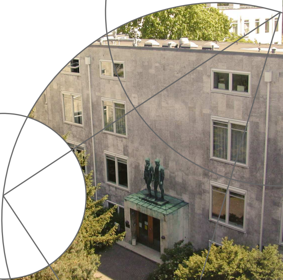
Linear Classification

Machine Learning

Christian Igel
Department of Computer Science



@christian_igel

Outline

1. Logistic Regression

2. Linear Classification and Margins

3. Perceptron Learning

4. Convergence of Perceptron Learning

5. Summary

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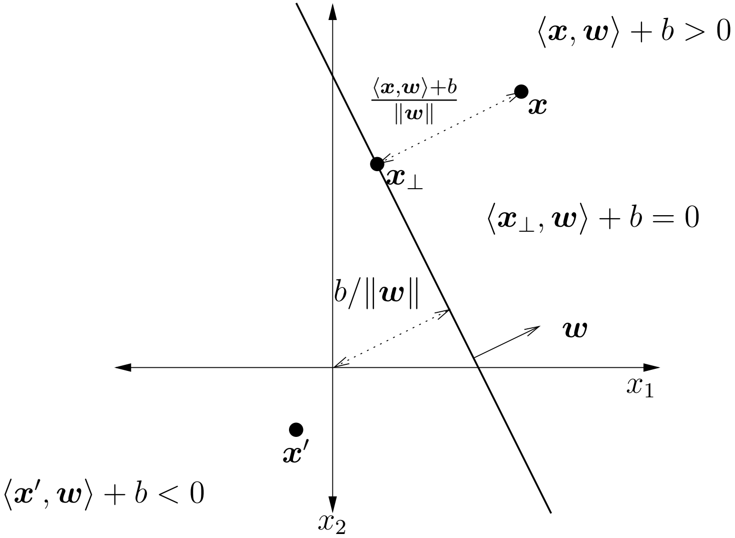
Linear functions

$$f(\boldsymbol{x}) = \langle \boldsymbol{x}, \boldsymbol{w} \rangle + b$$


$\langle \boldsymbol{x}, \boldsymbol{w} \rangle + b > 0$
$\frac{\langle \boldsymbol{x}, \boldsymbol{w} \rangle + b}{\|\boldsymbol{w}\|}$
$\boldsymbol{x}$
$\boldsymbol{x}_\perp$
$\langle \boldsymbol{x}_\perp, \boldsymbol{w} \rangle + b = 0$
$b/\|\boldsymbol{w}\|$
$\boldsymbol{w}$
x_1
$\boldsymbol{x}'$
$\langle \boldsymbol{x}', \boldsymbol{w} \rangle + b < 0$
x_2

Decision functions

- Classification assigns an input $x \in \mathcal{X}$ to one of a finite set of classes $\mathcal{Y} = \{\mathcal{C}_1, \dots, \mathcal{C}_m\}$, $2 \leq m$.

- One approach is to learn *discriminant functions* $\delta_k : \mathcal{X} \to \mathbb{R}$, $1 \leq k \leq m$, and assign a pattern x to class $\hat{y}$ using

$$\hat{y} = h(x) = \operatorname{argmax}_k \delta_k(x) \quad .$$

Linear classification

- We build affine linear decision functions

$$\delta(\boldsymbol{x}) = \sum_{i=1}^{d} w_i x_i + b = \boldsymbol{w}^{\mathsf{T}} \boldsymbol{x} + b$$

with $\boldsymbol{w} \in \mathbb{R}^d$ and $b \in \mathbb{R}$.

- For convenience, we define $\tilde{\boldsymbol{x}}_i^{\mathsf{T}} = (x_1, \ldots, x_d, 1)$ for $i = 1, \ldots, N$ and $\tilde{\boldsymbol{w}}^{\mathsf{T}} = (w_1, \ldots, w_d, b)$ and consider the equivalent formulation

$$\delta(\tilde{\boldsymbol{x}}) = \sum_{i=1}^{d+1} \tilde{w}_i \tilde{x}_i = \tilde{\boldsymbol{w}}^{\mathsf{T}} \tilde{\boldsymbol{x}} \quad .$$

We omit the tilde in the following.

