

CS 474/574 Machine Learning

5. Regression

Prof. Dr. Forrest Sheng Bao
Dept. of Computer Science
Iowa State University
Ames, IA, USA

February 28, 2023

Agenda

- ▶ Linear Regression
- ▶ Logistic Regression (that can be used for classification)
- ▶ SVM Regression
- ▶ Loss functions
- ▶ Something about regularization

Regression vs. Classification

- ▶ The very first demo ($h = \frac{1}{2}gt^2$) is regression.
- ▶ Regression is also supervised ML, thus given an $f = f(x)$, we want to construct another \hat{f} such that \hat{y} and y is very close.
- ▶ The only difference is that in Classification, the y is usually discrete.
- ▶ While in Regression, the y is in a range - could be as large as the entire real number domain.
- ▶ Hence in regression, the output is usually not called **labels** but **targets**.
- ▶ And thus, the model is not called a **classifier** but a **regressor**.

Linear Regression

- ▶ We assume a linear relationship between two sets of variables \mathbf{x} and \mathbf{y}
- ▶ Thus, the prediction is the same as in classification $\hat{y} = \mathbf{w}^T \mathbf{x}$.
- ▶ How do we count the loss? We could use mean squared error (MSE) again:

$$\sum_i (\mathbf{w}^T \mathbf{x}_i - y)^2$$

- ▶ A criterion often used to judge a regression model is **correlation coefficient**.

Logistic Regression I

- ▶ Logistic regression is nonlinear. It was not originally proposed for ML, but as a way to model the probability of a random events.
- ▶ It is frequently used for classification but its nature is regression.
- ▶ The log odds, or logit (**logistic unit**) for an event A of probability $P(A)$ is $\log\left(\frac{P(A)}{1-P(A)}\right)$.
- ▶ Use a linear model to fit the log odds: $\log\left(\frac{P(A)}{1-P(A)}\right) = b_0 + b_1x_1 + b_2x_2 + \dots$.
- ▶ Solve it, we can express the probability as $P(A) = 1 / \left(1 + e^{-(b_0+b_1x_1+b_2x_2+\dots)}\right)$
- ▶ If we set a threshold on $P(A)$, e.g., $P(\text{the fruit is a banana}) > 0$, then we can use this function as a classifier.
- ▶ The fraction part is often called the **sigmoid** or **logistic** function

$$\sigma(z) = \frac{1}{1 + e^{-z}} = \frac{e^z}{1 + e^z},$$

where the z can be a result of a linear transform $\mathbf{w}^T \mathbf{x}$ (\mathbf{x} is augmented to include the bias).

- ▶ Properties of the sigmoid function: Range is $(0, 1)$.

Logistic Regression II

- ▶ Note that in some context, the word “sigmoid” is used to describe any S-shape functions. And the function symbol $\sigma()$ could be used for other functions. ..And, the logarithm can be of any base.
- ▶ To use logistic regression for classification, the class labels should be 0 and 1 instead of any arbitrary number, such as $+1$ and -1 we have been doing in class. In cross-entropy loss, only one term will be activated depending on the label.
- ▶ The loss function used for using logistic regression for classification is usually **cross-entropy**, also called **log loss**:

$$J = \sum_i [-y_i \log(\hat{y}_i) - (1 - y_i) \log(1 - \hat{y}_i)],$$

where $\hat{y}_i = \sigma(\mathbf{w}^T \mathbf{x}_i)$ is the prediction and y_i is the target for the i -th sample.

- ▶ That is

$$\begin{cases} -\log(\sigma(\mathbf{w}^T \mathbf{x}_i)) & \text{if } y = 1, \\ -\log(1 - \sigma(\mathbf{w}^T \mathbf{x}_i)) & \text{if } y = 0, \end{cases}$$

