Linear Regression (continued)

Professor Ameet Talwalkar

Outline

Announcements

- HW2 will be returned in section on Friday
- HW3 due in class next Monday
- Midterm is next Wednesday (will review in more detail next class)

Outline

Perceptron Main idea

Consider a linear model for binary classification

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

We use this model to distinguish between two classes $\{-1, +1\}$.

One goal

$$\varepsilon = \sum_{n} \mathbb{I}[y_n \neq \mathsf{sign}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n)]$$

i.e., to minimize errors on the training dataset.

Hard, but easy if we have only one training example

How can we change $\boldsymbol{w}$ such that

$$y_n = \text{sign}(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n)$$

Two cases

- If $y_n = \text{sign}(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n)$, do nothing.
- If $y_n \neq \text{sign}(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n)$, $\boldsymbol{w}^{\mathrm{NEW}} \leftarrow \boldsymbol{w}^{\mathrm{OLD}} + y_n \boldsymbol{x}_n$
  - Gauranteed to make progress, i.e., to get us closer to $y(\boldsymbol{w}^{\top} \boldsymbol{x}) > 0$

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What does update do?

$$y_n[(\boldsymbol{w} + y_n\boldsymbol{x}_n)^{\mathrm{T}}\boldsymbol{x}_n] = y_n\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n + y_n^2\boldsymbol{x}_n^{\mathrm{T}}\boldsymbol{x}_n$$

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We are adding a positive number, so it's possible that $y_n(\boldsymbol{w}^{\mathrm{NEW}\,\mathrm{T}}\boldsymbol{x}_n) > 0$

Perceptron algorithm

Iteratively solving one case at a time

- REPEAT
- Pick a data point $\boldsymbol{x}_n$ (can be a fixed order of the training instances)
- Make a prediction $y = \text{sign}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n)$ using the *current* $\boldsymbol{w}$
- If $y = y_n$, do nothing. Else,

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + y_n \boldsymbol{x}_n$$

- UNTIL converged.

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Properties

- This is an online algorithm.
- If the training data is linearly separable, the algorithm stops in a finite number of steps (we proved this).
- The parameter vector is always a linear combination of training instances (requires initialization of $\boldsymbol{w}_0 = 0$).

