

Machine Learning

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Chapter 1

Formal Setup

1.1 Definitions

Definition. Let \mathcal{X} be the domain. Let Y be the label set. We define a **classifier**, denoted by h , to be a function from X to Y .

Definition (Error). Let \mathcal{X} denote the domain. Let \mathcal{D} be a probability distribution on X . Let f be the true labeling function on X . Let h be a classifier. We define the **error** of h , with respect to \mathcal{D} and f , denoted by $\mathcal{L}_{\mathcal{D},f}$, to be a probability given by

$$\mathcal{L}_{\mathcal{D},f}(h) := \mathcal{D}\{x \in \mathcal{X} : h(x) \neq f(x)\}.$$

- We are never sure about the true error. We only approximate the true error.
- Note that there is no label set in this definition. What we have is the true labeling function f .

1.2 Empirical Risk Minimization (ERM)

Definition (Empirical Error). Let \mathcal{S} be a training data. Let h be a classifier. We define the **empirical error**, with respect to \mathcal{S} , denoted by $L_{\mathcal{S}}$, to be a proportion given by

$$L_{\mathcal{S}}(h) := \frac{|\{i : h(x_i) \neq y_i\}|}{|\mathcal{S}|}.$$

Definition (The Realizability Assumption). Assume that $\exists h^* \in \mathcal{H}$ such that $\mathcal{L}_{\mathcal{D},f}(h^*) = 0$.

Theorem 1. *Assume that the data are independent and identically distributed. Assume realizability. Then if \mathcal{H} is a finite class of classifiers, the $ERM(H)$ algorithm is guaranteed to succeed.*

Intuitively, the training set S is a window through which the learner gets partial information about the distribution D over the world and the labeling function, f . The larger the sample gets, the more likely it is to reflect more accurately the distribution and labeling used to generate it.

Proof Idea. Given some error rate ε and a sample of size m , what is the probability that $ERM(H)$ will have error ε .

$$\Pr(\mathcal{L}_{D,f}(A[S]) > \varepsilon).$$

Let's call a sample S "BAD" if $\exists h \in H$ such that $L_S(h) = 0$ but $L_{D,f}(h) > \varepsilon$. Let's show that the probability of picking a BAD sample is small. For every given h , such that $L_{D,f}(h) > \varepsilon$, the probability of picking x on which h is correct is $\leq 1 - \varepsilon$. So by independence,

$$D^m\{S : S \text{ is BAD w.r.t. this } h\} \leq (1 - \varepsilon)^m.$$

Given a BAD h , the probability of S failing to show that this h is BAD $\leq (1 - \varepsilon)^m$. The probability that S is BAD, S fails any $h \in H$, by the Union Bound, is $\leq \sum_{BAD h \in H} \Pr[S \text{ fails to alert on } h] \leq |H| \cdot (1 - \varepsilon)^m$.

Conclusion

The prob of picking an S that will mislead $ERM(H)$ to pick some h with true error $> \varepsilon$ is at most $|H| \cdot (1 - \varepsilon)^m$. So

$$\Pr(\mathcal{L}_{D,f}(ERM(H)(S)) > \varepsilon) < |H| \cdot (1 - \varepsilon)^m \xrightarrow{m \rightarrow \infty} 0.$$

■

Formal Proof. Let \mathcal{X} denote the domain. Let \mathcal{Y} denote the labeling set. Let \mathcal{D} be some probability distribution on \mathcal{X} . Let f be some true labeling function from \mathcal{X} to \mathcal{Y} . Let \mathcal{H} be a finite class of classifiers. Define for each sample S a classifier h_S as $h_S := \operatorname{argmin}_{h \in \mathcal{H}} \mathcal{L}_{S,f}(h)$. The realizability assumption implies that $\mathcal{L}_{S,f}(h_S) = 0$. Define a set \mathcal{H}_B as

