CSC 311: Introduction to Machine Learning

Lecture 4 - ~~Bias-Variance Decomposition,~~
~~Ensemble Method I: Bagging,~~
Linear Classification

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Classification with Linear Models

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.
    - $t \in \{0, 1\}$ or $t \in \{-1, +1\}$ is for computational convenience.
- **linear:** model is a linear function of $\mathbf{x}$, followed by a threshold r:

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

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

Some Simplifications

Eliminating the threshold

- We can assume without loss of generality (w.l.o.g.) that the threshold is $r = 0$:

$$\mathbf{w}^T\mathbf{x} + b \geq r \quad \iff \quad \mathbf{w}^T\mathbf{x} + \underbrace{b - r}_{\triangleq w_0} \geq 0.$$

Eliminating the bias

- Add a dummy feature x_0 which always takes the value 1. The weight $w_0 = b$ is equivalent to a bias (same as linear regression)

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 us 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: $z = w_0 x_0 + w_1 x_1 > 0 \iff w_0 > 0$
  - When $x_1 = 1$, need: $z = w_0 x_0 + w_1 x_1 < 0 \iff w_0 + w_1 < 0$
- 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

$$z = w_0 x_0 + w_1 x_1 + w_2 x_2$$

$$\text{need: } w_0 < 0$$

$$\text{need: } w_0 + w_2 < 0$$

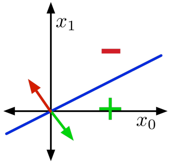
$$\text{need: } w_0 + w_1 < 0$$

$$\text{need: } w_0 + w_1 + w_2 > 0$$

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

The Geometric Picture

Input Space, or Data Space for NOT example

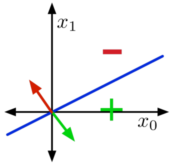


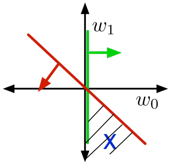
x_0	x_1	t
1	0	1
1	1	0

- Training examples are points
- Weights (hypotheses) $\mathbf{w}$ 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 is a line, but think of it as a hyperplane
- If the training examples can be perfectly separated by a linear decision rule, we say data is linearly separable.

The Geometric Picture

Weight Space





$w_0 > 0$

$w_0 + w_1 < 0$

- Weights (hypotheses) $\mathbf{w}$ are points
- Each training example $\mathbf{x}$ specifies a half-space $\mathbf{w}$ must lie in to be correctly classified: $\mathbf{w}^T\mathbf{x} > 0$ if $t = 1$.
- 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, otw it is infeasible.

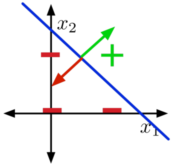
The Geometric Picture

- 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.
  - Feasible set will always have a corner at the origin.

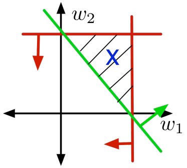
The Geometric Picture

Visualizations of the **AND** example

Data Space



Weight Space



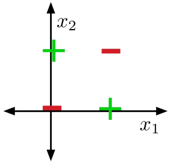
- Slice for $x_0 = 1$ and
- example sol: $w_0 = -1.5$, $w_1 = 1$, $w_2 = 1$
- decision boundary:

$w_0x_0 + w_1x_1 + w_2x_2 = 0$
$\implies -1.5 + x_1 + x_2 = 0$

- Slice for $w_0 = -1.5$ for the constraints
- $w_0 < 0$
- $w_0 + w_2 < 0$
- $w_0 + w_1 < 0$
- $w_0 + w_1 + w_2 > 0$

The Geometric Picture

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



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
  - data is almost never separable in real life.

Loss Functions

- Instead: define loss function then try to minimize the resulting cost function
  - Recall: cost is loss averaged (or summed) 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

- Usually, the cost $\mathcal{J}$ is the averaged loss over training examples; for 0-1 loss, this is the misclassification rate/error:

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

Attempt 1: 0-1 Loss

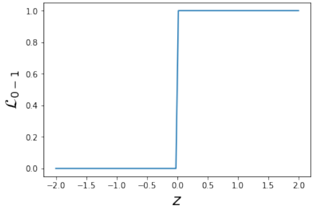
- Problem: how to optimize? In general, a hard problem (can be NP-hard)
- This is due to the step function (0-1 loss) not being nice (continuous/smooth/convex etc)

Attempt 1: 0-1 Loss

- Minimum of a function will be at its critical points.
- Let's try to find the critical point of 0-1 loss
- 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 is defined!



  - $\partial \mathcal{L}_{0-1} / \partial w_j = 0$ means that changing the weights by a very small amount has no effect on the loss (whenever the gradient of the loss is defined)
  - Almost any point has 0 gradient!

