CSCI567 Machine Learning (Fall 2021)

Prof. Haipeng Luo

U of Southern California

Sep 2, 2021

Administrative stuff

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

HW1 to be released today.

Programming project:

- invitation to enroll is out
- all six tasks available now, with detailed description
- collaboration not allowed, for questions talk to graders

Outline

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

Outline

1. Review of last lecture
2. Linear regression
3. Linear regression with nonlinear basis
4. 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

- N samples/instances: $\mathcal{D}^{\text{TRAIN}} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \cdots, (\boldsymbol{x}_{\mathsf{N}}, y_{\mathsf{N}})\}$
- 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).

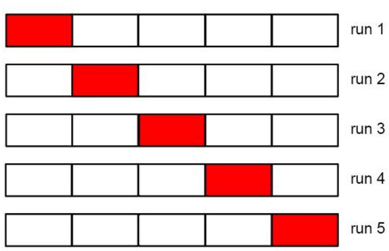
These three sets should *not* overlap!

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: $\mathsf{S} = \mathsf{N}$, 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.

How to do the *red part* exactly?

Today: from a simple example to a general recipe

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
- ...

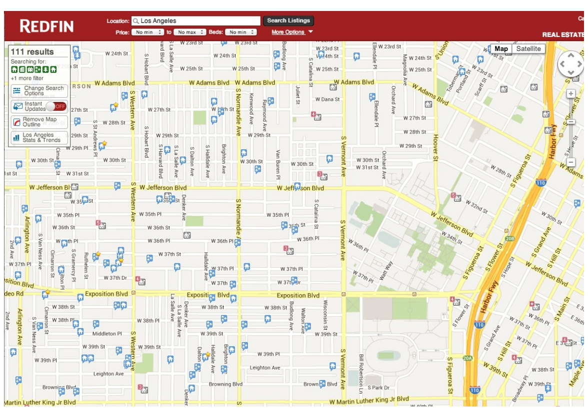
Key difference from classification

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

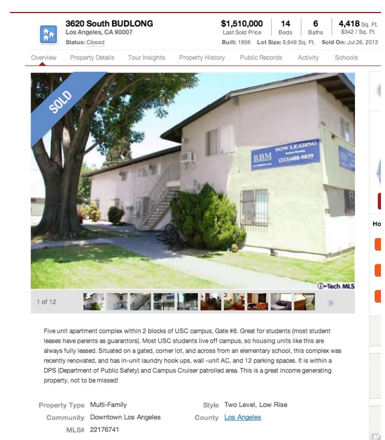
Linear Regression: regression with linear models

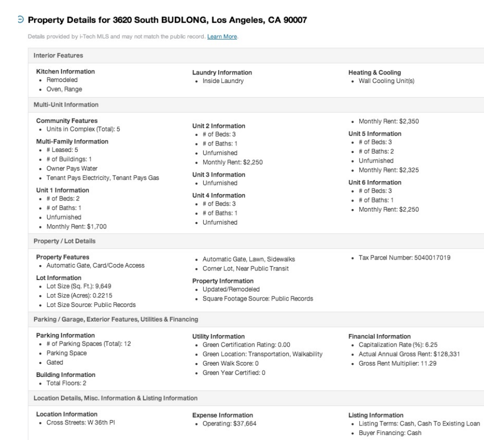
Ex: Predicting the sale price of a house

Retrieve historical sales records (training data)

