Regression

Motivation

H^L is one of the most useful families of hypothesis classes.

Many models that are used in practice rely on linear predictors.

There exist many types of linear models, including:

- Perceptron(classification).
- Linear regression. $\boldsymbol{y} \in \mathbb{R}$
- Logistic regression. $\text{output}\, \boldsymbol{probability}\, \boldsymbol{p} \in \ (\mathbf{0}, \mathbf{1}) \boldsymbol{and\ input}\ \boldsymbol{y} \in \{-1, +1\}$

Motivation

Let's define the class of affine functions L=L_d: input = $\boldsymbol{x}$

$$H^{L_d} = \{h_{w,b} : \boldsymbol{w} \in \mathbb{R}^{\boldsymbol{d}} \ \boldsymbol{and}\ \boldsymbol{b} \in \mathbb{R}\} \quad |H^{L_d}| = \infty$$

Where:

$$\boldsymbol{h_{w,b}(x_i)} = \langle \boldsymbol{w}, \boldsymbol{x_i} \rangle + \boldsymbol{b} = \sum_{\boldsymbol{j=1}}^{\boldsymbol{d}} \boldsymbol{w_j} x_i^j + \boldsymbol{b} = \boldsymbol{y_i}$$

To simplify the notation, we will integrate the bias as an extra coordinate into w:

$$x_i = (x_i^1, \dots, x_i^d) \in \mathbb{R}^d \longleftarrow x = (1, x_i) \in \mathbb{R}^{d+1}, w \longleftarrow (b, w) \in \mathbb{R}^{d+1}$$

$$\boldsymbol{h_w}(x_i) = \sum_{\boldsymbol{j=0}}^{\boldsymbol{d}} \boldsymbol{w_j} x_i^j \ \boldsymbol{avec} \quad \boldsymbol{x_i^0} = \boldsymbol{1}\ \boldsymbol{and}\ \boldsymbol{w_0} = \boldsymbol{b}$$

Hence, the class of affine functions is called « homogenous affine functions »

$$H^{L_d} = \boldsymbol{L_d} = \{\boldsymbol{h_w} : \boldsymbol{w} \in \mathbb{R}^{\boldsymbol{d+1}}\} \to |L_d| = \infty$$

h(x)=y

Motivation

Therefore, we can generate different hypothesis classes H^L, defining different models, by using the composition of φ over L_d such that: ($\boldsymbol{h_w} \in L_d$)

$$\varphi : \mathbb{R} \rightarrow Y$$

Perceptron(classification):

$$\varphi_p(x) = sign(x) \text{ and } Y = \{-1, +1\}$$

$$H_p = sing(\varphi_p \circ L_d = \left\{\varphi_p \circ \boldsymbol{h_w}(\boldsymbol{x}) : \boldsymbol{h_w} \in L_d\right\})$$

Linear regression:

$$\varphi_{reg}(x) = Id(x) = x \text{ and } Y = \mathbb{R}$$

$$H_{reg} = \varphi_{reg} \circ L_d = \left\{\varphi_p \circ \boldsymbol{h_w}(\boldsymbol{x}) : \boldsymbol{h_w} \in L_d\right\} = \{\boldsymbol{h_w}(\boldsymbol{x}) : \boldsymbol{h_w} \in L_d\}$$

Logistic regression:

$$\boldsymbol{\varphi_{sig}(x) = \frac{1}{1+e^{-x}}} \text{ and } Y = \{-1, +1\}, \boldsymbol{\varphi_{sig}\left(h_w\left(x_j^i\right) = \sum_{i=0}^{d} w_i x_j^i\right) = \frac{1}{1+e^{-\sum_{i=0}^{d} w_i x_i}}}$$

$$\boldsymbol{H_{sig} = \varphi_{sig} \circ L_d(x) = \frac{1}{1 + e^{-\sum_{i=0}^{d} w_i x_i}}}$$

Linear Regression

Definition:
Linear regression is a type of model used for regression tasks by studying the relationship between some explanatory variables and some real valued outcome.