Regression

Predicting a continuous outcome variable

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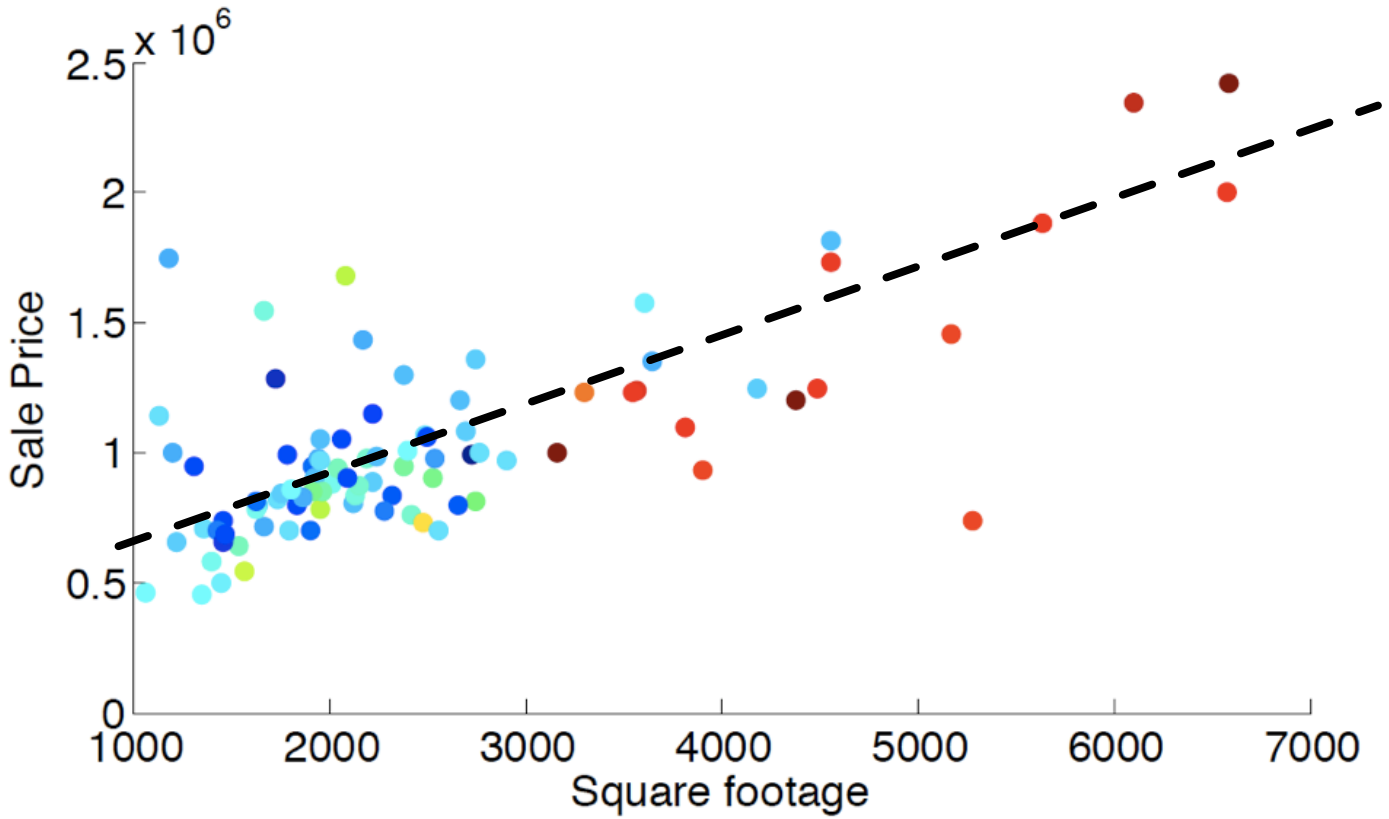
Key difference from classification

- We can measure 'closeness' of prediction and labels
  - Predicting shoe size: better to be off by one size than by 5 sizes
  - Predicting song year: better to be off by one year than by 20 years
- As opposed to 0-1 classification error, we will focus on squared difference, i.e., $(\hat{y} - y)^2$

1D example: predicting the sale price of a house



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

Minimize squared errors

Our model

Sale price = price_per_sqft $\times$ square_footage + fixed_expense + unexplainable_stuff

Training data

sqft	sale price	prediction	error	squared error
2000	810K	720K	90K	8100
2100	907K	800K	107K	107^2
1100	312K	350K	38K	38^2
5500	2,600K	2,600K	0	0
...	...			
Total				$8100 + 107^2 + 38^2 + 0 + \cdots$

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Aim

Adjust price_per_sqft and fixed_expense such that the sum of the squared error is minimized — i.e., unexplainable_stuff is minimized.

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: $f : \boldsymbol{x} \to y$, with $f(\boldsymbol{x}) = w_0 + \sum_d w_d x_d = w_0 + \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}$

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  - $\boldsymbol{w} = [w_1 \; w_2 \; \cdots \; w_{\mathrm{D}}]^{\mathrm{T}}$: *weights*, *parameters*, or *parameter vector*
  - w_0 is called *bias*
  - We also sometimes call $\tilde{\boldsymbol{w}} = [w_0 \; w_1 \; w_2 \; \cdots \; w_{\mathrm{D}}]^{\mathrm{T}}$ 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'

Probabilistic interpretation

- Noisy observation model

$$Y = w_0 + w_1 X + \eta$$

where $\eta \sim N(0, \sigma^2)$ is a Gaussian random variable

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- Likelihood of one training sample (x_n, y_n)

$$p(y_n|x_n) = N(w_0 + w_1 x_n, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{[y_n - (w_0 + w_1 x_n)]^2}{2\sigma^2}}$$

