Overfitting, Bias / Variance Analysis

Professor Ameet Talwalkar

Slide Credit: Professor Fei Sha

Outline

Announcements

- HW2 (and remaining HW1) will be returned today after class (see Nikos and Amogh)
- HW3 and HW4 due on Thursday
- No new HW assigned on Thursday (to give you time to work on project proposal)
- Project proposal guideline posted on course website last week

CS260: Project Proposal

Professor Ameet Talwalkar

Due: 11/5/15

Project proposals should be 1-2 pages long and contain the following information:

- **Motivation**: What high-level problem are you studying? Why is it important?
- **Background**: What previous work exists on your topic? How does your proposed project differ from these existing works? Note: If you have prior experience working on this problem, please clearly describe how your proposed work for this class project differs from your prior work.
- **Proposed Work**: What do you plan to do? What methods will you use and why will you use them?
- **Timeline**: What is your timeline for performing this work?
- **Deliverables / Evaluation**: What is the expected outcome of your work? How will you evaluate the quality of your work?
- **Data**: If your project involves data, what data are you using? How did you obtain this data? Why is this data interesting / relevant to your problem? What computing resources will you be using to analyze this data?
- **Software Tools / Libraries**: What (if any) software will be used for this project? Please describe any third-party software libraries you plan to use.
- **Team**: Who is working on this project (at most two students can work on a project)?
- **Prior Discussion**: You are required to discuss this project with Professor Talwalkar or one of the TAs prior to submitting your proposal. Please list who you spoke with and when. Note: You are also encouraged to speak with us as you continue working on the project if you have questions.

Outline

Linear regression 1D

Setup

- Input: $\boldsymbol{x} \in \mathbb{R}^{\mathsf{D}}$ (covariates, predictors, features, etc)
- Output: $y \in \mathbb{R}$ (responses, targets, outcomes, outputs, etc)
- Training data: $\mathcal{D} = \{(\boldsymbol{x}_n, y_n), n = 1, 2, \ldots, \mathsf{N}\}$
- Model: $f : \boldsymbol{x} \rightarrow y$, with $f(\boldsymbol{x}) = w_0 + \sum_d w_d x_d = w_0 + \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}$

  We also sometimes call $\tilde{\boldsymbol{w}} = [w_0 \; w_1 \; w_2 \; \cdots \; w_{\mathsf{D}}]^{\mathrm{T}}$ parameters too!

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Least Mean Squares (LMS) Objective: Minimize squared difference on training data (or residual sum of squares)

$$RSS(\tilde{\boldsymbol{w}}) = \sum_n [y_n - f(\boldsymbol{x}_n)]^2 = \sum_n [y_n - (w_0 + \sum_d w_d x_{nd})]^2$$

1D Solution: Identify stationary points by taking derivative with respect to parameters and setting to zero, yielding 'normal equations'

LMS when $\boldsymbol{x}$ is D-dimensional

$RSS(\tilde{w})$ in matrix form

$$RSS(\tilde{\boldsymbol{w}}) = \sum_n [y_n - (w_0 + \sum_d w_d x_{nd})]^2 = \sum_n [y_n - \tilde{\boldsymbol{w}}^{\mathrm{T}} \tilde{\boldsymbol{x}}_n]^2$$

where we have redefined some variables (by augmenting)

$$\tilde{\boldsymbol{x}} \leftarrow [1 \; x_1 \; x_2 \; \ldots \; x_{\mathsf{D}}]^{\mathrm{T}}, \quad \tilde{\boldsymbol{w}} \leftarrow [w_0 \; w_1 \; w_2 \; \ldots \; w_{\mathsf{D}}]^{\mathrm{T}}$$

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which leads to

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

$RSS(\tilde{\boldsymbol{w}})$ in new notation

Design matrix and target vector

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

Compact expression

$$RSS(\tilde{\boldsymbol{w}}) = ||\tilde{\boldsymbol{X}}\tilde{\boldsymbol{w}} - \boldsymbol{y}||_2^2 = \left\{ \tilde{\boldsymbol{w}}^{\mathrm{T}} \tilde{\boldsymbol{X}}^{\mathrm{T}} \tilde{\boldsymbol{X}} \tilde{\boldsymbol{w}} - 2 \left(\tilde{\boldsymbol{X}}^{\mathrm{T}} \boldsymbol{y} \right)^{\mathrm{T}} \tilde{\boldsymbol{w}} \right\} + \text{const}$$

Solution in matrix form

Compact expression

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Gradients of Linear and Quadratic Functions

- $\nabla_{\boldsymbol{x}} \boldsymbol{b}^{\top} \boldsymbol{x} = \boldsymbol{b}$
- $\nabla_{\boldsymbol{x}} \boldsymbol{x}^{\top} \boldsymbol{A} \boldsymbol{x} = 2\boldsymbol{A}\boldsymbol{x}$ (symmetric $\boldsymbol{A}$)

Normal equation

$$\nabla_{\tilde{\boldsymbol{w}}} RSS(\tilde{\boldsymbol{w}}) \propto \tilde{\boldsymbol{X}}^{\mathrm{T}} \tilde{\boldsymbol{X}} \boldsymbol{w} - \tilde{\boldsymbol{X}}^{\mathrm{T}} \boldsymbol{y} = 0$$

