

Bayesian Machine Learning

Course 67564

Solution To Exercise 1: Bayesian Statistics and Gaussians

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10/11/2022

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1 Bayesian Statistics

1.1 MSE and BMSE

1.1.1 Q1 $\text{MSE} [\hat{\theta}] = \text{bias}^2 (\hat{\theta}) + \text{var} [\hat{\theta}]$

Note

$$\text{bias}^2 (\hat{\theta}) = \left(E_D [\hat{\theta}(D)] - \theta \right)^2 = E_D [\hat{\theta}(D)]^2 - 2E_D [\hat{\theta}(D)] \theta + \theta^2$$

and so:

$$\text{bias}^2 (\hat{\theta}) + \text{var} [\hat{\theta}] = E_D [\hat{\theta}(D)^2] - 2E_D [\hat{\theta}(D)] \theta + \theta^2$$

Moreover:

$$\begin{aligned} \left\| \theta - \hat{\theta}(D) \right\|^2 &= \left\langle \theta - \hat{\theta}(D), \theta - \hat{\theta}(D) \right\rangle \\ &= \left\langle \theta, \theta - \hat{\theta}(D) \right\rangle - \left\langle \hat{\theta}(D), \theta - \hat{\theta}(D) \right\rangle \\ &= \langle \theta, \theta \rangle - \left\langle \theta, \hat{\theta}(D) \right\rangle - \left\langle \hat{\theta}(D), \theta \right\rangle + \left\langle \hat{\theta}(D), \hat{\theta}(D) \right\rangle \\ &= \langle \theta, \theta \rangle - 2 \left\langle \theta, \hat{\theta}(D) \right\rangle + \left\langle \hat{\theta}(D), \hat{\theta}(D) \right\rangle \\ &= \left\langle \hat{\theta}(D), \hat{\theta}(D) \right\rangle - 2 \left\langle \theta, \hat{\theta}(D) \right\rangle + \langle \theta, \theta \rangle \end{aligned}$$

Now, from linearity of E:

$$E_D \left\| \theta - \hat{\theta}(D) \right\|^2 = E_D [\hat{\theta}(D)^2] - 2E_D [\left\langle \theta, \hat{\theta}(D) \right\rangle] + E_D [\theta^2]$$

Because θ is constant with regards to D , E_D is not effected by θ and so

$$E_D \left[\left\| \theta - \hat{\theta}(D) \right\|^2 \right] = E_D [\hat{\theta}(D)^2] - 2E_D [\hat{\theta}(D)] \theta + \theta^2 = \text{bias}^2 (\hat{\theta}) + \text{var} [\hat{\theta}]$$

Q.E.D.

1.1.2 Q2 $\hat{\theta}_a = a \cdot \underset{\tilde{\theta}}{\text{argmin}} \sum_{i=1}^N (y_i - \tilde{\theta})^2$, $\text{MSE} [\hat{\theta}_a] = ?$

First we can compute $\hat{\theta}_a$ by finding the minima of $MD(\tilde{\theta}) \triangleq \sum_{i=1}^N (y_i - \tilde{\theta})^2$ (we know there is such a unique term as $MD(\tilde{\theta})$ is convex). So:

$$\frac{\partial MD(x)}{\partial x} = \frac{\partial}{\partial x} \sum_{i=1}^N (y_i - x)^2 = \sum_{i=1}^N \frac{\partial}{\partial x} (y_i - x)^2 = -2 \sum_{i=1}^N (y_i - x) = 2 \sum_{i=1}^N (x - y_i) = 2 \left(Nx - \sum_{i=1}^N y_i \right)$$

So, $\frac{\partial MD(x)}{\partial x} = 0$ iff $Nx - \sum_{i=1}^N y_i = 0$ iff $x = \sum_{i=1}^N \frac{y_i}{N}$. We get:

$$\hat{\theta}_a = a \cdot \underset{\tilde{\theta}}{\text{argmin}} \sum_{i=1}^N (y_i - \tilde{\theta})^2 = \frac{a}{N} \sum_{i=1}^N y_i$$

