CS-E4710 Machine Learning: Supervised Methods

Lecture 4: Linear classification

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Course topics

- Part I: Theory
  - Introduction
  - Generalization error analysis & PAC learning
  - Rademacher Complexity & VC dimension
- Part II: Algorithms and models
  - **Linear classification**
  - Support vector machines
  - Kernel methods
  - Boosting
  - Neural networks (MLPs)
- Part III: Additional learning models
  - Feature learning, selection and sparsity
  - Multi-class classification
  - Preference learning, ranking
  - Multi-output learning

Linear classification

Linear classification

- Input space $X \subset \mathbb{R}^d$, each $\mathbf{x} \in X$ is a d-dimensional real-valued vector, output space: $\mathcal{Y} = \{-1, +1\}$
- Target function or concept $f : X \mapsto \mathcal{Y}$ assigns a (true) label to each example
- Training sample $S = \{(x_1, y_1), \ldots, (x_m, y_m)\}$, with $y_i = f(x_i)$ drawn from an unknown distribution D
- Hypothesis class $\mathcal{H} = \{\mathbf{x} \mapsto \operatorname{sgn}\left(\sum_{j=1}^d w_j x_j + b\right) | \mathbf{w} \in \mathbb{R}^d, b \in \mathbb{R}\}$ consists of functions $h(\mathbf{x}) = \operatorname{sgn}\left(\sum_{j=1}^d w_j x_j + b\right)$ that map each example in one of the two classes
- $\operatorname{sgn}(a) = \begin{cases} +1, & a \geq 0 \\ -1 & a < 0 \end{cases}$ is the sign function

Linear classifiers

Linear classifiers

$$h(\mathbf{x}) = \operatorname{sgn}\left(\sum_{j=1}^{d} w_j x_j + b\right)$$

have several attractive properties

- They are fast to evaluate and takes small space to store ($O(d)$ time and space)
- Easy to understand: $|w_j|$ shows the importance of variable x_j and its sign tells if the effect is positive or negative
- Linear models have relatively low complexity (e.g. $VCdim = d + 1$) so they can be reliably estimated from limited data

Good practise is to try a linear model before something more complicated

Generalizing a linear model

We can generalize the linear model by considering pairwise interactions of variables

- Let w_{ij} be the importance of the product $x_i x_j$
- The model

  $$g(\mathbf{x}) = \sum_{i=1}^{d} \sum_{j=1}^{d} w_{ij} x_i x_j + \sum_{j=1}^{d} w_j x_j + w_0$$

  is now a **quadratic function**
- However, we have now $O(d^2)$ parameters to estimate, affecting time and space complexity, and generally requires more data in order to achieve low generalization error

Basis functions

Alternatively we can generalize a linear model through using non-linear basis functions in the original

- A basis function $\phi(\mathbf{x}) : X \mapsto \mathbb{R}$ computes a non-linear transformation of the original data
- Through the use of basis functions we can write model as

$$g(\mathbf{x}) = \sum_{k=1}^{d} w_k \phi_k(\mathbf{x})$$

- The model is a linear model in the new space defined by the basis functions
- But it can represent a **non-linear model** in the original space, e.g. choose $\phi_k(\mathbf{x}) = x_i x_j$ where $k = d(i-1) + j$, to obtain a quadratic model

Basis functions

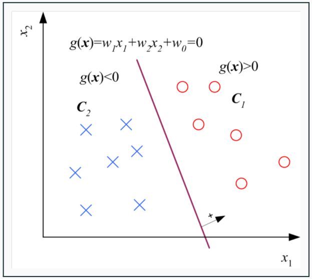
There is a wide variety of potentially useful basis functions, for example:

- Polynomials of degree k: $\phi(\mathbf{x}) = x_{i_1} x_{i_2} \cdots x_{i_k}$ where $1 \leq i_j \leq d$
- Radial basis functions: $\phi(\mathbf{x}) = \exp(-(\mathbf{x} - \mathbf{m})/c)$
- Rectilinear functions: $\phi(\mathbf{x}) = \max(0, \mathbf{a}^T \mathbf{x} + b)$
- In signal processing: Wavelet and Fourier basis functions

Basis functions are important building block of neural networks and kernel-based models