Maximum likelihood estimation

- Maximize over w_0 and w_1

$$\max \ \log P(\mathcal{D}) \Leftrightarrow \min \ \sum_n [y_n - (w_0 + w_1 x_n)]^2 \leftarrow \text{That is RSS}(\tilde{\boldsymbol{w}})!$$

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- Maximize over $s = \sigma^2$

$$\frac{\partial \log P(\mathcal{D})}{\partial s} = -\frac{1}{2}\left\{-\frac{1}{s^2}\sum_n [y_n - (w_0 + w_1 x_n)]^2 + \mathsf{N}\frac{1}{s}\right\} = 0$$

$$\rightarrow \sigma^{*2} = s^* = \frac{1}{\mathsf{N}}\sum_n [y_n - (w_0 + w_1 x_n)]^2$$

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- It gives a solid footing to our intuition: minimizing $\text{RSS}(\tilde{\boldsymbol{w}})$ is a sensible thing based on reasonable modeling assumptions
- Estimating σ^* tells us how much noise there could be in our predictions. For example, it allows us to place confidence intervals around our predictions.

Outline

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

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

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

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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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LMS when x is D-dimensional

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Matrix Multiplication via Inner Products

Each entry of output matrix is result of inner product of inputs matrices

$$\begin{bmatrix} 9 & 3 & 5 \\ 4 & 1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 3 & -5 \\ 2 & 3 \end{bmatrix} = \begin{bmatrix} & \\ & \end{bmatrix}$$

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Output matrix is **sum of outer products** between corresponding rows and columns of input matrices

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$RSS(\tilde{\boldsymbol{w}})$ 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

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

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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 $\boldsymbol{A}$)

Solution in matrix form

Compact expression

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

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

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

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

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

Mini-Summary

- Linear regression is the linear combination of features
  $f : \boldsymbol{x} \rightarrow y$, with $f(\boldsymbol{x}) = w_0 + \sum_d w_d x_d = w_0 + \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}$
- If we minimize residual sum of squares as our learning objective, we get a closed-form solution of parameters
- Probabilistic interpretation: maximum likelihood if assuming residual is Gaussian distributed

Computational complexity

Bottleneck of computing the solution?

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How many operations do we need?

- $O(\mathsf{ND}^2)$ for matrix multiplication
- $O(\mathsf{D}^3)$ (e.g., using Gauss-Jordan elimination) or $O(\mathsf{D}^{2.373})$ (recent theoretical advances) for matrix inversion
- Impractical for very large D or N

Alternative method: an example of using numerical optimization

(Batch) Gradient descent

- Initialize $\tilde{\boldsymbol{w}}$ to $\tilde{\boldsymbol{w}}^{(0)}$ (e.g., randomly); set $t = 0$; choose $\eta > 0$

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What is the complexity of each iteration?

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$\tilde{\boldsymbol{X}}^{\mathrm{T}} \tilde{\boldsymbol{X}}$ is positive semidefinite, because for any $\boldsymbol{v}$

$$\boldsymbol{v}^{\mathrm{T}} \tilde{\boldsymbol{X}}^{\mathrm{T}} \tilde{\boldsymbol{X}} \boldsymbol{v} = \| \tilde{\boldsymbol{X}}^{\mathrm{T}} \boldsymbol{v} \|_2^2 \geq 0$$

Stochastic gradient descent

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How does the complexity per iteration compare with gradient descent?

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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

Mini-summary

- Batch gradient descent computes the exact gradient.
- Stochastic gradient descent approximates the gradient with a single data point; Its expectation equals the true gradient.
- Mini-batch variant: trade-off between accuracy of estimating gradient and computational cost
- Similar ideas extend to other ML optimization problems.
  - For large-scale problems, stochastic gradient descent often works well.

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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.

