Logistic Regression

Based on slides by Daniel Lowd, Vibhav Gogate,
Carlos Guestrin, Luke Zettlemoyer and Dan Weld.

Predicting Probabilities

- We have mainly talked about binary classification
- Our decision rule always give one type with 100% confidence for a given example (e.g., Spam nor Not)
- What if an email has a 60% chance of being spam?
- What if there is a 30% chance of rain?
- What if a mushroom has a 10% probability of being poisonous?

- **We want to be able to talk about uncertainty or the probability of a type given an example.**

Logistic Regression

- Predict class probabilities $P(Y|X)$ with a linear model: still compute a linear predictor (based on the linear combination of parameters), then transform it into a probability
- How do we turn (w x + b) into a probability?

Linear models in general

- By linear models, we mean that the hypothesis function $h_w(x)$ is a linear function of the parameters w, not the linear function of the input vector x
- Generalized linear model

  - Logistic regression is a special case of a generalized linear model:

$$E[Y \mid \mathbf{x}] = g^{-1}(\mathbf{w}^\top \mathbf{x}).$$

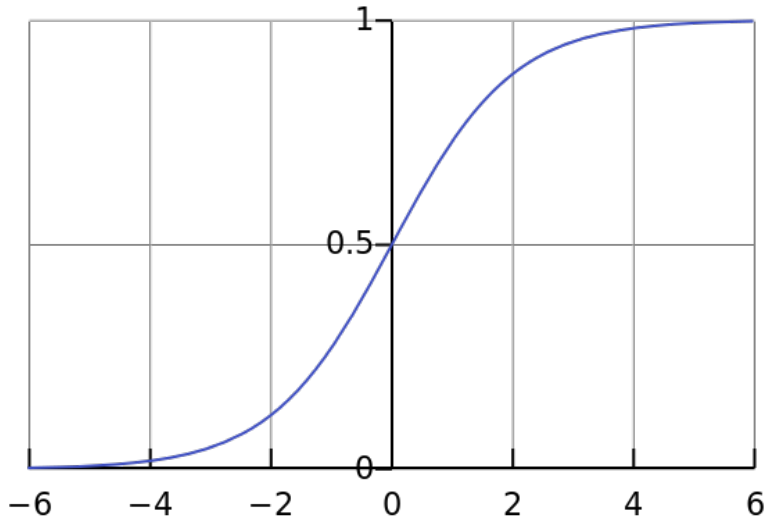
    g is called the *link function*, it relates the mean of the response to the linear predictor.
  - Linear regression: $E[Y \mid \mathbf{x}] = E[\mathbf{w}^\top \mathbf{x} + \varepsilon \mid \mathbf{x}] = \mathbf{w}^\top \mathbf{x}$ (g is the identity).
  - Logistic regression: $E[Y \mid \mathbf{x}] = P(Y = 1 \mid \mathbf{x}) = \sigma(\mathbf{w}^\top \mathbf{x})$
  - Poisson regression: $E[Y \mid \mathbf{x}] = \exp(\mathbf{w}^\top \mathbf{x})$ (for count data)
  - ...

The logit function $\text{Log}\ \frac{z}{1-z}$

The Logistic Function

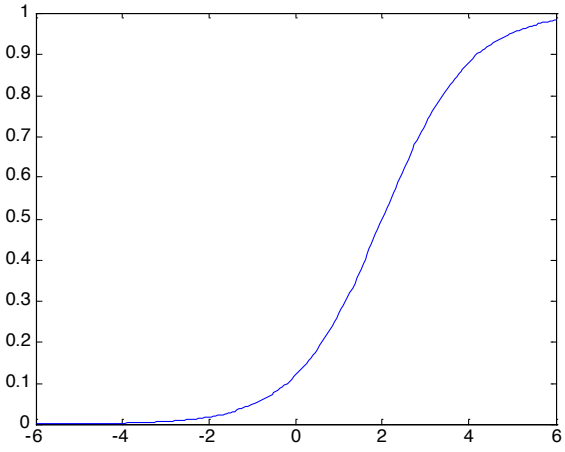
The **logistic function** squashes a real number in the range (-∞,+∞) into the range (0,1) (inverse of the logit function).