This leads to the least-mean-square (LMS) solution

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

Practical concerns

Bottleneck of computing the LMS solution

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

Matrix multiply of $\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}} \in \mathbb{R}^{(\mathsf{D}+1)\times(\mathsf{D}+1)}$
Inverting the matrix $\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}}$

Scalable methods

- Batch gradient descent
- Stochastic gradient descent

Stochastic gradient descent

Widrow-Hoff rule: update parameters using one example at a time

- Initialize $\tilde{\boldsymbol{w}}$ to $\tilde{\boldsymbol{w}}^{(0)}$ (anything reasonable is fine); set $t = 0$; choose $\eta > 0$
- Loop *until convergence*
  1. random choose a training a sample $\boldsymbol{x}_t$
  2. Compute its contribution to the gradient

$$\boldsymbol{g}_t = (\tilde{\boldsymbol{x}}_t^{\mathrm{T}} \tilde{\boldsymbol{w}}^{(t)} - y_t)\tilde{\boldsymbol{x}}_t$$

  3. Update the parameters $\tilde{\boldsymbol{w}}^{(t+1)} = \tilde{\boldsymbol{w}}^{(t)} - \eta \boldsymbol{g}_t$

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How does the complexity per iteration compare with gradient descent?

- $O(\mathrm{ND})$ for gradient descent versus $O(\mathrm{D})$ for SGD

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

Can you think of any reasons why that could happen?

Answer 1: N $<$ D. Intuitively, not enough data to estimate all the parameters.

Answer 2: $\boldsymbol{X}$ columns are not linearly independent. Intuitively, there are two features that are perfectly correlated. In this case, solution is not unique.

Ridge regression

For $\tilde{X}^{\mathrm{T}}\tilde{X}$ that is not invertible

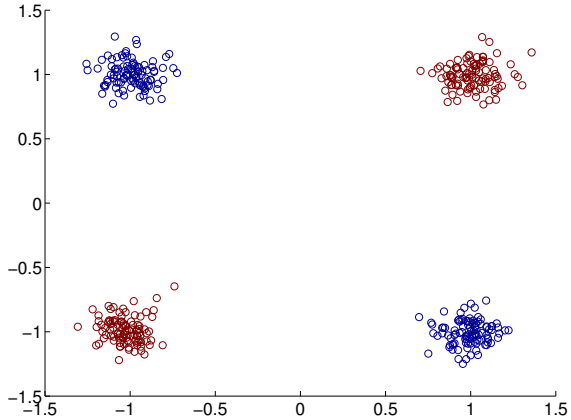
$$\tilde{\boldsymbol{w}} = \left(\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}} + \lambda \boldsymbol{I}\right)^{-1} \tilde{\boldsymbol{X}}^{\mathrm{T}}\boldsymbol{y}$$

This is equivalent to adding an extra term to $RSS(\tilde{\boldsymbol{w}})$

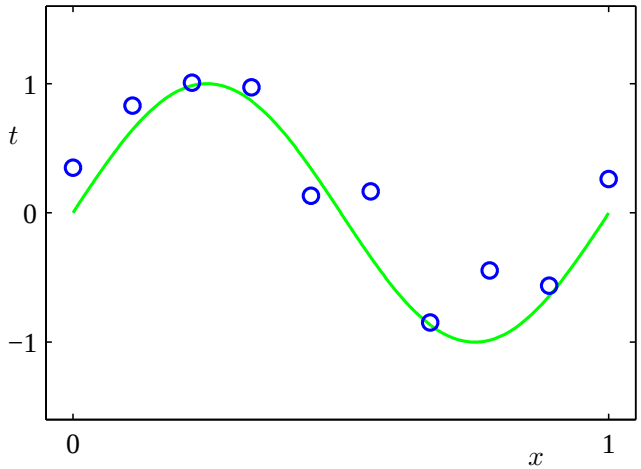
$$\overbrace{\frac{1}{2}\left\{\tilde{\boldsymbol{w}}^{\mathrm{T}}\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}}\tilde{\boldsymbol{w}} - 2\left(\tilde{\boldsymbol{X}}^{\mathrm{T}}\boldsymbol{y}\right)^{\mathrm{T}}\tilde{\boldsymbol{w}}\right\}}^{RSS(\tilde{\boldsymbol{w}})} + \underbrace{\frac{1}{2}\lambda\|\tilde{w}\|_2^2}_{\text{regularization}}$$

What if data is not linearly separable or fits to a line

Example of nonlinear classification



Example of nonlinear regression



General nonlinear basis functions

We can use a nonlinear mapping

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

where M is the dimensionality of the new feature/input $\boldsymbol{z}$ (or $\boldsymbol{\phi}(\boldsymbol{x})$). Note that M could be either greater than D or less than or the same.

With the new features, we can apply our learning techniques to minimize our errors on the transformed training data

- linear methods: prediction is based on $\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x})$
- other methods: nearest neighbors, decision trees, etc

Regression with nonlinear basis

Residual sum squares

$$\sum_n [\boldsymbol{w}^{\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x}_n) - y_n]^2$$

where $\boldsymbol{w} \in \mathbb{R}^M$, the same dimensionality as the transformed features $\boldsymbol{\phi}(\boldsymbol{x})$.

