Introduction to Statistical Learning

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Likelihood and posterior distribution

- $X_i \sim Ber(\theta)$
- Θ: Probability of heads (uncertain value).
- N: Number of coin flips
- $\mathscr{D} := \{N_1$ heads, N_0 tails$\}$ (observed data)
- $\mathbf{D}$: Random variable that represents data, i.e., random number of heads and tails given N coin flips.
- Observe that $\mathbf{D}$ follows Binomial Distribution. $\mathbf{D} \sim Binomial(\theta, N)$ and $N = N_1 + N_0$

Likelihood and posterior distribution

likelihood:

$$p_{\mathbf{D}|\Theta}(\mathscr{D}|\theta) = \binom{N_1 + N_0}{N_1} \theta^{N_1} (1-\theta)^{N_0}$$

Posterior distribution:

$$p_{\Theta|\mathbf{D}}(\theta|\mathscr{D}) = \frac{p_{\mathbf{D}|\Theta}(\mathscr{D}|\theta) p_{\Theta}(\theta)}{p_{\mathbf{D}}(\mathscr{D})}$$

$$= \frac{\binom{N_1+N_0}{N_1}}{\underbrace{p_{\mathbf{D}}(\mathscr{D})}_{\text{constant}}} \theta^{N_1} (1-\theta)^{N_0} p_{\Theta}(\theta)$$

$$\propto \theta^{N_1} (1-\theta)^{N_0} \underbrace{p_{\Theta}(\theta)}_{prior}$$

Computing the posterior

- We want a close-form expression for $p_{\Theta|\mathbf{D}}(\theta|\mathscr{D})$
- Take $\Theta \sim Beta(a, b)$
- Recall:

$$\Theta \sim \text{Beta}(a, b) \Rightarrow P_{\Theta}(\theta) = \underbrace{\frac{1}{B(a, b)}}_{constant} \theta^{a-1}(1-\theta)^{b-1} \quad \text{for } \theta \in [0, 1]$$

Hence:

$$\begin{aligned} p_{\Theta|\mathbf{D}}(\theta|\mathscr{D}) &\propto \theta^{N_1}(1-\theta)^{N_0}\theta^{a-1}(1-\theta)^{b-1} \\ &\propto \theta^{N_1+a-1}(1-\theta)^{N_0+b-1} \\ &\Rightarrow \Theta|\mathscr{D} \sim Beta(N_1 + a, N_0 + b) \end{aligned}$$

Computing the posterior

- Beta(a,b): our prior belief about Θ
- Nothing known a priori: $a = 1, b = 1 \Rightarrow$ Beta(1,1) $=$ Unif([0,1])

Maximum likelihood estimation (MLE)

Goal: Infer Θ from $\mathscr{D}$

MLE:

$$p(\mathscr{D}|\theta) \propto \theta^{N_1}(1-\theta)^{N_0}$$

$$\hat{\theta}_{MLE} := arg_{\theta} \max p(\mathscr{D}\theta)$$

For the example:

$$\hat{\theta}_{MLE} := arg_{\theta \in [0,1]} \max \theta^{N_1}(1-\theta)^{N_0}$$

MAP estimation

$$\hat{\theta}_{MAP} := arg_{\theta} \max p(\theta|\mathscr{D})$$

For the example:

$$\hat{\theta}_{MAP} = arg_{\theta\in[0,1]} \max \theta^{a+N_1}(1-\theta)^{b+N_0-1}$$

What happens when we start with a uniform prior, i.e., Beta(1; 1)?

Posterior mean

Posterior mean: $E[\Theta|\mathscr{D}]$
For the example:

$$E[\Theta|\mathscr{D}] = \frac{a + N_1}{a + b + N_0 + N_1}$$

Since for $X \sim \text{beta}(x, y)$ we have

$$E[X] = \frac{x}{x + y}$$

Hence, in general $\hat{\theta}_{MLE}, \hat{\theta}_{MAP}$ and $E[\Theta|\mathscr{D}]$ are different.

Is MAP a good estimate?

- MAP = point estimate (does not measure uncertainty)

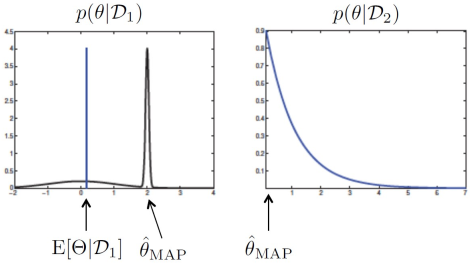

Figure: Murphy, 2012

What does MAP really optimize?

- Assume θ is the true parameter (realization Θ)
- Loss: $L(\theta, \hat{\theta}) = I(\theta \neq \hat{})$
- $\hat{\theta}_{MAP}$ is the optimal estimate

Bayesian linear regression

- Least squares, ridge regression, lasso all produce point estimates, i.e., they output a single solution (least squares = MLE, ridge and lasso = posterior mode (MAP))
- Bayesian linear regression provides a posterior for β
- We can specify any prior and likelihood on β!
- But we assume that both prior and likelihood is Gaussian for analytical tractability!