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

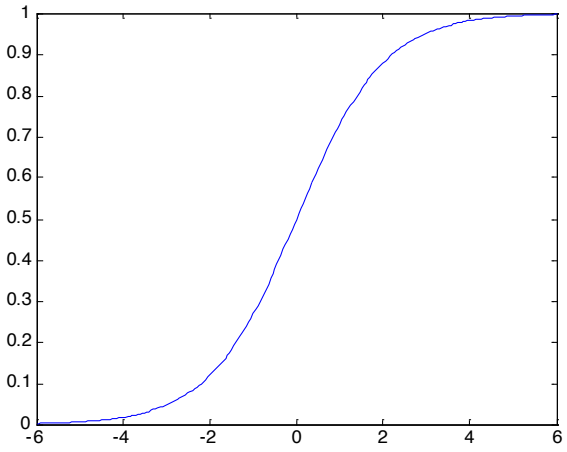


Understanding Sigmoids

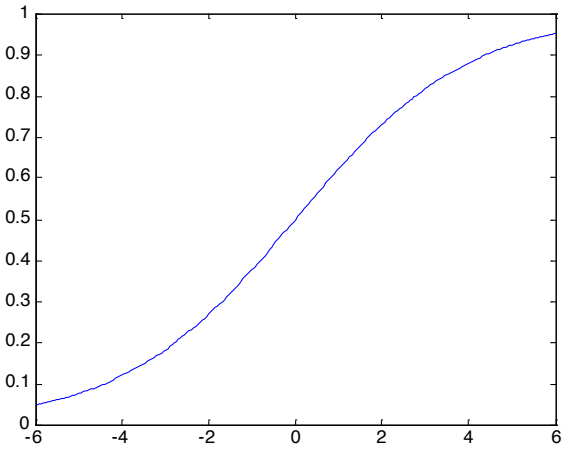
$$\sigma(w_1 x_1 + b) = \frac{1}{1 + \exp(-(w_1 x_1 + b))}$$



w_1=1, b=-2



w_1=1, b = 0

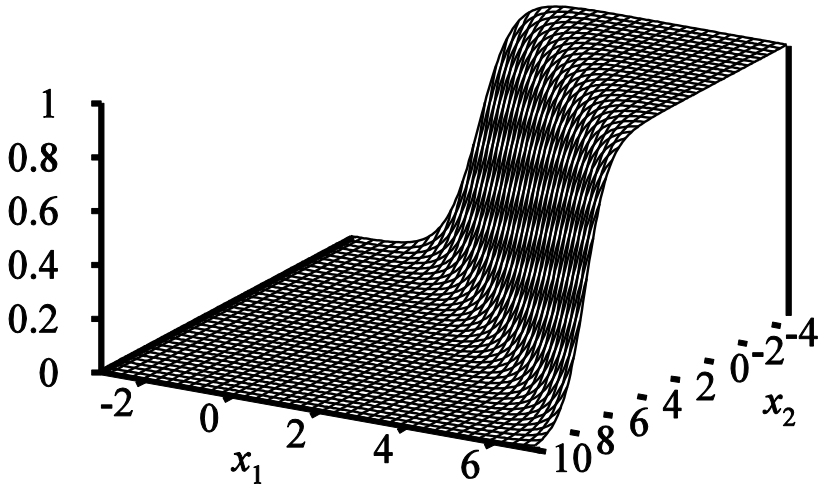


w_1= 0.5, b = 0

Logistic Regression

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

Example: Logistic function for two input features x_1 and x_2:



Very convenient for two classes

$$P(Y=1|X=<X_1,...X_n>)=\frac{1}{1+exp(w_0+\sum_i w_i X_i)}$$

implies

$$P(Y=0|X=<X_1,...X_n>)=\frac{exp(w_0+\sum_i w_i X_i)}{1+exp(w_0+\sum_i w_i X_i)}$$

implies

$$\frac{P(Y=0|X)}{P(Y=1|X)}=exp(w_0+\sum_i w_i X_i)$$

implies

$$\ln\frac{P(Y=0|X)}{P(Y=1|X)}=w_0+\sum_i w_i X_i$$

linear classification rule!

