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

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

- Normal equation

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

Proof.

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

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

3. Regularized Logistic Regression

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

4. MLE & MAP

Preliminaries

- Assume data are generated via $d\sim p(d;\theta)$
- $D=\{d^{(i)}\}_{i=1,2,\cdots,m}$, 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 $l(\theta)$.
- $\theta_{MLE} = \text{arg max}_{\theta} \ \sum_{i=1}^{m} \text{log} p(d^{(i)}; \theta)$

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 prbability of θ, where $p(D)$ is probability of the data.
- MAP usually maximizes the log of the posteriori probability
- $\theta_{MAP} = \text{arg max}_{\theta} \ \left(\text{log} p(\theta) + \sum_{i=1}^{m} \text{log} p(d^{(i)}|\theta)\right)$

Linear Regression

1. MLE

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

2. MAP

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

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

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.