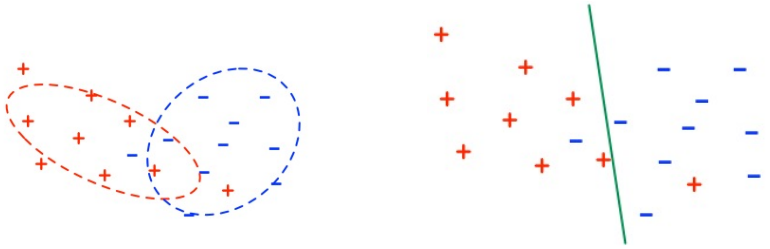
Classification with discriminative models

CSE 250B

Classification with parametrized models

Classifiers with a fixed number of parameters can represent a limited set of functions. Learning a model is about picking a good approximation.

Typically the x's are points in p-dimensional Euclidean space, $\mathbb{R}^p$.



Two ways to classify:

- **Generative**: model the individual classes.
- **Discriminative**: model the decision boundary between the classes.

Generative models: pros and cons

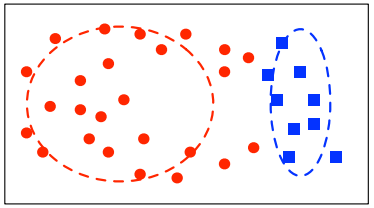
Advantages:

- Multiclass is a breeze
- Special density models (such as Bayes nets or hidden Markov models) can model temporal and other dependencies
- Returns not just a classification but also a confidence $\Pr(y|x)$
- For many common models: converges fast

Disadvantages:

- Formula for $\Pr(y|x)$ assumes the class-specific density models are perfect, but this is never true
- If we only care about classification, shouldn't we focus on the decision boundary rather than trying to model other aspects of the distribution of x?

Generative versus discriminative



The generative way:

- Fit: π_0, π_1, P_0, P_1
- This determines a full joint distribution $\Pr(x, y)$
- Use Bayes' rule to obtain $\Pr(y|x)$

Discriminative: model $\Pr(y|x)$ directly
In our earlier terminology: forget about the μ, just learn the η

The logistic regression model

What model to use for $\Pr(y|x)$?

- Say $\mathcal{Y} = \{-1, 1\}$. Recall: for Gaussians with common covariance,

$$\ln \frac{\Pr(y = 1 \mid x)}{\Pr(y = -1 \mid x)} = \underbrace{w \cdot x + \theta}_{\text{linear}}$$

- Can drop θ by adding an extra feature to x.
- Then $\Pr(y = 1 \mid x) = \Pr(y = -1 \mid x)\, e^{w \cdot x}$, whereupon

$$\Pr(y = -1 \mid x) = \frac{1}{1 + e^{w \cdot x}}$$

$$\Pr(y = 1 \mid x) = 1 - \frac{1}{1 + e^{w \cdot x}} = \frac{e^{w \cdot x}}{1 + e^{w \cdot x}} = \frac{1}{1 + e^{-w \cdot x}}$$

- More concisely,

$$\Pr(y \mid x) = \frac{1}{1 + e^{-y(w \cdot x)}}$$

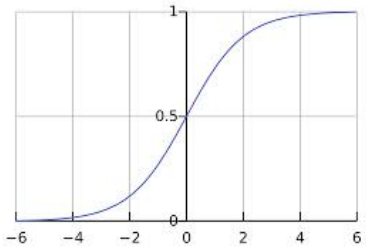
This is the **logistic regression model**, parametrized by w.

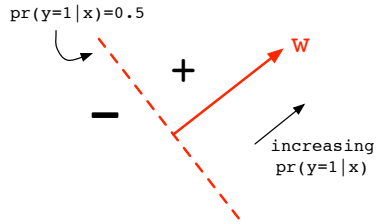
The squashing function

Take $\mathcal{X} = \mathbb{R}^p$ and $\mathcal{Y} = \{-1, 1\}$. The model specified by $w \in \mathbb{R}^p$ is

$$\Pr_w(y \mid x) = \frac{1}{1 + e^{-y(w \cdot x)}} = g(y(w \cdot x)),$$

where $g(z) = 1/(1 + e^{-z})$ is the *squashing function*.





