Logistic Regression

Lecture 12 (b)

Machine Learning
Fall 2015

THE UNIVERSITY OF UTAH

Where are we?

We have seen the following ideas

- Linear models
- Learning as loss minimization
- Bayesian learning criteria (MAP and MLE estimation)
- The Naïve Bayes classifier

This lecture

- Logistic regression
- Connection to Naïve Bayes
- Training a logistic regression classifier
- Back to loss minimization

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Logistic Regression: Setup

- The setting
  - Binary classification
  - Inputs: Feature vectors $\mathbf{x} \in \Re^{\mathrm{d}}$
  - Labels: $\mathbf{y} \in \{-1, +1\}$
- Training data
  - S = $\{(\mathbf{x}_i, \mathbf{y}_i)\}$, m examples

Classification, but…

The output y is discrete valued (-1 or 1)

Instead of predicting the output, let us try to predict P(y = 1 | **x**)

Expand hypothesis space to functions whose output is [0-1]

- Original problem: $\Re^{\mathrm{d}} \rightarrow \{-1, 1\}$
- Modified problem: $\Re^{\mathrm{d}} \rightarrow [0\text{-}1]$
- Effectively make the problem a regression problem

Many hypothesis spaces possible

The Sigmoid function

The hypothesis space for logistic regression: All functions of the form

$$h_{\mathbf{w}}(\mathbf{x}) = \sigma(\mathbf{w}^T\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^T\mathbf{x})}$$

That is, a linear function, composed with a sigmoid function (the logistic function) σ

