Logistic Regression

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Vineeth N Balasubramanian

आई आई टी हैदराबाद
IIT Hyderabad

Classification Methods

- k-Nearest Neighbors
- Decision Trees
- Naïve Bayes
- Support Vector Machines
- Logistic Regression
- Neural Networks
- Ensemble Methods (Boosting, Random Forests)

Regression Formulation

Given *x*, want to predict an estimate *ŷ* of *y*, which minizes the discrepancy (*L*) between *ŷ* and *y*.

$$L(\hat{y}; y) := |\hat{y} - y|$$ ***Absolute error***

$$:= (\hat{y} - y)^2$$ ***Squared error***

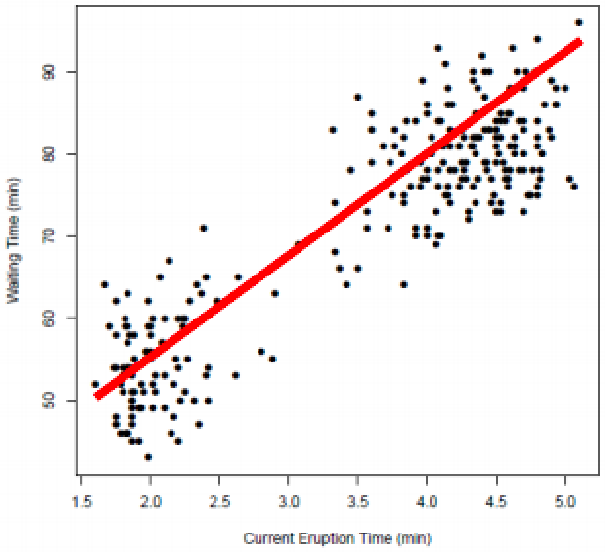
Loss

A **linear predictor** *f*, can be defined by the slope *w* and the intercept w_0 :

$$\hat{f}(\vec{x}) := \vec{w} \cdot \vec{x} + w_0$$

which minimizes the prediction loss.

$$\min_{w, w_0} \mathbb{E}_{\vec{x}, y} \left[L(\hat{f}(\vec{x}), y) \right]$$



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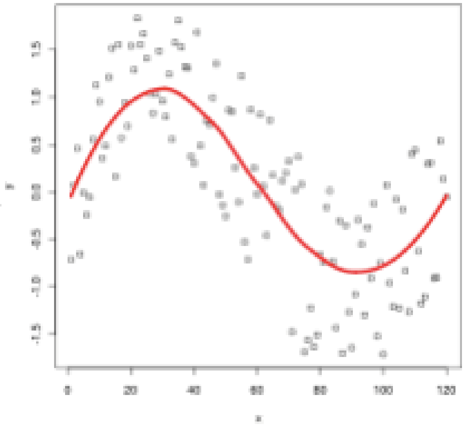
Parametric (vs) Non-parametric Regression

If we assume a particular form of the regressor:

Parametric regression

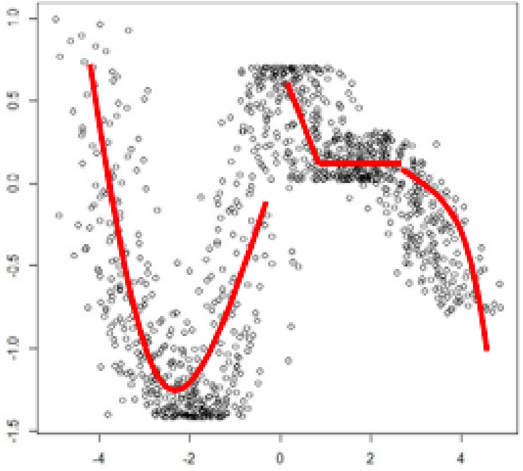
Goal: to learn the parameters which yield the minimum error/loss



If no specific form of regressor is assumed:

Non-parametric regression

Goal: to learn the predictor directly from the input data that yields the minimum error/loss



