CSCI567 Machine Learning (Fall 2020)

Prof. Haipeng Luo

U of Southern California

Sep 3, 2020

Outline

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Administrative stuff

Please enroll in Piazza (163/202 as of this morning).

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- #submissions updated *from* 10 *to* ∞

Outline

1. Administration
2. Review of last lecture
3. Linear regression
4. Linear regression with nonlinear basis
5. Overfitting and preventing overfitting

Multi-class classification

Training data (set)

- N samples/instances: $\mathcal{D}^{\text{TRAIN}} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \cdots, (\boldsymbol{x}_{\mathsf{N}}, y_{\mathsf{N}})\}$
- Each $\boldsymbol{x_n} \in \mathbb{R}^{\mathsf{D}}$ is called a feature vector.
- Each $y_n \in [\mathsf{C}] = \{1, 2, \cdots, \mathsf{C}\}$ is called a label/class/category.
- They are used to learn $f : \mathbb{R}^{\mathsf{D}} \to [\mathsf{C}]$ for future prediction.

Special case: binary classification

- Number of classes: $\mathsf{C} = 2$
- Conventional labels: $\{0, 1\}$ or $\{-1, +1\}$

K-NNC: predict the majority label within the K-nearest neighbor set

Datasets

Training data

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- They are used to learn $f(\cdot)$

Test data

- M samples/instances: $\mathcal{D}^{\text{TEST}} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \cdots, (\boldsymbol{x}_{\mathsf{M}}, y_{\mathsf{M}})\}$
- They are used to evaluate how well $f(\cdot)$ will do.

Development/Validation data

- L samples/instances: $\mathcal{D}^{\text{DEV}} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \cdots, (\boldsymbol{x}_{\mathsf{L}}, y_{\mathsf{L}})\}$
- They are used to optimize hyper-parameter(s).

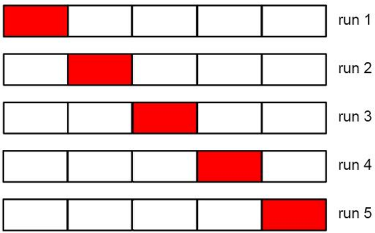
These three sets should *not* overlap!

S-fold Cross-validation

What if we do not have a development set?

- Split the training data into S equal parts.
- Use each part *in turn* as a development dataset and use the others as a training dataset.
- Choose the hyper-parameter leading to best *average* performance.

S $= 5$: 5-fold cross validation



Special case: S = N, called leave-one-out.

High level picture

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.

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How to do the *red part* exactly?

Outline

Regression

Predicting a continuous outcome variable using past observations

- Predicting future temperature (last lecture)
- Predicting the amount of rainfall
- Predicting the demand of a product
- Predicting the sale price of a house
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Key difference from classification

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

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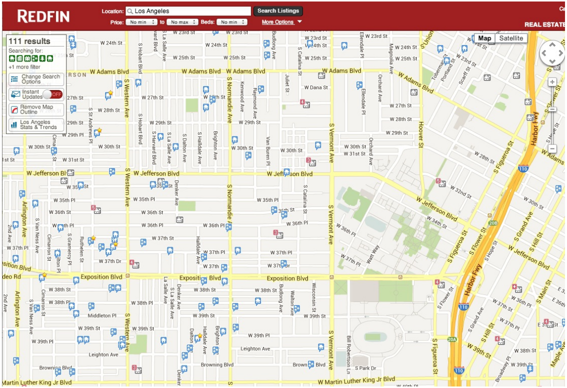
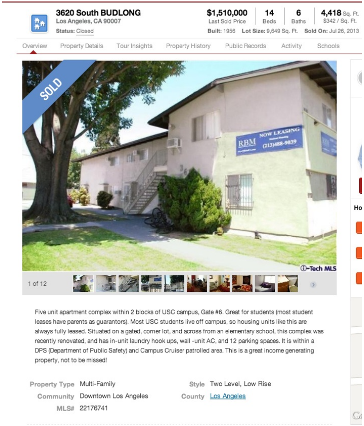
Linear Regression: regression with linear models

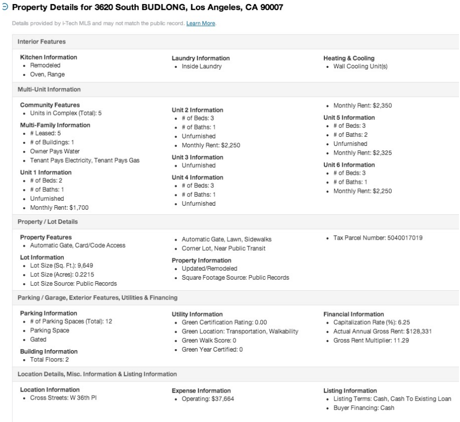
Ex: Predicting the sale price of a house