$$\mathcal{H}_B := \{h \in \mathcal{H} : \mathcal{L}_{D,f}(h) > \varepsilon\}.$$

i.e., \mathcal{H}_B is the set of bad hypotheses. Define a set M as

$$M := \{S \in \mathcal{X}^m : \exists h \in \mathcal{H}, \mathcal{L}_{D,f}(h) > \varepsilon \text{ and } \mathcal{L}_{S,f}(h) = 0\}.$$

i.e., M is the set of misleading samples. Note that

$$\{S \in \mathcal{X}^m : \mathcal{L}_{D,f}(h_S) > \varepsilon\} \subseteq M.$$

So

$$\begin{aligned}
\mathcal{D}^m\{S \in \mathcal{X}^m : \mathcal{L}_{\mathcal{D},f}(h_S) > \varepsilon\} &\leq \mathcal{D}^m(M) \\
&= \mathcal{D}^m \bigcup_{h \in \mathcal{H}_B} \{S \in \mathcal{X}^m : \mathcal{L}_{S,f}(h) = 0\} \\
&\leq \sum_{h \in \mathcal{H}_B} \mathcal{D}^m\{S \in \mathcal{X}^m : \mathcal{L}_{S,f}(h) = 0\} \\
&= \sum_{h \in \mathcal{H}_B} \mathcal{D}^m\{S \in \mathcal{X}^m : \forall x \in S, h(x) = f(x)\} \\
&= \sum_{h \in \mathcal{H}_B} \mathcal{D}^m \prod_{i=1}^m \{x \in \mathcal{X} : h(x) = f(x)\} \\
&= \sum_{h \in \mathcal{H}_B} \prod_{i=1}^m \mathcal{D}\{x \in \mathcal{X} : h(x) = f(x)\} \\
&= \sum_{h \in \mathcal{H}_B} \prod_{i=1}^m (1 - \mathcal{L}_{\mathcal{D},f}(h)) \\
&\leq \sum_{h \in \mathcal{H}_B} \prod_{i=1}^m (1 - \varepsilon) \\
&= \sum_{h \in \mathcal{H}_B} (1 - \varepsilon)^m \\
&= |\mathcal{H}|(1 - \varepsilon)^m.
\end{aligned}$$

■

Chapter 2

Probably Approximately Correct Learning

Chapter 3

Uniform Convergence

3.1 Definitions

Definition (ε Representative). *We say a sample S is ε -representative, with respect to H and p , if*

$$\forall h \in H, \quad |L_p(h) - L_S(h)| < \varepsilon.$$

Intuitively, this property tells you that you can trust on sample S on estimating p for any h in H .

Definition (Uniform Convergence Property). *Let Z be the domain set. We say that a class H has the **uniform convergence property** if $\exists m : (0,1)^2 \rightarrow \mathbb{N}$ such that for any probability distribution p over $Z = X \times Y$, for any $m \geq m_0 = m(\varepsilon, \delta)$, we have*

$$\Pr_{S \sim p^m} [S \text{ is not } \varepsilon\text{-representative with respect to } H \text{ and } p] < \delta.$$

A class has the uniform convergence property if when I take samples which are big enough, the probability that it is not an representative is small, no matter what p is.

Proposition 3.1.1. *If a sample S is $\frac{\varepsilon}{2}$ -representative with respect to p and a class H , then if A is an ERM_H function, we get*

$$L_p(A(S)) \leq \min_{h \in H} \{L_p(h)\} + \varepsilon.$$

This connects being representative to the success of an ERM algorithm.

