CSCI567 Machine Learning (Spring 2025)

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Administrative stuff

Please enroll in Piazza (still missing some of you).

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HW1 to be released today.

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Programming project:

- invitation to enroll is out

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Programming project:

- invitation to enroll is out
- six tasks available now, four more to come

Outline

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

Outline

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 $f : \mathbb{R}^\mathsf{D} \rightarrow [\mathsf{C}]$ 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).

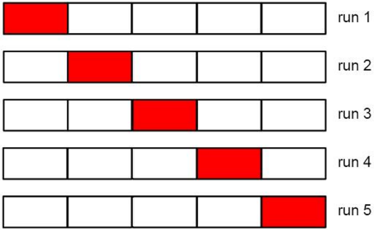
These three sets should *not* overlap!

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.

$\mathsf{S} = 5$: 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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Today: from a simple example to a general recipe

Outline

1. Review of last lecture
2. Linear regression
   - Motivation
   - Setup and Algorithm
   - Discussions
3. Linear regression with nonlinear basis
4. Overfitting and preventing overfitting

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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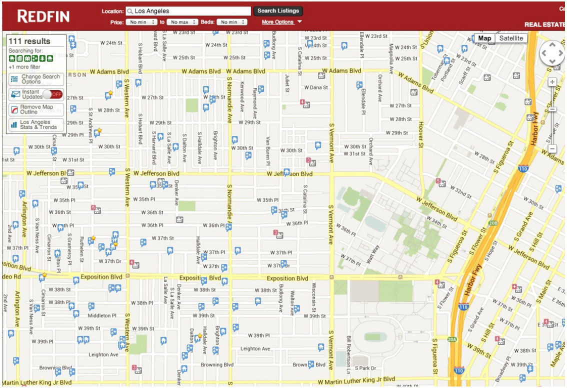
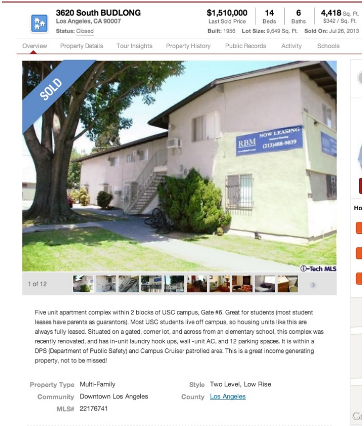
Linear Regression: regression with linear models

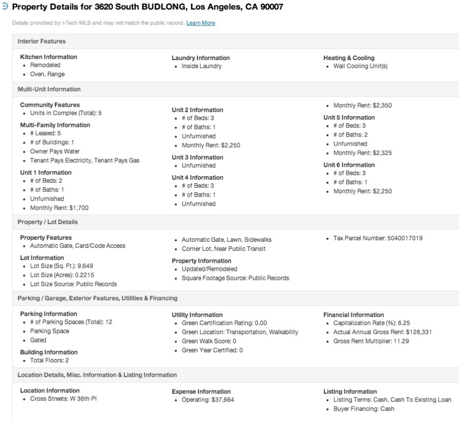
Ex: Predicting the sale price of a house

Retrieve historical sales records (training data)