Here we have: $x = (1, x) \in X$

$$X \subset \mathbb{R}^{d+1} \text{ for some } d$$

And

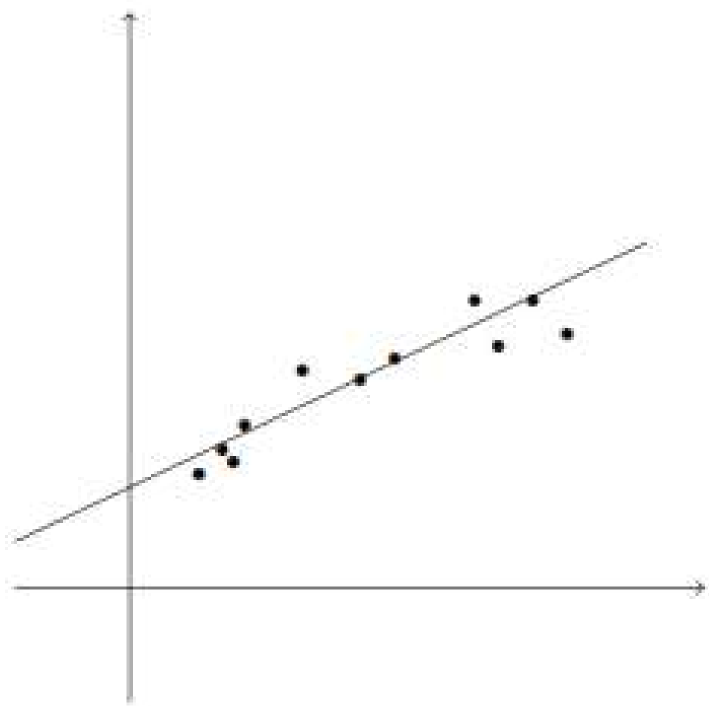
$$Y = \mathbb{R}$$

Objective:
Learn a linear predictor $h_w \in L_d$ that best approximate the relationship between our variables:

$$\begin{array}{llcl} h_w: & \mathbb{R}^{d+1} & \longrightarrow & \mathbb{R} \\ & x & \longrightarrow & h_w(x) = w^t x = y \end{array}$$

Linear Regression

Example:
Predicting the weight of a baby as a function of his age and weight at birth.
Here, $d = 1$.



Linear Regression

The hypothesis class for linear regression model:

In linear regression model, we have:

$$\varphi_{regL}(x) = Id(x) = x \Longrightarrow \varphi_{regL} \circ \boldsymbol{h_w}(\mathrm{x}) = \mathrm{Id}(\boldsymbol{h_w}(\mathrm{x})) = \boldsymbol{h_w}(\mathrm{x})$$

The hypothesis class of linear regression predictors is simply the set of linear functions:

$$H_{regL} = \varphi \circ L_d = L_d = \left\{\varphi_{regL} \circ \boldsymbol{h_w} : \boldsymbol{h_w} \in \ L_d\right\}$$

$$\boldsymbol{H_{reg}} = \{\boldsymbol{h_w} : \ \boldsymbol{x} \longmapsto \langle \boldsymbol{w}, \boldsymbol{x} \rangle \ : \boldsymbol{w} \in \mathbb{R}^{\boldsymbol{d+1}}\} \rightarrow \left|\boldsymbol{H_{reg}}\right| \approx \infty$$

- $\varepsilon = 0,02$
- $Min\ f(x) = |x| \rightarrow |x| = \varepsilon = 0,02$
- $Min\ g(x) = x^2 \rightarrow x^2 = \varepsilon \rightarrow x = \sqrt{0,02} = 0,14$

Linear Regression

The loss function for linear regression model:
It measures how much the model should be penalized for the discrepancy between $h_w(x)$ and y. One common way is to use the squared-loss function:

$$0 \approx d(h_w(x), y) = l\big(h_w, (x, y)\big) = (h_w(x) - y)^2$$

For this loss function, the empirical risk is called the Mean Squared Error:

$$L_S(h_w) = E_{empi}\Big(l\big(h_w, (x, y)\big)\Big) = \frac{1}{m}\sum_{i=1}^{m}(h_w(x_i) - y_i)^2$$