The geometry of the linear classifier

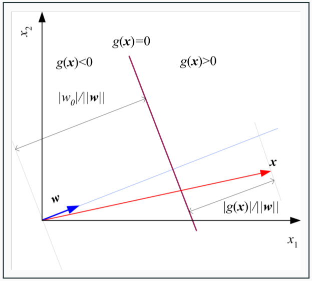
- The points $\{\mathbf{x} \in X | g(\mathbf{x}) = \mathbf{w}^T\mathbf{x} - b = 0\}$ define a hyperplane in $\mathbb{R}^d$, where d is the number of variables in $\mathbf{x}$
- The hyperplane $g(\mathbf{x}) = \mathbf{w}^T\mathbf{x} - b = 0$ splits the input space into two half-spaces. The linear classifier predicts $+1$ for points in the halfspace $\{\mathbf{x} \in X | g(\mathbf{x}) = \mathbf{w}^T\mathbf{x} - b \geq 0\}$ and -1 for points in $\{\mathbf{x} \in X | g(\mathbf{x}) = \mathbf{w}^T\mathbf{x} - b < 0\}$



In the figure $w_0 = -b$

The geometry of the linear classifier

- **w** is the **normal vector** of the hyperplane $\mathbf{w}^T\mathbf{x} - b = 0$
- The distance of the hyperplane from the origin is $|b| / \|\mathbf{w}\|$
- If $b < 0$ the hyperplane lies in the direction of **w** from origin, otherwise it lies in the direction of $-\mathbf{w}$
- The distance of a point **x** from the hyperplane is $|g(\mathbf{x})| / \|\mathbf{w}\|$
- If $g(\mathbf{x}) > 0$, **x** lies in the halfspace that is in the direction of **w** from the hyperplane, otherwise it lies in the direction of $-\mathbf{w}$ from the hyperplane



In the figure $w_0 = -b$

Learning linear classifiers

Change of representation

- Consider learning the parameters of the linear discriminant $g(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0$
- For presentation is is convenient to subsume term w_0 into the weight vector

$$\mathbf{w} \Leftarrow \begin{bmatrix} \mathbf{w} \\ w_0 \end{bmatrix}$$

  and augment all inputs with a constant 1:

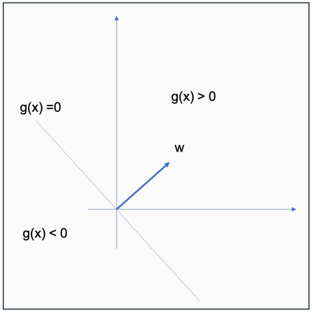
$$\mathbf{x} \Leftarrow \begin{bmatrix} \mathbf{x} \\ 1 \end{bmatrix}$$

- The models have the same value for the discriminant:

$$\begin{bmatrix} \mathbf{w} \\ w_0 \end{bmatrix}^T \begin{bmatrix} \mathbf{x} \\ 1 \end{bmatrix} = \mathbf{w}^T\mathbf{x} + w_0$$

Geometric interpretation

- Geometrically, the hyperplane defined by the discriminant goes now through origin
- The positive points have an **acute angle** with $\mathbf{w}$: $\mathbf{w}^T\mathbf{x} > 0$
- The negative points have an **obtuse angle** with $\mathbf{w}$: $\mathbf{w}^T\mathbf{x} <= 0$



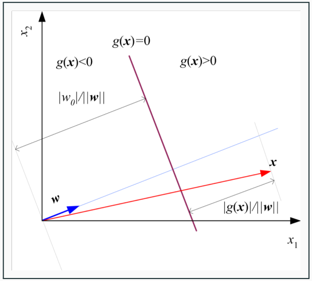
Checking for prediction errors

- When the labels are $\mathcal{Y} = \{-1, +1\}$ for a training example $(\mathbf{x}, y)$ we have for $g(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$,
  $\operatorname{sgn}(g(\mathbf{x})) = \begin{cases} y & \text{if } \mathbf{x} \text{ is correctly classified} \\ -y & \text{if } \mathbf{x} \text{ is incorrectly classified} \end{cases}$
- Alternative we can just multiply with the correct label to check for misclassification:

$$yg(\mathbf{x}) = \begin{cases} \geq 0 & \text{if } \mathbf{x} \text{ is correctly classified} \\ < 0 & \text{if } \mathbf{x} \text{ is incorrectly classified} \end{cases}$$