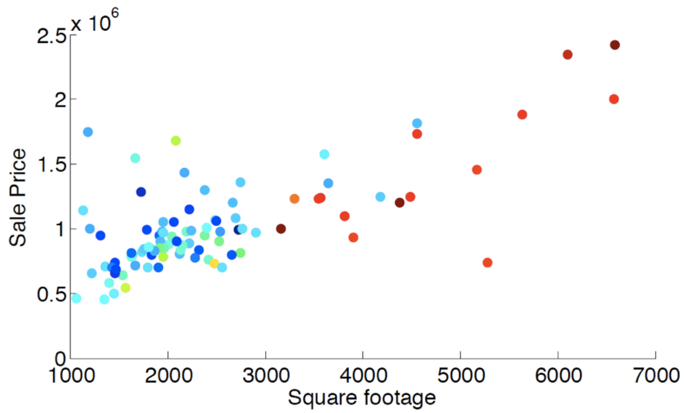


Features used to predict



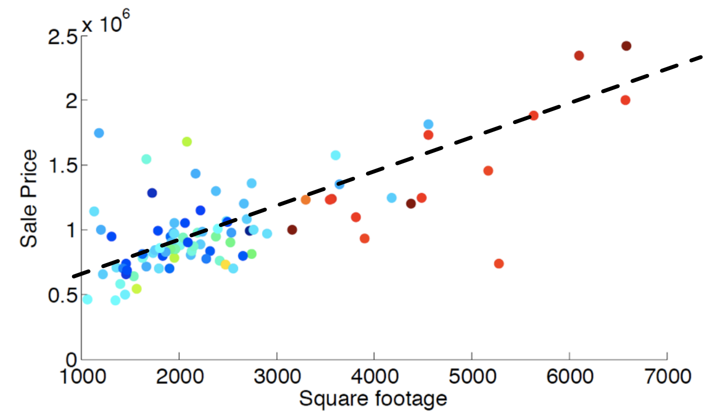


Correlation between square footage and sale price



Possibly linear relationship

Sale price $\approx$ **price_per_sqft** $\times$ square_footage + **fixed_expense**
(*slope*) (*intercept*)



How to learn the unknown parameters?

How to measure error for one prediction?

- The classification error (0-1 loss, i.e. *right* or *wrong*) is *inappropriate* for continuous outcomes.
- We can look at
  - *absolute* error: | prediction - sale price |
  - or *squared* error: (prediction - sale price)^2 (**most common**)

Goal: pick the model (unknown parameters) that minimizes the average/total prediction error, but *on what set*?

- test set, ideal but we *cannot use test set while training*
- training set ✓

Example

Predicted price = **price_per_sqft** $\times$ 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, predictors, etc)

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

Training data: $\mathcal{D} = \{(\boldsymbol{x}_n, y_n), n = 1, 2, \ldots, \mathsf{N}\}$

Linear model: $f : \mathbb{R}^{\mathsf{D}} \to \mathbb{R}$, with $f(\boldsymbol{x}) = w_0 + \sum_{d=1}^{D} w_d x_d = w_0 + \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$ (superscript ^{T} stands for transpose), i.e. a *hyper-plane* parametrized by

- $\boldsymbol{w} = [w_1 \; w_2 \; \cdots \; w_{\mathsf{D}}]^{\mathrm{T}}$ (weights, weight vector, parameter vector, etc)
- bias w_0

NOTE: for notation convenience, very often we

- append 1 to each x as the first feature: $\tilde{\boldsymbol{x}} = [1 \; x_1 \; x_2 \; \ldots \; x_{\mathsf{D}}]^{\mathrm{T}}$
- let $\tilde{\boldsymbol{w}} = [w_0 \; w_1 \; w_2 \; \cdots \; w_{\mathsf{D}}]^{\mathrm{T}}$, a concise representation of all $D + 1$ parameters
- the model becomes simply $f(\boldsymbol{x}) = \tilde{\boldsymbol{w}}^{\mathrm{T}}\tilde{\boldsymbol{x}}$
- sometimes just use $\boldsymbol{w}, \boldsymbol{x}, \mathsf{D}$ for $\tilde{\boldsymbol{w}}, \tilde{\boldsymbol{x}}, \mathsf{D} + 1$!

Goal

Minimize total squared error

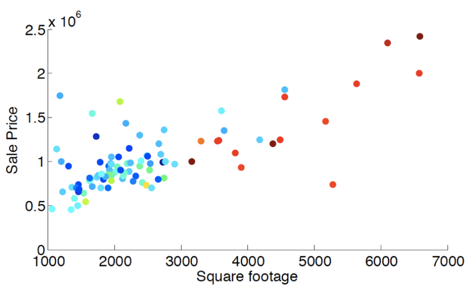
- **Residual Sum of Squares** (RSS), a function of $\tilde{\boldsymbol{w}}$

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

- find $\tilde{\boldsymbol{w}}^* = \operatorname*{argmin}_{\tilde{\boldsymbol{w}} \in \mathbb{R}^{\mathsf{D}+1}} \mathrm{RSS}(\tilde{\boldsymbol{w}})$, i.e. **least squares solution** (more generally called **empirical risk minimizer**)
- *reduce machine learning to optimization*
- in principle can apply any optimization algorithm, but linear regression admits a *closed-form solution*

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

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



f is a horizontal line, where should it be?

