Course Notes

EECS 445

Introduction to Machine Learning

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Contents

Abstract

Theory and implementation of state-of-the-art machine learning algorithms for large-scale real-world applications. Topics include supervised learning (regression, classification, kernel methods, neural networks, and regularization) and unsupervised learning (clustering, density estimation, and dimensionality reduction).

1 Introduction

- Formal definition: A computer program A is said to learn from experience E with respect to some class of tasks T and performance measure P , if its performance at tasks in T, as measured by P, improves with experience E
- Informal definition: Algorithms that improve their prediction performance at some task with experience (or data)
- e.g., spam filtering, handwritten digit recognition
- **Training**: given some example data you update parameters of your machine learning algorithm
- **Testing**: evaluating how well your algorithm performs on new data
- Machine learning tasks:
  - Supervised learning:
    - Classification
    - Regression
  - Unsupervised learning:
    - Clustering
    - Density estimation
    - Dimensionality reduction
  - Reinforcement Learning
    - Learning to act

1.1 Supervised Learning

- Goal:
  - Given data X in feature space and the labels Y
  - Learn to predict Y from X
- Labels could be discrete or continuous
  - Discrete labels: classification
  - Continuous labels: regression
- Classification:
  - Given a feature space (e.g., words in a document)
  - Predict a label space (e.g., topic of document)
- Regression:
  - Given a continuous feature space (e.g., market infromation up to time t)
  - Predict a label space (e.g., shapre price "$24.50")

1.2 Unsupervised Learning

- Goal:
  - Given data X without any labels
  - Learn the structures of the data
- "Learning without teacher"
- Clustering:
  - "Grouping into similar examples"
  - TODO: Image
- Lecture cut early, possibly add skipped here.

1.3 Feature Extraction

- Represent data in terms of vectors
  - Featurs are statistics or attributes that describe the data
  - Practitioners tend to tern this data into a feature space
  - e.g., For housing data useful features may be: number of rooms, square footage, etc.
- You can also consider domain knowledge, namely, use knowledge of how the task work to inject features into the domain
  - e.g., for OCR, aspect ratio of tight bounding boxes, existence of of vertical/horizontal strokes

2 Linear Regression

2.1 Notation

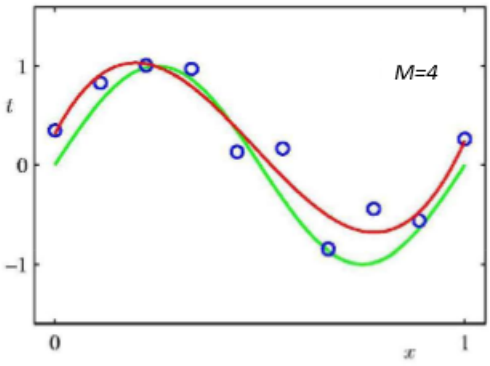
- $x \in \mathbb{R}^D$: data
- $\phi(x) \in \mathbb{R}^M$: features for $\vec{x}$
- $t \in \mathbb{R}$: continuous-valued labels
- $\vec{x}^{(n)} \equiv \vec{x}_n$: n-th training example
- $\vec{t}^{(n)} \equiv \vec{t}_n$: n-th targe value

2.2 1D Inputs

- In the 1D case ($x \in \mathbb{R}^1$)
- Given a set of observations $x^{(1)}, \ldots, x^{(N)}$ and corresponding targe values $t^{(1)}, \ldots, t^{(N)}$
- We want to learn a function $y(\vec{x}, W) \approx t$ to predict future values

$$y(\vec{x}, \vec{w}) = \sum_{j=0}^{M-1} \vec{w}_j \phi_j(\vec{x}) = \vec{w}^T \phi(x)$$

– e.g., (green = solution, red = 3-rd polynomial approximation)



– For simplicity, we add a *bias function*: $\phi_0(\vec{x}) = 1$

$$\vec{\phi} = 1, x, x^2, x^3, \ldots$$

2.3 Basis Function

– Function to construct features from raw data.

