

Lecture 1 - Linear Regression

Model Selection

When 2 models both fit the training data equally well, which one should we choose?

- use validation data and choose the better one
 - 一般来说 train : valid : test = 8:1:1
 - 一般over-fit时error on validation data会上升
- choose a simpler one (if without validation data)
 - Occam's Razor(奥卡姆剃刀准则): 如无必要, 勿增实体
 - Inductive bias

Bias-Variance Decomposition

- D is a training set and $D = \{(x_1, y_1), \dots, (x_n, y_n)\}$ ($D \sim P(D)$)
 - 也就是说用由分布 $P(D)$ 采样出来的 D 训练一个模型 $f(x; D)$
- 对于一个测试数据 (x, y) , 平方误差的期望为 $E_D(f(x; D) - y)^2$
 - which means average error of $f(x; D)$ over infinitely many $D \sim P(D)$
 - we define $\bar{f}(x) := E_D(f(x; D) - y)$
 - now we have:

$$\begin{aligned} E_D(f(x; D) - y)^2 &= E_D[f(x; D) - \bar{f}(x) + \bar{f}(x) - y]^2 \\ &= E_D[f(x; D) - \bar{f}(x)]^2 + 2E_D[f(x; D) - \bar{f}(x)][\bar{f}(x) - y] + E_D[\bar{f}(x) - y]^2 \\ &= E_D[f(x; D) - \bar{f}(x)]^2 + (\bar{f}(x) - y)^2 \\ &= \text{Variance} + \text{Bias}^2 \\ (E_D[f(x; D) - \bar{f}(x)] &= 0) \end{aligned}$$

- Variance: error caused by over-fitting particular D can be decreased by increasing the size n of D
简单来说即是测试的预测与平均预测之差的平方
- Bias: error caused by the model's ability to fit the data, or the model is not complex enough
即平均预测与标签也就是实际值之差
- Trade-off
 - simple model: high bias, low variance
 - complex model: low bias, high variance
- One more thing
 - $\bar{f}(x) = E_D(f(x; D))$ is an average model over infinitely sample small D
 - $\hat{f}(x) = f(x; D, |D| \rightarrow \infty)$ is a model trained over an infinitely large D
 - 虽然上述推导使用了第一个函数, 但在实际过程中数据自然越多越好, 那么也就是第二个模型往往表现更好
 - example:

$$P(D) = \begin{cases} 1/3 & \{(-1, 1), (0, 0)\} \\ 1/3 & \{(1, 1), (0, 0)\} \\ 1/3 & \{(-1, 1), (1, 1)\} \end{cases}$$

- $\bar{f}(x) = 1/3, \text{variance} > 0, \text{bias}^2 = 1$
- $\hat{f}(x) = 2/3, \text{variance} = 0, \text{bias}^2 = 2/3$

Linear Regression

Basic Model

- D is a training set and $D = \{(x_1, y_1), \dots, (x_n, y_n)\}$. $x_i \in \mathbb{R}^d$, $y_i \in \mathbb{R}$, $i = 1, 2, \dots, n$
- we are going to train a model $y = w^T x + b$, $w \in \mathbb{R}^d$, $b \in \mathbb{R}$
- How to determine w, b
 - ERM(Empirical Risk Minimization)
- Loss function
 - squared loss $(f(x_i) - y_i)^2$
- 优化目标

$$\min_{w,b} \sum_{i=1}^n (f(x_i) - y_i)^2$$
$$= \min_{w,b} \sum_{i=1}^n (w^T x_i + b - y_i)^2 := L(w, b)$$

- 求梯度

$$\frac{\partial L}{\partial w} = 2 \sum_{i=1}^n (w^T x_i + b - y_i) x_i$$
$$\frac{\partial L}{\partial b} = 2 \sum_{i=1}^n (w^T x_i + b - y_i)$$

注意这里是一个向量对标量求梯度，结果还是一个向量

- Gradient Descent

$$w \leftarrow w - \alpha \frac{\partial L}{\partial w}$$
$$b \leftarrow b - \alpha \frac{\partial L}{\partial b}$$

α is the **learning rate** and it's a **hyperparameter**

- 常用公式

$$w \in \mathbb{R}^d$$
$$\frac{\partial w^T w}{\partial w} = 2w$$
$$\frac{\partial w^T x}{\partial x} = w$$
$$\frac{\partial x^T A x}{\partial x} = (A + A^T)x$$

Least Squares

- Least squares actually has closed-form solution! (which also regards as **Normal Equation**)
- we need some vectorized variables:

$$x = \begin{bmatrix} x_1^T, 1 \\ x_2^T, 1 \\ \dots \\ x_n^T, 1 \end{bmatrix} \in \mathbb{R}^{n \times (d+1)}$$
$$\hat{w} = \begin{bmatrix} w \\ b \end{bmatrix} \in \mathbb{R}^{d+1}$$
$$y = \begin{bmatrix} y_1 \\ \dots \\ y_n \end{bmatrix} \in \mathbb{R}^n$$