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

Optimization objective becomes

$$\begin{aligned} \mathrm{RSS}(w_0) &= \sum_n (w_0 - y_n)^2 \qquad \text{(it's a } \textit{quadratic } aw_0^2 + bw_0 + c\text{)} \\ &= N w_0^2 - 2\left(\sum_n y_n\right) w_0 + \text{cnt.} \\ &= N\left(w_0 - \frac{1}{N}\sum_n y_n\right)^2 + \text{cnt.} \end{aligned}$$

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

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

Warm-up: D = 1

Optimization objective becomes

$$\mathrm{RSS}(\tilde{\boldsymbol{w}}) = \sum_n (w_0 + w_1 x_n - y_n)^2$$

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

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

$$\Rightarrow \begin{aligned} N w_0 + w_1 \textstyle\sum_n x_n &= \textstyle\sum_n y_n \\ w_0 \textstyle\sum_n x_n + w_1 \textstyle\sum_n x_n^2 &= \textstyle\sum_n y_n x_n \end{aligned} \quad \text{(a linear system)}$$

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

Least square solution for 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)

Are stationary points minimizers?

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

General least square solution

Objective

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

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

$$\begin{aligned} \nabla \mathrm{RSS}(\tilde{\boldsymbol{w}}) &= 2 \sum_n \tilde{\boldsymbol{x}}_n (\tilde{\boldsymbol{x}}_n^{\mathrm{T}} \tilde{\boldsymbol{w}} - y_n) \propto \left(\sum_n \tilde{\boldsymbol{x}}_n \tilde{\boldsymbol{x}}_n^{\mathrm{T}} \right) \tilde{\boldsymbol{w}} - \sum_n \tilde{\boldsymbol{x}}_n y_n \\ &= (\tilde{\boldsymbol{X}}^{\mathrm{T}} \tilde{\boldsymbol{X}}) \tilde{\boldsymbol{w}} - \tilde{\boldsymbol{X}}^{\mathrm{T}} \boldsymbol{y} = \boldsymbol{0} \end{aligned}$$

where

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

General least square solution

$$(\tilde{\boldsymbol{X}}^{\mathrm{T}} \tilde{\boldsymbol{X}}) \tilde{\boldsymbol{w}} - \tilde{\boldsymbol{X}}^{\mathrm{T}} \boldsymbol{y} = \boldsymbol{0} \quad \Rightarrow \quad \tilde{\boldsymbol{w}}^* = (\tilde{\boldsymbol{X}}^{\mathrm{T}} \tilde{\boldsymbol{X}})^{-1} \tilde{\boldsymbol{X}}^{\mathrm{T}} \boldsymbol{y}$$

assuming $\tilde{\boldsymbol{X}}^{\mathrm{T}} \tilde{\boldsymbol{X}}$ (**covariance matrix**) is invertible for now.

Again by convexity $\tilde{\boldsymbol{w}}^*$ is the minimizer of RSS.

Verify the solution when D = 1:

$$\tilde{\boldsymbol{X}}^{\mathrm{T}} \tilde{\boldsymbol{X}} = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_{\mathsf{N}} \end{pmatrix} \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \cdots & \cdots \\ 1 & x_{\mathsf{N}} \end{pmatrix} = \begin{pmatrix} N & \sum_n x_n \\ \sum_n x_n & \sum_n x_n^2 \end{pmatrix}$$

when 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:

$$
\begin{aligned}
\mathrm{RSS}(\tilde{\boldsymbol{w}}) &= \sum_n (\tilde{\boldsymbol{w}}^{\mathrm{T}}\tilde{\boldsymbol{x}}_n - y_n)^2 = \|\tilde{\boldsymbol{X}}\tilde{\boldsymbol{w}} - \boldsymbol{y}\|_2^2 \\
&= \left(\tilde{\boldsymbol{X}}\tilde{\boldsymbol{w}} - \boldsymbol{y}\right)^{\mathrm{T}} \left(\tilde{\boldsymbol{X}}\tilde{\boldsymbol{w}} - \boldsymbol{y}\right) \\
&= \tilde{\boldsymbol{w}}^{\mathrm{T}}\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}}\tilde{\boldsymbol{w}} - \boldsymbol{y}^{\mathrm{T}}\tilde{\boldsymbol{X}}\tilde{\boldsymbol{w}} - \tilde{\boldsymbol{w}}^{\mathrm{T}}\tilde{\boldsymbol{X}}^{\mathrm{T}}\boldsymbol{y} + \text{cnt.} \\
&= \left(\tilde{\boldsymbol{w}} - (\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}})^{-1}\tilde{\boldsymbol{X}}^{\mathrm{T}}\boldsymbol{y}\right)^{\mathrm{T}} \left(\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}}\right) \left(\tilde{\boldsymbol{w}} - (\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}})^{-1}\tilde{\boldsymbol{X}}^{\mathrm{T}}\boldsymbol{y}\right) + \text{cnt.}
\end{aligned}
$$

