Deep Learning - Foundations and Concepts

Chapter 5. Single-layer Networks: Classification

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Outline

1 Discriminant Functions

2 Decision Theory

3 Generative Classifiers

Discriminant functions

- The goal in classification is to take an input vector $x \in \mathbb{R}^D$ and assign it to one of K discrete classes $\mathcal{C}_k$.
- A discriminant is a function that takes an input vector x and assigns it to one of K classes, denoted $\mathcal{C}_k$.
- We will restrict attention to linear discriminants, for which the decision surfaces are hyperplaines.

Two classes

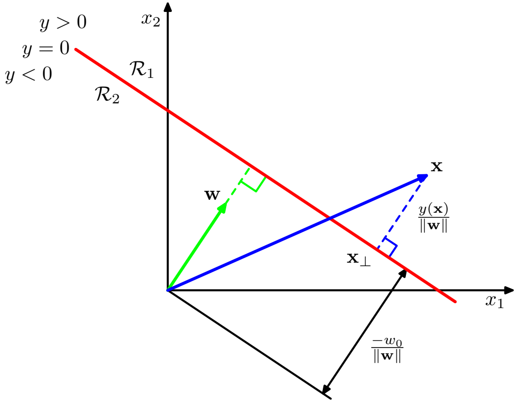
Taking a linear function of the input vector:

$$y(x) = w^T x + w_0$$

- An input vector is assigned to class $\mathcal{C}_1$ if $y(x) \geq 0$ and to class $\mathcal{C}_2$ otherwise.
- The decision boundary is a $(D-1)$-dimensional hyperplane.

Two classes

Figure: The geometry of a linear discriminant function in two dimensions



Two classes

It's easy to see that:

- w is orthogonal to the decision surface.
- w points to the direction of the increase of y.

Also the value of $y(x)$ gives a signed measure of the perpendicular distance r of the point x from the decision surface:

$$
\begin{aligned}
x &= x_\perp + r\frac{w}{||w||} \\
y(x) &= w^T x + w_0 = w^T x_\perp + w_0 + r||w|| = r||w|| \\
r &= \frac{y(x)}{||w||}
\end{aligned}
$$

In particular, the signed distance of the origin from the decision surface is given by $\frac{w_0}{||w||}$.

Multiple classes

Building a K-class discriminant by combining a number of two-class discriminant functions usually doens't work:

- One-versus-the-rest.
- One-versus-one.

Multiple classes

Consider a single K-class discriminant comprising K linear functions of the form:

$$y_k(x) = w_k^T x + w_{k0}$$

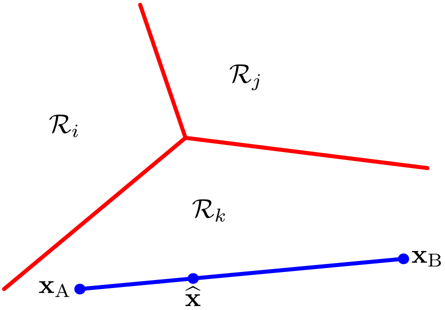
Assign a point x to class $\mathcal{C}_k$ if $y_k(x) > y_j(x)$ for all $j \neq k$. The decision boundary between class $\mathcal{C}_k$ and $\mathcal{C}_j$ is given by $y_k(x) = y_j(x)$ and corresponds to a $(D-1)$-dimensional hyperplane:

$$(w_k - w_j)^T x + (w_{k0} - w_{j0}) = 0$$

The decision regions of such a discriminant are always singly connected and convex.

Multiple classes

Figure: The decision regions for a multi-class linear discriminant



Linear squares for classification

Consider a general classification problem with K classes:

- There are N input data: $x^1, \ldots, x^N$, where $x^n \in \mathbb{R}^D$.
- There are N target data: $t^1, \ldots, t^N$ using a 1-of-K binary coding scheme, thus $t^n \in \mathbb{R}^K$.
  - Let $T = \begin{pmatrix} t^1 & t^2 & \ldots & t^N \end{pmatrix}^T \in \mathbb{R}^{N \times K}$.
- Each class $\mathcal{C}_k$ is described by its own linear model so that $y_k(x) = w_k^T x + w_{k0}$.
  - Let $\tilde{w}_k = \begin{pmatrix} w_{k0} \\ w_k \end{pmatrix}$ and $\tilde{W} = \begin{pmatrix} \tilde{w}_1 & \tilde{w}_2 & \ldots & \tilde{w}_K \end{pmatrix} \in \mathbb{R}^{(D+1) \times K}$.
  - Let $\tilde{x} = \begin{pmatrix} 1 \\ x \end{pmatrix}$ and $\tilde{X} = \begin{pmatrix} \tilde{x}^1 & \tilde{x}^2 & \ldots & \tilde{x}^N \end{pmatrix}^T \in \mathbb{R}^{N \times (D+1)}$.
  - Then $y_k(x) = \tilde{w}_k^T \tilde{x}$ and $y(x) = \tilde{W}^T \tilde{x}$.

