Lecture 2 Part B: Loss functions

Pranabendu Misra Chennai Mathematical Institute

Advanced Machine Learning 2022

(based on slides by Madhavan Mukund)

Supervised learning estimates parameters for a model based on training data

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- Parameter estimate is through gradient descent
 - Define a loss function measuring the error with respect to training data
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- Typical loss functions include mean squared error (MSE) and cross entropy
- How do arrive at these loss functions?

■ Build a model M from training data $D = \{(x_1, y_1,), (x_2, y_2,), \dots, (x_n, y_n)\}$



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- Likelihood is $\prod_{i=1}^{n} P_{\text{model}}(y_i \mid x_i, \theta)$
- Find *M* that maximizes the likelihood

Log likelihood

■ Maximize the likelihood $\prod_{i=1} P_{\text{model}}(y_i \mid x_i, \theta)$

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$$\log \left(\prod_{i=1}^{n} P_{\text{model}}(y_i \mid x_i, \theta) \right) = \sum_{i=1}^{n} \log(P_{\text{model}}(y_i \mid x_i, \theta))$$

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■ Define
$$P_{\text{data}}(y \mid x_i)$$
 as follows: $P_{\text{data}}(y \mid x_i) = \begin{cases} 1 & \text{if } y = y_i \\ 0 & \text{otherwise} \end{cases}$

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- For each x_i , $P_{\text{data}}(y_i \mid x_i) = 1$, so rewrite log likelihood as

$$\sum_{i=1}^{n} \log(P_{\text{model}}(y_i \mid x_i, \theta)) = \sum_{i=1}^{n} P_{\text{data}}(y_i \mid x_i) \cdot \log(P_{\text{model}}(y_i \mid x_i, \theta))$$

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$$\mathcal{L}(\theta) = \sum_{i=1}^{n} P_{\mathsf{data}}(y_i \mid x_i) \log(P_{\mathsf{model}}(y_i \mid x_i, \theta))$$

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Log likelihood is a function of the learned parameters θ

$$\mathcal{L}(\theta) \neq \sum_{i=1}^{n} P_{\text{data}}(y_i \mid x_i) \log(P_{\text{model}}(y_i \mid x_i, \theta))$$

■ To maximize, find an optimum value of $\theta \left(\frac{\partial \mathcal{L}(\theta)}{\partial \theta} = 0 \right)$



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■ Let $X = \{x_1, x_2, ..., x_k\}$ with a probability distribution P



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- Let $X = \{x_1, x_2, \dots, x_k\}$ with a probability distribution $P(x_1, x_2, \dots, x_k)$
- Entropy is defined as $H(P) = -\sum_{i=1}^{k} P(x_i) \log P(x_i)$
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- Imagine an encoding based on Q where true distribution is P
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- Note that cross entropy is not symmetric: $H(P,Q) \neq H(Q,P)$

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■ Maximum likelihood estimator (MLE) — maximize

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- Minimizing cross entropy is the same as maximizing likelihood
- The "cross entropy loss function" is a special form of this generic observation

- Training input is $\{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$
 - Noisy outputs from a linear function
 - $y_i = w^T x_i + \epsilon$
 - ullet $\epsilon \sim \mathcal{N}(0,\sigma^2)$: Gaussian noise, mean 0, fixed variance σ^2
 - $y_i \sim \mathcal{N}(\mu_i, \sigma^2), \ \mu_i = w^T x_i$

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Log likelihood

$$\mathcal{L}(\theta) = \sum_{i=1}^{n} \log \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y-w^T x_i)^2}{2\sigma^2}} \right)$$



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- Log likelihood (assuming natural logarithm)

$$\mathcal{L}(\theta) = \sum_{i=1}^{n} \log \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y-w^T x_i)^2}{2\sigma^2}} \right) = n \log \left(\frac{1}{\sqrt{2\pi\sigma^2}} \right) - \sum_{i=1}^{n} \frac{(y-w^T x_i)^2}{2\sigma^2}$$



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$$\hat{w}_{\mathsf{MSE}} = \underset{w}{\mathsf{arg\,max}} \left[-\sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \right]$$

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$$\hat{w}_{MSE} = \underset{w}{arg max} \left[-\sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \right] = \underset{w}{arg min} \left[\sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \right]$$

 Assuming data points are generated by linear function and then perturbed by Gaussian noise, MSE is the "correct" loss function to maximize likelihood (and minimize cross entropy)

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- Cross entropy: $\sum_{i=1}^{n} \sum_{j \in \{0,1\}} P_{\text{data}}(y_i = j) \log(P_{\text{model}}(y_i = j \mid x_i, \theta))$



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- Expand:

$$\sum_{i=1}^{n} P_{\mathsf{data}}(y_{i} = 0) \log P_{\mathsf{model}}(y_{i} = 0 \mid x_{i}, \theta) + P_{\mathsf{data}}(y_{i} = 1) \log P_{\mathsf{model}}(y_{i} = 1 \mid x_{i}, \theta)$$



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■ Equivalently, $\sum_{i=1}^{n} (1-y_i) \cdot \log(1-a_i) + y_i \cdot \log a_i$



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- Equivalently, $\sum_{i=1}^{n} (1-y_i) \cdot \log(1-a_i) + y_i \cdot \log a_i$
- Recommended loss function, directly minimizes cross entropy

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- Finding MLE is equivalent to minimizing cross entropy $H(P_{data}, P_{model})$

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- Finding MLE is equivalent to minimizing cross entropy $H(P_{data}, P_{model})$
- Applying this to a given situation, we arrive at concrete loss functions
 - Mean square error for regression
 - "Cross entropy" for binary classification



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