Note: $\boldsymbol{u}^{\mathrm{T}}\left(\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}}\right)\boldsymbol{u} = \left(\tilde{\boldsymbol{X}}\boldsymbol{u}\right)^{\mathrm{T}}\tilde{\boldsymbol{X}}\boldsymbol{u} = \|\tilde{\boldsymbol{X}}\boldsymbol{u}\|_2^2 \geq 0$ and is 0 if $\boldsymbol{u} = 0$.
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 $\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}} \in \mathbb{R}^{(\mathsf{D}+1)\times(\mathsf{D}+1)}$

- naively need $O(\mathsf{D}^3)$ time
- there are many faster approaches (such as conjugate gradient)

What if $\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}}$ is not invertible

What does that imply?

Recall $\left(\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}}\right)\boldsymbol{w}^* = \tilde{\boldsymbol{X}}^{\mathrm{T}}\boldsymbol{y}$. If $\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}}$ not invertible, this equation has

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

What if $\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}}$ is not invertible

Why would that happen?

One situation: $\mathsf{N} < \mathsf{D}+1$, i.e. not enough data to estimate all parameters.

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?

D $= 1$, N $= 2$

sqft	sale price
1000	500K
1000	600K

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

D $= 2$, N $= 3$**?**

sqft	#bedroom	sale price
1000	2	500K
1500	3	700K
2000	4	800K

Again *infinitely many minimizers*.

How to resolve this issue?

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

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

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

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

i.e. just invert the eigenvalues

How to solve this problem?

Non-invertible $\Rightarrow$ some eigenvalues are 0.

One natural fix: add something positive

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

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

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

Fix the problem

The solution becomes

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

- not a minimizer of the original RSS
- more than an arbitrary hack (as we will see soon)

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

Comparison to NNC

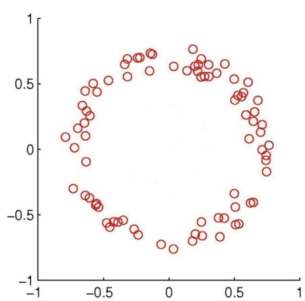
Non-parametric versus Parametric

- **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.
- **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



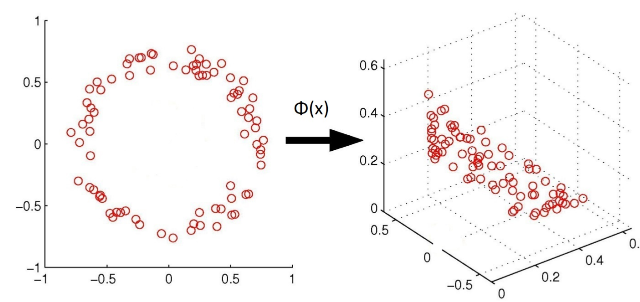
Solution: nonlinearly transformed features

1. Use a nonlinear mapping

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

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

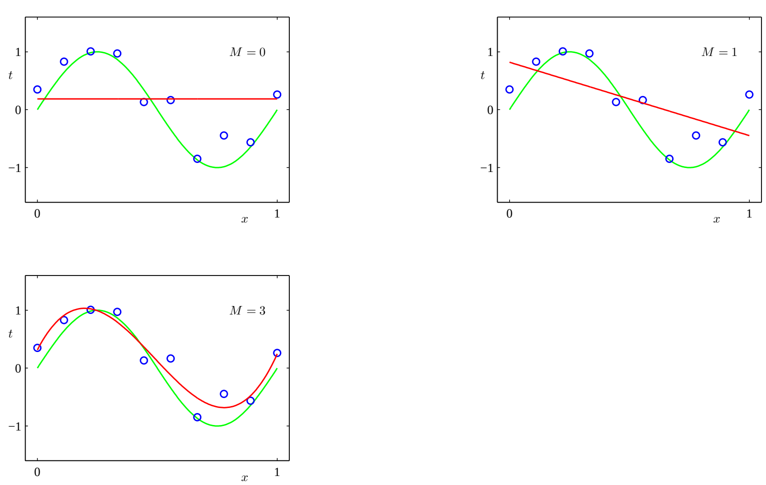
Polynomial basis functions for $\mathsf{D} = 1$

