Logistic Regression and MaxEnt

Wei Wang @ CSE, UNSW

April 9, 2020

Generative vs. Discriminative Learning

- Generative models:

$$\begin{aligned}\mathbf{Pr}[y \mid \mathbf{x}] &= \frac{\mathbf{Pr}[\mathbf{x} \mid y]\mathbf{Pr}[y]}{\mathbf{Pr}[\mathbf{x}]} \\ &\propto \mathbf{Pr}[\mathbf{x} \mid y]\mathbf{Pr}[y] = \mathbf{Pr}[\mathbf{x}, y]\end{aligned}$$

  - The key is to model the generative probability: $\mathbf{Pr}[\mathbf{x} \mid y]$.
  - Example: Naive Bayes.
- Discriminative models:
  - models $\mathbf{Pr}[y \mid \mathbf{x}]$ directly as $g(\mathbf{x}; \boldsymbol{\theta})$.
  - Example: Decision tree, Logistic Regression.
- Instance-based Learning.
  - Example: kNN classifier.

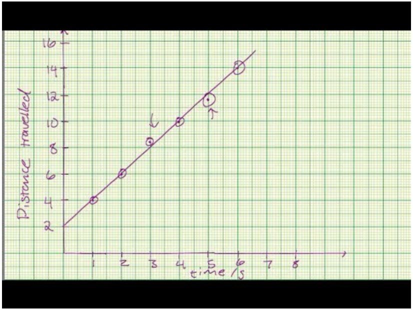


Figure: Linear Regression

Task

- Input: $(x^{(i)}, y^{(i)})$ pairs $(1 \leq i \leq n)$
- Preprocess: let $\mathbf{x^{(i)}} = \begin{bmatrix} 1 & x^{(i)} \end{bmatrix}^\top$
- Output: The best $\mathbf{w} = \begin{bmatrix} w_0 & w_1 \end{bmatrix}^\top$ such that $\hat{y} = \mathbf{w}^\top \mathbf{x}$ best explains the observations

Least Square Fit

The criterion for "best":

- Individual error: $\epsilon_i = \hat{y}^{(i)} - y^{(i)}$
- Sum squared error: $\ell = \sum_{i=1}^{n} \epsilon_i^2$

Find $\mathbf{w}$ such that ℓ is minimized.

Minimizing a Function

Taylor Series of $f(x)$ at point a

$$f(x) = \sum_{n=0}^{+\infty} \frac{f^{(i)}(a)}{n!}(x-a)^n \tag{1}$$

$$= f(a) + f'(a) \cdot (x-a) + \frac{f''(a)}{2}(x-a)^2 + o((x-a)^2) \tag{2}$$

- Intuitively, $f(x)$ is almost $f(a) + f'(a) \cdot (x-a)$ for all a if it is close to x.
- If $f(x)$ has local minimum x^*, then
  - $f'(x^*) = 0$, and
  - $f''(x^*) > 0$.

  Minimum of the local minima is the global minimum if it is smaller than the function values at all the boundary points.
- Intuitively, $f(x)$ is almost $f(a) + \frac{f''(a)}{2}(x-a)^2$ if a is close to x^*.

Find the Least Square Fit for Linear Regression

$$
\begin{aligned}
\frac{\partial \ell}{\partial w_j} &= \sum_{i=1}^{n} 2\epsilon_i \frac{\partial \epsilon_i}{\partial w_j} = \sum_{i=1}^{n} 2\epsilon_i \frac{\partial \mathbf{w}^\top \mathbf{x}^{(\mathbf{i})}}{\partial w_j} \\
&= \sum_{i=1}^{n} 2\epsilon_i x_j^{(i)} = 2 \sum_{i=1}^{n} (\hat{y}^{(i)} - y^{(i)}) x_j^{(i)}
\end{aligned}
$$

By setting the above to 0, this essentially requires, for all j

$$
\boxed{\sum_{i=1}^{n} \hat{y}^{(i)} x_j^{(i)}} = \boxed{\sum_{i=1}^{n} y^{(i)} x_j^{(i)}}
$$

what the model predicts

what the data says

Find the Least Square Fit for Linear Regression

In the simple 1D case, we have only two parameters in $\mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}$

$$\sum_{i=1}^{n} (w_0 + w_1 x_1^{(i)}) x_0^{(i)} = \sum_{i=1}^{n} y^{(i)} x_0^{(i)}$$

$$\sum_{i=1}^{n} (w_0 + w_1 x_1^{(i)}) x_1^{(i)} = \sum_{i=1}^{n} y^{(i)} x_1^{(i)}$$

Since $x_0^{(i)} = 1$, they are essentially

$$\sum_{i=1}^{n} (w_0 + w_1 x_1^{(i)}) \cdot 1 = \sum_{i=1}^{n} y^{(i)} \cdot 1$$

$$\sum_{i=1}^{n} (w_0 + w_1 x_1^{(i)}) \cdot x_1^{(i)} = \sum_{i=1}^{n} y^{(i)} \cdot x_1^{(i)}$$