The LMS solution can be formulated with the new design matrix

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

Example with regression

Polynomial basis functions

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

Example with regression

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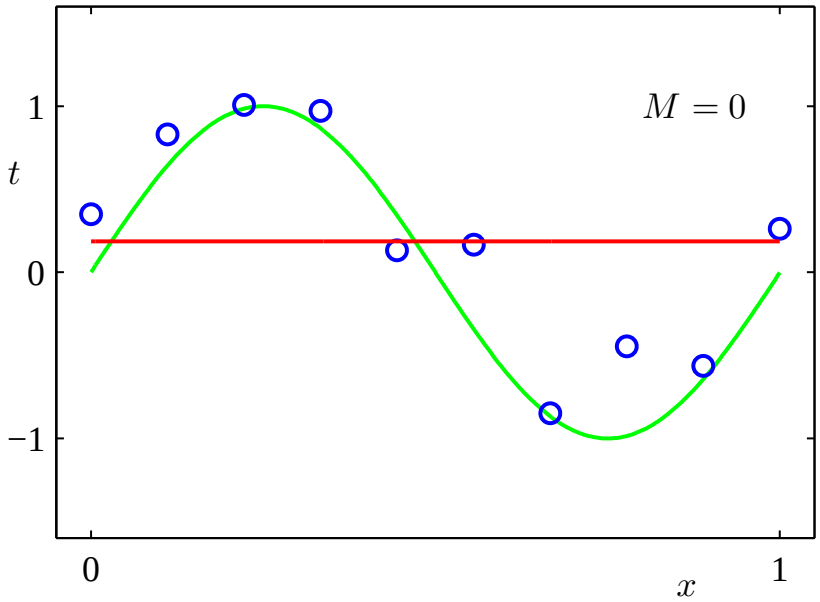
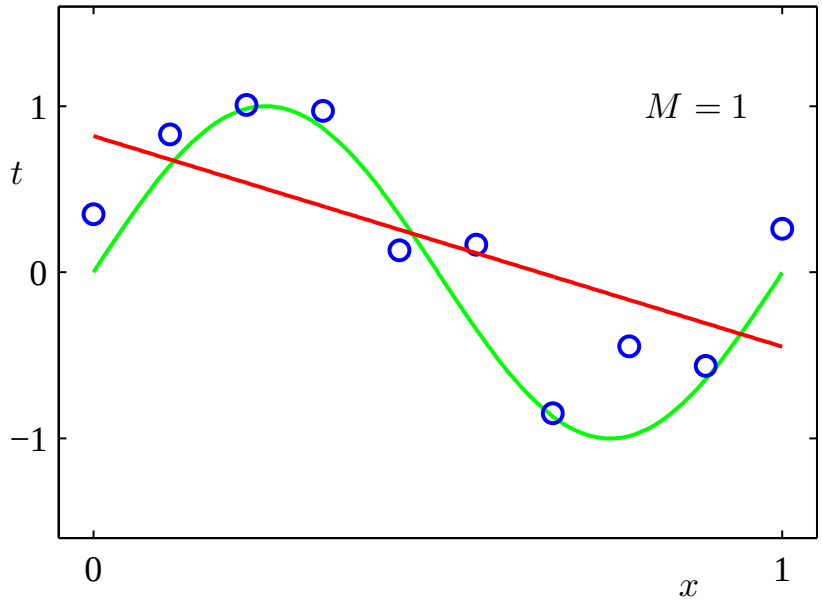
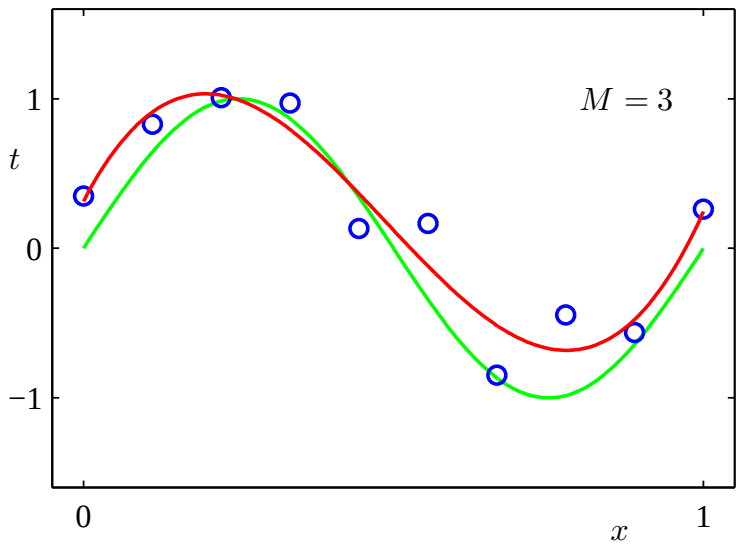
Fitting samples from a sine function: *underrfitting* as $f(x)$ is too simple





