Chapter 5. Machine Learning Basics

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August 25th, 2018

Outline

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- The Task, T: Classification, Regression, Transcription, Structured output, Anomaly detection, Denoising, Density estimation, etc.
- The Performance Measure, P: Error rate (the expected 0-1 loss), MSE, etc.
- The Experience, E: Supervised learning, Unsupervised learning, Reinforcement learning (fixed dataset or not), etc.

An Example: Linear Regression

- T: To build a linear system that can take a vector $\mathbf{x} \in \mathbb{R}^n$ as input and predict the value of a scalar $y \in \mathbb{R}^n$ as its output as

$$\hat{y} = \mathbf{w}^T \mathbf{x}, \tag{1}$$

  where $\mathbf{w} \in \mathbb{R}^n$ is a vector of parameters.

- P: To compute MSE of the model on the test set:

$$\mathrm{MSE}_{\mathrm{test}} = \frac{1}{m} \|\hat{\mathbf{y}}^{\mathrm{test}} - \hat{\mathbf{y}}^{\mathrm{test}}\|_2^2. \tag{2}$$

- E: To design an algorithm that will improve the weights $\mathbf{w}$ in a way that reduce $\mathrm{MSE}_{\mathrm{test}}$ when the algorithm can observe a training set $\{\mathbf{X}^{\mathrm{test}}, \mathbf{y}^{\mathrm{test}}\}$. (Solved by the normal equations)

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Capacity, Overfitting and Underfitting

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- Two factors correspond to underfitting and overfitting:
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  2. Make the gap between training and test error small.
- Capacity is defined by the ability to fit a wide variety of functions. We can control whether a model is more likely to be overfit or underfit by altering its capacity.

Capacity, Overfitting and Underfitting

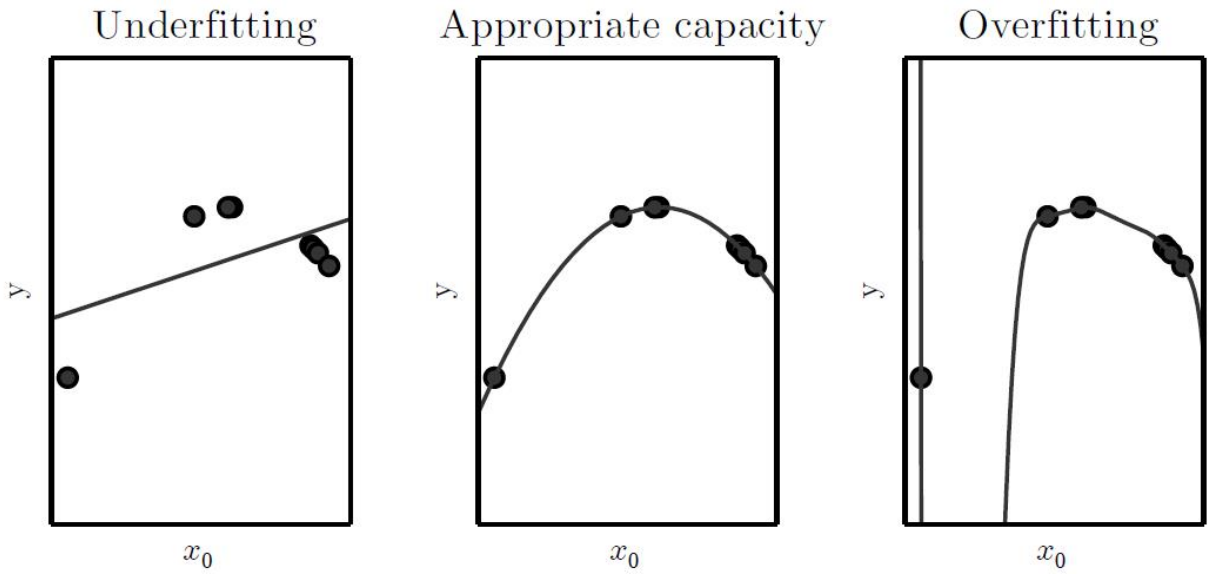

Figure: (Left)A linear function fit to the date suffers from underfitting. (Center)A quadratic function fit to the date generalizes well to unseen points. (Right)A polynomial of degree 9 fit to the data suffers from overfitting.

