HONG KONG BAPTIST UNIVERSITY 香港浸會大學

DEPARTMENT OF COMPUTER SCIENCE 計算機科學系

COMP7015 Artificial Intelligence

Lecture 5: Machine Learning I — Linear Models and Decision Tree

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Logistics

- Piazza for course Q&A:
  `https://piazza.com/hkbu.edu.hk/fall2022/comp7015/home`
- You are encouraged to post questions & feedback in Piazza. Usually you get quikcer response in Piazza than in email.
- You can also creat a post there to look for teammates for course project.
- Quiz on Oct. 20, covering:
  - Searching
  - Logics
  - Machine Learning Basics

Toy example: how to build a system to detect cats?

List out all rules that specifie the physical characteristics of a cat?

Not feasible:

- Not possible to enumerate all rules.
- Hard to distinguish with similar species.
- Cannot map image pixles to the rules.

How we learned to recognize a cat?

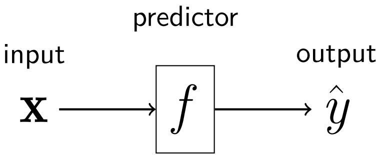
- We did not start from learning a set of rules that define a cat.
- We started by seeing cats and non-cats, in real life, in catoon, etc.

vs.

- **Machine Learning: the same intuitive idea**

$$\boxed{\text{Data}} \xrightarrow{\textit{Learning}} \boxed{\text{Model}}$$

Abstraction of reflex-based models



- Machine learning learns a *model (predictor)* from a collection of *data*.
- With the *model*, we can perform inference to make *predictions*.
- We focus on relfex-based models, which make inference by a fixed set of fast and feedforward operations.
- a reflex-based model (*predictor*) takes some *input* $\mathbf{x}$ and generates some *output* $\hat{y}$.

Types of Machine Learning

- **Supervised Learning**
  - Training with *labeled data*.
  - Dataset: $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$, where $\mathbf{x}$ is the *feature* and y is the *label*.
  - Example: training a cat detector with images of cats and other animals.
- **Unsupervised Learning**
  - Training with *unlabeled data*.
  - Dataset: $\mathcal{D} = \{x_1, \ldots, x_n\}$, where $\mathbf{x}$ is the feature.
  - Example: given a set of images of animals, group images of the same species.
- Semi-supervised Learning
  - A combination of supervised and unsupervised learning.
  - Training with a small amount of *labeled data* and a large amount of *unlabeled data*.
  - Dataset: $\mathcal{D} = \{x_1, \ldots, x_n\} \cup \{(x_1, y_1), \ldots, (x_m, y_m)\}$.

Supervised Learning: Regression

input — predictor — output

$$\mathbf{x} \longrightarrow \boxed{f} \longrightarrow \hat{y} \in \mathbb{R}$$

- The output is a scalar.
- Example: information about house (location, area, etc.) $\rightarrow$ Price

Supervised Learning: Binary classification

predictor (classifier)

input

output (label)

$$\mathbf{x} \longrightarrow \boxed{f} \longrightarrow \hat{y} \in \{+1, -1\}$$

- The output is a binary label of positive ($+1$) or negative (-1).
- Example:
  - Credit card application: information abut applicants $\rightarrow$ Approve or Reject
  - Cat classification: an image $\rightarrow$ Is a cat or Not a cat
  - COVID-19 diagnosis: CT image $\rightarrow$ Has COVID-19 or Does not have COVID-19

Supervised Learning: Multiclass classification

predictor (classifier)

input $\qquad$ output (label)

$$\mathbf{x} \longrightarrow \boxed{f} \longrightarrow \hat{y} \in \{1, 2, \ldots, K\}$$

- The output is one of K possibilities.
- Example:
  - Digit recognition: image of handwritten digit $\rightarrow$ one of $\{0, 1, 2, 3, 4, 5, 6, 7, 8, 9\}$
  - Animal classification: an image $\rightarrow$ one of $\{$Cat, Dog, Wolf, $\ldots\}$
  - COVID-19 diagnosis: CT image $\rightarrow$ Has COVID-19 or Does not have COVID-19

Application: house price prediction (1-dimensional)

- Suppose you have a house and want to sell it.
- How should you price it?
- Intuition: price of a house should be propotional to its area.

