Machine Learning & its Application

Linear Models

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Outline

- Introduction
- Linear Regression
- Linear Classification
- Unified Framework
- Conclusion

- The easiest problem to begin with are linear problems.
- In the linear case, we suppose that the data is linear.
- We can have 2 use cases:
 - Regression: we suppose there is a line that fits the data.
 - Classification: we suppose there is a line that separates the data.
- We will present and solve each problem apart.

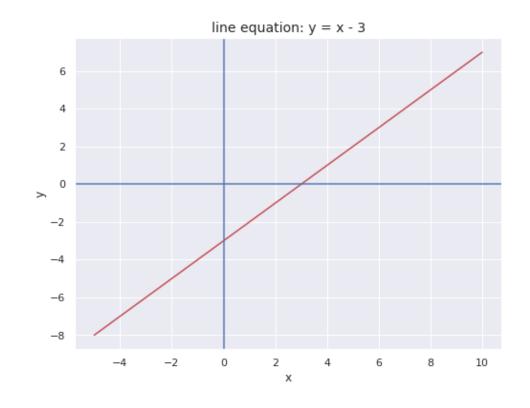
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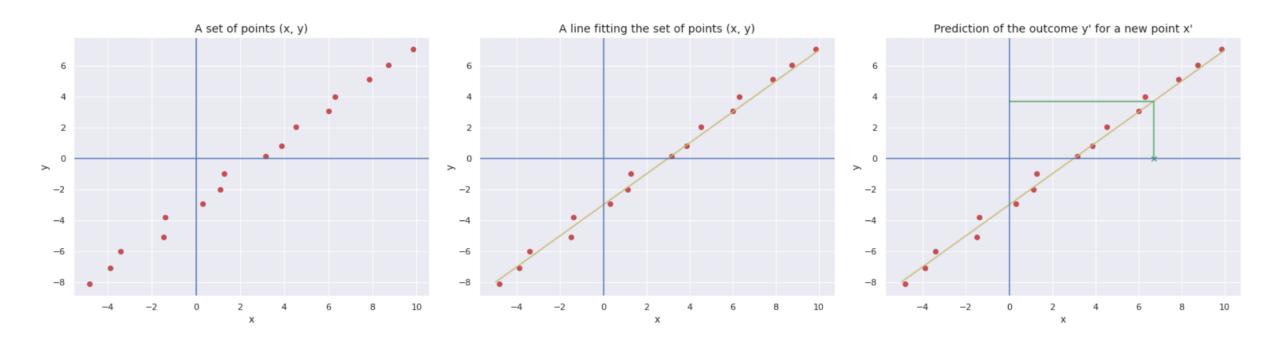
Linear Regression

- Introduction
- Line of best fit
- High dimensional space
- The normal equation
- Exercise

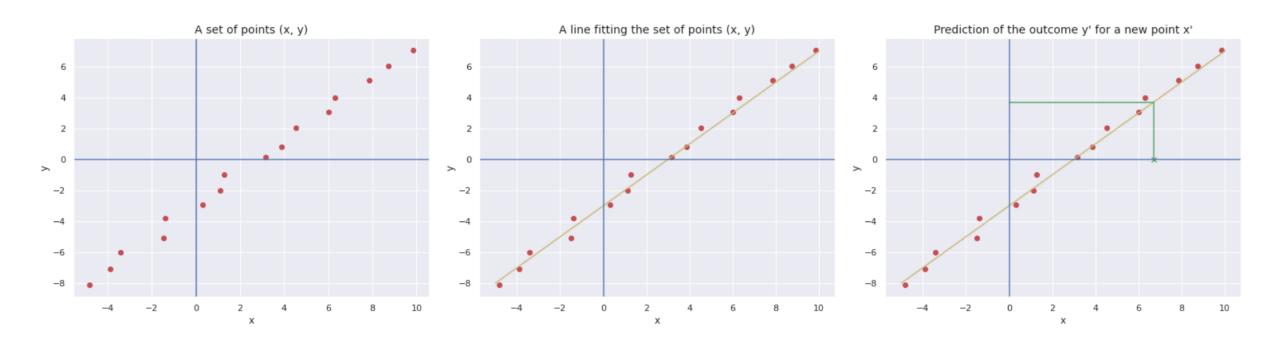
- We will begin in 2D for simplicity.
- A line equation has the form: y=ax+b
- We can draw a line using 2 points only.
- But what can we do with a line?