Retrieve historical sales records (training data)

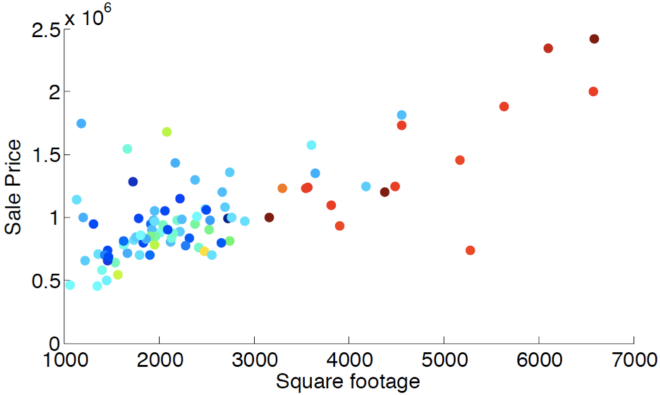


Features used to predict



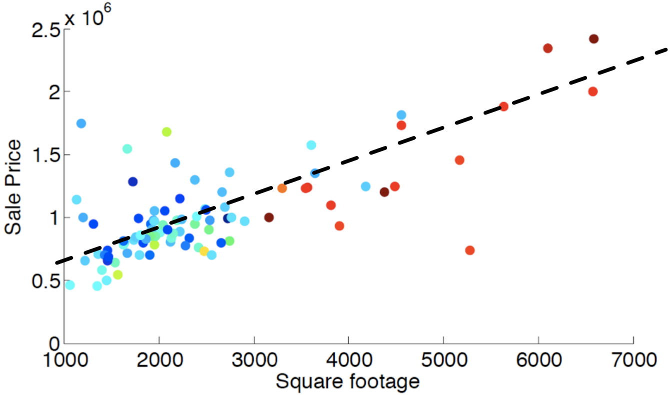


Correlation between square footage and sale price



Possibly linear relationship

Sale price ≈ **price_per_sqft** × square_footage + **fixed_expense**



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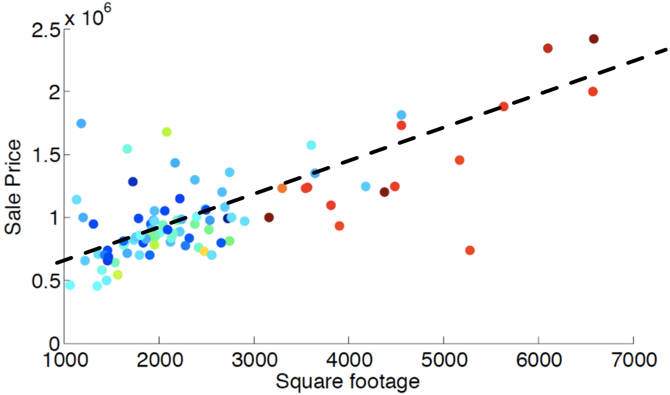
Sale price $\approx$ **price_per_sqft** $\times$ square_footage + **fixed_expense**

(*slope*) (*intercept*)



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- training set ✓

Example

Predicted price = **price_per_sqft** × square_footage + **fixed_expense**

one model: price_per_sqft = 0.3K, fixed_expense = 210K

sqft	sale price (K)	prediction (K)	squared error
2000	810	810	0
2100	907	840	67^2
1100	312	540	228^2
5500	2,600	1,860	740^2
...	...	...	...
Total			$0 + 67^2 + 228^2 + 740^2 + \cdots$

Adjust price_per_sqft and fixed_expense such that the total squared error is minimized.

Formal setup for linear regression

Input: $\boldsymbol{x} \in \mathbb{R}^{\mathsf{D}}$ (features, covariates, context, predictors, etc)

Output: $y \in \mathbb{R}$ (responses, targets, outcomes, etc)

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- append 1 to each x as the first feature: $\tilde{\boldsymbol{x}} = [1 \ x_1 \ x_2 \ \ldots \ x_{\mathsf{D}}]^{\mathrm{T}}$

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- sometimes just use $\boldsymbol{w}, \boldsymbol{x}, \mathsf{D}$ for $\tilde{\boldsymbol{w}}, \tilde{\boldsymbol{x}}, \mathsf{D} + 1$!