Ridge regression

Intuition: what does a non-invertible $\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}}$ mean? Consider the SVD of this matrix:

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$$\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}} = \boldsymbol{U}\begin{bmatrix} \lambda_1 & 0 & 0 & \cdots & 0 \\ 0 & \lambda_2 & 0 & \cdots & 0 \\ 0 & \cdots & \cdots & \cdots & 0 \\ 0 & \cdots & \cdots & \lambda_r & 0 \\ 0 & \cdots & \cdots & 0 & 0 \end{bmatrix}\boldsymbol{U}^{\top}$$

where $\lambda_1 \geq \lambda_2 \geq \cdots \lambda_r > 0$ and $r <$ D.

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where $\lambda_1 \geq \lambda_2 \geq \cdots \lambda_r > 0$ and $r <$ D.

Fix the problem by ensuring all singular values are non-zero

$$\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}} + \lambda\boldsymbol{I} = \boldsymbol{U}\mathrm{diag}(\lambda_1 + \lambda, \lambda_2 + \lambda, \cdots, \lambda)\boldsymbol{U}^{\top}$$

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

Regularized least square (ridge regression)

Solution

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

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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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Benefits

- Numerically more stable, invertible matrix
- Prevent overfitting — more on this later

How to choose λ?

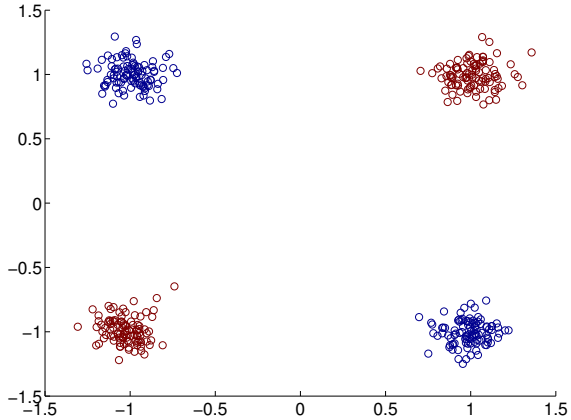
λ is referred as *hyperparameter*

- In contrast $\boldsymbol{w}$ is the parameter vector
- Use validation set or cross-validation to find good choice of λ

Outline

Is a linear modeling assumption always a good idea?

Example of nonlinear classification



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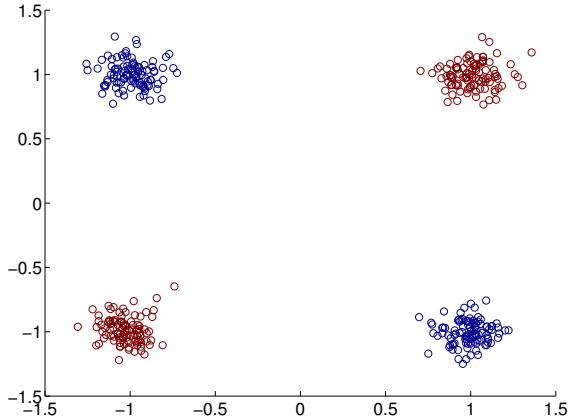
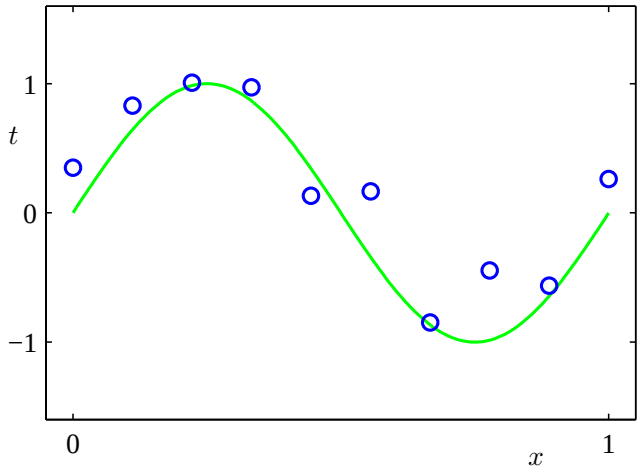