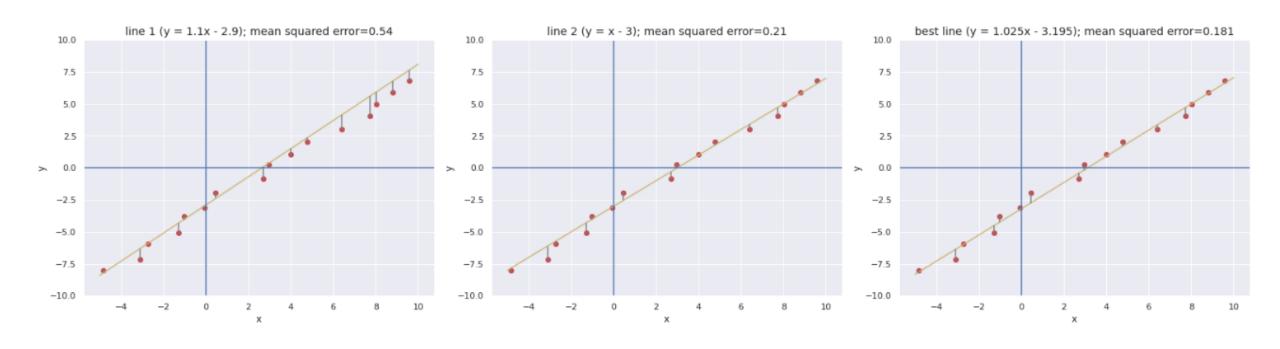
- Imagine we have a set of points (x, y): x is the area of a house and y its price.
- We want to find the line that fits those points (x, y).
- Thus, if we get a new point x' (house area), we can predict the outcome y' (its price).



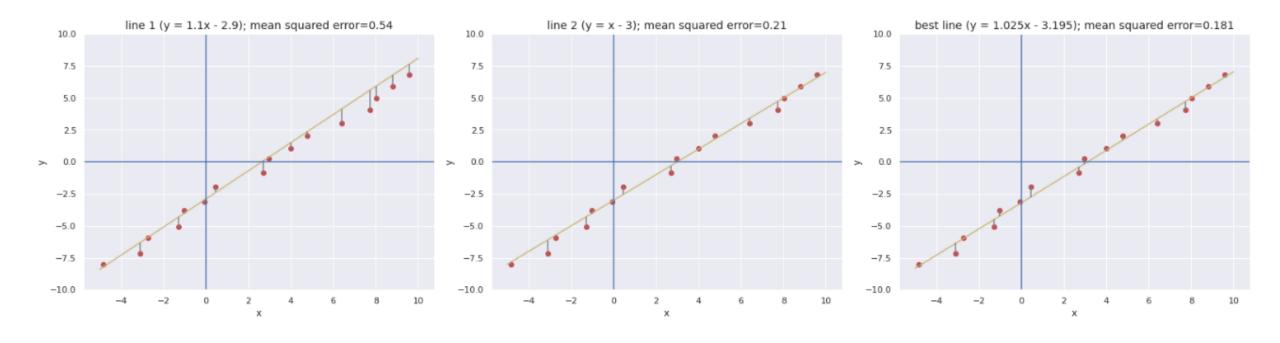
- The data is not perfectly aligned, it has some noise.
- Thus, we cannot use any 2 points to find the line.
- We need to find the line that fits best the data, a.k.a the line of best fit.



- The word "best" should be defined with respect to a metric.
- Let's take 3 lines (for different values of a and b).
- We need to compute an error metric in order to find which line is better.



- The error should represent how much a point is far from the line on average
- It should a positive value, so the values don't cancel each other.
- One choice is to use mean squared error. And thus, line 3 is better than lines 1 and 2.