Now:

$$E_D \left[\hat{\theta}_a(D) \right] = E_D \left[\frac{a}{N} \sum_{i=1}^N y_i \right] = \frac{a}{N} \sum_{i=1}^N E_D [y_i]$$

Because y_i 's are sampled from θ we get $E_D [y_i] = \theta$ for each i and so:

$$E_D \left[\hat{\theta}_a(D) \right] = \frac{a}{N} \sum_{i=1}^N \theta = \frac{a}{N} N\theta = a\theta$$

And the bias is:

$$\text{bias}(\hat{\theta}) = E_D \left[\hat{\theta}_a(D) \right] - \theta = a\theta - \theta = \theta(a - 1)$$

And so:

$$\text{bias}^2(\hat{\theta}) = \theta^2(a - 1)^2$$

And the variance is:

$$E_D \left[\left(\hat{\theta}_a(D) \right)^2 \right] = E_D \left[\left(\frac{a}{N} \sum_{i=1}^N y_i \right)^2 \right] = \left(\frac{a}{N} \right)^2 E_D \left[\left(\sum_{i=1}^N y_i \right)^2 \right]$$

$$\text{var} \left[\hat{\theta}_a(D) \right] = \text{var} \left[\frac{a}{N} \sum_{i=1}^N y_i \right] = \left(\frac{a}{N} \right)^2 \text{var} \left[\sum_{i=1}^N y_i \right] = \left(\frac{a}{N} \right)^2 \sum_{i=1}^N \text{var} [y_i]$$

Where the last transition is due to the fact the y_i 's are disjoint. Since $y_i \sim N(\theta, \sigma^2)$ we get $\text{var} [y_i] = \sigma^2$ For each i . Hence:

$$\text{var} \left[\hat{\theta}_a(D) \right] = \frac{a^2}{N^2} N\sigma^2 = \frac{a^2\sigma^2}{N}$$

Now, using Q1:

$$\begin{aligned} \text{MSE} \left[\hat{\theta} \right] &= \text{bias}^2(\hat{\theta}) + \text{var} \left[\hat{\theta} \right] \\ &= \theta^2(a - 1)^2 + \frac{a^2\sigma^2}{N} \end{aligned}$$

As $\text{MSE} \left[\hat{\theta} \right]$ depends on a we're left to determine which a is optimal, if any. We look for the extrema:

$$\begin{aligned} \frac{\partial}{\partial a} \text{MSE} \left[\hat{\theta} \right] &= \frac{\partial}{\partial a} \theta^2(a - 1)^2 + \frac{\partial}{\partial a} \frac{a^2\sigma^2}{N} = \theta^2 \frac{\partial}{\partial a} (a - 1)^2 + \frac{\sigma^2}{N} \frac{\partial}{\partial a} a^2 \\ &= \theta^2 \cdot 2(a - 1) + \frac{\sigma^2}{N} \cdot 2a = 2a\theta^2 - 2\theta^2 + \frac{2a\sigma^2}{N} = 2a \left(\theta^2 + \frac{\sigma^2}{N} \right) - 2\theta^2 \end{aligned}$$

Now $\frac{\partial}{\partial a} \text{MSE} \left[\hat{\theta} \right] = 0$ iff

$$a^{MSE} = \frac{2\theta^2}{2 \left(\theta^2 + \frac{\sigma^2}{N} \right)} = \frac{\theta^2}{N\theta^2 + \sigma^2} \cdot \frac{1}{\frac{1}{N}} = \frac{N\theta^2}{N\theta^2 + \sigma^2}$$

Since a^{MSE} is a function of θ , we can't say a single value of a is globally optimal.

