Machine Learning

Linear Models

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Linear Predictors and Affine Functions

Consider $\mathcal{X} = \mathbb{R}^d$

"Linear" (affine) functions:

$$L_d = \{h_{\mathbf{w},b} : \mathbf{w} \in \mathbb{R}^d, b \in \mathbb{R}\}$$

where

$$h_{\mathbf{w},b}(\mathbf{x}) = \langle \mathbf{w}, \mathbf{x} \rangle + b = \left(\sum_{i=1}^{d} w_i x_i\right) + b$$

Note:

- each member of L_d is a function $\mathbf{x} \to \langle \mathbf{w}, \mathbf{x} \rangle + b$
- b: bias

Linear Models

Hypothesis class $\mathcal{H}: \phi \circ L_d$, where $\phi: \mathbb{R} \to \mathcal{Y}$

- $h \in \mathcal{H}$ is $h : \mathbb{R}^d \to \mathcal{V}$
- ϕ depends on the learning problem

Example

- binary classification, $\mathcal{Y} = \{-1, 1\} \Rightarrow \phi(z) = \operatorname{sign}(z)$
- regression, $\mathcal{Y} = \mathbb{R} \Rightarrow \phi(z) = z$

Equivalent Notation

Given $\mathbf{x} \in \mathcal{X}$, $\mathbf{w} \in \mathbb{R}^d$, $b \in \mathbb{R}$, define:

- $\mathbf{w}' = (b, w_1, w_2, \dots, w_d) \in \mathbb{R}^{d+1}$
- $\mathbf{x}' = (1, x_1, x_2, \dots, x_d) \in \mathbb{R}^{d+1}$

Then:

$$h_{\mathbf{w},b}(\mathbf{x}) = \langle \mathbf{w}, \mathbf{x} \rangle + b = \langle \mathbf{w}', \mathbf{x}' \rangle$$
 (1)

 \Rightarrow we will consider bias term as part of **w** and assume $\mathbf{x} = (1, x_1, x_2, \dots, x_d)$ when needed, with $h_{\mathbf{w}}(\mathbf{x}) = \langle \mathbf{w}, \mathbf{x} \rangle$

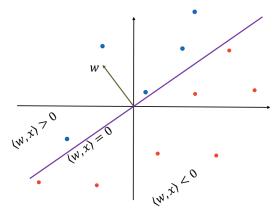
Linear Classification

$$\mathcal{X} = \mathbb{R}^d$$
, $\mathcal{Y} = \{-1, 1\}$, 0-1 loss

Hypothesis class = halfspaces

$$HS_d = \operatorname{sign} \circ L_d = \{\mathbf{x} \to \operatorname{sign}(h_{\mathbf{w},b}(\mathbf{x})) : h_{\mathbf{w},b} \in L_d\}$$

Example: $\mathcal{X} = \mathbb{R}^2$



Finding a Good Hypothesis

Linear classification with hypothesis set $\mathcal{H} = \text{halfspaces}$.

How do we find a good hypothesis?

Good = minimizes the training error (ERM)

⇒ Perceptron Algorithm (Rosenblatt, 1958)

Note:

if $y_i \langle \mathbf{w}, \mathbf{x}_i \rangle > 0$ for all $i = 1, ..., m \Rightarrow$ all points are classified correctly by model $\mathbf{w} \Rightarrow realizability assumption$ for training set

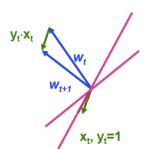
Linearly separable data: there exists **w** such that: $y_i \langle \mathbf{w}, \mathbf{x}_i \rangle > 0$

Perceptron

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Input: training set (\mathbf{x}_1, y_1), \dots, (\mathbf{x}_m, y_m) initialize \mathbf{w}^{(1)} = (0, \dots, 0); for t = 1, 2, \dots do

if \exists i \ s.t. \ y_i \langle \mathbf{w}^{(t)}, \mathbf{x}_i \rangle \leq 0 then \mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} + y_i \mathbf{x}_i; else return \mathbf{w}^{(t)};
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Interpretation of update:



Note that:

$$y_i \langle \mathbf{w}^{(t+1)}, \mathbf{x}_i \rangle = y_i \langle \mathbf{w}^{(t)} + y_i \mathbf{x}_i, \mathbf{x}_i \rangle$$

= $y_i \langle \mathbf{w}^{(t)}, \mathbf{x}_i \rangle + ||\mathbf{x}_i||^2$

 \Rightarrow update guides **w** to be "more correct" on (\mathbf{x}_i, y_i) .

