

5.17

$$\begin{aligned}
E &= \frac{1}{2} \int \int \{y(\mathbf{x}, \mathbf{w}) - t\}^2 p(\mathbf{x}, t) d\mathbf{x} dt \\
\Rightarrow \frac{\partial E}{\partial w_s} &= \int \int \{y(\mathbf{x}, \mathbf{w}) - t\} \left(\frac{\partial y(\mathbf{x}, \mathbf{w})}{\partial w_s} \right) p(\mathbf{x}, t) d\mathbf{x} dt \\
\Rightarrow \frac{\partial^2 E}{\partial w_r \partial w_s} &= \int \int \left(\left(\frac{\partial y(\mathbf{x}, \mathbf{w})}{\partial w_r} \right) \left(\frac{\partial y(\mathbf{x}, \mathbf{w})}{\partial w_s} \right) \right. \\
&\quad \left. + \{y(\mathbf{x}, \mathbf{w}) - t\} \left(\frac{\partial^2 y(\mathbf{x}, \mathbf{w})}{\partial w_r \partial w_s} \right) \right) p(\mathbf{x}, t) d\mathbf{x} dt \\
&= \int \int \left(\frac{\partial y(\mathbf{x}, \mathbf{w})}{\partial w_r} \right) \left(\frac{\partial y(\mathbf{x}, \mathbf{w})}{\partial w_s} \right) p(\mathbf{x}, t) d\mathbf{x} dt \\
&\quad + \int \int \{y(\mathbf{x}, \mathbf{w}) - t\} \left(\frac{\partial^2 y(\mathbf{x}, \mathbf{w})}{\partial w_r \partial w_s} \right) p(\mathbf{x}, t) d\mathbf{x} dt \\
&= \int \left(\frac{\partial y(\mathbf{x}, \mathbf{w})}{\partial w_r} \right) \left(\frac{\partial y(\mathbf{x}, \mathbf{w})}{\partial w_s} \right) p(\mathbf{x}) d\mathbf{x} \\
&\quad + \int \int y(\mathbf{x}, \mathbf{w}) \left(\frac{\partial^2 y(\mathbf{x}, \mathbf{w})}{\partial w_r \partial w_s} \right) p(\mathbf{x}, t) d\mathbf{x} dt \\
&\quad - \int \int t \left(\frac{\partial^2 y(\mathbf{x}, \mathbf{w})}{\partial w_r \partial w_s} \right) p(\mathbf{x}, t) d\mathbf{x} dt
\end{aligned}$$

Simplifying the second term by integrating out t :

$$\begin{aligned}
&\int \int y(\mathbf{x}, \mathbf{w}) \left(\frac{\partial^2 y(\mathbf{x}, \mathbf{w})}{\partial w_r \partial w_s} \right) p(\mathbf{x}, t) d\mathbf{x} dt \\
&= \int \int y(\mathbf{x}, \mathbf{w}) \left(\frac{\partial^2 y(\mathbf{x}, \mathbf{w})}{\partial w_r \partial w_s} \right) p(\mathbf{x}) d\mathbf{x}
\end{aligned}$$

Simplifying the third term:

$$\int \int t \left(\frac{\partial^2 y(\mathbf{x}, \mathbf{w})}{\partial w_r \partial w_s} \right) p(\mathbf{x}, t) d\mathbf{x} dt$$

$$\begin{aligned}
&= \int \int t \left(\frac{\partial^2 y(\mathbf{x}, \mathbf{w})}{\partial w_r \partial w_s} \right) p(t|\mathbf{x}) p(\mathbf{x}) d\mathbf{x} dt \\
&= \int \left(\frac{\partial^2 y(\mathbf{x}, \mathbf{w})}{\partial w_r \partial w_s} \right) \left(\int t p(t|\mathbf{x}) dt \right) p(\mathbf{x}) d\mathbf{x} \\
&= \int \left(\frac{\partial^2 y(\mathbf{x}, \mathbf{w})}{\partial w_r \partial w_s} \right) \mathbb{E}[t|\mathbf{x}] p(\mathbf{x}) d\mathbf{x}
\end{aligned}$$

From Section 1.5.5, we know that the optimal function that minimizes a sum-of-squares loss is the conditional average of the target data. This means that $y(\mathbf{x}, \mathbf{w}) = \mathbb{E}[t|\mathbf{x}]$.

Therefore, the second and third terms cancel out, and we get:

$$\frac{\partial^2 E}{\partial w_r \partial w_s} = \int \left(\frac{\partial y(\mathbf{x}, \mathbf{w})}{\partial w_r} \right) \left(\frac{\partial y(\mathbf{x}, \mathbf{w})}{\partial w_s} \right) p(\mathbf{x}) d\mathbf{x}$$

which is the result in 5.194 that we wanted.