Adding high-order terms

M=3



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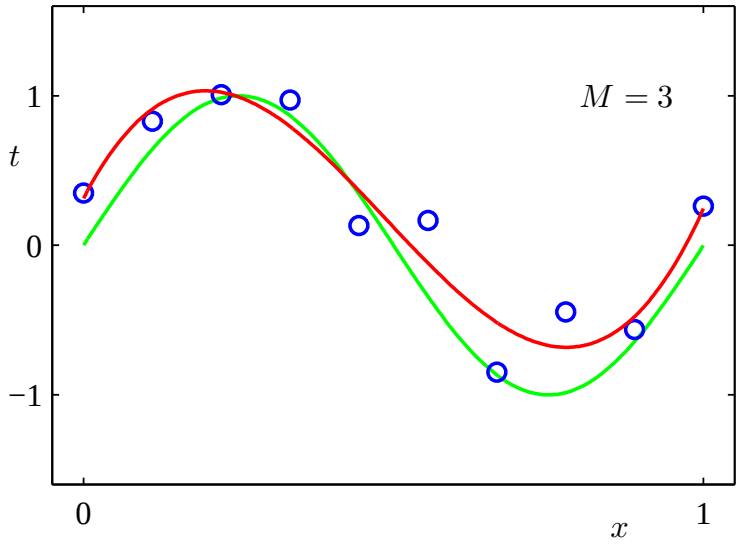
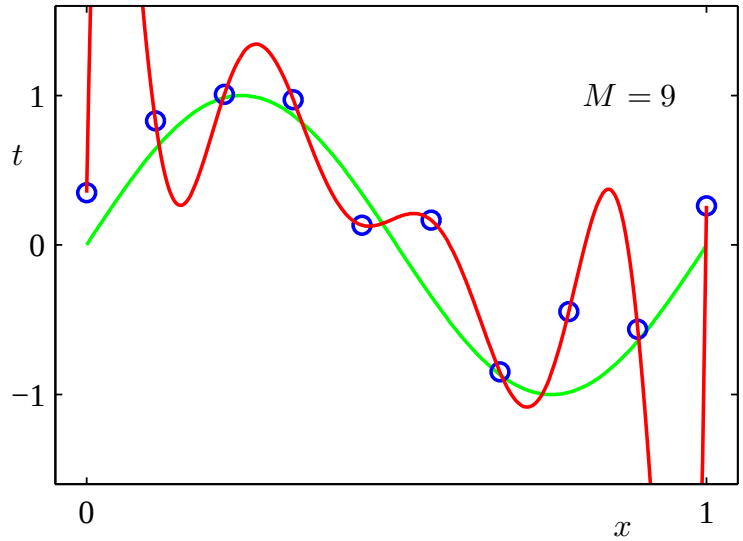


M=9: *overfitting*



More complex features lead to better results on the training data, but potentially worse results on new data, e.g., test data!

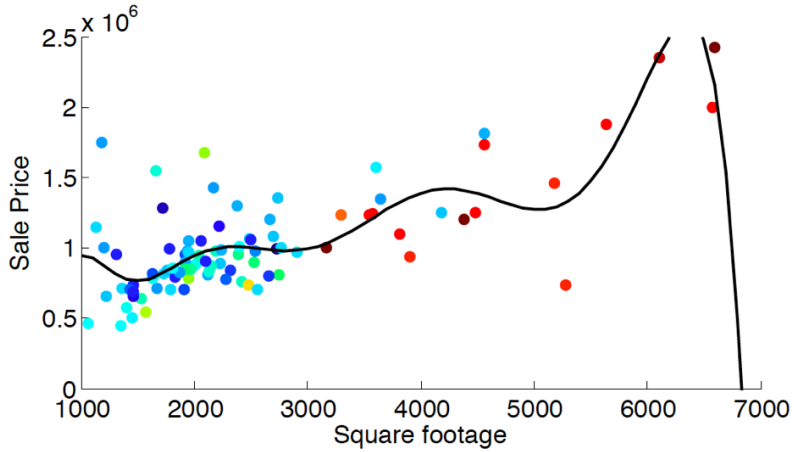
Overfitting

Parameters for higher-order polynomials are very large

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

Overfitting can be quite disastrous

Fitting the housing price data with $M = 3$



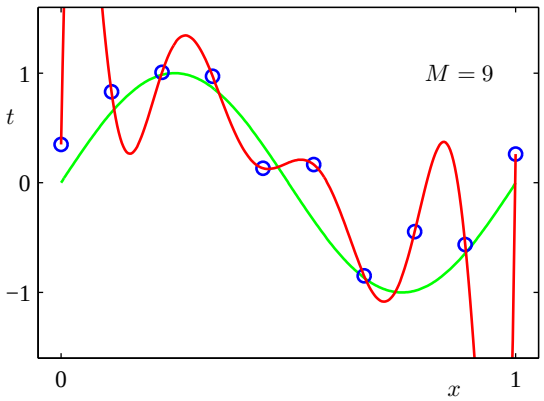
Note that the price would goes to zero (or negative) if you buy bigger ones! This is called poor generalization/overfitting.

How might we prevent overfitting?