Margin

- The geometric margin of an example $\mathbf{x}$ is given by $\gamma(\mathbf{x}) = yg(\mathbf{x}) / \|\mathbf{w}\|$
- It takes into account both the distance $|\mathbf{w}^T\mathbf{x}| / \|\mathbf{w}\|$ from the hyperplane, and whether $\mathbf{x}$ is on the correct side of the hyperplane
- The unnormalized version of the margin is sometimes called the **functional margin** $\gamma(\mathbf{x}) = yg(\mathbf{x})$
- Often the term **margin** is used for both variants, assuming the context makes clear which one is meant



The perceptron algorithm

- The perceptron algorithm (Rosenblatt, 1958) a learns a hyperplane separating two classes
$$g(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$$
- It processes incrementally a set of training examples
    - At each step, it finds a training example $\mathbf{x}_i$ that is incorrectly classified by the current model
    - It updates the model by adding the example to the current weight vector together with the label: $\mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} + y_i\mathbf{x}_i$
    - This process is continued until incorrectly predicted training examples are not found

The perceptron algorithm

```
**Input:** Training set $S = \{(\mathbf{x}_i, y_i)\}_{i=1}^m, \mathbf{x} \in \mathbb{R}^d, y \in \{-1, +1\}$
  Initialize $w^{(1)} \leftarrow (0, \dots, 0), t \leftarrow 1$, $stop \leftarrow FALSE$
  repeat
    if exists $i$, s.t. $y_i {\mathbf{w}^{(t)}}^T \mathbf{x}_i \leq 0$ then
      $\mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} + y_i \mathbf{x}_i$
    else
      $stop \leftarrow TRUE$
    end if
    $t \leftarrow t + 1$
  until $stop$
```

Understanding the update rule

- Let us examine the update rule

$$\mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} + y_i\mathbf{x}_i$$

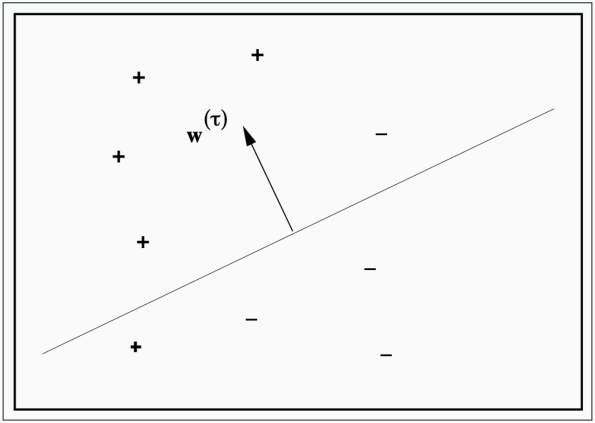
- We can see that the margin of the example $(\mathbf{x}_i, y_i)$ increases after the update

$$\begin{aligned} y_i g^{(t+1)}(\mathbf{x}_i) &= y_i {\mathbf{w}^{(t+1)}}^T\mathbf{x}_i = y_i(\mathbf{w}^{(t)} + y_i\mathbf{x}_i)^T\mathbf{x}_i \\ &= y_i {\mathbf{w}^{(t)}}^T\mathbf{x}_i + y_i^2\mathbf{x}_i^T\mathbf{x}_i = y_i g^{(t)}(\mathbf{x}_i) + \|\mathbf{x}_i\|^2 \\ \geq y_i g^{(t)}(\mathbf{x}_i) \end{aligned}$$

- Note that this does not guarantee that $y_i g^{(t+1)}(\mathbf{x}_i) > 0$ after the update, further updates may be required to achieve that

