

1  $\ell_1$ - and  $\ell_2$ -Regularization

Consider sample points  $X_1, X_2, \dots, X_n \in \mathbb{R}^d$  and associated values  $y_1, y_2, \dots, y_n \in \mathbb{R}$ , an  $n \times d$  design matrix  $X = [X_1 \dots X_n]^\top$  and an  $n$ -vector  $y = [y_1 \dots y_n]^\top$ .

For the sake of simplicity, assume (1) that the sample data have been centered (i.e each feature has mean 0) and (2) that the sample data have been whitened, meaning a linear transformation is applied to the original data matrix so that the resulting features have variance 1 and the features are uncorrelated; i.e.,  $X^\top X = nI$ .

For this question, we will not use a fictitious dimension nor a bias term; our linear regression function will output zero for  $x = 0$ .

Consider linear least-squares regression with regularization in the  $\ell_1$ -norm, also known as Lasso. The Lasso cost function is

$$J(w) = \|Xw - y\|_2^2 + \lambda \|w\|_1$$

where  $w \in \mathbb{R}^d$  and  $\lambda > 0$  is the regularization parameter. Let  $w^* = \operatorname{argmin}_{w \in \mathbb{R}^d} J(w)$  denote the weights that minimize the cost function.

In the following steps, we will explore the sparsity-promoting property of the  $\ell_1$ -norm and compare this with the  $\ell_2$ -norm.

1. We use the notation  $X_{*i}$  to denote column  $i$  of the design matrix  $X$ , which represents the  $i^{\text{th}}$  feature. Write  $J(w)$  in the following form for appropriate functions  $g$  and  $f$ .

$$J(w) = g(y) + \sum_{i=1}^d f(X_{*i}, w_i, y, \lambda)$$

$$\begin{aligned} J(w) &= \|Xw - y\|_2^2 + \lambda \|w\|_1 = (Xw - y)^\top (Xw - y) + \lambda \|w\|_1 = (w^\top X^\top - y^\top) (Xw - y) + \lambda \|w\|_1 \\ &= w^\top X^\top Xw - y^\top Xw - w^\top X^\top y + y^\top y + \lambda \|w\|_1 \\ &= nw^\top w - y^\top Xw - w^\top X^\top y + y^\top y + \lambda \|w\|_1 \\ &= y^\top y - 2 \sum_{i=1}^d w_i (y^\top X_{*i}) + \lambda \|w\|_1 + nw^\top w \\ g(y) &= y^\top y \\ f(X_{*i}, w_i, y, \lambda) &= -2w_i (y^\top X_{*i}) + \lambda |w_i| + nw_i^2 \end{aligned}$$

2. If  $w_i^* > 0$ , solve for the optimal value  $w_i^*$ . *Hint: use your answer in the previous part.*

$$w_i^* = \underset{w_i \in \mathbb{R}_+}{\operatorname{argmin}} f(x_{*i}, w_i, y, \lambda) = n w_i^2 + (\lambda - 2y^T x_{*i}) \cdot w_i$$

$$w_i^* = \frac{2y^T x_{*i} - \lambda}{2n}$$

3. If  $w_i^* < 0$ , solve for the optimal value  $w_i^*$ .

$$w_i^* = \underset{w_i \in \mathbb{R}_-}{\operatorname{argmin}} f(x_{*i}, w_i, y, \lambda) = n w_i^2 - (\lambda + 2y^T x_{*i}) \cdot w_i$$

$$w_i^* = \frac{2y^T x_{*i} + \lambda}{2n}$$

4. Considering parts 2 and 3, what is the condition for  $w_i^*$  to be zero?

$$\begin{cases} 2y^T x_{*i} - \lambda \leq 0 \\ 2y^T x_{*i} + \lambda \geq 0 \end{cases}$$

$$|2y^T x_{*i}| \leq \lambda$$

5. Now consider ridge regression, which uses the  $\ell_2$  regularization term  $\lambda |w|^2$ . How does this change the function  $f(\cdot)$  from part 1? What is the new condition in which  $w_i^* = 0$ ? How does it differ from the condition you obtained in part 4?

$$f(\cdot) = -2(y^T x_{*i}) \cdot w_i + (\lambda + n) w_i^2$$

$$w_i^* = \frac{y^T x_{*i}}{\lambda + n}$$

$$\text{if } w_i^* = 0, \text{ it means } y^T x_{*i} = 0$$

## 2 Probabilistic Interpretation of Lasso

Let's start with the probabilistic interpretation of least squares. Start with labels  $y \in \mathbb{R}$ , data  $\mathbf{x} \in \mathbb{R}^d$ , and noise  $z \sim \mathcal{N}(0, \sigma^2)$ , where  $y = \mathbf{w}^\top \mathbf{x} + z$ . Recall from lecture that we then have

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

However, maximum likelihood estimates (MLE) can overfit by picking parameters that mirror the training data. To ameliorate this issue, we can assume a Laplace prior on  $w_j \sim \text{Laplace}(0, t)$ , i.e.

$$\begin{aligned} P(w_j) &= \frac{1}{2t} e^{-|w_j|/t} \\ P(\mathbf{w}) &= \prod_{j=1}^D P(w_j) = \left(\frac{1}{2t}\right)^D \cdot e^{-\sum |w_j|/t} \end{aligned}$$

Here, we will see that this modification results in the Lasso objective function.