Fitting w

The maximum-likelihood principle: given a data set

$$(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)}) \in \mathbb{R}^p \times \{-1, 1\},$$

pick the $w \in \mathbb{R}^p$ that maximizes

$$\prod_{i=1}^{n} \Pr_w(y^{(i)} \mid x^{(i)}).$$

Easier to work with sums, so take log to get **loss function**

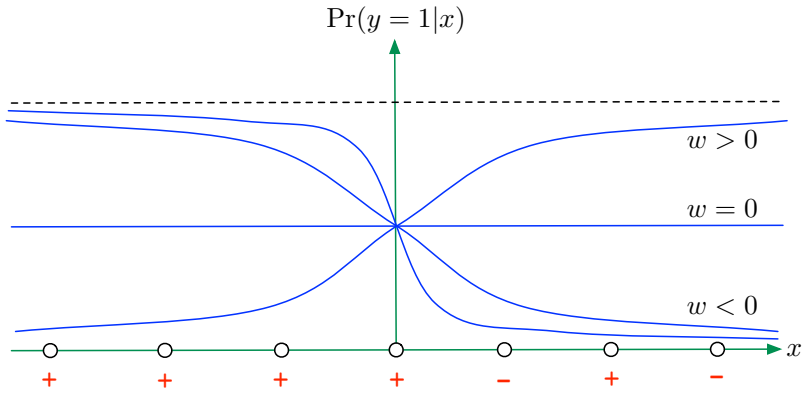
$$L(w) = -\sum_{i=1}^{n} \ln \Pr_w(y^{(i)} \mid x^{(i)}) = \sum_{i=1}^{n} \ln(1 + e^{-y^{(i)}(w \cdot x^{(i)})})$$

Our goal is to minimize $L(w)$.

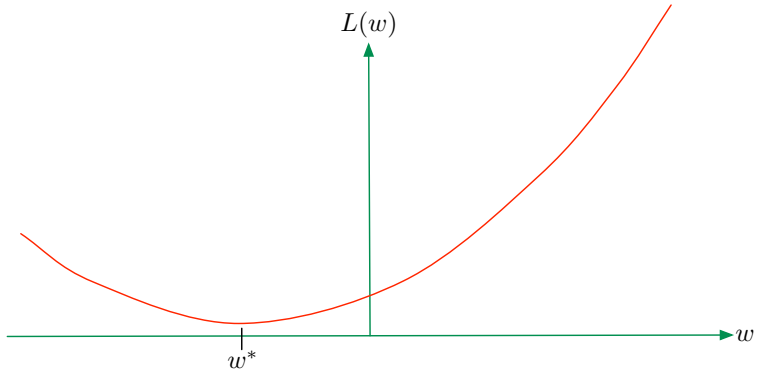
The good news: $L(w)$ is **convex** in w.

One dimensional example

$$\Pr_w(y \mid x) = \frac{1}{1 + e^{-ywx}}, \quad w \in \mathbb{R}$$



Example, cont'd



How to find the minimum of this convex function? A variety of options:

- Gradient descent
- Newton-Raphson

and many others.

Gradient descent procedure for logistic regression

Given $(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)}) \in \mathbb{R}^p \times \{-1, 1\}$, find

$$\arg\min_{w \in \mathbb{R}^p} L(w) = \sum_{i=1}^{n} \ln(1 + e^{-y^{(i)}(w \cdot x^{(i)})})$$

- Set $w_0 = 0$
- For $t = 0, 1, 2, \ldots$, until convergence:

$$w_{t+1} = w_t + \eta_t \sum_{i=1}^{n} y^{(i)} x^{(i)} \underbrace{\Pr_{w_t}(-y^{(i)}|x^{(i)})}_{\text{doubt}_t(x^{(i)}, y^{(i)})},$$

where η_t is a step size chosen by line search to minimize $L(w_{t+1})$.