Example of nonlinear regression



Nonlinear basis for classification

Transform the input/feature

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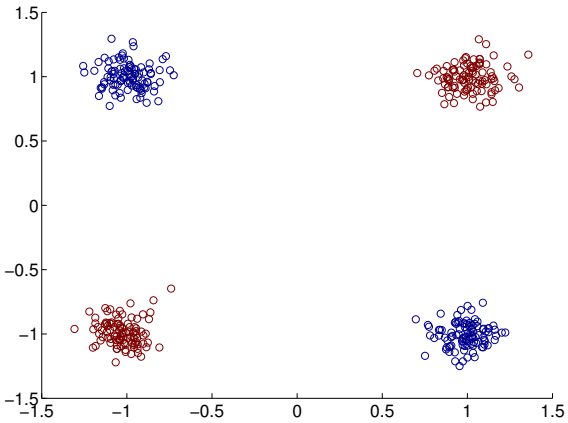
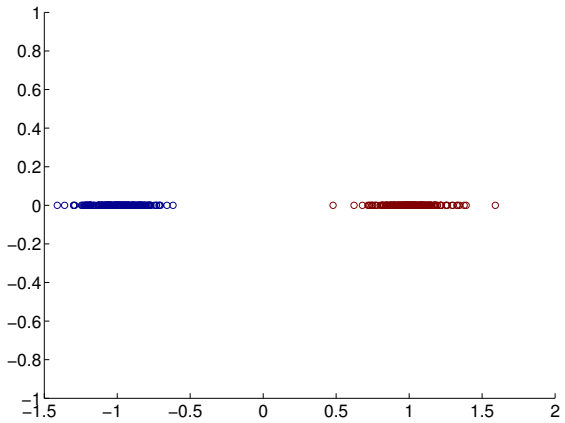
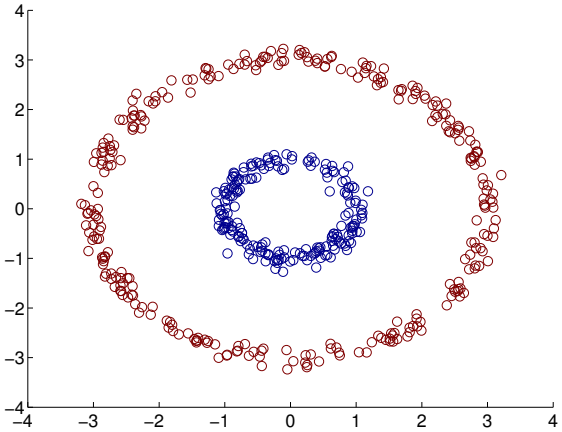
Transformed training data: linearly separable!





Another example



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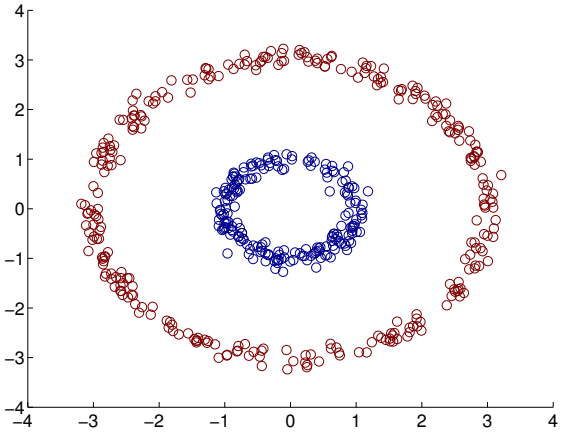

How to transform the input/feature?

$$\boldsymbol{\phi}(\boldsymbol{x}) : \boldsymbol{x} \in \mathbb{R}^2 \rightarrow \boldsymbol{z} = \begin{bmatrix} x_1^2 \\ x_1 \cdot x_2 \\ x_2^2 \end{bmatrix} \in \mathbb{R}^3$$