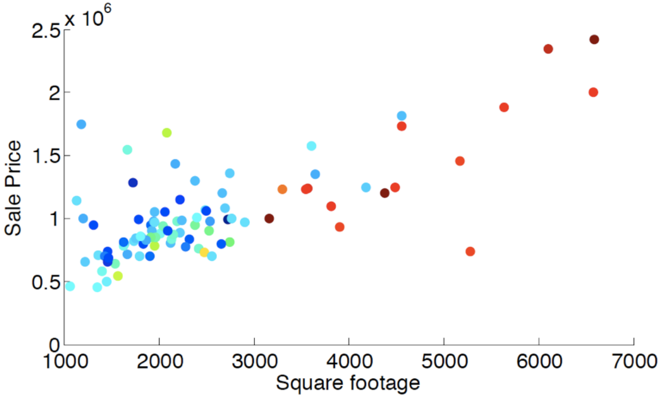


Features used to predict



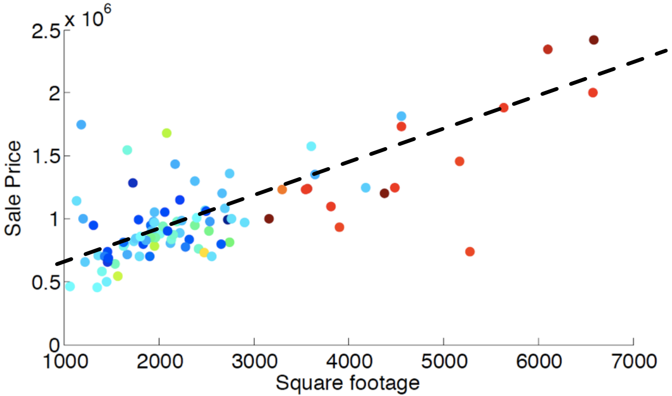


Correlation between square footage and sale price



Possibly linear relationship

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



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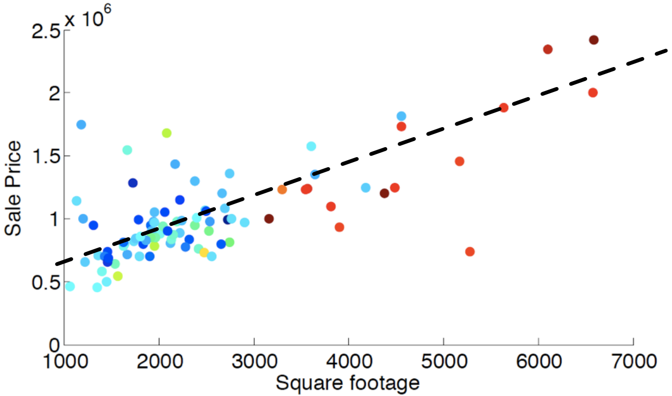
(*slope*) (*intercept*)



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- test set, ideal but we *cannot use test set while training*
- 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
$\cdots$	$\cdots$	$\cdots$	$\cdots$
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, 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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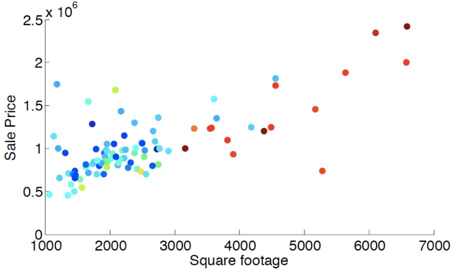
- *reduce machine learning to optimization*

- 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: 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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$$\begin{aligned}\mathrm{RSS}(w_0) &= \sum_n (w_0 - y_n)^2 \qquad \text{(it's a \textit{quadratic} } aw_0^2 + bw_0 + c\text{)} \\ &= Nw_0^2 - 2\left(\sum_n y_n\right) w_0 + \text{cnt.}\end{aligned}$$

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

Warm-up: $\mathsf{D} = 1$

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

$$\begin{cases} \frac{\partial \mathrm{RSS}(\tilde{\boldsymbol{w}})}{\partial w_0} = 0 \\ \frac{\partial \mathrm{RSS}(\tilde{\boldsymbol{w}})}{\partial w_1} = 0 \end{cases} \Rightarrow \begin{array}{ll} \sum_n (w_0 + w_1 x_n - y_n) & = 0 \\ \sum_n (w_0 + w_1 x_n - y_n) x_n & = 0 \end{array}$$

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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 $\mathsf{D} = 1$

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

(assuming the matrix is invertible)

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Are stationary points minimizers?

Least square solution for D $= 1$

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

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- not true in general

General least square solution

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A compact form:

$$\mathrm{RSS}(\tilde{\boldsymbol{w}}) = \|\tilde{\boldsymbol{X}} \tilde{\boldsymbol{w}} - \boldsymbol{y}\|_2^2$$

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Verify the solution when $\mathsf{D} = 1$:

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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**, so let's complete the square:

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

sqft	#bedroom	sale price
1000	2	500K
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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 invert the eigenvalues

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

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

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

Comparison to NNC

Non-parametric versus Parametric

- **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.

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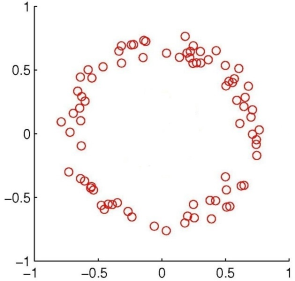
  - e.g. NNC, the training set itself needs to be kept in order to predict. Thus, the size of the model is the size of the training set.

- **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.

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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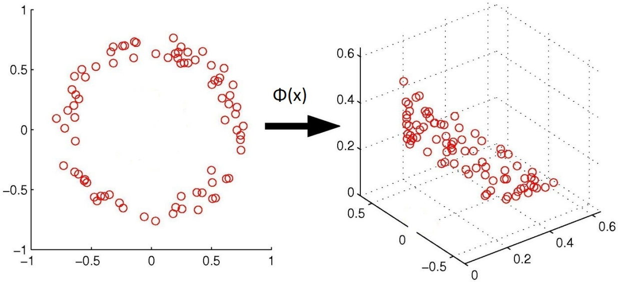

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Model: $f(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x})$ where $\boldsymbol{w} \in \mathbb{R}^M$

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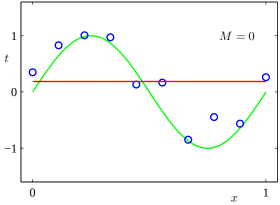
Learning a linear model in the new space
= learning an *M-degree polynomial model* in the original space

Example

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



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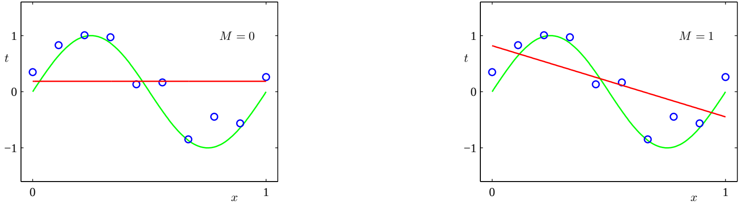

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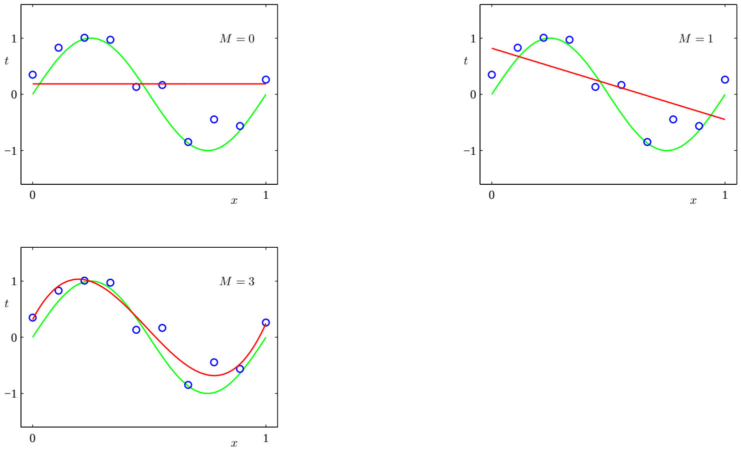

Why nonlinear?

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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No, it basically *does nothing* since

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

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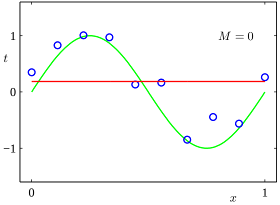
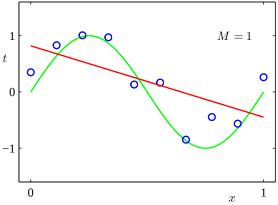
We will see more nonlinear mappings soon.

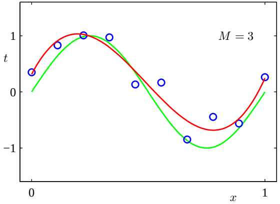
Outline

Should we use a very complicated mapping?

Ex: fitting a noisy sine function with a polynomial:







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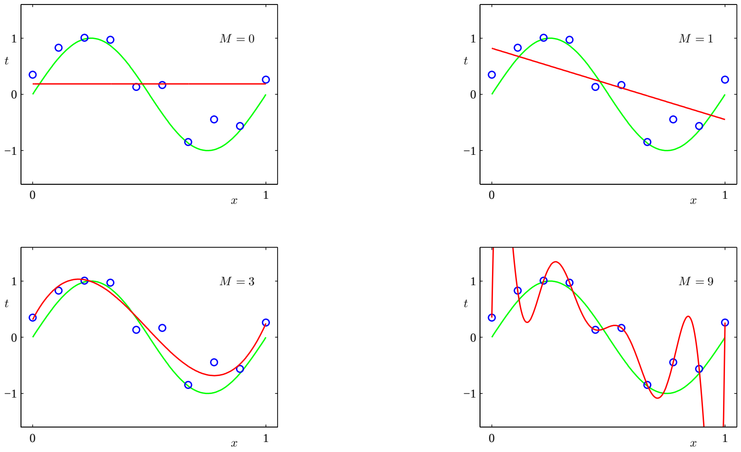

Underfitting and Overfitting

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

- large training error
- large test error

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

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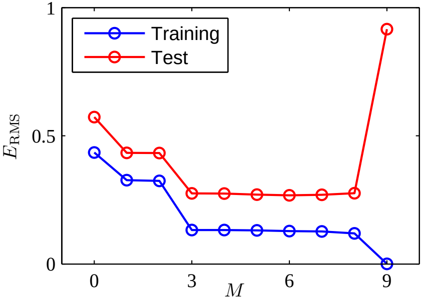