Linear squares for classification

Let's determine the parameter matrix $\tilde{W}$ by minimizing a sum-of-squares error function:

$$
\begin{aligned}
E_D(\tilde{W}) &= \frac{1}{2}\sum_{i,j}(\tilde{X}\tilde{W} - T)_{ij}^2 \\
&= \frac{1}{2}\mathrm{tr}((\tilde{X}\tilde{W} - T)^T(\tilde{X}\tilde{W} - T)) \\
DE_D(\tilde{W})H &= \mathrm{tr}((\tilde{X}\tilde{W} - T)^T\tilde{X}H) \\
\tilde{W}_* &= (\tilde{X}^T\tilde{X})^{-1}\tilde{X}^T T
\end{aligned}
$$

Linear squares for classification

What property does $y(x) = \tilde{W}_*^T \tilde{x}$ has? Because t^n is using a 1-of-K binary coding scheme, we know:

$$\begin{pmatrix} 1 & 1 & \dots & 1 \end{pmatrix} t^n = 1$$

Thus we have:

$$\begin{aligned}
\begin{pmatrix} 1 & 1 & \dots & 1 \end{pmatrix} y(x) &= \begin{pmatrix} 1 & 1 & \dots & 1 \end{pmatrix} \tilde{W}_*^T \tilde{x} \\
&= \begin{pmatrix} 1 & 1 & \dots & 1 \end{pmatrix} T^T \tilde{X} (\tilde{X}^T \tilde{X})^{-1} \tilde{x} \\
&= \begin{pmatrix} 1 & 1 & \dots & 1 \end{pmatrix} \tilde{X} (\tilde{X}^T \tilde{X})^{-1} \tilde{x} \\
&= \mathrm{e}_1^T \tilde{X}^T \tilde{X} (\tilde{X}^T \tilde{X})^{-1} \tilde{x} = \mathrm{e}_1^T \tilde{x} = 1
\end{aligned}$$

That is, the predictions made by the model will have the property that the elements of $y(x)$ will sum to 1 for any value of x.

Linear squares for classification

- The model outputs cannot be interpreted as probabilities because they are not contrained to lie within the interval $(0, 1)$.
- If the true distribution of the data is markedly different from being Gaussian, the least squares can give poor results.
- Least squares is very sensitive to the presence of outliers (a.k.a., lack robustness).

Misclassification rate

To minimize the chance of assigning x to the wrong class, intuitively we would choose the class having the higher posterior probability.

- Divide the input space into regions $\mathcal{R}_k$ called decision regions.
- All points in $\mathcal{R}_k$ are assigned to class $\mathcal{C}_k$.

We want to maximize the probability of being correct:

$$p(\text{correct}) = \sum_{k=1}^{K} p(x \in \mathcal{R}_k, \mathcal{C}_k) = \sum_{k=1}^{K} \int_{\mathcal{R}_k} p(\mathcal{C}_k|x)p(x)\mathrm{d}x$$

It's easy to see that this is maximized when the regions $\mathcal{R}_k$ are chosen such that each x is assigned to the class for which $p(\mathcal{C}_k|x)$ is largest. So the intuition is indeed correct.

Expected loss

- Sometimes, our objective will be more complex than minimizing the number of misclassifications.
- We can introduce a loss function which measure loss incurred in taking any of the available decisions or actions and minimize the total loss.

If the true class for x is $\mathcal{C}_k$ and we assign x to $\mathcal{C}_j$, we incur some level of loss denoted by L_{kj}. Because we do not know the true class, instead of minimizing the loss function, we minimize its average:

$$E(L) = \sum_k \sum_j \int_{\mathcal{R}_j} L_{kj} p(x, \mathcal{C}_k) \mathrm{d}x = \sum_j \int_{\mathcal{R}_j} \sum_k L_{kj} p(\mathcal{C}_k|x) p(x) \mathrm{d}x$$

The decision rule that minimizes the expected loss assigns x to the class j for which $\sum_k L_{kj} p(\mathcal{C}_k|x)$ is a minimum.

The reject option

- Classification errors arise when the largest of the posterior probabilities is significantly less than 1.
- Reject option: Avoid making decisions on such cases to obtain a lower error rate.
- Introduce a threshold θ and reject inputs x when the largest of the posterior probabilities is less than or equal to θ:
  - $\theta = 1$: All examples are rejected.
  - $\theta < \frac{1}{K}$: No examples are rejected.