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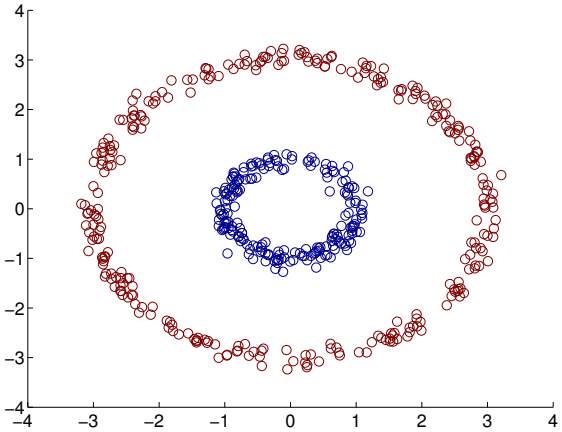

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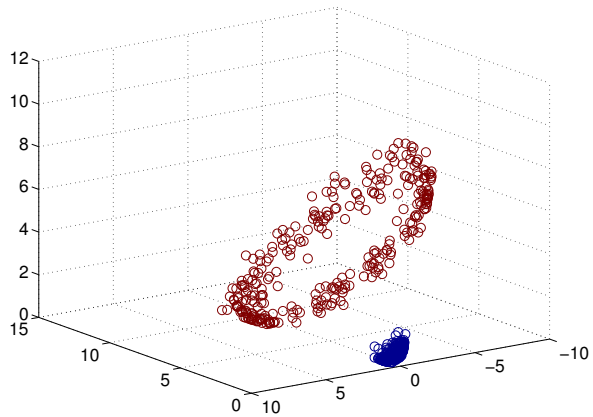

General nonlinear basis functions

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 $\boldsymbol{\phi}(\boldsymbol{x})$).

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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 $\boldsymbol{\phi}(\boldsymbol{x})$.

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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

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

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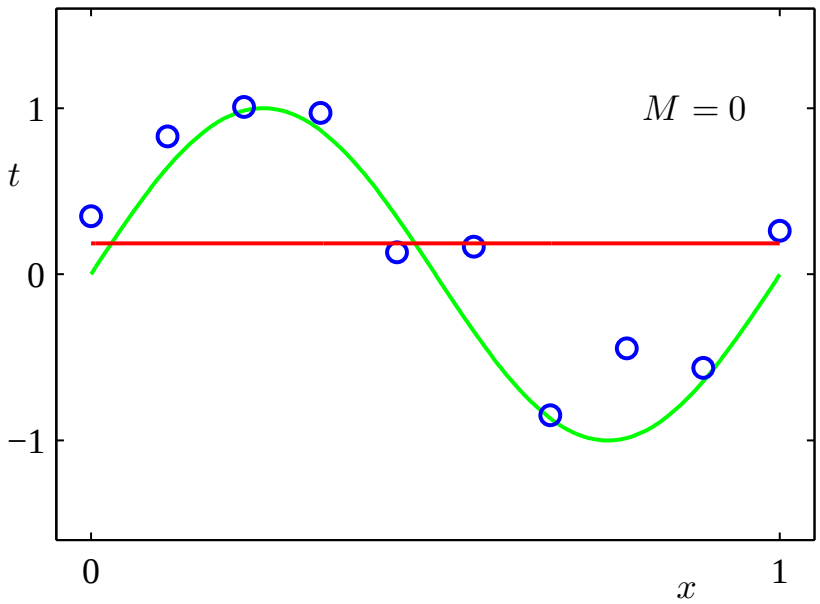
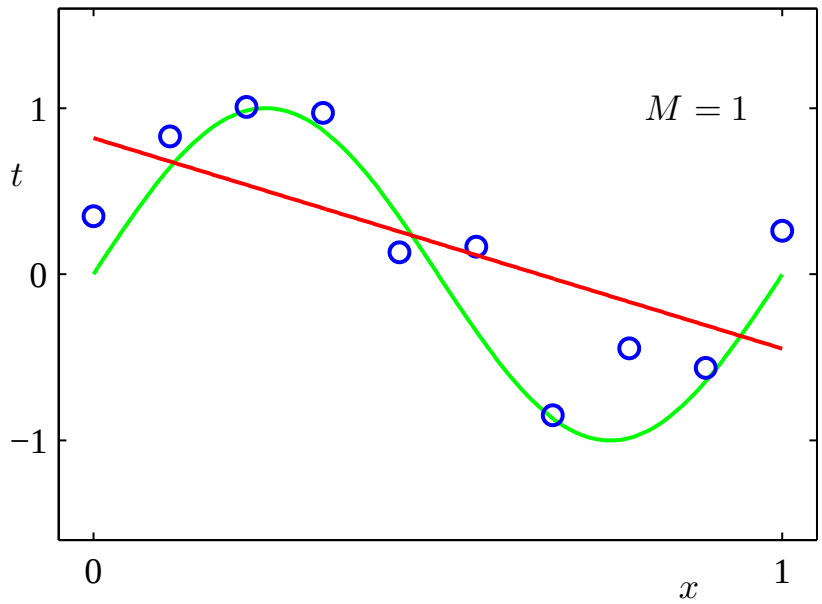
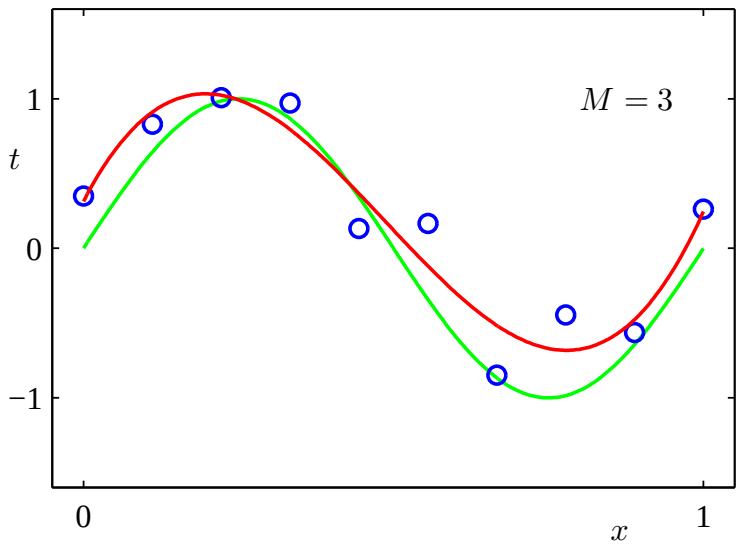
Fitting samples from a sine function: *underrfitting* as $f(x)$ is too simple





