Overfitting, Bias / Variance Analysis

Professor Ameet Talwalkar

Outline

1. Administration
2. Review of last lecture
3. Basic ideas to overcome overfitting
4. Bias/Variance Analysis

Announcements

- HW2 will be returned in section on Friday
- HW3 due in class next Monday
- Midterm is next Wednesday

Midterm

- Next Wednesday in class from 10am - 11:50am
- Completely closed-book (no notes allowed)
- Will include roughly 6 short answer questions and 3 long questions
  - Short questions should take 5 minutes on average
  - Long questions should take 15 minutes each
- Covers all material through (and including) today's lecture
  - Goal is to test conceptual understanding of the course material
  - Suggestion: carefully review lecture notes and problem sets
- Office hours / Section (see timing on course website)

Outline

Linear regression

Setup

- Input: $\boldsymbol{x} \in \mathbb{R}^{\mathsf{D}}$ (covariates, predictors, features, etc)
- Output: $y \in \mathbb{R}$ (responses, targets, outcomes, outputs, etc)
- Model: $f : \boldsymbol{x} \rightarrow y$, with $f(\boldsymbol{x}) = w_0 + \sum_d w_d x_d = w_0 + \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$
  - $\boldsymbol{w} = [w_1 \ w_2 \ \cdots \ w_{\mathsf{D}}]^{\mathrm{T}}$: *weights*, *parameters*, or *parameter vector*
  - w_0 is called *bias*
  - 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)

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

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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

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

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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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\end{aligned}$$

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

From previous slide

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

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Design matrix and target vector

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

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Solution in matrix form

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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 $\boldsymbol{A}$)

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Normal equation

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

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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

(Batch) Gradient Descent

- Initialize $\tilde{\boldsymbol{w}}$ to $\tilde{\boldsymbol{w}}^{(0)}$ (e.g., randomly); set $t = 0$; choose $\eta > 0$
- Loop *until convergence*
  1. Compute the gradient
     $\nabla RSS(\tilde{\boldsymbol{w}}) = \tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}}\tilde{\boldsymbol{w}}^{(t)} - \tilde{\boldsymbol{X}}^{\mathrm{T}}\boldsymbol{y}$
  2. Update the parameters
     $\tilde{\boldsymbol{w}}^{(t+1)} = \tilde{\boldsymbol{w}}^{(t)} - \eta\nabla RSS(\tilde{\boldsymbol{w}})$
  3. $t \leftarrow t + 1$

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What is the complexity of each iteration? $O(\text{ND})$

Why does this work? $RSS(\tilde{\boldsymbol{w}})$ is convex (Hessian is PSD)

Stochastic gradient descent

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

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

Answer 2: Columns of $\boldsymbol{X}$ are not linearly independent, e.g., some features are perfectly correlated. In this case, solution is not unique.

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- Add regularizer so that all singular values are at least $\lambda > 0$!
- This is equivalent to adding an extra term to $RSS(\tilde{\boldsymbol{w}})$

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

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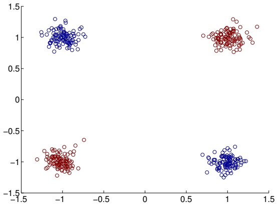
Solution

- Can derive normal equations as before
- Solution is of the form:

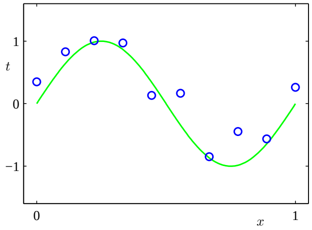
$$\tilde{\boldsymbol{w}} = \left(\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}} + \lambda\boldsymbol{I}\right)^{-1}\tilde{\boldsymbol{X}}^{\mathrm{T}}\boldsymbol{y}$$

Is a linear modeling assumption always a good idea?