– e.g.,

– Polynomial: $\phi_j(x) = x^j$

– Gaussian: $\phi_j(x) = exp(-\frac{(x-\mu_j)^2}{2s^2})$

– Sigmoid: $\phi_j(x) = \sigma(\frac{x-\mu_j}{s})$

2.4 Objective Function

– We will use of sum-of-square errors:

$$E(w) = \frac{1}{2}\sum_{n=1}^{N}(y(x^{(n)}, w) - t^{(n)})^2$$

2.5 Batch Gradient Descent

– Given data (x, y) initial w, repeat until convergence:

$$\vec{w} = \vec{w} - \eta\nabla_{\vec{w}}E(\vec{w})$$

$$\nabla_{\vec{w}}E(w) = \sum_{n=1}^{N}\left(\sum_{k=0}^{M-1} w_k\phi_k(\vec{x}^{(n)}) - t^{(n)}\right)\phi(\vec{x}^{(n)}) = \sum_{n=1}^{N}\left(\vec{w}^T\phi(\vec{x}^{(n)}) - \vec{t}^{(n)}\right)\phi(x^{(n)})$$

2.6 Overfitting

- An implicit way to tell is when the coeffecients become unreasonably large
- Solutions:
  - Reduce order
  - Add more data point
  - Reselect features, some may be harming you
- If you have a small number of data points, then you should use low order polynomial (small number of features)
- As you obtain more data points, you can gradually increase the order of the polynomial (more features)
- Controlling model complexity: **regularization**

3 Linear Regression Pt. 2

3.1 Probability

- **Experiment**: procedure that yields an outcome
- **Sample space**: set of all possible outcomes in the experiment, denoted as Ω (or S)
- **Event**: subset of the sample space Ω (i.e., an event is a set consisting of individual outcomes)
- **Probability measure**: function from events to probability levels
- **Probability space**: $(\Omega, \mathcal{F}, P)$

Axioms of Probability

- $P(A) \geq 0, \forall A \in \mathcal{F}$
- $P(\Omega) = 1$
- If $A_1, A_2, \ldots$ are disjoint events, then:

$$P(\Cup_i A_i) = \sum_i P(A_i)$$

Set probabilities

- $A \subset B \rightarrow P(A) \leq P(B)$
- $P(A \cap B) \leq min(P(A), P(B))$
- $P(A \cup B) \leq P(A) + P(B)$
- $P(\Omega$
  $A) = 1 - P(A)$

– If $A_1, \ldots, A_k$ are a set of disjoint events such that $\biguplus_{i=1}^{k} A_i = \Omega$, then:

$$\sum_{i=1}^{k} P(A_k) = 1$$

Conditional Probability

– For events $A, B \in \mathcal{F}$ with $P(B) > 0$, we may write the conditional probability of A given B:

$$TODO$$

3.2 Bayes' Rule

– Using chain rule we may see **Bayes' rule**:

$$P(B|A) = \frac{P(A|B)P(B)}{P(A)}$$

– Often written:

$$P(B_i|A) = \frac{P(A|B_i)P(B_i)}{\sum_i P(A|B_i)P(B_i)}$$

– Where B_i are a partition of Ω (note the bottom is just the law of total probability)

–

3.3 Likelihood Functions

– Bayes' allows us to compute the posterior of w given data D:

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

$$p(D) = \sum_w p(D|w)p(w)$$

– The likelihood unction $p(D|w)$ is evaluated for observbed data D as a function of w.

– Namely,

$$posterior \propto likelihood \times prior$$

$$p(\vec{w}|D) \propto p(D|\vec{w})p(\vec{w})$$

– We do this because we typically have a model ($p(\vec{w})$), and then we can improve our likelihood of prediction by observing data ($p(D|\vec{w})$

3.4 Maximum Likelihood

- Maximum likelihood:
  - choose parameter setting w that maximizes likelihood function $p(D|w)$
  - Choose the value of w that maximizes the probability of observed data
  - The negative log of the likelihood is called the negative log-likelihood (e.g., a loss function to minimize)
  - Maximizing likelihood is equivalent to minimizing the loss
- MAP (maximum a posteriori) estimation
  - Equivalent to mazimizing $p(w|D) \propto p(D|w)p(w)$