Termination? Depends on the realizability assumption!

Perceptron with Linearly Separable Data

If data is linearly separable one can prove that the perceptron terminates.

Proposition

Assume that $(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_m, y_m)$ is linearly separable, let:

- $B = \min\{||\mathbf{w}|| : y_i \langle \mathbf{w}, \mathbf{x}_i \rangle \ge 1 \ \forall i, i = 1, \dots, m, \}$, and
- $R = \max_i ||\mathbf{x}_i||$.

Then the Perceptron algorithm stops after at most $(RB)^2$ iterations (and when it stops it holds that $\forall i, i \in \{1, ..., m\} : y_i \langle \mathbf{w}^{(t)}, \mathbf{x}_i \rangle > 0$).

Perceptron: Notes

- simple to implement (but some details are not described in the pseudocode...)
- for separable data
 - termination is guaranteed
 - may require a number of iterations that is exponential in d...
 ⇒ other approaches (e.g., ILP Integer Linear Programming) may be better to find ERM solution in such cases
 - potentially multiple solutions, which one is picked depends on starting values
- non separable data?
 - run for some time and keep best solution found up to that point (pocket algorithm)

Perceptron: A Modern View

The previous presentation of the Perceptron is the standard one.

However, we can derive the Perceptron in a different way...

Assume you want to solve a:

- binary classification problem: $\mathcal{X} = \mathbb{R}^d$, $\mathcal{Y} = \{-1, 1\}$
- with linear models
- with loss $\ell(\mathbf{w}, (\mathbf{x}, y)) = \max\{0, -y\langle \mathbf{w}, \mathbf{x}\rangle\}$.

Approach: ERM \Rightarrow need to find the model/hypothesis with smallest training error

How?

Note: this is a common framework in all of machine learning!

Gradient Descent (GD)

General approach for *minimizing* a differentiable convex function $f(\mathbf{w})$

Let $f: \mathbb{R}^d \to \mathbb{R}$ be a differentiable function

Definition

The gradient $\nabla f(\mathbf{w})$ of f at $\mathbf{w} = (w_1, \dots, w_d)$ is

$$\nabla f(\mathbf{w}) = \left(\frac{\partial f(\mathbf{w})}{\partial w_1}, \dots, \frac{\partial f(\mathbf{w})}{\partial w_d}\right)$$

Intuition: the gradient points in the direction of the greatest rate of increase of f around w

Let $\eta \in \mathbb{R}, \eta > 0$ be a parameter.

GD algorithm:



Notes:

- output vector could also be $\mathbf{w}^{(T)}$ or $\arg\min_{\mathbf{w}^{(t)} \in \{1,...,T\}} f(\mathbf{w}^{(t)})$
- returning w
 is useful for nondifferentiable functions (using subgradients instead of gradients...) and for stochastic gradient descent...
- η : learning rate; sometimes a time dependent $\eta^{(t)}$ is used (e.g., "move" more at the beginning than at the end)

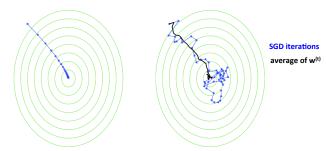
Note: there are guarantees on the number of iterations required by GD to return a *good* value of $\overline{\mathbf{w}}$ under some assumptions on \mathbf{f} (see the book for details)

Stochastic Gradient Descent (SGD)

Idea: instead of using exactly the gradient, we take a (random) vector with *expected value* equal to the gradient direction.

