CSCI567 Machine Learning (Spring 2021)

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Outline

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Logistics

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

Outline

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

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

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

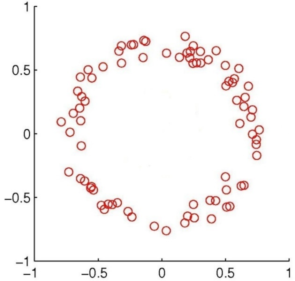
Two approaches to find the minimum:

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

Outline

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

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

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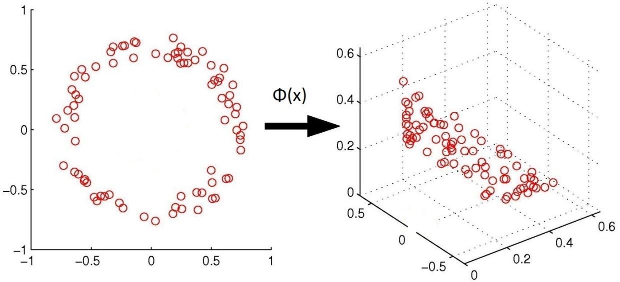

Regression with nonlinear basis

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

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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 $\mathsf{D} = 1$

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

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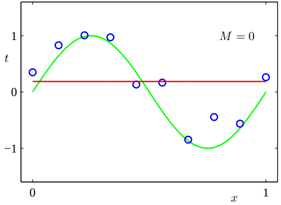
Learning a linear model in the new space
= learning an *M-degree polynomial model* in the original space

Example

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



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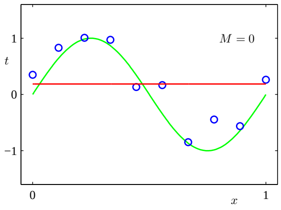

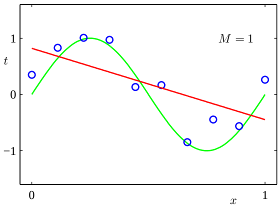

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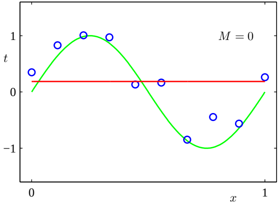

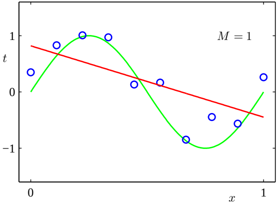

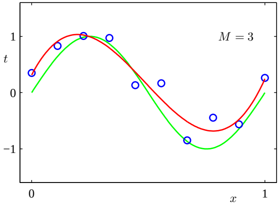

Why nonlinear?

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

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

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We will see more nonlinear mappings soon.

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Should we use a very complicated mapping?

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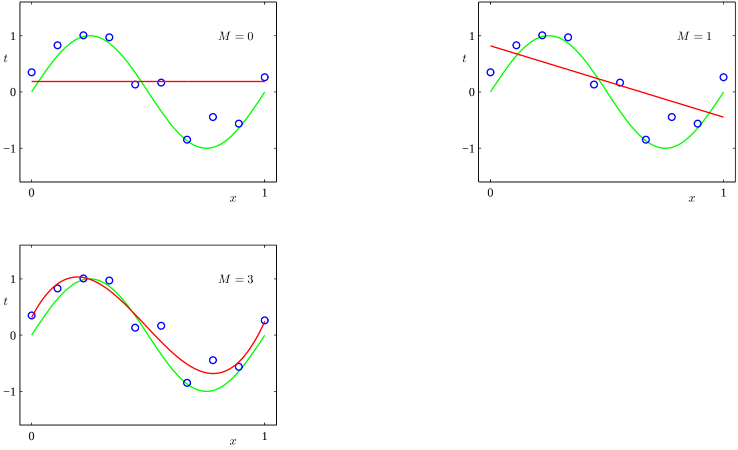

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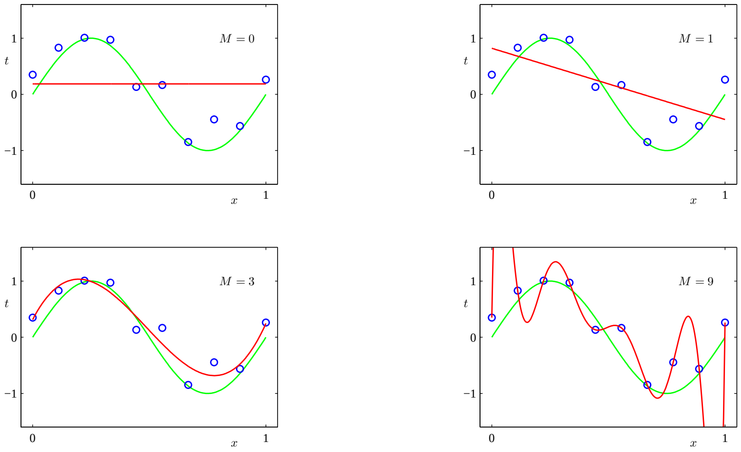