Binary decision functions

- If we have only two classes, we can consider a single function

  $$\delta(x) = \delta_1(x) - \delta_2(x)$$

  and the hypothesis

  $$h(x) = \begin{cases} \mathcal{C}_1 & \text{if } \delta(x) > 0 \\ \mathcal{C}_2 & \text{otherwise} \end{cases} .$$

- For $\mathcal{Y} = \{-1, 1\}$ this is equal to

  $$h(x) = \operatorname{sgn}(\delta(x)) = \begin{cases} 1 & \text{if } \delta(x) > 0 \\ -1 & \text{otherwise} \end{cases} .$$

Decision functions and class posteriors

- If we know the class posteriors $P(Y \mid X)$ we can perform optimal classification: a pattern x is assigned to class $\mathcal{C}_k$ with maximum $P(Y = \mathcal{C}_k \mid X = x)$, i.e.,

  $$\hat{y} = h(x) = \operatorname{argmax}_k P(Y = \mathcal{C}_k \mid X = x)$$

  or in the binary case with $\mathcal{Y} = \{-1, 1\}$

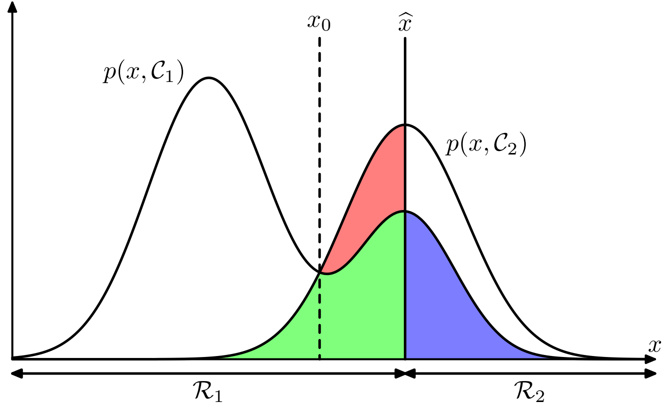
  $$\delta(x) = P(Y = \mathcal{C}_1 \mid X = x) - P(Y = \mathcal{C}_2 \mid X = x)$$

  and $\hat{y} = h(x) = \operatorname{sgn}(\delta(x))$.

- $P(Y = \mathcal{C}_k \mid X = x)$ is proportional to the class-conditional density $p(X = x \mid Y = \mathcal{C}_k)$ times the class prior $P(Y = \mathcal{C}_k)$:

  $$P(Y = \mathcal{C}_k \mid X = x) = \frac{p(X = x \mid Y = \mathcal{C}_k) P(Y = \mathcal{C}_k)}{p(X = x)}$$

Joint probabilities



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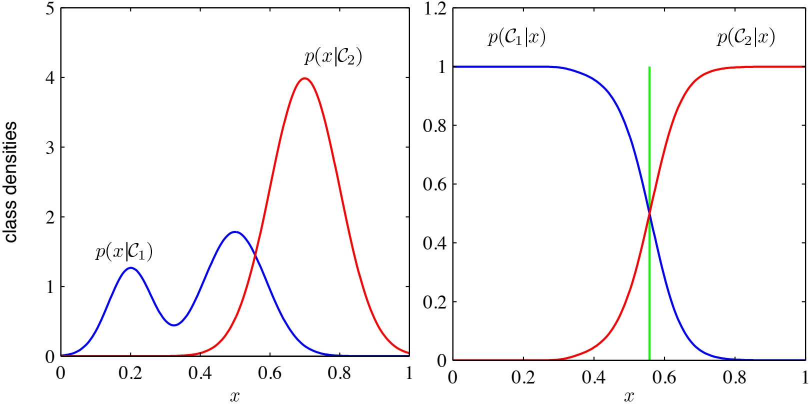
Class-conditional densities