Inference and decision

There are three distinct approaches to solving decision problems:

- Generative models:
  - Solve the inference problem of determining the class-conditional densities $p(x|\mathcal{C}_k)$.
  - Infer the prior class probabilities $p(\mathcal{C}_k)$.
  - Find the posterior class probabilities $p(\mathcal{C}_k|x) = \frac{p(x|\mathcal{C}_k)p(\mathcal{C}_k)}{p(x)}$.
  - Use decision theory to determine the class membership for each new input x.
- Discriminative models:
  - Solve the inference problem of determining the posterior class probabilities $p(\mathcal{C}_k|x)$.
  - Use decision theory to assign each new x to one of the classes.
- Discriminant functions:
  - Find a function that maps each input x directly onto a class label.

Inference and decision

There are many reasons for wanting to compute the posterior probabilities:

- Minimizing risk: What if the loss matrix are subjected to revision from time to time?
- Reject option.
- Compensating for class priors: What if one class occupies 99.9% of the cases (we want a balanced data set to find a more accurate model)?
- Combining models:
  - Combine the outputs of smaller models use the rules of probability.
  - Models can easily be made differentiable with respect to adjustable parameters, which allows them to be composed and trained jointly.

Classifier accuracy

Consider a cancer screening example:

- True positive: The classifier predicts that a person has cancer and is correct.
- False positive (type 1 errors): The classifier predicts that a person has cancer and is wrong.
- True negative: The classifier predicts that a person does not have cancer and is correct.
- False negative (type 2 errors): The classifier predicts that a person does not have cancer and is wrong.

Classifier accuracy

$$
\begin{aligned}
\text{Accuracy} &= \frac{N_{TP} + N_{TN}}{N_{TP} + N_{FP} + N_{TN} + N_{FN}} \\
\text{Precision} &= \frac{N_{TP}}{N_{TP} + N_{FP}} \\
\text{Recall} &= \frac{N_{TP}}{N_{TP} + N_{FN}} \\
\text{False positive rate} &= \frac{N_{FP}}{N_{FP} + N_{TN}} \\
\text{False discovery rate} &= \frac{N_{FP}}{N_{FP} + N_{TP}}
\end{aligned}
$$

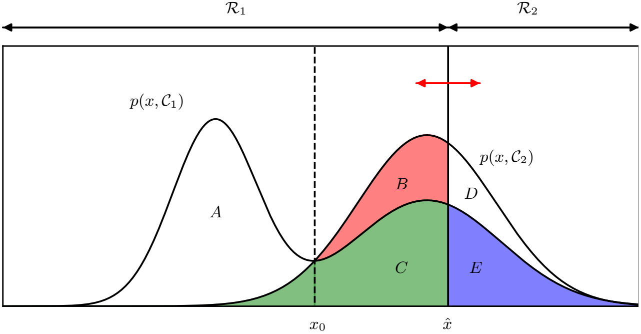
ROC curve

There is a trade-off between type 1 errors and type 2 errors. To better understand this trade-off, it is useful to plot the ROC (receiver operating characteristic) curve:

- x-axis: $\text{False positive rate} = \frac{N_{FP}}{N_{FP}+N_{TN}}$.
- y-axis: $\text{True positive rate} = \frac{N_{TP}}{N_{TP}+N_{FN}}$.

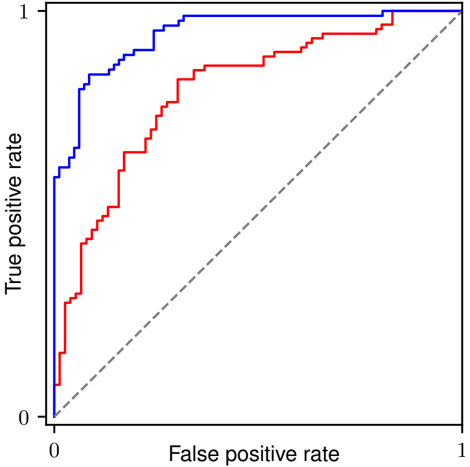
ROC curve

Figure: As the decision boundary is moved from ∞ to $-\infty$, the ROC curve is traced out



ROC curve

Figure: The ROC (receiver operating characteristic) curve



ROC curve

Some observations:

- The bottom left corner represents a classifier that always outputs negative.
- The top left corner represents the best possible classifier.
- The top right corner represents a classifier that always outputs positive.
- The diagonal line represents a simple random classifier.