Adding high-order terms

M=3



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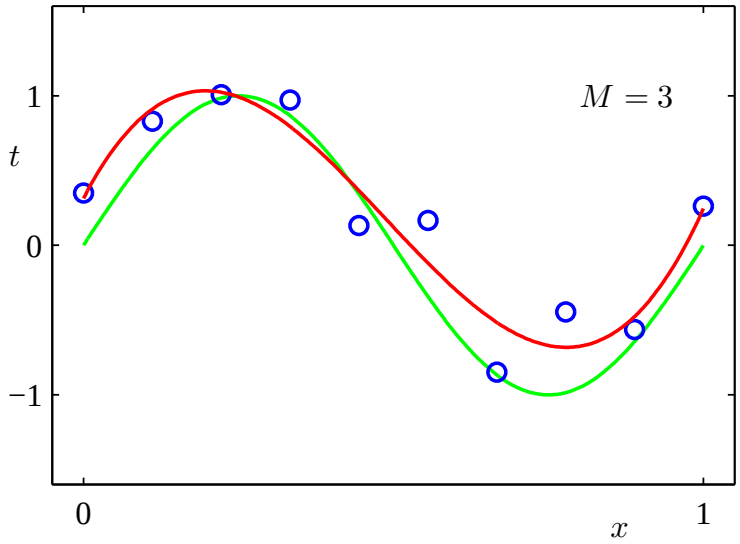
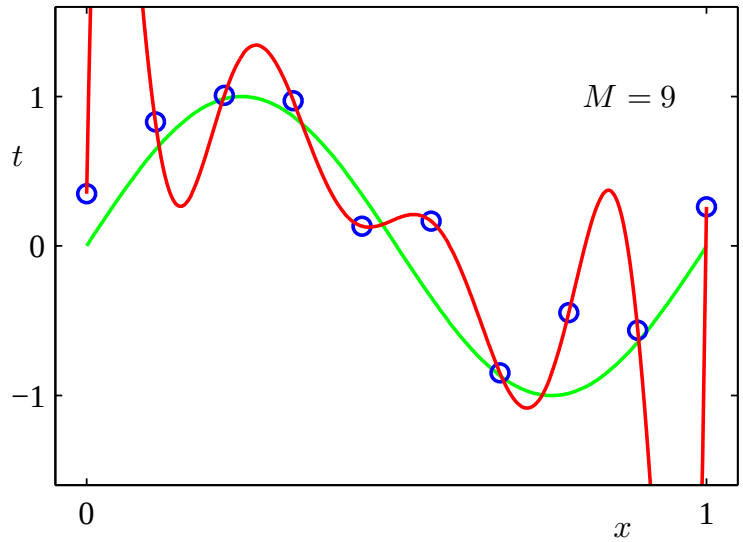


