MLSS 2014 – Introduction to Machine Learning Lecture 2

J. Zico Kolter

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Outline

Other machine learning algorithms

Unsupervised learning

Probabilistic models

Evaluating machine learning algorithms

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Kernel methods

- Kernel methods are a very popular approach to non-linear classification, though they are still "linear" in some sense

$$h_\theta(x) = \sum_{i=1}^{m} \theta_i K(x, x^{(i)})$$

  where $K : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is a *kernel function* that measures the similarity between x and $x^{(i)}$ (larger values for more similar)

- For certain K, can be interpreted as working in a high dimensional feature space without explicitly forming features

- Still linear in θ, can use many of the same algorithms as before

- **Important**: $\theta \in \mathbb{R}^m$, as many parameters as examples (*non-parametric* approach)

Nearest neighbor methods

- Predict output based upon closest example in training set

$$h_\theta(x) = y^{(\text{argmin}_i \, \|x - x^{(i)}\|^2)}$$

  where $\|x\|^2 = \sum_{i=1}^{n} x_i^2$

- Can also average over k closest examples: k-nearest neighbor

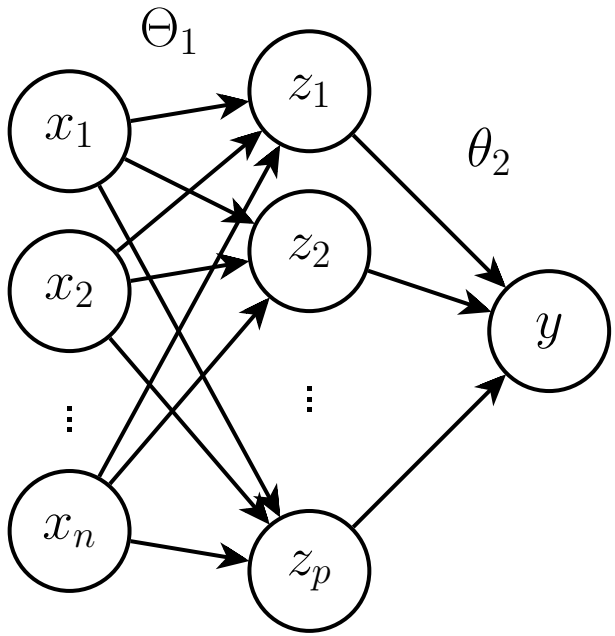
- Requires no separate "training" phase, but (like kernel methods) it is non-parametric, requires that we keep around all the data

Neural networks

- Non-linear hypothesis class

$$h_\theta(x) = \sigma(\theta_2^T \sigma(\Theta_1^T x))$$

for a 2-layer network, where $\theta = \{\Theta_1 \in \mathbb{R}^{n \times p}, \theta_2 \in \mathbb{R}^p$ and $\sigma : \mathbb{R} \to \mathbb{R}$ is an sigmoid function $\sigma(z) = 1/(1 + \exp(-z))$ (applied elementwise to vector)

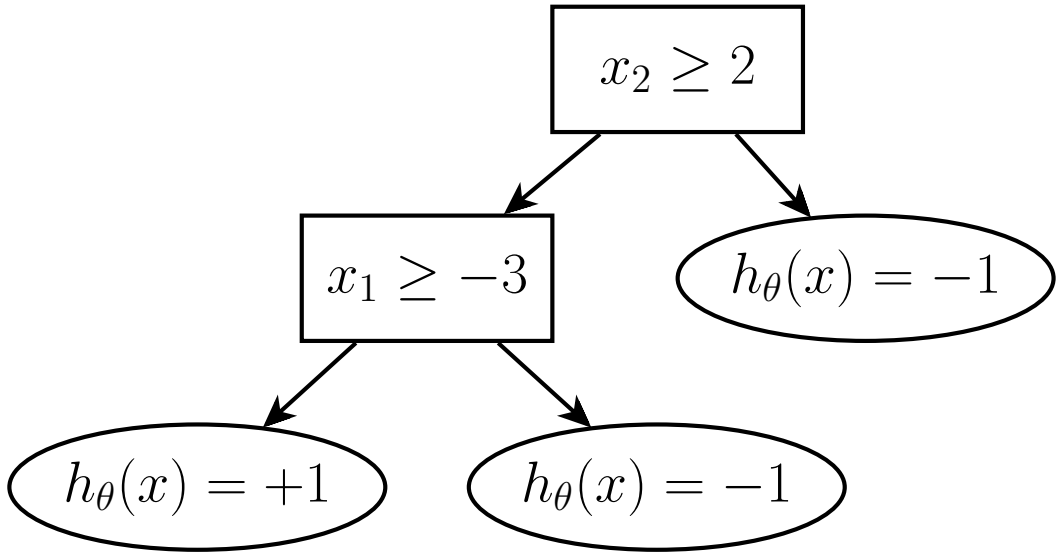


- Non-convex optimization, but smooth (gradient and similar methods can work very well)

