Supervised Learning

Carlos Valle

Departamento de Informática
Universidad Técnica Federico Santa María

cvalle@inf.utfsm.cl

December 3, 2015

Overview

Motivation

- Suppose we have a dataset giving weight, gender and calorie consumption a day from 40 people.

Weight (Kg)	Gender (M/F)	calorie cons. (cal)
85	M	2075
58	F	1757
52	M	2783
55	F	3500
⋮	⋮	⋮

- We would like to predict the calorie consumption per day of other people.
- In this case, weight and gender are called input features. Each vector input $\mathbf{x}_m$ has these two features.
- A calorie consumption per day y_m is called target.
- A pair $(\mathbf{x}_m, y_m)$ is called a train example. A training set is a group of M training examples $S_M = \{(\mathbf{x}_m, y_m)\}, m = 1 \ldots M$.

Preliminary definitions

- Features can be either numerical or categorical.
- Let $\mathcal{X}$ be the feature space, and $\mathcal{Y}$ the output space.
- Our goal is to obtain a mapping $f : \mathcal{X} \to \mathcal{Y}$, commonly called the *hypothesis* or learner), $\mathcal{X} \subseteq \mathbb{R}^n$, $y \in Y \subseteq \mathbb{R}$.
- Let $\mathcal{S}$ the space that spans the possible samples, drawn from an unknown distribution $P(\mathbf{x}, y)$.
- A *learning algorithm* is a map from the space of training sets to the hypothesis space $\mathcal{H}$ of possible functional solutions

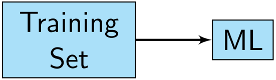
$$\begin{aligned} \mathcal{A} \quad : \quad & \mathcal{S} \to \mathcal{H} \\ & S_M \to \mathcal{A}(S_M) = f. \end{aligned} \tag{1}$$

Learning process

Training Set

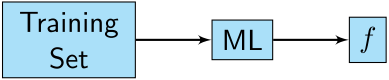
- If the target is continuous, we have a regression problem
- If the target can take a finite number k of discrete values, we have a classification problem. In particular $k = 2$ the problem is called binary classification.

Learning process



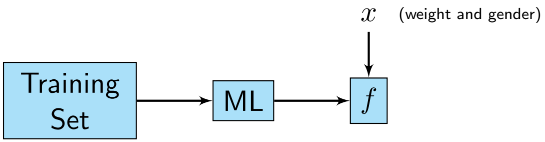
- If the target is continuous, we have a regression problem
- If the target can take a finite number k of discrete values, we have a classification problem. In particular $k = 2$ the problem is called binary classification.

Learning process



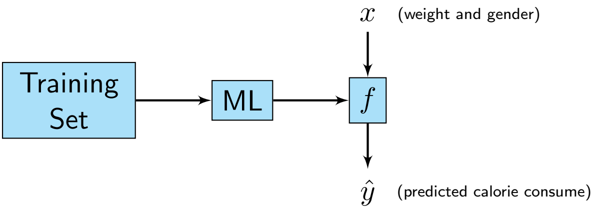
- If the target is continuous, we have a regression problem
- If the target can take a finite number k of discrete values, we have a classification problem. In particular $k = 2$ the problem is called binary classification.

Learning process



- If the target is continuous, we have a regression problem
- If the target can take a finite number k of discrete values, we have a classification problem. In particular $k = 2$ the problem is called binary classification.

Learning process



- If the target is continuous, we have a regression problem
- If the target can take a finite number k of discrete values, we have a classification problem. In particular $k = 2$ the problem is called binary classification.

Learning process (2)

- A main challenge is to construct an automatic method or algorithm able to estimate future examples based on the observed phenomenon in the training set.
- This key property of an algorithm is known as the generalization ability.
- The algorithms that memorize the training samples but have poor predictive performance with unknown examples, this undesirable problem is well-known as overfitting.