1.1.3 Q3 $\text{BMSE}[\hat{\theta}] = \int p(\theta), \text{MSE}[\hat{\theta}] d\theta, \theta \sim N(0, 1)$

Note

$$\text{BMSE}[\hat{\theta}] = E_{\theta}[\text{MSE}[\hat{\theta}]] = E_{\theta}\left[\theta^2(a-1)^2 + \frac{a^2\sigma^2}{N}\right] = (a-1)^2 E_{\theta}[\theta^2] + \frac{a^2\sigma^2}{N}$$

Also, as we can write $p(\theta)$ explicitly and use Wolfram Alpha, we get - $E_{\theta}[\theta^2] = \int p(\theta)\theta^2 d\theta = 1$, than:

$$\text{BMSE}[\hat{\theta}] = (a-1)^2 + \frac{a^2\sigma^2}{N}$$

Again, we look for the max by a:

$$\begin{aligned} \frac{\partial}{\partial a} \text{BMSE}[\hat{\theta}] &= \frac{\partial}{\partial a} (a-1)^2 + \frac{\partial}{\partial a} \frac{a^2\sigma^2}{N} \\ &= 2a - 2 + \frac{2a\sigma^2}{N} = 2a \left(1 - \frac{\sigma^2}{N}\right) - 2 \stackrel{?}{=} 0 \\ \iff a^{MMSE} &= \frac{1}{(1 - \frac{\sigma^2}{N})} = \frac{N}{(N - \sigma^2)} \end{aligned}$$

Hence we can find an optimal a regardless of θ , i.e. a globally optimal a .

1.2 Prior, Likelihood and Posterior

1.2.1 Q4 $\theta \sim U[a, b], y|\theta \sim U([\theta - \delta, \theta + \delta])$

So for a single data point y , we get $p(y|\theta) = \frac{1}{2\delta}$ and - $p(\theta) = \frac{1}{b-a}$. Using Bayes' law:

$$\begin{aligned} p(\theta|y) &= \frac{1}{c} \cdot \begin{cases} \frac{p(y|\theta)}{b-a} & \theta \in [a, b] \\ 0 & \text{else} \end{cases} = \frac{1}{c} \cdot \begin{cases} \frac{1}{2\delta(b-a)} & \theta \in [a, b] \text{ and } y \in [\theta - \delta, \theta + \delta] \\ 0 & \text{else} \end{cases} \\ &= \frac{1}{c} \cdot \begin{cases} \frac{1}{2\delta(b-a)} & a \leq \theta \leq b \text{ and } \theta - \delta \leq y \leq \theta + \delta \\ 0 & \text{else} \end{cases} = \star \end{aligned}$$

As $\theta - \delta \leq y \leq \theta + \delta$ iff $y - \delta \leq \theta \leq y + \delta$ we can rewrite the condition for $p(\theta|y) \neq 0$ as: $\min\{a, y - \delta\} \leq \theta \leq \max\{y + \delta, b\}$. Hence:

$$\star = \frac{1}{c} \cdot \begin{cases} \frac{1}{2\delta(b-a)} & \min\{a, y - \delta\} \leq \theta \leq \max\{y + \delta, b\} \\ 0 & \text{else} \end{cases}$$

Now we know the PDF function holds the condition: $\int_{-\infty}^{\infty} p(\theta|y) d\theta = 1$ so c above must be a normlization factor in the range $[\min\{a, y - \delta\}, \max\{y + \delta, b\}]$ so we can say $p(\theta|y)$ is continues uniform in the range $[\min\{a, y - \delta\}, \max\{y + \delta, b\}]$, i.e.:

$$p(y|\theta) \sim U(\theta | [\min\{a, y - \delta\}, \max\{y + \delta, b\}])$$

1.2.2 Q5 $\theta \sim U[a, b]$, $y|\theta \sim N(\theta, \lambda^2)$

We have - $p(\theta) = \frac{1}{b-a}$ and $p(y|\theta) = \frac{1}{\sqrt{2\pi\lambda^2}} \exp\left(-\frac{1}{2\lambda^2} \|y - \theta\|^2\right)$. Using Bayes' law:

$$p(\theta|y) = \frac{1}{c} \cdot \begin{cases} \frac{1}{b-a} \cdot \frac{1}{\sqrt{2\pi\lambda^2}} \exp\left(-\frac{1}{2\lambda^2} \|y - \theta\|^2\right) & \theta \in [a, b] \\ 0 & else \end{cases}$$

where $c = P(y) = \int_{\theta} p(\theta)p(y|\theta)d\theta$ and because $p(\theta) = 0$ outside the range $[a, b]$ we get:

$$c = \frac{1}{b-a} \int_a^b p(y|\theta)d\theta = \frac{1}{b-a} \int_a^b \frac{1}{\sqrt{2\pi\lambda^2}} \exp\left(-\frac{1}{2\lambda^2} \|y - \theta\|^2\right) d\theta$$