Proof.

$$L_p(A(S)) \leq L_S(A(S)) + \varepsilon/2, \text{ since } S \text{ is } \frac{\varepsilon}{2}\text{-representative}$$

$$\begin{aligned}
&= \min_{h \in H} \{L_S(h)\} + \varepsilon/2 \\
&\leq \min_{h \in H} \{L_p(h) + \varepsilon/2\} + \varepsilon/2, \text{ since } S \text{ is } \frac{\varepsilon}{2}\text{-representative again} \\
&= \min_{h \in H} \{L_p(h)\} + \varepsilon.
\end{aligned}$$

That is,

$$L_p(A(S)) \leq \min_{h \in H} \{L_p(h)\} + \varepsilon.$$

■

Proposition 3.1.2. *If a class H has the uniform convergence property, then H is agnostically PAC learnable. Further more, any ERM_H function will be a successful learner in such a case.*

Theorem 2. *Every finite H has the uniform convergence property.*

Proof. Step 1: Showing that for any fixed h , we can find $m(\varepsilon, \delta)$ that guarantees $|L_p(h) - L_S(h)| < \varepsilon$.

Let θ_i denote the loss $\ell(h, (x_i, h_I))$. Then $L_S(h) = \frac{1}{m} \sum_{i=1}^m \theta_i$. Let μ denote $L_p(h)$. By the Hoeffding's inequality, we have

$$\Pr(|L_S(h) - L_p(h)| > \varepsilon) \leq 2 \exp(-2m\varepsilon^2).$$

For any fixed h , large enough samples are likely to be ε -representative for that H .

Step 2: Using the union bound we extend this to every finite H .

■

Corollary. *Every finite H is agnostically PAC learnable.*

Chapter 4

Perceptron

4.1 The Perceptron Algorithm

Algorithm 1: The Perceptron Algorithm (Rosenblatt 1958)

Input: Dataset $\mathcal{D} = \{(\mathbf{x}_i, y_i) \in \mathbb{R}^d \times \{\pm 1\} : i = 1..n\}$, initialization $\mathbf{w} \in \mathbb{R}^d$ and $b \in \mathbb{R}$, threshold $\delta \geq 0$.

Output: Approximate solutions \mathbf{w} and b so that $\forall i \in \{1..n\}, y_i(\mathbf{w}^\top \mathbf{x}_i + b) > 0$.

```
1 while true do
2   receive training example index  $i \in \{1..n\}$ ;
3   if  $y_i(\mathbf{w} \cdot \mathbf{x}_i + b) \leq \delta$  then
4      $\mathbf{w} \leftarrow \mathbf{w} + y_i \mathbf{x}_i$ ;
5      $b \leftarrow b + y_i$ ;
```

Remark. *We only perform updates when we make a mistake, and this is a necessary rule.*

Theorem 3. *Assume there exists some \mathbf{z} such that $A^\top \mathbf{z} > 0$, then the perceptron algorithm converges to some \mathbf{z}^* . If each column of A is selected indefinitely often, then $A^\top \mathbf{z}^* > \delta$.*

Corollary. *Let $\delta = 0$ and $\mathbf{z}_0 = \mathbf{0}$. Then the perceptron algorithm converges after at most $(R/\gamma)^2$ steps, where R and γ are dataset properties given by*

$$R := \|A\|_{2,\infty} = \max_i \|\mathbf{a}_i\|_2 \quad \text{and} \quad \gamma := \max_{\|\mathbf{z}\|_2 \leq 1} \min_i \langle \mathbf{z}, \mathbf{a}_i \rangle.$$

Note that the parameters R and γ are independent of the dataset size n .

Theorem 4. *The iterate $\mathbf{z} = (\mathbf{w}; b)$ of the perceptron algorithm is always bounded. In particular, if there is no separating hyperplane, then perceptron cycles.*

Chapter 5

Logistic Regression

5.1 Logit Transform

Definition (Logit Transform).

$$\log \frac{p(\mathbf{x}; \mathbf{w})}{1 - p(\mathbf{x}; \mathbf{w})} = \mathbf{w}^\top \mathbf{x}.$$

Or equivalently,

$$p(\mathbf{x}; \mathbf{w}) = \frac{1}{1 + \exp(-\mathbf{w}^\top \mathbf{x})}.$$

This $p(\mathbf{x}; \mathbf{w})$ is the confidence in the prediction.