Collect some transaction records in the neighbourhood:

$$\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\} \qquad \textit{(Dataset)}$$

x_i: area of the i-th house; y_i: price of the i-th house; n: number of data samples

Fitting a linear regression: $f(x_i) = wx_i + b$, such that $f(x_i)$ is close to y_i.

coefficient/weight *bias*

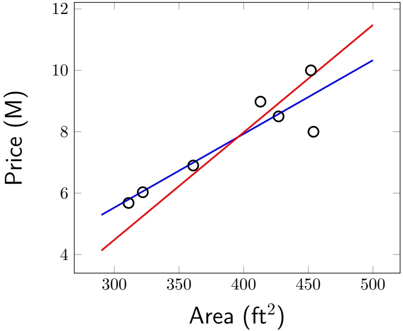
Loss function: how good is a predictor?

Fitting a linear regression: $f(x_i) = wx_i + b$, such that $f(x_i)$ is close to y_i.

- Hypothesis class (a set of all possible hypotheses):

$$\mathcal{F} = \{f_{w,b} : w \in \mathbb{R}, b \in \mathbb{R}\}$$

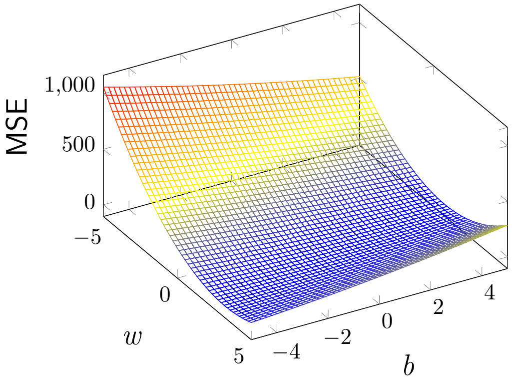
  - Hypothesis 1: $f(x) = 0.024x - 1.67$
  - Hypothesis 2: $f(x) = 0.035x - 6.02$
- Which one to choose?



The **square loss**: $\ell(x_i, y_i, w, b) = (\underbrace{f_{w,b}(x_i) - y_i}_{\text{residual}})^2$

The **mean squared loss (error)**: $\mathrm{MSE}(w, b) = \frac{1}{n} \sum_{(x_i,y_i)\in\mathcal{D}} (f_{w,b}(x_i) - y_i)^2$

Loss function: a visualization of the 1-dimensional MSE



$$\mathrm{MSE}(w, b) = \frac{1}{n} \sum_{(x_i, y_i) \in \mathcal{D}} (f_{w,b}(x_i) - y_i)^2 = \frac{1}{n} \sum_{(x_i, y_i) \in \mathcal{D}} (wx_i + b - y_i)^2$$

Loss minimization framework: how to solve for the best w and b

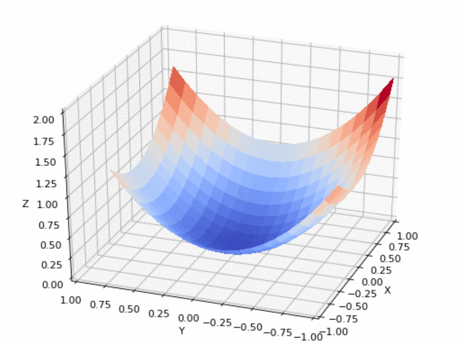
- 1-dimensioanl linear regression: $f_{w,b}(x_i) = wx_i + b$.
- Our goal: to make the mean square loss (MSE) as small as possible.
- **Convert it to the optimization problem:**

$$\begin{aligned}(w^*, b^*) &= \arg\min_{w,b} \mathrm{MSE}(w, b) \\ &= \arg\min_{w,b} \frac{1}{n} \sum_{(x_i, y_i) \in \mathcal{D}} (wx_i + b - y_i)^2\end{aligned}$$

- Algorithm to use: Gradient descent.