Loss function

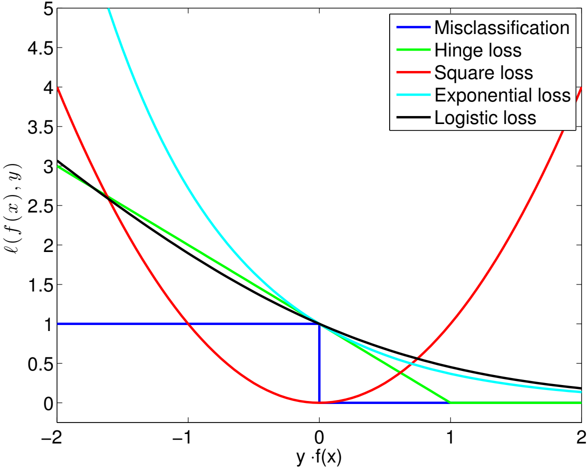
- The quality of the algorithm $\mathcal{A}$ is measured by the loss function given by $\ell : \mathbb{R} \times \mathcal{Y} \to [0, \infty)$, which quantifies the accuracy of the observed response $f(\mathbf{x})$ with respect to the true or desired response y.
- This function does not penalize the exact predictions, i.e., $\ell(y, f(\mathbf{x})) = 0$ if and only if $y = f(\mathbf{x})$.
- ℓ is a non-negative function, hence, the hypothesis will never profit from additional good predictions.
- In regression settings we use the quadratic loss function $\ell(y, f(\mathbf{x})) = (y - f(\mathbf{x}))^2$
- While in classification we have the misclassification loss function

$$\ell(f(\mathbf{x}), y) = \begin{cases} 0 & \text{if } f(\mathbf{x}) = y \\ 1 & \text{if } f(\mathbf{x}) \neq y \end{cases}.$$

Loss function (2)

- However, In binary classification problem (where $y \in \{-1, 1\}$), the margin $yf(\mathbf{x})$ is introduced as a quality measure.
- This quality amount leads to several loss functions such as the *hinge loss*
$$\ell(f(\mathbf{x}), y) = \max(1 - yf(\mathbf{x}), 0) = |1 - yf(\mathbf{x})|_+.$$
- The *logistic loss* $\ell(f(\mathbf{x}), y) = \log_2\left(1 + e^{-yf(\mathbf{x})}\right)$
- The *exponential loss* $\ell(f(\mathbf{x}), y) = e^{-yf(\mathbf{x})}$.
- Note that the square loss can be arranged as $\ell(f(\mathbf{x}), y) = (y - f(\mathbf{x}))^2 = (1 - yf(\mathbf{x}))^2$ taking into account that $y^2 = 1$.
- And the misclassification loss can be written as $\ell(f(\mathbf{x}), y) = I(yf(\mathbf{x}) < 0)$, where $I(\cdot)$ is the indicator function.

Loss function (3)



- Logistic Loss and exponential loss can be viewed as a continuous approximation of the misclassification function

Motivation

- We want to predict the total daily travel time of a trucker considering both the distance traveled and the number of deliveries made as input features:

Distance travel time (km)	Number of deliveries	Travel time (hr)
50	4	8.4
75	10	12.3
34	3	6.5
62	5	10.0
$\vdots$	$\vdots$	$\vdots$

- Here the inputs $\mathbf{x}$ are bi-dimensional vectors. We let $\mathbf{x}_m^{(i)}$ denote the feature i of the m-th example.

Linear model

- We could approximate the total daily travel time y as a linear function of the distance traveled and the number of deliveries made:

$$f(x) = \beta_0 + \beta_1 x^{(1)} + \beta_2 x^{(2)},$$

- where $\beta_i, i = 0, 1, 2$ are the parameters of the linear model.
- Thus, the space of linear functions mapping from $\mathcal{X}$ to $\mathcal{Y}$ is parametric.
- We define $x^{(0)} = 1$ to define the linear model in matrix form:

$$f(x) = \sum_{i=0}^{I} \beta_i x^{(i)} = \beta^T \mathbf{x}, \qquad (2)$$

- where I is the number of features.

How do we select the β 's?

- We can get the parameters of the model by minimizing the quadratic loss funcion over the training set:

$$J(\beta) = \frac{1}{2}\sum_{m=1}^{M}\left(f\left(\mathbf{x}_m\right) - y_m\right)^2 \tag{3}$$

- where $\beta = (\beta_1, \beta_2, \ldots, \beta_I)^T$.
- We need to choose β which minimizes $J(\beta)$.

LMS Algorithm

- This problem can be expressed in matrix form:

$$\frac{1}{2}J(\beta) = (y - X\beta)^T(y - X\beta),$$

- where X is an $N \times (I+1)$ matrix.