Example of nonlinear classification



Example of nonlinear regression



General nonlinear basis functions

We can use a nonlinear mapping

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

- M is dimensionality of new features $\boldsymbol{z}$ (or $\phi(\boldsymbol{x})$)
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We can apply existing learning methods on the transformed 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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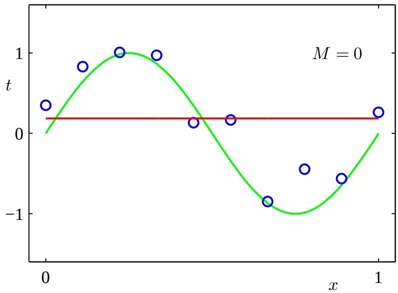
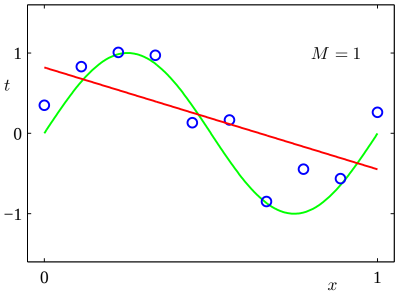
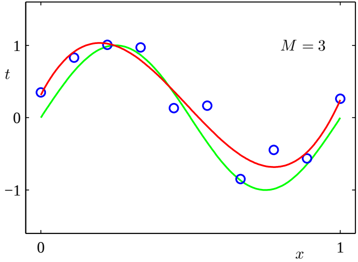
Fitting samples from a sine function: *underfitting* as $f(x)$ is too simple





Adding high-order terms

M=3



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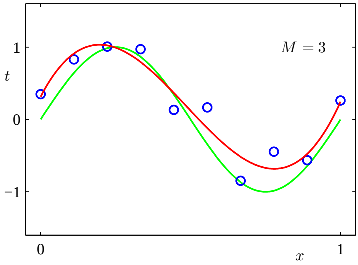
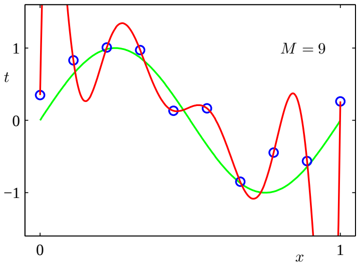


M=9: *overfitting*



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

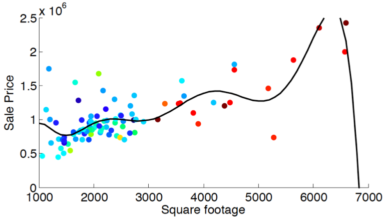
Overfitting

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 large M



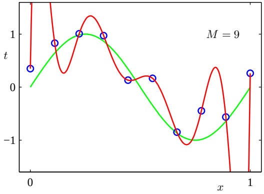
Predicted price goes to zero (and is ultimately negative) if you buy a big enough house!

How might we prevent overfitting?

Outline

Use more training data to prevent over fitting

The more, the merrier



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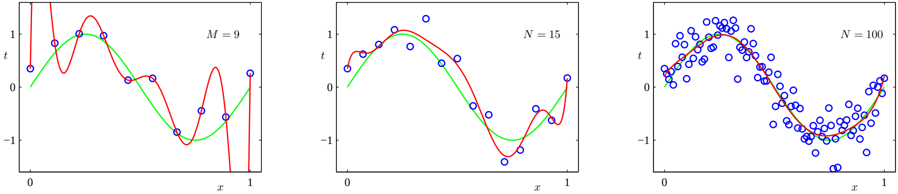
The more, the merrier



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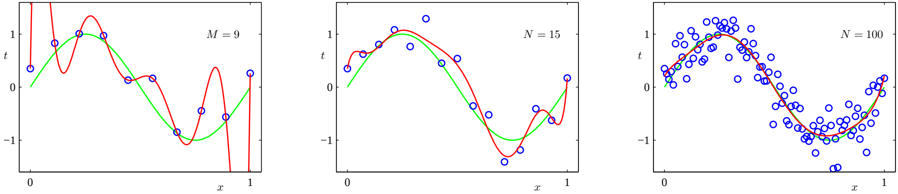

What if we do not have a lot of data?