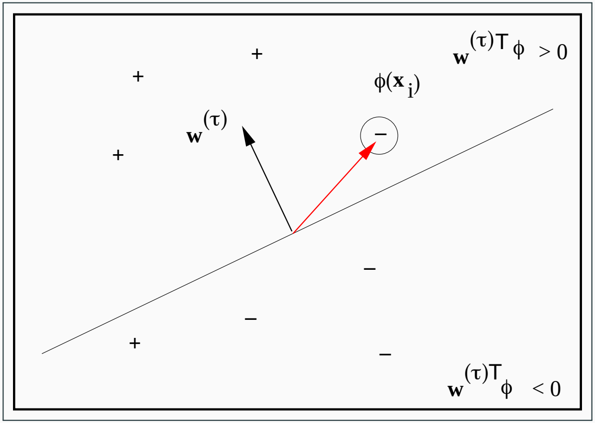
Perceptron animation

- Assume $\mathbf{w}^{(t)}$ has been found by running the algorithm for t steps
- We notice two misclassified examples



Perceptron animation

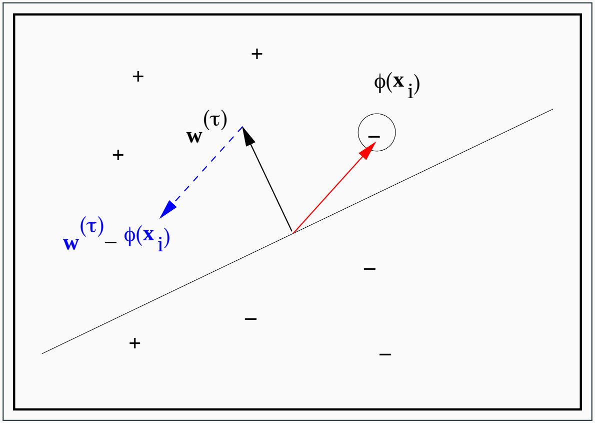
- Select the misclassified example $(\phi(\mathbf{x}_i), -1)$
- Note: $\phi(\mathbf{x}_i)$ is here some transformation of $\mathbf{x}_i$ e.g. with some basis functions but it could be identity $\phi(\mathbf{x}) = \mathbf{x}$



$\mathbf{w}^{(\tau)T}\phi > 0$
$\phi(\mathbf{x}_i)$
$\mathbf{w}^{(\tau)}$
$\mathbf{w}^{(\tau)T}\phi < 0$

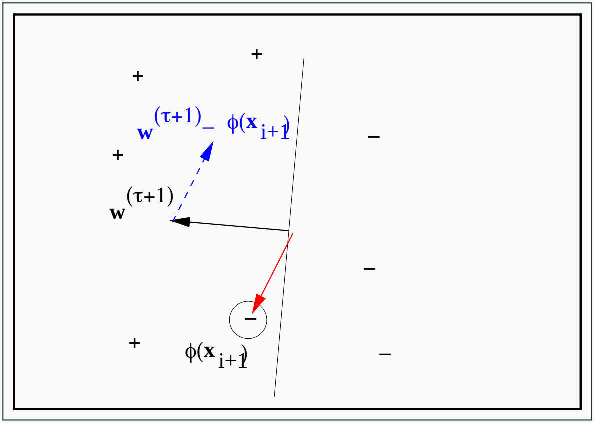
Perceptron animation

- Update the weight vector: $\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} + y_i \phi(\mathbf{x}_i)$



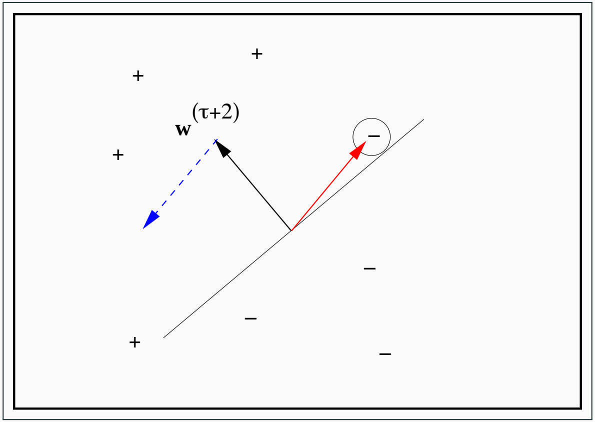
Perceptron animation

- The update tilts the hyperplane to make the example "more correct", i.e. more negative
- We repeat the process by finding the next misclassified example $\phi(\mathbf{x}_{i+1})$ and update: $\mathbf{w}^{(t+2)} = \mathbf{w}^{(t+1)} + y_{i+1}\phi(\mathbf{x}_{i+1})$