Gradient descent algorithm

- **Graident**: the gradient $\nabla_w f(w)$ is the direction of the greatest increase of $f(w)$.
- Start from an initial location, move a bit along the opposite direction of the gradient.



"Rolling a ball down the hill"

- **Graident descent algorithm**

  Initialize $w = 0$ and $b = 0$;

  For $t = 1, \ldots, T$, do

$$w \leftarrow w - \eta \nabla_w \mathrm{MSE}(w, b)$$

$$b \leftarrow b - \eta \nabla_b \mathrm{MSE}(w, b)$$

  - η: step size (how much do we move in each step);
  - $\nabla_w \mathrm{MSE}(w, b)$ and $\nabla_b \mathrm{MSE}(w, b)$: gradient of MSE with respect to w and b, respectively.

Gradient Computation

$$\mathrm{MSE}(w, b) = \frac{1}{n} \sum_{(x_i, y_i) \in \mathcal{D}} (f_{w,b}(x_i) - y_i)^2 = \frac{1}{n} \sum_{(x_i, y_i) \in \mathcal{D}} (wx_i + b - y_i)^2$$

$$\begin{aligned}
\frac{\partial}{\partial w} \mathrm{MSE}(w, b) &= \frac{\partial}{\partial w} \left[\frac{1}{n} \sum_{(x_i, y_i) \in \mathcal{D}} (wx_i + b - y_i)^2 \right] \\
&= \frac{1}{n} \sum_{(x_i, y_i) \in \mathcal{D}} \frac{\partial}{\partial w} (wx_i + b - y_i)^2 \\
\textit{(By chain rule)} \qquad &= \frac{1}{n} \sum_{(x_i, y_i) \in \mathcal{D}} 2(wx_i + b - y_i) \cdot \frac{\partial}{\partial w} (wx_i + b - y_i) \\
&= \frac{1}{n} \sum_{(x_i, y_i) \in \mathcal{D}} 2(wx_i + b - y_i) \cdot x_i
\end{aligned}$$

Summary so far

- **Dataset**: $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$;
- **Linear regression (1-dimensional)**: $f_{w,b}(x_i) = wx_i + b$;
- **Hypothesis class**: $\mathcal{F} = \{f_{w,b} : w \in \mathbb{R}, b \in \mathbb{R}\}$
- **Mean squared loss**: $\mathrm{MSE}(w, b) = \frac{1}{n} \sum_{(x_i,y_i)\in\mathcal{D}} (f_{w,b}(x_i) - y_i)^2$
- **Gradient descent algorithm**: $w \leftarrow w - \eta \nabla_w \mathrm{MSE}(w, b)$

Linear regression for d-dimensional data

- House pricing example: price is also related to the location, building age, facing, etc.
- We represent each data sample by a d dimensional *column vector*: $\mathbf{x} \in \mathbb{R}^d$.
- We say that the data samples have d *features*.
- The dataset: $\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$
- d-dimensioanl linear regression: $f_{\mathbf{w},b}(x_i) = \mathbf{w}^\top \mathbf{x}_i + b$ or $f_{\hat{\mathbf{w}}}(x_i) = \hat{\mathbf{w}}^\top \hat{\mathbf{x}}_i$.

  We can absorb the bias term into the weight vector:

$$\underbrace{\begin{bmatrix} w_1 & w_2 & w_3 & b \end{bmatrix}}_{\hat{\mathbf{w}}=[\mathbf{w};b]\in\mathbb{R}^{d+1}} \cdot \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ 1 \end{bmatrix}}_{\hat{\mathbf{x}}\in\mathbb{R}^{d+1}} = w_1 x_1 + w_2 x_2 + w_3 x_3 + b$$

Linear regression for d-dimensional data

- **Dataset**: $\mathcal{D} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$;
- **Linear regression**: $f_{\mathbf{w}}(\mathbf{x}_i) = \mathbf{w}^\top \mathbf{x}_i$