- We found the best line over 3 possible values of a and b.
- However, we have an infinite number of possibilities.
- We can't compare all possible values, we need a way to find the smallest mean square error.
- The problem is to find the minimum of a function, which we know how to solve:

Compute the derivative and set it to zero

Let's formalize the problem and define the optimization to solve:

given *n* data points $X = \{x_1, x_2, ..., x_n\}$ and $Y = \{y_1, y_2, ..., y_n\}$; $x_i, y_i \in R$

$$\min_{a,b} (Y' - Y)^2 = \min_{a,b} \frac{1}{n} \sum_{i=1}^{n} (ax_i + b - y_i)^2$$

• We want to find (a, b) that gives minimum average distance between the line and all points (xi, yi).

$$\frac{\partial \frac{1}{n} \sum_{i}^{n} (ax_{i} + b - y_{i})^{2}}{\partial a} = \frac{2}{n} \sum_{i}^{n} (ax_{i} + b - y_{i})^{2} x_{i} = 0$$

$$\frac{\partial \frac{1}{n} \sum_{i}^{n} (ax_{i} + b - y_{i})^{2}}{\partial b} = \frac{2}{n} \sum_{i}^{n} (ax_{i} + b - y_{i})^{2} = 0$$

- We have 2 equations with 2 unknowns.
- By rearranging the terms, we can find the line of best fit.

$$a = \frac{\sum_{i}^{n} (x_{i} - \overline{x})(y_{i} - \overline{y})}{\sum_{i}^{n} (x_{i} - \overline{x})^{2}} ; b = \overline{y} - a\overline{x}$$

where
$$\overline{x} = \frac{1}{n} \sum_{i=1}^{n} x_i$$
; $\overline{y} = \frac{1}{n} \sum_{i=1}^{n} y_i$

- We solved the problem in a simple setting when \mathbf{x} and \mathbf{y} are both scalars.
- For the example of house pricing, many features contribute to estimating the price.
- We call each feature a "dimension", and thus x is a vector no more a scalar.
- We also may want to predict multiple quantity not only the price.
- We will take the general case when X and Y are both vectors, of different dimensions.

- We can still define the relationship between a data point Xi and Yi as: Yi = AXi + b.
- To be able to relate Xi and Yi, A should be a matrix and b a vector, as follows:

$$\begin{pmatrix} Y_{i1} \\ Y_{i2} \\ \vdots \\ Y_{iq} \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1p} \\ A_{21} & A_{22} & \dots & A_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ A_{q1} & A_{q2} & \dots & A_{qp} \end{pmatrix} \begin{pmatrix} X_{i1} \\ X_{i2} \\ \vdots \\ X_{ip} \end{pmatrix} + \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_q \end{pmatrix}$$

• Yi a vector of dimension q, Xi of dimension p, b of dimension q, A a matrix of size (q, p).

- The relationship between all data points can also be expressed as: Y = AX + b.
- A and b are the same because they are independent of the number of examples.
- X and Y are now matrices containing all the data points, as follows:

$$\begin{pmatrix} Y_{11} & Y_{21} & \dots & Y_{n1} \\ Y_{12} & Y_{22} & \dots & Y_{n2} \\ \vdots & \vdots & \ddots & \vdots \\ Y_{1q} & Y_{2q} & \dots & Y_{nq} \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1p} \\ A_{21} & A_{22} & \dots & A_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ A_{q1} & A_{q2} & \dots & A_{qp} \end{pmatrix} \begin{pmatrix} X_{11} & X_{21} & \dots & X_{n1} \\ X_{12} & X_{22} & \dots & X_{n2} \\ \vdots & \vdots & \ddots & \vdots \\ X_{1p} & X_{2p} & \dots & X_{np} \end{pmatrix} + \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_q \end{pmatrix}$$

• X is of shape (p, n) and Y of shape (q, n).

- A final trick to make the equation easier is to set A and b into a single matrix.
- We can easily prove that the following formulation is equivalent:

$$\begin{pmatrix} Y_{11} & Y_{21} & \dots & Y_{n1} \\ Y_{12} & Y_{22} & \dots & Y_{n2} \\ \vdots & \vdots & \ddots & \vdots \\ Y_{1q} & Y_{2q} & \dots & Y_{nq} \end{pmatrix} = \begin{pmatrix} b_1 & A_{11} & A_{12} & \dots & A_{1p} \\ b_2 & A_{21} & A_{22} & \dots & A_{2p} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ b_q & A_{q1} & A_{q2} & \dots & A_{qp} \end{pmatrix} \begin{pmatrix} 1 & 1 & \dots & 1 \\ X_{11} & X_{21} & \dots & X_{n1} \\ X_{12} & X_{22} & \dots & X_{n2} \\ \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ X_{1p} & X_{2p} & \dots & X_{np} \end{pmatrix}$$

• We can write the equation as Y = AX, where A contains b as well.