From matrix calculus

- If x is a column vector:
- $\frac{\partial u^T v}{\partial x} = \frac{\partial u}{\partial x} \cdot v + \frac{\partial v}{\partial x} \cdot u$
- $\frac{\partial Ax}{\partial x} = A^T$

LMS Algorithm (2)

- Then,

$$\begin{aligned}\frac{\partial J(\beta)}{\partial \beta} &= -X^T(y - X\beta)\\ \frac{\partial^2 J(\beta)}{\partial \beta \partial \beta^T} &= X^T X\end{aligned}$$

- Equalizing the first derivative to zero we get the normal equations:

$$X^T(y - X\beta) = 0 \Longrightarrow \widehat{\beta} = (X^T X)^{-1} X^T y$$

Gradient descent algorithm

- Let consider the gradient descent algorithm which start with some initial β and repeatedly performs:

$$\beta_i^{p+1} = \beta_i^p - \alpha \frac{\partial}{\partial \beta_i} J(\beta)$$

- Let's calculate the derivative of the loss function for a single training example $(\mathbf{x}_m, y_m)$:

$$\begin{aligned}
\frac{\partial}{\partial \beta_i} J(\beta) &= \frac{\partial}{\partial \beta_i} \frac{1}{2} \left(f\left(\mathbf{x}_m\right) - y_m\right)^2 \\
&= \left(f\left(\mathbf{x}_m\right) - y_m\right) \cdot \frac{\partial}{\partial \beta_i} \left(\sum_{i=0}^{I} \beta_i x^{(i)} \right) \\
&= \left(f\left(\mathbf{x}_m\right) - y_m\right) \mathbf{x}_m^{(i)}
\end{aligned}$$

Gradient descent algorithm (2)

- Then, for a single example:

$$\beta_i^{p+1} = \beta_i^p - \alpha(f(\mathbf{x}_m) - y_m)\,\mathbf{x}_m^{(i)}$$

- This rule is called Widrow-Hoff learning rule.
- Note that the amount of the update is proportional to the error: $(f(\mathbf{x}_m) - y_m)$

Batch gradient descent algorithm

- We can apply the learning rule above for the training set:

Algorithm 1 Batch gradient descent algorithm

1: **repeat**
2: $\beta_i^{p+1} = \beta_i^p - \alpha \sum_{m=1}^{M} \left(f\left(\mathbf{x}_m\right) - y_m \right) \mathbf{x}_m^{(i)}$ (for every i)
3: **until** Convergence

- In general, gradient descent can reach a local minimum.
- However, J is a convex function. Thus, the optimization problem has only one global optimum.

Stochastic gradient descent algorithm

- We can modify the learning rule above for each example:

Algorithm 2 Stochastic gradient descent algorithm

1: **repeat**
2:     **for** $m := 1$ to M **do**
3:         $\beta_i^{p+1} := \beta_i^p - \alpha(f(\mathbf{x}_m) - y_m)\,\mathbf{x}_m^{(i)}$ (for every i)
4:         $\beta_i^p := \beta_i^{p+1}$
5:     **end for**
6: **until** Convergence

- This method is called stochastic or online gradient descent.
- Usually, this technique converge faster than batch gradient descent.
- However, using a fixed value for α it may never converge to the minimum of $J(\beta)$, oscillating around it.
- To avoid this behavior, it is recommended to slowly decrease α to zero along the iterations.

Motivation (Matrix derivatives)

- When we find the parameter vector that minimize a loss function, we need to take its derivatives respect to this vector and set them to zero.
- In order to do this, we need to learn some tools fro doing matrix calculus.

Matrix derivatives

- Let $f : \mathbb{R}^{P\times Q} \mapsto \mathbb{R}$ be a function which maps from $P \times Q$ matrices to the real numbers.
- We define the derivative of f with respect to A as:

$$\nabla_A f(A) = \begin{bmatrix} \frac{\partial f}{\partial A_{11}} & \cdots & \frac{\partial f}{\partial A_{1Q}} \\ \vdots & \ddots & \vdots \\ \frac{\partial f}{\partial A_{P1}} & \cdots & \frac{\partial f}{\partial A_{PQ}} \end{bmatrix}$$

- Thus, the gradient $\nabla_A f(A)$ is an $P \times Q$ matrix where its (i,j) element is $\frac{\partial f}{\partial A_{ij}}$
- For example: Let $A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$, and $f(x) = 3A_{11}^2 + A_{12}A_{21} + \frac{1}{2}A_{22}$
- Then the gradient is $\nabla_A f(A) = \begin{bmatrix} 6A_{11} & A_{21} \\ A_{12} & \frac{1}{2} \end{bmatrix}$

Matrix derivatives (2)

- Since our loss functions are in $\mathbb{R}$, we will use the trace operator to compute the derivatives with respect to the parameter vector.
- Now we will define this operator and we will study its properties.
- After that, we will apply trace derivatives in order to minimize $J(\beta)$.

