CSC 411: Lecture 4 - Logistic regression

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Key Concepts:

- Logistic Regression
- Regularization
- Cross validation

note: we are still talking about binary classification (with $\{0, 1\}$ labels)

So far: Turned a real score $\mathbf{w}^T\mathbf{x} = w_0 \cdot 1 + \sum_{i=1}^{d} w_i \cdot x_i$ to binary decision by thresholding.

Alternative: Model the probability $P(y = 1|\mathbf{x})$.

Need to squash $\mathbf{w}^T\mathbf{x}$ into $[0, 1]$, $p(y = 1|\mathbf{x}) = f(\mathbf{w}^T\mathbf{x})$.

What about $P(y = -1|\mathbf{w})$? $P(y = -1|\mathbf{w}) = 1 - P(y = 1|\mathbf{w}) = 1 - f(\mathbf{w}^T\mathbf{x})$

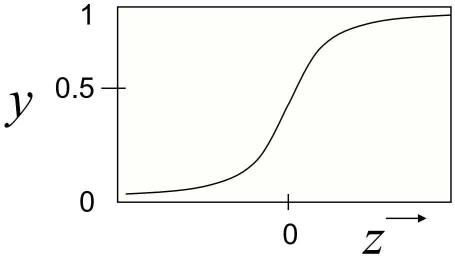
How to chose label? Pick the most probable (when shouldn't you do that?).

Benefits:

- Models uncertainty (in a limited manor)
- Can use probability for decision making.
- Can use probabilistic objective (ML/MAP).

Useful squashing function: sigmoid or logistic function

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

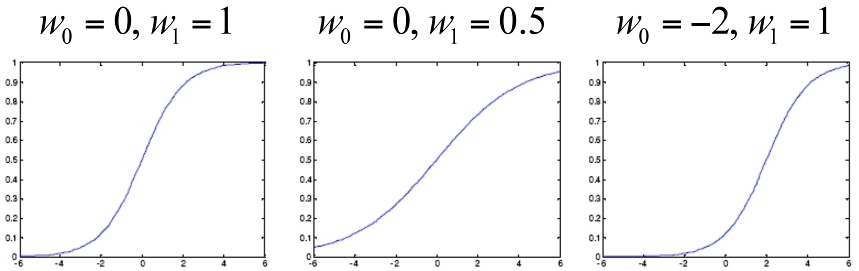


- Smooth function.
- Monotonic increasing.
- $\sigma(0) = 0.5$
- $\sigma(z) \xrightarrow{z \to -\infty} = 0$, $\sigma(z) \xrightarrow{z \to \infty} = 1$

Sigmoid

- Let's look at how modifying $\mathbf{w}$ changes the shape of the function
- 1D example:

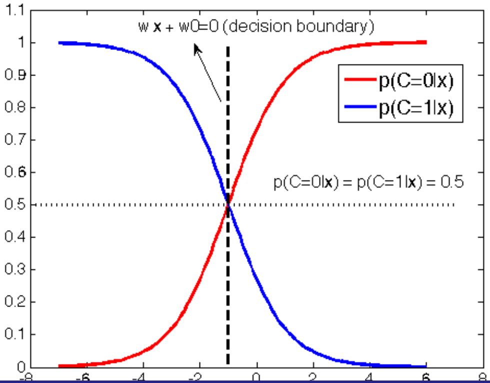
$$y = \sigma\left(w_1 x + w_0\right)$$



The magnitude of $\mathbf{w}_{[1:]}$ decides the slope.

It can be seen as a smooth alternative to the step function.

- What is the decision boundary for logistic regression?
- $p(y=1|\mathbf{x},\mathbf{w}) = \sigma(\mathbf{w}^T\mathbf{x}) \geq 0.5 \Rightarrow \mathbf{w}^T\mathbf{x} \geq 0$
- Decision boundary: $\mathbf{w}^T\mathbf{x} = w_0 + \sum_{j=1}^{d} w_j x_j = 0.$
- Logistic regression has a linear decision boundary
- The decision boundary is invariant to scaling but the probability isn't.