Thus we can write

$$p(\theta|y) = \begin{cases} \frac{N(\theta|y, \lambda^2)}{\int_a^b \frac{1}{\sqrt{2\pi\lambda^2}} \exp\left(-\frac{1}{2\lambda^2} \|y - \theta\|^2\right) d\theta} & \theta \in [a, b] \\ 0 & else \end{cases}$$

1.2.3 Q6 $\theta \sim N(\mu, \sigma^2)$, $y|\theta \sim N(h\theta, \lambda^2)$

We have - $p(\theta) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2} \|\theta - \mu\|^2\right)$ and $p(y|\theta) = \frac{1}{\sqrt{2\pi\lambda^2}} \exp\left(-\frac{1}{2\lambda^2} \|y - h\theta\|^2\right)$. Using Bayes' law:

$$\begin{aligned} p(\theta|y) &= \frac{1}{c} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2} \|\theta - \mu\|^2\right) \frac{1}{\sqrt{2\pi\lambda^2}} \exp\left(-\frac{1}{2\lambda^2} \|y - h\theta\|^2\right) \\ &= \frac{1}{c} \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \frac{1}{\sqrt{2\pi\lambda^2}} \exp\left(-\frac{1}{2\sigma^2} \|\theta - \mu\|^2 - \frac{1}{2\lambda^2} \|y - h\theta\|^2\right) \\ &= \frac{1}{z} \exp(-\Delta) \end{aligned}$$

As Δ is a quadratic term of θ and we saw in the recitation this indicates $p(\theta|y)$ is indeed a Gaussian, we're left to find its mean and variance and can use the derivative trick to do so. So:

$$\begin{aligned} \frac{\partial \Delta}{\partial \theta} &= \frac{1}{\sigma^2} (\theta - \mu) - \frac{h}{\lambda^2} (y - h\theta) \\ &= \frac{\lambda^2 \theta - \lambda^2 \mu - \sigma^2 h y + \sigma^2 h^2 \theta}{(\sigma \lambda)^2} \\ &= \frac{(\lambda^2 + \sigma^2 h^2) \theta - \lambda^2 \mu - \sigma^2 h y}{(\sigma \lambda)^2} \\ &= \frac{(\lambda^2 + \sigma^2 h^2)}{(\sigma \lambda)^2} \left(\theta - \frac{\lambda^2 \mu + \sigma^2 h y}{(\lambda^2 + \sigma^2 h^2)} \right) \end{aligned}$$

Hence -

$$p(\theta|y) \sim N\left(\frac{(\lambda^2 \mu + \sigma^2 h y)}{(\lambda^2 + \sigma^2 h^2)}, \left(\frac{(\lambda^2 + \sigma^2 h^2)}{(\sigma \lambda)^2}\right)^{-1}\right)$$

2 Gaussians

2.1 Sampling from a Multivariate Normal

2.1.1 Q7

First note that - $f^{-1}(y) = A^{-1}(y - b)$. Now:

$$\frac{\partial}{\partial y} f^{-1}(y) = \frac{\partial}{\partial y} A^{-1}(y - b) = \frac{\partial}{\partial y} (y - b) \cdot \frac{\partial}{\partial (y - b)} A^{-1}(y - b) = 1 \cdot A^{-1} = A^{-1}$$