Y=0 if the RHS>0

Learning Logistic Regression

Key idea: Choose a model where reality is probable.

Probability of the true labels given the data:

$$\prod_{(x,y)\in D} \hat{P}(y|x) = \prod_{(x,y)\in D} \frac{1}{1+\exp(-y(w^T x + b))}$$

$$\log \prod_{(x,y)\in D} \hat{P}(y|x) = \sum_{(x,y)\in D} -\log(1+\exp(-y(w^T x + b)))$$

Conditional log-likelihood

(Negative) logistic loss

Maximize the log-likelihood
= Minimize negative log-likelihood
= Minimize logistic loss

Why logistic loss?

- How's about the 0/1 loss: $\min_{w,b} \sum_n \mathbf{1}[y_n(\boldsymbol{w} \cdot \boldsymbol{x}_n + b) > 0]$
- 0-1 loss is non-smooth – a small change in a parameter could lead to a BIG change in accuracy! (How?)
- What do we want beyond smoothness?

Convex functions

- A function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if for all $\mathbf{a}, \mathbf{b} \in \mathbb{R}^d$, $\lambda \in [0, 1]$:

$$f(\lambda \mathbf{a} + (1 - \lambda)\mathbf{b}) \leq \lambda f(\mathbf{a}) + (1 - \lambda) f(\mathbf{b}).$$

- If f and g are convex functions, $\alpha f + \beta g$ is also convex for any real numbers α and β.
- *First-order* characterization:

$$f \text{ is convex} \Leftrightarrow \text{for all } \mathbf{a}, \mathbf{b}: \quad f(\mathbf{a}) \geq f(\mathbf{b}) + \nabla f(\mathbf{b})^\top (\mathbf{a} - \mathbf{b})$$

(the function is globally above the tangent at $\mathbf{b}$).

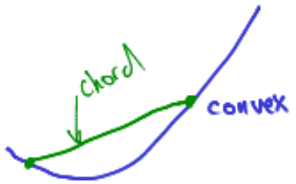
- *Second-order* characterization:

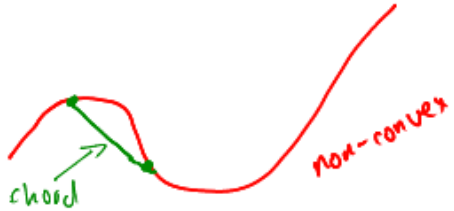
$$f \text{ is convex} \Leftrightarrow \text{the Hessian of } f \text{ is positive semi-definite.}$$

The Hessian contains the second-order derivatives of f:

$$\mathbf{H}_{i,j} = \frac{\partial^2 f}{\partial x_i \partial x_j}.$$

It is positive semi-definite if $\mathbf{a}^\top \mathbf{H} \mathbf{a} \geq 0$ for all $\mathbf{a} \in \mathbb{R}^d$.