Capacity, Overfitting and Underfitting

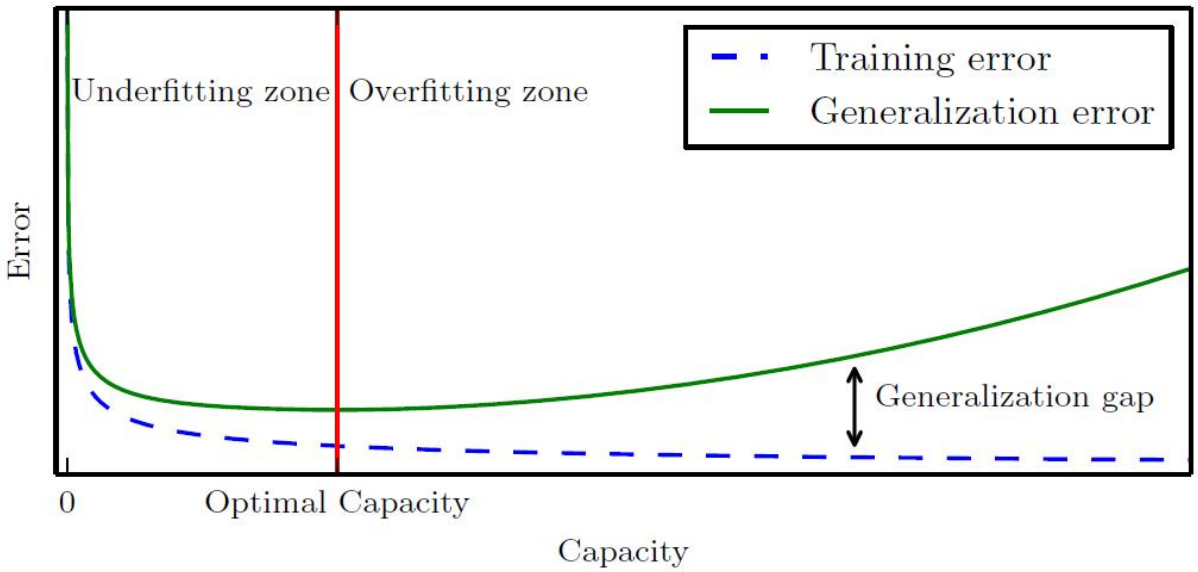

Figure: Typical relationship between capacity and error.

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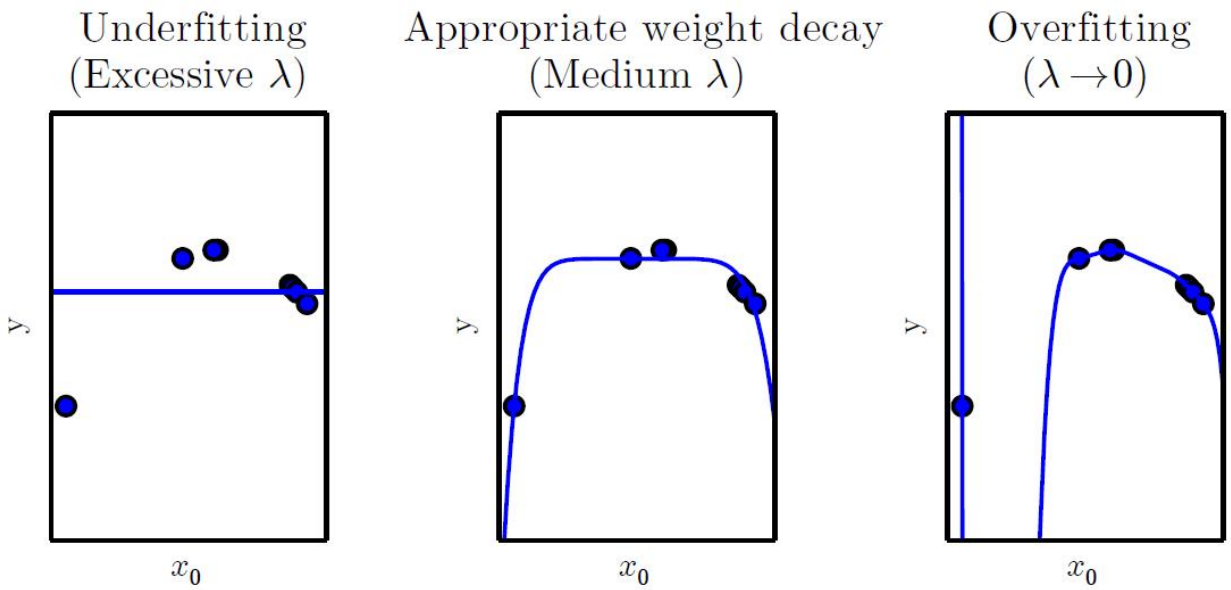

Figure: Example: Fit a high-degree polynomial regression model. The true function is quadratic, but here we use only models with degree 9. We vary the amount of weight decay to prevent these high-degree models from overfitting.