- Some major recent success stories in speech recognition, image classification

Decision trees

- Hypothesis class partitions space into different regions



- Can also have linear predictors (regression or classification) at the leaves

- Greedy training find nodes that best separate data into distinct classes

Ensemble methods

- Combine a number of different hypotheses

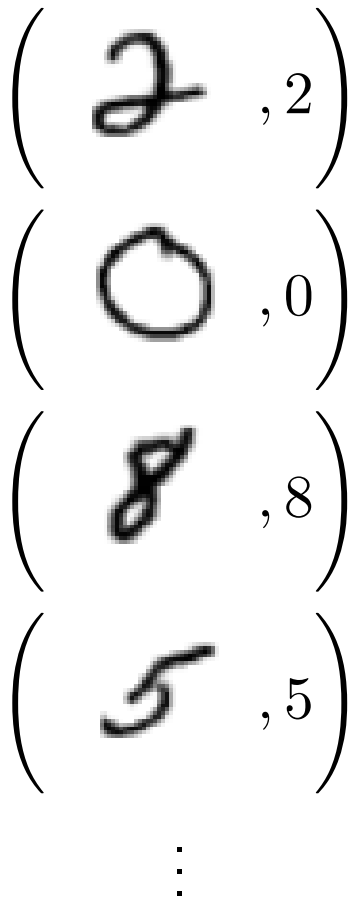
$$h_\theta(x) = \sum_{i=1}^{k} \theta_i \text{sign}(h_i(x))$$

- Popular instances
  - Random forests: ensemble of decision trees built from different subsets of training data
  - Boosting: iteratively train multiple classifiers/regressors on reweighted examples based upon performance of the previous hypothesis

Outline

Supervised learning

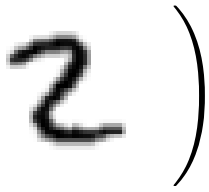
Training Data

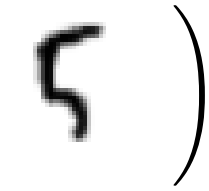


Machine Learning

$\longrightarrow$ Hypothesis function h_θ

Deployment

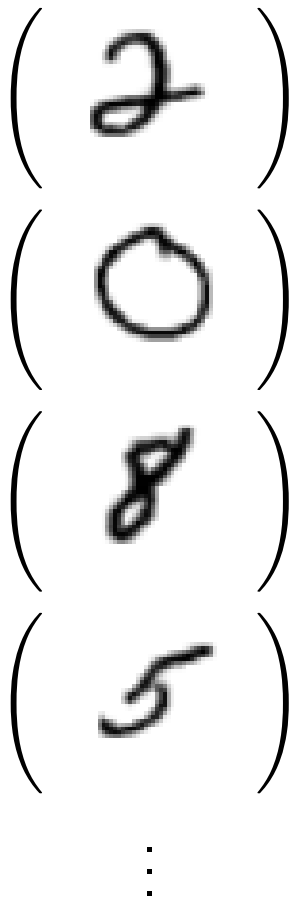
Prediction $= h_\theta$ 

Prediction $= h_\theta$ 

$\vdots$

Unsupervised learning

Training Data



Machine Learning

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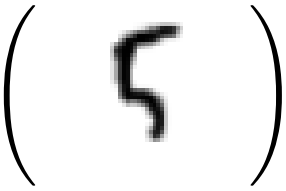
Prediction $= h_\theta$ 

$\vdots$

Problem setting

- **Input features**: $x^{(i)} \in \mathbb{R}^n, \quad i = 1, \ldots, m$
- **Model parameters**: $\theta \in \mathbb{R}^k$
- How do we specify a hypothesis class or loss function without outputs?

- One way to interpret many unsupervised learning algorithms is that they try to "re-create" the input using a limited hypothesis class

- **Hypothesis function**: $h_\theta : \mathbb{R}^n \to \mathbb{R}^n$
  - Want $h_\theta(x^{(i)}) \approx x^{(i)}$ for all training data

- **Loss function**: $\ell : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}_+$
  - E.g., $\ell(h_\theta(x), x) = \|h_\theta(x) - x\|^2$

- In order to prevent the trivial solution $h_\theta(x) = x$, we need to restrict the class of allowable functions h_θ

k-means

- Parameters are a set of k "centers" in the data

$$\theta = \{\mu^{(1)}, \ldots, \mu^{(k)}\}, \ \mu^{(i)} \in \mathbb{R}^k$$

- Hypothesis class picks the closest center

$$h_\theta(x) = \mu^{(\text{argmin}_i \, \|x - \mu^{(i)}\|^2)}$$

- With this framework, training looks the same as supervised learning

$$\underset{\theta}{\text{minimize}} \sum_{i=1}^{m} \|x^{(i)} - h_\theta(x^{(i)})\|^2$$

