2 + \lambda \|\boldsymbol{w}\|_2^2$$

where $\lambda > 0$. This extra term $\|\boldsymbol{w}\|_2^2$ is called regularization/regularizer and controls the model complexity.

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- If $\lambda \to +\infty$, then $\boldsymbol{w}$ approaches $\mathbf{0}$.

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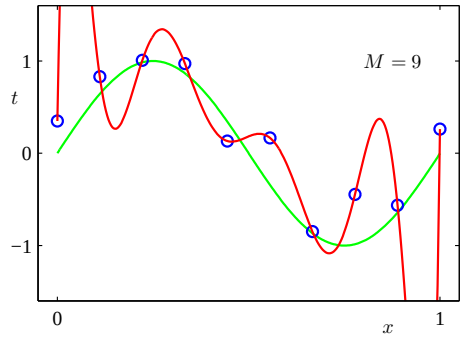
Intuition

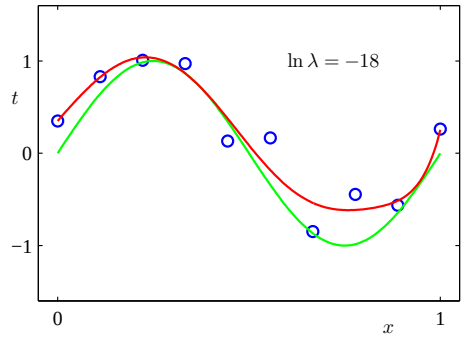
- If $\lambda \to +\infty$, then $\boldsymbol{w}$ approaches $\mathbf{0}$.
- If $\lambda \to 0$, then we approach the standard LMS solution

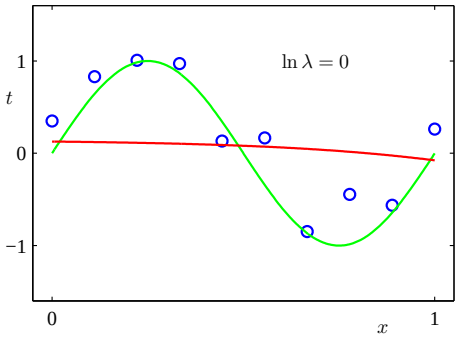
$$\arg\min \sum_n (\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n - y_n)^2$$

Overfitting in terms of λ

Overfitting is reduced from complex model to simpler one with the help of increasing regularizers







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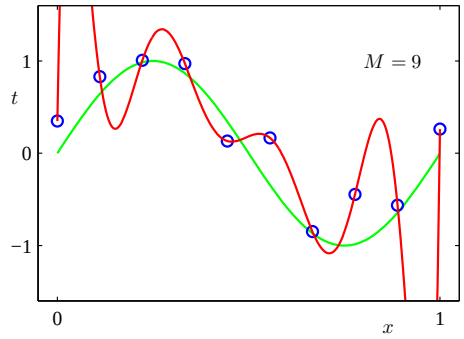
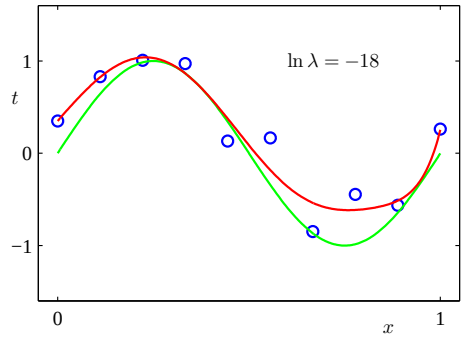
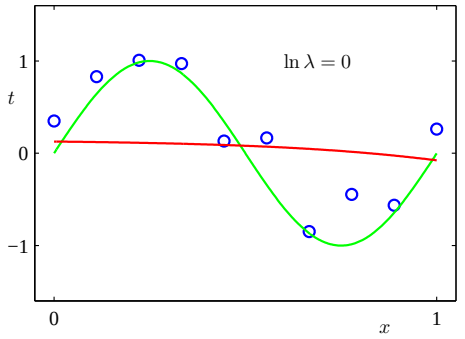
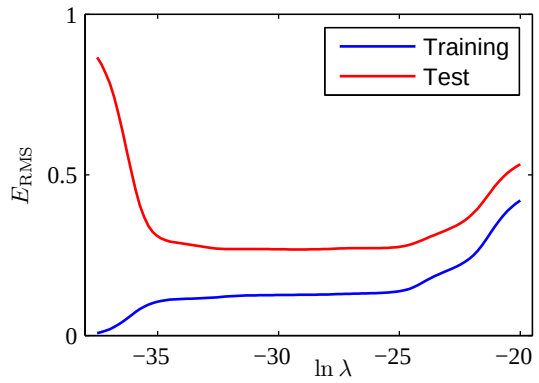