Newton-Raphson procedure for logistic regression

- Set $w_0 = 0$
- For $t = 0, 1, 2, \ldots$, until convergence:

$$w_{t+1} = w_t + \eta_t (X^T D_t X)^{-1} \sum_{i=1}^{n} y^{(i)} x^{(i)} \Pr_{w_t}(-y^{(i)}|x^{(i)}),$$

where

- X is the $n \times p$ data matrix with one point per row
- D_t is an $n \times n$ diagonal matrix with (i, i) entry

$$D_{t,ii} = \Pr_{w_t}(1|x^{(i)}) \Pr_{w_t}(-1|x^{(i)})$$

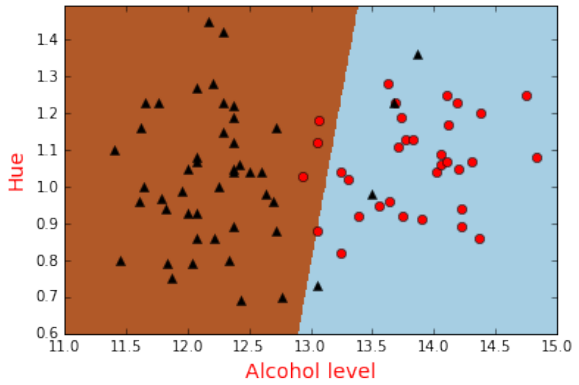
- η_t is a step size that is either fixed to 1 ("iterative reweighted least squares") or chosen by line search to minimize $L(w_{t+1})$.

Example: "wine" data set

Recall: data from three wineries from the same region of Italy.

- 13 attributes: hue, color intensity, flavanoids, ash content, ...
- 178 instances in all: split into 118 train, 60 test

Pick two classes and just two attributes (hue, alcohol content).



Test error using logistic regression: 10%.

A closer look at the logistic loss

For $(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)}) \in \mathbb{R}^p \times \{-1, +1\}$,

$$L(w) \;=\; \sum_{i=1}^{n} \ln(1 + e^{-y^{(i)}(w \cdot x^{(i)})}).$$

Can't we just minimize this by calculus?

First derivative. There are p partial derivatives $\partial L / \partial w_j$. Put into a vector:

$$\nabla L(w) = \left(\frac{\partial L}{\partial w_1}, \ldots, \frac{\partial L}{\partial w_p} \right).$$

$$\frac{\partial L}{\partial w_j} = \sum_{i=1}^{n} \frac{e^{-y^{(i)}(w \cdot x^{(i)})}}{1 + e^{-y^{(i)}(w \cdot x^{(i)})}} (-y^{(i)} x_j^{(i)}) = -\sum_{i=1}^{n} y^{(i)} x_j^{(i)} \frac{1}{1 + e^{y^{(i)}(w \cdot x^{(i)})}}$$

$$\nabla L(w) = -\sum_{i=1}^{n} y^{(i)} x^{(i)} \frac{1}{1 + e^{y^{(i)}(w \cdot x^{(i)})}}$$

We know $\nabla L(w) = 0$ iff w is a local optimum. But we want a **global** optimum.

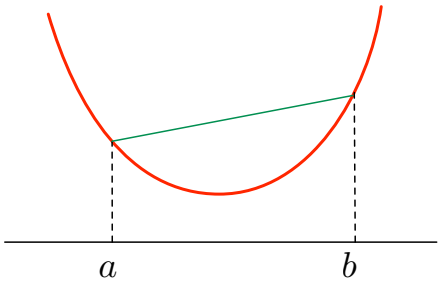
Good news: $L(w)$ is **convex**, so local optimum implies global optimum.

Quick quiz

Compute the first derivative of the following functions on $\mathbb{R}^p$.