Sometimes it is useful to have a single number that characterises the whole ROC curve:

- The AUC (area under the curve):
  - 0.5: Random guessing.
  - 1.0: Perfect classifier.
- The F-score: $F = \frac{2\times\text{precision}\times\text{recall}}{\text{precision}+\text{recall}} = \frac{2N_{TP}}{2N_{TP}+N_{FP}+N_{FN}}$.

Activation functions

In linear regression, the model prediction is given by:

$$y(x; w) = w^T x + w_0$$

which gives a continuous-valued output in the range $(-\infty, +\infty)$. For classification problems, we wish to predict posterior probabilities in the range $(0, 1)$, which could be achieved using an activation function:

$$y(x; w) = f(w^T x + w_0)$$

We see that the decision surfaces are linear functions of x. For this reason, these models are called generalized linear models.

Activation functions

For two classes, we can use the logistic sigmoid function $\sigma(a) = \frac{1}{1+\exp(-a)}$ as the activation function:

$$p(\mathcal{C}_1|x) = \sigma(a(x)) = \frac{1}{1+\exp(-a(x))}$$

Compare with:

$$\begin{aligned} p(\mathcal{C}_1|x) &= \frac{p(x|\mathcal{C}_1)p(\mathcal{C}_1)}{p(x|\mathcal{C}_1)p(\mathcal{C}_1) + p(x|\mathcal{C}_2)p(\mathcal{C}_2)} \\ &= \frac{1}{1+\frac{p(x|\mathcal{C}_2)p(\mathcal{C}_2)}{p(x|\mathcal{C}_1)p(\mathcal{C}_1)}} \end{aligned}$$

We see that:

$$a(x) = \log \frac{p(x|\mathcal{C}_1)p(\mathcal{C}_1)}{p(x|\mathcal{C}_2)p(\mathcal{C}_2)}$$

Activation functions

The softmax function is defined by:

$$\mathrm{softmax}(a) = \frac{1}{\sum_{k=1}^{K} \exp(a_k)} \begin{pmatrix} \exp(a_1) \\ \vdots \\ \exp(a_K) \end{pmatrix}$$

For multiple classes, we can use the softmax function as the activation function:

$$\begin{pmatrix} p(\mathcal{C}_1|x) \\ \vdots \\ p(\mathcal{C}_K|x) \end{pmatrix} = \mathrm{softmax}(a_1(x), \ldots, a_K(x))$$

Compare with:

$$p(\mathcal{C}_k|x) = \frac{p(x|\mathcal{C}_k)p(\mathcal{C}_k)}{\sum_j p(x|\mathcal{C}_j)p(\mathcal{C}_j)}$$

We see that:

$$a_k(x) = \log(p(x|\mathcal{C}_k)p(\mathcal{C}_k))$$

Continuous inputs

Let's assume that the class-conditional densities are Guassian. To start with, we will assume that all classes share the same covariance matrix Σ:

$$p(x|\mathcal{C}_k) = \frac{1}{(2\pi)^{\frac{D}{2}}(\det\Sigma)^{\frac{1}{2}}}\exp(-\frac{1}{2}(x-\mu_k)^T\Sigma^{-1}(x-\mu_k))$$

We will see that this lead to generalized linear models.

Continuous inputs

For two classes:

$$p(\mathcal{C}_1|x) = \sigma(a(x))$$

where:

$$\begin{aligned} a(x) &= w^T x + w_0 \\ w &= \Sigma^{-1}(\mu_1 - \mu_2) \\ w_0 &= -\frac{1}{2}\mu_1^T \Sigma^{-1}\mu_1 + \frac{1}{2}\mu_2^T \Sigma^{-1}\mu_2 + \log \frac{p(\mathcal{C}_1)}{p(\mathcal{C}_2)} \end{aligned}$$

Continuous inputs

For multiple classes:

$$\begin{pmatrix} p(\mathcal{C}_1|x) \\ \vdots \\ p(\mathcal{C}_K|x) \end{pmatrix} = \mathrm{softmax}(a_1(x), \ldots, a_K(x))$$

where:

$$\begin{aligned} a_k(x) &= w_k^T x + w_{k0} \\ w_k &= \Sigma^{-1}\mu_k \\ w_{k0} &= -\frac{1}{2}\mu_k^T \Sigma^{-1}\mu_k + \log p(\mathcal{C}_k) \end{aligned}$$

Maximum likelihood solution

- There are N input data: $x^1, \ldots, x^N$, where $x^n \in \mathbb{R}^D$.
- There are N target data: $t^1, \ldots, t^N$ using a 1-of-K binary coding scheme, thus $t^n \in \mathbb{R}^K$.
- The total number of data points in class $\mathcal{C}_k$ is denoted by N_k.
- Prior class probabilities are denoted by $\pi_k = p(\mathcal{C}_k)$.
- Class-conditional densities are Gaussian: $p(x|\mathcal{C}_k) = \mathcal{N}(x; \mu_k, \Sigma)$.

