CSCI567 Machine Learning (Spring 2021)

Sirisha Rambhatla

University of Southern California

Jan 27, 2021

Outline

1. Logistics
2. Review of Last Lecture
3. Linear regression with nonlinear basis
4. Overfitting and preventing overfitting

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Logistics

- The schedule of lectures is available at `https://sirisharambhatla.com/CSCI567/index.html`

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Regression

Predicting a continuous outcome variable using past observations

- temperature, amount of rainfall, house price, etc.

Key difference from classification

- continuous vs discrete
- measure *prediction errors* differently.
- lead to quite different learning algorithms.

Linear Regression: regression with linear models: $f(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$

Least square solution

$$\begin{aligned}\boldsymbol{w}^* &= \underset{\boldsymbol{w}}{\operatorname{argmin}} \operatorname{RSS}(\boldsymbol{w}) \\ &= \underset{\boldsymbol{w}}{\operatorname{argmin}} \|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|_2^2 \\ &= \left(\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}\right)^{-1}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{y}\end{aligned}$$

$$\boldsymbol{X} = \begin{pmatrix} \boldsymbol{x}_1^{\mathrm{T}} \\ \boldsymbol{x}_2^{\mathrm{T}} \\ \vdots \\ \boldsymbol{x}_{\mathsf{N}}^{\mathrm{T}} \end{pmatrix}, \quad \boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{\mathsf{N}} \end{pmatrix}$$

Two approaches to find the minimum:

- find **stationary points** by setting gradient $= \mathbf{0}$
- "**complete the square**"

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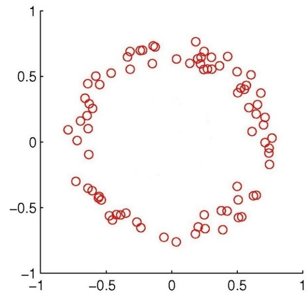
What if linear model is not a good fit?

Example: a straight line is a bad fit for the following data



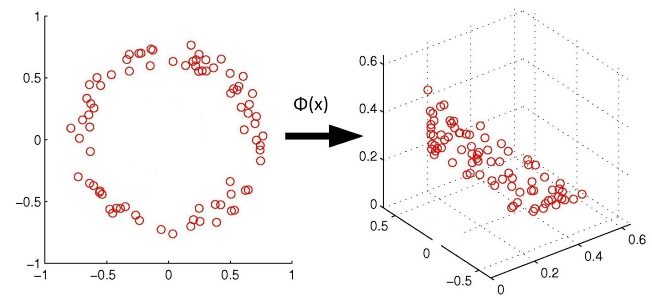
Solution: nonlinearly transformed features

1. Use a nonlinear mapping

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

to transform the data to a more complicated feature space

2. Then apply linear regression (hope: linear model is a better fit for the new feature space).



Regression with nonlinear basis

Model: $f(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x})$ where $\boldsymbol{w} \in \mathbb{R}^M$

Objective:

$$\mathrm{RSS}(\boldsymbol{w}) = \sum_n \left(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) - y_n\right)^2$$

Similar least square solution:

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

Example

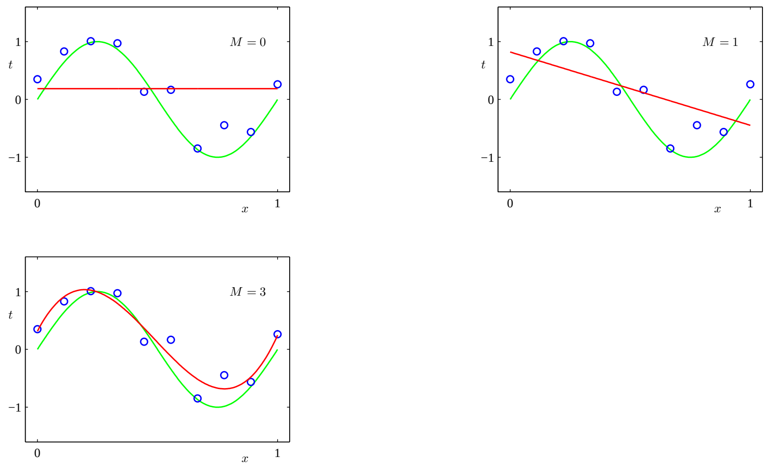
Polynomial basis functions for $\mathrm{D} = 1$

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

Learning a linear model in the new space
= learning an *M-degree polynomial model* in the original space

Example

Fitting a noisy sine function with a polynomial ($M = 0, 1,$ or 3):



Why nonlinear?