λ **vs. residual error** shows the difference of the model performance on training and testing dataset



Closed-form solution

For regularized linear regression (RLS): the solution changes very little (in form) from the LMS solution

$$\arg\min \sum_n (\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n - y_n)^2 + \lambda \|\boldsymbol{w}\|_2^2 \Rightarrow \boldsymbol{w}^{\mathrm{RLS}} = \left(\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X} + \lambda \boldsymbol{I}\right)^{-1} \boldsymbol{X}^{\mathrm{T}}\boldsymbol{y}$$

and reduces to the LMS solution when $\lambda = 0$, as expected.

Note that this form is the same as the proposed solution when the matrix $\boldsymbol{X}^T\boldsymbol{X}$ is not invertible

The effect of λ

Large λ attenuating parameters towards 0

	$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
w_0	0.35	0.35	0.13
w_1	232.37	4.74	-0.05
w_2	-5321.83	-0.77	-0.06
w_3	48568.31	-31.97	-0.06
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w_8	-557682.99	-91.53	0.00
w_9	125201.43	72.68	0.01

How to choose the right amount of regularization?

Can we tune λ on the training dataset?

No: as this will set λ to zero, i.e., without regularization, defeating our intention to use it to control model complexity and to gain better generalization.

λ is thus a hyperparmeter. To tune it,

- We can use a development/holdout dataset independent of training and testing dataset.
- We can do leave-one-out (LOO)

The procedure is similar to choose K in the nearest neighbor classifiers.

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For different λ, we get $\boldsymbol{w}^{\mathrm{RLS}}$ and evaluate the model on the development/holdout dataset (or, the samples being left in LOO).

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For different λ, we get $\boldsymbol{w}^{\mathrm{RLS}}$ and evaluate the model on the development/holdout dataset (or, the samples being left in LOO).

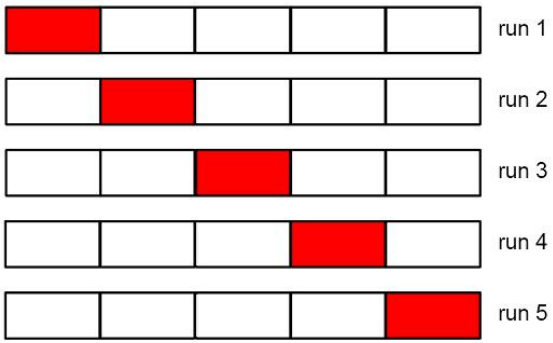
We then plot the curve λ versus prediction error (accuracy, classification error) and find the place that the performance on the holdout/LOO is the best.

Use cross-validation to choose λ

Procedure

- Randomly partition training data into K *disjoint* parts
  Normally, K is chosen to be 10, 5, etc.
- For each possible value of λ
  1. Use one part as holdout; use other $(K-1)$ parts as training
  2. Evaluate the model on the holdout
  3. Do this K times, and average the performance on the holdouts
- Choose the λ with the best performance

When $K = N$ (the number of training examples), this becomes LOO.