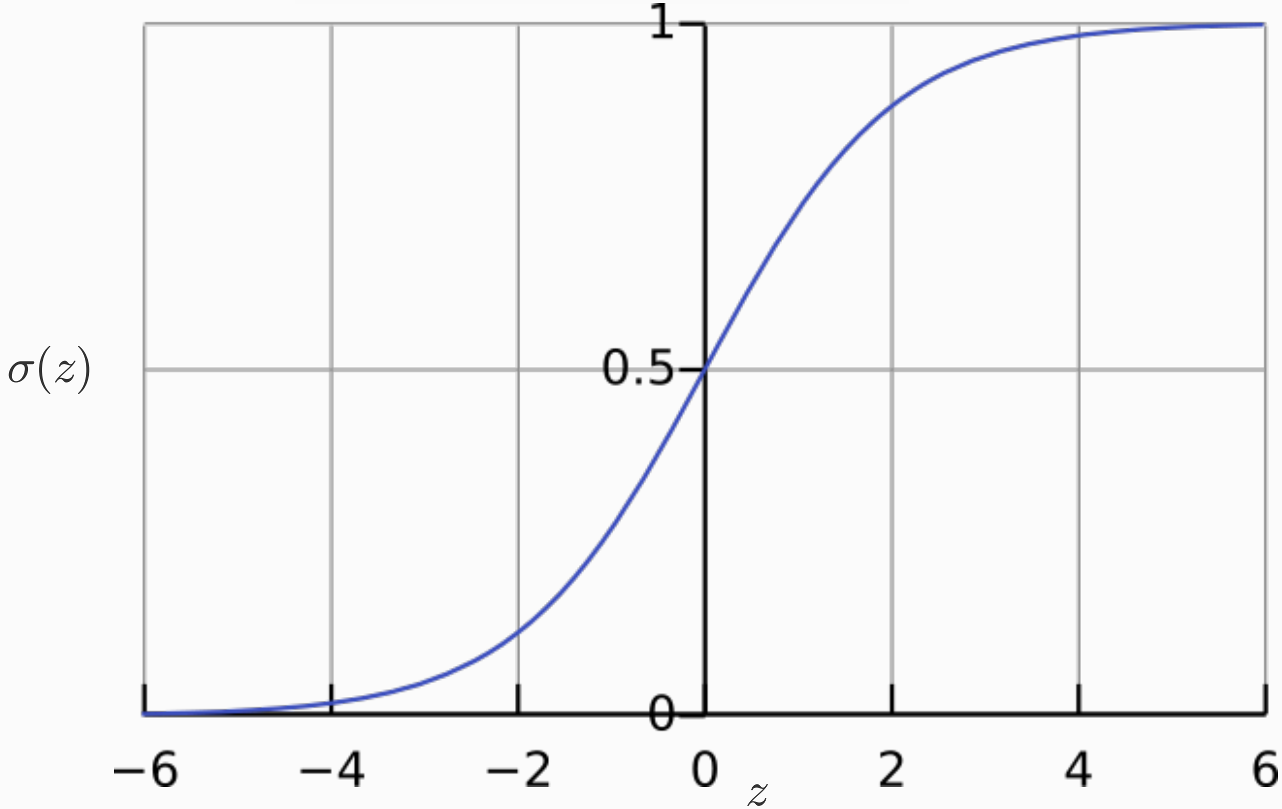
$$\sigma(z) = \frac{1}{1 + \exp(-z)}$$

What is the domain and the range of the sigmoid function?

This is a reasonable choice. We will see why later

The Sigmoid function

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



The Sigmoid function

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

What is its derivative with respect to z?

$$\frac{d\sigma}{dz} = \frac{d}{dz}\frac{1}{1+\exp(-z)}$$

The Sigmoid function

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What is its derivative with respect to z?

$$\begin{aligned}
\frac{d\sigma}{dz} &= \frac{d}{dz}\frac{1}{1+\exp(-z)} \\
&= \frac{1}{(1+\exp(-z))^2} \cdot \exp(-z)
\end{aligned}$$

The Sigmoid function

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What is its derivative with respect to z?

$$\begin{aligned}
\frac{d\sigma}{dz} &= \frac{d}{dz}\frac{1}{1 + \exp(-z)} \\
&= \frac{1}{(1 + \exp(-z))^2} \cdot \exp(-z) \\
&= \left(1 - \frac{1}{1 + \exp(-z)}\right) \cdot \frac{1}{1 + \exp(-z)} \\
&= \sigma(z)\left(1 - \sigma(z)\right).
\end{aligned}$$

Predicting probabilities

According to the logistic regression model, we have

$$P(y = 1|\mathbf{x}; \mathbf{w}) = \sigma(\mathbf{w}^T\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^T\mathbf{x})}$$

$$P(y = -1|\mathbf{x}; \mathbf{w}) = 1 - \sigma(\mathbf{w}^T\mathbf{x}) = \frac{\exp(-\mathbf{w}^T\mathbf{x})}{1 + \exp(-\mathbf{w}^T\mathbf{x})}$$

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$$\frac{1}{1+\exp(\mathbf{w}^T\mathbf{x})}$$

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Or equivalently

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

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Note that we are directly modeling P(y | x) rather than P(x |y) and P(y)

Or equivalently

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

Predicting a label with logistic regression

$$P(y = 1|\mathbf{x}; \mathbf{w}) = \sigma(\mathbf{w}^T\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^T\mathbf{x})}$$

- Compute P(y =1 | x; w)

- If this is greater than half, predict 1 else predict -1
  - What does this correspond to in terms of $\mathbf{w}^T\mathbf{x}$?

  - Prediction = sgn($\mathbf{w}^T\mathbf{x}$)

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Naïve Bayes and Logistic regression

Remember that the naïve Bayes decision is a linear function

$$\log \frac{P(y = -1|\mathbf{x})}{P(y = 1|\mathbf{x})} = \mathbf{w}^T\mathbf{x}$$

Here, the P's represent the naïve Bayes probabilities

Naïve Bayes and Logistic regression

Remember that the naïve Bayes decision is a linear function

$$\log \frac{P(y = -1|\mathbf{x})}{P(y = 1|\mathbf{x})} = \mathbf{w}^T\mathbf{x}$$

But we also know that $P(y = -1|\mathbf{x}) = 1 - P(y = 1|\mathbf{x})$

Naïve Bayes and Logistic regression

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But we also know that $P(y = -1|\mathbf{x}) = 1 - P(y = 1|\mathbf{x})$

Substituting in the above expression, we get

$$P(y = 1|\mathbf{x}; \mathbf{w}) = \sigma(\mathbf{w}^T \mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^T \mathbf{x})}$$