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Linear Regression

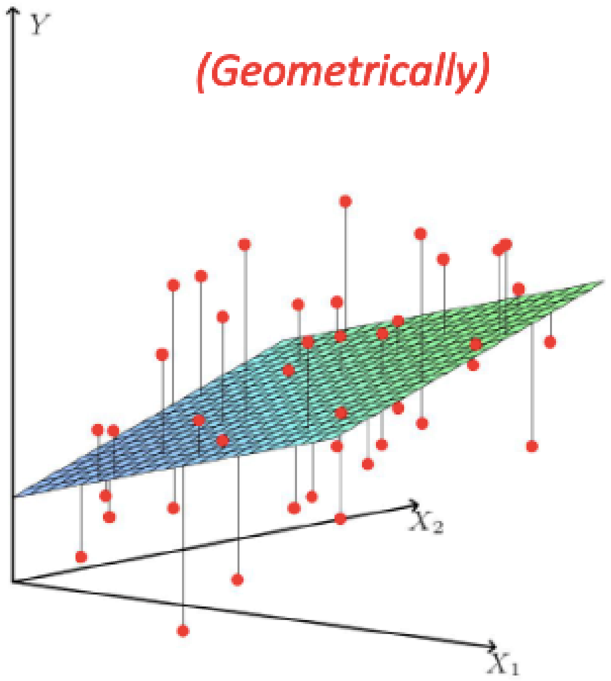
Want to find a **linear predictor** *f*, i.e., *w* (intercept w_0 absorbed via lifting):

$$\hat{f}(\vec{x}) := \vec{w} \cdot \vec{x}$$

which minimizes the prediction loss over the population.

$$\min_{\vec{w}} \mathbb{E}_{\vec{x},y}\left[L(\hat{f}(\vec{x}), y)\right]$$

(Geometrically)



We estimate the parameters by minimizing the corresponding loss on the training data:

$$\arg\min_{w} \frac{1}{n}\sum_{i=1}^{n}\left[L(\vec{w}\cdot\vec{x}_i, y_i)\right]$$
$$= \arg\min_{w} \frac{1}{n}\sum_{i=1}^{n}\left(\vec{w}\cdot\vec{x}_i - y_i\right)^2$$

for squared error

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Linear Regression

Linear predictor with squared loss:

$$\arg\min_{w} \frac{1}{n} \sum_{i=1}^{n} \left(\vec{w} \cdot \vec{x}_i - y_i \right)^2$$

$$= \arg\min_{w} \left\| \begin{pmatrix} \dots \mathrm{x}_1 \dots \\ \dots \mathrm{x}_i \dots \\ \dots \mathrm{x}_n \dots \end{pmatrix} \begin{pmatrix} w \end{pmatrix} - \begin{pmatrix} y_1 \\ y_i \\ y_n \end{pmatrix} \right\|^2$$

$$= \arg\min_{w} \left\| X\vec{w} - \vec{y} \right\|_2^2$$

Unconstrained problem!

Can take the gradient and examine the stationary points!

Why need not check the second order conditions?

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Linear Regression

Best fitting *w*:

$$\frac{\partial}{\partial \vec{w}} \left\| X\vec{w} - \vec{y} \right\|^2 = 2X^\top (X\vec{w} - \vec{y})$$

$$X^\top X \vec{w} = X^\top \vec{y}$$

At a stationary point

$$\implies \vec{w}_{\text{ols}} = (X^\top X)^\dagger X^\top \vec{y}$$

Pseudo-inverse

Also called the Ordinary Least Squares (OLS)

The solution is unique and stable when $X^T X$ is invertible

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Regularized Least-Squared Regression

- Complex models (lots of parameters) often prone to overfitting.
- Overfitting can be reduced by imposing a constraint on the overall magnitude of the parameters.
- Two common types of regularization in linear regression:
  - **L$_2$ regularization (a.k.a. ridge regression):** Find **w** which minimizes:

$$\sum_{j=1}^{N}(y_j - \sum_{i=0}^{d} w_i \cdot x_i)^2 + \lambda \sum_{i=1}^{d} w_i^{\ 2}$$

