

1 MLE vs. MAP

Let D denote the observed data and θ 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 θ 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:

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

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 θ , but this is oftentimes intractable or very computationally expensive.

Now suppose we have a coin with unknown bias θ . We are trying to find the bias of the coin by maximizing the underlying distribution. 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 θ ?

(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 0.8.¹ What is the MAP estimation of θ ? You can leave your result as a polynomial equation on θ .

¹This 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 $N(0.8, 1)$? How does the difference between MAP and MLE change and why?

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

2 Tikhonov Regularization

As defined in the homework, Tikhonov regularized regression is a generalization of ridge regression specified by the optimization problem

$$\arg \min_{\mathbf{w}} \frac{1}{2} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2 + \lambda \|\mathbf{\Gamma}\mathbf{w}\|_2^2,$$

For some full rank matrix $\mathbf{\Gamma} \in \mathbb{R}^{d \times d}$.

In this problem, we look at Tikhonov regularization from a probabilistic standpoint and how it relates to the MAP estimator for a certain choice of prior on the parameters \mathbf{w} .

Let $\mathbf{x} \in \mathbb{R}^d$ be a d -dimensional vector and $Y \in \mathbb{R}$ be a one-dimensional random variable. Assume a linear-Gaussian model: $Y|\mathbf{x}, \mathbf{w} \sim N(\mathbf{x}^\top \mathbf{w}, 1)$. Suppose that $\mathbf{w} \in \mathbb{R}^d$ is a d -dimensional Gaussian random vector $\mathbf{w} \sim N(0, \mathbf{\Sigma})$, where $\mathbf{\Sigma}$ is a known symmetric positive-definite covariance matrix.

- (a) Let us assume that we are given n training data points $\{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \dots, (\mathbf{x}_n, y_n)\}$. Derive the posterior distribution of \mathbf{w} given the training data. What is the MAP estimate of \mathbf{w} ? Compare this result to the solution you achieve in your homework. Comment on how Tikhonov regularization is a generalization of ridge regression from a probabilistic perspective.

[Hint: You may find the following lemma useful. If the probability density function of a random variable is of the form

$$f(\mathbf{v}) = C \cdot \exp \left\{ -\frac{1}{2} \mathbf{v}^\top \mathbf{A} \mathbf{v} + \mathbf{b}^\top \mathbf{v} \right\},$$

where C is some constant to make $f(\mathbf{v})$ integrate to 1 and \mathbf{A} is a symmetric positive definite matrix, then \mathbf{v} is distributed as $N(\mathbf{A}^{-1}\mathbf{b}, \mathbf{A}^{-1})$.

- (b) Let us extend this result from the previous part to the case where the observation noise variables Z_i are no longer independent across samples, i.e. \mathbf{Z} is no longer $N(\mathbf{0}, \mathbb{I}_n)$ but instead distributed as $N(\boldsymbol{\mu}_z, \boldsymbol{\Sigma}_z)$ for some mean $\boldsymbol{\mu}_z$ and some covariance $\boldsymbol{\Sigma}_z$ (still independent of the parameter \mathbf{w}). We make the reasonable assumption that the $\boldsymbol{\Sigma}_z$ is invertible. Derive the posterior distribution of \mathbf{w} by appropriately changing coordinates.

(Hint: Write \mathbf{Z} as a function of a standard normal Gaussian vector $\mathbf{V} \sim N(\mathbf{0}, \mathbb{I}_n)$ and use the result in (a) for an equivalent model of the form $\tilde{\mathbf{y}} = \tilde{\mathbf{X}}\mathbf{w} + \mathbf{V}$.)