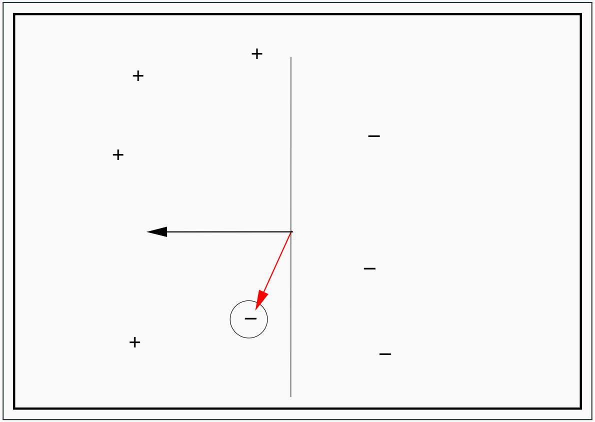
Perceptron animation

- Next iteration



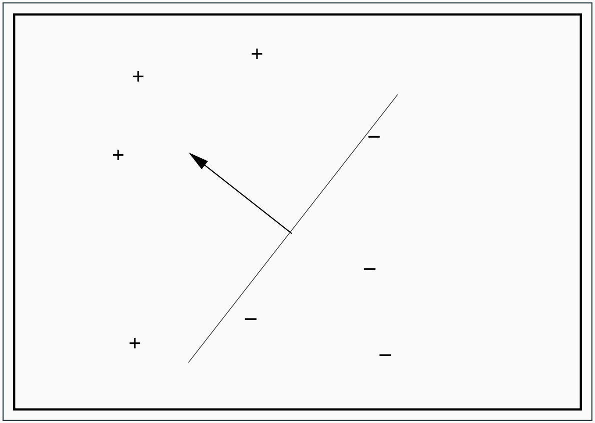
Perceptron animation

- Next iteration



Perceptron animation

- Finally we have found a hyperplane that correctly classify the training points
- We can stop the iteration and output the final weight vector

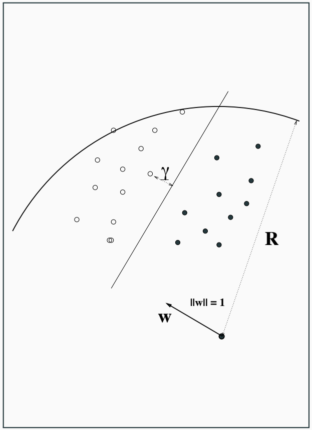


Convergence of the perceptron algorithm

- The perceptron algorithm can be shown to eventually converge to a consistent hyperplane if the two classes are **linearly separable**, that is, if there exists a hyperplane that separates the two classes
- Theorem (Novikoff):
    - Let $S = \{(\mathbf{x}_i, y_i)\}_{i=1}^{m}$ be a linearly separable training set.
    - Let $R = \max_{\mathbf{x}_i \in S} \|\mathbf{x}_i\|$.
    - Let there exist a vector $\mathbf{w}_*$ that satisfies $\|\mathbf{w}_*\| = 1$ and $y_i \mathbf{w}_*^T \mathbf{x}_i + b_{opt} \geq \gamma$ for $i = 1 \ldots, m$.
    - Then the perceptron algorithm will stop after at most $t \leq (\frac{2R}{\gamma})^2$ iterations and output a weight vector $\mathbf{w}^{(t)}$ for which $y_i \mathbf{w}^{(t)} \mathbf{x}_i \geq 0$ for all $i = 1 \ldots, m$

Convergence of the perceptron algorithm

- The number of iterations in the bound $t \leq (\frac{2R}{\gamma})^2$ depend on
  - γ: The largest achievable geometric margin so that all training examples have at least that margin
  - R: The smallest radius of the d-dimensional ball that encloses the training data
  - Intuitively: how large the margin in is relative to the distances of the training points