Examples of Loss Functions

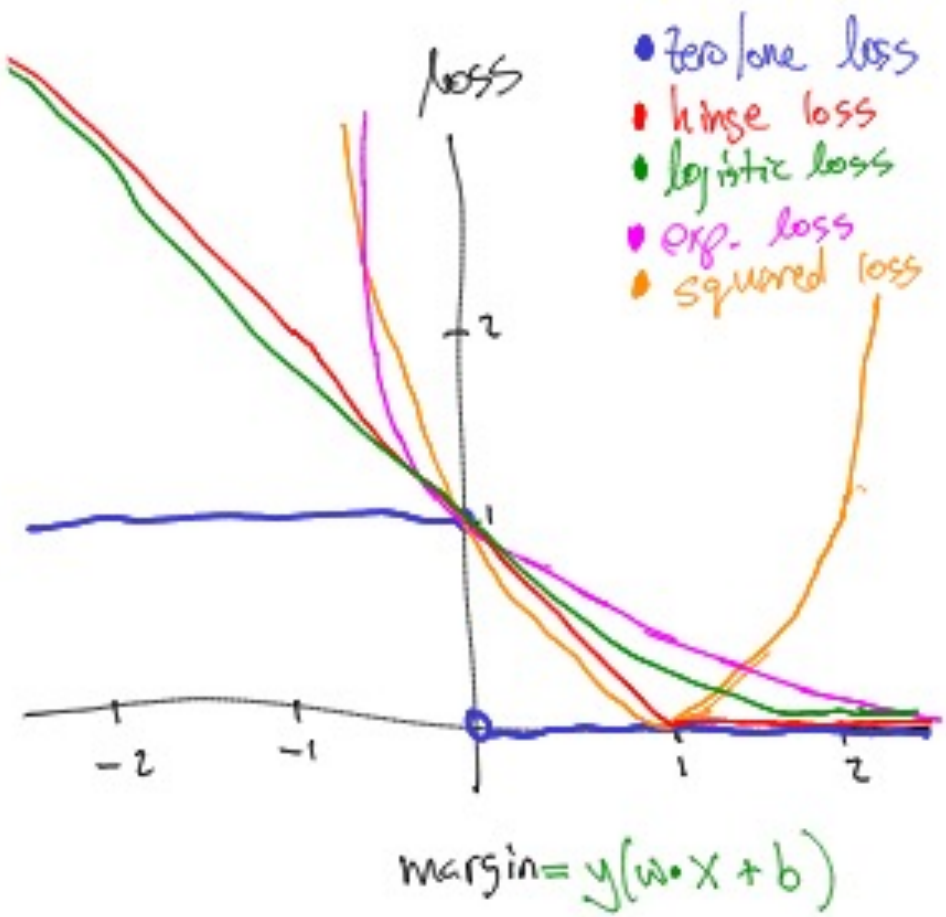
Zero/one: $$\ell^{(0/1)}(y, \hat{y}) = \mathbf{1}[y\hat{y} \leq 0] \tag{6.3}$$

Hinge: $$\ell^{(\text{hin})}(y, \hat{y}) = \max\{0, 1 - y\hat{y}\} \tag{6.4}$$

Logistic: $$\ell^{(\log)}(y, \hat{y}) = \frac{1}{\log 2} \log\left(1 + \exp[-y\hat{y}]\right) \tag{6.5}$$

Exponential: $$\ell^{(\exp)}(y, \hat{y}) = \exp[-y\hat{y}] \tag{6.6}$$

Squared: $$\ell^{(\text{sqr})}(y, \hat{y}) = (y - \hat{y})^2 \tag{6.7}$$


loss
zero/one loss
hinge loss
logistic loss
exp. loss
squared loss
2
1
-2
-1
1
2
margin = y(w·x + b)

Learning Logistic Regression

- Given the training data, how can we find the model parameters that would minimize the negative log-likelihood?
- Bad news: no closed-form solution to maximize the negative log-likelihood
- Good news: The negative log-likelihood function is concave function of **w**!
  - No local minima
  - Concave functions easy to optimize
- Optimization techniques: finding the minimum/maximum of multivariate functions.
- So, machine learning is sort of

  Model + Cost function + Optimization technique

Gradient Descent

Q: Suppose you want to avoid a flood. How do you find a high place?

A: Walk uphill!

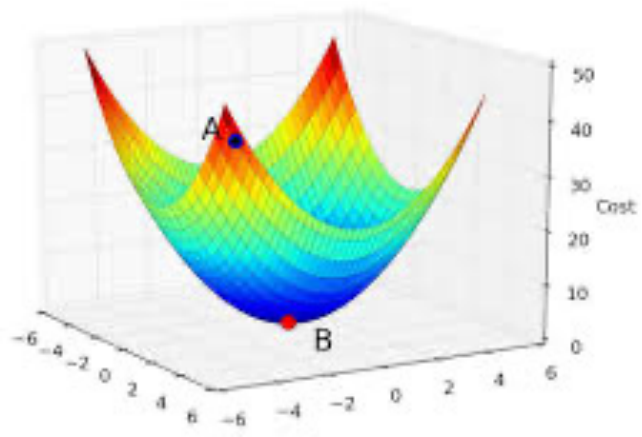
Q: And if you want to find a low place?