- When we have a d-dim input $\mathbf{x} \in \Re^d$
- How should we learn the weights $\mathbf{w} = (w_0, w_1, \cdots, w_d)$?
- We have a probabilistic model
- Let's use maximum likelihood

Optimization

- Assume $y \in \{0,1\}$, we can write the probability distribution of each of our training points $p(y^{(1)}, \cdots, y^{(N)} | \mathbf{x}^{(1)}, \cdots \mathbf{x}^{(N)}; \mathbf{w})$
- Assuming that the training examples are sampled IID: independent and identically distributed, we can write the *likelihood function*:

$$L(\mathbf{w}) = p(y^{(1)}, \cdots, y^{(N)} | \mathbf{x}^{(1)}, \cdots \mathbf{x}^{(N)}; \mathbf{w}) = \prod_{i=1}^{N} p(y^{(i)} | \mathbf{x}^{(i)}; \mathbf{w})$$

- We can write each probability as (will be useful later):

$$\begin{aligned} p(y^{(i)} | \mathbf{x}^{(i)}; \mathbf{w}) &= p(y=1 | \mathbf{x}^{(i)}; \mathbf{w})^{y^{(i)}} p(y=0 | \mathbf{x}^{(i)}; \mathbf{w})^{1-y^{(i)}} \\ &= p(y=1 | \mathbf{x}^{(i)}; \mathbf{w})^{y^{(i)}} \left(1 - p(y=1 | \mathbf{x}^{(i)}; \mathbf{w}\right)^{1-y^{(i)}} \end{aligned}$$

- We can learn the model by maximizing the likelihood

$$\max_{\mathbf{w}} L(\mathbf{w}) = \max_{\mathbf{w}} \prod_{i=1}^{N} p(y^{(i)} | \mathbf{x}^{(i)}; \mathbf{w})$$

- Easier to maximize the log likelihood $\log L(\mathbf{w})$

Optimization

$$\begin{aligned} L(\mathbf{w}) &= \prod_{i=1}^{N} p(y^{(i)}|\mathbf{x}^{(i)}) \qquad \text{(likelihood)} \\ &= \prod_{i=1}^{N} \left(1 - p(y=1|\mathbf{x}^{(i)})\right)^{1-y^{(i)}} p(y=1|\mathbf{x}^{(i)})^{y^{(i)}} \end{aligned}$$

- We can convert the maximization problem into minimization the negative log-likelihood (NLL):

$$L_{log}(\mathbf{w}) = -\log L(\mathbf{w}) = -\sum_{i=1}^{N} \log p(y^{(i)}|\mathbf{x}^{(i)}; \mathbf{w})$$

$$\begin{aligned} L_{log}(\mathbf{w}) &= -\log L(\mathbf{w}) \\ &= -\sum_{i=1}^{N} y^{(i)} \log(p(y=1|\mathbf{x}^{(i)}, \mathbf{w})) - \sum_{i=1}^{N} (1 - y^{(i)}) \log p(y=0|\mathbf{x}^{(i)}; \mathbf{w}) \end{aligned}$$

- Is there a closed form solution?

$$\min_{\mathbf{w}} L(\mathbf{w}) = \min_{\mathbf{w}} \left\{ -\sum_{i=1}^{N} y^{(i)} \log p(y=1|\mathbf{x}^{(i)}, \mathbf{w}) - \sum_{i=1}^{N} (1-y^{(i)}) \log(1 - p(y=1|\mathbf{x}^{(i)}, \mathbf{w})) \right\}$$

- Gradient descent: iterate and at each iteration compute steepest direction towards optimum, move in that direction, step-size λ

$$w_j^{(t+1)} \leftarrow w_j^{(t)} - \lambda \frac{\partial L(\mathbf{w})}{\partial w_j}$$