  (from now on, we directly use $\mathbf{w} \in \mathbb{R}^{d+1}$ *instead of* $\hat{\mathbf{w}}$ *for simplicity)*;
- **Hypothesis class**: $\mathcal{F} = \{f_{\mathbf{w}} : \mathbf{w} \in \mathbb{R}^{d+1}\}$
- **Mean squared loss** (objective function):

$$\mathrm{MSE}(\mathbf{w}) = \frac{1}{n} \sum_{(\mathbf{x}_i, y_i) \in \mathcal{D}} (\mathbf{w}^\top \mathbf{x}_i - y_i)^2$$

- **Gradient descent algorithm**: $\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla_{\mathbf{w}} \mathrm{MSE}(\mathbf{w})$

Linear regression for d-dimensional data

- Writing it the matrix form:

$$\mathbf{X} = \begin{bmatrix} \mathbf{x_1}^\top & 1 \\ \mathbf{x_2}^\top & 1 \\ \vdots & \vdots \\ \mathbf{x_n}^\top & 1 \end{bmatrix} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1d} & 1 \\ x_{21} & x_{22} & \cdots & x_{2d} & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nd} & 1 \end{bmatrix} \in \mathbb{R}^{n\times(d+1)}$$

$$\mathbf{y} = \begin{bmatrix} y_1 & y_2 & \cdots & y_n \end{bmatrix}^\top \in \mathbb{R}^n$$

- Each row of $\mathbf{X}$: a *data sample*
- Each column of $\mathbf{X}$: a *feature*
- The mean squared loss can then be written as: $\mathrm{MSE}(\mathbf{w}) = (\mathbf{Xw} - \mathbf{y})^\top(\mathbf{Xw} - \mathbf{y})$
- Gradient in matrix form: $\nabla_{\mathbf{w}} \mathrm{MSE}(\mathbf{w}) = 2\mathbf{X}^\top(\mathbf{Xw} - \mathbf{y})$

Linear regression for d-dimensional data

$$\mathrm{MSE}(\mathbf{w}) = (\mathbf{X}\mathbf{w} - \mathbf{y})^\top (\mathbf{X}\mathbf{w} - \mathbf{y})$$

Gradient in matrix form:

$$\begin{aligned}
\nabla_{\mathbf{w}} \mathrm{MSE}(\mathbf{w}) &= \nabla_{\mathbf{w}} \left[(\mathbf{X}\mathbf{w} - \mathbf{y})^\top (\mathbf{X}\mathbf{w} - \mathbf{y}) \right] \\
&= \nabla_{\mathbf{w}} \left[(\mathbf{X}\mathbf{w})^\top (\mathbf{X}\mathbf{w}) - (\mathbf{X}\mathbf{w})^\top \mathbf{y} - \mathbf{y}^\top (\mathbf{X}\mathbf{w}) + \mathbf{y}^\top \mathbf{y} \right] \\
&= \nabla_{\mathbf{w}} \left[\mathbf{w}^\top (\mathbf{X}^\top \mathbf{X}) \mathbf{w} - 2 (\mathbf{X}^\top \mathbf{y})^\top \mathbf{w} \right] \\
&= 2\mathbf{X}^\top \mathbf{X}\mathbf{w} - 2\mathbf{X}^\top \mathbf{y} \\
&= 2\mathbf{X}^\top (\mathbf{X}\mathbf{w} - \mathbf{y})
\end{aligned}$$

Summary of Linear Regression

input $\quad$ predictor $\quad$ output

$$\mathbf{X} \longrightarrow \boxed{f_{\mathbf{w}}} \longrightarrow \hat{\mathbf{y}} \in \mathbb{R}^n \xleftrightarrow{\text{loss function}} \mathbf{y} \in \mathbb{R}^n$$

$$\mathrm{MSE}(\mathbf{w}) = (\mathbf{X}\mathbf{w} - \mathbf{y})^\top (\mathbf{X}\mathbf{w} - \mathbf{y})$$

- Learning $\mathbf{w}$ by minimizing the loss function.
- Minimizing the loss function using gradient descent.