Example

Using the same example in https://en.wikipedia.org/wiki/Linear_least_squares_(mathematics)

$$\mathbf{X} = \begin{bmatrix} — & (x^{(1)})^\top & — \\ — & (x^{(2)})^\top & — \\ — & (x^{(3)})^\top & — \\ — & (x^{(4)})^\top & — \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix} \quad \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} 6 \\ 5 \\ 7 \\ 10 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix} \qquad \begin{bmatrix} 6 \\ 5 \\ 7 \\ 10 \end{bmatrix} \qquad = \qquad \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix} \qquad \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \hat{y}_3 \\ \hat{y}_4 \end{bmatrix}$$

Generalization to m-dim

- Easily generalizes to more than 2-dim:

$$\mathbf{X} = \begin{bmatrix} 1 & x_1^{(1)} & \dots & x_m^{(1)} \\ 1 & \dots & \dots & \dots \\ 1 & x_1^{(i)} & \dots & x_m^{(i)} \\ 1 & \dots & \dots & \dots \\ 1 & x_1^{(n)} & \dots & x_m^{(n)} \end{bmatrix} \qquad \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ \dots \\ w_m \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} y^{(1)} \\ \dots \\ y^{(i)} \\ \dots \\ y^{(n)} \end{bmatrix}$$

- How to perform polynomial regression for one dimensional x?
  - $\hat{y} = w_0 + w_1 x + w_2 x^2 \ldots + w_m x^m$.
  - Let $x_j^{(i)} = (x_1^{(i)})^j \implies$ Polynomial least square fitting (`http://mathworld.wolfram.com/LeastSquaresFittingPolynomial.html`)

High-level idea:

- Observations (i.e., training data) are noisy
  - $P(y^{(i)} \mid \hat{y}^{(i)}) = \qquad\qquad\qquad\qquad = f_i(\mathbf{w})$
- Any $\mathbf{w}$ is possible, but some $\mathbf{w}$ is most likely.
  - Assuming independence of training examples, the likelihood of the training dataset is $\prod_i f_i(\mathbf{w})$.
  - We shall choose the $\mathbf{w}^*$ that maximizes the likelihood.
    - Maximum likelihood estimation (MLE)
    - If we also incorporate some prior on $\mathbf{w}$, this becomes Maximum Posterior Estimation (MAP): If we assume some Gaussian prior on $\mathbf{w}$, this will add a ℓ_2 regularization term to the objective function.
- Many models and their variants can be deemed as different ways of estimating $P(y^{(i)} \mid \hat{y}^{(i)})$

Geometric Interpretation and the Closed Form Solution

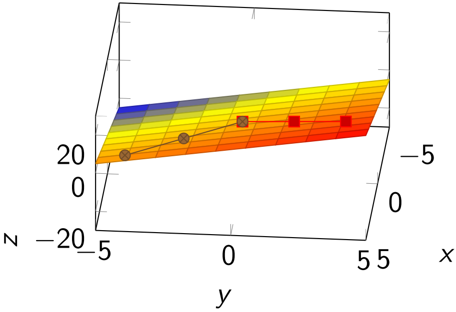
Find $\mathbf{w}$ such that $\|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2$ is minimized.

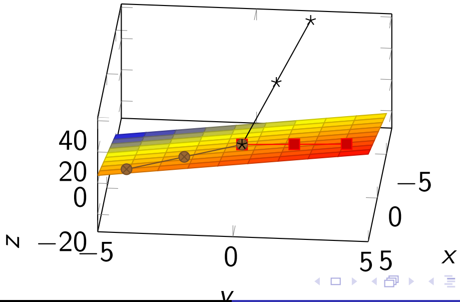
- What is $\mathbf{X}\mathbf{w}$ when $\mathbf{X}$ is fixed?
    - It is the hyperplane spanned by the d column vectors of $\mathbf{X}$.
- $\mathbf{y}$ in general is a vector outside the hyperplane. So the minimum distance is achieved when $\mathbf{X}\mathbf{w}^*$ is exactly the projection of $\mathbf{y}$ on the hyperplane. This means (denote i-th column of $\mathbf{X}$ as X_i)

$$\left.\begin{aligned} X_1^\top(\mathbf{y} - \mathbf{X}\mathbf{w}) &= 0 \\ X_2^\top(\mathbf{y} - \mathbf{X}\mathbf{w}) &= 0 \\ \ldots\ldots &= 0 \\ X_d^\top(\mathbf{y} - \mathbf{X}\mathbf{w}) &= 0 \end{aligned}\right\} \Longrightarrow \mathbf{X}^\top(\mathbf{y} - \mathbf{X}\mathbf{w}) = \mathbf{0}$$

- $\mathbf{w} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y} = \mathbf{X}^+\mathbf{y}$ $\qquad$ ($\mathbf{X}^+$: pseudo inverse of $\mathbf{X}$)

Illustration





Special case: $y^{(i)} \in \{0, 1\}$.