1. $F(w) = u \cdot w$, where $u \in \mathbb{R}^p$
2. $F(w) = w^T w$

Convexity



A function $f : \mathbb{R}^p \to \mathbb{R}$ is **convex** if for all $a, b \in \mathbb{R}^p$ and $0 < \theta < 1$,

$$f(\theta a + (1 - \theta) b) \;\leq\; \theta f(a) + (1 - \theta) f(b).$$

It is **strictly convex** if strict inequality holds for all $a \neq b$.

f is **concave** (resp., **strictly concave**) iff $-f$ is convex (resp., strictly convex).

Second-derivative test for convexity

A function $f : \mathbb{R}^p \to \mathbb{R}$ has p^2 second partial derivatives $\frac{\partial^2 f}{\partial z_j \partial z_k}$ at any $z \in \mathbb{R}^p$ (assuming these exist).

Assemble into a $p \times p$ matrix, the **Hessian** $H(z)$:

$$H_{jk} \;=\; \frac{\partial^2 f}{\partial z_j \partial z_k}.$$

Useful fact. Suppose that for $f : \mathbb{R}^p \to \mathbb{R}$, the second partial derivatives exist everywhere and are continuous functions of z. Then:

1. $H(z)$ is a symmetric matrix.
2. f is convex if and only if $H(z)$ is positive semidefinite for all $z \in \mathbb{R}^p$.

Quick quiz

Is this function $f : \mathbb{R}^p \to \mathbb{R}$ convex?

$$f(z) = (u \cdot z)^2$$

(Here u is some fixed vector in $\mathbb{R}^p$.)

Convexity of logistic regression loss function

Recall the loss function: for data $(x^{(i)}, y^{(i)}) \in \mathbb{R}^p \times \{-1, +1\}$,

$$L(w) = \sum_{i=1}^{n} \ln(1 + e^{-y^{(i)}(w \cdot x^{(i)})}).$$

We already know the first derivative:

$$\frac{\partial L}{\partial w_j} = -\sum_{i=1}^{n} y^{(i)} x_j^{(i)} \frac{1}{1 + e^{y^{(i)}(w \cdot x^{(i)})}}.$$

Second derivative: the (j, k) entry of the Hessian $H(w)$ is

$$\frac{\partial L}{\partial w_k \partial w_j} = -\sum_{i=1}^{n} y^{(i)} x_j^{(i)} (-1) \frac{e^{y^{(i)}(w \cdot x^{(i)})}}{(1 + e^{y^{(i)}(w \cdot x^{(i)})})^2} y^{(i)} x_k^{(i)}$$

$$= \sum_{i=1}^{n} x_j^{(i)} x_k^{(i)} \frac{e^{y^{(i)}(w \cdot x^{(i)})}}{(1 + e^{y^{(i)}(w \cdot x^{(i)})})^2} = \sum_{i=1}^{n} x_j^{(i)} x_k^{(i)} \frac{1}{1 + e^{w \cdot x^{(i)}}} \frac{1}{1 + e^{-w \cdot x^{(i)}}}$$

This is $u_j \cdot u_k$, where vectors $u_1, \ldots, u_p \in \mathbb{R}^n$ are defined as follows:

$$u_j \text{ has } i\text{th coordinate } x_j^{(i)} \sqrt{\frac{1}{(1 + e^{w \cdot x^{(i)}})(1 + e^{-w \cdot x^{(i)}})}}.$$

Therefore $H(w) = UU^T$, where U is the matrix with rows u_j $\Rightarrow$ **convex**.

Gradient descent

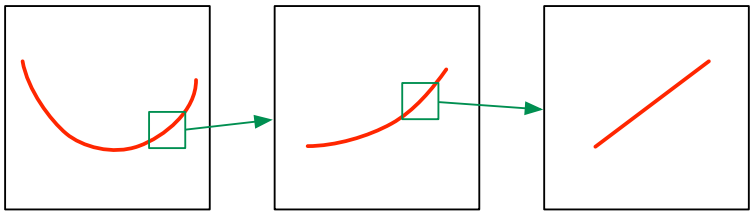
For minimizing a function $L(w)$:

- $w_o = 0, t = 0$
- while $\nabla L(w_t) \not\approx 0$:
  - $w_{t+1} = w_t - \eta_t \nabla L(w_t)$
  - $t = t + 1$

Here η_t is the *step size* at time t.