Validation Sets

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- Cross-validation: When the dataset is small, repeating the training and testing computation on different randomly chosen subsets or splits of the original sets.

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- Examples: Logistic Regression, Support Vector Machines, $k-NN$, Decision Tree.

Logistic Regression

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- Probabilistic interpretation:

  Classes $y \in \{0, 1\}$;
  Function $z = \mathbf{w}^T \mathbf{x}$;
  Hypothesis logistic sigmoid function $\sigma(z) = \frac{1}{1+e^{-z}}$.

- Decision rules:

$$\hat{y} = \begin{cases} 1, & z > 0 \\ 0, & z \leq 0 \end{cases}.$$

Logistic Regression

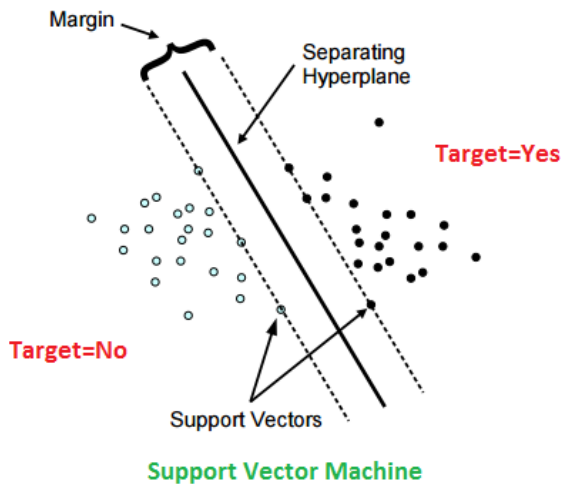
- Define $\pi_i = \sigma(\mathbf{w}^T \mathbf{x}_i)$, then $p(y_i|\mathbf{x}_i, \mathbf{w}) = \pi_i^{y_i} \cdot (1 - \pi_i)^{1-y_i}$.
- Loglikelihood of all data: $\ell(\mathbf{w}) = \sum_i \log p(y_i|\mathbf{x}_i, \mathbf{w})$.
- MLE: $\mathbf{w}^* = \text{argmax}_{\mathbf{w}}\, \ell(\mathbf{w})$.
  1. No close-form solution;
  2. Gradient ascent / SGD (first-order);
  3. Newton-Raphson method (second-order).

Support Vector Machines

- Non-probabilistic interpretation:

$$\begin{aligned} \text{Classes} \quad & y \in \{-1, 1\}; \\ \text{Function} \quad & z = \mathbf{w}^T \mathbf{x} + b; \\ \text{Decision rules} \quad & \hat{y} = sign(z). \end{aligned}$$

`http://www.saedsayad.com/support_vector_machine.htm`



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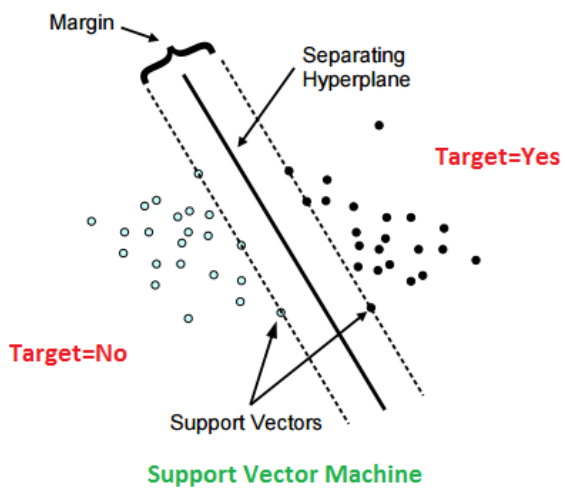


- Assumption: Data set $\{(\mathbf{x}_i, y_i)\}$ are linearly separable.