Goal

Minimize total squared error

$$\sum_n (f(\boldsymbol{x}_n) - y_n)^2 = \sum_n (\tilde{\boldsymbol{x}}_n^{\mathrm{T}} \tilde{\boldsymbol{w}} - y_n)^2$$

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- **Residual Sum of Squares** (RSS), a function of $\tilde{\boldsymbol{w}}$

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- find $\tilde{\boldsymbol{w}}^* = \underset{\tilde{\boldsymbol{w}} \in \mathbb{R}^{\mathsf{D}+1}}{\operatorname{argmin}} \mathrm{RSS}(\tilde{\boldsymbol{w}})$, i.e. **least (mean) squares solution**
  (more generally called **empirical risk minimizer**)

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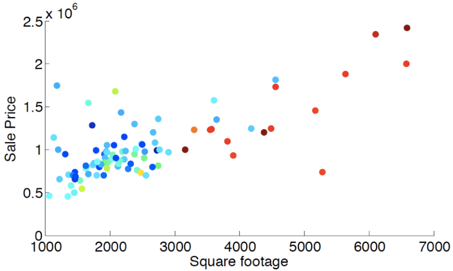
- *reduce machine learning to optimization*

- in principle can apply any optimization algorithm, but linear regression admits a *closed-form solution*

Warm-up: $D = 0$

Only one parameter w_0: constant prediction $f(x) = w_0$



f is a horizontal line, where should it be?

Warm-up: $\mathrm{D} = 0$

Optimization objective becomes

$$\mathrm{RSS}(w_0) = \sum_n (w_0 - y_n)^2$$ (it's a *quadratic* $aw_0^2 + bw_0 + c$)

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$$= N\left(w_0 - \frac{1}{N}\sum_n y_n\right)^2 + \text{cnt.}$$

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It is clear that $w_0^* = \frac{1}{N}\sum_n y_n$, i.e. the **average**

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Exercise: what if we use absolute error instead of squared error?

Warm-up: D $= 1$

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General approach: find *stationary points*, i.e., points with *zero gradient*

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$$\Rightarrow \begin{array}{ll} N w_0 + w_1 \sum_n x_n & = \sum_n y_n \\ w_0 \sum_n x_n + w_1 \sum_n x_n^2 & = \sum_n y_n x_n \end{array}$$ (**a linear system**)

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$$\Rightarrow \begin{pmatrix} N & \sum_n x_n \\ \sum_n x_n & \sum_n x_n^2 \end{pmatrix} \begin{pmatrix} w_0 \\ w_1 \end{pmatrix} = \begin{pmatrix} \sum_n y_n \\ \sum_n x_n y_n \end{pmatrix}$$

Least square solution for $\mathrm{D} = 1$

$$\Rightarrow \begin{pmatrix} w_0^* \\ w_1^* \end{pmatrix} = \begin{pmatrix} N & \sum_n x_n \\ \sum_n x_n & \sum_n x_n^2 \end{pmatrix}^{-1} \begin{pmatrix} \sum_n y_n \\ \sum_n x_n y_n \end{pmatrix}$$

(assuming the matrix is invertible)

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Are stationary points minimizers?

Least square solution for $\mathrm{D} = 1$

$$\Rightarrow \begin{pmatrix} w_0^* \\ w_1^* \end{pmatrix} = \begin{pmatrix} N & \sum_n x_n \\ \sum_n x_n & \sum_n x_n^2 \end{pmatrix}^{-1} \begin{pmatrix} \sum_n y_n \\ \sum_n x_n y_n \end{pmatrix}$$

(assuming the matrix is invertible)

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- yes for **convex** objectives (RSS is convex in $\tilde{\boldsymbol{w}}$)
- not true in general

General least square solution

Objective

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

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Again, find stationary points (**multivariate calculus**)

$$\nabla \mathrm{RSS}(\tilde{\boldsymbol{w}}) = 2 \sum_n \tilde{\boldsymbol{x}}_n (\tilde{\boldsymbol{x}}_n^{\mathrm{T}} \tilde{\boldsymbol{w}} - y_n)$$

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where

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when $\mathsf{D} = 0$**:** $(\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}})^{-1} = \frac{1}{N}$, $\tilde{\boldsymbol{X}}^{\mathrm{T}}\boldsymbol{y} = \sum_n y_n$

Another approach

RSS is a quadratic:

$$\mathrm{RSS}(\tilde{\boldsymbol{w}}) = \sum_n (\tilde{\boldsymbol{w}}^{\mathrm{T}} \tilde{\boldsymbol{x}}_n - y_n)^2 = \|\tilde{\boldsymbol{X}} \tilde{\boldsymbol{w}} - \boldsymbol{y}\|_2^2$$

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So $\tilde{\boldsymbol{w}}^* = (\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}})^{-1}\tilde{\boldsymbol{X}}^{\mathrm{T}}\boldsymbol{y}$ is the minimizer.