M=9: *overfitting*



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

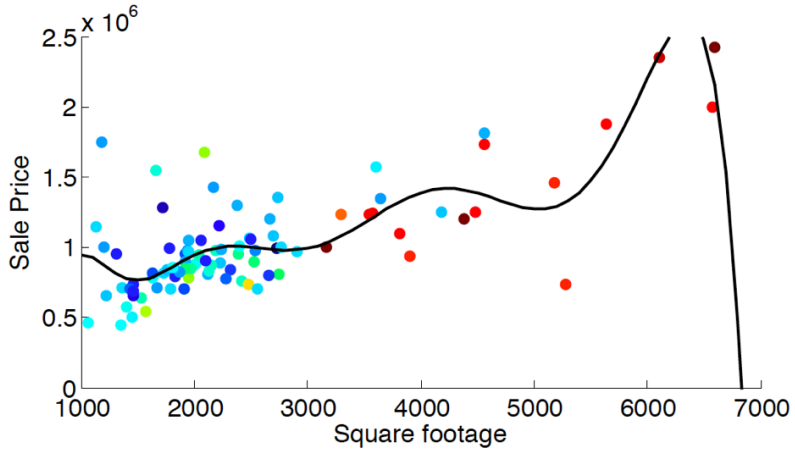
Overfiting

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



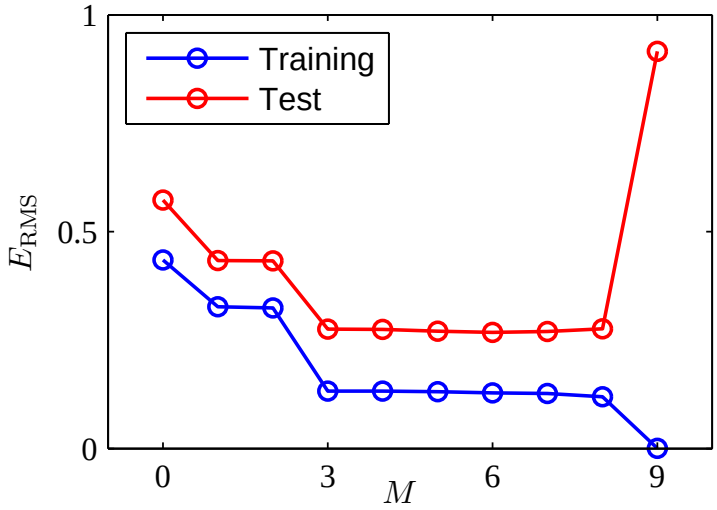
Predicted price goes to zero (and is ultimately negative) if you buy a big enough house!

This is called poor generalization/overfitting.

Detecting overfitting

Plot model complexity versus objective function

- X axis: model complexity, e.g., M
- Y axis: error, e.g., RSS, RMS (square root of RSS), 0-1 loss



As a model increases in complexity:

- Training error keeps improving
- Test error may first improve but eventually will deteriorate