Linear Classification

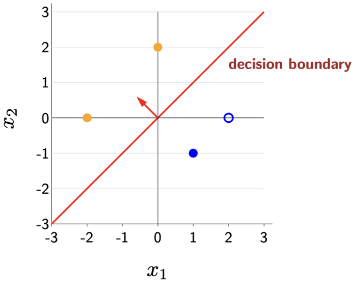
Can we use linear regression for classification?.

predictor (classifier)

input

output (label)

$$\mathbf{x} \longrightarrow \boxed{f} \longrightarrow \hat{y} \in \{+1, -1\}$$



The **decision boundary** devides the data space into two regions: one would have output of $+1$ and the other would have output of -1.

But our output from linear regression is a real number, instead of a binary label.

Unit-step function

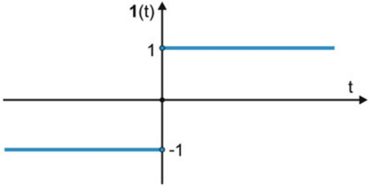
We need to transform the real number output $\hat{y} \in \mathbb{R}$ to a binary value $\hat{y} \in \{+1, -1\}$.

Unit-step function:

$$f(\mathbf{x}) = \text{sign}(\underbrace{\mathbf{w}^\top \mathbf{x}}_{\text{Score}})$$

The score on an example $(\mathbf{x}, y)$ is $\mathbf{w}^\top \mathbf{x}$: how confident we are in predicting $+1$.

$$\text{sign}(t) = \begin{cases} +1 & \text{if } t > 0, \\ -1 & \text{if } t < 0, \\ 0 & \text{if } t = 0 \end{cases}$$



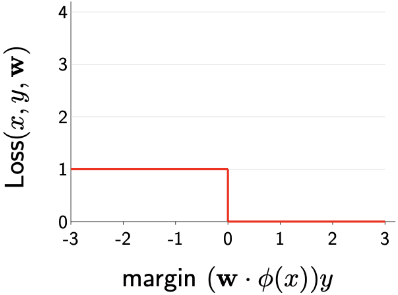
Zero-one loss function

Predicted label: $f(\mathbf{x}) = \text{sign}(\mathbf{w}^\top \mathbf{x})$
Target label: y

We define the **zero-one loss** as:

$$\text{Loss}_{0-1}(\mathbf{x}, y, \mathbf{w}) = \underbrace{\mathbb{1}\left[f_{\mathbf{w}}(\mathbf{x}) \neq y\right]}_{\text{counting how many mistakes we make}}$$

$$= \mathbb{1}\left[\underbrace{(\mathbf{w}^\top \mathbf{x})y}_{\text{margin}} \leq 0\right]$$



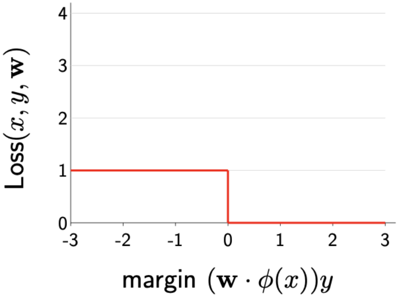
The margin on an example $(\mathbf{x}, y)$ is $(\mathbf{w}^\top \mathbf{x})y$: how correct we are.

Optimization: gradient descent with zero-one loss?

$$\text{Loss}_{0-1}(\mathbf{x}, y, \mathbf{w}) = \mathbb{1}\left[(\mathbf{w}^\top \mathbf{x})y \le 0\right]$$

What is the gradient w.r.t. $\mathbf{w}$ in the **zero-one loss**?

Almost zero everywhere!



What went wrong?

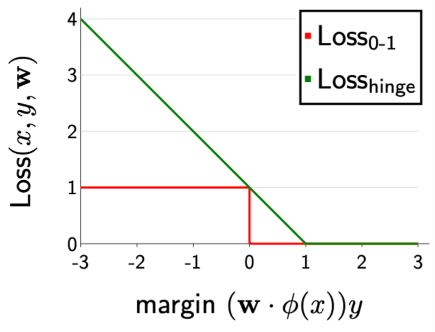
- In MSE, when we move $\mathbf{w}$ a little bit, the residuals will change. The loss of some data points get smaller while some others get larger.
- In zero-one loss, moving $\mathbf{w}$ a tiny bit changes very little the loss, until we make a big change that makes an example cross the decision boundary.