- Now it is time to find A and b the fits well the data as we did for the scalar case.
- We will define an optimization problem and set the derivative to zero as usual.
- The problem can be expressed as follows:

$$\min_{A} || Y' - Y ||_{2}^{2} = \min_{A} || AX - Y ||_{2}^{2} = \min_{A} \sum_{i=1}^{n} \sum_{j=1}^{n} ((AX)_{ij} - Y_{ij})^{2}$$

However, computing the matrices derivative is not easy, we will define some properties.

The Normal Equation

For a given matrix M of shape (n, n), and Q of shape (n, p)

1. We define the trace (tr) of **M** as the sum of its diagonal elements. The trace of a matrix is a scalar value:

$$tr(M) = \sum_{i} M_{ii}$$

2. The transpose of a matrix is the swapping of its rows and columns. Then, the shape of transpose Q is (p, n):

$$Q = \begin{pmatrix} Q_{11} & Q_{12} & \cdots & Q_{1p} \\ Q_{21} & Q_{22} & \cdots & Q_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ Q_{n1} & Q_{n2} & \cdots & Q_{np} \end{pmatrix}; Q^{T} = \begin{pmatrix} Q_{11} & Q_{21} & \cdots & Q_{n1} \\ Q_{12} & Q_{22} & \cdots & Q_{n2} \\ \vdots & \vdots & \ddots & \vdots \\ Q_{1p} & Q_{2p} & \cdots & Q_{np} \end{pmatrix}; (MQ)^{T} = Q^{T}M^{T}$$

3. The L2 norm square of a matrix equals the trace of the matrix times its transpose:

$$||Q||_2^2 = \operatorname{tr}(Q, Q^T) = \operatorname{tr}(Q^T, Q)$$

4. The derivative of the trace of a matrix with respect to itself is the identity matrix:

$$\frac{\partial \operatorname{tr}(M)}{\partial M} = I$$

- 5. The derivative of scalar **b** with respect to a matrix **M** is a matrix of the same dimension as **M** (point 4 is an example).
- 6. Some useful rules:

$$\frac{\partial MQ}{\partial M} = Q^T; \frac{\partial MQ^T}{\partial Q} = M; \frac{\partial MM^T}{\partial M} = 2M; \frac{\partial MZM^T}{\partial M} = MZ + MZ^T; (QQ^T)^T = QQ^T$$

The Normal Equation

- We want to compute the derivative with respect to A.
- We will use the aforementioned properties to solve it step by step.

$$\frac{\partial \operatorname{tr}((AX - Y)(AX - Y)^{T})}{\partial A} = \frac{\partial (AX - Y)(AX - Y)^{T}}{\partial A} \cdot \frac{\partial \operatorname{tr}((AX - Y)(AX - Y)^{T})}{\partial (AX - Y)(AX - Y)^{T}} \text{ (chain rule)}$$

$$\frac{\partial \operatorname{tr}((AX - Y)(AX - Y)^{T})}{\partial (AX - Y)(AX - Y)^{T}} = I \text{ (property 4)}$$

$$\frac{\partial \operatorname{tr}((AX - Y)(AX - Y)^{T})}{\partial A} = \frac{\partial (AX - Y)(AX - Y)^{T}}{\partial A}$$

The Normal Equation

- We simplified the expression in order to compute the derivatives.
- This equation is known as the **normal equation**.

$$(AX - Y)(AX - Y)^{T} = (AX - Y)(X^{T}A^{T} - Y^{T}) = AXX^{T}A^{T} - AXY^{T} - YX^{T}A^{T} + YY^{T}$$

$$\frac{\partial(AXX^{T}A^{T} - AXY^{T} - YX^{T}A^{T} + YY^{T})}{\partial A} = AXX^{T} + AXX^{T} - YX^{T} - YX^{T} = 2AXX^{T} - 2YX^{T} = 0$$

$$AXX^{T} = YX^{T}$$

$$A = YX^{T}(XX^{T})^{-1}$$

N.B.: You may find a slightly different formulation in most references. This is due to the way we define the matrices X and Y. In this derivation, we defined X and Y as matrices of shape (number_of_features, number_of_samples). In practice, we use (number_of_samples, number_of_features). Thus the difference.