Gaussian likelihood:

$$\mathbf{Y} = \begin{bmatrix} Y_1 \\ \vdots \\ Y_n \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} \mathbf{x}_1^T \\ \vdots \\ \mathbf{x}_n^T \end{bmatrix} \quad \beta = \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_n \end{bmatrix}$$

What is the likelihood of $\mathbf{Y} = \mathbf{y}$ given that the true parameter vector is β and data $\mathbf{X}$ is observed?

$$L(\beta) = p(\mathscr{D}|\beta) \underbrace{=}_{\text{Since } \mathbf{X} \text{ is fixed}} p(\mathbf{y}|\mathbf{X}, \beta) = \prod_{i=1}^{n} p(y_i|\mathbf{x}_i, \beta)$$

$$= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} exp(-\frac{(y_i - \beta^T \mathbf{x}_i)^2}{2\sigma^2})$$

$$\sim \mathcal{N}(\mathbf{X}\beta, \sigma^2 \mathbf{I}_n)$$

- $\mathbf{I}_n$ is the $n * n$ identity matrix

Gaussian posterior

- Gaussian prior + Gaussian likelihood $\Rightarrow$ Gaussian posterior

General formula for Gaussian posterior:

1. $p(\beta) \sim \mathscr{N}(\mu_0, \Sigma_0)$
2. $p(\mathscr{D}|\beta) \sim \mathscr{N}(\mathbf{X}\beta, \Sigma_{\mathscr{D}})$
3. 1&2 implies that $p(\beta|\mathscr{D}) \sim \mathscr{N}(\mu_{\beta|\mathscr{D}}, \Sigma_{\beta|\mathscr{D}})$

We have

- $\Sigma_{\beta|\mathscr{D}}^{-1} = \Sigma_0^{-1} + \mathbf{X}^T \Sigma_{\mathscr{D}}^{-1} \mathbf{X}$
- $\mu_{\beta|\mathscr{D}} = \Sigma_{\beta|\mathscr{D}}(\mathbf{X}^T \Sigma_{\mathscr{D}}^{-1} \mathbf{y} + \Sigma_0^{-1} \mu_0)$

Example 3.1

- How can we use $p(\beta|\mathscr{D}) \sim \mathcal{N}(\mu_{\beta|\mathscr{D}}, \Sigma_{\beta|\mathscr{D}})$?
- Assume we trained our model and fixed $p(\beta|\mathscr{D})$. We can use this to learn the distrbution of Y given that we observe a new data instance $\mathbf{x}$.

Posterior predictive density at test point x:

$$p(y|\mathbf{x}, \mathscr{D}) = \int_\beta \underbrace{p(y|\mathbf{x}, \beta)}_{\sim \mathcal{N}(\mathbf{x}^T\beta, \sigma^2)} \; p(\beta, \mathscr{D}) d\beta$$

$$\Rightarrow Y \sim \mathcal{N}(\underbrace{\mu_{\beta|\mathscr{D}}^T \mathbf{x}}_{mean}, \underbrace{\sigma^2 + \mathbf{x}^T \Sigma_{\beta|\mathscr{D}} \mathbf{x}}_{variance})$$

- σ^2: variance of the noise term
- $\Sigma_{\beta|\mathscr{D}}$: covariance of the parameters

Example 3.1 cont.

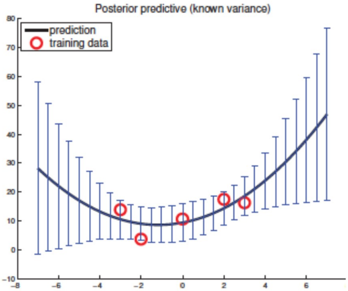

Figure: Murphy, 2012

- Y-axis: Y values, X-axis: X values
- Red circles are training points
- Black curve is the posterior mean of Y given $\mathscr{D}$ and $X = x$
- Error bars (vertical bars): two standard deviations range for the posterior predictive density

Example 3.1 cont.

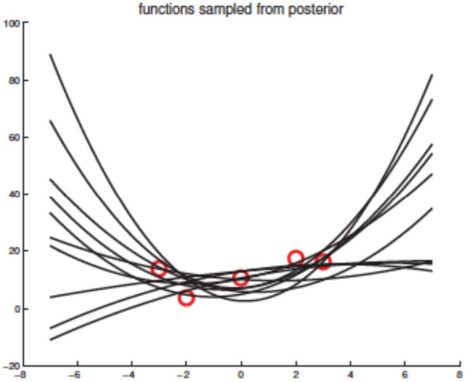

Figure: Murphy, 2012

References

Murphy, K. (2012). *Machine learning: A probabilistic perspective*. MIT Press.
https://books.google.fr/books?id=NZP6AQAAQBAJ