Outline

Use more training data to prevent over fitting

The more, the merrier



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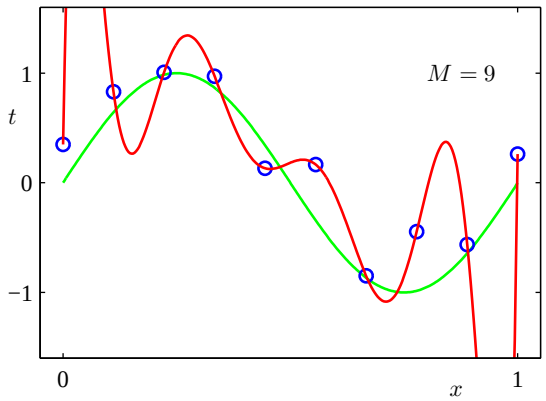

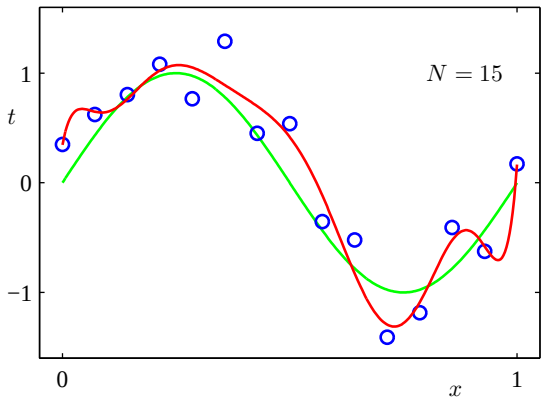

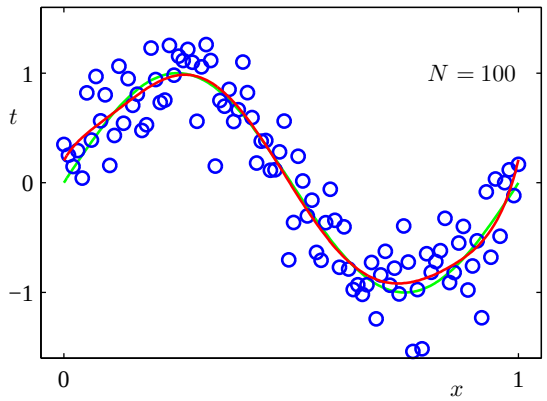

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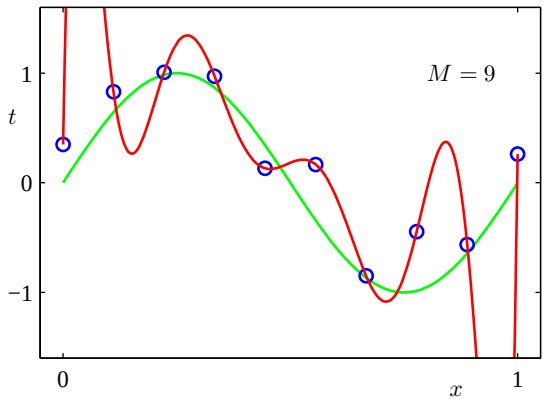

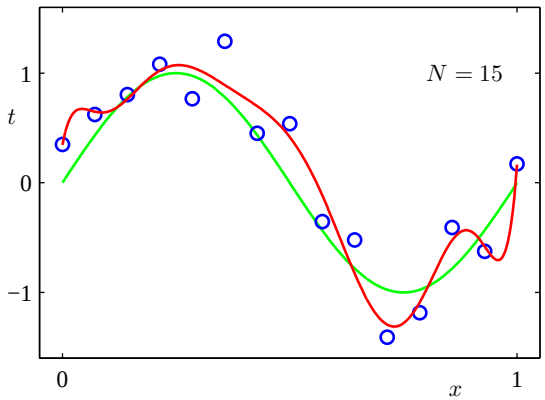

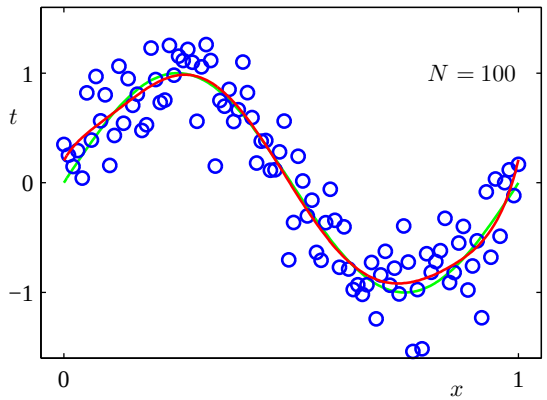

What if we do not have a lot of data?

Regularization methods

Intuition: For a linear model for regression

$$\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$$

we can try to identify 'simpler' models. But what does it mean for a model to *be simple*?

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Assumption We can place a *prior* on our weights, assuming that w_d is centered around zero.

With this reasoning, we will interpret $\boldsymbol{w}$ as a random variable and we will use the observed data $\mathcal{D}$ to update our prior belief on $\boldsymbol{w}$

Review: Probabilistic interpretation for LMS

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- LMS model: $Y = \boldsymbol{w}^\top \boldsymbol{X} + \eta$
  - $\eta \sim N(0, \sigma_0^2)$ is a Gaussian random variable
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- The likelihood function maps parameters to probabilities

$$L : \boldsymbol{w}, \sigma_0^2 \mapsto p(\boldsymbol{y}|\mathcal{D}, \boldsymbol{w}, \sigma_0^2) = \prod_n p(y_n|\boldsymbol{x}_n, \boldsymbol{w}, \sigma_0^2)$$

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- Maximizing likelihood with respect to $\boldsymbol{w}$ minimizes RSS and yields the LMS solution:

$$\boldsymbol{w}^{\text{LMS}} = \boldsymbol{w}^{\text{ML}} = \arg\max_{\boldsymbol{w}} L(\boldsymbol{w}, \sigma_0^2)$$

Probabilistic interpretation of Ridge Regression

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- Ridge Regression model: $Y = \boldsymbol{w}^\top \boldsymbol{X} + \eta$
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- To find $\boldsymbol{w}$ given data $\mathcal{D}$, we can compute posterior distribution of $\boldsymbol{w}$:

$$p(\boldsymbol{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\boldsymbol{w})p(\boldsymbol{w})}{p(\mathcal{D})}$$

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- Maximum a posterior (MAP) estimate:

$$\boldsymbol{w}^{\text{MAP}} = \arg\max_{\boldsymbol{w}} p(\boldsymbol{w}|\mathcal{D}) = \arg\max_{\boldsymbol{w}} p(\mathcal{D}, \boldsymbol{w})$$

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  - $w_d \sim N(0, \sigma^2)$ are i.i.d. Gaussian random variables (unlike before)
  - Note that all w_d share the same variance σ^2
- $\boldsymbol{w}$ is a random variable with a prior distribution (*Bayesian* interpretation)
- To find $\boldsymbol{w}$ given data $\mathcal{D}$, we can compute posterior distribution of $\boldsymbol{w}$:

$$p(\boldsymbol{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\boldsymbol{w})p(\boldsymbol{w})}{p(\mathcal{D})}$$

- Maximum a posterior (MAP) estimate:

$$\boldsymbol{w}^{\text{MAP}} = \arg\max_{\boldsymbol{w}} p(\boldsymbol{w}|\mathcal{D}) = \arg\max_{\boldsymbol{w}} p(\mathcal{D}, \boldsymbol{w})$$

- What's the relationship between MAP and MLE?

Probabilistic interpretation of Ridge Regression

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- What's the relationship between MAP and MLE?
  - MAP reduces to MLE if we assume uniform prior for $p(\boldsymbol{w})$

Estimating $\boldsymbol{w}$

- Let $X_1, \ldots, X_N$ be IID with $y|\boldsymbol{w}, \boldsymbol{x} \sim N(\boldsymbol{w}^\top \boldsymbol{x}, \sigma_0^2)$
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Joint likelihood of data and parameters (given σ_0, σ)

$$p(\mathcal{D}, \boldsymbol{w}) = p(\mathcal{D}|\boldsymbol{w})p(\boldsymbol{w}) \quad = \prod_n p(y_n|\boldsymbol{x}_n, \boldsymbol{w}) \prod_d p(w_d)$$

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MAP estimate: $\boldsymbol{w}^{\mathrm{MAP}} = \arg\max_{\boldsymbol{w}} \log p(\mathcal{D}, \boldsymbol{w})$

- As with LMS, set gradient equal to zero and solve (for $\boldsymbol{w}$)

Maximum a posterior (MAP) estimate

Regularized linear regression: a new error to minimize

$$\mathcal{E}(\boldsymbol{w}) = \sum_n (\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n - y_n)^2 + \lambda \|\boldsymbol{w}\|_2^2$$

where $\lambda > 0$ is used to denote σ_0^2/σ^2. This extra term $\|\boldsymbol{w}\|_2^2$ is called regularization/regularizer and controls the model complexity.

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- If $\lambda \to 0$, then we trust our data more. Numerically,

$$\boldsymbol{w}^{\mathrm{MAP}} \to \boldsymbol{w}^{\mathrm{LMS}} = \arg\min \sum_n (\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n - y_n)^2$$

Closed-form solution

For regularized linear regression: the solution changes very little (in form) from the LMS solution

$$\arg\min \sum_n (\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n - y_n)^2 + \lambda \|\boldsymbol{w}\|_2^2 \Rightarrow \boldsymbol{w}^{\mathrm{MAP}} = \left(\boldsymbol{X}^{\mathrm{T}} \boldsymbol{X} + \lambda \boldsymbol{I}\right)^{-1} \boldsymbol{X}^{\mathrm{T}} \boldsymbol{y}$$

and reduces to the LMS solution when $\lambda = 0$, as expected.

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and reduces to the LMS solution when $\lambda = 0$, as expected.

If we have to use numerical procedure, the gradients and the Hessian matrix would change nominally too,

$$\nabla \mathcal{E}(\boldsymbol{w}) = 2(\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}\boldsymbol{w} - \boldsymbol{X}^{\mathrm{T}}\boldsymbol{y} + \lambda \boldsymbol{w}), \qquad \boldsymbol{H} = 2(\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X} + \lambda \boldsymbol{I})$$

As long as $\lambda \geq 0$, the optimization is convex.