Exercise

- We will do a small exercise on Google Colab.
- The goal is to implement a linear regression function in Python.
- We will code the scalar version and the matrix version for higher dimensional data.
- We will compare the result to sklearn <u>LinearRegression</u> class.

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Linear Classification

- Introduction
- Binary classification
 - Probabilistic modelling
 - Maximum likelihood estimation
 - Binary classification as Bernoulli distribution
- Multiclass classification

- Classification is assigning a label yi to an input xi, where yi is a discrete value.
- In case yi can take only 2 values (e.g. cat vs dog) we call it binary classification.
- If yi can take more than 2 values, we call it multiclass classification.
- In both cases, we suppose that an input xi can take only a single label yi.
- We call this problem single label classification (against multi label classification).
- An example of multilabel classification is movie type prediction, where a movie
 can belong to multiple type at the same time. It is out of the scope of this course.

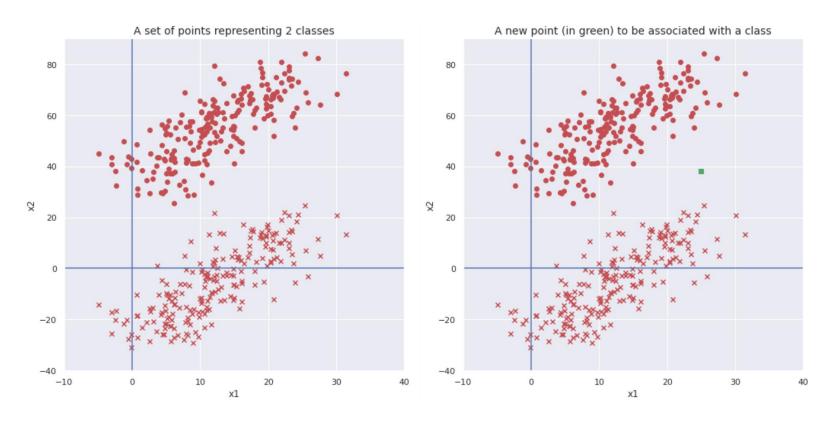
Binary Classification

Let's take a simple binary classification problem as illustrated below.

• Given a set of linearly separable points (x, y), we want to assign for a new point

x' a label y'.

• Here y is a circle or cross.



Binary Classification

- There are two main approaches to solve this problem:
 - 1. Find the line that maximize the margin between the 2 set of points.
 - 2. Learn a probabilistic model to predict a probability of belonging to one of the classes.
- One well-known classical algorithm that follows the first approach is SVM.
- The problem with this approach is that it doesn't give a confidence measurement.
- Deep Learning algorithms follow the second approach.
- We will present a probabilistic linear classifier known as logistic regression.

Probabilistic Modeling

- Probabilistic classifiers should output a probability of belonging to one class.
- Thus, the output of a binary classifier is not 0 or 1 but a value in the range [0-1].
- To be able to define a probability, we need to define random variables.
- Let x be a random variable that can take on different realizations Xi.
- Let y be a function of x and some unknown parameters A, y=f(x; A).
- Thus, **y** is also a random variable that can take different realization **Yi**.

Probabilistic Modeling

- We define the data-generating process, p(x, y) that can generate any (x, y) value.
- We suppose that the data is independent and identically distributed (iid).
- Our goal is to compute the probability of a label y, given x and A: p(y/x; A).
- For instance, for the green point x', based on the learned knowledge A:
 - Compute p(y=circle/x'; A) and p(y=cross/x'; A)
 - If p(y=circle/x'; A) > p(y=cross/x'; A) then x' is a circle with a given probability.
- To solve this problem we should have 2 things:
 - 1. The value of the parameter **A**.
 - 2. The expression of p(y/x; A).