5.2 Hypothesis Representation

Logistic Regression Model

Want $0 \leq h_\theta(x) \leq 1$.

$$h_\theta(x) = g(\theta^\top x)$$

where

$$g(z) = \frac{1}{1 + e^{-z}}.$$

So

$$h_\theta(x) = \frac{1}{1 + e^{-\theta^\top x}}.$$

Sigmoid function (logistic function)

$$g(z) = \frac{1}{1 + e^{-z}}.$$

Properties:

- $g(0) = 0.5$.
- $\lim_{z \rightarrow +\infty} g(z) = 1$.
- $\lim_{z \rightarrow -\infty} g(z) = 0$.

Interpretation of the Hypothesis Output

$h_\theta(x)$ is the probability that $y = 1$ on input x . i.e. $h_\theta(x) = P(y = 1 \mid x; \theta)$, the probability that $y = 1$, given x , parameterized by θ .

Since y is either 0 or 1,

$$P(y = 0 \mid x; \theta) + P(y = 1 \mid x; \theta) = 1, \text{ or}$$

$$P(y = 0 \mid x; \theta) = 1 - P(y = 1 \mid x; \theta).$$

5.3 Decision Boundary

Proposition 5.3.1. *The decision boundary \mathcal{D} of logistic regression with parameter $\mathbf{w} \in \mathbb{R}^n$ is*

$$\mathcal{D} = \{x \in \mathbb{R}^n : \mathbf{w}^\top \mathbf{x} = 0\}.$$

Proof. Predict $y = 1$ if $h_{\mathbf{w}}(x) \geq 0.5$ and predict $y = 0$ if $h_{\mathbf{w}}(x) < 0.5$. Notice

$$h_{\mathbf{w}}(x) = 0.5 \iff \mathbf{w}^\top \mathbf{x} = 0.$$

So the model predicts $\hat{y} = \text{sign}(\mathbf{w}^\top \mathbf{x})$ but with confidence $p(\mathbf{x}; \mathbf{w})$. ■

Example 5.3.1. Consider $\theta = \begin{bmatrix} -3 \\ 1 \\ 1 \end{bmatrix}$. Predict “ $y = 1$ ” if $\theta^\top \mathbf{x} = -3 + x_1 + x_2 \geq 0$. That

is, $x_2 \geq 3 - x_1$. This gives a “half space” in \mathbb{R}^2 . The line $x_1 + x_2 = 3$ separates \mathbb{R}^2 into a region where the model predicts “ $y = 0$ ” and a region where the model predicts “ $y = 1$ ”.

5.4 Maximum Likelihood Estimation

Proposition 5.4.1 (Maximum Likelihood Estimation of the Parameter \mathbf{w}). *The maximum likelihood estimation of \mathbf{w} is given by the following update rule:*

$$\mathbf{w}_{k+1} = \mathbf{w}_k - (\mathbf{X} \mathbf{W} \mathbf{X}^\top)^{-1} \mathbf{X}^\top (\mathbf{y} - \mathbf{p})$$

where

$$\mathbf{p} = \left[\frac{\exp(\mathbf{w}^\top \mathbf{x}_i)}{1 + \exp(\mathbf{w}^\top \mathbf{x}_i)} \right]_{i=1}^n \quad \text{and} \quad \mathbf{W} = \text{diag}(p_i(1 - p_i))_{i=1}^n.$$

Proof. The maximum likelihood function \mathcal{L} is:

$$\begin{aligned}\mathcal{L}(\mathbf{x}_1, \dots, \mathbf{x}_n; \mathbf{w}) &= \prod_{i=1}^n f_i(\mathbf{x}_i; \mathbf{w}) \\ &= \prod_{i=1}^n \begin{cases} \Pr(y = 1 \mid \mathbf{X} = \mathbf{x}_i), & \text{if } y_i = 1 \\ \Pr(y = 0 \mid \mathbf{X} = \mathbf{x}_i), & \text{if } y_i = 0 \end{cases} \\ &= \prod_{i=1}^n [\Pr(y = 1 \mid \mathbf{X} = \mathbf{x}_i)^{y_i} \Pr(y = 0 \mid \mathbf{X} = \mathbf{x}_i)^{1-y_i}].\end{aligned}$$

So the log maximum likelihood function ℓ is:

$$\begin{aligned}\ell(\mathbf{x}_1, \dots, \mathbf{x}_n; \mathbf{w}) &= \log \mathcal{L}(\mathbf{x}_1, \dots, \mathbf{x}_n; \mathbf{w}) \\ &= \log \prod_{i=1}^n [\Pr(y = 1 \mid \mathbf{X} = \mathbf{x}_i)^{y_i} \Pr(y = 0 \mid \mathbf{X} = \mathbf{x}_i)^{1-y_i}] \\ &= \sum_{i=1}^n \log [\Pr(y = 1 \mid \mathbf{X} = \mathbf{x}_i)^{y_i} \Pr(y = 0 \mid \mathbf{X} = \mathbf{x}_i)^{1-y_i}] \\ &= \sum_{i=1}^n [y_i \log \Pr(y = 1 \mid \mathbf{X} = \mathbf{x}_i) + (1 - y_i) \log \Pr(y = 0 \mid \mathbf{X} = \mathbf{x}_i)] \\ &= \sum_{i=1}^n \left[y_i \log \frac{\exp(\mathbf{w}^\top \mathbf{x}_i)}{1 + \exp(\mathbf{w}^\top \mathbf{x}_i)} + (1 - y_i) \log \frac{1}{1 + \exp(\mathbf{w}^\top \mathbf{x}_i)} \right] \\ &= \sum_{i=1}^n \left[y_i [\mathbf{w}^\top \mathbf{x}_i - \log(1 + \exp(\mathbf{w}^\top \mathbf{x}_i))] - (1 - y_i) [\log(1 + \exp(\mathbf{w}^\top \mathbf{x}_i))] \right] \\ &= \sum_{i=1}^n \left[y_i \mathbf{w}^\top \mathbf{x}_i - \log(1 + \exp(\mathbf{w}^\top \mathbf{x}_i)) \right].\end{aligned}$$

So the derivative of ℓ , with respect to \mathbf{w} , is:

$$\begin{aligned}\frac{\partial}{\partial \mathbf{w}} \ell(\mathbf{x}_1, \dots, \mathbf{x}_n; \mathbf{w}) &= \frac{\partial}{\partial \mathbf{w}} \sum_{i=1}^n \left[y_i \mathbf{w}^\top \mathbf{x}_i - \log(1 + \exp(\mathbf{w}^\top \mathbf{x}_i)) \right] \\ &= \sum_{i=1}^n \left[\frac{\partial}{\partial \mathbf{w}} y_i \mathbf{w}^\top \mathbf{x}_i - \frac{\partial}{\partial \mathbf{w}} \log(1 + \exp(\mathbf{w}^\top \mathbf{x}_i)) \right] \\ &= \sum_{i=1}^n \left[y_i \mathbf{x}_i^\top - \frac{1}{1 + \exp(\mathbf{w}^\top \mathbf{x}_i)} \exp(\mathbf{w}^\top \mathbf{x}_i) \mathbf{x}_i^\top \right] \\ &= \sum_{i=1}^n \left[y_i - \frac{\exp(\mathbf{w}^\top \mathbf{x}_i)}{1 + \exp(\mathbf{w}^\top \mathbf{x}_i)} \right] \mathbf{x}_i^\top \\ &= \mathbf{X}^\top (\mathbf{y} - \mathbf{p}).\end{aligned}$$

So the second derivative of ℓ , with respect to \mathbf{w} , is:

$$\frac{\partial^2}{\partial \mathbf{w} \partial \mathbf{w}^\top} \ell(\mathbf{x}_1, \dots, \mathbf{x}_n; \mathbf{w}) = \frac{\partial}{\partial \mathbf{w}^\top} \frac{\partial}{\partial \mathbf{w}} \ell(\mathbf{x}_1, \dots, \mathbf{x}_n; \mathbf{w})$$

$$\begin{aligned}
&= \frac{\partial}{\partial \mathbf{w}^\top} \sum_{i=1}^n \left[y_i - \frac{\exp(\mathbf{w}^\top \mathbf{x}_i)}{1 + \exp(\mathbf{w}^\top \mathbf{x}_i)} \right] \mathbf{x}_i^\top \\
&= - \sum_{i=1}^n \frac{\partial}{\partial \mathbf{w}^\top} \frac{\exp(\mathbf{w}^\top \mathbf{x}_i)}{1 + \exp(\mathbf{w}^\top \mathbf{x}_i)} \mathbf{x}_i^\top \\
&= - \sum_{i=1}^n \frac{\exp(-\mathbf{w}^\top \mathbf{x}_i) \mathbf{x}_i}{(1 + \exp(-\mathbf{w}^\top \mathbf{x}_i))^2} \mathbf{x}_i^\top \\
&= - \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^\top \frac{\exp(\mathbf{w}^\top \mathbf{x}_i)}{1 + \exp(\mathbf{w}^\top \mathbf{x}_i)} \frac{1}{1 + \exp(\mathbf{w}^\top \mathbf{x}_i)} \\
&= \mathbf{X} \mathbf{W} \mathbf{X}^\top.
\end{aligned}$$

So the update rule is:

$$\begin{aligned}
\mathbf{w}_{k+1} &= \mathbf{w}_k - \left(\frac{\partial^2 \ell}{\partial \mathbf{w} \partial \mathbf{w}^\top} \right)^{-1} \left(\frac{\partial \ell}{\partial \mathbf{w}} \right) \\
&= \mathbf{w}_k - (\mathbf{X} \mathbf{W} \mathbf{X}^\top)^{-1} \mathbf{X}^\top (\mathbf{y} - \mathbf{p}).
\end{aligned}$$

■

5.5 Cost Function

Training set: $\{(x^{(1)}, y^{(1)}), \dots, (x^{(m)}, y^{(m)})\}$. $x_0 = 1$. $x = \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{bmatrix} \in \mathbb{R}^{n+1}$. $y \in \{0, 1\}$.

If

$$cost(h_\theta(x^{(i)}, y^{(i)})) = \frac{1}{2} (h_\theta(x^{(i)}) - y^{(i)})^2$$

as in linear regression, then the cost function is non-convex.

Logistic Regression Cost Function

$$cost(h_\theta(x), y) := \begin{cases} -\log(h_\theta(x)), & \text{if } y = 1 \\ -\log(1 - h_\theta(x)), & \text{if } y = 0. \end{cases}$$

Property:

- If $y = 1$ and $h_\theta(x) \uparrow 1$, then $cost(h_\theta(x), y) \approx 0$.
- If $y = 1$ and $h_\theta(x) \downarrow 0$, then $cost(h_\theta(x), y) \rightarrow +\infty$.
- Similar for $y = 0$.

Captures intuition that if $h_\theta(x) = 0$ (the model predicts $P(y = 1 \mid x; \theta) = 0$), but $y = 1$, we'll penalize the learning algorithm by a very large cost.

Cost Function for the Training Set

$$J(\theta) := \frac{1}{m} \sum_{i=1}^m \text{cost}(h_\theta(x^{(i)}), y^{(i)})$$

where cost is the function given above.

Rewrite the cost function:

$$\text{cost}(h_\theta(x), y) = -y \log(h_\theta(x)) - (1 - y) \log(1 - h_\theta(x)).$$

So

$$J(\theta) = -\frac{1}{m} \sum_{i=1}^m \left[y^{(i)} \log(h_\theta(x^{(i)})) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)})) \right].$$

To fit parameter θ : $\min_\theta J(\theta)$.

5.6 Optimization

Gradient Descent

$$\frac{\partial}{\partial \theta_j} J(\theta) = \sum_{i=1}^m (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}.$$

This looks identical to linear regression.