SGD algorithm:

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\begin{aligned} \mathbf{w}^{(0)} &\leftarrow \mathbf{0}; \\ \text{for } t \leftarrow 0 \text{ to } T - 1 \text{ do} \\ & \text{choose } \mathbf{v}_t \text{ at random from distribution such that } \mathbf{E}[\mathbf{v}_t | \mathbf{w}^{(t)}] \in \nabla f(\mathbf{w}^{(t)}); \\ & /* \ \mathbf{v}_t \text{ has } expected \text{ value equal to the gradient of } f(\mathbf{w}^{(t)}) \text{ */} \\ & \mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} - \eta \mathbf{v}_t; \\ \text{return } \bar{\mathbf{w}} &= \frac{1}{T} \sum_{t=1}^T \mathbf{w}^{(t)}; \end{aligned}
```



Note: there are guarantees on the number of iterations required by GD to return a *good*, *in expectation*, value of $\bar{\mathbf{w}}$ under some assumptions on f (see the book for details)

Why should we use SGD instead of GD?

Question: when do we use GD in the first place?

Answer: for example to find **w** that minimizes $L_S(\mathbf{w})$

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That is: we use GD for f(\mathbf{w}) = L_S(\mathbf{w})

\Rightarrow \nabla f(\mathbf{w}) depends on all pairs (\mathbf{x}_i, y_i) \in S, i = 1, ..., m: may require long time to compute it!
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What about SGD?

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We need to pick \mathbf{v}_t such that \mathbf{E}[\mathbf{v}_t|\mathbf{w}^{(t)}] \in \nabla f(\mathbf{w}^{(t)}): how?
Pick a random (\mathbf{x}_i, y_i) \in S \Rightarrow \text{pick } \mathbf{v}_t \in \nabla \ell(\mathbf{w}^{(t)}, (\mathbf{x}_i, y_i)):
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- satisfies the requirement!
- requires much less computation than GD

Analogously we can use SGD for regularized losses, etc.

Back to Our Linear Classification Problem

- binary classification problem: $\mathcal{X} = \mathbb{R}^d$, $\mathcal{Y} = \{-1, 1\}$
- with linear models
- with loss $\ell(\mathbf{w}, (\mathbf{x}, y)) = \max\{0, -y\langle \mathbf{w}, \mathbf{x}\rangle\}$.

How to find the ERM solution? SGD!

SGD for Linear Classification

Linear Regression

$$\mathcal{X} = \mathbb{R}^d$$
, $\mathcal{Y} = \mathbb{R}$

Hypothesis class:

$$\mathcal{H}_{reg} = L_d = \{ \mathbf{x} \to \langle \mathbf{w}, \mathbf{x} \rangle + b : \mathbf{w} \in \mathbb{R}^d, b \in \mathbb{R} \}$$

Note: $h \in \mathcal{H}_{reg} : \mathbb{R}^d \to \mathbb{R}$

Commonly used loss function: squared-loss

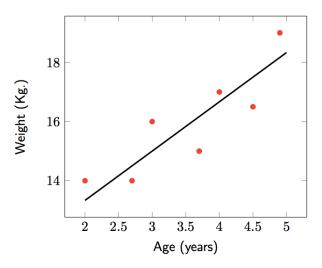
$$\ell(h, (\mathbf{x}, y)) \stackrel{\text{def}}{=} (h(\mathbf{x}) - y)^2$$

⇒ empirical risk function (training error): Mean Squared Error

$$L_S(h) = \frac{1}{m} \sum_{i=1}^{m} (h(\mathbf{x}_i) - y_i)^2$$

Linear Regression - Example

d = 1



Least Squares

How to find a ERM hypothesis? Least Squares algorithm

Best hypothesis:

$$\arg\min_{\mathbf{w}} L_{S}(h_{\mathbf{w}}) = \arg\min_{\mathbf{w}} \frac{1}{m} \sum_{i=1}^{m} (\langle \mathbf{w}, \mathbf{x}_{i} \rangle - y_{i})^{2}$$

Equivalent formulation: \mathbf{w} minimizing Residual Sum of Squares (RSS), i.e.

