Deep Learning - Foundations and Concepts

Chapter 4. Single-layer Networks: Regression

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Outline

Basis functions

Consider the linear combinations of fixed nonlinear functions of the input variables:

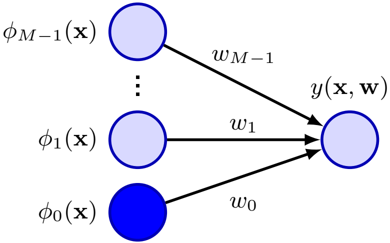
$$y(x;w) = w_0 + \sum_{m=1}^{M-1} w_m \phi_m(x)$$

where $\phi_m(x)$ are known as basis functions. The parameter w_0 allows for any fixed offset in the data and is sometimes called a bias parameter. If we define $\phi_0(x) = 1$ then $y(x;w)$ becomes:

$$y(x;w) = \sum_{m=0}^{M-1} w_m \phi_m(x) = w^T \phi(x)$$

Basis function

Figure: The linear regression model as a single-layer network



Basis function

Here are some possible choices of basis functions:

- Polynomial: $\phi_m(x) = x^m$.
- Gaussian: $\phi_m(x) = \exp(-\frac{(x-\mu_m)^2}{2s^2})$.
- Sigmoidal: $\phi_m(x) = \frac{1}{1+\exp(-\frac{x-\mu_m}{s})}$.

Maximum likelihood

Consider a data set of inputs $\{x^1, \ldots, x^N\}$ with corresponding target values $t_1, \ldots, t_N$. Assume that given the value of x^n, the corresponding value of t_n has a Gaussian distribution. The likelihood function takes the form:

$$p(t_1, \ldots, t_N | x^1, \ldots, x^N; w, \sigma^2) = \prod_{n=1}^{N} \mathcal{N}(t_n; w^T \phi(x^n), \sigma^2 I)$$

The negative log of the likelihood function is given by:

$$\begin{aligned} L &= -\log p(t_1, \ldots, t_N | x^1, \ldots, x^N; w, \sigma^2) \\ &= \frac{N}{2} \log(2\pi) + \frac{N}{2} \log \sigma^2 + \frac{1}{2\sigma^2} \sum_{n=1}^{N} (t_n - w^T \phi(x^n))^2 \end{aligned}$$

Maximum likelihood

Let's maximize the likelihood function (for simplicity, we will denote $\phi(x^n)$ by ϕ_n):

$$\frac{\partial L}{\partial w} = \frac{1}{\sigma^2}(w^T \sum_{n=1}^{N} \phi_n \phi_n^T - \sum_{n=1}^{N} t_n \phi_n^T) = \frac{1}{\sigma^2}(w^T \Phi^T \Phi - t^T \Phi)$$

where:

$$\Phi = \begin{pmatrix} \phi_1 & \phi_2 & \dots & \phi_N \end{pmatrix}^T$$

We see that:

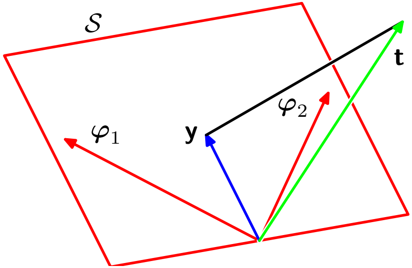
$$w_{ML} = (\Phi^T \Phi)^{-1} \Phi^T t$$

The quantity $(\Phi^T \Phi)^{-1} \Phi^T$ is known as the Moore-Penrose pseudo-inverse of the matrix Φ. It's easy to calculate σ_{ML}^2 as well:

$$\sigma_{ML}^2 = \frac{1}{N} \sum_{n=1}^{N} (t_n - w_{ML}^T \phi_n)^2$$

Geometry of least squares

Figure: Geometrical interpretation of the least squares solution



Geometry of least squares

Let Φ_m be the mth column of the matrix Φ, and let $y_{ML} \in \mathbb{R}^N$ be the best approximation to t we obtained by maximizing the likelihood function:

$$y_{ML} = \begin{pmatrix} w_{ML}^T \phi_1 \\ w_{ML}^T \phi_2 \\ \vdots \\ w_{ML}^T \phi_N \end{pmatrix} = \Phi w_{ML} = \sum_{m=0}^{M-1} (w_{ML})_m \Phi_m$$

Here we clearly see that $y_{ML} \in \mathrm{span}(\Phi_0, \ldots, \Phi_{M-1})$. In addition, we have:

$$\Phi^T y_{ML} = \Phi^T \Phi w_{ML} = (\Phi^T \Phi)(\Phi^T \Phi)^{-1} \Phi^T t = \Phi^T t$$
$$(t - y_{ML})^T \Phi = 0 \qquad (t - y_{ML})^T \Phi_m = 0$$

That is, $t - y_{ML}$ is orthogonal to each Φ_m, or put another way, y_{ML} is the orthogonal projection of t.

Sequential learning

The maximum likelihood estimator for w involves processing the entire training set in one go. Sometimes we want the data points to be considered one at a time and the model parameters updated after each such presentation. The technique of stochastic (sequential) gradient descent:

- The error function comprises a sum over data points: $E = \sum_n E_n$.
- After presentation of data point n, updates the parameter w using: $w^{(\tau+1)} = w^{(\tau)} - \eta \nabla E_n$.
- τ denotes the iteration number, and η is a training rate parameter.

