

Regularization

1. Overfitting

- Underfitting, or high bias, is when the form of our hypothesis function h maps poorly to the trend of the data.
- Overfitting, or high variance, is caused by a hypothesis function that fits the available data but does not generalize well to predict new data.

Addressing

- Reduce the number of features (manually select, model selection).
- Regularization (keep all the features, but reduce the magnitude of parameters).

2. Regularized Linear Regression

$$\min_{\theta} \frac{1}{2m} \left[\sum_{i=1}^m (h_{\theta}(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{j=1}^n \theta_j^2 \right], \text{ where } h_{\theta}(x) = \theta^T x$$

- Normal equation

$$\theta = (X^T X + \lambda \cdot L)^{-1} X^T y \text{ where } L = \begin{bmatrix} 0 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix}$$

Proof.

$$\begin{cases} \frac{\partial}{\partial \theta_j} J(\theta) = \frac{1}{m} \sum_{k=1}^m (\theta^T x^{(k)} - y^{(k)}) x_j^{(k)} & (j = 0) \\ \frac{\partial}{\partial \theta_j} J(\theta) = \frac{1}{m} \sum_{k=1}^m (\theta^T x^{(k)} - y^{(k)}) x_j^{(k)} + \frac{\lambda}{m} \theta_j & (j \in N^+) \end{cases}$$

$$\Rightarrow \nabla_{\theta} J(\theta) = \frac{1}{m} (X^T X \theta - X^T y) + \frac{\lambda}{m} L \theta$$

3. Regularized Logistic Regression

$$\min_{\theta} \left[-\frac{1}{m} \sum_{i=1}^m (y^{(i)} \log h_{\theta}(x^{(i)}) + (1 - y^{(i)}) \log(1 - h_{\theta}(x^{(i)}))) + \frac{\lambda}{2m} \sum_{j=1}^n \theta_j^2 \right]$$

4. MLE & MAP

Preliminaries

- Assume data are generated via $d \sim p(d; \theta)$
- $D = \{d^{(i)}\}_{i=1,2,\dots,m}$, where $d^{(i)}$ is i.i.d. (independent of others and same distribution).
- Goal: Estimate parameter θ that best models the data.

Maximum Likelihood Estimation (MLE)

- Likelihood: $L(\theta) = p(D; \theta) = \prod_{i=1}^m p(d^{(i)}; \theta)$
- MLE typically maximizes the log-likelihood $l(\theta)$.
- $\theta_{MLE} = \arg \max_{\theta} \sum_{i=1}^m \log p(d^{(i)}; \theta)$

Maximum-a-Posteriori Estimation (MAP)

- Posterior probability of θ is $p(\theta|D) = \frac{p(\theta)p(D|\theta)}{p(D)}$
- $p(\theta)$ is prior probability of θ , where $p(D)$ is probability of the data.
- MAP usually maximizes the log of the posterior probability
- $\theta_{MAP} = \arg \max_{\theta} (\log p(\theta) + \sum_{i=1}^m \log p(d^{(i)}|\theta))$

Linear Regression

1. MLE

- Suppose $y^{(i)} = \theta^T x^{(i)} + \epsilon^{(i)}$, where $\epsilon \sim \mathcal{N}(0, \sigma^2)$
 - Normal Distribution $p(x; \mu, \sigma) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp(-\frac{1}{2\sigma^2}(x - \mu)^2)$
- $p(d^{(i)}; \theta) = \frac{1}{\sigma\sqrt{2\pi}} \exp(-\frac{1}{2\sigma^2}(y^{(i)} - \theta^T x^{(i)})^2) \Rightarrow \log p(d^{(i)}; \theta) = \log \frac{1}{\sigma\sqrt{2\pi}} - \frac{1}{2\sigma^2}(y^{(i)} - \theta^T x^{(i)})^2$
- $\theta_{MLE} = \arg \min_{\theta} \sum_{i=1}^m (y^{(i)} - \theta^T x^{(i)})^2$

2. MAP

- Suppose $\epsilon \sim \mathcal{N}(0, \sigma^2)$, $\theta \sim \mathcal{N}(0, \lambda^2 I)$
 - Multivariate normal distribution $p(x; \mu, \Sigma) = \frac{1}{(2\pi)^{n/2} |\Sigma|^{1/2}} \exp(-\frac{1}{2}(x - \mu)^T \Sigma^{-1}(x - \mu))$
 - where $\mu \in \mathbb{R}^n$, $\Sigma \in \mathbb{R}^{n \times n}$ is symmetric and positive semidefinite
- $p(\theta) = \frac{1}{(\sqrt{2\pi}\lambda)^n} \exp(-\frac{1}{2\lambda^2} \theta^T \theta) \Rightarrow \log p(\theta) = n \log \frac{1}{\sqrt{2\pi}\lambda} - \frac{\theta^T \theta}{2\lambda^2}$
- $\theta_{MAP} = \arg \min_{\theta} \left\{ \sum_{i=1}^m (y^{(i)} - \theta^T x^{(i)})^2 + \frac{\theta^T \theta}{2\lambda^2} \right\}$

3. MLE vs MAP

- MLE (unregularized solution) vs MAP (regularized solution)
- The prior distribution acts as a regularizer in MAP estimation

Logistic Regression

1. MLE

- Suppose $p(d^{(i)}; \theta) = h_{\theta}(y^{(i)} x^{(i)}) = \frac{1}{1 + \exp(-y^{(i)} \theta^T x^{(i)})} \Rightarrow \log p(d^{(i)}; \theta) = -\log(1 + \exp(-y^{(i)} \theta^T x^{(i)}))$
- $\theta_{MLE} = \arg \min_{\theta} \sum_{i=1}^m \log(1 + \exp(-y^{(i)} \theta^T x^{(i)}))$

2. MAP

- Suppose $\theta \sim \mathcal{N}(0, \lambda^2 I)$

- $\theta_{MAP} = \arg \min_{\theta} \left\{ \sum_{i=1}^m (\log(1 + \exp(-y^{(i)} \theta^T x^{(i)}))) + \frac{\theta^T \theta}{2\lambda^2} \right\}$

3. MLE vs MAP

- Similar conclusion as linear regression.