Attempt 2: Linear Regression

- Sometimes we can replace the loss function we care about with one that is easier to optimize. This is known as relaxation with a smooth surrogate loss function.
- One problem with $\mathcal{L}_{0-1}$ is that it is 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: $z = \mathbf{w}^T\mathbf{x} + b$

Attempt 2: Linear Regression

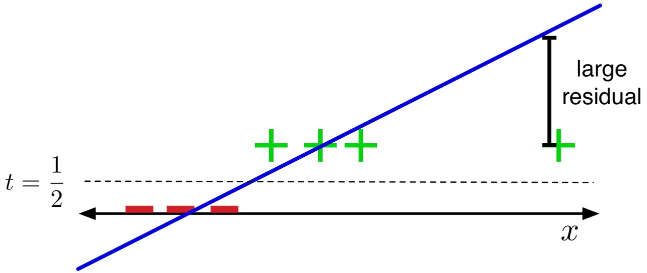
- We already know how to fit a linear regression model using the squared error loss. Can we use the same squared error loss instead?

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

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

Attempt 2: Linear Regression

The problem:



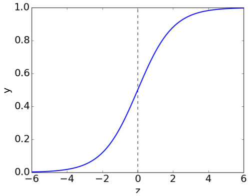
- The loss function penalizes you when you make correct predictions with high confidence!
- If $t = 1$, the loss is larger when $z = 10$ than when $z = 0$.

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 sigmoid, or S-shaped function:

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



- $\sigma^{-1}(y) = \log(y/(1-y))$ is called the logit.
- A linear model with a logistic nonlinearity is known as log-linear:

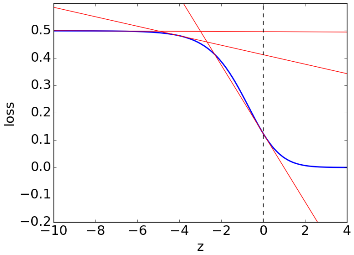
$$z = \mathbf{w}^\top \mathbf{x} + b$$
$$y = \sigma(z)$$
$$\mathcal{L}_{\mathrm{SE}}(y, t) = \frac{1}{2}(y - t)^2.$$

- Used in this way, σ is called an activation function.

Attempt 3: Logistic Activation Function

The problem:

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



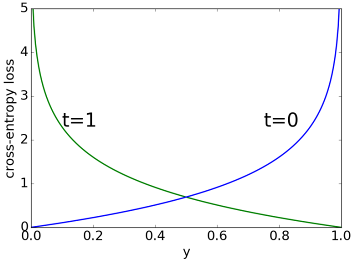
$$\frac{\partial \mathcal{L}}{\partial w_j} = \frac{\partial \mathcal{L}}{\partial z} \frac{\partial z}{\partial w_j}$$

- For $z \ll 0$, we have $\sigma(z) \approx 0$.
- $\frac{\partial \mathcal{L}}{\partial z} \approx 0$ (check!) $\implies \frac{\partial \mathcal{L}}{\partial w_j} \approx 0 \implies$ derivative w.r.t. w_j is small $\implies w_j$ is like a critical point
- If the prediction is really wrong, you should be far from a critical point (which is your candidate solution).

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 (aka log loss) captures this intuition:

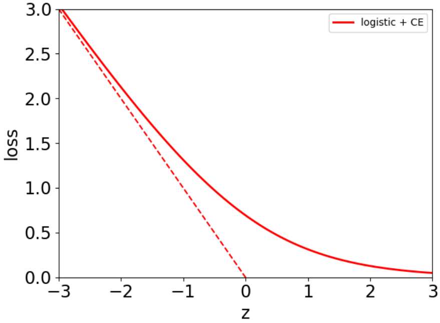
$$\begin{aligned}\mathcal{L}_{\mathrm{CE}}(y, t) &= \begin{cases} -\log y & \text{if } t = 1 \\ -\log(1 - y) & \text{if } t = 0 \end{cases} \\ &= -t \log y - (1 - t) \log(1 - y)\end{aligned}$$



Logistic Regression

Logistic Regression:

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



Plot is for target $t = 1$.

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.