$$\arg\min_{\mathbf{w}} \sum_{i=1}^{m} (\langle \mathbf{w}, \mathbf{x}_i \rangle - y_i)^2$$

RSS: Matrix Form

Let

$$\mathbf{X} = \begin{bmatrix} \cdots & \mathbf{x}_1 & \cdots \\ \cdots & \mathbf{x}_2 & \cdots \\ \cdots & \vdots & \cdots \\ \cdots & \mathbf{x}_m & \cdots \end{bmatrix}$$

X: design matrix

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}$$

⇒ we have that RSS is

$$\sum_{i=1}^{m} (\langle \mathbf{w}, \mathbf{x}_i \rangle - y_i)^2 = (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w})$$

Want to find **w** that minimizes RSS (=objective function):

$$\underset{\mathbf{w}}{\operatorname{arg \, min}} \, RSS(\mathbf{w}) = \underset{\mathbf{w}}{\operatorname{arg \, min}} \, (\mathbf{y} - \mathbf{X}\mathbf{w})^T \, (\mathbf{y} - \mathbf{X}\mathbf{w})$$

How?

Compute gradient $\frac{\partial RSS(\mathbf{w})}{\partial \mathbf{w}}$ of objective function w.r.t \mathbf{w} and compare it to 0.

$$\frac{\partial RSS(\mathbf{w})}{\partial \mathbf{w}} = -2\mathbf{X}^T(\mathbf{y} - \mathbf{X}\mathbf{w})$$

Then we need to find w such that

$$-2\mathbf{X}^{T}(\mathbf{y}-\mathbf{X}\mathbf{w})=0$$

$$-2\mathbf{X}^T(\mathbf{y} - \mathbf{X}\mathbf{w}) = 0$$

is equivalent to

$$\mathbf{X}^T \mathbf{X} \mathbf{w} = \mathbf{X}^T \mathbf{y}$$

If $\mathbf{X}^T\mathbf{X}$ is invertible \Rightarrow solution to ERM problem is:

$$\mathbf{w} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

Complexity Considerations

We need to compute

$$(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Algorithm:

- ① compute $\mathbf{X}^T \mathbf{X}$: product of $(d+1) \times m$ matrix and $m \times (d+1)$ matrix
- 2 compute $(\mathbf{X}^T\mathbf{X})^{-1}$ inversion of $(d+1)\times(d+1)$ matrix
- 3 compute $(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$: product of $(d+1)\times(d+1)$ matrix and $(d+1)\times m$ matrix
- **4** compute $(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$: product of $(d+1)\times m$ matrix and $m\times 1$ matrix

Most expensive operation? Inversion!

$$\Rightarrow$$
 done for $(d+1) \times (d+1)$ matrix

$$\mathbf{X}^T\mathbf{X}$$
 not invertible?

How do we get w such that

$$\mathbf{X}^T \mathbf{X} \mathbf{w} = \mathbf{X}^T \mathbf{y}$$

if $\mathbf{X}^{\mathsf{T}}\mathbf{X}$ is not invertible? Let

$$\mathbf{A} = \mathbf{X}^T \mathbf{X}$$

Let A^+ be the generalized inverse of A, i.e.:

$$AA^+A=A$$

Proposition

If $\mathbf{A} = \mathbf{X}^T \mathbf{X}$ is not invertible, then $\hat{w} = \mathbf{A}^+ \mathbf{X}^T \mathbf{y}$ is a solution to $\mathbf{X}^T \mathbf{X} \mathbf{w} = \mathbf{X}^T \mathbf{y}$.

Computing the Generalized Inverse of A

Note $\mathbf{A} = \mathbf{X}^T \mathbf{X}$ is symmetric \Rightarrow eigenvalue decomposition of \mathbf{A} :

$$A = VDV^T$$

with

- D: diagonal matrix (entries = eigenvalues of A)
- **V**: orthonormal matrix ($\mathbf{V}^T\mathbf{V} = \mathbf{I}_{d\times d}$)

Define D⁺ diagonal matrix such that:

$$\mathbf{D}_{i,i}^{+} = \begin{cases} 0 & \text{if } \mathbf{D}_{i,i} = 0\\ \frac{1}{\mathbf{D}_{i,i}} & \text{otherwise} \end{cases}$$

