

## Problem Set 10, Nov 23, 2023 (Solutions to Theory Questions)

### 1 Vector Calculus

1. We have  $\nabla f(\mathbf{x}) = (\mathbf{A} + \mathbf{A}^\top)\mathbf{x} + \mathbf{b}$ . One way to see this is to explicitly expand out the expression. We have

$$f(\mathbf{x}) = \sum_{i,j} A_{i,j} x_i x_j + \sum_i b_i x_i + c.$$

If we now take the derivative with respect to  $x_k$  we get

$$\frac{\partial f(\mathbf{x})}{\partial x_k} = \sum_j A_{k,j} x_j + \sum_i A_{i,k} x_i + b_k.$$

2.  $\nabla^2 f(\mathbf{x}) = \mathbf{A} + \mathbf{A}^\top$ . Taking the derivative of  $\frac{\partial f(\mathbf{x})}{\partial x_k}$ , as given in the previous expression, with respect to  $x_l$  we get

$$\frac{\partial^2 f(\mathbf{x})}{\partial x_k \partial x_l} = A_{k,l} + A_{l,k}.$$

## 2 Maximum Likelihood Principle

1. The likelihood is given by

$$\begin{aligned}\mathbb{P}[X_1, \dots, X_N | \mu, \sigma^2] &= \prod_{n=1}^N \mathbb{P}[X_n | \mu, \sigma^2] \\ &= \prod_{n=1}^N \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(X_n - \mu)^2}{2\sigma^2}\right) \\ &= \left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^N \exp\left(-\frac{\sum_{n=1}^N (X_n - \mu)^2}{2\sigma^2}\right)\end{aligned}$$

2. It might be easier to work with the negative log-likelihood, given by

$$\begin{aligned}-\log \mathbb{P}[X_1, \dots, X_N | \mu, \sigma^2] &= -\log \left[ \left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^N \exp\left(-\frac{\sum_{n=1}^N (X_n - \mu)^2}{2\sigma^2}\right) \right] \\ &= \frac{N}{2} \log(2\pi\sigma^2) + \frac{1}{2\sigma^2} \sum_{n=1}^N (X_n - \mu)^2 \\ &= \frac{N}{2} \log(2\pi) + \frac{N}{2} \log(\sigma^2) + \frac{1}{2\sigma^2} \sum_{n=1}^N (X_n - \mu)^2\end{aligned}$$

The derivative with respect to  $\mu$  is

$$\begin{aligned}-\frac{\partial \log \mathbb{P}[X_1, \dots, X_N | \mu, \sigma^2]}{\partial \mu} &= \frac{1}{2\sigma^2} \frac{\partial \left( \sum_{n=1}^N (X_n^2 - 2X_n\mu + \mu^2) \right)}{\partial \mu} \\ &= \frac{1}{2\sigma^2} \sum_{n=1}^N (-2X_n + 2\mu) \\ &= \frac{1}{\sigma^2} \sum_{n=1}^N (-X_n + \mu)\end{aligned}$$

Setting this expression to 0, we get  $\hat{\mu} = \frac{1}{N} \sum_{n=1}^N X_n$ .

The derivative with respect to  $\sigma^2$  is

$$\begin{aligned}-\frac{\partial \log \mathbb{P}[X_1, \dots, X_N | \mu, \sigma^2]}{\partial \sigma^2} &= \frac{N}{2} \frac{\partial \log(\sigma^2)}{\partial \sigma^2} + \frac{\partial \frac{1}{\sigma^2}}{\partial \sigma^2} \frac{1}{2} \sum_{n=1}^N (X_n - \mu)^2 \\ &= \frac{N}{2} \frac{1}{\sigma^2} - \frac{1}{\sigma^4} \frac{1}{2} \sum_{n=1}^N (X_n - \mu)^2\end{aligned}$$

Setting this expression to 0, and replacing the unknown quantity  $\mu$  by the estimate  $\hat{\mu}$  we get

$$\hat{\sigma}^2 = \frac{1}{N} \sum_{n=1}^N (X_n - \hat{\mu})^2.$$

3. By linearity of expectation, we get  $\mathbb{E}[\hat{\mu}] = \frac{1}{N} \sum_{n=1}^N \mathbb{E}[X_n] = \mu$ . So indeed, this estimate is *unbiased*.

4. We get that

$$\begin{aligned}
\mathbb{E}[\hat{\sigma}^2] &= \mathbb{E} \left[ \frac{1}{N} \sum_{n=1}^N (X_n - \hat{\mu})^2 \right] \\
&= \mathbb{E} \left[ \frac{1}{N} \sum_{n=1}^N ((X_n - \mu) - (\hat{\mu} - \mu))^2 \right] \\
&= \mathbb{E} \left[ \frac{1}{N} \sum_{n=1}^N \left( (X_n - \mu) - \frac{1}{N} \sum_{j=1}^N (X_j - \mu) \right)^2 \right] \\
&= \mathbb{E} \left[ \frac{1}{N} \sum_{n=1}^N \left( \frac{N-1}{N} (X_n - \mu) - \frac{1}{N} \sum_{j \neq n} (X_j - \mu) \right)^2 \right] \\
&= \frac{1}{N} \sum_{n=1}^N \mathbb{E} \left[ \left( \frac{N-1}{N} (X_n - \mu) - \frac{1}{N} \sum_{j \neq n} (X_j - \mu) \right)^2 \right].
\end{aligned}$$

Since the variables  $X_i - \mu$  and  $X_j - \mu$  for  $i \neq j$  are independent and have mean  $= 0$ , we can separate out the expectations as

$$\begin{aligned}
\mathbb{E}[\hat{\sigma}^2] &= \frac{1}{N} \sum_{n=1}^N \mathbb{E} \left[ \left( \frac{N-1}{N} (X_n - \mu) - \frac{1}{N} \sum_{j \neq n} (X_j - \mu) \right)^2 \right] \\
&= \frac{1}{N} \sum_{n=1}^N \mathbb{E} \left[ \left( \frac{N-1}{N} (X_n - \mu) \right)^2 \right] + \frac{1}{N} \sum_{n=1}^N \sum_{j \neq n} \mathbb{E} \left[ \left( \frac{1}{N} (X_j - \mu) \right)^2 \right] \\
&= \frac{(N-1)^2}{N^3} \sum_{n=1}^N \mathbb{E} [(X_n - \mu)^2] + \frac{1}{N^3} \sum_{n=1}^N \sum_{j \neq n} \mathbb{E} [(X_j - \mu)^2] \\
&= \frac{(N-1)^2}{N^3} \sum_{n=1}^N \sigma^2 + \frac{1}{N^3} \sum_{n=1}^N \sum_{j \neq n} \sigma^2 \\
&= \frac{(N-1)^2}{N^2} \sigma^2 + \frac{N-1}{N^2} \sigma^2 \\
&= \frac{N^2 - 2N + 1 - 1 + N}{N^2} \sigma^2 \\
&= \frac{N-1}{N} \sigma^2.
\end{aligned}$$

We see that the ML estimate of the variance is biased (but asymptotically as  $N \rightarrow \infty$  it is unbiased).