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

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

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

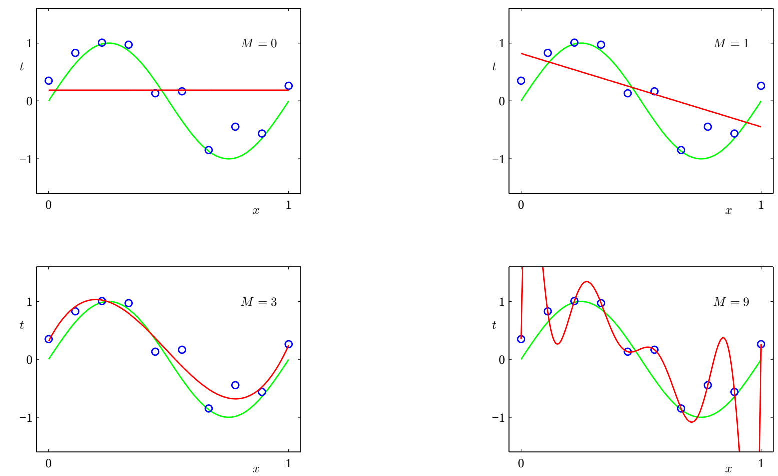
We will see more nonlinear mappings soon.

Outline

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

Should we use a very complicated mapping?

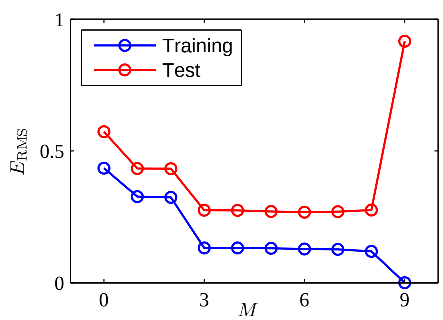
Ex: fitting a noisy sine function with a polynomial:



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**

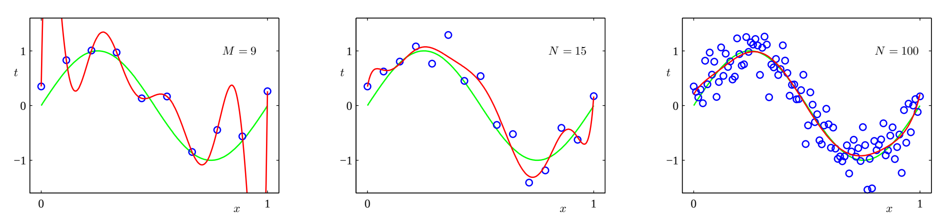


More complicated models ⇒ larger gap between training and test error

How to prevent overfitting?

Method 1: use more training data

The more, the merrier



More data ⇒ 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

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

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

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

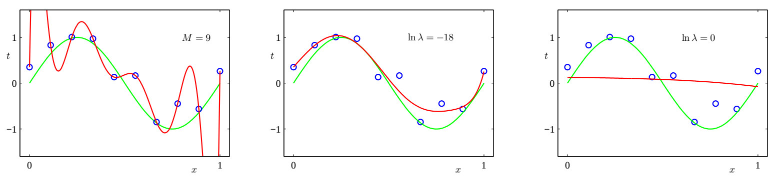
The effect of λ

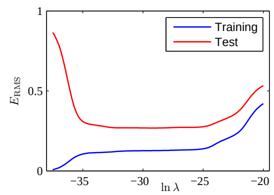
when we increase regularization coefficient λ

	$\ln\lambda = -\infty$	$\ln\lambda = -18$	$\ln\lambda = 0$
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 $R(\boldsymbol{w}) = \|\boldsymbol{w}\|_2^2$:

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

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

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

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

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)**:

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

or **regularized empirical risk minimizer**:

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

ML becomes optimization