    - λ is the regularization parameter: bigger λ imposes more constraint
  - **L$_1$ regularization (a.k.a. lasso):** Find **w** which minimizes:

$$\sum_{j=1}^{N}(y_j - \sum_{i=0}^{d} w_i \cdot x_i)^2 + \lambda \sum_{i=1}^{d} | w_i |$$

k-NN Regression

- Calculate the mean value of the *k* nearest training examples rather than calculate their most common value

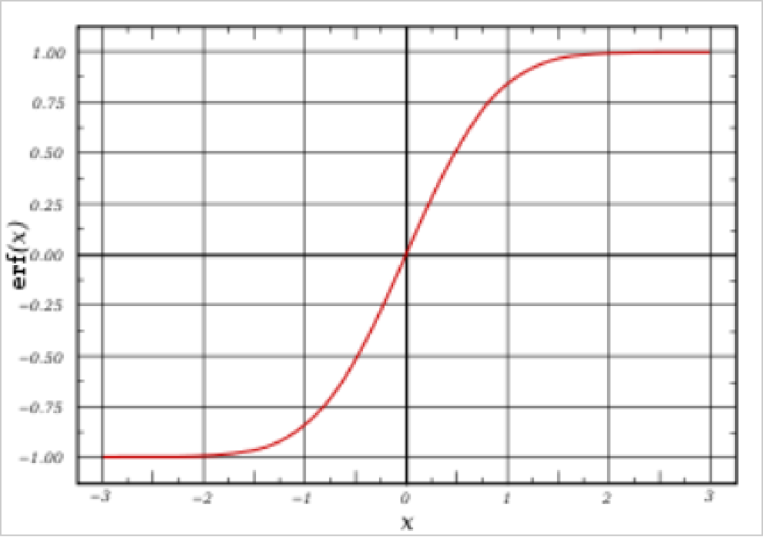
$$f : \Re^d \rightarrow \Re$$

$$\hat{f}(x_q) \neg \frac{\overset{k}{\underset{i=1}{\text{å}}} f(x_i)}{k}$$

Logistic Regression

- To predict an outcome variable that is categorical from one or more categorical or continuous predictor variables.
- Used because having a categorical outcome variable violates the assumption of linearity in normal regression.

- Let X be the data instance, and Y be the class label: Learn P(Y|X) directly
  - Let W = (W_1, W_2, … W_n), X=(X_1, X_2, …, X_n), **W.X** is the dot product
  - Sigmoid function: $P(Y=1|\mathbf{X}) = \dfrac{1}{1+e^{-\mathbf{wx}}}$



Logistic Regression

- Generative or Discriminative?

Logistic Regression

- Generative classifier, e.g., Naïve Bayes:
  - Assume some functional form for **P(X|Y), P(Y)**
  - Estimate parameters of P(X|Y), P(Y) directly from training data
  - Use Bayes rule to calculate P(Y|X=x)
  - This is 'generative' model
    - Indirect computation of P(Y|X) through Bayes rule
    - But, can generate a sample of the data, $P(X) = \sum_{y} P(y)P(X \mid y)$
- Discriminative classifier, e.g., Logistic Regression:
  - Assume some functional form for **P(Y|X)**
  - Estimate parameters of P(Y|X) directly from training data
  - This is the 'discriminative' model
    - Directly learn P(Y|X)

Logistic Regression

- In logistic regression, we learn the conditional distribution P(y|x)
- Let $p_y(x;w)$ be our estimate of P(y|x), where w is a vector of adjustable parameters.
- Assume there are two classes, y = 0 and y = 1 and

$$p_1(\mathbf{x};\mathbf{w}) = \frac{1}{1+e^{-\mathbf{wx}}} \qquad p_0(\mathbf{x};\mathbf{w}) = 1 - \frac{1}{1+e^{-\mathbf{wx}}}$$

- This is equivalent to $\log \frac{p_1(\mathbf{x};\mathbf{w})}{p_0(\mathbf{x};\mathbf{w})} = \mathbf{wx}$

- That is, the log odds of class 1 is a linear function of x
- Q: How to find **W**?