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Basic and important machine learning concepts

Supervised learning

We aim to build a function $f(\boldsymbol{x})$ to predict the true value y associated with $\boldsymbol{x}$. If we make a mistake, we incur a *loss*

$$L(f(\boldsymbol{x}), y)$$

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Supervised learning

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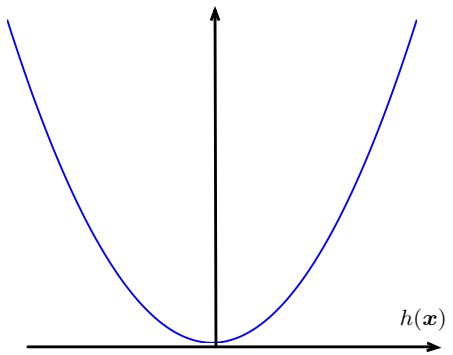
Example: quadratic loss function for regression when y is continuous

$$L(f(\boldsymbol{x}), y) = [f(\boldsymbol{x}) - y]^2$$

Ex: when $y = 0$

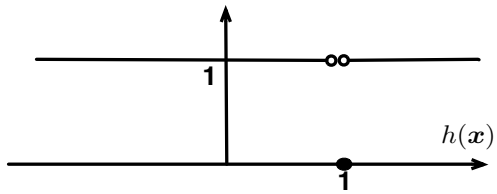


Other types of loss functions

For classification: $0/1$ loss

$$L(f(\boldsymbol{x}), y) = \mathbb{I}[f(\boldsymbol{x}) \neq y]$$

Ex: when $y = 1$



Measure how good our predictor is

Risk: assume we know the true distribution of data $p(\boldsymbol{x}, y)$, the *risk* is

$$R[f(\boldsymbol{x})] = \int L(f(\boldsymbol{x}), y) p(\boldsymbol{x}, y) d\boldsymbol{x} d\, y$$

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However, we cannot compute $R[f(\boldsymbol{x})]$, so we use *empirical risk*, given a training dataset $\mathcal{D}$

$$R^{\text{EMP}}[f(\boldsymbol{x})] = \frac{1}{N} \sum_n L(f(\boldsymbol{x}_n), y_n)$$

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$$R^{\text{EMP}}[f(\boldsymbol{x})] = \frac{1}{N} \sum_n L(f(\boldsymbol{x}_n), y_n)$$

Intuitively, as $N \to +\infty$,

$$R^{\text{EMP}}[f(\boldsymbol{x})] \to R[f(\boldsymbol{x})]$$

How this relates to what we have learned?

So far, we have been doing empirical risk minimization (ERM)

- For linear regression, $f(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$, and we use squared loss, which leads to *residual sum squares*

How this relates to what we have learned?

So far, we have been doing empirical risk minimization (ERM)

- For linear regression, $f(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$, and we use squared loss, which leads to *residual sum squares*

ERM might be problematic

- If $f(\boldsymbol{x})$ is complicated enough,

$$R^{\mathrm{EMP}}[f(\boldsymbol{x})] \to 0$$

- But then $f(\boldsymbol{x})$ is unlikely to do well in predicting things out of the training dataset $\mathcal{D}$
  This is called *poor generalization* or *overfitting*. We have seen how to fix that problem.

The root of overfitting

Intuition

- Given a specific dataset $\mathcal{D}$, the learned function $f_{\mathcal{D}}(x)$ has two types of errors
  - $f_{\mathcal{D}}(x)$ fluctuates around the best possible $f(x)$ if $\mathcal{D}$ is infinitely large. This error is called *variance*
  - $f_{\mathcal{D}}(x)$ or $f(x)$ is a specific type of function (eg. linear), thus, it might not be able to model complex relations. This error is called *bias*
- The total error is the *sum of variance and bias*
- Simpler models (functions $f(x)$) has a smaller variance but a larger bias
- Complex models (functions $f(x)$) has a larger variance but a smaller bias

Thus, one needs to balance bias and variance.

Regularized models reduces variance (because they lead to simpler models) but then increase the bias.

Summary

- We can extend linear regression to nonlinear regression by using nonlinear basis functions to compose features.
- However, *we have never suggested how to choose the right nonlinear basis functions to use*
- Furthermore, with complex nonlinear basis functions, we increase the risk of *overfitting*
- Overfitting leads to poor generalization error, which means we have a bad tradeoff between variance and bias.

Outline

1. Review of Last Lecture
2. Nonlinear basis functions
3. Basic ideas of overcome overfitting
4. Bias/Variance Analysis
5. Maximum Likelihood Estimation
   - Maximum Likelihood Estimation
   - Optimization
   - Multivariate Optimization

Maximum Likelihood Estimation

- Example: Coin Toss
  - You observe me throwing a coin five times.
  - You count three heads, two tails.
  - What is the chance of a heads for next flip?