Notice:
There are a variety of other loss functions that one can use, for example, the absolute value loss function:

$$l\big(h_w, (x, y)\big) = |h_w(x) - y| \Longrightarrow \boldsymbol{\partial l\big(h_w, (x, y)\big)}\ \boldsymbol{is\ a\ set}\ \textbf{if}\ h_w(x) = y$$

Linear Regression

The learning algorithm for linear regression model:
The learning algorithm follows ERM_H learning rule.

Least squares:
Least squares is the algorithm that solves the ERM_H problem for the hypothesis class of linear regression predictors with respect to squared loss.

$$\underset{w}{\operatorname{argmin}} L_S(h_w) = \underset{w}{\operatorname{argmin}} \left(\frac{1}{m} \sum_{i=1}^{m} (\langle w, x_i \rangle - y_i)^2 \right)$$

To solve this problem, we calculate the gradient of the objective function and compare it to zero. That is, we need to solve:

$$\nabla L_S(h_w) = \frac{2}{m} \sum_{i=1}^{m} (\langle w, x_i \rangle - y_i) x_i = 0 \longrightarrow \boldsymbol{\nabla^2 L_S(h_w) = cte}$$

Linear Regression

We can rewrite the problem as the problem :

$$\nabla L_S(h_w) = \frac{2}{m}\sum_{i=1}^{m}(\langle w, x_i\rangle - y_i)x_i = 0 \Rightarrow \sum_{i=1}^{m}(\langle w, x_i\rangle x_i) - \sum_{i=1}^{m} y_i x_i = 0$$

$$\Leftrightarrow Aw = b \Longrightarrow \boldsymbol{\nabla^2 L_S(h_w) = A}$$

Where:

$$A = \left(\sum_{i=1}^{m} x_i . x_i^T\right)$$

And

$$b = \sum_{i=1}^{m} y_i x_i$$

Linear Regression

Or in matrix form:

$$A^T = A = \begin{pmatrix} \vdots & & \vdots \\ x_1 & \dots & x_m \\ \vdots & & \vdots \end{pmatrix} \begin{pmatrix} \vdots & & \vdots \\ x_1 & \dots & x_m \\ \vdots & & \vdots \end{pmatrix}^T = square\ order\ matrix\ d \times d$$

And

$$b = \begin{pmatrix} \vdots & & \vdots \\ x_1 & \dots & x_m \\ \vdots & & \vdots \end{pmatrix} \begin{pmatrix} y_1 \\ \vdots \\ y_m \end{pmatrix}$$

If A is invertible, then the solution to the ERM problem is:

$$w = A^{-1}b$$

- $x_1^T = (1,0,0), x_2^T = (1,1,0), x_3^T = (0,1,0), if\, x_3^T = (0,0,1)$ A is inver
- $A = \left(\sum_{i=1}^{3} x_i . x_i^T\right) = x_1 . x_1^T + x_2 . x_2^T + x_3 . x_3^T$
- $= \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} (1,0,0) + \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} (1,1,0) + \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} (0,1,0)$
- $= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 2 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

Linear Regression

If A is not invertible, we require a few standard tools from linear algebra.

A is not invertible when the training data do not cover the entire space of $\mathbb{R}^d$.
Even if A is not invertible, we can always find a solution to the system:

$$Aw = b$$

because b is in the range of A.

Indeed, since A is symmetric, then we can write it using its eigenvalue decomposition as:

$$A = VDV^T$$

Where:
D is a diagonal matrix.
V is an orthonormal matrix (because $V^T V = I$ which is a $d \times d$ matrix).