Trace

- Let A a $P \times P$ matrix.
- The trace of A is an linear $M(\mathbb{R}^P) \mapsto \mathbb{R}$ operator defined as:

$$\text{tr}(A) = \sum_{p=1}^{P} A_{pp}$$

- Thus, $\text{tr}(A + B) = \text{tr}(A) + \text{tr}(B)$
- And $\text{tr}(cA) = c\text{tr}(A)$, where $c \in \mathbb{R}$
- Also note that $\text{tr}(c) = c$

Trace properties

- Transposition of dependent variables:

$$\text{tr}(\mathbf{A}) = \text{tr}(\mathbf{A}^T). \tag{4}$$

- Hence,

$$\frac{\partial \text{tr}(\mathbf{A})}{\partial \mathbf{X}} = \frac{\partial \text{tr}(\mathbf{A}^T)}{\partial \mathbf{X}}$$

- Cyclic permutation: Let $\mathbf{A}$,$\mathbf{B}$ be two matrices such that $\mathbf{AB}$ is square. Then, $\text{tr}(\mathbf{AB}) = \text{tr}(\mathbf{BA})$ Thus,

$$\frac{\partial \text{tr}(\mathbf{AB})}{\partial \mathbf{X}} = \frac{\partial \text{tr}(\mathbf{BA})}{\partial \mathbf{X}}$$

- Moreover, $\text{tr}(\mathbf{ABC}) = \text{tr}(\mathbf{CAB}) = \text{tr}(\mathbf{BCA})$

Trace properties (2)

- Transposition of independent variables:

$$\nabla_{\mathbf{A}} f(\mathbf{A}) = \frac{\partial f}{\partial A_{pq}}, p = 1, \ldots, P, q = 1, \ldots, Q.$$

- Thus,

$$\nabla_{\mathbf{A}^T} f(\mathbf{A}) = \frac{\partial f}{\partial A_{qp}}, p = 1, \ldots, P, q = 1, \ldots, Q. = \left(\nabla_{\mathbf{A}} f(\mathbf{A})\right)^T \quad (5)$$

- Property 2:

$$\nabla_{\mathbf{B}} \mathrm{tr}(\mathbf{AB}) = \mathbf{A}^T \quad (6)$$

- This came from the fact that

$$D_Y f(\mathbf{X}) = \lim_{t \to 0} \frac{f(\mathbf{X} + t\mathbf{Y}) - f(\mathbf{X})}{t} = \mathrm{tr}(\mathbf{Y}^T \mathbf{U})$$

- where $U = \nabla_X f(X)$

Trace properties (3)

- Setting $f(\mathbf{B}) = \text{tr}(\mathbf{AB})$ we have

$$
\begin{aligned}
D_{\mathbf{Y}}\text{tr}(\mathbf{AB}) &= \lim_{t\to 0} \frac{\text{tr}(\mathbf{A}(\mathbf{B}+t\mathbf{Y})) - \text{tr}(\mathbf{AB})}{t} \\
&= \lim_{t\to 0} \frac{\text{tr}(\mathbf{AB}+t\mathbf{AY}) - \text{tr}(\mathbf{AB})}{t} \\
&= \lim_{t\to 0} \frac{\text{tr}(\mathbf{AB}) + t\text{tr}(\mathbf{AY}) - \text{tr}(\mathbf{AB})}{t} \\
&= \lim_{t\to 0} \frac{t\text{tr}(\mathbf{AY})}{t} \\
&= \text{tr}(\mathbf{AY}) \\
&= \text{tr}((\mathbf{AY})^T) \\
&= \text{tr}(\mathbf{Y}^T\mathbf{A}^T)
\end{aligned}
$$

- Thus, $\nabla_{\mathbf{B}}\text{tr}(\mathbf{AB}) = \mathbf{A}^T$.

Product rule

- We can generalize the product rule of scalars to matrices:
- $$\frac{\partial UV}{\partial x} = \frac{\partial U}{\partial x}V + U\frac{\partial V}{\partial x}$$
- Besides, from the definition of the gradient we have
$$\text{tr}\left(\frac{\partial Y}{\partial x}\right) = \frac{\partial(\text{tr}(Y))}{\partial x}$$
- Then,
$$\frac{\partial \text{tr}(UV)}{\partial x_{ij}} = \frac{\partial \text{tr}(UV_c)}{\partial x_{ij}} + \frac{\partial \text{tr}(U_c V)}{\partial x_{ij}}$$
- Where the subscript "c" means constant for purposes of differentiation.
- From the last two equations we obtain
$$\frac{\partial \text{tr}(UV)}{\partial X} = \frac{\partial \text{tr}(UV_c)}{\partial X} + \frac{\partial \text{tr}(U_c V)}{\partial X}$$

Product rule (2)

- $$\begin{aligned}\nabla_A(\mathrm{tr}(ABA^TC)) &= \nabla_A(\mathrm{tr}(A(BA^TC)_c)) + \nabla_A(\mathrm{tr}(A_cBA^TC)) \\ &= \nabla_A(\mathrm{tr}((BA^TC)_c)A) + \nabla_A(\mathrm{tr}(A^TCAB)) \\ &= C^TAB^T + CAB\end{aligned}$$

- $$\nabla_A(\mathrm{tr}(|A|)) = |A|(A^{-1})^T \qquad (7)$$

- For a detailed proof of the properties above refer to "With(out) A Trace Matrix Derivatives the Easy Way". Steven W. Nydick.