Recall that the MLE objective finds the parameters that maximize the likelihood of the data,

$$\begin{aligned} \mathbf{w}^* &= \underset{\mathbf{w}}{\operatorname{argmax}} L(\mathbf{w}) \\ &= \underset{\mathbf{w}}{\operatorname{argmax}} P(Y_1, \dots, Y_n | \mathbf{w}, \mathbf{X}_1, \dots, \mathbf{X}_n, \sigma^2) \\ &= \underset{\mathbf{w}}{\operatorname{argmax}} \prod_{i=1}^n P(Y_i | \mathbf{X}_i, \mathbf{w}, \sigma^2). \end{aligned}$$

When working in a Bayesian framework, we instead focus on the posterior distribution of the parameters conditioned on the data,  $P(\mathbf{w} | Y_1, \dots, Y_n, \mathbf{X}_1, \dots, \mathbf{X}_n, \sigma^2)$ . To pick a single model, we can choose the  $\mathbf{w}$  that is most likely according to the posterior,

$$\begin{aligned} \mathbf{w}^* &= \underset{\mathbf{w}}{\operatorname{argmax}} P(\mathbf{w} | Y_1, \dots, Y_n, \mathbf{X}_1, \dots, \mathbf{X}_n, \sigma^2) \\ &= \underset{\mathbf{w}}{\operatorname{argmax}} \frac{P(\mathbf{w}, Y_1, \dots, Y_n | \mathbf{X}_1, \dots, \mathbf{X}_n, \sigma^2)}{P(Y_1, \dots, Y_n | \mathbf{X}_1, \dots, \mathbf{X}_n, \sigma^2)} \\ &= \underset{\mathbf{w}}{\operatorname{argmax}} \frac{P(Y_1, \dots, Y_n | \mathbf{w}, \mathbf{X}_1, \dots, \mathbf{X}_n, \sigma^2) P(\mathbf{w})}{P(Y_1, \dots, Y_n | \mathbf{X}_1, \dots, \mathbf{X}_n, \sigma^2)} \\ &= \underset{\mathbf{w}}{\operatorname{argmax}} \frac{L(\mathbf{w}) P(\mathbf{w})}{P(Y_1, \dots, Y_n)} \\ &= \underset{\mathbf{w}}{\operatorname{argmax}} L(\mathbf{w}) P(\mathbf{w}) \quad \text{since } P(Y_1, \dots, Y_n | \mathbf{X}_1, \dots, \mathbf{X}_n, \sigma^2) \text{ does not depend on } \mathbf{w}. \end{aligned}$$

We call  $\mathbf{w}^*$  the Maximum a posteriori (MAP) estimate.

(a) Write the log-likelihood for this MAP estimate.

$$\begin{aligned}
 (a) \quad \omega^* &= \underset{\omega}{\operatorname{argmax}} L(\omega) \cdot P(\omega) \\
 &= \underset{\omega}{\operatorname{argmin}} \quad -\log L(\omega) - \log P(\omega) \\
 &= \underset{\omega}{\operatorname{argmin}} \quad - \sum_{i=1}^n \log P(Y_i | X_i, \omega, \sigma^2) + D \log 2t + \frac{\sum |w_j|}{t} \\
 &= \underset{\omega}{\operatorname{argmin}} \quad - \sum_{i=1}^n \log \left( \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(Y_i - \omega^T X_i)^2}{2\sigma^2}\right) \right) + D \log 2t + \frac{\sum |w_j|}{t} \\
 &= \underset{\omega}{\operatorname{argmin}} \quad \frac{1}{2\sigma^2} \sum (Y_i - \omega^T X_i)^2 + \frac{1}{t} \sum |w_j| + \cancel{D \log 2t + n \log(\sqrt{2\pi}\sigma)}
 \end{aligned}$$

(b) We already have the log-likelihood for MAP. Show that the MAP you derived in the previous part (in this case, Gaussian noise with a Laplace prior) is equivalent to minimizing the following objective. Additionally, identify the constant  $\lambda$ . Note that  $\|\mathbf{w}\|_1 = \sum_{j=1}^D |w_j|$ .