Let
$$\mathbf{A}^+ = \mathbf{V}\mathbf{D}^+\mathbf{V}^T$$

Then

$$\mathbf{A}\mathbf{A}^{+}\mathbf{A} = \mathbf{V}\mathbf{D}\mathbf{V}^{T}\mathbf{V}\mathbf{D}^{+}\mathbf{V}^{T}\mathbf{V}\mathbf{D}\mathbf{V}^{T}$$

$$= \mathbf{V}\mathbf{D}\mathbf{D}^{+}\mathbf{D}\mathbf{V}^{T}$$

$$= \mathbf{V}\mathbf{D}\mathbf{V}^{T}$$

$$= \mathbf{A}$$

 \Rightarrow **A**⁺ is a generalized inverse of **A**.

In practice: the Moore-Penrose generalized inverse \mathbf{A}^\dagger of \mathbf{A} is used, since it can be efficiently computed from the Singular Value Decomposition of \mathbf{A} .

Exercise

Consider a linear regression problem, where $\mathcal{X} = \mathbb{R}^d$ and $\mathcal{Y} = \mathbb{R}$, with mean squared loss. The hypothesis set is the set of *constant* functions, that is $\mathcal{H} = \{h_a : a \in \mathbb{R}\}$, where $h_a(\mathbf{x}) = a$. Let $S = ((\mathbf{x}_1, y_1), \dots, (\mathbf{x}_m, y_m))$ denote the training set.

- Derive the hypothesis $h \in \mathcal{H}$ that minimizes the training error.
- Use the result above to explain why, for a given hypothesis \hat{h} from the set of all linear models, the coefficient of determination $R^2 = 1 \frac{\sum_{i=1}^m (\hat{h}(x_i) y_i)^2}{\sum_{i=1}^m (y_i \bar{y})^2}$ where \bar{y} is the average of the $y_i, i = 1, \ldots, m$ is a measure of how well \hat{h} performs (on the training set).

Polynomial Models

Consider a regression problem.

Can we as hypothesis set the set of polynomials of degree *r* with the tools we have already developed for linear regression?

Logistic Regression

Learn a function h from \mathbb{R}^d to [0,1].

What can this be used for?

Classification!

Example: binary classification $(\mathcal{Y} = \{-1, 1\}) - h(\mathbf{x}) = probability$ that label of \mathbf{x} is 1.

For simplicity of presentation, we consider binary classification with $\mathcal{Y}=\{-1,1\}$, but similar considerations apply for multiclass classification.

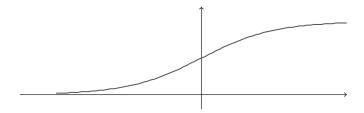
Logistic Regression: Model

Hypothesis class \mathcal{H} : $\phi_{\text{sig}} \circ L_d$, where $\phi_{\text{sig}} : \mathbb{R} \to [0,1]$ is sigmoid function

Sigmoid function = "S-shaped" function

For logistic regression, the sigmoid ϕ_{sig} used is the *logistic regression*:

$$\phi_{\mathsf{sig}}(z) = \frac{1}{1 + e^{-z}}$$



Therefore

$$H_{\text{sig}} = \phi_{\text{sig}} \circ L_d = \{\mathbf{x} \to \phi_{\text{sig}}(\langle \mathbf{w}, \mathbf{x} \rangle) : \mathbf{w} \in \mathbb{R}^{d+1}\}$$

and $h_{\mathbf{w}}(\mathbf{x}) \in H_{\text{sig}}$ is:

$$h_{\mathbf{w}}(\mathbf{x}) = \frac{1}{1 + e^{-\langle \mathbf{w}, \mathbf{x} \rangle}}$$

Main difference with binary classification with halfspaces: when $\langle {\bf w}, {\bf x} \rangle \approx 0$

- halfspace prediction is deterministically 1 or -1
- $\phi_{\rm Sig}(\langle {f w}, {f x} \rangle) pprox 1/2 \Rightarrow$ uncertainty in predicted label

Loss Function

Need to define how bad it is to predict $h_{\mathbf{w}}(\mathbf{x}) \in [0,1]$ given that true label is $y=\pm 1$