Other Optimization Algorithms

- Conjugate Gradient
- BFGS
- L-BFGS

Advantages:

- No need to pick learning rate α .
- Often faster than gradient descent.

5.7 Multiclass Classification

One-vs-rest

$$h_{\theta}^{(i)}(x) = P(y = i \mid x; \theta) \quad i = 1, 2, 3.$$

Train a logistic regression classifier for each i to predict the probability that $y = i$. On a new input x , pick class $i = \operatorname{argmax}_i h_{\theta}^{(i)}(x)$.

Softmax

$$\mathbb{P}(Y = k \mid \mathbf{x}; \mathbf{W}) = \frac{\exp(\mathbf{w}_k^{\top} \mathbf{x})}{\sum_{l=1}^C \exp(\mathbf{w}_l^{\top} \mathbf{x})}.$$

5.8 Introducing Non-linearity

Consider

$$h_{\theta}(x) = g(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2)$$

and $\theta = \begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$. Then the model predicts “ $y = 1$ ” if $-1 + x_1^2 + x_2^2 \geq 0$. That is, if $x_1^2 + x_2^2 \geq 1$.

5.9 Beyond Logistic Regression

The logit transform is just one choice among the others. What we need is a function Q from $[0, 1]$ onto \mathbb{R} . The inverse of any cumulative distribution function can be used as the Q function. e.g. the probit regression which uses the inverse of the CDF of a standard normal distribution.

Definition (Logistic Distribution). *We define the **logistic distribution** to be a probability distribution with CDF given by*

$$F(x; \mu; s) := \frac{1}{1 + \exp(-\frac{x-\mu}{s})}.$$

Proposition 5.9.1 (Mean of Logistic Distribution). *Let $X \sim F(x; \mu; s)$. Then*

$$\mathbb{E}[X] = \mu.$$

Proposition 5.9.2. *Let $X \sim F(x; \mu; s)$. Then*

$$\operatorname{var}[X] = \frac{s^2 \pi^2}{3}.$$

Chapter 6

Dimensionality Reduction

6.1 Motivations

- Data compression.
- Data visualization.

6.2 Principal Component Analysis

PCA is trying to find a lower dimensional surface onto which to project the data so as to minimize squared projection error.

Principal component analysis vs. linear regression:

- Linear regression tries to minimize residuals. PCA tries to minimize projection error.
- In linear regression, we try to predict one feature with other features. In PCA, all features are equivalent.

Algorithm: (from n dimensions to k dimensions)

- Preprocessing: mean normalization and feature scaling (standardization).
- Compute covariance matrix

$$\Sigma = \frac{1}{m} \sum_{i=1}^m (x^{(i)})(x^{(i)})^T.$$

- Compute the eigenvalues of Σ .

$$\Sigma = U S V.$$

Let U_{reduce} denote the first k columns of U . Then $z = U_{reduce}^T x$.

Choosing k :

- Average squared projection error:

$$\frac{1}{m} \sum_{i=1}^m \|x^{(i)} - x_{approx}^{(i)}\|^2.$$

- Total variation in the data:

$$\frac{1}{m} \sum_{i=1}^m \|x^{(i)}\|^2.$$

- Typically, we choose k to be the smallest value so that

$$\frac{\text{average squared projection error}}{\text{total variation}} < 0.01,$$

i.e. 99% of variance is retained.