Hinge loss function

The margin on an example $(\mathbf{x}, y)$ is $(\mathbf{w}^\top \mathbf{x})y$: how correct we are.

$$\mathrm{Loss}_{\text{hinge}}(\mathbf{x}, y, \mathbf{w}) = \max\{1 - (\mathbf{w}^\top \mathbf{x})y, 0\}$$

- In order to get zero loss, the model has to classify all points correctly and confidently (margin ≥ 1).
- If the model makes confident error, it incurs a linearly increasing penalty.
- Application: Support Vector Machine (SVM)

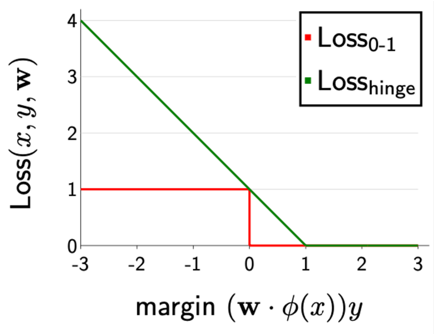


Optimization: gradient descent with hinge loss

$$\text{Loss}_{\text{hinge}}(\mathbf{x}, y, \mathbf{w}) = \max\{1 - (\mathbf{w}^\top \mathbf{x})y, 0\}$$

$$\nabla \text{Loss}_{\text{hinge}}(\mathbf{x}, y, w) = \begin{cases} -\mathbf{w}y & \text{if}(\mathbf{w}^\top \mathbf{x})y < 1 \\ 0 & \text{otherwise} \end{cases}$$

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \left[\frac{1}{n} \sum_{(\mathbf{x}_i, y_i) \in \mathcal{D}} \nabla \text{Loss}_{\text{hinge}}(\mathbf{x}, y, w) \right]$$



Sigmoid function

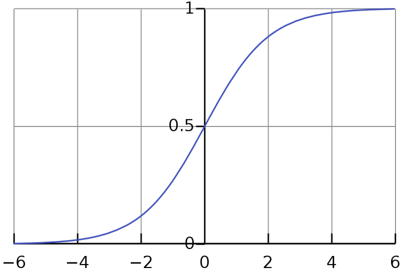
The sigmoid function (logistic function) maps a real value to be between $(0, 1)$:

$$y = \sigma(z) = \frac{1}{1 + e^{-z}} = \frac{e^z}{1 + e^z}$$

Substitute z with our score $\mathbf{w}^\top \mathbf{x}$, we have:

$$f_{\mathbf{w}}(\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^\top \mathbf{x})}$$

This model is called **logistic regression**.

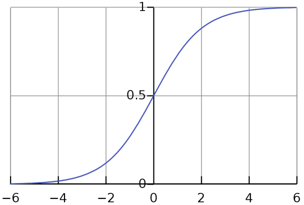


the sigmoid function

Logistic regression

Consider this transfromation retruns a "probability":

- $p(y=+1|x) = \sigma(\mathbf{w}^\top \mathbf{x}) = \frac{1}{1+\exp(-\mathbf{w}^\top \mathbf{x})}$
- $p(y=-1|x) = 1 - \sigma(\mathbf{w}^\top \mathbf{x}) = \frac{\exp(-\mathbf{w}^\top \mathbf{x})}{1+\exp(-\mathbf{w}^\top \mathbf{x})} = \frac{1}{1+\exp(+\mathbf{w}^\top \mathbf{x})}$



- The *likelihood* (probability of observing all data samples):

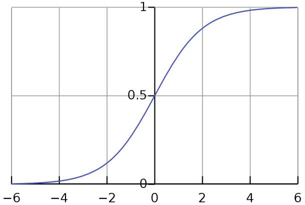
$$\prod_{(\mathbf{x}_i, y_i)\in\mathcal{D}} p(y_i=+1|\mathbf{x})^{\mathbb{1}[y_i=+1]} p(y_i=-1|\mathbf{x})^{\mathbb{1}[y_i=-1]}$$

- The *log likelihood* (numerically more stable):

$$\ell(\mathbf{w}) = \sum_{(\mathbf{x}_i, y_i)\in\mathcal{D}} \mathbb{1}[y_i=+1]\log p(y_i=+1|\mathbf{x}) + \mathbb{1}[y_i=-1]\log p(y_i=-1|\mathbf{x})$$

Logistic regression

Consider this transfromation retruns a "probability":



- $p(y=+1|x) = \sigma(\mathbf{w}^\top \mathbf{x}) = \frac{1}{1+\exp(-\mathbf{w}^\top \mathbf{x})}$
- $p(y=-1|x) = 1-\sigma(\mathbf{w}^\top \mathbf{x}) = \frac{\exp(-\mathbf{w}^\top \mathbf{x})}{1+\exp(-\mathbf{w}^\top \mathbf{x})} = \frac{1}{1+\exp(+\mathbf{w}^\top \mathbf{x})}$

- The *log likelihood* (numerically more stable):

$$\ell(\mathbf{w}) = \sum_{(\mathbf{x}_i, y_i)\in\mathcal{D}} \mathbb{1}[y_i=+1]\log p(y_i=+1|\mathbf{x}) + \mathbb{1}[y_i=-1]\log p(y_i=-1|\mathbf{x})$$

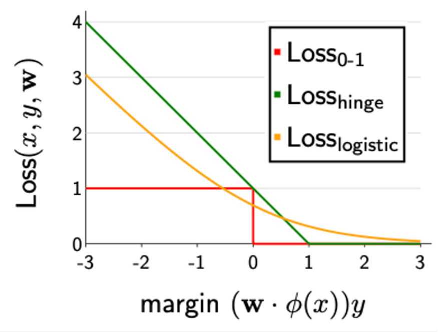
- We can maximize the likelihood, or equivalently, minimize the negative likelihood:

$$\text{Loss}(\mathbf{x}, y, \mathbf{w}) = \log(1+\exp(-(\mathbf{w}^\top \mathbf{x})y))$$

Logistic regression

$$\text{Loss}_{\text{logistic}}(\mathbf{x}, y, \mathbf{w}) = \log(1 + \exp(-(\mathbf{w}^\top \mathbf{x})y))$$

$$\text{TrainLoss}_{\text{logistic}}(\mathbf{w}) = \sum_{(\mathbf{x},y)\in\mathcal{D}_{\text{train}}} \log(1 + \exp(-(\mathbf{w}^\top \mathbf{x})y))$$



- Try to increase margin even when it already exceeds 1.
- Always have non-zero loss.
- Use gradient descent as in previous examples: $\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla_{\mathbf{w}} \text{TrainLoss}(\mathbf{w})$

Exercise: compute the gradient

- For the loss function of logistic regression:

$$\mathrm{TrainLoss}_{\mathsf{logistic}}(\mathbf{w}) = \sum_{(\mathbf{x},y)\in\mathcal{D}_{\mathsf{train}}} \log(1+\exp(-(\mathbf{w}^\top\mathbf{x})y))$$

- Compute its gradient $\nabla_{\mathbf{w}} \mathrm{TrainLoss}(\mathbf{w})$

$$\nabla_{\mathbf{w}} \mathrm{TrainLoss}(\mathbf{w}) = -\sum_{(\mathbf{x},y)\in\mathcal{D}_{\mathsf{train}}} y\frac{\exp(-(\mathbf{w}^\top\mathbf{x})y)}{1+\exp(-(\mathbf{w}^\top\mathbf{x})y)}\mathbf{x}$$

Summary of Part 1 (Linear Models)

$$\underbrace{\mathbf{w} \cdot \phi(x)}_{\text{score}}$$

	Regression	Classification
Prediction $f_{\mathbf{w}}(x)$	score	sign(score)
Relate to target y	residual (score $- y$)	margin (score y)
Loss functions	squared absolute deviation	zero-one hinge logistic
Algorithm	gradient descent	gradient descent