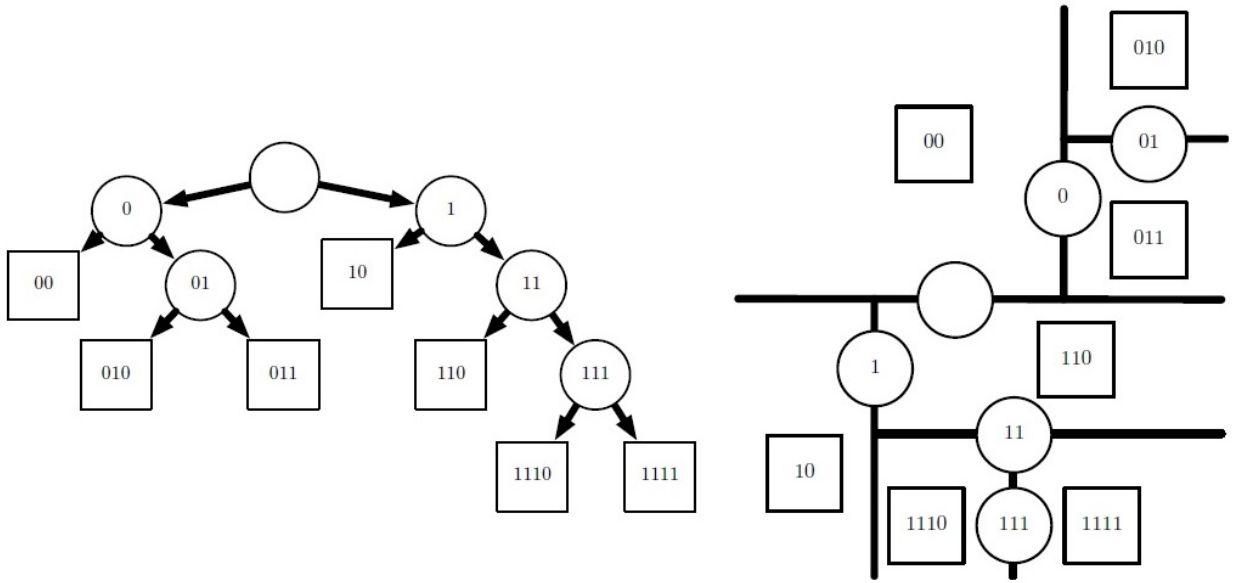
  Margin: Distance from boundary to the closet point in training sets as

$$\gamma = \min_i \frac{|\mathbf{w}^T \mathbf{x}_i + b|}{\|\mathbf{w}\|} = \min_i \frac{y_i(\mathbf{w}^T \mathbf{x}_i + b)}{\|\mathbf{w}\|}. \tag{3}$$

  Idea: To maximize the margin. Solved by Quadratic Programming.

k-NN and Decision Tree

- k-nearest neighbors (k-NN) algorithm: When we want to produce an output y for a new test input $\mathbf{x}$, we find the k-nearest neighbors to $\mathbf{x}$ in the training data $\mathbf{X}$. We then return the average of the corresponding y values in the training set.
- Decision Tree:



Unsupervised Learning

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- A classic unsupervised learning task is to find the "best" representation of the data.
- Three common representations
  1. Low-dimensional representations: Compress as much information as possible;
  2. Sparse representations: Entries are mostly zeros;
  3. Independent representations: Disentangle the source of variation underlying the data distribution such that the dimensions of the representation are statistically independent.

Principle component analysis

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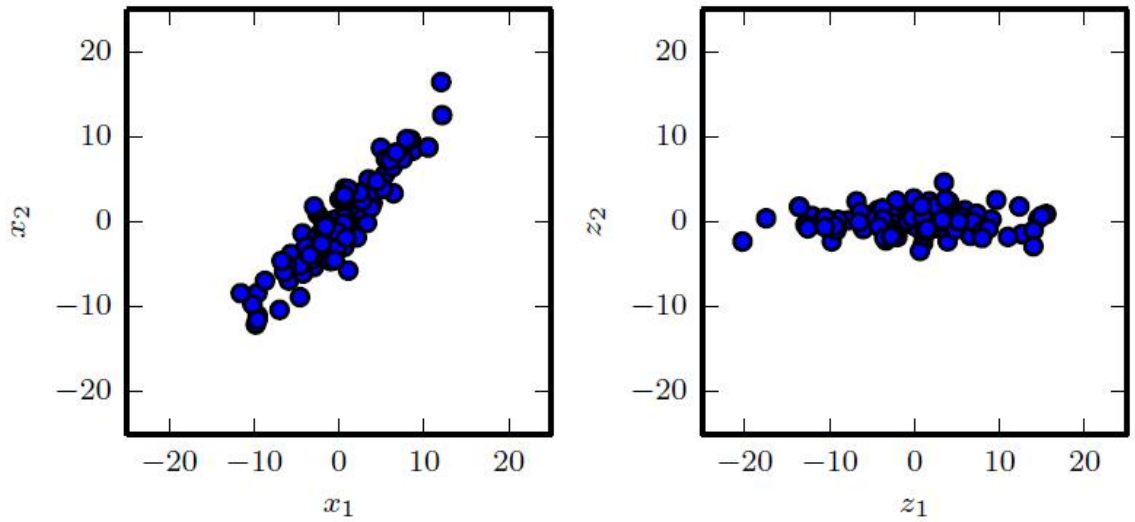

Figure: (Left)The original data consist of samples of $\boldsymbol{x}$. In this space, the variance might occur along directions that are not axis aligned. (Right) The transformed data $\boldsymbol{z} = \boldsymbol{x}^T \boldsymbol{W}$ now varies most along the axis z_1. The direction of second-most variance is now along z_2.