Naïve Bayes and Logistic regression

Remember that the naïve Bayes decision is a linear function

$$\log \frac{P(y=-1|\mathbf{x})}{P(y=1|\mathbf{x})} = \mathbf{w}^T\mathbf{x}$$

But we a

That is, both naïve Bayes and logistic regression try to compute the same posterior distribution over the outputs

Naïve Bayes is a generative model

Logistic Regression is the discriminative version

Substitut

$$P(y=1|\mathbf{x};\mathbf{w}) = \sigma(\mathbf{w}^T\mathbf{x}) = \frac{1}{1+\exp(-\mathbf{w}^T\mathbf{x})}$$

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Maximum likelihood estimation

Let's get back to the problem of learning

- Training data
  - S = $\{(\mathbf{x}_i, \mathbf{y}_i)\}$, m examples
- What we want
  - Find a **w** such that P(S | **w**) is maximized
  - We know that our examples are drawn independently and are identically distributed (i.i.d)
  - How do we proceed?

Maximum likelihood estimation

$$\arg\max_{\mathbf{w}} P(S|\mathbf{w}) = \arg\max_{\mathbf{w}} \prod_{i=1}^{m} P(y_i|\mathbf{x}_i, \mathbf{w})$$

The usual trick: Convert products to sums by taking log

Recall that this works only because log is an increasing function and the maximizer will not change

Maximum likelihood estimation

$$\arg\max_{\mathbf{w}} P(S|\mathbf{w}) = \arg\max_{\mathbf{w}} \prod_{i=1}^{m} P(y_i|\mathbf{x}_i, \mathbf{w})$$

Equivalent to solving

$$\max_{\mathbf{w}} \sum_{i=1}^{m} \log P(y_i|\mathbf{x}_i, \mathbf{w})$$

Maximum likelihood estimation

$$\arg\max_{\mathbf{w}} P(S|\mathbf{w}) = \arg\max_{\mathbf{w}} \prod_{i=1}^{m} P(y_i|\mathbf{x}_i, \mathbf{w})$$

$$\max_{\mathbf{w}} \sum_{i=1}^{m} \log P(y_i|\mathbf{x}_i, \mathbf{w})$$

But (by definition) we know that

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

Maximum likelihood estimation

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$$\max_{\mathbf{w}} \sum_{i=1}^{m} \log P(y_i|\mathbf{x}_i, \mathbf{w})$$

Equivalent to solving

$$\max_{\mathbf{w}} \sum_{i=1}^{m} -\log\left(1 + \exp(-y_i \mathbf{w}^T \mathbf{x}_i)\right)$$

Maximum a posteriori estimation

We could also add a prior on the weights

Suppose each weight in the weight vector is drawn independently from the normal distribution with zero mean and standard deviation σ^2

$$p(\mathbf{w}) = \prod_i p(w_i) = \prod_i \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{w_i^2}{\sigma^2}\right)$$

MAP estimation for logistic regression

Maximum likelihood estimation

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$$\Big\downarrow \boxed{\text{Equivalent to solving}}$$

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Equivalent to solving

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Learning by solving

$$\max_{\mathbf{w}} P(S|\mathbf{w})p(\mathbf{w})$$

MAP estimation for logistic regression

Maximum likelihood estimation

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$$\max_{\mathbf{w}} \sum_{i=1}^{m} \log P(y_i|\mathbf{x}_i, \mathbf{w}) + \sum_{i=1}^{d} -\frac{\mathbf{w}_i^2}{\sigma^2}$$

MAP estimation for logistic regression

Maximum likelihood estimation

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Learning by solving

$$\max_{\mathbf{w}} P(S|\mathbf{w})p(\mathbf{w})$$

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$$\max_{\mathbf{w}} \sum_{i=1}^{m} \log P(y_i|\mathbf{x}_i, \mathbf{w}) + \sum_{i=1}^{d} -\frac{\mathbf{w}_i^2}{\sigma^2}$$

$$\max_{\mathbf{w}} \sum_{i=1}^{m} -\log\left(1 + \exp(-y_i \mathbf{w}^T \mathbf{x}_i)\right) - \frac{1}{\sigma^2}\mathbf{w}^T\mathbf{w}$$

Learning a logistic regression classifier

Learning a logistic regression classifier is equivalent to solving

$$\min_{\mathbf{w}} \sum_{i=1}^{m} \log\left(1 + \exp(-y_i \mathbf{w}^T \mathbf{x}_i)\right) + \frac{1}{\sigma^2}\mathbf{w}^T\mathbf{w}$$

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Where have we seen this before?

