

Chapter 4 Linear Model

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This part corresponds to **Chapter 1,3,4 of PRML, Chapter of UML**, and mainly answers the following questions:

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1 Linear classification

In the last chapter, we stop at the linear classification of binary classification task,

$$y = h(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + w_0 = \sum_{j=1}^d w_j x_j + w_0 \quad (1)$$

in which \mathbf{w} is weight vector, and w_0 is bias. The input vector is assigned to class C_1 iff. $h(\mathbf{x}) \geq 0$ and to class C_2 otherwise.

Consider two points $\mathbf{x}_1, \mathbf{x}_2$ on the decision boundary, i.e., $\mathbf{w}^\top (\mathbf{x}_1 - \mathbf{x}_2) = 0$, hence \mathbf{w} is orthogonal to the decision boundary. And the distance from the origin to the decision boundary is

$$\frac{\mathbf{w}^\top \mathbf{x}}{\|\mathbf{w}\|} = \frac{-w_0}{\|\mathbf{w}\|} \quad (2)$$

It is usually convenient to use a more compact notation in which we introduce an additional input value $x_0 = 1$ and then define $\tilde{\mathbf{w}} = (w_0, \mathbf{w})$ and $\tilde{\mathbf{x}} = (x_0, \mathbf{x})$ so that $h(\mathbf{x}) = \tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}$. For simplification, we neglect the ‘tilde’ symbol below.

1.1 Extend to multiple classes

- *one-versus-the-rest* For each class $k = 1, 2, \dots, K$, each classifier judge whether an example is C_k or not. So there are K classifiers needed.
- *one-versus-one* An alternative is to introduce $K(K-1)/2$ binary discriminant functions, one for every pair of classes (but will lead to ambiguous region).

1.2 Fisher’s linear discriminant

One way to view a linear classification model is in terms of dimensionality reduction. By adjusting the components of the weight vector \mathbf{w} , we can select a projection that maximizes the class separation. To begin with, consider a two-class problem in which there are N_1 points of class C_1 and N_2 points of class C_2 , so that the mean vectors of the two classes are given by

$$\mathbf{m}_1 = \frac{1}{N_1} \sum_{\mathbf{x}_n \in C_1} \mathbf{x}_n, \quad \mathbf{m}_2 = \frac{1}{N_2} \sum_{\mathbf{x}_n \in C_2} \mathbf{x}_n \quad (3)$$

The simplest measure of the separation of the classes, when projected onto \mathbf{w} , is the separation of the projected class means. This suggests that we might choose w so as to maximize

$$m_2 - m_1 = \mathbf{w}^\top (\mathbf{m}_2 - \mathbf{m}_1) \quad (4)$$

where $m_k = \mathbf{w}^\top \mathbf{m}_k$ is the mean of the projected data from class C_k .

This expression can be made arbitrarily large simply by increasing the magnitude of \mathbf{w} . To solve this problem, we could constrain \mathbf{w} to have unit length, i.e., $\|\mathbf{w}\|_2 = 1$. Using a Lagrange multiplier, it turns to maximize $\mathbf{w}^\top (\mathbf{m}_2 - \mathbf{m}_1) + \lambda(1 - \|\mathbf{w}\|_2^2)$, which leads to $\mathbf{w} \propto \mathbf{m}_2 - \mathbf{m}_1$

2 Linear regression

In linear regression model, the model is the same except that the learning target y is continuous but not discrete. And the learning goal is the sum-of-square (SSE) loss

$$\min_{\mathbf{w}} L_S(h) = \sum_{i=1}^m (h(\mathbf{x}_i) - y_i)^2 = \sum_{i=1}^m (\mathbf{w}^\top \mathbf{x}_i - y_i)^2 \quad (5)$$

Suppose the fitting error $\epsilon_i = y_i - \mathbf{w}^\top \mathbf{x}_i$ is Gaussian noise, i.e., $\epsilon_i \sim \mathcal{N}(0, \beta)$. Then the log likelihood function of the training sequence is

$$\log \mathcal{L} = -\frac{m}{2} \log 2\pi\beta - \sum_{i=1}^m \frac{(y_i - \mathbf{w}^\top \mathbf{x}_i)^2}{2\beta} \quad (6)$$

Obviously, MLE is equivalent to linear regression.

remark1: Since linear regression is not a binary prediction task, we cannot analyse its sample complexity using the VC-dimension. One possible analysis of the sample complexity of linear regression is by relying on the "discretization trick". However, to apply the sample complexity bounds from Chapter 2 we also need that the loss function will be bounded.