Regularization methods

Intuition: Give preference to 'simpler' models

- How do we define a simple linear regression model — $\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$?

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Our Strategy: Place a *prior* on our weights

- Interpret $\boldsymbol{w}$ as a random variable
- Assume that each w_d is centered around zero
- Use observed data $\mathcal{D}$ to update our prior belief on $\boldsymbol{w}$

Review: Probabilistic interpretation for LMS

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

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

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- What's the relationship between MAP and MLE?
  - MAP reduces to MLE if we assume uniform prior for $p(\boldsymbol{w})$
- Fully Bayesian treatment considers entire posterior, not just the mode

Estimating $\boldsymbol{w}$

- Let $X_1, \ldots, X_N$ be IID with $y|\boldsymbol{w}, \boldsymbol{x} \sim N(\boldsymbol{w}^\top \boldsymbol{x}, \sigma_0^2)$
- Let w_d be IID with $w_d \sim N(0, \sigma^2)$

Joint likelihood of data and parameters (given σ_0, σ)

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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 $\lambda \rightarrow 0$, then we trust our data more. Numerically,

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

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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Gradients and Hessian 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

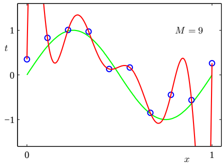
$$y = \sum_{m=1}^{M} w_m x^m$$

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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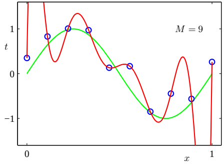

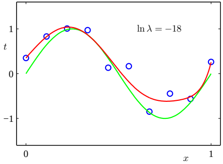

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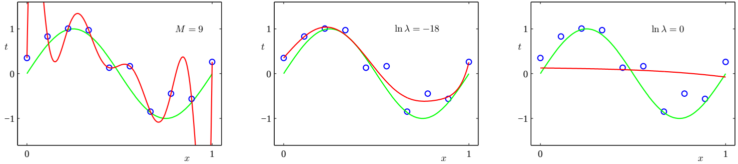

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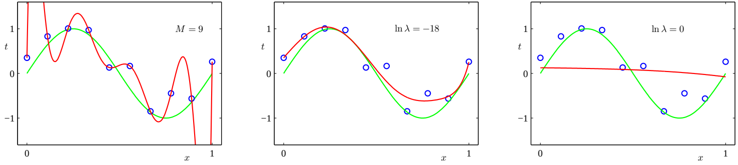
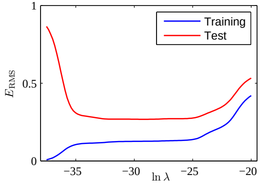


λ **vs. residual error** shows the difference of the model performance on training and testing dataset



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 change marginally and can be easily derived.

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Can we tune λ on the training dataset?

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Can we tune λ on the training dataset?

No: as this will always set λ to zero, i.e., no regularization, defeating our intention of controlling model complexity

λ is thus a hyperparemeter. To tune it,

- We can use a validation set or do cross validation (as previously discussed)

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*

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

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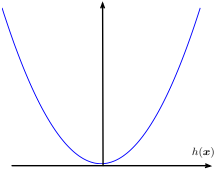
Example: quadratic loss function for regression when y is continuous

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

Ex: when $y = 0$

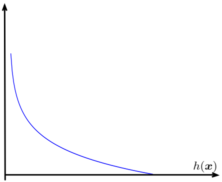


Other types of loss functions

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

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

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

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
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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

ERM might be problematic

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

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

- 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.
- We'll explore 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

$$\mathbb{E}_{\mathcal{D}} R[h_{\mathcal{D}}(\boldsymbol{x})] = \textsc{variance} + \textsc{bias}^2 + \textsc{noise}$$

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