Solutions: GPs / NNs Optional Practice Problems

Due: Friday 25/02/22 4pm

Problem 1: Gaussian Process Regression

(a) The mean and covariance of the GP prior are defined by the mean and covariance functions given, and are independent of Y. Thus, the prior will have mean $\begin{bmatrix} 0 & 0 & 0 \end{bmatrix}^T$ and covariance

$$\begin{bmatrix} 4 & 0 & 1 \\ 0 & 4 & 9 \\ 1 & 9 & 25 \end{bmatrix}$$

(b) The GP posterior is defined as a normal distribution with mean and covariance as follows.

$$K(X_*, X)K(X, X)^{-1}Y$$

$$K(X_*, X_*) - K(X_*, X)K(X, X)^{-1}K(X, X_*)$$

where the function $K(X, X')$ defines a matrix K such that $K_{ij} = k(X_i, X'_j)$. Accordingly, the relevant matrices are:

$$Y = \begin{bmatrix} 5 & 5 & 8 \end{bmatrix}^T$$

$$K(X, X) = \begin{bmatrix} 4 & 0 & 1 \\ 0 & 4 & 9 \\ 1 & 9 & 25 \end{bmatrix}$$

$$K(X_*, X) = \begin{bmatrix} 9 & 1 & 9 \\ 1 & 1 & 1 \end{bmatrix} = K(X, X_*)^T$$

$$K(X_*, X_*) = \begin{bmatrix} 25 & 1 \\ 1 & 1 \end{bmatrix}$$

Accordingly, we can compute the posterior mean and covariance, which are (respectively)

$$\begin{bmatrix} 8 & 4 \end{bmatrix}^T$$

$$\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$

which matches exactly to the target values at each of the test points.

Problem 2: RELU-network

(a) To find the decision boundary, we will first express $\sigma(z)$ in terms of x_1, x_2. Using the weights and architecture given:

$$\begin{bmatrix} h_1 \\ h_2 \end{bmatrix} = \begin{bmatrix} 1 & -1 & 0 \\ -1 & -1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ 1 \end{bmatrix}$$

$$h_1 = x_1 - x_2$$

$$h_2 = -x_1 - x_2$$

$$
\begin{aligned}
z &= \begin{bmatrix} 1 & 1 & -2 \end{bmatrix} \begin{bmatrix} f(h_1) \\ f(h_2) \\ 1 \end{bmatrix} \\
&= f(h_1) + f(h_2) - 2
\end{aligned}
$$

Putting this all together, we see that:

$$
\begin{aligned}
t &= \sigma(z) \\
&= \sigma(f(h_1) + f(h_2) - 2) \\
&= \sigma(f(x_1 - x_2) + f(-x_1 - x_2) - 2) \\
&= \frac{1}{1 + e^{-(max(0, x_1 - x_2) + max(0, -x_1 - x_2) - 2)}}
\end{aligned}
$$

If you do this by hand, you can split the equation into the cases in which:

- $x_1 > x_2$ *and* $x_1 + x_2 > 0$
- $x_1 > x_2$ *and* $x_1 + x_2 < 0$
- $x_1 < x_2$ *and* $x_1 + x_2 > 0$
- $x_1 < x_2$ *and* $x_1 + x_2 < 0$

For all of these, you get the following equations:

- $\frac{1}{1+e^{-(x_1 - x_2 - 2)}}$
- $\frac{1}{1+e^{2(x_2+1)}}$
- $\frac{1}{1+e^{2}}$
- $\frac{1}{1+e^{x_1+x_2+2}}$

Graphing this with Wolfram Alpha gives us:

Input:

$$0.5 = \frac{1}{1 + e^{-(\max(0, x-y) + \max(0, -x-y) - 2)}}$$

Implicit plot:

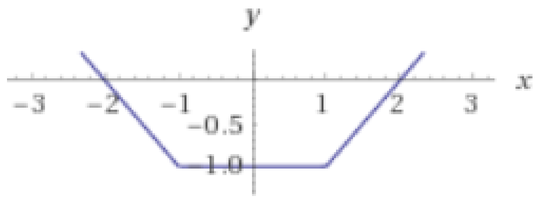

Figure 1: Decision Boundary for the RELU Network

The top is classified negative, and the bottom is positive. (See Part B for more information.)

(b) Plugging values into the equation from Part A, we see that the prediction for the point $\begin{bmatrix} 1 & 1 \end{bmatrix}^T$ is $\frac{1}{1+e^2} \approx 0.11920$. Since this is less than the decision boundary of 0.5, we classify this point as negative.

(c) Notice that $\frac{\partial t}{\partial z} = t(1-t)$

For i=1,2:

$$\frac{\partial l}{\partial v_i} = \frac{\partial l}{\partial t} \cdot \frac{\partial t}{\partial z} \cdot \frac{\partial z}{\partial v_3} = (\frac{-y}{t} + \frac{1-y}{1-t}) \cdot (t \cdot (1-t)) \cdot f(h_i) = (t-y) \cdot f(h_i)$$

For i=3:

$$\frac{\partial l}{\partial v_3} = \frac{\partial l}{\partial t} \cdot \frac{\partial t}{\partial z} \cdot \frac{\partial z}{\partial v_3} = (\frac{-y}{t} + \frac{1-y}{1-t}) \cdot (t \cdot (1-t)) \cdot 1 = t - y$$

For j=1,2:

$$\begin{aligned} \frac{\partial l}{\partial w_{ij}} &= \frac{\partial l}{\partial t} \cdot \frac{\partial t}{\partial z} \cdot \frac{\partial z}{\partial f(h_i)} \cdot \frac{\partial f(h_i)}{\partial h_i} \cdot \frac{\partial h_i}{\partial w_{ij}} \\ &= (\frac{-y}{t} + \frac{1-y}{1-t}) \cdot (t \cdot (1-t)) \cdot v_i \cdot I(h_i > 0) \cdot x_j \\ &= (t-y) \cdot v_i \cdot I(h_i > 0) \cdot x_j \end{aligned}$$

For j=3:

$$\begin{aligned} \frac{\partial l}{\partial w_{i3}} &= \frac{\partial l}{\partial t} \cdot \frac{\partial t}{\partial z} \cdot \frac{\partial z}{\partial f(h_i)} \cdot \frac{\partial f(h_i)}{\partial h_i} \cdot \frac{\partial h_i}{\partial w_{i3}} \\ &= (\frac{-y}{t} + \frac{1-y}{1-t}) \cdot (t \cdot (1-t)) \cdot I \cdot I(h_i > 0) \cdot 1 \\ &= (t-y) \cdot v_i \cdot I(h_i > 0) \end{aligned}$$