Can I use a fancy **linear feature map**?

$$\boldsymbol{\phi}(\boldsymbol{x}) = \begin{bmatrix} x_1 - x_2 \\ 3x_4 - x_3 \\ 2x_1 + x_4 + x_5 \\ \vdots \end{bmatrix} = \boldsymbol{A}\boldsymbol{x} \quad \text{for some } \boldsymbol{A} \in \mathbb{R}^{\mathsf{M}\times\mathsf{D}}$$

No, it basically *does nothing* since

$$\min_{\boldsymbol{w}\in\mathbb{R}^{\mathsf{M}}} \sum_n \left(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{A}\boldsymbol{x}_n - y_n\right)^2 = \min_{\boldsymbol{w}'\in\mathsf{Im}(\boldsymbol{A}^{\mathrm{T}})\subset\mathbb{R}^{\mathsf{D}}} \sum_n \left(\boldsymbol{w}'^{\mathrm{T}}\boldsymbol{x}_n - y_n\right)^2$$

We will see more nonlinear mappings soon.

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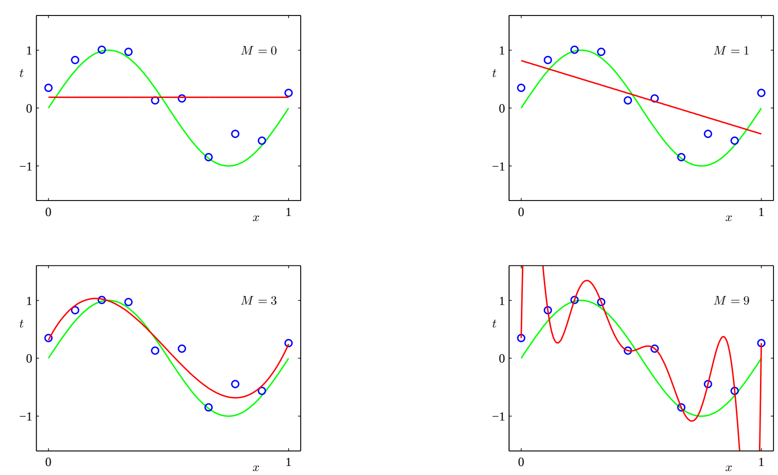
Should we use a very complicated mapping?

Ex: fitting a noisy sine function with a polynomial:



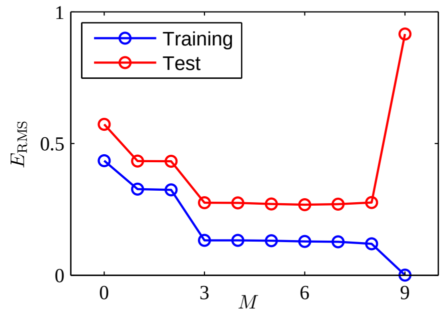
Underfitting and Overfitting

$M \leq 2$ is *underfitting* the data

- large training error
- large test error

$M \geq 9$ is *overfitting* the data

- small training error
- **large test error**

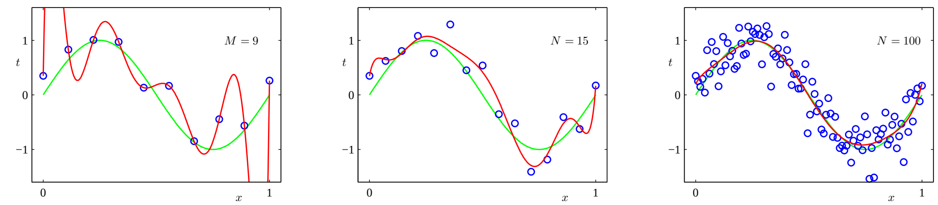


More complicated models $\Rightarrow$ larger gap between training and test error

How to prevent overfitting?

Method 1: use more training data

The more, the merrier



More data $\Rightarrow$ smaller gap between training and test error

Method 2: control the model complexity

For polynomial basis, the **degree** M clearly controls the complexity

- use cross-validation to pick hyper-parameter M

When M or in general Φ is fixed, are there still other ways to control complexity?

Magnitude of weights

Least square solution for the polynomial example:

	$M = 0$	$M = 1$	$M = 3$	$M = 9$
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

Intuitively, **large weights $\Rightarrow$ more complex model**

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

Regularized linear regression: new objective

$$\mathcal{E}(\boldsymbol{w}) = \mathrm{RSS}(\boldsymbol{w}) + \lambda R(\boldsymbol{w})$$