Exercise: Write down the stochastic gradient descent algorithm for this?

Historically, other training algorithms exist. In particular, you might run into LBFGS

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Learning as loss minimization

- The setup
  - Examples $\mathbf{x}$ drawn from a fixed, unknown distribution D
  - Hidden oracle classifier f labels examples
  - We wish to find a hypothesis h that mimics f
- The ideal situation
  - Define a function L that penalizes bad hypotheses
  - **Learning:** Pick a function h $\in$ H to minimize expected loss

$$\min_{h \in H} E_{\mathbf{x} \sim D} \left[L\left(h(\mathbf{x}), f(\mathbf{x})\right)\right]$$

But distribution D is unknown

- Instead, minimize *empirical loss* on the training set

$$\min_{h \in H} \frac{1}{m} \sum_i L(h(\mathbf{x}_i), f(\mathbf{x}_i))$$

Empirical loss minimization

Learning = minimize *empirical loss* on the training set

$$\min_{h \in H} \frac{1}{m} \sum_i L(h(\mathbf{x}_i), f(\mathbf{x}_i))$$

Is there a problem here? Overfitting!

We need something that biases the learner towards simpler hypotheses

Achieved using a regularizer, which penalizes complex hypotheses

Regularized loss minimization

- Learning: $\min_{h \in H} \text{regularizer}(h) + C\frac{1}{m}\sum_i L(h(\mathbf{x}_i), f(\mathbf{x}_i))$
- With linear classifiers: $\min_{\mathbf{w}} \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_i L(y_i, \mathbf{x}_i, \mathbf{w})$
  (using $l2$ regularization)
- What is a loss function?
  - Loss functions should penalize mistakes
  - We are minimizing average loss over the training data
- What is the ideal loss function for classification?

The 0-1 loss

Penalize classification mistakes between true label y and prediction y'

$$L_{0\text{-}1}(y, y') = \begin{cases} 1 & \text{if } y \neq y', \\ 0 & \text{if } y = y'. \end{cases}$$

- For linear classifiers, the prediction y' = sgn($\mathbf{w}^T\mathbf{x}$)
  - Mistake if y $\mathbf{w}^T\mathbf{x} \leq 0$

$$L_{0\text{-}1}(y, \mathbf{x}, \mathbf{w}) = \begin{cases} 1 & \text{if } y\ \mathbf{w}^T\mathbf{x} \leq 0, \\ 0 & \text{otherwise.} \end{cases}$$

Minimizing 0-1 loss is intractable. Need surrogates

$$\min_{h \in H} \text{regularizer}(h) + C\frac{1}{m}\sum_i L(h(\mathbf{x}_i), f(\mathbf{x}_i))$$

The loss function zoo

Many loss functions exist

- Perceptron loss

$$L_{Perceptron}(y, \mathbf{x}, \mathbf{w}) = \max(0, -y\mathbf{w}^T\mathbf{x})$$

- Hinge loss (SVM)

$$L_{Hinge}(y, \mathbf{x}, \mathbf{w}) = \max(0, 1 - y\mathbf{w}^T\mathbf{x})$$

- Exponential loss (AdaBoost)

$$L_{Exponential}(y, \mathbf{x}, \mathbf{w}) = e^{-y\mathbf{w}^T\mathbf{x}}$$

- Logistic loss (logistic regression)

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

$$\min_{h \in H} \text{regularizer}(h) + C\frac{1}{m}\sum_i L(h(\mathbf{x}_i), f(\mathbf{x}_i))$$