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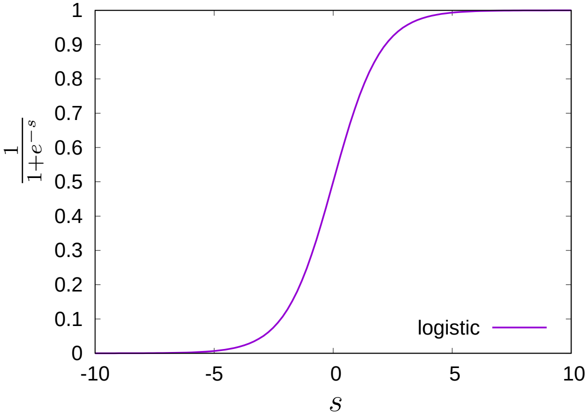
Logistic function



$$\theta(s) = \frac{1}{1 + e^{-s}}$$

Predicting probabilities

- Instead of predicting the class label, we want to learn

  $$f(\boldsymbol{x}) = P(Y = 1 \,|\, X = \boldsymbol{x})$$

  assuming that the data is generated by

  $$P(Y = y \,|\, X = \boldsymbol{x}) = \begin{cases} f(\boldsymbol{x}) & \text{for } y = 1 \\ 1 - f(\boldsymbol{x}) & \text{for } y = -1 \end{cases} .$$

- In the binary case, our model takes the form $h : \mathcal{X} \rightarrow [0, 1]$:

  $$h(\boldsymbol{x}) = \theta(\boldsymbol{w}^{\mathsf{T}} \boldsymbol{x})$$

Log-odds

Choice of logistic function is not arbitrary, it guarantees that the (affine) linear part of the model encodes the log-odds:

$$\boldsymbol{w}^{\mathsf{T}}\boldsymbol{x} = \ln \frac{P(Y=1 \,|\, X=\boldsymbol{x})}{P(Y=-1 \,|\, X=\boldsymbol{x})}$$

That is, $\boldsymbol{w}^{\mathsf{T}}\boldsymbol{x}$ encodes on log-scale how frequent class 1 occurs relative to class 0-1.

Likelihood function

- Our hypothesis h describes the probability distribution:

$$P(Y = y \,|\, X = \boldsymbol{x}; \boldsymbol{w}) = \theta(y\boldsymbol{w}^\mathsf{T}\boldsymbol{x}) = \begin{cases} \theta(\boldsymbol{w}^\mathsf{T}\boldsymbol{x}) & \text{for } y = 1 \\ 1 - \theta(\boldsymbol{w}^\mathsf{T}\boldsymbol{x}) & \text{for } y = -1 \end{cases}$$

- $S = \{(\boldsymbol{x}_1, y_1), \dots, (\boldsymbol{x}_N, y_N)\} \subseteq (\mathbb{R}^n \times \{-1, 1\})^N$
- Likelihood (function) of the parameters $\boldsymbol{w}$ given training data S is the probability of observing S when the data is generated by h with parameters $\boldsymbol{w}$.
- Likelihood for i.i.d. S:

$$\prod_{i=1}^{N} P(Y = y_i \,|\, X = \boldsymbol{x}_i; h) \text{ or short } \prod_{i=1}^{N} P(y_i \,|\, \boldsymbol{x}_i)$$

Maximum likelihood

- Learning principle: Maximize the likelihood function!
- Equivalently, we can minimize the negative logarithmic likelihood.
- Negative log-likelihood (divided by N):

$$-\frac{1}{N}\ln\left(\prod_{i=1}^{N} P(y_i \,|\, \boldsymbol{x}_i)\right) = -\frac{1}{N}\sum_{i=1}^{N}\ln\left(P(y_i \,|\, \boldsymbol{x}_i)\right)$$

- Plugging in our linear hypothesis gives the error function:

$$-\frac{1}{N}\sum_{n=1}^{N}\ln\left(\theta(y_n\boldsymbol{w}^{\mathsf{T}}\boldsymbol{x}_n)\right) = \frac{1}{N}\sum_{n=1}^{N}\ln\left(1+e^{-y_n\boldsymbol{w}^{\mathsf{T}}\boldsymbol{x}_n}\right)$$

Recall: Gradient

- The *gradient*

$$\nabla f(\boldsymbol{x}) = \left(\frac{\partial f(\boldsymbol{x})}{\partial x_1}, \frac{\partial f(\boldsymbol{x})}{\partial x_2}, \ldots, \frac{\partial f(\boldsymbol{x})}{\partial x_d} \right)^{\mathsf{T}}$$

points in the direction $\nabla f(\boldsymbol{x}) / \|\nabla f(\boldsymbol{x})\|$ giving maximum rate of change $\|\nabla f(\boldsymbol{x})\|$.

Gradient descent

- Consider learning by iteratively changing the parameters:

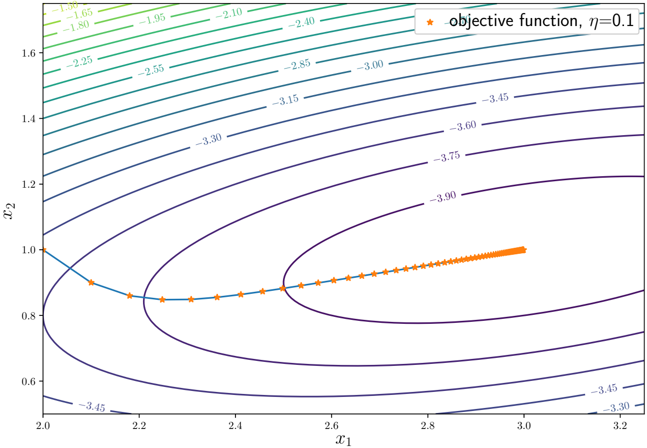
$$\boldsymbol{w} \leftarrow \boldsymbol{w} + \Delta\boldsymbol{w}$$

- Simplest choice is (steepest) gradient descent

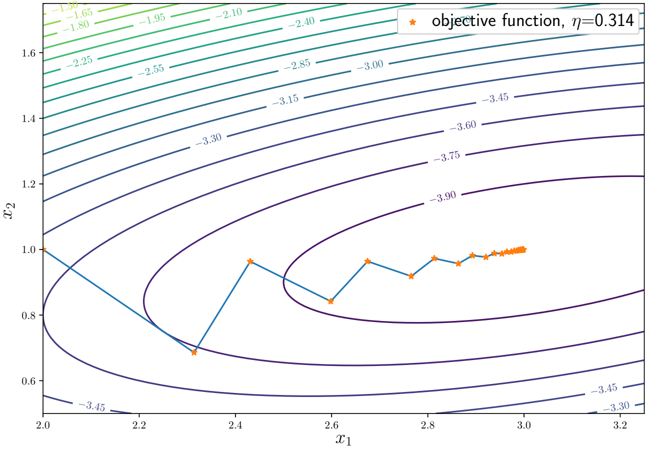
$$\Delta\boldsymbol{w} = -\eta\nabla f|_{\boldsymbol{w}}$$

with learning rate $\eta > 0$.

Gradient descent example, small learning rate



Gradient descent, larger learning rate



Gradient for training logistic regression

- For data $\{(\boldsymbol{x}_1, y_1), \dots, (\boldsymbol{x}_N, y_N)\} \subseteq (\mathbb{R}^n \times \{-1, 1\})^N$, we have the following gradient of the negative log-likelihood:

$$-\frac{1}{N}\sum_{n=1}^{N} \frac{y_n \boldsymbol{x}_n}{1 + e^{y_n \boldsymbol{w}^\mathsf{T} \boldsymbol{x}_n}}$$

- This equals:

$$-\frac{1}{N}\sum_{n=1}^{N} \left[\frac{y_n + 1}{2} - \theta(\boldsymbol{w}^\mathsf{T} \boldsymbol{x}_n)\right] \boldsymbol{x}_n$$

- Thus, for $\{(\boldsymbol{x}_1, y_1), \dots, (\boldsymbol{x}_N, y_N)\} \subseteq (\mathbb{R}^n \times \{0, 1\})^N$, we have the gradient:

$$-\frac{1}{N}\sum_{n=1}^{N} \left[y_n - \theta(\boldsymbol{w}^\mathsf{T} \boldsymbol{x}_n)\right] \boldsymbol{x}_n$$

Logistic regression algorithm (steepest descent)

```
Algorithm 1: Logistic regression
Input: data $\{(\boldsymbol{x}_1, y_1), \dots, \boldsymbol{x}_N, y_N)\} \subseteq (\mathbb{R}^n \times \{-1, 1\})^N$,
       learning rate $\eta$
Output: weights of linear hypothesis $h(\boldsymbol{x}) = \langle \boldsymbol{w}, \boldsymbol{x} \rangle$
initialize $\boldsymbol{w}$
repeat
    // gradient of negative log-likelihood over N
    $\boldsymbol{g} \leftarrow -\frac{1}{N} \sum_{n=1}^{N} \frac{y_n \boldsymbol{x}_n}{1+e^{y_n \boldsymbol{w}^{\mathsf{T}} \boldsymbol{x}_n}}$
    // model parameter update
    $\boldsymbol{w} \leftarrow \boldsymbol{w} - \eta \boldsymbol{g}$
until stopping criterion is met
```

Logistic regression algorithm (stochastic gradient descent, SGD)

```
Algorithm 2: Logistic regression
Input: data $\{(\boldsymbol{x}_1, y_1), \dots\} \subseteq (\mathbb{R}^n \times \{-1, 1\})^N$, learning
       rate $\eta$
Output: weights of linear hypothesis $h(\boldsymbol{x}) = \langle \boldsymbol{w}, \boldsymbol{x} \rangle$
initialize $\boldsymbol{w}$
repeat
    pick $(\boldsymbol{x}, y) \in S$
    $\boldsymbol{w} \leftarrow \boldsymbol{w} + \eta \frac{y\boldsymbol{x}}{1+e^{y\boldsymbol{w}^\mathsf{T}\boldsymbol{x}}}$
until stopping criterion is met
```

Logistic regression algorithm (mini-batch gradient descent)

Algorithm 3: Logistic regression

```
Input: data $\{(\boldsymbol{x}_1, y_1), \dots\} \subseteq (\mathbb{R}^n \times \{-1, 1\})^N$, learning
       rate $\eta$
Output: weights of linear hypothesis $h(\boldsymbol{x}) = \langle \boldsymbol{w}, \boldsymbol{x} \rangle$
initialize $\boldsymbol{w}$
repeat
    pick $S' \subset S$
    $\boldsymbol{g} \leftarrow -\frac{1}{|S'|} \sum_{(\boldsymbol{x},y) \in S'} \frac{y\boldsymbol{x}}{1+e^{y\boldsymbol{w}^\mathsf{T}\boldsymbol{x}}}$
    $\boldsymbol{w} \leftarrow \boldsymbol{w} - \eta \boldsymbol{g}$
until stopping criterion is met
```

Multiple classes

- Binary, single discriminant function, $y \in \{0, 1\}$:

$$P(Y = 1 \,|\, \boldsymbol{x}) = \frac{1}{1 + e^{-\delta(\boldsymbol{x})}} = \frac{e^{\delta(\boldsymbol{x})}}{1 + e^{\delta(\boldsymbol{x})}}$$

- Binary, two discriminant functions, $y \in \{1, 2\}$:

$$P(Y = y \,|\, \boldsymbol{x}) = \frac{e^{\delta_y(\boldsymbol{x})}}{e^{\delta_1(\boldsymbol{x})} + e^{\delta_2(\boldsymbol{x})}} = \frac{e^{\delta_y(\boldsymbol{x})+C}}{e^{\delta_1(\boldsymbol{x})+C} + e^{\delta_2(\boldsymbol{x})+C}}$$

  for every constant C, thus logistic function is special case for $C = -\delta_1(\boldsymbol{x})$.

- Multiple classes, $y \in \{1, \ldots, m\}$:

$$P(Y = y \,|\, \boldsymbol{x}) = \underbrace{\frac{e^{\delta_y(\boldsymbol{x})}}{\sum_{i=1}^{m} e^{\delta_i(\boldsymbol{x})}}}_{\text{softmax function}}$$

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2. Linear Classification and Margins
3. Perceptron Learning
4. Convergence of Perceptron Learning
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Margins I

The functional margin of an example $(\boldsymbol{x}_i, y_i)$ with respect to a hyperplane $(\boldsymbol{w}, b)$ is