Goal: find $\boldsymbol{w}^* = \mathrm{argmin}_w \, \mathcal{E}(\boldsymbol{w})$

- $R : \mathbb{R}^{\mathsf{D}} \to \mathbb{R}^+$ is the *regularizer*
  - measure how complex the model $\boldsymbol{w}$ is
  - common choices: $\|\boldsymbol{w}\|_2^2$, $\|\boldsymbol{w}\|_1$, etc.
- $\lambda > 0$ is the *regularization coefficient*
  - $\lambda = 0$, no regularization
  - $\lambda \to +\infty$, $\boldsymbol{w} \to \mathrm{argmin}_w \, R(\boldsymbol{w})$
  - i.e. control **trade-off** between training error and complexity

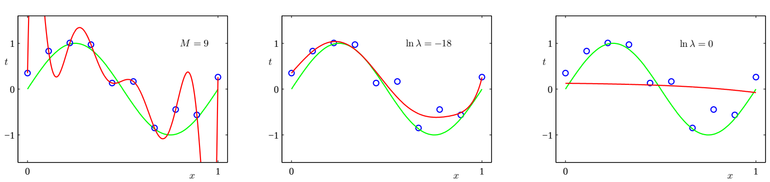
The effect of λ

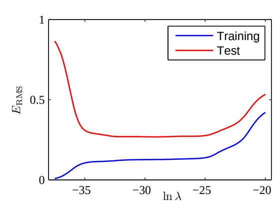
when we increase regularization coefficient λ

	$\ln\lambda = -\infty$	$\ln\lambda = -18$	$\ln\lambda = 0$
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
w_4	-231639.30	-3.89	-0.03
w_5	640042.26	55.28	-0.02
w_6	-1061800.52	41.32	-0.01
w_7	1042400.18	-45.95	-0.00
w_8	-557682.99	-91.53	0.00
w_9	125201.43	72.68	0.01

The trade-off

when we increase regularization coefficient λ





How to solve the new objective?

Simple for $R(\boldsymbol{w}) = \|\boldsymbol{w}\|_2^2$:

$$\mathcal{E}(\boldsymbol{w}) = \mathrm{RSS}(\boldsymbol{w}) + \lambda\|\boldsymbol{w}\|_2^2 = \|\boldsymbol{\Phi w} - \boldsymbol{y}\|_2^2 + \lambda\|\boldsymbol{w}\|_2^2$$

$$\nabla\mathcal{E}(\boldsymbol{w}) = 2(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi w} - \boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{y}) + 2\lambda\boldsymbol{w} = 0$$
$$\Rightarrow \left(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi} + \lambda\boldsymbol{I}\right)\boldsymbol{w} = \boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{y}$$
$$\Rightarrow \boldsymbol{w}^* = \left(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi} + \lambda\boldsymbol{I}\right)^{-1}\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{y}$$

Note the same form as in the fix when $\boldsymbol{X}^T\boldsymbol{X}$ is not invertible!

For other regularizers, as long as it's **convex**, standard optimization algorithms can be applied.

Equivalent form

Regularization is also sometimes formulated as

$$\underset{\boldsymbol{w}}{\operatorname{argmin}} \operatorname{RSS}(w) \quad \textbf{subject to } R(\boldsymbol{w}) \leq \beta$$

where β is some hyper-parameter.

Finding the solution becomes a *constrained optimization problem*.

Choosing either λ or β can be done by cross-validation.

Summary

$$\boldsymbol{w}^* = \left(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi} + \lambda \boldsymbol{I}\right)^{-1} \boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{y}$$

Important to understand the derivation than remembering the formula

Overfitting: small training error but large test error

Preventing Overfitting: more data + regularization

Recall the question

Typical steps of developing a machine learning system:

- Collect data, split into training, development, and test sets.
- *Train a model with a machine learning algorithm.* Most often we apply cross-validation to tune hyper-parameters.
- Evaluate using the test data and report performance.
- Use the model to predict future/make decisions.

How to do the *red part* exactly?

General idea to derive ML algorithms

1. Pick a set of **models** $\mathcal{F}$
   - e.g. $\mathcal{F} = \{f(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} \mid \boldsymbol{w} \in \mathbb{R}^{\mathsf{D}}\}$
   - e.g. $\mathcal{F} = \{f(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{\Phi}(\boldsymbol{x}) \mid \boldsymbol{w} \in \mathbb{R}^{\mathsf{M}}\}$
2. Define **error/loss** $L(y', y)$
3. Find **empirical risk minimizer (ERM)**:

$$\boldsymbol{f}^* = \underset{f \in \mathcal{F}}{\operatorname{argmin}} \sum_{n=1}^{N} L(f(x_n), y_n)$$

or **regularized empirical risk minimizer**:

$$\boldsymbol{f}^* = \underset{f \in \mathcal{F}}{\operatorname{argmin}} \sum_{n=1}^{N} L(f(x_n), y_n) + \lambda R(f)$$

ML becomes optimization