Probabilistic Modeling

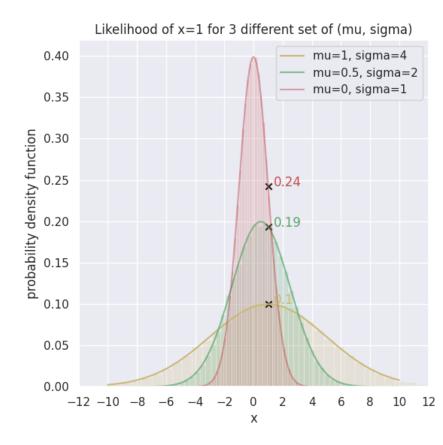
- Finding the value of A is also called parameter estimation.
- We need to find an estimator of A. An estimator in general is a function of the data.
- For instance, an estimator of the expectation is the average value.
- But how can we find estimators? The answer is maximum likelihood principle.

- Maximum likelihood is a way to find estimators. Let's take an example.
- Imagine we have a set of points generated from a Gaussian distribution of unknown mean and variance.
- The probability density function of a Gaussian distribution is as follows:

$$p(x; \ \mu, \sigma) = \frac{1}{\sigma \sqrt{2\pi}} \exp\left(-\frac{1}{2} \frac{(x - \mu)^2}{\sigma^2}\right)$$

 The question to answer is "what are the parameters that highly likely generated our data"?

- Let's take the first data point, let it be X=1 and plot 3 different Gaussians.
- For each we want to see which μ and σ are more likely to generate X=1.
- Among all curves, the red one has a bigger likelihood.
- We say that we will choose the parameters that maximize the likelihood.



- However, here we compared only 3 possible values.
- In addition, we should choose the maximum likelihood for all data points not only X=1.
- Thus, we can write the optimization problem as:

$$\max_{A} P(X; A) = \max_{A} P(X_1, X_2, ..., X_n; A) = \max_{A} \prod_{i=1}^{n} P(X_i; A)$$

- However, it is hard to optimize a product. We can transform it to sum with a log.
- Thus, an equivalent optimization problem is the log likelihood:

$$\max_{A} \prod_{i}^{n} P(X_{i}; A) \equiv \max_{A} \sum_{i}^{n} \log P(X_{i}; A)$$

• Now let's apply maximum log likelihood to estimate μ and σ .

$$P(X_i; A = (\mu, \sigma)) = \frac{1}{\sigma \sqrt{2\pi}} \exp\left(-\frac{1}{2} \left(\frac{X_i - \mu}{\sigma}\right)^2\right)$$
$$\log P(X_i; A = (\mu, \sigma)) = \log\left(\frac{1}{\sigma \sqrt{2\pi}}\right) - \frac{1}{2} \left(\frac{X_i - \mu}{\sigma}\right)^2$$

$$\sum_{i=1}^{n} \log P(X_{i}; A = (\mu, \sigma)) = -n \log(\sigma \sqrt{2\pi}) - \frac{1}{2\sigma^{2}} \sum_{i=1}^{n} (X_{i} - \mu)^{2}$$

$$\frac{\partial \sum_{i}^{n} \log P(X_{i}; A = (\mu, \sigma))}{\partial \mu} = \frac{1}{\sigma^{2}} \sum_{i}^{n} (X_{i} - \mu) = 0; \mu = \frac{1}{n} \sum X_{i} = \overline{X}; \sigma \neq 0$$

$$\frac{\partial \sum_{i}^{n} \log P(X_{i}; A = (\mu, \sigma))}{\partial \sigma} = -n\frac{1}{\sigma} + \frac{1}{\sigma^{3}} \sum_{i}^{n} (X_{i} - \mu)^{2} = 0; \sigma^{2} = \frac{1}{n} \sum_{i}^{n} (X_{i} - \overline{X})^{2}$$

Binary Classification as Bernoulli

- Let's get back to binary classification.
- We mentioned that the goal is to compute p(y/x; A).
- We showed how maximum likelihood can be used to estimate the parameters A.
- What remain is to find the expression of the p(y/x; A).
- Binary classification is similar to a coin flipping task when the outcome is 1 or 0.
- Thus, it can be modeled with a Bernoulli distribution.