Maximum likelihood solution

$$p(t^n|x^n) = \prod_{k=1}^{K} p(\mathcal{C}_k|x^n)^{t_k^n} = \prod_{k=1}^{K} (\frac{p(x^n|\mathcal{C}_k)\pi_k}{p(x^n)})^{t_k^n}$$

$$= \frac{1}{p(x^n)} \prod_{k=1}^{K} \pi_k^{t_k^n} \prod_{k=1}^{K} \mathcal{N}(x^n; \mu_k, \Sigma)^{t_k^n}$$

$$-\log p(t^n|x^n) = -\sum_{k=1}^{K} t_k^n \log \pi_k$$

$$+ \frac{1}{2} \log \det \Sigma + \frac{1}{2} \sum_{k=1}^{K} t_k^n (x^n - \mu_k)^T \Sigma^{-1} (x^n - \mu_k)$$

$$+ \log p(x^n) + \frac{D}{2} \log 2\pi$$

Maximum likelihood solution

$$
\begin{aligned}
L &= -\log p(t^1, \ldots, t^N | x^1, \ldots, x^N) = -\sum_{n=1}^{N} \log p(t^n | x^n) \\
&= -\sum_{k=1}^{K} N_k \log \pi_k \\
&+ \frac{N}{2} \log \det \Sigma + \frac{1}{2} \sum_{k=1}^{K} \sum_{n=1}^{N} t_k^n (x^n - \mu_k)^T \Sigma^{-1} (x^n - \mu_k) \\
&+ \sum_{n=1}^{N} \log p(x^n) + \frac{ND}{2} \log 2\pi
\end{aligned}
$$

Maximum likelihood solution

$$\frac{\partial L}{\partial \pi_k} = \frac{N_K}{\pi_K} - \frac{N_k}{\pi_k} \qquad \pi_k = \frac{N_k}{N}$$

$$\frac{\partial L}{\partial \mu_k} = (N_k \mu_k - \sum_{x^n \in \mathcal{C}^k} x^n)^T \Sigma^{-1} \qquad \mu_k = \frac{1}{N_k} \sum_{x^n \in \mathcal{C}_k} x^n$$

$$\frac{\partial L}{\partial \Lambda}(\Lambda)H = \frac{1}{2}\mathrm{tr}((\sum_{k=1}^{K} \sum_{x^n \in \mathcal{C}_k} (x^n - \mu_k)(x^n - \mu_k)^T - N\Sigma)H)$$

$$\Sigma = \sum_{k=1}^{K} \frac{N_k}{N} S_k \qquad S_k = \frac{1}{N_k} \sum_{x^n \in \mathcal{C}_k} (x^n - \mu_k)(x^n - \mu_k)^T$$

Discrete features

Suppose $x \in \mathbb{R}^D$ is a feature vector, where each feature $x_d \in \{0, 1\}$. And further suppose that the different features are independent when conditioned on the class $\mathcal{C}_k$. So we have:

$$p(x|\mathcal{C}_k) = \prod_{d=1}^{D} p(x_d|\mathcal{C}_k) = \prod_{d=1}^{D} \mu_{dk}^{x_d}(1 - \mu_{dk})^{1-x_d}$$

Using a softmax activation function, we see that:

$$a_k(x) = \sum_{d=1}^{D}(x_d \log \mu_{dk} + (1 - x_d)\log(1 - \mu_{dk})) + \log p(\mathcal{C}_k)$$

which again are linear functions of the input values x.

Exponential family

If the class-conditional densities $p(x|\mathcal{C}_k)$ are members of the subset of the exponential family of distributions given by:

$$p(x|\mathcal{C}_k; \lambda_k, s) = \frac{1}{s} h(\frac{1}{s} x) g(\lambda_k) \exp(\frac{1}{s} \lambda_k^T x)$$

the resulting model will be a generalized linear model. For two classes using the logistic sigmoid activation function:

$$a(x) = \frac{1}{s}(\lambda_1 - \lambda_2)^T x + \log \frac{g(\lambda_1)}{g(\lambda_2)} + \log \frac{p(\mathcal{C}_1)}{p(\mathcal{C}_2)}$$

For multiple classes using the softmax activation function:

$$a_k(x) = \frac{1}{s} \lambda_k^T x + \log g(\lambda_k) + \log p(\mathcal{C}_k)$$