- Not appropriate to directly regress $y^{(i)}$.
- Rather, model $y^{(i)}$ as the observed outcome of a Bernoulli trial with an unknown parameter p_i
- How to model p_i
  - We assume that p_i depends on $\mathbf{x} \triangleq \mathbf{X}_{i\bullet} \implies$ rename p_i to $p_{\mathbf{x}}$.
  - Still hard to estimate $p_{\mathbf{x}}$ reliably.
    - MLE: $p_{\mathbf{x}} = \mathbf{E}[y = 1 \mid \mathbf{x}]$
  - What can we say about $p_{\mathbf{x}+\epsilon}$ when $p_{\mathbf{x}}$ is given?
- Answer: we impose a linear relationship between $p_{\mathbf{x}}$ and $\mathbf{x}$
  - What about a simple linear model $p_{\mathbf{x}} = \mathbf{w}^\top \mathbf{x}$ for some $\mathbf{w}$? (Note: all points share the same parameter $\mathbf{w}$)
  - Problem: mismatch of the domains: vs
  - Solution: mean function / inverse of link function: $g^{-1} : \Re \to \text{params}$

Solution

- Solution: Link function $g(\text{parameters}) \to \Re$

$$g(p) = \mathrm{logit}(p) \triangleq \log \frac{p}{1-p} \qquad = \mathbf{w}^\top \mathbf{x} \tag{3}$$

- Equivalently, solve for p.

$$p = \frac{e^{\mathbf{w}^\top \mathbf{x}}}{1 + e^{\mathbf{w}^\top \mathbf{x}}} = \frac{1}{1 + e^{-\mathbf{w}^\top \mathbf{x}}} = \sigma(\mathbf{w}^\top \mathbf{x}) \tag{4}$$

  Where $\sigma(z) = \frac{1}{1+\exp(-z)}$.
  Recall that $p_{\mathbf{x}} = \mathbf{E}[y = 1 \mid \mathbf{x}]$.

- Decision boundary is $p \geq 0.5$.
  - Equivalent to whether $\mathbf{w}^\top \mathbf{x} \geq 0$. Hence, LR is a linear classifier.

Learning the Parameter $\mathbf{w}$

- Consider a training data point $\mathbf{x^{(i)}}$.
  - Recall that the conditional probability ($\mathbf{Pr}[y^{(i)} = 1 \mid \mathbf{x^{(i)}}]$) computed by the model is denoted by the shorthand notation p (which is a function of $\mathbf{w}$ and $\mathbf{x^{(i)}}$).
  - The likelihood of $\mathbf{x^{(i)}}$ is $\begin{cases} p & \text{, if } y^{(i)} = 1 \\ 1 - p & \text{, otherwise} \end{cases}$, or equivalently, $p^{y^{(i)}}(1-p)^{1-y^{(i)}}$.
- Hence, the likelihood of the whole training dataset is

$$L(\mathbf{w}) = \prod_{i=1}^{n} p(\mathbf{x^{(i)}})^{y^{(i)}}(1 - p(\mathbf{x^{(i)}}))^{1-y^{(i)}}.$$

- Log-likelihood is (assume $\log \triangleq \ln$)

$$\ell(\mathbf{w}) = \sum_{i=1}^{n} y^{(i)} \log p(\mathbf{x^{(i)}}) + (1 - y^{(i)}) \log (1 - p(\mathbf{x^{(i)}})) \quad (5)$$

Learning the Parameter $\mathbf{w}$

- To maximize ℓ, notice that it is concave. So take its partial derivatives

$$\frac{\partial \ell(\mathbf{w})}{\partial \mathbf{w}_j} = \sum_{i=1}^{n} \left(y^{(i)} \frac{1}{p(\mathbf{x^{(i)}})} \frac{\partial p(\mathbf{x^{(i)}})}{\partial \mathbf{w}_j} + (1 - y^{(i)}) \frac{1}{1 - p(\mathbf{x^{(i)}})} \frac{\partial (1 - p(\mathbf{x^{(i)}}))}{\partial \mathbf{w}_j} \right)$$

$$= \sum_{i=1}^{n} \left(\mathbf{x^{(i)}}_j y^{(i)} - \mathbf{x^{(i)}}_j p(\mathbf{x^{(i)}}) \right)$$