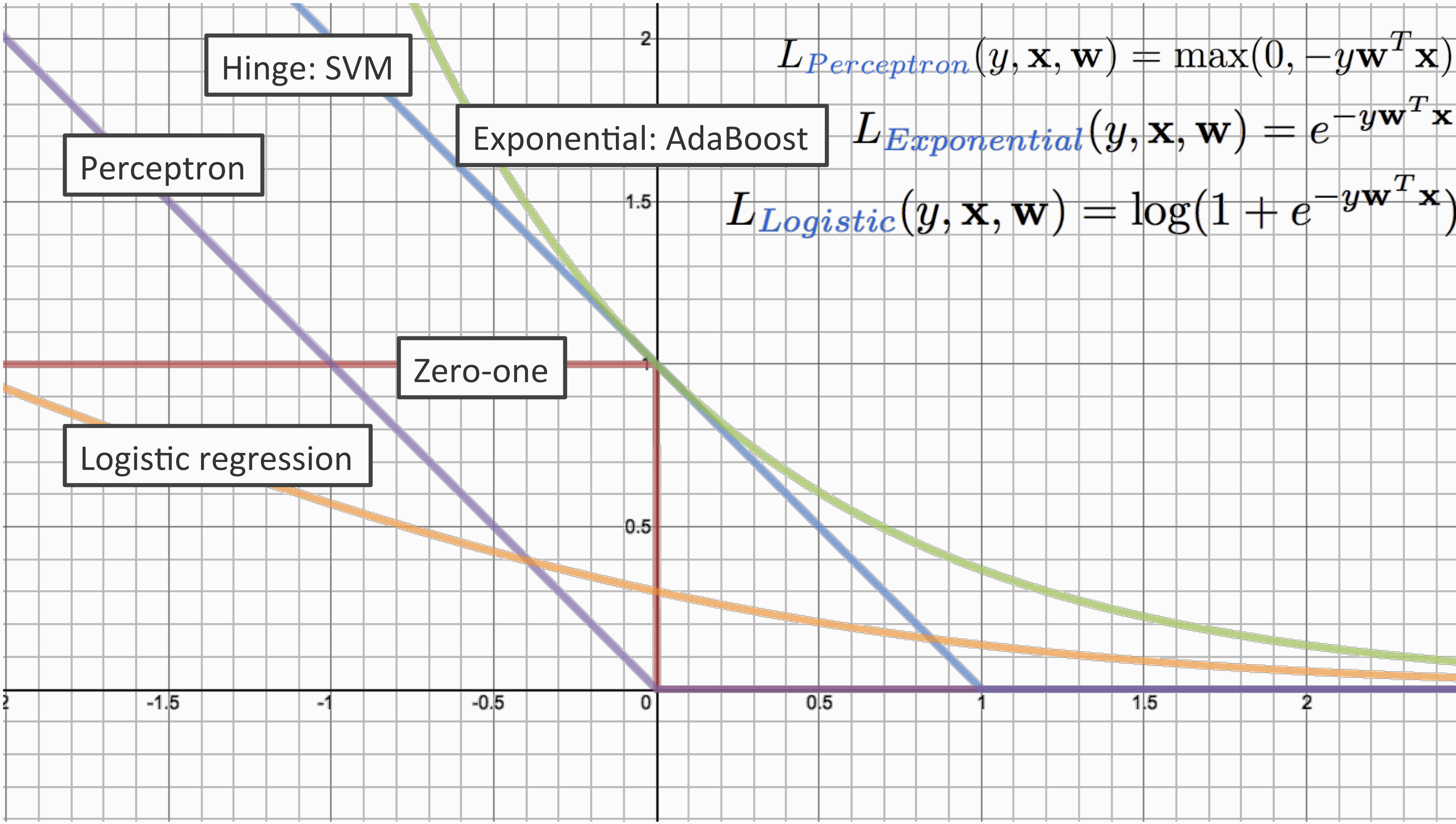
The loss function zoo

$$L_{Hinge}(y, \mathbf{x}, \mathbf{w}) = \max(0, 1 - y\mathbf{w}^T\mathbf{x})$$

$$L_{Perceptron}(y, \mathbf{x}, \mathbf{w}) = \max(0, -y\mathbf{w}^T\mathbf{x})$$

$$L_{Exponential}(y, \mathbf{x}, \mathbf{w}) = e^{-y\mathbf{w}^T\mathbf{x}}$$

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



Logistic regression is…

- A classifier that predicts the probability that the label is +1 for a particular input

- The discriminative counter-part of the naïve Bayes classifier

- A discriminative classifier that can be trained via MAP or MLE estimation

- A discriminative classifier that minimizes the logistic loss over the training set