- You can write this in vector form

$$\bigtriangledown L(\mathbf{w}) = \left[\frac{\partial L(\mathbf{w})}{\partial w_0}, \cdots, \frac{\partial L(\mathbf{w})}{\partial w_k} \right]^T \qquad \mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} - \lambda \nabla_{\mathbf{w}} L(\mathbf{w}^{(t)})$$

- But where is $\mathbf{w}$?

$$p(y=1|\mathbf{x}) = \frac{1}{1+\exp(-\mathbf{w}^T\mathbf{x})}, \quad p(y=0|\mathbf{x}) = \frac{\exp(-\mathbf{w}^T\mathbf{x})}{1+\exp(-\mathbf{w}^T\mathbf{x})}$$

- The loss is

$$L_{log-loss}(\mathbf{w}) = -\sum_{i=1}^{N} y^{(i)} \log p(y=1|\mathbf{x}^{(i)},\mathbf{w}) - \sum_{i=1}^{N}(1-y^{(i)}) \log p(y=0|\mathbf{x}^{(i)},\mathbf{w})$$

  where the probabilities are

$$p(y=1|\mathbf{x},\mathbf{w}) = \frac{1}{1+\exp(-z)} \qquad p(y=0|\mathbf{x},\mathbf{w}) = \frac{\exp(-z)}{1+\exp(-z)} = \frac{1}{1+\exp(z)}$$

  and $z = \mathbf{w}^T\mathbf{x}$
- We can simplify

$$\begin{aligned} L(\mathbf{w})_{log-loss} &= \sum_i y^{(i)} \log(1+\exp(-z^{(i)})) + \sum_i (1-y^{(i)}) z^{(i)} + \sum_i (1-y^{(i)}) \log(1+\exp(-z^{(i)})) \\ &= \sum_i \log(1+\exp(-z^{(i)})) + \sum_i (1-y^{(i)}) z^{(i)} \end{aligned}$$

- Now it's easy to take derivatives

Optimization

$$L(\mathbf{w}) = \sum_i (1 - y^{(i)}) z^{(i)} + \sum_i \log(1 + \exp(-z^{(i)}))$$

- Now it's easy to take derivatives
- Remember $z = \mathbf{w}^T \mathbf{x} \Rightarrow \frac{\partial z}{\partial w_j} = x_j$

$$\frac{\partial \ell}{\partial w_j} = \frac{\partial \ell}{\partial z} \cdot \frac{\partial z}{\partial w_j} = \sum_i x_j^{(i)} \left(1 - y^{(i)} - \frac{\exp(-z^{(i)})}{1 + \exp(-z^{(i)})}\right) = \sum_i x_j^{(i)} \left(\frac{1}{1 + \exp(-z^{(i)})} - y^{(i)}\right)$$

- What's $x_j^{(i)}$? The $j-$th dimension of the $i-$th training example $\mathbf{x}^{(i)}$
- And simplifying

$$\frac{\partial \ell}{\partial w_j} = \sum_i x_j^{(i)} \left(p(y = 1 | \mathbf{x}^{(i)}; \mathbf{w}) - y^{(i)}\right)$$

- Don't get confused with indices: j for the weight that we are updating and i for the training example

- Putting it all together (plugging the update into gradient descent): Gradient descent for logistic regression:

$$w_j^{(t+1)} \leftarrow w_j^{(t)} - \lambda \sum_i x_j^{(i)} \left(p(y = 1 | \mathbf{x}^{(i)}; \mathbf{w}) - y^{(i)} \right)$$

where:

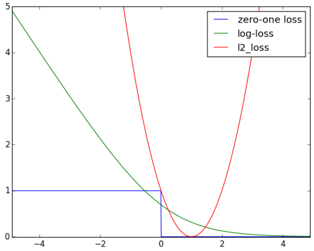
$$p(y = 1 | \mathbf{x}^{(i)}; \mathbf{w}) = \frac{1}{1 + \exp\left(-\mathbf{w}^T \mathbf{x}\right)}$$

- This is all there is to learning in logistic regression. Simple, huh?