Principle Component Analysis

- Consider a zero-mean data matrx $\boldsymbol{X}$, the covariance matrix associated with $\boldsymbol{X}$ is given by

$$\mathrm{Var}[\boldsymbol{x}] = \frac{1}{m-1}\boldsymbol{X}^T\boldsymbol{X}. \tag{4}$$

  PCA finds a representation $\boldsymbol{z} = \boldsymbol{W}^T\boldsymbol{x}$, where $\mathrm{Var}[\boldsymbol{x}]$ is diagonal.

- The principle components of a design matrix $\boldsymbol{X}$ are given by the eigenvectors of $\boldsymbol{X}^T\boldsymbol{X}$.

k-means Clustering

- The $k-$means clustering algorithm divides the training set into k different clusters of examples that are near each other.

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- Initializing k different centroids $\{\boldsymbol{\mu}^{(1)}, ..., \boldsymbol{\mu}^{(k)}\}$, the k-means algorithm alternates between the following two different steps until convergence:

  1. Each training example is assigned to cluster i, where i is the index of the nearest centroid $\boldsymbol{\mu}^{(i)}$.
  2. Each centroid $\boldsymbol{\mu}^{(i)}$ is updated to the mean of all training examples $\boldsymbol{x}^{(i)}$ assigned to cluster i.

Outline

Stochastic Gradient Descent

- The cost function used by a machine learning algorithm often decomposes as a sum over training examples of some per-example loss function, such as

$$J(\boldsymbol{\theta}) = \mathbb{E}_{\mathbf{x},y\sim\hat{p}_{data}} L(\mathbf{x}, y, \boldsymbol{\theta}) = \frac{1}{m}\sum_{i=1}^{m} L(\mathbf{x}^{(i)}, y^{(i)}, \boldsymbol{\theta}), \tag{5}$$

where L is the per-example loss $L(\mathbf{x}^{(i)}, y^{(i)}, \boldsymbol{\theta}) = -\log p(y^{(i)}|\mathbf{x}^{(i)}, \boldsymbol{\theta})$.

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- Gradient descent requires computing

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = \frac{1}{m}\sum_{i=1}^{m} \nabla_{\boldsymbol{\theta}} L(\mathbf{x}^{(i)}, y^{(i)}, \boldsymbol{\theta}). \tag{6}$$

As the size m grows to billions, a single gradient step becomes computational prohibitive.

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- On each step of the algorithm, we can sample a minibatch of examples $\mathbb{B} = \{\mathbf{x}^{(1)}, ..., \mathbf{x}^{(m')}\}$ drawn uniformly from the training set.
- The estimate of the gradient is formed as

$$\mathbf{g} = \frac{1}{m'} \sum_{i=1}^{m'} \nabla_{\boldsymbol{\theta}} L(\mathbf{x}^{(i)}, y^{(i)}, \boldsymbol{\theta}) \tag{7}$$

The SGD algorithm then follows $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \epsilon \mathbf{g}$ with ϵ being the learning rate.

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Building a Machine Learning Algorithm

- Recipe: Combine a specification of a dataset, a cost function, an optimization procedure and a model.

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- For example, the linear regression combines a dataset consisting of $\boldsymbol{X}$ and $\boldsymbol{y}$, the cost function

$$J(\boldsymbol{w}, b) = -\mathbb{E}_{\boldsymbol{x},y\sim\hat{p}_{\text{data}}} \log p_{\text{model}}(y|\boldsymbol{x}), \tag{8}$$

the model specification $p_{\text{model}}(y|\boldsymbol{x}) = \mathcal{N}(y; \boldsymbol{x}^T\boldsymbol{w} + b, 1)$, and the optimization algorithm. is solving the normal equations for the gradient of the cost being zero.

Challenges Motivating Deep Learning

- The Curse of Dimensionality

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- Local Constancy and Smoothness Regularization

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- The Curse of Dimensionality
- Local Constancy and Smoothness Regularization
- Manifold Learning

Thanks!

Q&A

Aug 25, 2018