Example: fitting data with polynomials

Our regression model

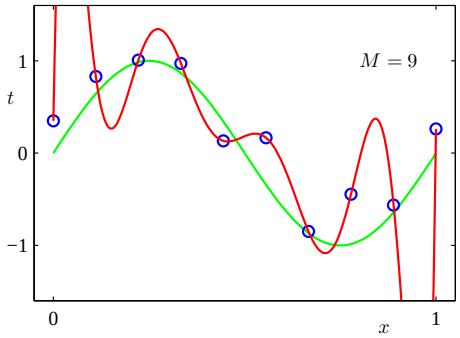
$$y = \sum_{m=1}^{M} w_m x^m$$

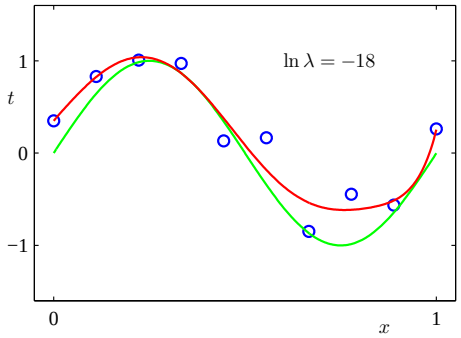
Regularization would discourage large parameter values as we saw with the LMS solution, thus potentially preventing overfitting.

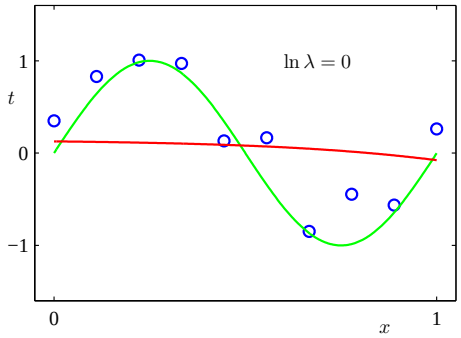
	$M=0$	$M=1$	$M=3$	$M=9$
w_0	0.19	0.82	0.31	0.35
w_1		-1.27	7.99	232.37
w_2			-25.43	-5321.83
w_3			17.37	48568.31
w_4				-231639.30
w_5				640042.26
w_6				-1061800.52
w_7				1042400.18
w_8				-557682.99
w_9				125201.43

Overfitting in terms of λ

Overfitting is reduced from complex model to simpler one with the help of increasing regularizers







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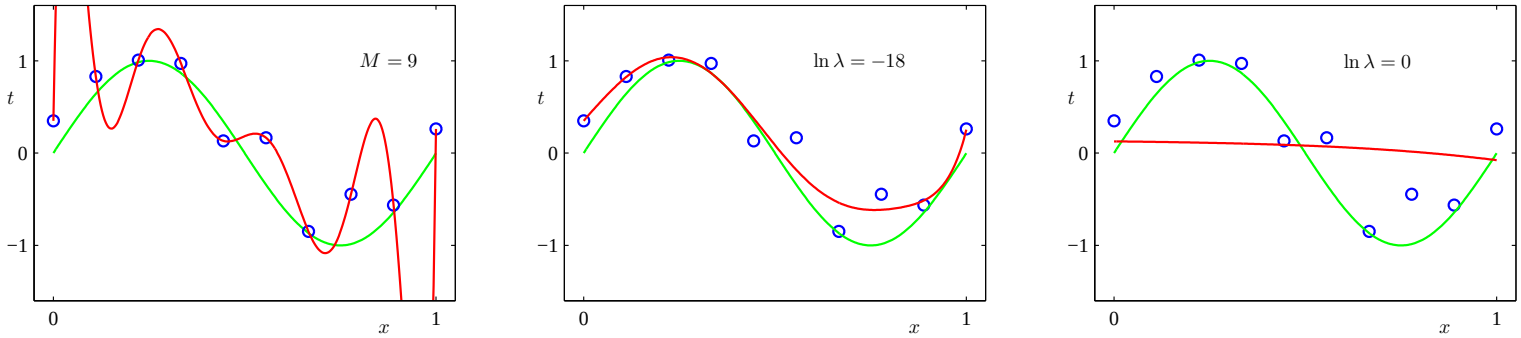
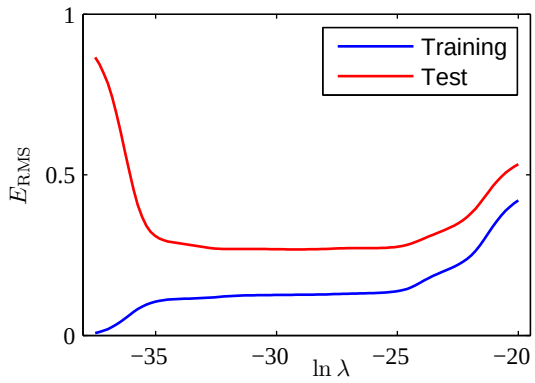


λ **vs. residual error** shows the difference of the model performance on training and testing dataset



The effect of λ

Large λ attenuates parameters towards 0

	$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
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

Regularized methods for classification

Adding regularizer to the cross-entropy functions used for binary and multinomial logistic regression

$$\mathcal{E}(\boldsymbol{w}) = -\sum_n \{y_n \log \sigma(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n) + (1-y_n)\log[1-\sigma(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n)]\} + \lambda\|\boldsymbol{w}\|_2^2$$

$$\mathcal{E}(\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_K) = -\sum_n \sum_k \log P(C_k|\boldsymbol{x}_n) + \lambda \sum_k \|\boldsymbol{w}_k\|_2^2$$

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Numerical optimization

- Objective functions remain to be convex as long as $\lambda \geq 0$.
- Gradients and Hessians are changed marginally and can be easily derived.

How to choose the right amount of regularization?

Can we tune λ on the training dataset?

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No: as this will set λ to zero, i.e., without regularization, defeating our intention to use it to control model complexity and to gain better generalization.