We are optimizing $\sum_i (1 - y^{(i)}) z^{(i)} + \sum_i \log(1 + \exp(-z^{(i)}))$.

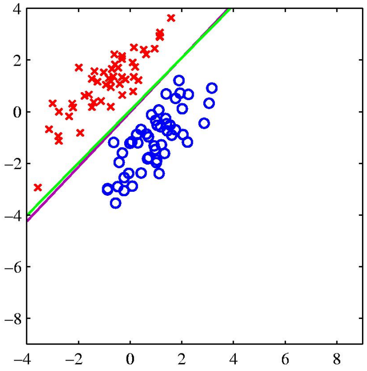
We can forget the probabilistic interpretation and just think about a surrogate loss function

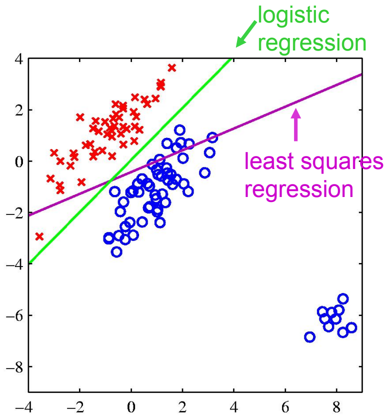
$$\ell(y, \hat{y}) = (1 - y)\hat{y} + \log(1 + \exp(-\hat{y})) = \begin{cases} \log(1 + \exp(-\hat{y})), & y = 1, \\ \log(1 + \exp(\hat{y})), & y = 0, \end{cases}$$



It is convex, so gradient descent converges to global minimum.

Logistic Regression vs Least Squares Regression:





If the right answer is 1 and the model says 1.5, it loses, so it changes the boundary to avoid being "too correct" (tilts away from outliers)

Regularization:

- We can also look at

$$p(\mathbf{w}|\{y\},\{\mathbf{x}\}) \propto p(\{y\}|\{\mathbf{x}\},\mathbf{w})\,p(\mathbf{w})$$

  with $\{y\} = (y^{(1)},\cdots,y^{(N)})$, and $\{\mathbf{x}\} = (\mathbf{x}^{(1)},\cdots,\mathbf{x}^{(N)})$
- We can define priors on parameters $\mathbf{w}$
- This is a form of regularization
- Helps avoid large weights and overfitting

$$\max_{\mathbf{w}} \log \left[p(\mathbf{w}) \prod_i p(y^{(i)}|\mathbf{x}^{(i)},\mathbf{w}) \right]$$

- This is called maximum-a-posteriori estimation (MAP)?
- What's $p(\mathbf{w})$?

Prior

- For example, define prior: normal distribution, zero mean and identity covariance $p(\mathbf{w}) \propto \mathcal{N}(0, \alpha^{-1}\mathbf{I})$ (best to exclude w_0)
- This prior pushes parameters towards zero (why is this a good idea?)
- Equivalent to L_2 regularization
- Including this prior the new gradient is

$$w_j^{(t+1)} \leftarrow w_j^{(t)} - \lambda \frac{\partial L(\mathbf{w})}{\partial w_j} - \lambda \alpha w_j^{(t)}$$