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

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

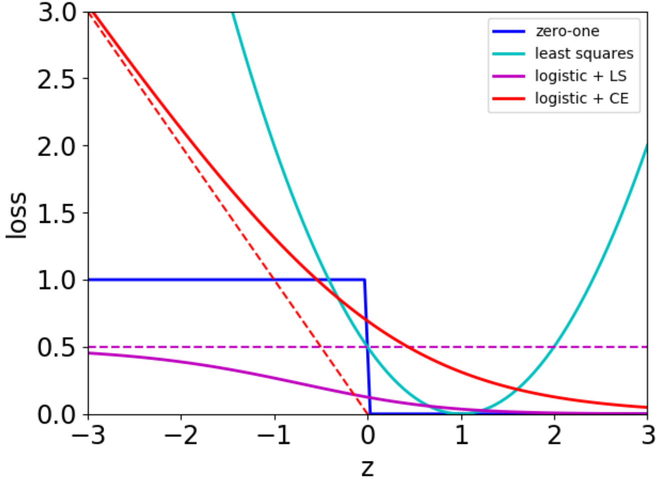
$$\mathcal{L}_{\text{LCE}}(z,t) = \mathcal{L}_{\text{CE}}(\sigma(z),t) = t\log(1+e^{-z}) + (1-t)\log(1+e^{z})$$

- Numerically stable computation:

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

Logistic Regression

Comparison of loss functions: (for $t = 1$)



Gradient Descent

- How do we minimize the cost $\mathcal{J}$ in this case? No direct solution.
  - Taking derivatives of $\mathcal{J}$ w.r.t. $\mathbf{w}$ and setting them to 0 doesn't have an explicit solution.
- Now let's see a second way to minimize the cost function which is more broadly applicable: gradient descent.
- Gradient descent is an iterative algorithm, which means we apply an update repeatedly until some criterion is met.
- We initialize the weights to something reasonable (e.g. all zeros) and repeatedly adjust them in the direction of steepest descent.

Gradient for Logistic Regression

Back to logistic regression:

$$\mathcal{L}_{\text{CE}}(y,t) = -\,t\log(y) - (1-t)\log(1-y)$$
$$y = 1/(1+e^{-z}) \quad \text{and} \quad z = \mathbf{w}^T\mathbf{x} + b$$

Therefore

$$\frac{\partial \mathcal{L}_{\text{CE}}}{\partial w_j} = \frac{\partial \mathcal{L}_{\text{CE}}}{\partial y}\cdot\frac{\partial y}{\partial z}\cdot\frac{\partial z}{\partial w_j} = \left(-\frac{t}{y} + \frac{1-t}{1-y}\right)\cdot y(1-y)\cdot x_j$$
$$= (y-t)x_j$$

Exercise: Verify this!

Gradient descent (coordinatewise) update to find the weights of logistic regression:

$$w_j \leftarrow w_j - \alpha\frac{\partial \mathcal{J}}{\partial w_j}$$
$$= w_j - \frac{\alpha}{N}\sum_{i=1}^{N}(y^{(i)} - t^{(i)})\,x_j^{(i)}$$

Logistic Regression

Comparison of gradient descent updates:

- Linear regression (verify!):

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

- Logistic regression:

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

- Not a coincidence! These are both examples of generalized linear models. But we won't go in further detail.
- Notice $\frac{1}{N}$ in front of sums due to averaged losses. This is why you need smaller learning rate when we optimize the sum of losses ($\alpha' = \alpha/N$).

Stochastic Gradient Descent

- So far, the cost function $\mathcal{J}$ has been the average loss over the training examples:

$$\mathcal{J}(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=1}^{N}\mathcal{L}^{(i)} = \frac{1}{N}\sum_{i=1}^{N}\mathcal{L}(y(\mathbf{x}^{(i)}, \boldsymbol{\theta}), t^{(i)}).$$

- By linearity,

$$\frac{\partial \mathcal{J}}{\partial \boldsymbol{\theta}} = \frac{1}{N}\sum_{i=1}^{N}\frac{\partial \mathcal{L}^{(i)}}{\partial \boldsymbol{\theta}}.$$

- Computing the gradient requires summing over *all* of the training examples. This is known as batch training.
- Batch training is impractical if you have a large dataset $N \gg 1$ (e.g. millions of training examples)!

Stochastic Gradient Descent

- Stochastic gradient descent (SGD): update the parameters based on the gradient for a single training example,
    1. Choose i uniformly at random
    2. $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \frac{\partial \mathcal{L}^{(i)}}{\partial \boldsymbol{\theta}}$
- Cost of each SGD update is independent of N.
- SGD can make significant progress before even seeing all the data!
- Mathematical justification: if you sample a training example uniformly at random, the stochastic gradient is an unbiased estimate of the batch gradient:

$$\mathbb{E}\left[\frac{\partial \mathcal{L}^{(i)}}{\partial \boldsymbol{\theta}}\right] = \frac{1}{N}\sum_{i=1}^{N} \frac{\partial \mathcal{L}^{(i)}}{\partial \boldsymbol{\theta}} = \frac{\partial \mathcal{J}}{\partial \boldsymbol{\theta}}.$$

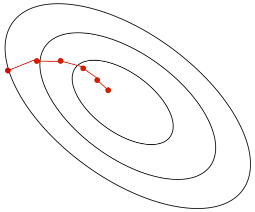
- Problems:
    - Variance in this estimate may be high
    - If we only look at one training example at a time, we can't exploit efficient vectorized operations.