Desiderata

- $h_{\mathbf{w}}(\mathbf{x})$ "large" if y = 1
- $1 h_{\mathbf{w}}(\mathbf{x})$ "large" if y = -1

Note that

$$1 - h_{\mathbf{w}}(\mathbf{x}) = 1 - \frac{1}{1 + e^{-\langle \mathbf{w}, \mathbf{x} \rangle}}$$
$$= \frac{e^{-\langle \mathbf{w}, \mathbf{x} \rangle}}{1 + e^{-\langle \mathbf{w}, \mathbf{x} \rangle}}$$
$$= \frac{1}{1 + e^{\langle \mathbf{w}, \mathbf{x} \rangle}}$$

Then reasonable loss function: increases monotonically with

$$\frac{1}{1 + e^{y\langle \mathbf{w}, \mathbf{x} \rangle}}$$

⇒ reasonable loss function: increases monotonically with

$$1 + e^{-y\langle \mathbf{w}, \mathbf{x} \rangle}$$

Loss function for logistic regression:

$$\ell(h_{\mathbf{w}}, (\mathbf{x}, y)) = \log\left(1 + e^{-y\langle \mathbf{w}, \mathbf{x}\rangle}\right)$$

Therefore, given training set $S = ((\mathbf{x}_1, y_1), \dots, (\mathbf{x}_m, y_m))$ the ERM problem for logistic regression is:

$$\arg\min_{\mathbf{w}\in\mathbb{R}^d}\frac{1}{m}\sum_{i=1}^m\log\left(1+e^{-y_i\langle\mathbf{w},\mathbf{x}_i\rangle}\right)$$

Notes: logistic loss function is a *convex function* \Rightarrow ERM problem can be solved efficiently

Definition may look a bit arbitrary: actually, ERM formulation is the same as the one arising from *Maximum Likelihood Estimation*

Maximum Likelihood Estimation (MLE) [UML, 24.1]

MLE is a statistical approach for finding the parameters that maximize the joint probability of a given dataset assuming a specific parametric probability function.

Note: MLE essentially assumes a generative model for the data

General approach:

- 1 given training set $S = ((\mathbf{x}_1, y_1), \dots, (\mathbf{x}_m, y_m))$, assume each (\mathbf{x}_i, y_i) is i.i.d. from some probability distribution of parameters θ
- 2 consider $\mathbb{P}[S|\theta]$ (likelihood of data given parameters)
- 3 log likelihood: $L(S; \theta) = \log(\mathbb{P}[S|\theta])$
- **4** maximum likelihood estimator: $\hat{\theta} = \arg\max_{\theta} L(S; \theta)$

Logistic Regression and MLE

Assuming $\mathbf{x}_1, \dots, \mathbf{x}_m$ are fixed, the probability that \mathbf{x}_i has label $y_i = 1$ is

$$h_{\mathbf{w}}(\mathbf{x}_i) = \frac{1}{1 + e^{-\langle \mathbf{w}, \mathbf{x}_i \rangle}}$$

while the probability that x_i has label $y_i = -1$ is

$$(1-h_{\mathbf{w}}(\mathbf{x}_i)) = rac{1}{1+e^{\langle \mathbf{w}, \mathbf{x}_i
angle}}$$

Then the likelihood for training set S is:

$$\prod_{i=1}^{m} \left(\frac{1}{1 + e^{-y_i \langle \mathbf{w}, \mathbf{x}_i \rangle}} \right)$$

Therefore the log likelihood is:

$$-\sum_{i=1}^{m}\log\left(1+e^{-y_{i}\langle\mathbf{w},\mathbf{x}_{i}\rangle}\right)$$

And note that the maximum likelihood estimator for w is:

$$\arg\max_{\mathbf{w}\in\mathbb{R}^d} - \sum_{i=1}^m \log\left(1 + e^{-y_i\langle\mathbf{w},\mathbf{x}_i\rangle}\right) = \arg\min_{\mathbf{w}\in\mathbb{R}^d} \sum_{i=1}^m \log\left(1 + e^{-y_i\langle\mathbf{w},\mathbf{x}_i\rangle}\right)$$

⇒ MLE solution is equivalent to ERM solution!

Bibliography

[UML] Chapter 9:

• no 9.1.1