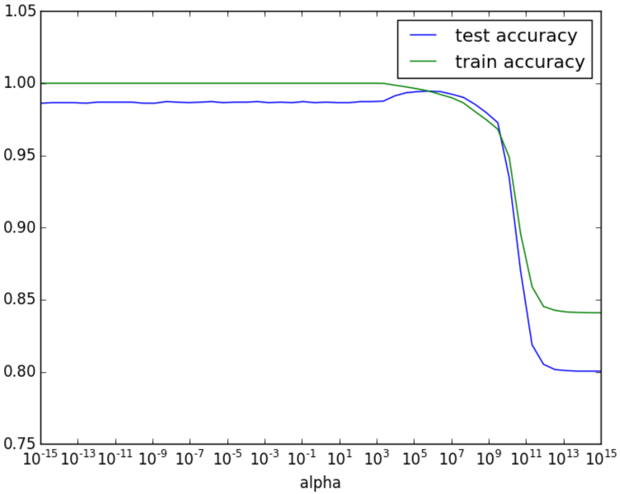
  where t here refers to iteration of the gradient descent
- The parameter α is the importance of the regularization, and it's a hyper-parameter
- How do we decide the best value of α (or a hyper-parameter in general)?

MNIST digit data-set: 60, 000 training 28×28 digit images, 10, 000 test images. Need to classify as 0-9.

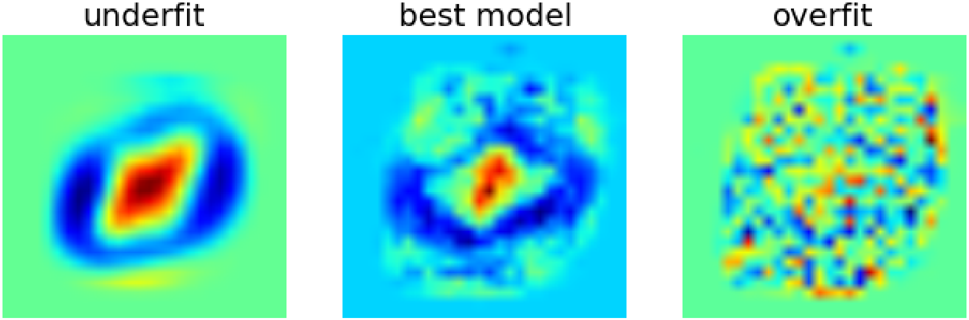
Only take zero and ones - binary classification.

Example

Train logistic regression with various regularization parameters-



How do the classifiers look?



(doesn't overfit that much, still great on test)

Tuning hyper-parameters:

- **Never use test data for tuning the hyper-parameters**
- We can divide the set of training examples into two disjoint sets: training and validation.
- Use the first set (i.e., training) to estimate the weights $\mathbf{w}$ for different values of α.
- Use the second set (i.e., validation) to estimate the best α, by evaluating how well the classifier does on this second set.
- This tests how well it generalizes to unseen data.
- Trade-off: Large validation set $\rightarrow$ less training data to use.
- Trade-off: Small validation set $\rightarrow$ less accurate estimation.
- Can overfit on the validation set!

- Leave-p-out cross-validation:
  - We use p observations as the validation set and the remaining observations as the training set.
  - This is repeated on all ways to cut the original training set.
  - It requires $\binom{n}{p}$ for a set of n examples
- Leave-1-out cross-validation: When $p = 1$, does not have this problem
- k-fold cross-validation:
  - The training set is randomly partitioned into k equal size subsamples.
  - Of the k subsamples, a single subsample is retained as the validation data for testing the model, and the remaining $k - 1$ subsamples are used as training data.
  - The cross-validation process is then repeated k times (the folds).
  - The k results from the folds can then be averaged (or otherwise combined) to produce a single estimate

Train your model:

- Leave-one-out cross-validation:
- k-fold cross-validation:

Logistic Regression wrap-up

Pros:

- Probabilistic view of class predictions
- Quick to train, convex loss
- Fast at classification
- Good accuracy for many simple data sets
- Resistant to overfitting (Rule of thumb: $\#data >= 10 \cdot \#features$)
- Can interpret model coefficients as indicators of feature importance

Cons:

- Linear decision boundary (too simple for more complex problems?)
- Very simple model of the conditional probabilities