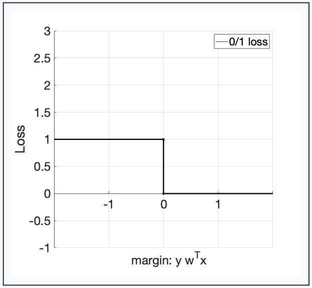
The non-separable case

- Perceptron algorithm does not stop on a non-separable training set, since there will always be a misclassified example that causes an update
- In general, finding a hyperplane that minimizes the number of classification errors is computationally hard (NP-hard to minimize empirical error)

The non-separable case

The main source of difficulty is the "step function" shape of the zero-one loss function

$$L(y, \mathbf{w}^T\mathbf{x})) = \begin{cases} 1 & \text{if } y\mathbf{w}^T\mathbf{x} < 0 \\ 0 & \text{otherwise} \end{cases}$$

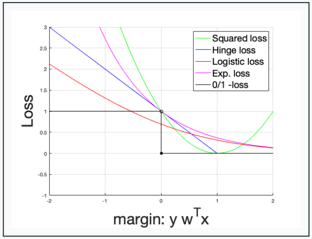


- It is non-differentiable, so cannot optimize using gradient approaches
- It is non-convex, so optimizer susceptible to fall in local minima

Surrogate loss functions for classification

There are multiple **surrogate** losses that are convex and differentiable upper bounds to zero-one loss

- Squared loss - used for regression, not optimal for classification
- Hinge loss - used in Support vector machines (Lecture 5)
- Exponential loss - used in Boosting
- **Logistic loss - used in Logistic regression**



Logistic regression

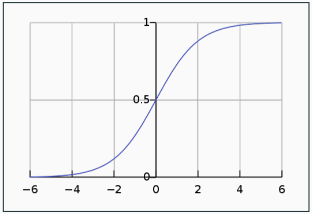
Logistic regression

Logistic regression is a classification technique (despite the name)

- it gets its name from the logistic function

  $$\phi_{logistic}(z) = \frac{1}{1+\exp(-z)} = \frac{\exp(z)}{1+\exp(z)}$$

  that maps a real valued input z onto the interval $0 < \phi_{logistic}(z) < 1$
- The function is an example of **sigmoid** ("S" shaped) functions



Logistic function: a probabilistic interpretation

- The logistic function $\phi_{logistic}(z)$ is the inverse of **logit function**
- The logit function is the logarithm of **odds ratio** of probability p of and event happening vs. the probability of the event not happening, $1 - p$;
$$z = logit(p) = \log \frac{p}{1-p} = \log p - \log(1-p)$$
- Thus the logistic function
$$\phi_{logistic}(z) = logit^{-1}(z) = \frac{1}{1 + \exp(-z)}$$
answer the question "what is the probability p that gives the log odds ratio of z"

Logistic regression

- Logistic regression model assumes a underlying conditional probability:

$$Pr(y|\mathbf{x}) = \frac{\exp(+\frac{1}{2}y\mathbf{w}^T\mathbf{x})}{\exp(+\frac{1}{2}y\mathbf{w}^T\mathbf{x}) + \exp(-\frac{1}{2}y\mathbf{w}^T\mathbf{x})}$$

where the denominator normalizes the right-hand side to be between zero and one.

- Dividing the numerator and denominator by $\exp(+\frac{1}{2}y\mathbf{w}^T\mathbf{x})$ reveals the logistic function

$$Pr(y|\mathbf{x}) = \phi_{logistic}(y\mathbf{w}^T\mathbf{x}) = \frac{1}{1+\exp(-y\mathbf{w}^T\mathbf{x})}$$

- The margin $z = y\mathbf{w}^T\mathbf{x}$ is thus interpreted as the log odds ratio of label y vs. label $-y$ given input $\mathbf{x}$:

$$y\mathbf{w}^T\mathbf{x} = \log \frac{Pr(y|\mathbf{x})}{Pr(-y|\mathbf{x})}$$

Logistic loss

- Consider the maximization of the likelihood of the observed input-output in the training data:

$$\mathbf{w}^* = \mathrm{argmax}_{\mathbf{w}} \prod_{i=1}^{m} P(y_i|\mathbf{x}_i) = \mathrm{argmax}_{\mathbf{w}} \prod_{i=1}^{m} \frac{1}{1+\exp(-y\mathbf{w}^T\mathbf{x})}$$