3.5 The Gaussian Distribution

$$\mathcal{N}(x|\mu, \sigma^2) = \frac{1}{(2\pi\sigma^2)^(1/2)} e^{-\frac{1}{2\sigma^2}(x-\mu)^2}$$

TODO INSERT FUNCTION AND GRAPH

- Expected value: $E(x) = \mu = \int p(x)xdx$
- Variance: $Var(x) = E(x^2) - E(x)^2 = \sigma^2$

3.6 Maximum Likelihood w

- Assume a stochastic model:
$$t = y(x, w) + \epsilon \text{ where } \epsilon \ \mathcal{N}(0, \beta^{-1})$$
- $\beta^{-1} = \sigma^2$
- This gives a likelihood function:
$$p(t|x, w, \beta) = \mathcal{N}(t|y(x, w), \beta^{-1})$$
- With inputs $X = \{x^{(1)}, \ldots, x^{(N}\}$ and targe values $t = \{t^{(1)}, \ldots, t^{(N)}\}$, the data likelihood is:
$$p(t|X, w, \beta) = \Pi_{n=1}^{N} \mathcal{N}(t^{(n)}|w^T\phi(x^{(n)}), \beta^{-1})$$
- Log likelihood is:
$$TODO - 16$$
- where:
$$TODO - 16$$

3.7 Log Likelihood

– The log likelihood is:

$$\ln p(\vec{t}|\vec{w},\beta) = \frac{N}{2}\ln\beta - \frac{N}{2}\ln(2\pi) - \beta E_D(\vec{w})$$

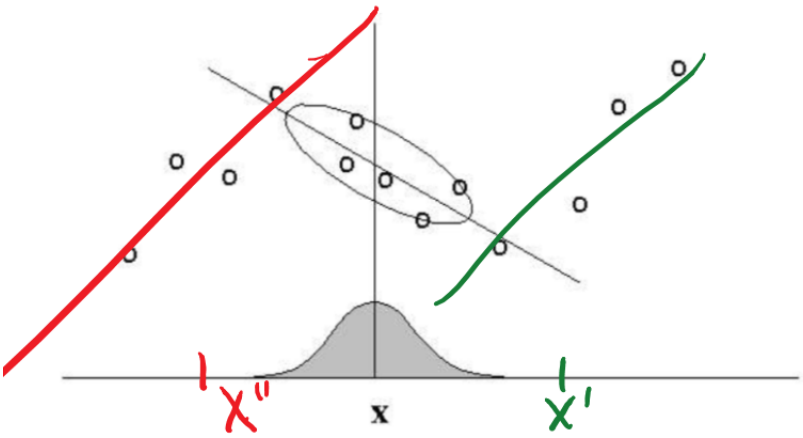
– Derivation:

$$\begin{aligned}
\log(P(t^{(1)},t^{(2)},\ldots,t^{(n)}|x^{(1)},x^{(2)},\ldots,x^{(n)},w)) &= \log P(\vec{t}|\vec{x},\vec{w}) \\
&= \log\left[\Pi_{i=1}^{N} P(t^{(i)}|x^{(i)},w)\right] \\
&= \log\left[\Pi_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{|t^{(i)}-w^T\phi(x^{(i)})|^2}{2\sigma^2}\right)\right] \\
&= \log\left[\Pi_{i=1}^{N} \frac{\sqrt{\beta}}{\sqrt{2\pi}}\exp\left(-\frac{1}{2}\beta|t^{(i)}-w^T\phi(x^{(i)})|^2\right)\right] \\
&= \sum_{i=1}^{N}\log\left(\frac{\sqrt{\beta}}{\sqrt{2\pi}}\right) + \log\left(\exp\left(-\frac{1}{2}\beta|t^{(i)}-w^T\phi(x^{(i)})|^2\right)\right) \\
&= \sum_{i=1}^{N}\log\left(\frac{\sqrt{\beta}}{\sqrt{2\pi}}\right) + -\frac{1}{2}\beta|t^{(i)}-w^T\phi(x^{(i)})|^2
\end{aligned}$$