Linear Regression

Let's define D^+ to be the diagonal matrix such that:

$$\begin{cases} D^+_{i,i} = 0 \quad if \quad D_{i,i} = 0 \\ D^+_{i,i} = \dfrac{1}{D_{i,i}} \quad if \quad D_{i,i} \neq 0 \end{cases} \Rightarrow DD^+ = I \setminus D_{i,i} = 0?$$

Now, define:

$$A^+ = VD^+V^T \text{ and } \hat{w} = A^+b$$

Let v_i denote the ith column of V. Then we have:

$$A\hat{w} = AA^+b = VDV^TVD^+V^Tb = VDD^+V^Tb = VV^Tb = \sum_{i\,:\,D_{i,i}\neq 0} v_i v_i^T b$$

This means that $A\hat{w}$ is the projection of b on the space of vectors v_i for which $D_{i,i} \neq 0$.

Linear Regression

Since the linear space of $(x_1, \dots, x_m)$ is the same as the linear space of those v_i.

And, since b is in the linear space of x_i.

We obtain that:

$$A\hat{w} = b$$

Then, $\hat{w}$ is a solution of $Aw = b$.

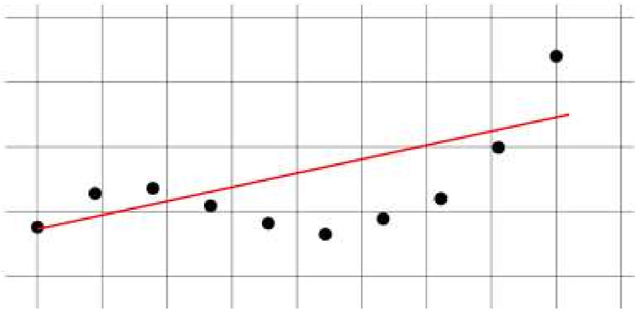
Linear Regression for polynomial regression tasks $x \in \mathbb{R}$

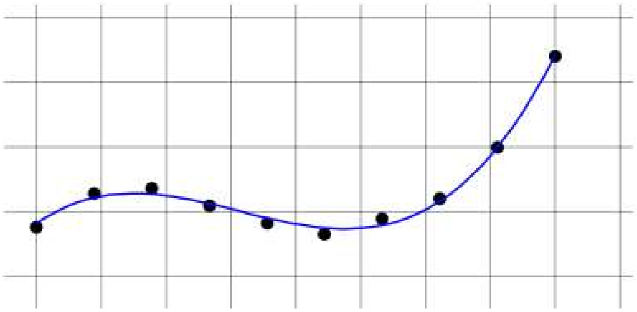
Some learning tasks call for nonlinear predictors, such as polynomial predictors.
Let's consider a one dimensional(one feature) polynomial function of degree n: $A_{\alpha}\ \ n = \alpha$

$$\boldsymbol{P_{w,n}(x) = w_0 + w_1 x + w_2 x^2 + \cdots + w_n x^n =}$$
$$\boldsymbol{P_w(Z) = w_0 * 1 + w_1 z_1 + w_2 z_2 + \cdots + w_n z_n}$$

With $\boldsymbol{Z = (1, z_1, \dots, z_n)}$

Where $(w_0, \dots, w_n)$ is a vector of coefficients of size $n + 1$.





Linear Regression for polynomial regression tasks

We will focus on the class of one dimensional, n-degree, polynomial regression hypotheses. Therefore, the class of polynomial hypotheses is:

$$\boldsymbol{H_{poly}^{n}} = \left\{\boldsymbol{P_{w,n=\alpha}}: \boldsymbol{X} \longmapsto \mathbb{R}: \boldsymbol{n} \in \mathbb{N}^{*}, \boldsymbol{w} \in \mathbb{R}^{\boldsymbol{n+1}}\right\} \Longrightarrow \left|\boldsymbol{H_{poly}^{n}}\right| = \infty$$

Where p is a one dimensional polynomial of degree n, parameterized by a vector of coefficients $(w_0, \dots, w_n)$.
In that case, we have:

$$X \in \mathbb{R} \quad \text{and} \quad Y \in \mathbb{R}$$

One way to learn the class H_{poly}^{n} is by reduction to the problem of linear regression.