Binary Classification as Bernoulli

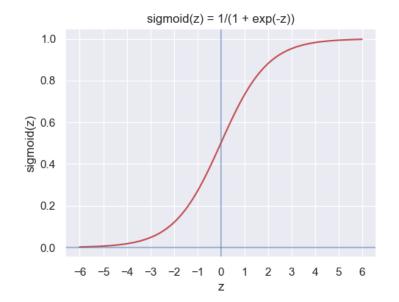
Bernoulli distribution is defined as follows:

$$P(Y = y_i) = \begin{cases} \theta & \text{if } y_i = 1 \\ 1 - \theta & \text{if } y_i = 0 \end{cases} = \theta^{y_i} (1 - \theta)^{1 - y_i}$$

- In coin flipping, \(\theta \) is the probability of having a head.
- It is sufficient to compute P(Y=1), because P(Y=0) = 1 P(Y=1).
- Thus, we can write Bernoulli as $P(Y=1) = \theta$.
- In our case, we don't have P(Y=1), instead we have $P(Y=1/x; A) = \theta$.
- But θ should be a function of x and A, thus $P(Y=1/x; A) = \theta(x; A)$.

Binary Classification as Bernoulli

- We begin by talking about linear classifiers, so we should have a linear relationship.
- $\theta(x; A)$ is a function of x and A, and should be between 0 and 1.
- We can define a linear relation Z=AX, then squash the values between 0 and 1.
- One function that do this is the sigmoid function, represented as follows:



Binary Classification as Bernoulli

- We finally get all the ingredients to solve linear classification problem.
- We have p(Y=1/X; A)=sigmoid(AX). This classifier is called logistic regression.
- We can apply maximum likelihood to find A, or equivalently the Negative Log

Likelihood (NLL) and set the derivative to 0.

$$P(Y = 1/X_i; A) = \sigma(AX_i); \text{ where } \sigma(x) = \frac{1}{1 + e^{-x}}$$

$$-\log P(Y = 1/X; A) = \log(1 + e^{-AX})$$

$$\min_{A} - \sum_{i}^{n} \log P(Y_i = 1/X_i; A) = \min_{A} \sum_{i}^{n} \log(1 + e^{-AX_i})$$

$$\frac{\partial \sum_{i}^{n} \log(1 + e^{-AX_i})}{\partial A} = \sum_{i}^{n} \frac{X_i e^{-AX_i}}{1 + e^{-AX_i}} = 0$$

Binary Classification as Bernoulli

- There is no closed-form solution for this equation.
- We need an iterative algorithm, like gradient descent, to solve it (next lesson).
- Note that, applying the NLL to a Bernoulli distribution give:

$$P(Y = y_i) = \theta^{y_i} (1 - \theta)^{1 - y_i}$$

$$-\log P(Y = y_i) = -\log \theta^{y_i} (1 - \theta)^{1 - y_i} = -y_i \log \theta - (1 - y_i) \log(1 - \theta)$$

- This is the well-known binary cross entropy loss.
- Cross entropy maximizes the likelihood of a binary classifier parameters to have generated the training data.

Multiclass Classification

- Everything we did for binary classification applies here as well with few exceptions.
- First, we can't model a multiclass problem with Bernoulli distribution.
- In addition, we can't use the sigmoid function.
- Multiclass problem is similar to a dice roll, where each face has a probability to occur.
- We can model it with a Multinoulli distribution, that is defined as follows:

Bernouilli:
$$P(Y = y_i) = \begin{cases} \theta & \text{if } y_i = 1 \\ 1 - \theta & \text{if } y_i = 0 \end{cases} = \theta^{y_i} (1 - \theta)^{1 - y_i}; y_i \in \{0, 1\}; 0 \leq \theta \leq 1$$

Multinouilli:
$$P(Y = y_i) = \prod_{j=1}^{k} \theta_j^{y_{ij}}$$
; $y_i \in \{0, 1\}^k$; $0 \le \theta_j \le 1$; $\sum_{j=1}^{k} \theta_j = 1$

Multiclass Classification

- The output of a k-class classifier is a vector of probability of size k.
- Each value represents the probability of a class to occur.
- In addition, the k value should sum to 1.
- To obtain this from a linear projection Z=AX, we can apply the softmax function:

$$\operatorname{softmax}(z_i) = \frac{\exp(z_i)}{\sum_{j=1}^{k} \exp(z_j)}; z = Ax; z \in \mathbb{R}^k; z_i \in \mathbb{R}$$

• Thus we can define our probabilistic classifier.