Underfitting and Overfitting

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

- large training error
- large test error

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

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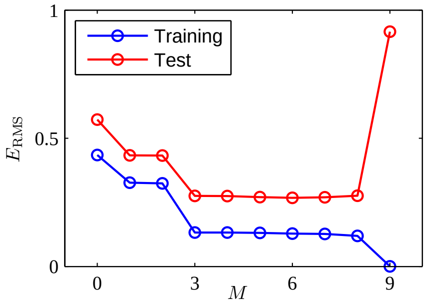

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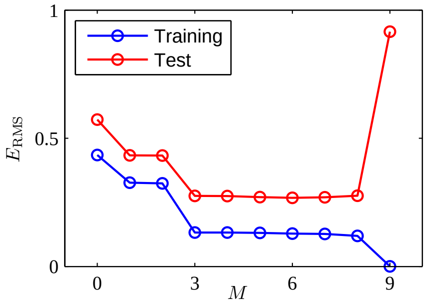

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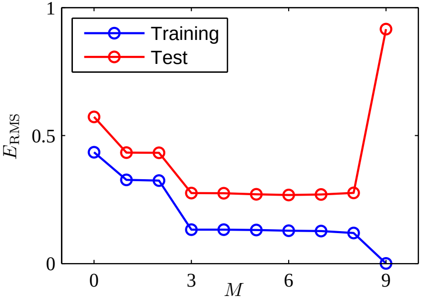

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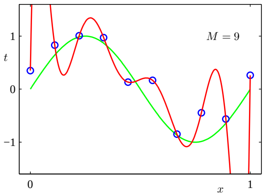
How to prevent overfitting?

Method 1: use more training data

The more, the merrier



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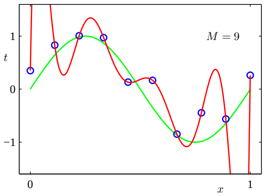

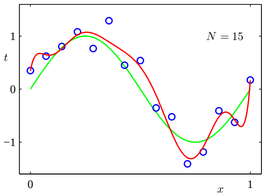

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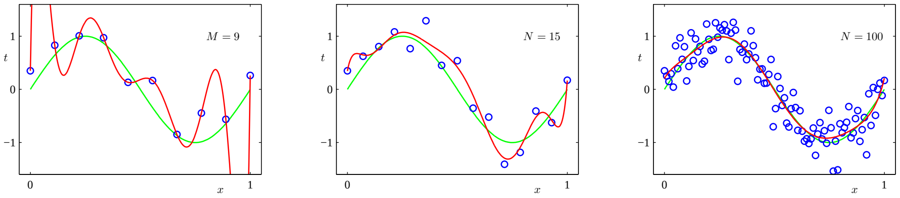

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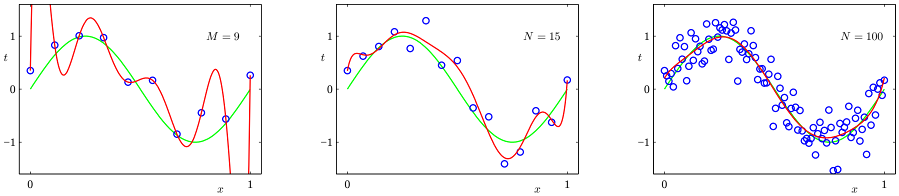

More data ⇒ smaller gap between training and test error

Method 2: control the model complexity

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

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- $R : \mathbb{R}^{\mathsf{D}} \to \mathbb{R}^+$ is the *regularizer*
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  - 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
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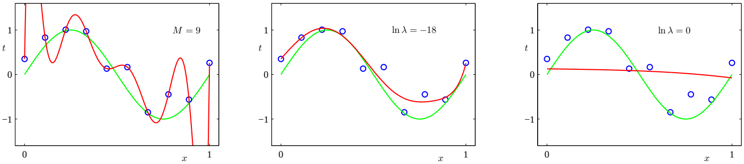

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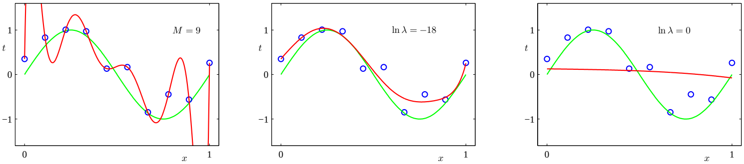

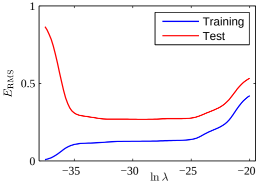

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For other regularizers, as long as it's **convex**, standard optimization algorithms can be applied.

Equivalent form

Regularization is also sometimes formulated as

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

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

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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. $\mathcal{F} = \{f(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} \mid \boldsymbol{w} \in \mathbb{R}^{\mathsf{D}}\}$
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3. Find **empirical risk minimizer (ERM)**:

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

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   - 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)**:

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

or **regularized empirical risk minimizer**:

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

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ML becomes optimization