- The above ratio can be computed in an easier way. Say

$$S = \begin{bmatrix} s_{11} & & O \\ & \ddots & \\ O & & s_{nn} \end{bmatrix}.$$

Then

$$\frac{\text{average squared projection error}}{\text{total variation}} = 1 - \frac{\sum_{i=1}^k s_{ii}}{\sum_{i=1}^n s_{ii}}.$$

So we can start with $k = 1$ and increase k and check whether

$$\frac{\sum_{i=1}^k s_{ii}}{\sum_{i=1}^n s_{ii}} > 0.99.$$

Chapter 7

Support Vector Machines

7.1 Hard-Margin SVM

Recall that the perceptron algorithm is

$$\begin{aligned} & \min 0 \\ & \text{subject to } \forall i, y_i(\mathbf{w}^\top \mathbf{x}_i + b) > 0. \end{aligned}$$

This is a feasibility problem.

$$\begin{aligned} & \max_{\mathbf{w}, b} \frac{1}{\|\mathbf{w}\|_2} \\ & \text{subject to } \forall i, y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1. \end{aligned}$$

The objective function is the margin between the hyperplanes $H_{+1} : \mathbf{w}^\top \mathbf{x}_i + b = 1$ and $H_{-1} : \mathbf{w}^\top \mathbf{x}_i + b = -1$.

Note that this problem is equivalent to

$$\begin{aligned} & \max_{\mathbf{w}, b} \frac{1}{2} \|\mathbf{w}\|_2^2 \\ & \text{subject to } \forall i, y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geq 1. \end{aligned}$$

This is a quadratic programming whereas the perceptron algorithm is a linear programming.

Definition (Support Vectors). *We define the **support vectors** to be the points that are on the hyperplanes H_{+1} and H_{-1} .*

Proposition 7.1.1 (Existence). *Assume that the data points are linearly separable. Then the minimizers \mathbf{w} and b exist.*

Proposition 7.1.2. *Assume that the data points are linearly separable. Then the minimizers \mathbf{w} and b exist and are unique.*

Proposition 7.1.3. *The Lagrangian dual problem is*

$$\begin{aligned} \max_{\alpha \geq 0} \quad & \sum_i \alpha_i - \frac{1}{2} \left\| \sum_i \alpha_i y_i \mathbf{x}_i \right\|_2^2 \\ \text{subject to} \quad & \sum_i \alpha_i y_i = 0, \end{aligned}$$

which is equivalent to

$$\begin{aligned} \min_{\alpha \geq 0} \quad & \frac{1}{2} \sum_i \sum_j \alpha_i \alpha_j y_i y_j \mathbf{x}_i^\top \mathbf{x}_j - \sum_k \alpha_k \\ \text{subject to} \quad & \sum_i \alpha_i y_i = 0. \end{aligned}$$

Proposition 7.1.4. *Define for any $d \in \mathbb{N}$ a set $\Delta \subseteq \mathbb{R}^d$ as*

$$\Delta := \{\mathbf{x} \in \mathbb{R}^d : \sum_i \mathbf{x}_i = 1\}.$$

$$\begin{aligned} \min_{\bar{\alpha} \in 2\Delta} \quad & \frac{1}{2} \left\| \sum_i \bar{\alpha}_i y_i \mathbf{x}_i \right\|_2^2 \\ \text{subject to} \quad & \sum_i \bar{\alpha}_i y_i = 0. \end{aligned}$$

Define sets P and N as

$$P := \{i : y_i = 1\} \text{ and } N := \{i : y_i = -1\}.$$

Define vectors μ and ν as

$$\mu := [\alpha_i]_{i \in P} \text{ and } \nu := [\alpha_i]_{i \in N}.$$

Then the problem is equivalent to

$$\min_{\mu \in \Delta, \nu \in \Delta} \quad \frac{1}{2} \left\| \sum_{i \in P} \mu_i \mathbf{x}_i - \sum_{j \in N} \nu_j \mathbf{x}_j \right\|_2.$$

Note that $\sum_{i \in P} \mu_i \mathbf{x}_i \in \text{conv}\{\mathbf{x}_i : i \in P\}$ and $\sum_{j \in N} \nu_j \mathbf{x}_j \in \text{conv}\{\mathbf{x}_i : i \in P\}$. So the objective function is the distance between the two convex hulls. So \mathbf{w} is in the direction of the line segment between the pair of points in the positive/negative convex hull with the minimum distance, and the hyperplane is the bisector of this line segment.