Computational complexity

Bottleneck of computing

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

is to invert the matrix $\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}} \in \mathbb{R}^{(\mathsf{D}+1)\times(\mathsf{D}+1)}$

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- there are many faster approaches (such as conjugate gradient)

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- no solution ($\Rightarrow$ RSS has no minimizer? ✗)
- or infinitely many solutions ($\Rightarrow$ infinitely many minimizers ✓)

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sqft	sale price
1000	500K

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Example: $\mathsf{D} = \mathsf{N} = 1$

sqft	sale price
1000	500K

Any line passing this single point is a minimizer of RSS.

How about the following?

$\mathsf{D} = 1, \mathsf{N} = 2$

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$D = 1, N = 2$

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Any line passing **the average** is a minimizer of RSS.

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$\mathsf{D} = 2, \mathsf{N} = 3$**?**

sqft	#bedroom	sale price
1000	2	500K
1500	3	700K
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$\mathsf{D} = 2, \mathsf{N} = 3$**?**

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Again *infinitely many minimizers*.

How to resolve this issue?

Intuition: what does inverting $\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}}$ do?

eigendecomposition: $$\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}} = \boldsymbol{U}^{\mathrm{T}} \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \lambda_{\mathsf{D}} & 0 \\ 0 & \cdots & 0 & \lambda_{\mathsf{D}+1} \end{bmatrix} \boldsymbol{U}$$

where $\lambda_1 \geq \lambda_2 \geq \cdots \lambda_{\mathsf{D}+1} \geq 0$ are **eigenvalues**.

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inverse: $$(\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}})^{-1} = \boldsymbol{U}^{\mathrm{T}} \begin{bmatrix} \frac{1}{\lambda_1} & 0 & \cdots & 0 \\ 0 & \frac{1}{\lambda_2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \frac{1}{\lambda_{\mathsf{D}}} & 0 \\ 0 & \cdots & 0 & \frac{1}{\lambda_{\mathsf{D}+1}} \end{bmatrix} \boldsymbol{U}$$

i.e. just inverse the eigenvalues

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One natural fix: add something positive

$$\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}} + \lambda \boldsymbol{I} = \boldsymbol{U}^{\mathrm{T}} \begin{bmatrix} \lambda_1 + \lambda & 0 & \cdots & 0 \\ 0 & \lambda_2 + \lambda & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \lambda_{\mathsf{D}} + \lambda & 0 \\ 0 & \cdots & 0 & \lambda_{\mathsf{D}+1} + \lambda \end{bmatrix} \boldsymbol{U}$$

where $\lambda > 0$ and $\boldsymbol{I}$ is the identity matrix.

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where $\lambda > 0$ and $\boldsymbol{I}$ is the identity matrix. Now it is invertible:

$$(\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}} + \lambda \boldsymbol{I})^{-1} = \boldsymbol{U}^{\mathrm{T}} \begin{bmatrix} \frac{1}{\lambda_1+\lambda} & 0 & \cdots & 0 \\ 0 & \frac{1}{\lambda_2+\lambda} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \frac{1}{\lambda_{\mathsf{D}}+\lambda} & 0 \\ 0 & \cdots & 0 & \frac{1}{\lambda_{\mathsf{D}+1}+\lambda} \end{bmatrix} \boldsymbol{U}$$

Fix the problem

The solution becomes

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

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λ is a *hyper-parameter*, can be tuned by cross-validation.

Comparison to NNC

Parametric versus non-parametric

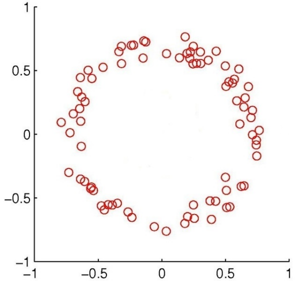
- **Parametric methods**: the size of the model does *not grow* with the size of the training set N.
  - e.g. linear regression, $D + 1$ parameters, independent of N.