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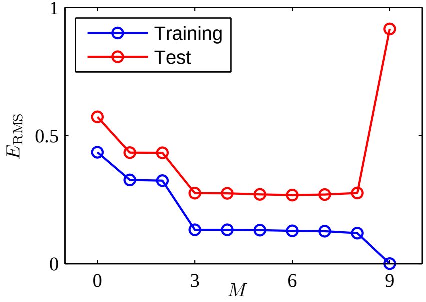

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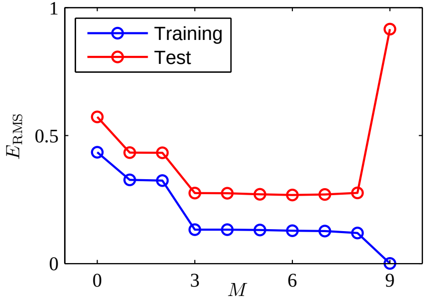

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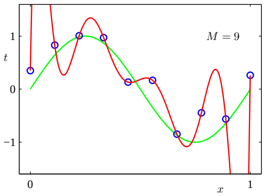
How to prevent overfitting?

Method 1: use more training data

The more, the merrier



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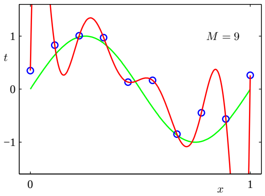

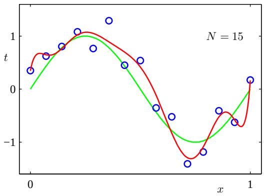

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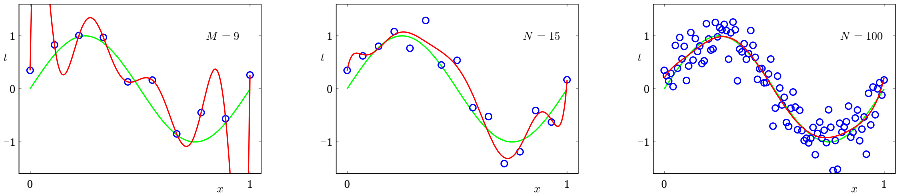

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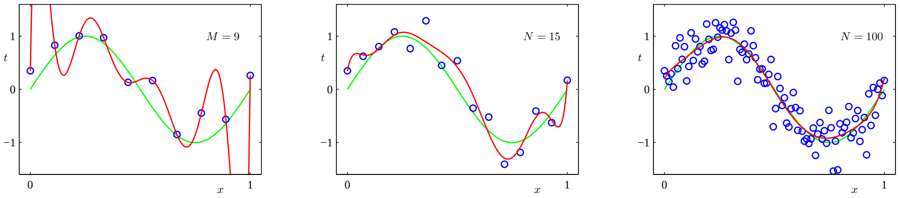

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Method 2: control the model complexity

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

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

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
  - $\lambda \rightarrow +\infty$, $\boldsymbol{w} \rightarrow \operatorname{argmin}_w R(\boldsymbol{w})$
  - i.e. control **trade-off** between training error and complexity

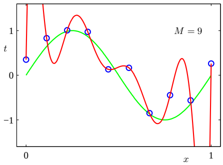
The effect of λ

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

The trade-off

when we increase regularization coefficient λ



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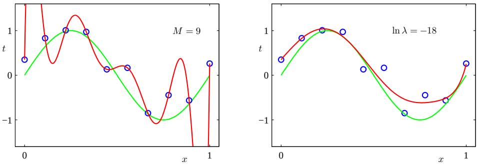

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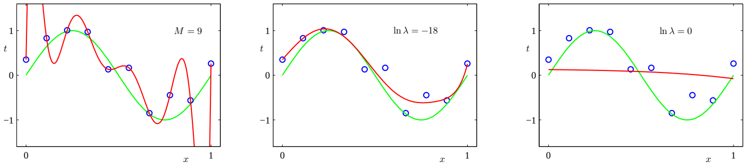

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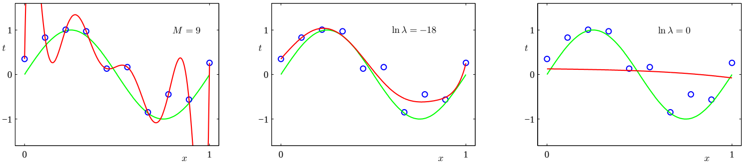

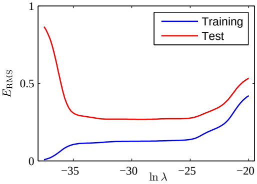

How to solve the new objective?

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

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

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For other regularizers, can apply general optimization algorithms (Lec 3).

Equivalent form

Regularization is also sometimes formulated as

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

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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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ML becomes optimization