Linear Regression for polynomial regression tasks

To translate a polynomial regression problem to a linear regression problem, we define the mapping:

$$\psi_n : \mathbb{R} \longrightarrow \mathbb{R}^{n+1}$$

Such that:

$$\boldsymbol{\psi_n(x) = (1, x, x^2, \dots, x^n)}$$

Then, we have that:

$$\boldsymbol{P_{w,n}\big(\psi_n(x)\big) = w_0 + w_1 x + w_2 x^2 + \cdots + w_n x^n = \langle w, \psi_n(x) \rangle \Longrightarrow \nabla_w P_{w,n} = \psi_n(x)}$$

Finally, we can find the optimal vector of coefficients w by using the Least Squares Algorithm.

Logistic Regression

Definition:
Logistic regression is a type of model used for classification tasks by studying the relationship between some explanatory variables and some binary outcome.

Here we have:

$$X \subset \mathbb{R}^d \text{ for some } d \quad \text{and } Y = \{-1, +1\}$$

Objective:
Learn a linear predictor that best approximate the relationship between our variables:

$$h_w : \mathbb{R}^d \longrightarrow [0,1]$$

We can interpret $h_w(x)$ as the probbability that the label of x is 1: $\mathbf{P}(\mathbf{y}|\mathbf{x}) = \mathbf{P}(\mathbf{y} = \mathbf{1} \vee \mathbf{y} = -\mathbf{1}|\mathbf{x}) = \mathbf{P}(\mathbf{y} = \mathbf{1}|\mathbf{x}) + \mathbf{P}(\mathbf{y} = -\mathbf{1}|\mathbf{x})$**=1**

$$\mathbf{h_w(x) = P(y = 1|x) = 1 - P(y = -1|x)}$$

Logistic Regression

The hypothesis class for logistic regression model:

In logistic regression model, we have:

$$\varphi_{sig}(x) = \frac{1}{1 + e^{-x}}$$

The hypothesis class of logistic regression predictors is the composition of a sigmoid function over the set of linear functions:

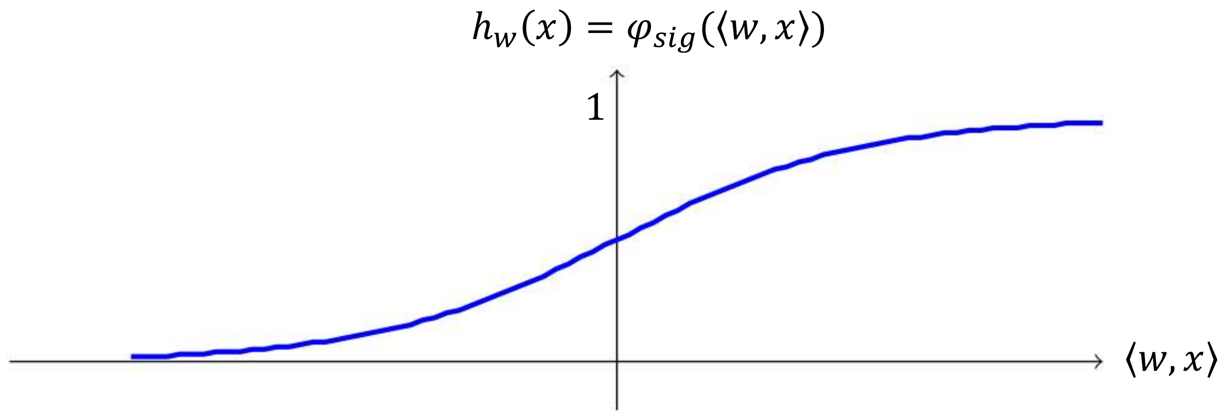
$$H_{sig} = \varphi \circ L_d$$

$$\boldsymbol{H_{sig}} = \{\boldsymbol{\varphi_{sig}}(\mathbf{h}_{\mathrm{w}}):\ \boldsymbol{x} \longmapsto \boldsymbol{\varphi_{sig}}(\langle \boldsymbol{w}, \boldsymbol{x} \rangle) = \frac{\mathbf{1}}{\mathbf{1} + \boldsymbol{e}^{-\langle \boldsymbol{w}, \boldsymbol{x} \rangle}} : \boldsymbol{w} \in \mathbb{R}^{\boldsymbol{d}+\mathbf{1}}\}$$

$$|\boldsymbol{H_{sig}}| = \infty$$

Logistic Regression

The name « sigmoid » means «S-shaped », referring to the plot of this function shown in the figure:



Logistic Regression

Logistic regression Vs Perceptron:

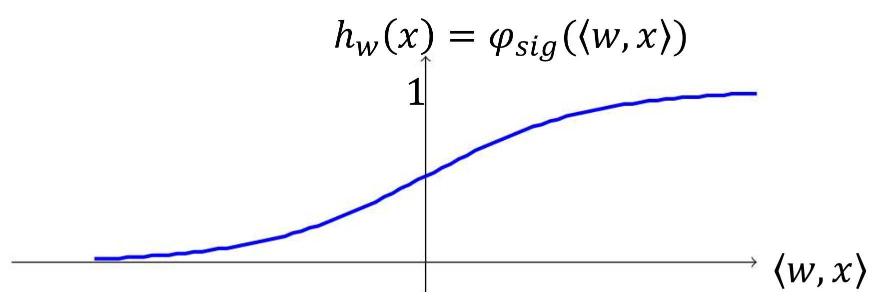
Whenever, $|\langle w, x\rangle|$ is large, the predictions of logistic regression hypothesis and perceptron hypothesis are similar.

However, whenever $|\langle w, x\rangle|$ is close to zero, we have that:

$$\boldsymbol{\varphi_{sig}(\langle w, x\rangle) \approx \frac{1}{2}} \quad \textbf{and} \quad \boldsymbol{\varphi_p(\langle w, x\rangle) = \mathbf{sign}(\langle w, x\rangle)}$$

The logistic regression hypothesis is not sure about the value of the label.

The perceptron hypothesis always outputs a deterministic prediction $\{-1, +1\}$, even if $|\langle w, x\rangle|$ is very close to zero.



Logistic Regression

The loss function for logistic regression model:
It measures how bad it is to predict some $h_w(x) \in [0,1]$ given that the true label is $y = \{\pm 1\}$.

Clearly, we want that:

$$P(y|x) = \begin{cases} h_w(x) \;\; if \;\; y = +1 \\ 1 - h_w(x) \;\; if \;\; y = -1 \end{cases} \Longrightarrow P(y|x) = P(y = 1|x) + P(y = -1|x) = 1$$

to be large.
We have:

$$P(y = 1|x) = h_w(x) = \frac{1}{1+e^{-\langle w,x \rangle}} \text{ and } P(y = -1|x) = 1 - h_w(x) = \frac{1}{1+e^{\langle w,x \rangle}}$$

Generally:

$$\boldsymbol{P(y|x) = \frac{1}{1 + e^{-y\langle w,x \rangle}}}$$

Logistic Regression

It is clear that the loss function will increase monotonically if the probability $P(y|x)$ decreases.

This implies that, it will increse monotonically if $1 + e^{-y\langle w,x \rangle}$ increases.

Therefore, the loss function used in logistic regression penalizes h_w based on the log of $1 + e^{-y\langle w,x \rangle}$, that is:

$$\boldsymbol{l(h_w, (x,y)) = log\left(1 + e^{-y\langle w,x \rangle}\right)}$$

(recall that the log is a monotonic function).
Therefore, given a training set $S = (x_1, y_1), \ldots, (x_m, y_m)$, the ERM problem associated with logistic regression is:

$$\underset{w}{\operatorname{argmin}} L_S(h_w) = \underset{w \in \mathbb{R}^d}{\operatorname{argmin}} \left(\frac{1}{m} \sum_{i=1}^{m} log\left(1 + e^{-y\langle w,x \rangle}\right) \right)$$

Logistic Regression

Notice:
It is clear that the loss function of the logistic regression is a convex function with respect to w.

So, the ERM_H problem for logisitic regression model can be solved using a gradient descent algorithm.