Introduction to Machine Learning

Bayesian Regression

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Outline

Linear Regression

- There is one scalar **target** variable y (instead of hidden)
- There is one vector **input** variable x
- Inductive bias:

$$y = \mathbf{w}^\top \mathbf{x}$$

Linear Regression Learning Task

Learn $\mathbf{w}$ given training examples, $\langle \mathbf{X}, \mathbf{y} \rangle$.

Probabilistic Interpretation

- y is assumed to be normally distributed

$$y \sim \mathcal{N}(\mathbf{w}^\top \mathbf{x}, \sigma^2)$$

- or, equivalently:

$$y = \mathbf{w}^\top \mathbf{x} + \epsilon$$

  where $\epsilon \sim \mathcal{N}(0, \sigma^2)$
- y is a *linear combination* of the input variables
- *Given* $\mathbf{w}$ *and* σ^2*, one can find the probability distribution of* y *for a given* $\mathbf{x}$

Learning Parameters - MLE Approach

- Find $\mathbf{w}$ and σ^2 that maximize the likelihood of training data

$$
\begin{aligned}
\widehat{\mathbf{w}}_{MLE} &= (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y} \\
\widehat{\sigma}^2_{MLE} &= \frac{1}{N}(\mathbf{y} - \mathbf{X}\mathbf{w})^\top(\mathbf{y} - \mathbf{X}\mathbf{w})
\end{aligned}
$$

Issues with Linear Regression

1. Not truly Bayesian
2. Susceptible to outliers
3. *Too simplistic* - Underfitting
4. No way to control overfitting
5. Unstable in presence of correlated input attributes
6. Gets "confused" by unnecessary attributes

Putting a Prior on $\mathbf{w}$

- "Penalize" large values of $\mathbf{w}$
- A zero-mean Gaussian prior

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|0, \tau^2 I)$$

- What is posterior of $\mathbf{w}$

$$p(\mathbf{w}|\mathcal{D}) \propto \prod_i \mathcal{N}(y_i|\mathbf{w}^\top \mathbf{x}_i, \sigma^2) p(\mathbf{w})$$

- Posterior is also Gaussian

Posterior Estimates of the Weight Vector

- Regularized least squares estimate of **w**

$$\arg\max_{\mathbf{w}} \sum_{i=1}^{N} log \mathcal{N}(y_i|\mathbf{w}^\top \mathbf{x}_i, \sigma^2) + \log \mathcal{N}(\mathbf{w}|0, \tau^2 I)$$

Parameter Estimation for Bayesian Regression

- Prior for $\mathbf{w}$

$$\mathbf{w} \sim \mathcal{N}(\mathbf{w}|\mathbf{0}, \tau^2\mathbf{I}_D)$$

- Posterior for $\mathbf{w}$

$$\begin{aligned} p(\mathbf{w}|\mathbf{y},\mathbf{X}) &= \frac{p(\mathbf{y}|\mathbf{X},\mathbf{w})p(\mathbf{w})}{p(\mathbf{y}|\mathbf{X})} \\ &= \mathcal{N}(\bar{\mathbf{w}} = (\mathbf{X}^\top\mathbf{X} + \frac{\sigma^2}{\tau^2}\mathbf{I}_N)^{-1}\mathbf{X}^\top\mathbf{y}, \sigma^2(\mathbf{X}^\top\mathbf{X} + \frac{\sigma^2}{\tau^2}\mathbf{I}_N)^{-1}) \end{aligned}$$

- Posterior distribution for $\mathbf{w}$ is also Gaussian
- What will be MAP estimate for $\mathbf{w}$?

Prediction with Bayesian Regression

- For a new $\mathbf{x}^*$, predict y^*
- Point estimate of y^*

$$y^* = \widehat{\mathbf{w}}_{MLE}^\top \mathbf{x}^*$$

- Treating y as a Gaussian random variable

$$p(y^*|\mathbf{x}^*) = \mathcal{N}(\widehat{\mathbf{w}}_{MLE}^\top \mathbf{x}^*, \widehat{\sigma}_{MLE}^2)$$

$$p(y^*|\mathbf{x}^*) = \mathcal{N}(\widehat{\mathbf{w}}_{MAP}^\top \mathbf{x}^*, \widehat{\sigma}_{MAP}^2)$$

Full Bayesian Treatment

- Treating y and $\mathbf{w}$ as random variables

$$p(y^*|\mathbf{x}^*) = \int p(y^*|\mathbf{x}^*, \mathbf{w})p(\mathbf{w}|\mathbf{X}, \mathbf{y})d\mathbf{w}$$

- This is also *Gaussian*!

Impact of outliers on regression

- Linear regression training gets impacted by the presence of outliers
- The square term in the exponent of the Gaussian pdf is the culprit
  - Equivalent to the square term in the loss
- How to handle this (*Robust Regression*)?
- Probabilistic:
  - Use a different distribution instead of Gaussian for $p(y|\mathbf{x})$
  - Robust regression uses Laplace distribution

$$p(y|\mathbf{x}) \sim Laplace(\mathbf{w}^\top \mathbf{x}, b)$$

- Geometric:
  - *Least absolute deviations* instead of least squares

$$J(\mathbf{w}) = \sum_{i=1}^{N} |y_i - \mathbf{w}^\top \mathbf{x}|$$

Generative vs. Discriminative Classifiers

- Probabilistic classification task:

$$p(Y = benign|\mathbf{X} = \mathbf{x}), p(Y = malicious|\mathbf{X} = \mathbf{x})$$

- How do you estimate $p(y|\mathbf{x})$?

$$p(y|\mathbf{x}) = \frac{p(y, \mathbf{x})}{p(\mathbf{x})} = \frac{p(\mathbf{x}|y)p(y)}{p(\mathbf{x})}$$

- Two step approach - Estimate generative model and then posterior for y (Naïve Bayes)
- Solving a more general problem [2, 1]
- Why not directly model $p(y|\mathbf{x})$? - **Discriminative approach**

Which is Better?