Also:

$$\begin{aligned} p_x(f^{-1}(y)) &= \frac{1}{\sqrt{(2\pi)^d |\Sigma|}} \exp \left(-\frac{1}{2} (f^{-1}(y) - \mu)^T \Sigma^{-1} (f^{-1}(y) - \mu) \right) \\ &= \frac{1}{\sqrt{(2\pi)^d |\Sigma|}} \exp \left(-\frac{1}{2} (A^{-1}(y - b) - \mu)^T \Sigma^{-1} (A^{-1}(y - b) - \mu) \right) \end{aligned}$$

So together:

$$\begin{aligned} p_y(y) &= p_x(f^{-1}(y)) \cdot \left| \frac{\partial}{\partial y} f^{-1}(y) \right| \\ &= \frac{|A|}{\sqrt{(2\pi)^d |\Sigma|}} \exp \left(-\frac{1}{2} (A^{-1}(y - b) - \mu)^T \Sigma^{-1} (A^{-1}(y - b) - \mu) \right) \end{aligned}$$

Denote $\Delta = -\frac{1}{2} (A^{-1}(y - b) - \mu)^T \Sigma^{-1} (A^{-1}(y - b) - \mu)$. As we saw in recitation, in order to show $y \propto N(\mu_y, \Sigma_y)$ it's enough to show ... From the chain rule:

$$\frac{\partial}{\partial y} \Delta = \frac{\partial f^{-1}(y)}{\partial y} \cdot \frac{\partial}{\partial f^{-1}(y)} \Delta$$

We know Δ is the term for the Mahalanobis distance and so $\frac{\partial}{\partial f^{-1}(y)} \Delta = \Sigma^{-1} (f^{-1}(y) - \mu)$ and we already saw $\frac{\partial}{\partial y} f^{-1}(y) = (A^{-1})^T = (A^T)^{-1}$. Together we get:

$$\begin{aligned} \frac{\partial}{\partial y} \Delta &= (A^{-1})^T \Sigma^{-1} (f^{-1}(y) - \mu) = (A^{-1})^T \Sigma^{-1} (A^{-1}(y - b) - \mu) \\ &= (A^{-1})^T \Sigma^{-1} A^{-1} (y - b - A\mu) \end{aligned}$$

So $\mu_y = b - A\mu$ and $\Sigma_y = A\Sigma A^T$. Lastly, we want to make sure Σ_y is indeed a PD. As A is invertible, it is infact a homomorphism from \mathbb{R}^n onto itself. Specifcly, A has a decomposition to eignvalues $\{a_i\}_{i=1}^n$ and the eigenvalues of Σ_y are $\{a_i^2 \lambda_i\}_{i=1}^n$. Since for each i $0 < a_i^2, \lambda_i$ we get that Σ_y is indeed a PD matrix. Hence we can write:

$$\frac{\partial}{\partial y} \Delta = \Sigma_y (y - \mu_y)$$

And so we get that $y \sim N(\mu_y, \Sigma_y)$ is a Gaussian.

2.1.2 Q8

In the terms of Q7 - we have \mathbf{x} as $\mathbf{y} \sim N(\mu_x, \Sigma_x)$, \mathbf{A} is \mathbf{R} for $\Sigma_x = \mathbf{R}\mathbf{R}^T$, \mathbf{b} as μ . we get $\Sigma_x = \mathbf{R}\Sigma_z\mathbf{R}^T = \mathbf{R}\mathbf{I}\mathbf{R}^T = \Sigma$ and $\mu_x = \mathbf{b} - \mathbf{A}\mu_z = \mu - 0$. If we pretend the double meaning of $\mathbf{x}, \mathbf{y}, \mathbf{z}$ here were not confusing, we get that by using $f(\mathbf{z}) = \mathbf{R}\mathbf{z} + \mu$ we're able to move from $N(0, \mathbf{I})$ To $N(\mu, \Sigma)$ ■

2.2 Product of Gaussians

$$x \sim N(\mu, \Sigma)$$

$$\eta \sim N(0, \Gamma)$$

$$y = Hx + \eta$$

2.2.1 Q9 $p(y|x)$

For a fixed \mathbf{x} , \mathbf{y} is an affine transformation of η . Hence - $p(\mathbf{y}|\mathbf{x}) \sim N(H\mathbf{x}, \Gamma)$.