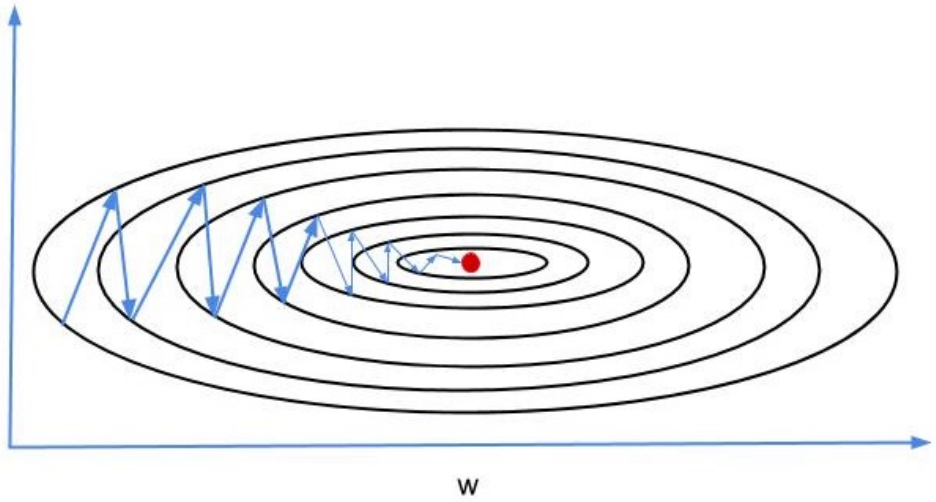
A: Walk downhill!

Q: And if you want to minimize a function?

A: Gradient descent!

Gradient Descent





Gradient Descent

Algorithm 22 GRADIENTDESCENT($\mathcal{F}$, K, η_1, ...)

1: $z^{(0)} \leftarrow \langle 0, 0, \ldots, 0 \rangle$ // initialize variable we are optimizing
2: **for** $k = 1 \ldots K$ **do**
3: $g^{(k)} \leftarrow \nabla_z \mathcal{F}|_{z^{(k-1)}}$ // compute gradient at current location
4: $z^{(k)} \leftarrow z^{(k-1)} - \eta^{(k)} g^{(k)}$ // take a step down the gradient
5: **end for**
6: **return** $z^{(K)}$

For logistic regression:

$$\mathcal{F} = -\log \prod_{(x,y) \in D} \hat{P}(y|x) = \sum_{(x,y) \in D} \log(1 + \exp(-y(w^T x + b)))$$

Gradient of Logistic Loss

$$\frac{\partial \mathcal{L}}{\partial w_i} = -\sum_{(x,y)\in D} \frac{1}{1+\exp(y(w^T x + b))} y\, x_i$$

$$\frac{\partial \mathcal{L}}{\partial b} = -\sum_{(x,y)\in D} \frac{1}{1+\exp(y(w^T x + b))} y$$

Try it!

Convergence Rate

For strongly convex functions:

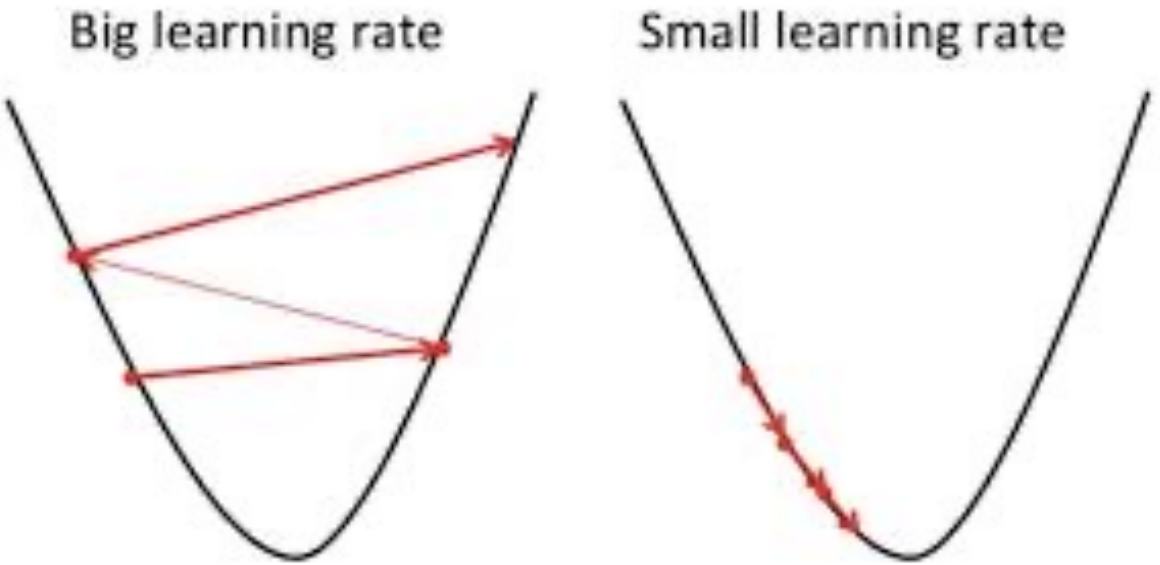
Theorem 7 (Gradient Descent Convergence). *Under suitable conditions[1], for an appropriately chosen constant step size (i.e., $\eta_1 = \eta_2, \cdots = \eta$), the* **convergence rate** *of gradient descent is $\mathcal{O}(1/k)$. More specifically, letting z^* be the global minimum of $\mathcal{F}$, we have: $\mathcal{F}(z^{(k)}) - \mathcal{F}(z^*) \leq \frac{2||z^{(0)} - z^*||^2}{\eta k)}$.*