- Not a convex problem, but can solve by iteratively finding the closest $\mu^{(i)}$ for each example, then setting $\mu^{(i)}$ to be the mean of all examples assigned to it

Principal component analysis

- Parameters are two matrices that reduce the effective dimension of the data, $\theta = \{\Theta_1 \in \mathbb{R}^{n \times k}, \Theta_2 \in \mathbb{R}^{k \times n}\}$ with $k < n$

- Hypothesis class $h_\theta(x) = \Theta_1 \Theta_2 x$

- Interpretation: to reconstruct data $\Theta_2 x \in \mathbb{R}^k$ needs to preserve most of the information in x, so that we can construct it (dimensionality reduction)

- Minimizing loss

$$\underset{\Theta_1, \Theta_2}{\text{minimize}} \sum_{i=1}^{m} \|x^{(i)} - \Theta_1 \Theta_2 x^{(i)}\|_2^2$$

  is not a convex problem, but can be solved (exactly) via an eigenvalue decomposition

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Probability in machine learning

- Probabilistic models lie behind many of the algorithms in machine learning

- Probabilistic models can make the predictions of many algorithms more interpretable in terms of the underlying uncertainty, and dictate certain choices of loss functions

- An example: why did we choose the squared loss function in the previous lecture on linear regression?

$$\ell(h_\theta(x), y) = (h_\theta(x) - y)^2$$

Squared loss and Gaussian likelihood

- Suppose that the each output y in our data really *is* equal to the hypothesis function for that example $h_\theta(x)$, just corrupted by Gaussian noise ϵ

$$y = h_\theta(x) + \epsilon$$

- The probability density of a Gaussian variable given by

$$p(\epsilon) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\epsilon^2}{2\sigma^2}\right)$$

- Subsituting terms, we can use this expression to write the probability of y *given* x (parameterized by θ)

$$p(y|x;\theta) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(h_\theta(x) - y)^2}{2\sigma^2}\right)$$

- Consider the joint probability of *all* training data (assuming samples are independent and identically distributed)

$$p(y^{(1)}, \ldots, y^{(m)} | x^{(1)}, \ldots, x^{(m)}; \theta) = \prod_{i=1}^{m} p(y^{(i)} | x^{(i)}; \theta)$$

- Find the parameters that θ maximize the probability of the data

$$\underset{\theta}{\text{maximize}} \prod_{i=1}^{m} p(y^{(i)} | x^{(i)}; \theta) \quad \equiv \quad \underset{\theta}{\text{minimize}} \; -\sum_{i=1}^{m} \log p(y^{(i)} | x^{(i)}; \theta)$$

$$\equiv \underset{\theta}{\text{minimize}} \sum_{i=1}^{m} \left(\log(\sqrt{2\pi}\sigma) + \frac{1}{2\sigma^2} (h_\theta(x^{(i)}) - y^{(i)})^2 \right)$$

$$\equiv \underset{\theta}{\text{minimize}} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2$$

- This is a procedure known as *maximum likelihood estimation*, a common statistical technique

- Note that we still just pushed the question of "which loss" to "which distribution"

  - But some distributions, like Gaussian, may have reasonable empirical or theoretical justifications for certain problems

Logistic regression

- Another example: for binary classification problem, suppose that

$$p(y|x;\theta) = \frac{1}{1+\exp(-y \cdot h_\theta(x))}$$

and for each data point $x^{(i)}$, $y^{(i)}$ is sampled randomly from this distribution

- Then

$$\begin{aligned}
&\underset{\theta}{\text{minimize}} \; -\sum_{i=1}^{m} \log p(y^{(i)}|x^{(i)};\theta) \\
&\equiv \underset{\theta}{\text{minimize}} \; \log\left(1+\exp\left(-y^{(i)} \cdot h_\theta(x^{(i)})\right)\right)
\end{aligned}$$

which was exactly our logistic loss function

- In both cases, probabilistic models gives both a loss function and a way to interpret predictions as measure of *uncertainty*

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Evaluating ML algorithms

- You have developed a machine learning approach to a certain task, and want to validate that it actually works well (or determine if it doesn't work well)

- Standard: approach, divide data into training and testing sets, train method on training set, and report results on the testing set

- Important: testing set is *not* the same as the validation test

- The proper way to evaluate an ML algorithm
  1. Break all data into training/testing sets (e.g., 70%/30%)
  2. Break training set into training/validation set (e.g., 70%/30% again)
  3. Choose hyperparameters using validation set
  4. (Optional) Once we have selected hyperparameters, retrain using all the training set
  5. Evaluate performance on the testing set