λ is thus a hyperparmeter. To tune it,

- We can use a development/holdout dataset independent of training and testing dataset.
- We can do leave-one-out (LOO)

The procedure is similar to choose K in the nearest neighbor classifiers.

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The procedure is similar to choose K in the nearest neighbor classifiers.

For different λ, we get $\boldsymbol{w}^{\text{MAP}}$ and evaluate the model on the development/holdout dataset (or, the samples being left in LOO).

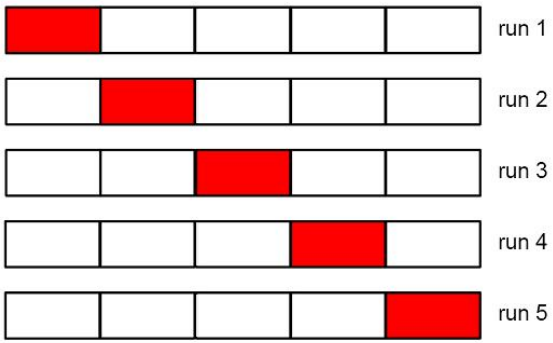
We then plot the curve λ versus prediction error (accuracy, classification error) and find the place that the performance on the holdout/LOO is the best.

Use cross-validation to choose λ

Procedure

- Randomly partition training data into K *disjoint* parts
  Normally, K is chosen to be 10, 5, etc.
- For each possible value of λ
  1. Use one part as holdout; use other $(K-1)$ parts as training
  2. Evaluate the model on the holdout
  3. Do this K times, and average the performance on the holdouts
- Choose the λ with the best performance

When $K = N$ (the number of training examples), this becomes LOO.



Outline

Basic and important machine learning concepts

Supervised learning

We aim to build a function $h(\boldsymbol{x})$ to predict the true value y associated with $\boldsymbol{x}$. If we make a mistake, we incur a *loss*

$$\ell(h(\boldsymbol{x}), y)$$

Basic and important machine learning concepts

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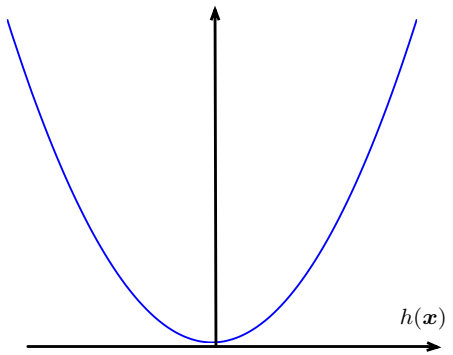
$$\ell(h(\boldsymbol{x}), y)$$

Example: quadratic loss function for regression when y is continuous

$$\ell(h(\boldsymbol{x}), y) = [h(\boldsymbol{x}) - y]^2$$

Ex: when $y = 0$

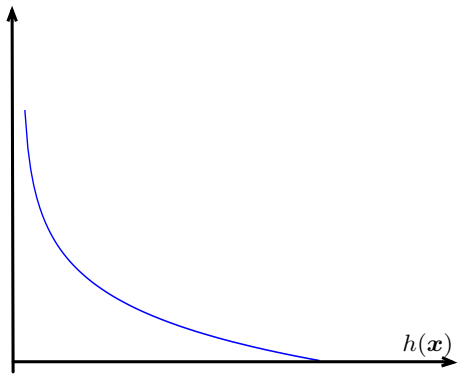


Other types of loss functions

For classification: cross-entropy loss (also called $logistic$ loss)

$$\ell(h(\boldsymbol{x}), y) = -y \log h(\boldsymbol{x}) - (1-y) \log[1-h(\boldsymbol{x})]$$

Ex: when $y = 1$



Measure how good our predictor is

Risk: assume we know the true distribution of data $p(\boldsymbol{x}, y)$, the *risk* is

$$R[h(\boldsymbol{x})] = \int_{\boldsymbol{x},y} \ell(h(\boldsymbol{x}), y) p(\boldsymbol{x}, y) d\boldsymbol{x} d\, y$$

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Intuitively, as $N \to +\infty$,

$$R^{\text{EMP}}[h(\boldsymbol{x})] \to R[h(\boldsymbol{x})]$$

How this relates to what we have learned?

So far, we have been doing empirical risk minimization (ERM)

- For linear regression, $h(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$, and we use squared loss
- For logistic regression, $h(\boldsymbol{x}) = \sigma(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x})$, and we use cross-entropy loss

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ERM might be problematic

- If $h(\boldsymbol{x})$ is complicated enough,

$$R^{\mathrm{EMP}}[h(\boldsymbol{x})] \to 0$$

- But then $h(\boldsymbol{x})$ is unlikely to do well in predicting things out of the training dataset $\mathcal{D}$
- This is called *poor generalization* or *overfitting*. We have just discussed approaches to address this issue.
- Let's try to understand why regularization might work from the context of the bias-variance tradeoff, focusing on regression / squared loss

Bias/variance tradeoff (Looking ahead)

Error decomposes into 3 terms

$$\mathbb{E}_{\mathcal{D}} R[h_{\mathcal{D}}(\boldsymbol{x})] = \text{VARIANCE} + \text{BIAS}^2 + \text{NOISE}$$

We will prove this result, and interpret what it means...