- the loss function now looks like this:

$$L(\hat{w}) = (y - x\hat{w})^T (y - x\hat{w})$$

because we know that:

$$x\hat{w} = \begin{bmatrix} f(x_1) \\ \dots \\ f(x_n) \end{bmatrix}$$

- to compute \hat{w} we want the gradient to be 0

$$\begin{aligned} \frac{\partial L(\hat{w})}{\partial \hat{w}} &= \frac{\partial [(y - x\hat{w})^T (y - x\hat{w})]}{\partial \hat{w}} \\ &= \frac{\partial (y^T y - y^T x\hat{w} - \hat{w}^T x^T y + \hat{w}^T x^T x\hat{w})}{\partial \hat{w}} \\ &= \frac{\partial (y^T y - 2y^T x\hat{w} + \hat{w}^T x^T x\hat{w})}{\partial \hat{w}} \\ &= -2x^T y + 2x^T x\hat{w} = 0 \end{aligned}$$

- now we focus on $x^T x$:
 - 我们知道 $x^T x$ 是一个实对称矩阵，那么它是半正定的，也就是说该矩阵的特征值都是大于等于0的
 - 如果 $x^T x$ 不满秩，那么显然这个方程里 \hat{w} 是可能有多于一个解的，造成这种结果的可能原因是：
 - $d+1 > n$:
 - $rank(x^T x) = rank(x) \leq \min\{d+1, n\}$
 - x has repeated columns or rows
 - 如果 $x^T x$ 满秩，则特征值都大于0，我们可以对其进行特征值分解：

$$\begin{aligned} x^T x &= U \Lambda U^T \\ &= U \begin{bmatrix} \lambda_1 & & \\ & \dots & \\ & & \lambda_{d+1} \end{bmatrix} U^T \\ (x^T x)^{-1} &= U \Lambda^{-1} U^T \\ &= U \begin{bmatrix} \lambda_1^{-1} & & \\ & \dots & \\ & & \lambda_{d+1}^{-1} \end{bmatrix} U^T \end{aligned}$$

- 那么这个方程有唯一解 $\hat{w} = (x^T x)^{-1} x^T y$
- 但依然有一个问题，就是 λ_{d+1} 可能很接近0，也就是 $x^T x$ 很接近一个非奇异矩阵，这就导致 λ_{d+1}^{-1} 会相当大，因此会导致计算上的问题 (**numerical issues and instability**)

L2 Regularization

- Linear Regression with L2 Regularization (Ridge Regression):

$$\min L(\hat{w}) + \lambda \|\hat{w}\|_2^2$$

- λ is a positive **constant hyperparameter** which can control the strength of regularization (weight decay)
- 简单来说就是避免某个 w 特别突出，使所有的 w 更平均一些
- loss function with L2 Regularization:

$$J(\hat{w}) = (y - x\hat{w})^T (y - x\hat{w}) + \lambda w^T w \quad (\lambda > 0)$$

- compute the gradient:

$$\begin{aligned} \frac{\partial J(\hat{w})}{\partial \hat{w}} &= -2x^T y + 2x^T x\hat{w} + 2\lambda \hat{w} \\ &= -2x^T y + 2(x^T x + \lambda I)\hat{w} = 0 \end{aligned}$$

- 这是我们对 $x^T x + \lambda I$ 进行特征值分解，就可以得到:

$$x^T x + \lambda I = U(\Lambda + \lambda I)U^T$$

$$= U \begin{bmatrix} \lambda_1 + \lambda & & \\ & \dots & \\ & & \lambda_{d+1} + \lambda \end{bmatrix} U^T$$

so $x^T x + \lambda I$ is always non-singular and \hat{w} is a unique solution!

$$\hat{w} = (x^T x + \lambda I)^{-1} x^T y$$

L1 Regularization

- Linear Regression with L1 Regularization (Lasso Regression):

$$\min L(\hat{w}) + \lambda \|\hat{w}\|_1$$

$$= \min L(\hat{w}) + \lambda \sum_{i=1}^{d+1} |\hat{w}_i|$$

- induce sparsity of \hat{w} (many dimensions of \hat{w} will be 0)
- Lasso stands for *Least Absolute Shrinkage and Selection Operator*
 - feature selection: 当参数很多时, 用L1正则化可以筛选出真正有用的参数

Geometric view of Linear Regression

- Ideally, we want $X\hat{W} = y$
- 但是显然我们没办法找到一个model可以fit任何数据
- Consider the column space of X , $col(X)$, spanned by columns of X
 - $X\hat{W}$ lies in $col(X)$, but y may not
 - let $X\hat{W} = \hat{y}$, this \hat{W} is the least square solution to $X\hat{W} = y$
 - Because \hat{y} minimizes $\|y - X\hat{W}\|^2$, which is the object of Linear Regression, $\hat{y}(X\hat{W})$ should satisfy $y - \hat{y} \perp col(X) \leftrightarrow X^T(y - \hat{y}) = 0 \leftrightarrow X^T X \hat{W} = X^T y$