Stochastic Gradient Descent

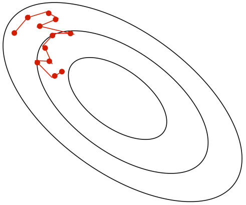
- Compromise approach: compute the gradients on a randomly chosen medium-sized set of training examples $\mathcal{M} \subset \{1, \dots, N\}$, called a mini-batch.
- Stochastic gradients computed on larger mini-batches have smaller variance. This is similar to bagging.
- The mini-batch size $|\mathcal{M}|$ is a hyperparameter that needs to be set.
  - Too large: takes more computation, i.e. takes more memory to store the activations, and longer to compute each gradient update
  - Too small: can't exploit vectorization, has high variance
  - A reasonable value might be $|\mathcal{M}| = 100$.

Stochastic Gradient Descent

- Batch gradient descent moves directly downhill. SGD takes steps in a noisy direction, but moves downhill on average.



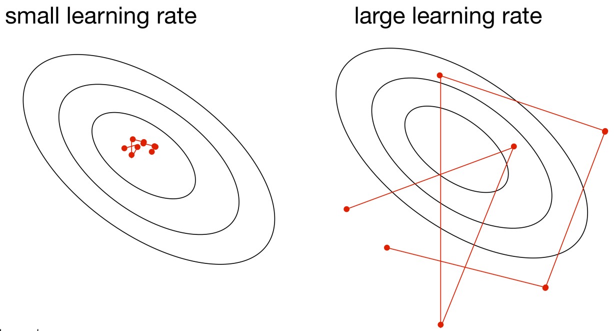
batch gradient descent



stochastic gradient descent

SGD Learning Rate

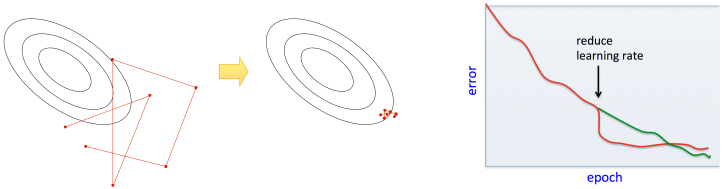
- In stochastic training, the learning rate also influences the fluctuations due to the stochasticity of the gradients.



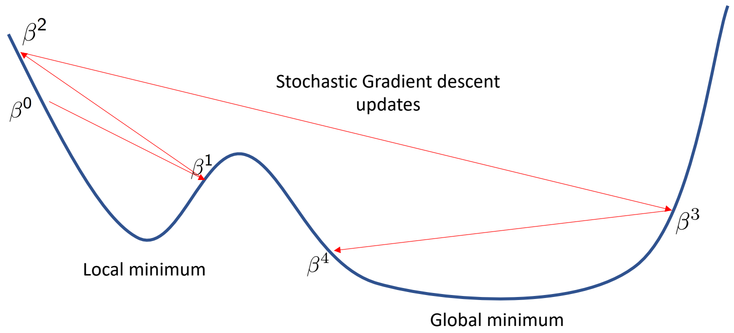
- Typical strategy:
  - Use a large learning rate early in training so you can get close to the optimum
  - Gradually decay the learning rate to reduce the fluctuations

SGD Learning Rate

- Warning: by reducing the learning rate, you reduce the fluctuations, which can appear to make the loss drop suddenly. But this can come at the expense of long-run performance.



SGD and Non-convex optimization



- Stochastic methods have a chance of escaping from bad minima.
- Gradient descent with small step-size converges to first minimum it finds.

Conclusion

- ~~Bias-Variance Decomposition~~
  - ~~The error of a machine learning algorithm can be decomposed to a bias term and a variance term.~~
  - ~~Hyperparameters of an algorithm might allow us to tradeoff between these two.~~
- ~~Ensemble Methods~~
  - ~~Bagging as a simple way to reduce the variance of an estimation method~~
- Binary Classification
  - $0-1$ loss is the difficult to work with
  - Use of surrogate loss functions such as the cross-entropy loss lead to computationally feasible solutions
  - Logistic regression as the result of using cross-entropy loss with a linear model going through logistic nonlinearity
  - No direct solution, but gradient descent can be used to minimize it
  - Stochastic gradient descent