- **Non-parametric methods**: the size of the model *grows* with the size of the training set.
  - e.g. NNC, the training set itself needs to be kept in order to predict. Thus, the size of the model is the size of the training set.

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

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

to transform the data to a more complicated feature space

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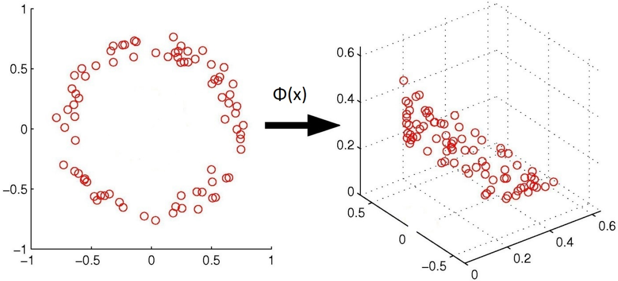

Regression with nonlinear basis

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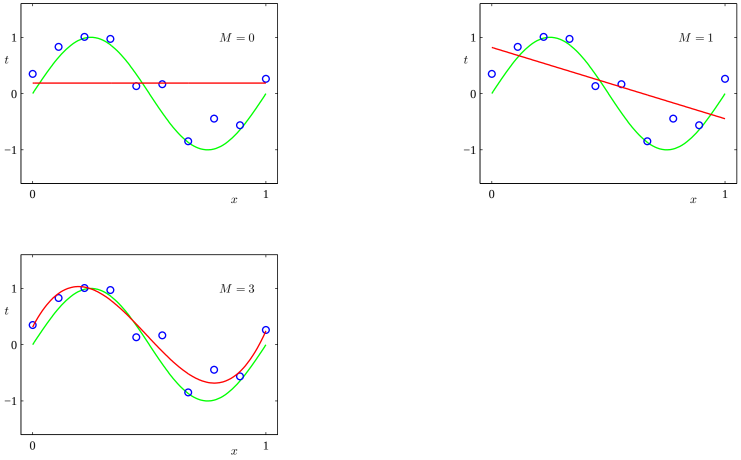
Learning a linear model in the new space
$=$ learning an *M-degree polynomial model* in the original space

Example

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



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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No, it basically *does nothing* since

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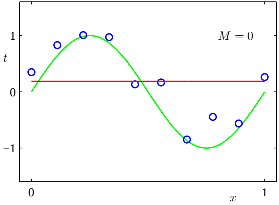
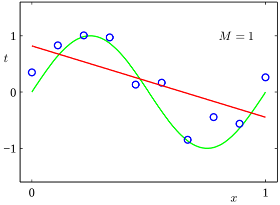
We will see more nonlinear mappings soon.

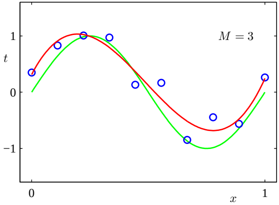
Outline

Should we use a very complicated mapping?

Ex: fitting a noisy sine function with a polynomial:







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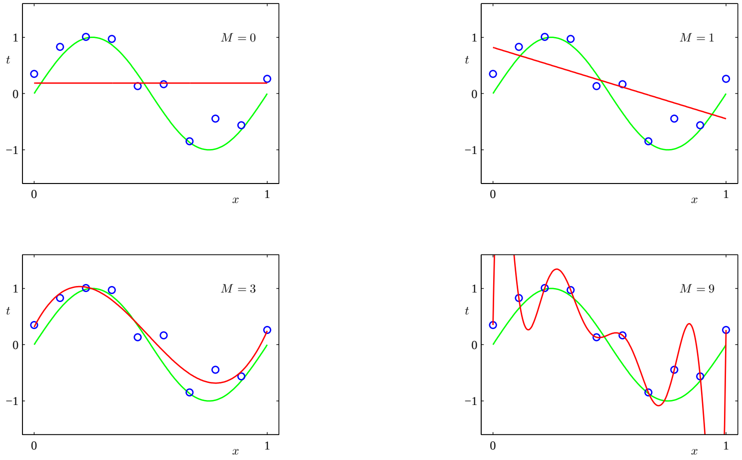

Underfitting and Overfitting

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

- large training error
- large test error

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

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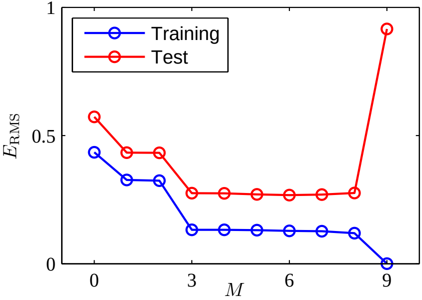