– Maximizing the likelihood is summarized as:

$$0 = (\phi^T t)^T - w^T(\phi^T\phi)$$

3.8 Locally weighted linear regression



– Main idea: when predicting $f(x)$, give high weights for "neighbors" of x

– In locally weighted regression, points are weighted by prioximity to the current x in question using a kernel. A regression is computed using the weighted points

– Use simple features, like when you're not sure what a good feature function would be

– Weighted based on proximity of neighbors

– Do linear regression at each position based on neighbors

- Approximation of local neighborhood
- Final curve is made by dragging x across and rerunning regression each time

Definition 3.1 (Locally-weighted linear regression)**.** 1. Fit $\vec{w}$ to minimize $\sum_i r^{(i)} \left(t^{(i)} - \vec{w}^T \phi(x^{(i)})\right)^2$

2. Predict: $\vec{w}^T \phi(x^{(i)})$

- Remarks:
  - Standard choice: $r^{(i)} = \exp\left(-\frac{||x^{(i)} - x||^2}{2\tau^2}\right)$, where $\tau =$"kernel width"
  - $r^{(i)}$ depends on x (query point), and you solve linear regression for each query point x
  - The problem can be formualted as a modified version of least squares

A Linear Algebra Review

Definition A.1 (Gradient (vector))**.**

$$f(x) : \mathbb{R}^{n \times n} \to \mathbb{R}$$

$$\nabla_x f(x) = \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{bmatrix}$$

Definition A.2 (Gradient (matrix))**.**

$$f(x) : \mathbb{R}^{n \times n} \to \mathbb{R}$$

$$\nabla_A f(A) = \begin{bmatrix} \frac{\partial f(A)}{\partial A_{11}} & \cdots & \frac{\partial f(A)}{\partial A_{1n}} \\ \vdots & \ddots & \vdots \\ \frac{\partial f(A)}{\partial A_{m1}} & \cdots & \frac{\partial f(A)}{\partial A_{mn}} \end{bmatrix}$$

Definition A.3 (Hessian)**.**

$$f : \mathbb{R}^n \to \mathbb{R}$$

$$\nabla_x^2 f(x) = \left[\frac{\partial^2 f(x)}{\partial x_r \partial x_c}\right]$$

A.1 Matrix Calculus Examples

- e.g.,

$$\vec{a}^T C \vec{b}; a \in \mathbb{R}^m, C \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^n$$

$$\sum_{i=1}^{m} a_i (Cb)^i$$

$$\sum_{i=1}^{m} a_i \sum_{j=1}^{n} C_{ij} b_j$$

$$\sum_{i=1}^{m} \sum_{j=1}^{n} C_{ij} a_i b_j$$

– e.g.,

$$\frac{\partial f(x)^T A g(x)}{\partial x}; f : \mathbb{R}^k \to \mathbb{R}^m, g : \mathbb{R}^k \to \mathbb{R}^n, A : m \times n$$

$$\begin{aligned}
\frac{\partial f(x)^T A g(x)}{\partial x_k} &= \frac{\partial}{\partial x_k} \left(\sum_{i=1}^{m} \sum_{j=1}^{n} A_{ij} f(x)_i g(x)_j \right) \\
&= \sum_{i=1}^{m} \sum_{j=1}^{n} A_{ij} \frac{\partial}{\partial x_k} f(x)_i g(x)_j \\
&= \sum_{i=1}^{m} \sum_{j=1}^{n} A_{ij} \left(g(x)_j \frac{\partial f(x)_i}{\partial x_k} + f(x)_i \frac{\partial g(x)_j}{\partial x_k} \right) \\
&= \sum_{i=1}^{m} \sum_{j=1}^{n} \left(A_{ij} g(x)_j \frac{\partial f(x)_i}{\partial x_k} \right) + \sum_{i=1}^{m} \sum_{j=1}^{n} \left(A_{ij} f(x)_i \frac{\partial g(x)_j}{\partial x_k} \right)
\end{aligned}$$