Gradient descent: rationale

"Differentiable" means "locally linear".



For *small* displacements $u \in \mathbb{R}^p$,

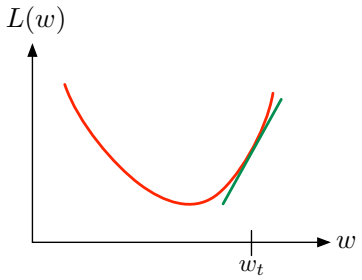
$$L(w + u) \approx L(w) + u \cdot \nabla L(w).$$

Therefore, if $u = -\eta \nabla L(w)$ is small,

$$L(w + u) \approx L(w) - \eta \|\nabla L(w)\|^2 < L(w).$$

The step size matters

Gradient descent update: $w_{t+1} = w_t - \eta_t \nabla L(w_t)$.



- Step size η_t too small: not much progress
- Too large: overshoot the mark

One option: pick η_t using a line search

$$\eta_t \;=\; \arg\min_{\alpha>0} L(w_t - \alpha \nabla L(w_t)).$$

Variant: stochastic gradient descent

Recall gradient descent update for logistic regression: at time t

$$w_{t+1} \;=\; w_t \;+\; \eta_t \sum_{i=1}^{n} y^{(i)} x^{(i)} \underbrace{\Pr_{w_t}(-y^{(i)}|x^{(i)})}_{\text{doubt}_t(x^{(i)},y^{(i)})}.$$

Each update involves the entire data set, which is inconvenient.

Stochastic gradient descent makes updates based on just one point:

- Get next data point (x, y) (e.g., keep cycling through the data set)
- $w_{t+1} \;=\; w_t \;+\; \eta_t\, y\, x \Pr_{w_t}(-y|x)$.

Convenient for very large data sets.

Another option: make updates based on "mini-batches" of data points.

Newton-Raphson

For minimizing a function $L(w)$:

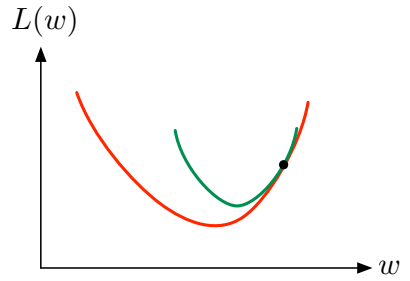
- $w_o = 0, t = 0$
- while $\nabla L(w_t) \not\approx 0$:
  - $w_{t+1} = w_t - \eta_t H^{-1}(w_t) \nabla L(w_t)$
  - $t = t + 1$

$H^{-1}(w)$ is the inverse of the Hessian at w.

Newton-Raphson: rationale

Second-order Taylor expansion: for small u,

$$L(w+u) \;\approx\; L(w) + u \cdot \nabla L(w) + \frac{1}{2} u^T H(w) u.$$



To minimize this quadratic approximation, set derivative to zero:

$$\nabla L(w) + H(w)u = 0 \;\Rightarrow\; u = -H^{-1}(w)\nabla L(w).$$

Variant: quasi-Newton methods

For optimizing a function over $\mathbb{R}^p$, the Newton update involves computing the $p \times p$ Hessian at each time step:

$$w_{t+1} = w_t - \eta_t H^{-1}(w_t) \nabla L(w_t).$$

Speed things up by using an approximation B_t of $H^{-1}(w_t)$:

- Initialize it to the identity, say.
- Efficiently update $B_t \to B_{t+1}$ using a second-order approximation based on $w_{t+1}, w_t, \nabla L(w_t), \nabla L(w_{t+1})$.

Example: the BFGS (Broyden-Fletcher-Goldfarb-Shanno) procedure.

Even better: instead of maintaining a *dense* matrix B_t, use an $O(p)$-sized approximation to it. Example: L-BFGS ("Limited memory BFGS").