$$J(\mathbf{w}) = \sum_{i=1}^n (Y_i - \mathbf{w}^T \mathbf{X}_i)^2 + \lambda \|\mathbf{w}\|_1$$

$$\begin{aligned}
 (b) \quad \omega^* &= \underset{\omega}{\operatorname{argmin}} \quad \sum (Y_i - \omega^T X_i)^2 + \frac{2\sigma^2}{t} \sum |w_j| \\
 \lambda &= \frac{2\sigma^2}{t}
 \end{aligned}$$

### 3 MLE vs. MAP

Let  $D$  denote the observed data and  $\theta$  the parameter. Whereas MLE only assumes and tries to maximize a likelihood distribution  $p(D|\theta)$ , MAP takes a more Bayesian approach. MAP assumes that the parameter  $\theta$  is also a random variable and has its own distribution. Recall that using Bayes' rule, the posterior distribution can be seen as the product of likelihood and prior:

$$p(\theta|D) = \frac{p(D|\theta)p(\theta)}{p(D)} \propto \underbrace{p(D|\theta)}_{\text{likelihood}} \underbrace{p(\theta)}_{\text{prior}}$$

Suppose that the data consists of  $n$  i.i.d. observations  $D = \{x_1, \dots, x_n\}$ . MAP tries to infer the parameter by maximizing the posterior distribution:

$$\begin{aligned}\theta_{\text{MAP}} &= \operatorname{argmax}_{\theta} p(\theta|D) \\ &= \operatorname{argmax}_{\theta} p(D|\theta)p(\theta) \\ &= \operatorname{argmax}_{\theta} \left[ \prod_{i=1}^n p(x_i|\theta) \right] p(\theta) \\ &= \operatorname{argmax}_{\theta} \left( \sum_{i=1}^n \log p(x_i|\theta) \right) + \log p(\theta)\end{aligned}$$

Note that since both of these methods are point estimates (they yield a value rather than a distribution), neither of them are completely Bayesian. A faithful Bayesian would use a model that yields a posterior distribution over all possible values of  $\theta$ , but this is oftentimes intractable or very computationally expensive.

Now suppose we have a coin with unknown bias  $\theta$  (probability of flipping heads in a single trial). We will estimate the bias of the coin using MLE and MAP. You tossed the coin  $n = 10$  times and 3 of the tosses came as heads.

(a) What is the MLE of the bias of the coin  $\theta$ ?

$$(a) \quad \theta_{MLE} = \underset{\theta}{\operatorname{argmax}} \sum_{i=1}^n \log p(x_i | \theta)$$

$$\hat{\theta}_{MLE} = 0.3$$

(b) Suppose we know that the bias of the coin is distributed according to  $\theta \sim N(0.8, 0.09)$ , i.e., we are rather sure that the bias should be around 0.8.<sup>1</sup> What is the MAP estimate of  $\theta$ ? You can leave your result as an equation of the form  $\frac{a}{\theta} - \frac{b}{1-\theta} - \frac{\theta-c}{d}$ .

$$(b) \quad \theta_{MAP} = \underset{\theta}{\operatorname{argmax}} \left( \sum_{i=1}^n \log p(x_i | \theta) \right) + \log p(\theta)$$

$$= \underset{\theta}{\operatorname{argmax}} \left( 7 \log(1-\theta) + 3 \log(\theta) + \left( -\frac{(\theta-0.8)^2}{2 \times 0.09} \right) \right)$$

$$f(\theta) = 7 \log(1-\theta) + 3 \log(\theta) - \frac{(\theta-0.8)^2}{2 \times 0.09}$$

$$\frac{df(\theta)}{d\theta} = \frac{3}{\theta} - \frac{7}{1-\theta} - \frac{\theta-0.8}{0.09}$$

<sup>1</sup>This is a somewhat strange choice of prior, since we know that  $0 \leq \theta \leq 1$ . However, we will stick with this example for illustrative purposes.

(c) What if our prior is  $\theta \sim N(0.5, 0.09)$  or  $N(0.8, 1)$ ? Write out the new equations using your previous answer, but you do not need to solve for the exact numeric value. How does the difference between MAP and MLE change and why?

(c) i.  $\theta \sim N(0.5, 0.09)$ :

$$\frac{3}{\theta} - \frac{7}{1-\theta} - \frac{\theta - 0.5}{0.09}$$

ii.  $\theta \sim N(0.8, 1)$

$$\frac{3}{\theta} - \frac{7}{1-\theta} - (\theta - 0.8)$$

(d) What if our prior is that  $\theta$  is uniformly distributed in the range  $(0, 1)$ ?

$$p(\theta) = 1$$

$$\text{MLE} = \text{MAP}$$