- Since the logarithm is monotonically increasing function, we can take the logarithm to obtain an equivalent objective:

$$\sum_{i=1}^{m} \log Pr(y_i|\mathbf{x}_I) = -\sum_{i=1}^{m} \log(1+\exp(-y_i\mathbf{w}^T\mathbf{x}_i))$$

- The right-hand side is the **logistic loss**:

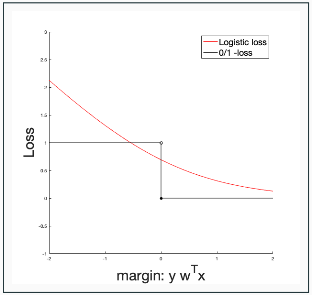
$$L_{logistic}(y, \mathbf{w}^T\mathbf{x}) = \log(1+\exp(-y\mathbf{w}^T\mathbf{x}))$$

- Minimizing the logistic loss correspond maximizing the likelihood of the training data

Geometric interpretation of Logistic loss

$$L_{logistic}(y, \mathbf{w}^T\mathbf{x}) = \log(1 + \exp(-y\mathbf{w}^T\mathbf{x}))$$

- Logistic loss is convex and differentiable
- It is a monotonically decreasing function of the margin $y\mathbf{w}^T\mathbf{x}$
- The loss changes fast when the margin is highly negative $\implies$ penalization of examples far in the incorrect halfspace
- It changes slowly for highly positive margins $\implies$ does not give extra bonus for being very far in the correct halfspace



Logistic regression optimization problem

- To train a logistic regression model, we need to find the **w** that minimizes the average logistic loss $J(\mathbf{w}) = \frac{1}{m}\sum_{i=1}^{m} L_{logistic}(y_i, \mathbf{w}^T\mathbf{x}_i)$ over the training set:

$$\min \quad J(\mathbf{w}) = \frac{1}{m}\sum_{i=1}^{m} \log(1 + \exp(-y_i \mathbf{w}^T \mathbf{x}_i))$$

$$w.r.t \text{ parameters } \mathbf{w} \in \mathbb{R}^d$$

- The function to be minimized is continuous and differentiable
- However, it is a non-linear function so it is not easy to find the optimum directly (e.g. unlike in linear regression)
- We will use **stochastic gradient descent** to incrementally step towards the direction where the objective decreases fastest, the **negative gradient**

Gradient

- The gradient is the vector of partial derivatives of the objective function $J(\mathbf{w})$ with respect to all parameters w_j

$$\nabla J(\mathbf{w}) = \frac{1}{m}\sum_{i=1}^{m} \nabla J_i(\mathbf{w}) = \frac{1}{m}\sum_{i=1}^{m} \left[\tfrac{\partial}{\partial w_1} J_i(\mathbf{w}), \ldots, \tfrac{\partial}{\partial w_d} J_i(\mathbf{w})\right]^T$$

- Compute the gradient by using the regular rules for differentiation. For the logistic loss we have

$$\begin{aligned}\frac{\partial}{\partial w_j} J_i(\mathbf{w}) &= \frac{\partial}{\partial w_j} \log(1+\exp(-y_i \mathbf{w}^T x_i)) = \frac{\exp(-y_i \mathbf{w}^T x_i)}{1+\exp(-y_i \mathbf{w}^T x_i)} \cdot (-y_i x_{ij}) \\ &= -\frac{1}{1+\exp(y_i \mathbf{w}^T x_i)} y_i x_{ij} = -\phi_{logistic}(-y_i \mathbf{w}^T x_i) y_i x_{ij}\end{aligned}$$

Stochastic gradient descent

- We collect the partial derivatives with respect to a single training example into a vector:

$$\nabla J_i(\mathbf{w}) = \begin{bmatrix} -(\phi_{logistic}(-y_i\mathbf{w}^T\mathbf{x}_i)y_i) \cdot x_{i1} \\ \vdots \\ -(\phi_{logistic}(-y_i\mathbf{w}^T\mathbf{x}_i)y_i) \cdot x_{ij} \\ \vdots \\ -(\phi_{logistic}(-y_i\mathbf{w}^T\mathbf{x}_i)y_i) \cdot x_{id} \end{bmatrix} = -\phi_{logistic}(-y_i\mathbf{w}^T\mathbf{x}_i)y_i \cdot \mathbf{x}_i$$