- Number of training examples needed to learn a PAC-learnable classifier $\propto$ *VC-dimension of the hypothesis space*
- VC-dimension of a probabilistic classifier $\propto$ Number of parameters [2] (or a small polynomial in the number of parameters)
- Number of parameters for $p(y, \mathbf{x})$ > Number of parameters for $p(y|\mathbf{x})$

Discriminative classifiers need lesser training examples to for PAC learning than generative classifiers

Logistic Regression

- $y|\mathbf{x}$ is a *Bernoulli* distribution with parameter $\theta = sigmoid(\mathbf{w}^\top \mathbf{x})$
- When a new input $\mathbf{x}^*$ arrives, we toss a coin which has $sigmoid(\mathbf{w}^\top \mathbf{x}^*)$ as the probability of heads
- If outcome is heads, the predicted class is 1 else 0
- Learns a linear boundary

Learning Task for Logistic Regression

Given training examples $\langle \mathbf{x}_i, y_i \rangle_{i=1}^D$, learn $\mathbf{w}$

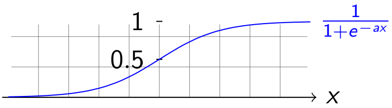
Logistic Regression

Bayesian Interpretation

- Directly model $p(y|\mathbf{x})$ ($y \in \{0, 1\}$)
- $p(y|\mathbf{x}) \sim Bernoulli(\theta = sigmoid(\mathbf{w}^\top \mathbf{x}))$

Geometric Interpretation

- Use regression to predict discrete values
- *Squash* output to $[0, 1]$ using sigmoid function
- Output less than 0.5 is one class and greater than 0.5 is the other



Learning Parameters

- MLE Approach
- Assume that $y \in \{0, 1\}$
- What is the likelihood for a bernoulli sample?
  - If $y_i = 1$, $p(y_i) = \theta_i = \frac{1}{1+exp(-\mathbf{w}^\top \mathbf{x}_i)}$
  - If $y_i = 0$, $p(y_i) = 1 - \theta_i = \frac{1}{1+exp(\mathbf{w}^\top \mathbf{x}_i)}$
  - In general, $p(y_i) = \theta_i^{y_i}(1-\theta_i)^{1-y_i}$

Log-likelihood

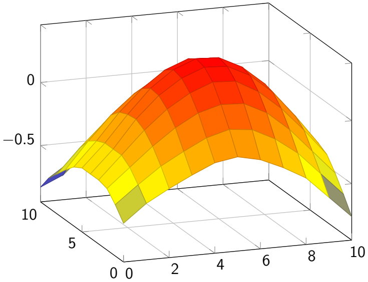
$$LL(\mathbf{w}) = \sum_{i=1}^{N} y_i \log \theta_i + (1 - y_i) \log (1 - \theta_i)$$

- No closed form solution for maximizing log-likelihood

Using Gradient Descent for Learning Weights

- Compute gradient of LL with respect to $\mathbf{w}$
- A convex function of $\mathbf{w}$ with a unique global maximum

$$\frac{d}{d\mathbf{w}} LL(\mathbf{w}) = \sum_{i=1}^{N} (y_i - \theta_i)\mathbf{x}_i$$



- Update rule:

$$\mathbf{w}_{k+1} = \mathbf{w}_k + \eta \frac{d}{d\mathbf{w}_k} LL(\mathbf{w}_k)$$

Using Newton's Method

- Setting η is sometimes *tricky*
- Too large – incorrect results
- Too small – slow convergence
- Another way to speed up convergence:

Newton's Method

$$\mathbf{w}_{k+1} = \mathbf{w}_k + \eta \mathbf{H}_k^{-1} \frac{d}{d\mathbf{w}_k} LL(\mathbf{w}_k)$$

What is the Hessian?

- Hessian or **H** is the second order derivative of the objective function
- Newton's method belong to the family of **second order optimization algorithms**
- For logistic regression, the Hessian is:

$$H = -\sum_i \theta_i(1-\theta_i)\mathbf{x}_i\mathbf{x}_i^\top$$

Regularization with Logistic Regression

- **Overfitting** is an issue, especially with large number of features
- Add a *Gaussian prior* $\sim \mathcal{N}(\mathbf{0}, \tau^2)$
- Easy to incorporate in the gradient descent based approach

$$LL'(\mathbf{w}) = LL(\mathbf{w}) - \frac{1}{2}\lambda\mathbf{w}^\top\mathbf{w}$$

$$\frac{d}{d\mathbf{w}}LL'(\mathbf{w}) = \frac{d}{d\mathbf{w}}LL(\mathbf{w}) - \lambda\mathbf{w}$$

$$H' = H - \lambda I$$

where I is the identity matrix.

Handling Multiple Classes

- $p(y|\mathbf{x}) \sim Multinoulli(\boldsymbol{\theta})$
- Multinoulli parameter vector $\boldsymbol{\theta}$ is defined as:

$$\theta_j = \frac{exp(\mathbf{w}_j^\top \mathbf{x})}{\sum_{k=1}^{C} exp(\mathbf{w}_k^\top \mathbf{x})}$$

- Multiclass logistic regression has C weight vectors to learn

Bayesian Logistic Regression

- How to get the posterior for $\mathbf{w}$?
- Not easy - *Why?*

Laplace Approximation

- We do not know what the true posterior distribution for $\mathbf{w}$ is.
- Is there a close-enough (approximate) Gaussian distribution?

References

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