2.2.2 Q10 $p(y)$

$$\begin{aligned} p(x)p(y|x) &= \frac{1}{z_1} \exp \left[-\frac{1}{2}(\mathbf{x} - \mu)^T \Sigma^{-1}(\mathbf{x} - \mu) \right] \cdot \frac{1}{z_2} \exp \left[-\frac{1}{2}(\mathbf{y} - H\mathbf{x})^T \Gamma^{-1}(\mathbf{y} - H\mathbf{x}) \right] \\ &= \frac{1}{z_1 z_2} \exp \left[-\frac{1}{2} \left((\mathbf{x} - \mu)^T \Sigma^{-1}(\mathbf{x} - \mu) + (\mathbf{y} - H\mathbf{x})^T \Gamma^{-1}(\mathbf{y} - H\mathbf{x}) \right) \right] \end{aligned}$$

Now we know $(\mathbf{x} - \mu)^T \Sigma^{-1}(\mathbf{x} - \mu)^T$ is a quadratic form and hence contains quadratic terms of \mathbf{x} . Moreover, $(\mathbf{y} - H\mathbf{x})^T \Gamma^{-1}(\mathbf{y} - H\mathbf{x})^T$ is also a quadratic form, this time of the linear combination $\mathbf{y} - H\mathbf{x}$. Using its linearity we'll get quadratic terms of \mathbf{x}, \mathbf{y} or their product. As we saw in class, having quadratic terms of the vector (\mathbf{x}, \mathbf{y}) in the exponent is enough in order to determine $p(\mathbf{x}, \mathbf{y}) = p(\mathbf{x})p(\mathbf{y}|\mathbf{x})$ is also a Gaussian. In turn, this implies $p(\mathbf{y})$ is also a Gaussian. This infact is enough to describe the distribution as $p(\mathbf{y}) \sim N(E[\mathbf{y}], \text{var}[\mathbf{y}])$. Remember that in exercise 0 we showed $\text{var}(\mathbf{y}) = H\Sigma H^T + \Gamma$ and from form linearity we get $E[\mathbf{y}] = HE[\mathbf{x}] + E[\eta] = H\mu + 0$. Thus we get:

$$\mathbf{y} \sim N(H\mu, H\Sigma H^T + \Gamma)$$

2.2.3 Q11 $p(x|y)$

Using Bayes' law we know $p(\mathbf{x}|\mathbf{y}) \propto p(\mathbf{x})p(\mathbf{y}|\mathbf{x})$. As we already know this is a Gaussian, we can use the derivative trick in order to bring the derivative of the term in the exponent the canonical form and deduce the mean and variance. Denote

$$\Delta = \frac{1}{2} \left((\mathbf{x} - \mu)^T \Sigma^{-1}(\mathbf{x} - \mu) + (\mathbf{y} - H\mathbf{x})^T \Gamma^{-1}(\mathbf{y} - H\mathbf{x}) \right)$$

Then:

$$\begin{aligned}\frac{\partial \Delta}{\partial x} &= \Sigma^{-1}(x - \mu) - H^T \Gamma^{-1}(y - Hx) \\ &= \Sigma^{-1}x - \Sigma^{-1}\mu - H^T \Gamma^{-1}y + H^T \Gamma^{-1}Hx \\ &= (\Sigma^{-1} + H^T \Gamma^{-1}H)x - \Sigma^{-1}\mu - H^T \Gamma^{-1}y \\ &= (\Sigma^{-1} + H^T \Gamma^{-1}H) \left(x - \frac{\Sigma^{-1}\mu + H^T \Gamma^{-1}y}{(\Sigma^{-1} + H^T \Gamma^{-1}H)} \right)\end{aligned}$$

Hence:

$$x \sim N \left[\frac{\Sigma^{-1}\mu + H^T \Gamma^{-1}y}{(\Sigma^{-1} + H^T \Gamma^{-1}H)}, (\Sigma^{-1} + H^T \Gamma^{-1}H)^{-1} \right]$$

Q.E.D.