Multiclass Classification

- Once we have the expression of p(y/x; A) we can apply Maximum likelihood to find A.
- Applying it to a Multinoulli distribution gives the following:

$$P(Y = y_i) = \prod_{j=1}^k \theta_j^{y_{ij}}$$

$$-\log P(Y = y_i) = -\log \prod_{j=1}^k \theta_j^{y_{ij}} = -\sum_{j=1}^k \log \theta_j^{y_{ij}} = -\sum_{j=1}^k y_{ij} \log \theta_j$$

- This is the well-known cross entropy loss.
- Similarly to binary classification, we need an iterative algorithm to find the solution.

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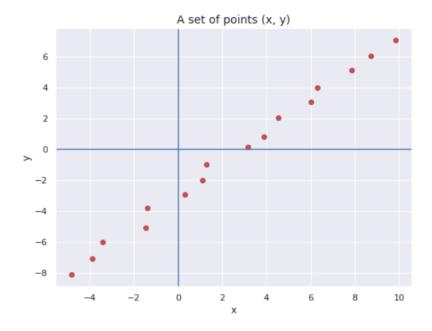
Unified Framework

- Let's summarize what we did in classification to solve the problem:
 - Define the distribution of p(y/x; A) (Bernoulli for binary, Multinoulli for multiclass).
 - Apply Maximum Likelihood principle to estimate the parameter A.
 - Compute the derivative to be used later with gradient descent (as there is no closed-form solution).
- We obtained the well-known cross entropy loss for classification.
- There are well-defined systemic steps to find classification solutions.
- It would be nice if we can have something similar to linear regression.

Unified Framework

- First, we need to define the probabilistic setting for linear regression.
- However, we should use a continuous distribution not a discrete one.
- Suppose there is a perfect line y=ax+b that should pass through all points.
- However, there is a noise term added to each point.
- We can express it as follows:

$$y = ax + b + \epsilon$$
; $\epsilon \sim N(0, \sigma)$



Unified Framework

• Thus, we can find p(y/x; A) and apply Negative Log likelihood as follows:

$$\epsilon = y - ax - b \sim N(0, \sigma) \rightarrow y \sim N(ax + b, \sigma) \rightarrow P(y/x; a, b) \sim N(ax + b, \sigma)$$

$$P(y/x; a, b) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2} \frac{(y - ax - b)^2}{\sigma^2}\right)$$

$$NLL: -\sum_{i} \log \frac{1}{\sigma \sqrt{2\pi}} \exp \left(-\frac{1}{2} \frac{(y - ax - b)^{2}}{\sigma^{2}} \right) = -\sum_{i} \log \frac{1}{\sigma \sqrt{2\pi}} - \frac{1}{2} \frac{(y_{i} - ax_{i} - b)^{2}}{\sigma^{2}} \propto -\sum_{i} (y_{i} - (ax_{i} + b))^{2}$$

- As we can see, we get the mean squared error as before.
- It means that mean squared error maximize the likelihood of the data being generated by a Gaussian distribution.

Exercise

• Show the importance of using sigmoid in binary classification from an optimization point of view.

Hints:

- Take the case where the correct label y=1 for simplicity.
- Plot the sigmoid function and the negative log likelihood applied to it.
- See what is the error when the model predict correctly and what is the error in the other case.
- The ideal behavior is to have very small error with correct prediction, and a proportional error otherwise.

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Conclusion

- We presented linear models for regression and classification.
- In the regression case, we derived and solved the normal equation in a closed-form.
- In classification, we had to define a probabilistic setting in order to output probability.
- The goal is to compute p(y/x; A):
 - We need to model the problem following a distribution (e.g. Bernoulli for binary case).
 - Then, we can apply the negative log likelihood to derive loss functions to get A.
- We applied the same framework for regression as well.
- We obtained the well-known loss functions for both classification and regression.