- The vector $-\nabla J_i(\mathbf{w})$ gives the update direction that fastest decreases the loss on training example $(\mathbf{x}_i, y_i)$

Stochastic gradient descent

- Evaluating the full gradient

$$\nabla J(\mathbf{w}) = \frac{1}{m}\sum_{i=1}^{n} \nabla J_i(\mathbf{w}) = -\frac{1}{m}\sum_{i=1}^{m} \phi_{logistic}(-y_i \mathbf{w}^T \mathbf{x}_i) y_i \cdot \mathbf{x}_i$$

  is costly since we need to process all training examples
- Stochastic gradient descent instead uses a series of smaller updates that depend on single randomly drawn training example $(\mathbf{x}_i, y_i)$ at a time
- The update direction is taken as $-\nabla J_i(\mathbf{w})$
- Its expectation is the full negative gradient:

$$-\mathbb{E}_{i=1\ldots,m}\left[\nabla J_i(\mathbf{w})\right] = -\nabla J(\mathbf{w})$$

- Thus on average, the updates match that of using the full gradient

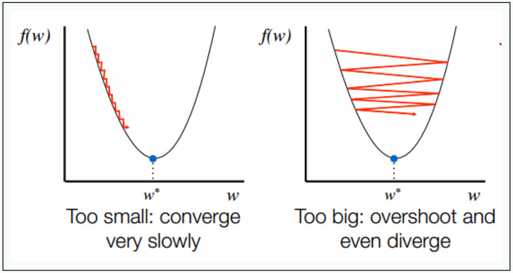
Stochastic gradient descent algorithm

```
Initialize $\mathbf{w} = 0$
**repeat**
    Draw a training example $(x_i, y_i)$ uniformly at random
    Compute the update direction corresponding to the training example:
    $\Delta\mathbf{w} = -\nabla J_i(\mathbf{w})$
    Determine a stepsize $\eta$
    Update $\mathbf{w} = \mathbf{w} - \eta\nabla J_i(\mathbf{w})$
**until** stopping criterion statisfied
Output $\mathbf{w}$
```

Stepsize selection

Consider the SGD update: $\mathbf{w} = \mathbf{w} - \eta \nabla J_i(\mathbf{w})$

- The stepsize parameter η, also called the **learning rate** is a critical one for convergence to the optimum value
- One uses small constant stepsize, the initial convergence may be unnecessarily slow
- Too large stepsize may cause the method to continually overshoot the optimum.


f(w)
w*
w
Too small: converge very slowly
f(w)
w*
w
Too big: overshoot and even diverge

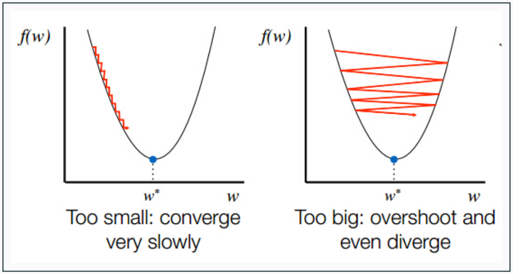
Source: https://dunglai.github.io/2017/12/21/gradient-descent/

Diminishing stepsize

- Initially larger but diminishing stepsize is one option:

$$\eta^{(t)} = \frac{1}{\alpha t}$$

  for some $\alpha > 0$, where t is the iteration counter
- Caution: In practice, finding a good value for parameter α requires experimenting with several values



f(w)
w*
w
Too small: converge very slowly
f(w)
w*
w
Too big: overshoot and even diverge

Source: https://dunglai.github.io/2017/12/21/gradient-descent/

Summary

- Linear classification model are and important class of machine learning models, they are used as standalone models and appear as building blocks of more complicated, non-liner models
- Perceptron is a simple algorithm to train linear classifiers on linearly separable data
- Logistic regression is a classification method that can be interpreted as maximizing odds ratios of conditional class probabilities
- Stochastic gradient descent is an efficient optimization method for large data that is nowadays very widely used