Maximum Likelihood Estimation

- Example: Coin Toss
  - You observe me throwing a coin five times.
  - You count three heads, two tails.
  - What is the chance of a heads for next flip?
- Model
  - Each toss is a Bernoulli Random Variable X
  - X can take two values: 1 (head) or 0 (tail)
  - $p(X = 1) = \theta$
    (θ is a parameter to be learned from the data)

Principles of MLE

Observation: $X_1 = 1$ $X_2 = 0$ $X_3 = 1$ $X_4 = 1$ $X_5 = 0$

Likelihood: θ $1 - \theta$ θ θ $1 - \theta$

$$\mathcal{L} = \theta^3 \cdot (1 - \theta)^2$$

Maximizing the Likelihood

$$\mathcal{L} = \theta^3 \cdot (1-\theta)^2 \rightarrow \theta^{\mathsf{MLE}} = \frac{3}{3+2}$$

More generally

- We have a model
  $X \sim P(X; \theta)$
- We have training data (observations)
  $\mathcal{D} = \{x_1, x_2, \ldots x_N\}$
- Maximum likelihood estimate

$$\mathcal{L}(\mathcal{D}) = \prod_{i=1}^{N} P(x_i; \theta)$$

$$\begin{aligned} \theta^{\mathsf{MLE}} &= \arg\max_\theta \mathcal{L}(\mathcal{D}) \\ &= \arg\max_\theta \sum_{i=1}^{N} \log P(x_i; \theta) \end{aligned}$$

Example

- We have a model

$$p(x) = \frac{1}{\sqrt{2\pi}\ \sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

- We have training data (observations)

$$\mathcal{D} = \{x_1, x_2, \ldots x_N\}$$

- Maximum likelihood estimate

$$\ell(\mu, \sigma) = \sum_{n=1}^{N} \left\{ -\frac{(x_n - \mu)^2}{2\sigma^2} - \log \sqrt{2\pi}\sigma \right\}$$

Solution

- We will solve the following later:

$$\arg\max_{\mu,\sigma} \ell(\mu, \sigma) = \sum_{n=1}^{N} \left\{ -\frac{(x_n - \mu)^2}{2\sigma^2} - \log \sqrt{2\pi}\sigma \right\}$$

- But the solution is:

$$\mu = \overline{x} = \frac{1}{N} \sum_{n=1}^{N} x_n \qquad \sigma^2 = \frac{1}{N} \sum_{n=1}^{N} (x_n - \overline{x})^2$$

Remember MLE for coin tosses?

- The objective function is:

$$\mathcal{L}(\theta) = \theta^3 \cdot (1-\theta)^2$$

- The gradient is:

$$\mathcal{L}'(\theta) = 3\theta^2(1-\theta)^2 - 2\theta^3(1-\theta)$$

- We set gradient to zero:

$$\mathcal{L}'(\theta) = 0 \rightarrow \theta = \frac{3}{3+2}$$

- Log-likelihood for Gaussian distribution

$$\arg\max_{\mu,\sigma} \ell(\mu, \sigma) = \sum_{n=1}^{N} \left\{ -\frac{(x_n - \mu)^2}{2\sigma^2} - \log \sqrt{2\pi}\sigma \right\}$$

- Partial derivatives

$$\frac{\partial \ell}{\partial \mu} = \sum_{n}^{N} -\frac{2(x_n - \mu)}{2\sigma^2}$$

$$\frac{\partial \ell}{\partial \sigma} = \sum_{n}^{N} \left\{ \frac{(x_n - \mu)^2}{\sigma^3} - \frac{1}{\sigma} \right\}$$

Stationary Points

$$\frac{\partial \ell}{\partial \mu} = 0 \rightarrow \mu = \frac{1}{N} \sum_n x_n$$

$$\frac{\partial \ell}{\partial \sigma} = 0 \rightarrow \sigma^2 = \frac{1}{N} \sum_n (x_n - \mu)^2$$