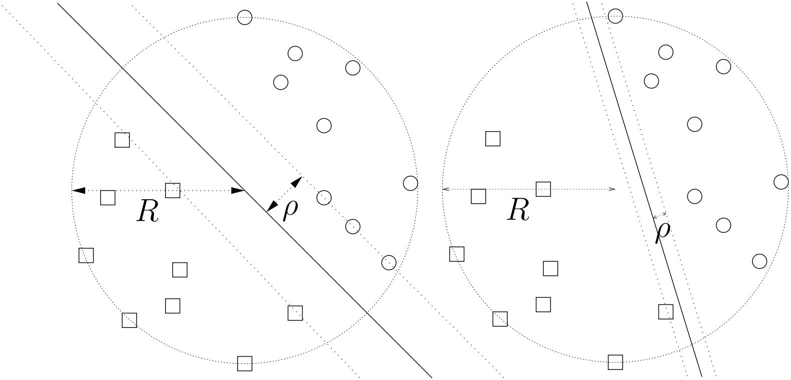
$$\gamma_i := y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b) \ .$$

The geometric margin of an example $(\boldsymbol{x}_i, y_i)$ with respect to a hyperplane $(\boldsymbol{w}, b)$ is

$$\rho_i := y_i(\langle \boldsymbol{w}, \boldsymbol{x}_i \rangle + b)/\|\boldsymbol{w}\| = \gamma_i/\|\boldsymbol{w}\| \ .$$

A positive margin implies correct classification.
The margin of a hyperplane $(\boldsymbol{w}, b)$ with respect to a training set S is $\min_i \rho_i$. The margin of a training set S is the maximum geometric margin over all hyperplanes. A hyperplane realizing this margin is called maximum margin hyperplane.

Margins II



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Analyzing the Perceptron

Why should we look at the Perceptron?

- Linear classifiers such as perceptrons are the basis of technical neurocomputing
- Support Vector Machines are basically linear classifiers
- Basic concepts of learning theory can be explained easily:
  - Margins
  - Dual representation
  - Bounds involving margins and the radius of the ball containing the data

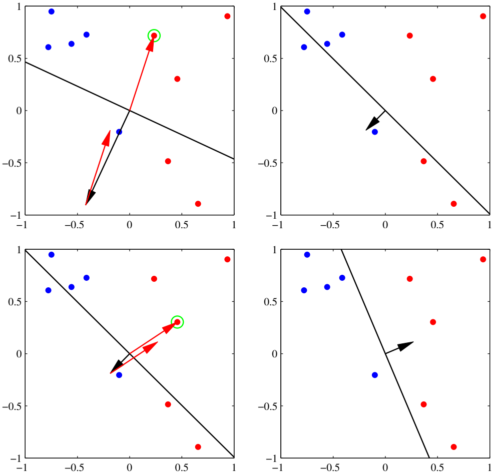
Perceptron learning algorithm (primal form)

For simplicity, consider hyperplanes with no bias ($b = 0$), i.e., $\mathcal{H} = \{h(\boldsymbol{x}) = \operatorname{sgn}(\langle \boldsymbol{w}, \boldsymbol{x} \rangle) \,|\, \boldsymbol{w} \in \mathbb{R}^n\}$.

Algorithm 4: Perceptron

```
Input: separable data $\{(\boldsymbol{x}_1, y_1), \dots\} \subseteq (\mathbb{R}^n \times \{-1, 1\})^N$
Output: hypothesis $h(\boldsymbol{x}) = \operatorname{sgn}(\langle \boldsymbol{w}_k, \boldsymbol{x} \rangle)$
$\boldsymbol{w}_0 \leftarrow \boldsymbol{0}; k \leftarrow 0$
repeat
    for $i = 1, \dots, N$ do
        if $y_i \langle \boldsymbol{w}_k, \boldsymbol{x}_i \rangle \leq 0$ then
            $\boldsymbol{w}_{k+1} \leftarrow \boldsymbol{w}_k + y_i \boldsymbol{x}_i$
            $k \leftarrow k + 1$
until no mistake made within for loop
```

Perceptron learning in pictures



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Novikoff

Theorem (Novikoff)