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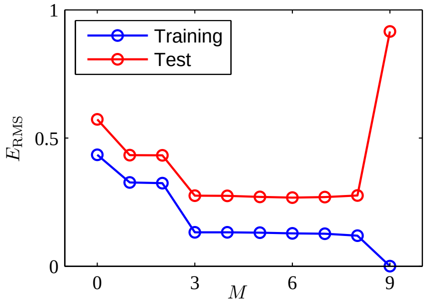

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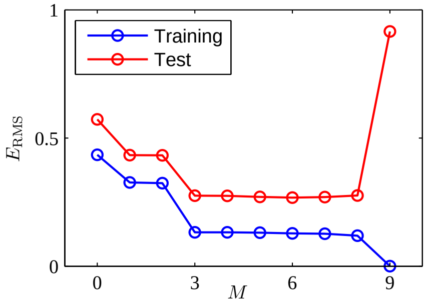

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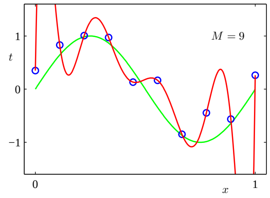
How to prevent overfitting?

Method 1: use more training data

The more, the merrier



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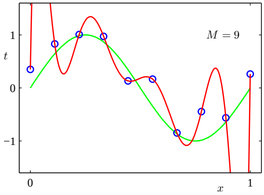

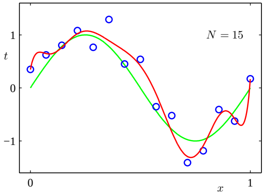

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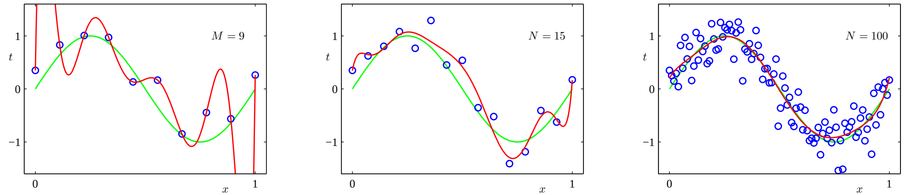

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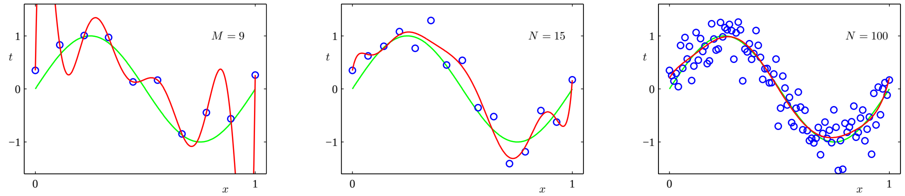

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For polynomial basis, the **degree** M clearly controls the complexity

- use cross-validation to pick hyper-parameter M

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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
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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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  - common choices: $\|\boldsymbol{w}\|_2^2$, $\|\boldsymbol{w}\|_1$, etc.
- $\lambda > 0$ is the *regularization coefficient*
  - $\lambda = 0$, no regularization
  - $\lambda \to +\infty$, $\boldsymbol{w} \to \operatorname{argmin}_w R(\boldsymbol{w})$
  - 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

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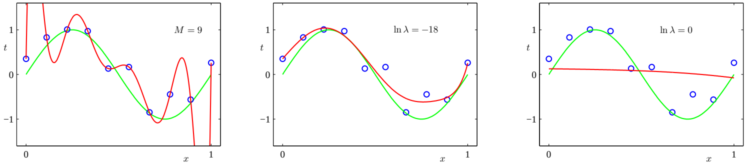

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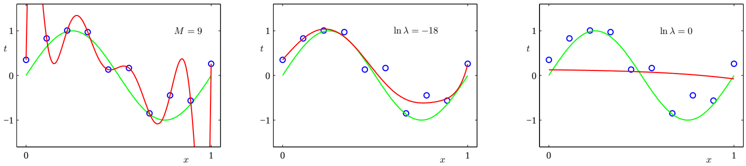

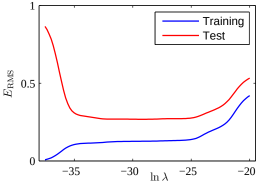

How to solve the new objective?

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

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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

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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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ML becomes optimization