Logistic Regression

- Conditional data likelihood - Probability of observed Y values in the training data, conditioned on corresponding X values.
- We choose parameters w that satisfy

$$\mathbf{w} = \arg\max_{\mathbf{w}} \prod_{l} P(y^l \mid \mathbf{x}^l, \mathbf{w})$$

- where
  - **w** = <w_0,w_1 ,…,w_n> is the vector of parameters to be estimated,
  - y^l denotes the observed value of Y in the *l* th training example, and
  - $\mathbf{x}^l$ denotes the observed value of **X** in the *l* th training example

Logistic Regression

- Equivalently, we can work with log of conditional likelihood:

$$\mathbf{w} = \arg\max_{\mathbf{w}} \sum_{l} \ln P(y^l \mid \mathbf{x}^l, \mathbf{w})$$

- Conditional data log likelihood, l(W), can be written as

$$l(\mathbf{w}) = \sum_{l} y^l \ln P(y^l = 1 \mid \mathbf{x}^l, \mathbf{w}) + (1 - y^l) \ln P(y^l = 0 \mid \mathbf{x}^l, \mathbf{w})$$

- Note here that Y can take only values 0 or 1, so only one of the two terms in the expression will be non-zero for any given y^l

Logistic Regression: Training

- We need to estimate:

$$\mathbf{w} = \arg\max_{\mathbf{w}} \sum_{l} \ln P(y^{l} \mid \mathbf{x}^{l}, \mathbf{w})$$

- Equivalently, we can minimize negative log likelihood

- This is convex – so, unique global minimum
- No closed-form solution though. Iterative method required.

Logistic Regression: Training

- Use gradient ascent (descent) for the maximization (min) problem
- The i th component of the vector gradient has the form

$$\frac{\partial}{\partial w_i} l(\mathbf{w}) = \sum_l x_i^l (y^l - \boxed{\hat{P}(y^l = 1 | \mathbf{x}^l, \mathbf{w})})$$

Logistic Regression prediction

- Beginning with initial weights, we repeatedly update the weights in the direction of the gradient, changing the i th weight according to

$$w_i \leftarrow w_i + \eta \sum_l x_i^l (y^l - \hat{P}(y^l = 1 | \mathbf{x}^l, \mathbf{w}))$$

Regularization in Logistic Regression

- Overfitting can arise especially when data has very high dimensions and is sparse.
- One approach -> modified "penalized log likelihood function," which penalizes large values of **w**, as before.

$$\mathbf{w} = \arg\max_{\mathbf{w}} \sum_l \ln P(y^l \mid \mathbf{x}^l, \mathbf{w}) - \frac{\lambda}{2} \|\mathbf{w}\|^2$$

- Derivative then becomes:

$$\frac{\partial}{\partial w_i} l(\mathbf{w}) = \sum_l x_i^l (y^l - \hat{P}(y^l = 1 | \mathbf{x}^l, \mathbf{w})) - \lambda w_i$$

Logistic Regression

- In general, NB and LR make different assumptions
  - NB: Features independent given class -> assumption on P(X|Y)
  - LR: Functional form of P(Y|X), no assumption on P(X|Y)
- LR is a linear classifier
  - decision rule is a hyperplane
- LR optimized by conditional likelihood
  - no closed-form solution
  - Concave (convex) -> global optimum with gradient ascent (descent)
- Extending logistic regression to multiple classes
  - Use softmax for each class k! $p(y=k|x) = \frac{\exp(\theta_k^\top x)}{\sum_{i=1}^K \exp(\theta_i^\top x)}$

Readings

- PRML Bishop, Chapter 4 (Sec 4.3)
- "Introduction to Machine Learning" by Ethem Alpaydin, Chapter 10