Revisited linear regression

- Let's compute the derivative of $J(\beta)$ with respect to β by using trace derivatives properties:

$$\begin{aligned}\nabla_\beta J(\beta) &= \frac{1}{2}\nabla_\beta (X\beta - Y)^T (X\beta - Y) \\ &= \frac{1}{2}\nabla_\beta (\beta^T X^T X\beta - \beta^T X^T Y - Y^T X\beta + Y^T Y\end{aligned}$$

- Note that $\nabla_\beta J(\beta)$ is a real number. Then,

$$\nabla_\beta J(\beta) = \frac{1}{2}\mathrm{tr}(\nabla_\beta (\beta^T X^T X\beta - \beta^T X^T Y - Y^T X\beta + Y^T Y).$$

From transposition of dependent variables property,

$$\nabla_\beta J(\beta) = \frac{1}{2}\left(\nabla_\beta (\mathrm{tr}\beta^T X^T X\beta - 2\mathrm{tr}(Y^T X\beta)\right).$$

Revisited linear regression (2)

- Using properties 2 (with $A^T = \beta$, $B = X^T X$ and $C = I$), and 3 we obtain

$$\begin{aligned}\nabla_\beta J(\beta) &= \frac{1}{2}\left(X^T X\beta + X^T X\beta - 2X^T Y\right) \\ &= X^T X\beta - X^T Y\end{aligned}$$

- Setting this to zero,

$$\beta = (X^T X)^{-1} X^T Y$$

Probabilistic linear model

- The use of equation (2) to model the regression problem is not flexible (we can't model underlying errors)
- Thus, we can fix it by introducing random variables:

$$y_m = \sum_{i=0}^{I} \beta_i x_m^{(i)} + \epsilon_m = \beta^T x_m + \epsilon_m$$

- Where ϵ_m represents either unmodeled effects or noise
- Using this new model we could assume that β is a random vector. Hence, we could measure the bias and the variance of β estimators. (We will do that later)

Probabilistic linear model (2)

- Now, let's assume that the ϵ_m are IID (independently and identically distributed) and $\epsilon_m \sim N(0, \sigma^2)$
- Then, the pdf of ϵ_m is given by

$$p(\epsilon_m) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{\epsilon_m^2}{2\sigma^2}}$$

- Thus,

$$p(y_m|x_m; \beta) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y_m - \beta^T x_m)^2}{2\sigma^2}}$$

Maximum likelihood

- Given the input (design) matrix X and the target vector Y. How we can choose β?
- It is reasonable to pick the β which maximizes the likelihood function:
- $$L(\beta) = \prod_{m=1}^{M} p(y_m|x_m;\beta) = \prod_{m=1}^{M} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y_m-\beta^T x_m)^2}{2\sigma^2}}$$
- As usual we will maximize the log likelihood $\ell(\beta)$ instead:

Maximum log likelihood

- As usual we will maximize the log likelihood $\ell(\beta)$ instead:
-

$$\begin{aligned}\ell(\beta) &= \sum_{m=1}^{M} \log \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y_m - \beta^T x_m)^2}{2\sigma^2}} \\ &= M \log \frac{1}{\sqrt{2\pi}\sigma} - \frac{1}{\sigma^2} \cdot \frac{1}{2} \sum_{m=1}^{M} (y_m - \beta^T x_m)^2\end{aligned}$$

- Hence, we obtain the same solution as minimizing (3).

Locally weighted linear regression

- Instead of minimizing $J(\beta)$, we want to minimize

$$= \frac{1}{2} \sum_{m=1}^{M} w_m (f(\mathbf{x}_m) - y_m)^2 \tag{8}$$

- A standard choice of w_m is:

$$w_m = e^{(-(x_m - x)^T (x_m - x)/(2\tau^2))},$$

- where τ is called bandwidth.
- $W = (w_1, \ldots, w_M)^T$
- Note that the weights depend on the particular point $\mathbf{x}$ that we are trying to evaluate.
- The solution is computed as $\beta = (X^T \mathrm{diag}(W) X)^{-1} X^T \mathrm{diag}(W) Y$.
- This is a non-parametric model.

Any questions?