Tian Han

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Week 5

- Generative and discriminative approach
- Linear Discriminant Function
- The Perceptron Algorithm
- Gradient Descent and its Variants.

Generative vs Discriminative

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- **Learning stage**: build model $p(C_k|\mathbf{x})$, C_k is the k-th class.
- **Decision stage**: use the obtained posterior $p(C_k|\mathbf{x})$ (together with the possible risk function) to make optimal decision/classification.

- Directly learn the class posterior probability $p(C_k|\mathbf{x})$.
- Logistic regression in last lecture.

Generative vs Discriminative

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Generative Approach

- Learn the class condition density $p(\mathbf{x}|C_k)$
- Estimate the class prior $P(C_k)$
- Use Bayes formula to get **class posterior**:

$$p(C_k|\mathbf{x}) = \frac{p(\mathbf{x}|C_k)P(C_k)}{p(x)}$$

where

$$p(x) = \sum_{k=1}^{K} p(\mathbf{x}|C_k) P(C_k)$$

Linear Discriminant Function

The Perceptron Algorithm

Two-class Discriminant Function

Recall we use *probabilistic discriminative* approach for classification by directly model the posterior $p(C_1|\mathbf{x})$ using some parametric form. (e.g., logistic regression, $p(C_1|\mathbf{x}) = \sigma(\mathbf{w}^T\mathbf{x})$)

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The simplest one would be *linear* discriminant function:

$$y(\mathbf{x}) = w_1 x_1 + w_2 x_2 + \dots + w_D x_D + w_0$$
$$= \mathbf{w}^T \mathbf{x} + w_0$$

where w is the weight vector, w_0 is the bias.

Two-class Discriminant Function

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where \mathbf{w} is the weight vector, w_0 is the bias.

Goal: classify x:

$$\mathbf{x} \rightarrow C_1$$
, if $y(\mathbf{x}) \ge 0$
 $\mathbf{x} \rightarrow C_2$, if $y(\mathbf{x}) < 0$

Given two vectors: $\mathbf{u} = (u_1, \dots, u_D)$ and $\mathbf{v} = (v_1, \dots, v_D)$, their dot product:

$$\mathbf{u} \cdot \mathbf{v} = <\mathbf{u}, \mathbf{v}> = \sum_{i=1}^{D} u_i v_i$$

- u, v in the same direction, the dot product grows large and positive.
- u, v in the opposite direction, the dot product grows large and negative.
- u, v perpendicular, dot product is zero.

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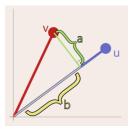


Figure: [from CIML]

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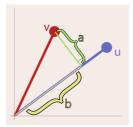


Figure: [from CIML]

The length of b is exactly $\mathbf{u} \cdot \mathbf{v} = 0.734$

Dot product as projections:

dot product between \mathbf{u} and \mathbf{v} is the "projection of \mathbf{v} onto \mathbf{u} ".

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Geometric Interpretation of decision boundary

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Think weight as vector w, then the decision boundary is simply the plane **perpendicular to** w. (on board)

From perspective of classification, the *scale* of the weight w is irrelevant. Really matters is the **SIGN** of $\mathbf{w}^T \mathbf{x} = \sum_{i=1}^{D} w_i x_i$.

Therefore, its common to work with **normalized** weight vector w which have length 1, i.e., $||\mathbf{w}|| = 1$.

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Therefore, its common to work with **normalized** weight vector \mathbf{w} which have length 1, i.e., $||\mathbf{w}|| = 1$.

Question: for any vector w, how to make it normalized?

Value $\mathbf{w} \cdot \mathbf{x}$ is just the distance of \mathbf{x} from the origin when projected onto the vector w. So can be considered as one-dimensional data. (on board)

Bias term as shift

Previously, without bias term (i.e., $w_0 = 0$), the threshold would be 0:

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- If w_0 is positive, the boundary is shift away w.
- If w_0 is negative, the boundary is shift towards w.

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

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The decision boundary between C_k and C_i is given by $y_k(\mathbf{x}) = y_i(\mathbf{x})$, i.e.,

$$(\mathbf{w}_k - \mathbf{w}_j)^T \mathbf{x} + (w_{k0} - w_{j0}) = 0$$

Geometry of decision region

- If x is D-dimensional, then decision boundary is (D-1)-dimensional hyperplane.
- The decision regions of linear discriminant are singly connected and convex.