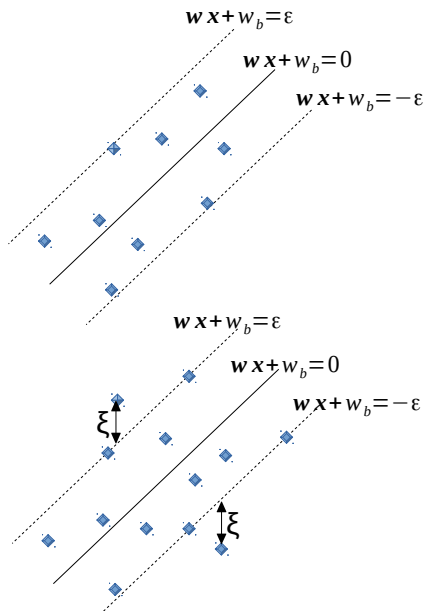
Logistic Regression III



$$\frac{\partial J}{\partial \mathbf{w}} = \frac{1}{m} \sum_i (\sigma(\mathbf{w}^T \mathbf{x}_i) - y) \mathbf{x}_i$$

SVM-based regression

- ▶ In (hard-margin) SVMs, samples need to be out of the margin.
- ▶ A inverse problem: Find a strip zone along the hyperplane, such that all samples are in the zone.
- ▶ Hence we can use SVM for regression but samples must be inside the “margin”.
$$\begin{cases} \min & \frac{1}{2} \|\mathbf{w}\|^2 \\ \text{s.t.} & |y_i - \mathbf{w}^T \mathbf{x}_i + w_b| \leq \epsilon, \forall \mathbf{x}_i. \end{cases}$$
- ▶ In regression a “hard margin” is often hard to achieve, so add the slack variables:
$$\begin{cases} \min & \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_i \xi_i \\ \text{s.t.} & |y_i - \mathbf{w}^T \mathbf{x}_i + w_b| \leq \epsilon + \xi_i, \forall \mathbf{x}_i \\ & \xi_i \geq 0. \end{cases}$$
- ▶ ϵ is a predefined value – how accurately you want the regression to be.
- ▶ Actually, we don't have margin here. IT's called ϵ -insensitive zone.
- ▶ This kind of SVMs are called ϵ -SVMs.



SVM-regression (cond.)

- ▶ ϵ -insensitive loss (very similar to hinge loss):
$$L(\mathbf{w}) = \begin{cases} 0 & \text{if } |y - \mathbf{w}^T \mathbf{x}| \leq \epsilon, \\ |y - \mathbf{w}^T \mathbf{x}| - \epsilon & \text{o/w,} \end{cases}$$
- ▶ What is the $\min \frac{1}{2} \|\mathbf{w}\|^2$ for? We don't have margins.
- ▶ It functions as an L2 regularizer.
- ▶ Good visuals:
 - ▶ <http://kernelsvm.tripod.com/>
 - ▶ https://www.saedsayad.com/support_vector_machine_reg.htm

Overfitting vs. Regularization

- ▶ **Overfitting:** A common problem in ML is that the model is very accurate on training data but not on test data
- ▶ A good example online
- ▶ In regression, this can be visualized as that the fitted curve matches training points very well, but misses test points.
- ▶ The cause is, for linear models, the magnitudes of elements in \mathbf{w} are too big.
- ▶ Dr. Chung's slides.
- ▶ A further extreme case is when the magnitudes of certain elements are substantially bigger than others. The model relies on certain features or certain components of the data too much.
- ▶ How to avoid overfitting? **regularization**.

L1 and L2 regularization (for linear models)

- ▶ L1 regularization (Lasso regularization): $J = \text{Error}(\hat{y}, y) + \alpha \|\mathbf{w}\|$
- ▶ L2 (ridge): $J = \text{Error}(\hat{y}, y) + \alpha \|\mathbf{w}\|^2$
- ▶ α is a constant weighing the regularization term. It's also a hyperparameter.
- ▶ Why they work?
- ▶ The new gradients:

$$\frac{\partial J_{L1}}{\partial \mathbf{w}} = \frac{\partial \text{Error}}{\partial \mathbf{w}} \pm \alpha$$

or

$$\frac{\partial J_{L2}}{\partial \mathbf{w}} = \frac{\partial \text{Error}}{\partial \mathbf{w}} + 2\alpha \mathbf{w}$$

- ▶ When using the new gradients to update \mathbf{w} , \mathbf{w} is not updated to what would be ideal.
- ▶ A good explanation online