Sequential learning

For the sum-of-squares error function:

$$E_n = \frac{1}{2}(t_n - w^T\phi_n)^2$$
$$\nabla E_n = -(t_n - w^T\phi_n)\phi_n$$
$$w^{(\tau+1)} = w^{(\tau)} + \eta(t_n - (w^{(\tau)})^T\phi_n)\phi_n$$

Regularized least squares

Adding a regularization term to an error function to control over-fitting:

$$E_D(w) + \lambda E_W(w)$$

For example, if we use the sum-of-squares error function, the total error function becomes:

$$\frac{1}{2}\sum_{n=1}^{N}(t_n - w^T\phi_n)^2 + \frac{\lambda}{2}w^T w$$

Minimizing this total error function, we obtain:

$$w_{ML} = (\lambda I + \Phi^T\Phi)^{-1}\Phi^T t$$

Multiple outputs

We have considered situations with a single target variable. In some applications, we may wish to predict $K > 1$ target variables. Let's first get the dimensions right:

- There are N input data: $x^1, \ldots, x^N$, where $x^n \in \mathbb{R}^D$.
- There are N target data: $t^1, \ldots, t^N$, where $t^n \in \mathbb{R}^K$.
  - Let $T = \begin{pmatrix} t_1 & t_2 & \ldots & t_N \end{pmatrix}^T \in \mathbb{R}^{N \times K}$
- There is a basis ϕ: $\mathbb{R}^D \to \mathbb{R}^M$, $x \to \phi(x)$. For simplicity, we denote $\phi(x^n)$ by ϕ_n.
  - Let $\Phi = \begin{pmatrix} \phi_1 & \phi_2 & \ldots & \phi_N \end{pmatrix}^T \in \mathbb{R}^{N \times M}$
- There is a matrix of parameters: $W \in \mathbb{R}^{M \times K}$.

Multiple outputs

Now, let's maximize the likelihood for $y(x; W) = W^T\phi(x)$:

$$\begin{aligned}
L &= -\log p(t^1, \ldots, t^N | x^1, \ldots, x^N; W, \sigma^2) \\
&= -\log \prod_{n=1}^{N} \mathcal{N}(t^n; W^T\phi_n, \sigma^2 I) \\
&= \frac{NK}{2}\log(2\pi\sigma^2) + \frac{1}{2\sigma^2}\sum_{n=1}^{N} ||t^n - W^T\phi_n||^2 \\
\frac{\partial L}{\partial W}(W)H &= \frac{1}{\sigma^2}\sum_{n=1}^{N}(\mathrm{tr}(W^T\phi_n\phi_n^T H) - \mathrm{tr}(t^n\phi_n^T H)) \\
&= \frac{1}{\sigma^2}\mathrm{tr}((W^T\Phi^T\Phi - T^T\Phi)H) \\
W_{ML} &= (\Phi^T\Phi)^{-1}\Phi^T T
\end{aligned}$$

Decision theory

- We have learned from data using maximum likelihood, and the result is a predictive distribution.
- However, for many practical applications we need to predict a specific value.
- In the inference stage, we use the training data to determine a predictive distribution.
- In the decision stage, we use this predictive distribution to determine a specific value.

Decision theory

Problem

Given a predictive distribution $p(t|x)$, determine a specific value $f(x)$, which will be dependent on the input x, that is optimal according to some criterion.

Decision theory

Because we do not know the true value of t, we cannot minimize the loss $L = (f(x) - t)^2$ itself, instead let's minimize the expected loss:

$$E(L) = \iint (f(x) - t)^2 p(x, t) \mathrm{d}x \mathrm{d}t$$

We want to find $f(x)$ that minimizes $E(L)$:

$$\frac{\delta E(L)}{\delta f(x)} = 2 \int (f(x) - t) p(x, t) \mathrm{d}t = 0$$

$$f(x) = \frac{\int t p(x, t) \mathrm{d}t}{\int p(x, t) \mathrm{d}t} = \frac{\int t p(x, t) \mathrm{d}t}{p(x)} = \int t p(t|x) \mathrm{d}t = E(t|x)$$

which is the conditional average of t conditioned on x and is known as the regression function.

Decision theory

Now that we know that the optimal solution is the conditional expectation, we can expand the square term as follows:

$$
\begin{aligned}
(f(x)-t)^2 &= ((f(x)-E(t|x))+(E(t|x)-t))^2 \\
&= (f(x)-E(t|x))^2+2(f(x)-E(t|x))(E(t|x)-t)+(E(t|x)-t)^2
\end{aligned}
$$

Decision theory

Let's examine the expectation for each term:

$$\iint (f(x) - E(t|x))^2 p(x,t)\mathrm{d}x\mathrm{d}t = \int (f(x) - E(t|x))^2 (\int p(x,t)\mathrm{d}t)\mathrm{d}x$$

$$= \int (f(x) - E(t|x))^2 p(x)\mathrm{d}x$$

$$\iint (f(x) - E(t|x))(E(t|x) - t)p(x,t)\mathrm{d}x\mathrm{d}t$$

$$= \int (f(x) - E(t|x))p(x)(\int (E(t|x) - t)p(t|x)\mathrm{d}t)\mathrm{d}x = 0$$

$$\iint (E(t|x) - t)^2 p(x,t)\mathrm{d}x\mathrm{d}t = \int p(x)(\int (t - E(t|x))^2 p(t|x)\mathrm{d}t)\mathrm{d}x$$

$$= \int \mathrm{var}(t|x)p(x)\mathrm{d}x$$

Decision theory

Let's interpret what we have derived here:

$$E(L) = \int (f(x) - E(t|x))^2 p(x) \mathrm{d}x + \int \mathrm{var}(t|x) p(x) \mathrm{d}x$$

- The first term shows that the optimal least-squares predictor is given by the conditional expectation.
- The second term is the variance of t averaged over x, and represents the intrinsic variability of the target data.