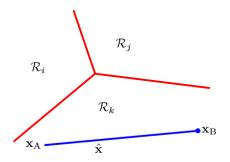


Figure: [Bishop 2006]

The Perceptron Algorithm •000000000

Perceptron Algorithm

Basic Settings

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Given N observations:
$$\{(\mathbf{x}_i, t_i), i = 1, \dots, N\}$$
, $t_i \in \{-1, +1\}$

The Perceptron Algorithm 000000000

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Build model:

$$y = sign(\mathbf{w}^T \mathbf{x})$$
$$= \begin{cases} +1, & \text{if } \mathbf{w}^T \mathbf{x} > 0 \\ -1, & \text{if } \mathbf{w}^T \mathbf{x} < 0 \end{cases}$$

• $\mathbf{w} = (w_0, w_1, \dots, w_D)^T$, $\mathbf{x} = (1, x_1, \dots, x_D)^T$

The Perceptron Algorithm 000000000

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Goal:

- Learn optimal/best \mathbf{w}^* from N observation to have minimum classification error.
- Make prediction: given new x, predict class using $sign(\mathbf{w}^{\star T}\mathbf{x})$

Key Observation

The Perceptron Algorithm 000000000

Note that:

$$t_i(\mathbf{w}^T\mathbf{x}_i) > 0 \iff \mathbf{x}_i \text{ is correctly classified}$$

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Note that:

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- Correctly classified means x_i is in the correct side of the hyperplane defined by w.
- Only valid when we define $t_i \in \{-1, 1\}$.
- If $t_i(\mathbf{w}^T\mathbf{x}_i) \leq 0$, what does it tell you?

Perceptron Algorithm [Rosenblatt 1957]

The Perceptron Algorithm 000000000

- 1. Initialize weight vector w, and set $\tau = 1$
- 2. Loop over the training data: given (\mathbf{x}_i, t_i) , if $t_i(\mathbf{w}^T \mathbf{x}_i) \leq 0$ (i.e., **mistake has been made**), then update w:
 - Mistake on positive, $\mathbf{w}^{(\tau+1)} \leftarrow \mathbf{w}^{(\tau)} + \mathbf{x}_i$
 - Mistake on negative. $\mathbf{w}^{(\tau+1)} \leftarrow \mathbf{w}^{(\tau)} \mathbf{x}_i$
 - Equivalently: $\mathbf{w}^{(\tau+1)} \leftarrow \mathbf{w}^{(\tau)} + t_i \mathbf{x}_i$
- 3. $\tau \leftarrow \tau + 1$ (going over whole dataset again and again, until no mistake)

Error-driven Learning

The Perceptron Algorithm 0000000000

The perceptron algorithm is error-driven, meaning that:

- If an element x is correctly classified with current model w, we do nothing about weight w.
- If an element x is misclassified using current model, we update weight w:

$$\mathbf{w} = \begin{cases} \mathbf{w} + \mathbf{x} & \text{if } \mathbf{x} \text{ from positive (t=+1) was classified to negative (-1)} \\ \mathbf{w} - \mathbf{x} & \text{if } \mathbf{x} \text{ from negative (t=-1) was classified to positive (+1)} \end{cases}$$

Error-driven learning

The goal of update is to adjust the parameters \mathbf{w} so that they are better for the current example.

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The Perceptron Algorithm 0000000000

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• 1^{st} case: x in positive class (+1) was classified as negative class (-1). The correct answer is (+1), which corresponds to: $\mathbf{w}^T \mathbf{x} > 0$, but we have $\mathbf{w}^T \mathbf{x} < 0$. We update \mathbf{w} to be $\mathbf{w}' = \mathbf{w} + \mathbf{x}$. then:

$$\mathbf{w}'^T\mathbf{x} = (\mathbf{w} + \mathbf{x})^T\mathbf{x} = \mathbf{w}^T\mathbf{x} + \mathbf{x}^T\mathbf{x} = \mathbf{w}^T\mathbf{x} + ||\mathbf{x}||^2$$
 because $||\mathbf{x}||^2 > 0$, so $\mathbf{w}'^T\mathbf{x} > \mathbf{w}^T\mathbf{x}$.

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• $\mathbf{2}^{nd}$ case: \mathbf{x} in negative class (-1) was classified as positive class (+1). The correct answer is (-1), which corresponds to: $\mathbf{w}^T\mathbf{x} < 0$, but we have $\mathbf{w}^T\mathbf{x} > 0$. We update \mathbf{w} to be $\mathbf{w}' = \mathbf{w} - \mathbf{x}$, then:

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The Perceptron Algorithm 0000000000

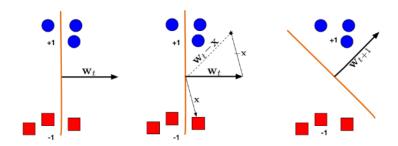


Figure: [Cornell cs4780]

Percetron: summary

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The Perceptron Algorithm 0000000000

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 Convergence theorem: regardless of the initial choice of weights, if the two classes are *linearly separable*, there exists w such that:

$$\begin{cases} \mathbf{w}^T \mathbf{x} > 0 & \text{if } \mathbf{x}_k \text{ in positive class} \\ \mathbf{w}^T \mathbf{x} \leq 0 & \text{if } \mathbf{x}_k \text{ in negative class} \end{cases}$$

then the learning rule will find such solution after a finite number of steps.

The Perceptron Algorithm 000000000

- The percetron algorithm can be successful if we have linearly separable classes.
- Examples:

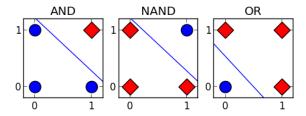


Figure: [Figures from Yue CS559-19S]

Power and Limitation

Non-linear separable dataset in general cannot computed by percetron algorithm. For example, the XOR problem (Minsky 1969).