2.1 Generalized linear regression

The model is just a linear function of the input variables, and this imposes significant limitations on it. Therefore, extended model considers **linear** combination of fixed **non-linear** functions of the input variables, of the form

$$h(\mathbf{x}) = w_0 + \sum_{j=1}^d w_j \phi_j(x) \quad (7)$$

where $\phi_j(x)$ are known as *basis functions*. Again, denote $\phi_0(\mathbf{x}) = 1$ so that $h(\mathbf{x}) = \tilde{\mathbf{w}}^\top \phi(\mathbf{x})$. For Simplification, we also neglect the 'tilde' symbol from now on.

Now, consider the closed-form solution for The gradient of the log likelihood. The gradient of the SSE loss takes the form

$$\nabla L_S(h) = \sum_{i=1}^m \{y_i - \mathbf{w}^\top \phi(\mathbf{x}_i)\} \phi^\top(\mathbf{x}_i)$$

Setting it to zero gives

$$\mathbf{w} = \Phi^\dagger \mathbf{y} = (\Phi^\top \Phi)^{-1} \Phi^\top \mathbf{y} \quad (8)$$

Here Φ is an $n \times d$ matrix, whose elements are given by $\Phi_{nj} = \Phi_j(\mathbf{x}_n)$. And Φ^\dagger is *Moore-Penrose pseudo-inverse*.

remark2, multiple-outputs: A more general case is multiple outputs, i.e., $\mathbf{y}_i \in \mathcal{R}^k, k > 1$. However, the solution to multiple-outputs regression problem decouples between the different target variables so we do not discuss it here.

remark3, on-line learning: Batch techniques involve processing the entire training set in one go, can be computationally costly for large data sets. For linear regression, stochastic gradient descent algorithm updates parameter using

$$\mathbf{w}^{t+1} = \mathbf{w}^t - lr * \nabla L_{(\mathbf{x}_t, y_t)}(h) = \mathbf{w}^t + lr * (y_i - (\mathbf{w}^t)^\top \phi(\mathbf{x}_t)) \phi(\mathbf{x}_t)$$

in which lr is the learning rate.

remark3, basis: There are three popular basis function: 1. **Polynomial basis**, 2. **Radical basis**, 3. **Fourier basis**.

2.2 Regularization *a.k.a* Bayesian linear regression

Recall the closed-form solution (Eq. 8) for linear regression problem, over-fitting

2.2.1 Ridge regression

Ridge regression addresses on over-fitting by penalizing the l_2 -norm of weight vector \mathbf{w} ,

$$\min_{\mathbf{w}} \sum_{i=1}^m (\mathbf{w} \phi_i(\mathbf{x}) - y_i)^2 + \lambda \|\mathbf{w}\|_2^2$$

If we assume a Gaussian prior for the weight vector, $\mathbf{w} \sim \mathcal{N}(0, \alpha^{-1} \mathbf{I})$, then the posterior of the training sequence is:

$$p(\mathbf{w}|S) \propto p(\mathbf{w})p(S|\mathbf{w}) \propto \exp\left(-\frac{\alpha}{2} \mathbf{w}^\top \mathbf{w}\right) \cdot \prod_{i=1}^N \exp\left(-\frac{(y_i - \mathbf{w} \mathbf{x}_i)^2}{2\beta}\right) \quad (9)$$

Maximizing the log posterior function is equivalent to the ridge regression.

2.2.2 Lasso

Lasso addresses on over-fitting by penalizing the l_1 -norm of weight vector \mathbf{w} ,

$$\min_{\mathbf{w}} \sum_{i=1}^m (\mathbf{w} \phi_i(\mathbf{x}) - y_i)^2 + \lambda \|\mathbf{w}\|_1$$

If we assume a Laplace prior for the weight vector, $p(\mathbf{w}) = \frac{1}{2\alpha} \exp\left(-\frac{\|\mathbf{w}\|_1}{\alpha}\right)$, then the posterior of the training sequence is:

$$p(\mathbf{w}|S) \propto p(\mathbf{w})p(S|\mathbf{w}) \propto \exp\left(-\frac{\|\mathbf{w}\|_1}{\alpha}\right) \cdot \prod_{i=1}^N \exp\left(-\frac{(y_i - \mathbf{w}\mathbf{x}_i)^2}{2\beta}\right) \quad (10)$$

Maximizing the log posterior function is equivalent to the Lasso model.

remark2:

