CSC 411: Introduction to Machine Learning

Lecture 7: Linear Classification

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Overview

- Classification: predicting a discrete-valued target
  - Binary classification: predicting a binary-valued target
- Examples
  - predict whether a patient has a disease, given the presence or absence of various symptoms
  - classify e-mails as spam or non-spam
  - predict whether a financial transaction is fraudulent

Overview

Binary linear classification

- **classification:** predict a discrete-valued target
- **binary:** predict a binary target $t \in \{0, 1\}$
  - Training examples with $t = 1$ are called positive examples, and training examples with $t = 0$ are called negative examples. Sorry.
- **linear:** model is a linear function of $\mathbf{x}$, followed by a threshold:

$$z = \mathbf{w}^T \mathbf{x} + b$$

$$y = \begin{cases} 1 & \text{if } z \geq r \\ 0 & \text{if } z < r \end{cases}$$

Some simplifications

Eliminating the threshold

- We can assume WLOG that the threshold $r = 0$:

$$\mathbf{w}^T\mathbf{x} + b \geq r \quad \iff \quad \mathbf{w}^T\mathbf{x} + \underbrace{b - r}_{\triangleq b'} \geq 0.$$

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Eliminating the bias

- Add a dummy feature x_0 which always takes the value 1. The weight w_0 is equivalent to a bias (i.e. $w_0 \equiv b$)

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Simplified model

$$z = \mathbf{w}^T\mathbf{x}$$

$$y = \begin{cases} 1 & \text{if } z \geq 0 \\ 0 & \text{if } z < 0 \end{cases}$$

Examples

- Let's consider some simple examples to examine the properties of our model
- Forget about generalization and suppose we just want to learn Boolean functions

Examples

NOT

x_0	x_1	t
1	0	1
1	1	0

- This is our "training set"
- What conditions are needed on w_0, w_1 to classify all examples?
  - When $x_1 = 0$, need: $w_0 x_0 + w_1 x_1 > 0 \iff w_0 > 0$
  - When $x_1 = 1$, need: $w_0 x_0 + w_1 x_1 < 0 \iff w_0 + w_1 < 0$
- Example solution: $w_0 = 1, w_1 = -2$
- Is this the only solution?

Examples

AND

x_0	x_1	x_2	t
1	0	0	0
1	0	1	0
1	1	0	0
1	1	1	1

Examples

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x_0	x_1	x_2	t
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need: $w_0 < 0$

Examples

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need: $w_0 < 0$

need: $w_0 + w_2 < 0$

Examples

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Examples

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need: $w_0 + w_1 + w_2 > 0$

Examples

AND

x_0	x_1	x_2	t
1	0	0	0
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1	1	0	0
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need: $w_0 < 0$

need: $w_0 + w_2 < 0$

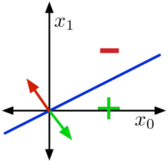
need: $w_0 + w_1 < 0$

need: $w_0 + w_1 + w_2 > 0$

Example solution: $w_0 = -1.5,\ w_1 = 1,\ w_2 = 1$

The Geometric Picture

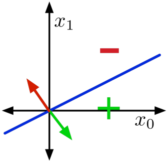
Input Space, or Data Space for NOT example

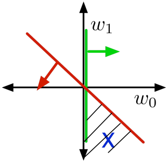


x_0	x_1	t
1	0	1
1	1	0

- Training examples are points
- Hypotheses **w** can be represented by half-spaces
  $H_+ = \{\mathbf{x} : \mathbf{w}^T\mathbf{x} \geq 0\}$, $H_- = \{\mathbf{x} : \mathbf{w}^T\mathbf{x} < 0\}$
  - The boundaries of these half-spaces pass through the origin (why?)
- The boundary is the decision boundary: $\{\mathbf{x} : \mathbf{w}^T\mathbf{x} = 0\}$
  - In 2-D, it's a line, but think of it as a hyperplane
- If the training examples can be separated by a linear decision rule, they are linearly separable.

Weight Space





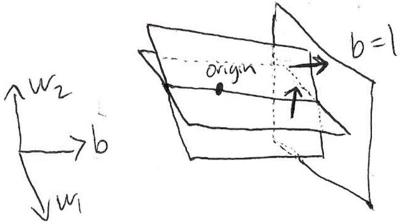
$w_0 > 0$

$w_0 + w_1 < 0$

- Hypotheses $\mathbf{w}$ are points
- Each training example $\mathbf{x}$ specifies a half-space $\mathbf{w}$ must lie in to be correctly classified
- For NOT example:
  - $x_0 = 1, x_1 = 0, t = 1 \implies (w_0, w_1) \in \{\mathbf{w} : w_0 > 0\}$
  - $x_0 = 1, x_1 = 1, t = 0 \implies (w_0, w_1) \in \{\mathbf{w} : w_0 + w_1 < 0\}$
- The region satisfying all the constraints is the feasible region; if this region is nonempty, the problem is feasible

The Geometric Picture

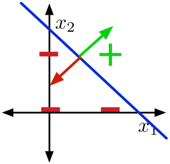
- The **AND** example requires three dimensions, including the dummy one.
- To visualize data space and weight space for a 3-D example, we can look at a 2-D slice:



- The visualizations are similar, except that the decision boundaries and the constraints need not pass through the origin.
  - The origin in our visualization may not have all coordinates set to 0!

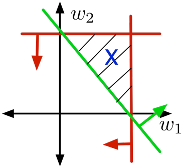
Visualizations of the **AND** example

Data Space



Slice for $x_0 = 1$

Weight Space

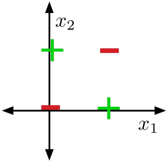


Slice for $w_0 = -1$

- Recall constraints:
  - $w_0 < 0$
  - $w_0 + w_2 < 0$
  - $w_0 + w_1 < 0$
  - $w_0 + w_1 + w_2 > 0$
- Why are only 3 constraints shown?

The Geometric Picture

Some datasets are not linearly separable, e.g. **XOR**



Proof coming next lecture...

Overview

- **Recall: binary linear classifiers.** Targets $t \in \{0, 1\}$

$$z = \mathbf{w}^T \mathbf{x} + b$$
$$y = \begin{cases} 1 & \text{if } z \geq 0 \\ 0 & \text{if } z < 0 \end{cases}$$

- How can we find good values for $\mathbf{w}, b$?
- If training set is separable, we can solve for $\mathbf{w}, b$ using linear programming
- If it's not separable, the problem is harder

Loss functions

- Instead: define loss function then try to minimize the resulting cost function
  - Recall: cost is loss averaged over the training set
- Seemingly obvious loss function: 0-1 loss

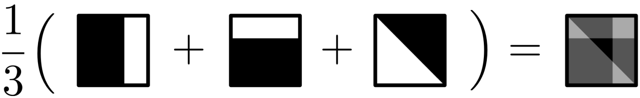
$$\begin{aligned} \mathcal{L}_{0-1}(y, t) &= \begin{cases} 0 & \text{if } y = t \\ 1 & \text{if } y \neq t \end{cases} \\ &= \mathbb{I}[y \neq t] \end{aligned}$$

Attempt 1: 0-1 loss

- As always, the cost $\mathcal{J}$ is the average loss over training examples; for 0-1 loss, this is the error rate:

$$\mathcal{J} = \frac{1}{N} \sum_{i=1}^{N} \mathbb{I}[y^{(i)} \neq t^{(i)}]$$

- Visualization of cost function in weight space for 3 examples:



Attempt 1: 0-1 loss

- Problem: how to optimize? In general, a hard problem
- (Guruswami and Raghavendra) "For arbitrary $\epsilon, \delta > 0$, we prove that given a set of examples-label pairs from the hypercube a fraction $(1 - \epsilon)$ of which can be explained by a halfspace, it is NP-hard to find a halfspace that correctly labels a fraction $(1/2 + \delta)$ of the examples."

Attempt 1: 0-1 loss

- Let's try the one optimization tool in our arsenal: gradient descent
- Chain rule:

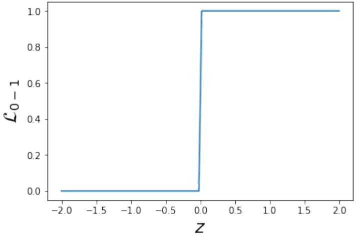
$$\frac{\partial \mathcal{L}_{0-1}}{\partial w_j} = \frac{\partial \mathcal{L}_{0-1}}{\partial z} \frac{\partial z}{\partial w_j}$$

Attempt 1: 0-1 loss

- Let's try the one optimization tool in our arsenal: gradient descent
- Chain rule:

$$\frac{\partial \mathcal{L}_{0-1}}{\partial w_j} = \frac{\partial \mathcal{L}_{0-1}}{\partial z} \frac{\partial z}{\partial w_j}$$

- But $\partial \mathcal{L}_{0-1} / \partial z$ is zero everywhere it's defined!



  - $\partial \mathcal{L}_{0-1} / \partial w_j = 0$ means that changing the weights by a very small amount probably has no effect on the loss.
  - The gradient descent update is a no-op.

Attempt 2: Linear Regression

- Sometimes we can replace the loss function we care about with one which is easier to optimize. This is known as a surrogate loss function.
- One problem with $\mathcal{L}_{0-1}$: defined in terms of final prediction, which inherently involves a discontinuity
- Instead, define loss in terms of $\mathbf{w}^T\mathbf{x} + b$ directly
  - Redo notation for convenience: $y = \mathbf{w}^T\mathbf{x} + b$

Attempt 2: Linear Regression

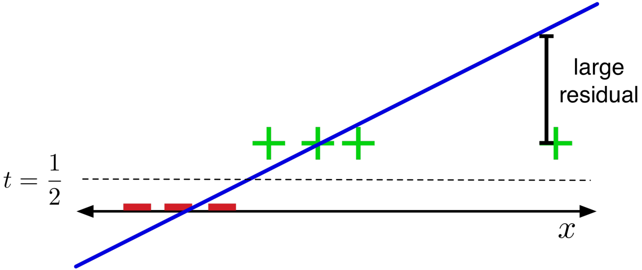
- We already know how to fit a linear regression model. Can we use this instead?

$$y = \mathbf{w}^\top \mathbf{x} + b$$
$$\mathcal{L}_{\mathrm{SE}}(y, t) = \frac{1}{2}(y - t)^2$$

- Doesn't matter that the targets are actually binary.
- For this loss function, it makes sense to make final predictions by thresholding y at $\frac{1}{2}$ (why?)

Attempt 2: Linear Regression

The problem:



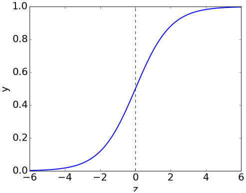
- The loss function hates when you make correct predictions with high confidence!
- If $t = 1$, it's more unhappy about $y = 10$ than $y = 0$.

Attempt 3: Logistic Activation Function

- There's obviously no reason to predict values outside [0, 1]. Let's squash y into this interval.

- The logistic function is a kind of sigmoidal, or S-shaped, function:

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



- A linear model with a logistic nonlinearity is known as log-linear:

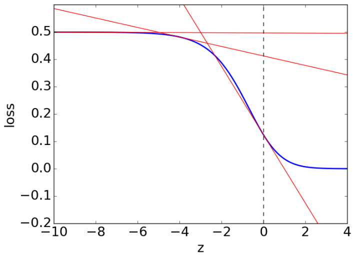
$$z = \mathbf{w}^\top \mathbf{x} + b$$
$$y = \sigma(z)$$
$$\mathcal{L}_{\mathrm{SE}}(y, t) = \frac{1}{2}(y - t)^2.$$

- Used in this way, σ is called an activation function, and z is called the logit.

Attempt 3: Logistic Activation Function

The problem:

(plot of $\mathcal{L}_{\mathrm{SE}}$ as a function of z, assuming $t = 1$)



$$\frac{\partial \mathcal{L}}{\partial w_j} = \frac{\partial \mathcal{L}}{\partial z} \frac{\partial z}{\partial w_j}$$

$$w_j \leftarrow w_j - \alpha \frac{\partial \mathcal{L}}{\partial w_j}$$

Attempt 3: Logistic Activation Function

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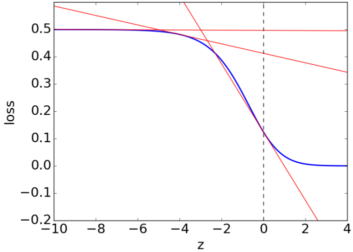


$$\frac{\partial \mathcal{L}}{\partial w_j} = \frac{\partial \mathcal{L}}{\partial z} \frac{\partial z}{\partial w_j}$$

$$w_j \leftarrow w_j - \alpha \frac{\partial \mathcal{L}}{\partial w_j}$$

- For $z << 0$, $\frac{\partial \mathcal{L}}{\partial z} \approx 0$ (check!) $\implies \frac{\partial \mathcal{L}}{\partial w_j} \approx 0 \implies$ update to w_j is small
- If the prediction is really wrong, shouldn't you take a large step?

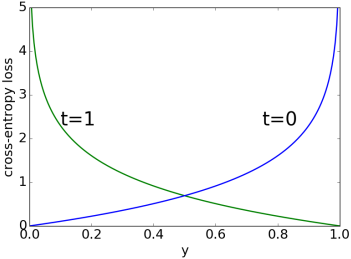
Logistic Regression

- Because $y \in [0, 1]$, we can interpret it as the estimated probability that $t = 1$.
- The pundits who were 99% confident Clinton would win were much more wrong than the ones who were only 90% confident.

Logistic Regression

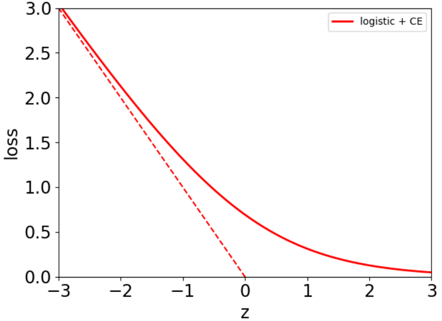
- Because $y \in [0, 1]$, we can interpret it as the estimated probability that $t = 1$.
- The pundits who were 99% confident Clinton would win were much more wrong than the ones who were only 90% confident.
- Cross-entropy loss captures this intuition:

$$\mathcal{L}_{\mathrm{CE}}(y, t) = \begin{cases} -\log y & \text{if } t = 1 \\ -\log(1 - y) & \text{if } t = 0 \end{cases}$$
$$= -t \log y - (1 - t) \log(1 - y)$$



Logistic Regression:

$$
\begin{aligned}
z &= \mathbf{w}^\top \mathbf{x} + b \\
y &= \sigma(z) \\
&= \frac{1}{1 + e^{-z}} \\
\mathcal{L}_{\mathrm{CE}} &= -t \log y - (1 - t) \log(1 - y)
\end{aligned}
$$



[[gradient derivation in the notes]]

Logistic Regression

- Problem: what if $t = 1$ but you're really confident it's a negative example ($z \ll 0$)?
- If y is small enough, it may be numerically zero. This can cause very subtle and hard-to-find bugs.

$$
\begin{aligned}
y &= \sigma(z) & \Rightarrow\ & y \approx 0 \\
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Logistic Regression

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$$\begin{aligned} y &= \sigma(z) & \Rightarrow y \approx 0 \\ \mathcal{L}_{\mathrm{CE}} &= -t \log y - (1-t) \log(1-y) & \Rightarrow \text{ computes } \log 0 \end{aligned}$$

- Instead, we combine the activation function and the loss into a single logistic-cross-entropy function.

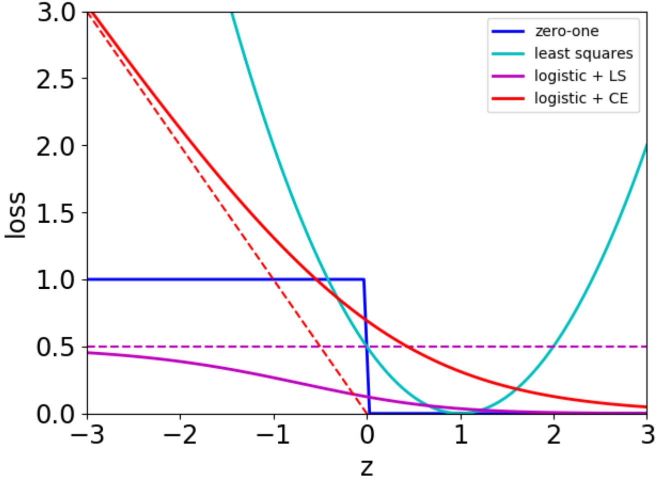
$$\mathcal{L}_{\mathrm{LCE}}(z, t) = \mathcal{L}_{\mathrm{CE}}(\sigma(z), t) = t \log(1 + e^{-z}) + (1-t) \log(1 + e^{z})$$

- Numerically stable computation:

```
E = t * np.logaddexp(0, -z) + (1-t) * np.logaddexp(0, z)
```

Logistic Regression

Comparison of loss functions:



Logistic Regression

Comparison of gradient descent updates:

- Linear regression:

$$\mathbf{w} \leftarrow \mathbf{w} - \frac{\alpha}{N} \sum_{i=1}^{N} (y^{(i)} - t^{(i)})\, \mathbf{x}^{(i)}$$

- Logistic regression:

$$\mathbf{w} \leftarrow \mathbf{w} - \frac{\alpha}{N} \sum_{i=1}^{N} (y^{(i)} - t^{(i)})\, \mathbf{x}^{(i)}$$

Logistic Regression

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- Not a coincidence! These are both examples of matching loss functions, but that's beyond the scope of this course.