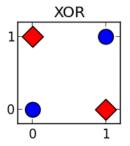


Figure: [Figure from Yue CS559-19S]

Recall:

 In previous chapter, we use probabilistic framework to describe models (e.g., linear regression, logistic regression etc) parameterized by w and given training set $\{(\mathbf{x}_1,t_1),(\mathbf{x}_2,t_2),\ldots,(\mathbf{x}_N,t_N)\}$, we learn such model using maximum likelihood or bayesian estimation.

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 - For linear regression, maximize likelihood is equivalent to minimize the sum-of-square loss function
 - For bayesian linear regression, maximize the posterior is equivalent to minimize the sum-or-square loss and the additional regularization term.
- Learn parameter w by minimizing (or maximizing) some loss functions.

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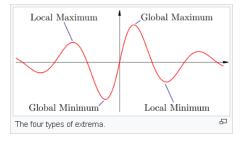


Figure: [From Wikibooks]

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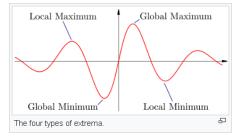


Figure: [From Wikibooks]

 Goal: (1) find the global optimum (feasible when objective function is convex), (2) find the "good" local optimum (in most non-convex problems and deep learning).

• Minimize loss $L(\mathbf{w})$, where the underlying model (i.e., hypothesis) is parameterized by w.

Gradient Descent

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- First-order optimization algorithm. More advanced techniques exist but may need second-order derivative information.

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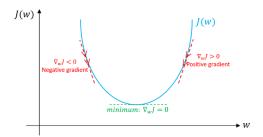


Figure: [From I. Dabbura]

• Initialization \mathbf{w}_0 :

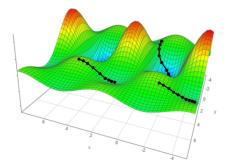


Figure: [From Offconvex.org]

• Learning rate η_{τ} :

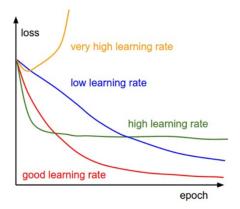


Figure: [From stanford cs231n]

Three types based on number of training data used for updating parameter w: suppose $\{(\mathbf{x}_1,t_1),(\mathbf{x}_2,t_2),\ldots,(\mathbf{x}_N,t_N)\}$

Variants of gradient descent

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• Batch gradient descent: use all data.

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 Mini-batch gradient descent: use relative small batch of data (e.g., batch size bs could be 16, 64 etc)

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta_{\tau} \nabla L(\mathbf{w}; \mathbf{x}_{i:bs}, t_{i:bs})$$

Variants of gradient descent

Three types based on number of training data used for updating parameter \mathbf{w} : suppose $\{(\mathbf{x}_1,t_1),(\mathbf{x}_2,t_2),\ldots,(\mathbf{x}_N,t_N)\}$

• Batch gradient descent: use **all** data.

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta_{\tau} \nabla L(\mathbf{w}; \mathbf{x}_{1:N}, t_{1:N})$$

 Mini-batch gradient descent: use relative small batch of data (e.g., batch size bs could be 16, 64 etc)

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• Stochastic gradient descent: use only **one** example (e.g., $\{\mathbf{x}_i, t_i\}$)

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 - Can be quite slow to converge, large variance for gradient estimation.

Illustration

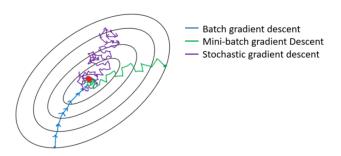


Figure: [From I. Dabbura]

SGD for linear regression

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- Equivalently, minimize the cross-entropy loss function:

$$L(\mathbf{w}) = -\sum_{i=1}^{N} [t_i \log y_i + (1 - t_i) \log(1 - y_i)]$$
$$y_i = \sigma(\mathbf{w}^T \mathbf{x}_i)$$

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$$l(\mathbf{w}; \mathbf{x}_i, t_i) = -[t_i \log y_i + (1 - t_i) \log(1 - y_i)]$$

SGD for logistic regression

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- However, above loss function cannot be optimized using gradient based learning methods (e.g., SGD).
- Perceptron criterion:

$$L(\mathbf{w}) = -\sum_{i=1}^{N} t_i(\mathbf{w}^T \mathbf{x}_i) \mathbb{I}(y_i \neq t_i)$$

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- Take learning rate $\eta_{\tau} = 1$, we get the perceptron algorithm discussed before.
 - If make mistake on positive example \mathbf{x}_i , $\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} + \mathbf{x}_i$.
 - If make mistake on negative example \mathbf{x}_i , $\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} \mathbf{x}_i$.

Part of the slides are based on A course in Machine Learning. Part of the materials are inspired by *Princeton COS495 S16*. Some figures are from *Cornell cs 4780*.