Let $S = \{(\boldsymbol{x}_1, y_1), \dots, (\boldsymbol{x}_N, y_N)\}$ *be a non-trivial training set (i.e., containing patterns of both classes),* $\boldsymbol{w}_0 = \mathbf{0}$*, and let*

$$R \leftarrow \max_{1 \le i \le N} \|\boldsymbol{x}_i\| \enspace .$$

Suppose that there exists $\boldsymbol{w}_{\textit{opt}}$ *and* $\rho > 0$ *such that* $\|\boldsymbol{w}_{\textit{opt}}\| = 1$ *and*

$$y_i \left\langle \boldsymbol{w}_{\textit{opt}}, \boldsymbol{x}_i \right\rangle \ge \rho > 0$$

for $1 \le i \le N$*. Then the number of updates* k *made by the online perceptron algorithm on* S *is at most*

$$\left(\frac{R}{\rho}\right)^2 \enspace .$$

Novikoff, sketch of proof I

Let i be the index of the example in update k

$$\begin{aligned}\left\|\boldsymbol{w}_{k+1}\right\|^2 &= \langle \boldsymbol{w}_k + y_i\boldsymbol{x}_i, \boldsymbol{w}_k + y_i\boldsymbol{x}_i\rangle\\ &= \left\|\boldsymbol{w}_k\right\|^2 + 2y_i\left\langle \boldsymbol{w}_k, \boldsymbol{x}_i\right\rangle + \left\|\boldsymbol{x}_i\right\|^2\\ &\leq \left\|\boldsymbol{w}_k\right\|^2 + R^2\\ &\leq (k+1)R^2\end{aligned}$$

Novikoff, sketch of proof II

$$\begin{aligned}\left\langle \boldsymbol{w}_{\mathsf{opt}}, \boldsymbol{w}_{k+1} \right\rangle &= \left\langle \boldsymbol{w}_{\mathsf{opt}}, \boldsymbol{w}_{k} \right\rangle + y_i \left\langle \boldsymbol{w}_{\mathsf{opt}}, \boldsymbol{x}_{i} \right\rangle \\ &\geq \left\langle \boldsymbol{w}_{\mathsf{opt}}, \boldsymbol{w}_{k} \right\rangle + \rho \\ &\geq (k+1)\rho\end{aligned}$$

$$k^2\rho^2 \leq \left\langle \boldsymbol{w}_{\mathsf{opt}}, \boldsymbol{w}_{k} \right\rangle^2 \leq \|\boldsymbol{w}_{\mathsf{opt}}\|^2 \|\boldsymbol{w}_{k}\|^2 \leq kR^2$$

$$k \leq \frac{R^2}{\rho^2}$$

Dual representation

- Weight vector of hyperplane computed by online perceptron algorithm can be written as

$$\boldsymbol{w} = \sum_{i=1}^{N} \alpha_i y_i \boldsymbol{x}_i$$

- Function $h(\boldsymbol{x}) = \operatorname{sgn}(\delta(\boldsymbol{x}))$ can be written in dual coordinates

$$\begin{aligned}\delta(\boldsymbol{x}) &= \langle \boldsymbol{w}, \boldsymbol{x} \rangle \\ &= \left\langle \sum_{i=1}^{N} \alpha_i y_i \boldsymbol{x}_i, \boldsymbol{x} \right\rangle \\ &= \sum_{i=1}^{N} \alpha_i y_i \langle \boldsymbol{x}_i, \boldsymbol{x} \rangle\end{aligned}$$

Perceptron learning algorithm (dual form)

Algorithm 5: Perceptron (dual form)

```
Input: separable data $\{(\boldsymbol{x}_1, y_1), \dots\} \subseteq (\mathbb{R}^n \times \{-1, 1\})^N$
Output: hypothesis $h(\boldsymbol{x}) = \operatorname{sgn}\left(\sum_{i=1}^{N} \alpha_i y_i \langle \boldsymbol{x}_i, \boldsymbol{x} \rangle\right)$
$\boldsymbol{\alpha} \leftarrow \boldsymbol{0}$
repeat
    for $i = 1, \dots, N$ do
        if $y_i \sum_{j=1}^{N} \alpha_j y_j \langle \boldsymbol{x}_j, \boldsymbol{x}_i \rangle \leq 0$ then
            $\alpha_i \leftarrow \alpha_i + 1$
until no mistake made within for loop
```

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Summary I

Logistic regression

- is easy to use, has in its simplest form no hyperparameters (not counting η),
- gives surprisingly good results, is highly recommended as baseline method,
- does typically not tend to overfit (assuming $d \ll N$), but does not capture non-linearities,
- can be used with non-linear transformations,
- can be parallelized and is applicable to “Big Data”.

Summary II

Hey, we also now know about

- perceptron learning,
- margins,
- dual representation,
- bounds involving margins and the radius of the ball containing the data.