- and set them to 0 essentially means, for all j

$$\sum_{i=1}^{n} \hat{y}^{(i)} \cdot \mathbf{x^{(i)}}_j = \boxed{\sum_{i=1}^{n} p(\mathbf{x^{(i)}}) \mathbf{x^{(i)}}_j} = \boxed{\sum_{i=1}^{n} y^{(i)} \cdot \mathbf{x^{(i)}}_j}$$

what the model predicts

what the data says

Understand the Equilibrium

- Consider one dimensional **x**. The above condition is simplified to

$$\sum_{i=1}^{n} p^{(i)} x^{(i)} = \sum_{i=1}^{n} y^{(i)} x^{(i)}$$

- The RHS is essentially the sum of x values **only** for the training data in class $Y = 1$.
- The LHS says: if we use our learned model to assign a probability (of belonging to the class $Y = 1$) for **every** training data, the LHS is the expected sum of x values.
- If this is still abstract, think of an example.

Numeric Solution

- There is no closed-form solution to maximize ℓ.
- Use the *Gradient Ascent* algorithm to maximize ℓ.
- There are faster algorithms.

(Stochastic) Gradient Ascent

- $\mathbf{w}$ is intialized to some random value (e.g., $\mathbf{0}$).
- Since the gradient gives the *steepest* direction to increase a function's value, we move a small step towards that direction, i.e.,

$$w_j \leftarrow w_j + \alpha \frac{\partial \ell(\mathbf{w})}{\partial \mathbf{w}_j} \qquad \text{, or}$$

$$w_j \leftarrow w_j + \alpha \sum_{i=1}^{n} (y^{(i)} - p(\mathbf{x^{(i)}}))\mathbf{x^{(i)}}_j$$

  where α (*learning rate*) is usually a small constant, or decreasing over the epochs.
- Stochastic version: using the gradient on a randomly selected training instance, i.e.,

$$w_j \leftarrow w_j + \alpha (y^{(i)} - p(\mathbf{x^{(i)}}))\mathbf{x^{(i)}}_j$$

Newton's Method

- Gradient Ascent moves to the "right" direction a tiny step a time. Can we find a good step size?
- Consider 1D case: **minimize** $f(x)$ and the current point is a.
  - $f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2}(x-a)^2$ for x near a.
  - To minimize $f(x)$, take $\frac{\partial f(x)}{\partial x} = 0$, i.e.,

$$
\begin{aligned}
& \frac{\partial f(x)}{\partial x} = 0 \\
\Leftrightarrow \quad & f'(a) \cdot 1 + \frac{f''(a)}{2} \cdot 2(x-a) \cdot 1 = f'(a) + f''(a)(x-a) = 0 \\
\Leftrightarrow \quad & x = a - \frac{f'(a)}{f''(a)}
\end{aligned}
$$

- Can be applied to multiple dimension cases too $\Rightarrow$ need to use ∇ (gradient) and Hess (Hessian).

Regularization

- Regularization is another method to deal with overfitting.
  - It is designed to penalize large values of the model parameters.
  - Hence it *encourages* simpler models, which are less likely to overfit.
- Instead of optimizing for $\ell(\mathbf{w})$, we optimize $\ell(\mathbf{w}) + \lambda R(\mathbf{w})$.
  - λ is a hyper-parameter that controls the strength of regularization.
    - It is usually determined by cross validating with a list of possible values (e.g., 0.001, 0.01, 0.1, 1, 10, ...)
    - Grid search: `http://scikit-learn.org/stable/modules/grid_search.html`
    - There are alternative methods.
  - $R(\mathbf{w})$ quantifies the "size" of the model parameters. Popular choices are:
    - L_2 regularization (Ridge LR) $R(\mathbf{w}) = \|w\|_2^2$
    - L_1 regularization (Lasso LR) $R(\mathbf{w}) = \|w\|_1$
    - L_1 regularization is more likely to result in sparse models.

- LR can be generalized to multiple classes $\implies$ MaxEnt.

$$\mathbf{Pr}[c \mid \mathbf{x}] \propto \exp\left(\mathbf{w}_c^\top \mathbf{x}\right) \quad \implies \quad \mathbf{Pr}[c \mid \mathbf{x}] = \frac{\exp\left(\mathbf{w}_c^\top \mathbf{x}\right)}{Z}$$

  - Z is the normalization constant. $= ?$
  - Let $\mathbf{c}^*$ be the last class in C, then $\mathbf{w}_{\mathbf{c}^*} = \mathbf{0}$.
- Derive LR from MaxEnt How?
- Both belong to *exponential* or *log-linear* classifiers.

Further Reading

- Andrew Ng's note: http://cs229.stanford.edu/notes/cs229-notes1.pdf
- Cosma Shalizi's note: http://www.stat.cmu.edu/~cshalizi/uADA/12/lectures/ch12.pdf
- Tom Mitchell's book chapter: https://www.cs.cmu.edu/~tom/mlbook/NBayesLogReg.pdf