← Doubling the number of iterations cuts the error in half.

The effect of learning rate

Q: What's an "appropriately chosen constant step size"?
A: 1/L where L is the curvature of the function.

Many variants – adaptive learning rates, line search, or momentum terms to speed up convergence.



The second order methods

- The Newton's method to find the zero of a function: g: $\mathbb{R} \rightarrow \mathbb{R}$

$$w^{i+1} = w^i - \frac{g(w^i)}{g'(w^i)}$$

- Applying to machine learning to minimize J, so finding the zero of the gradient J'

$$w^{i+1} = w^i - \frac{J'(w^i)}{J''(w^i)}$$

- So, no step size needed
- If the error function is quadratic, this will find the minimum in one step!
- But, we need to compute the second-order derivatives (the Hessian matrix)

$$\mathbf{H}_{ij} = \frac{\partial^2 J}{\partial w_i \partial w_j}$$

$$\mathbf{w} \leftarrow \mathbf{w} - \mathbf{H}^{-1} \nabla_{\mathbf{w}} J$$

Stochastic Gradient

- Perceptron algorithm: Update model immediately after each misprediction.
- Gradient descent: Compute gradient over all examples before updating.

What if we instead compute the gradient on a randomly chosen subset of the data?

Advantages?

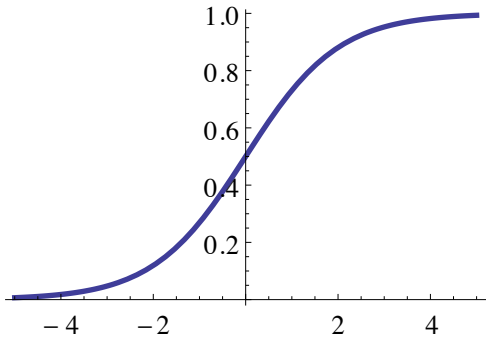
Disadvantages?

Mini batching

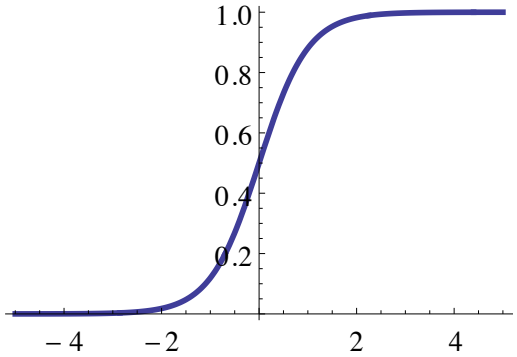
- A way to approximate the gradient computation over the whole training data
- Cons:
  - Not guaranteed to give us the steepest direction
- Pros:
  - Efficient (very often, you won't be able to load all your training data into memory for computation)
  - Less variance on gradient than stochastic gradient descent (batch size = 1)
  - Might be a way to jump out of shallow minima

Large parameters…

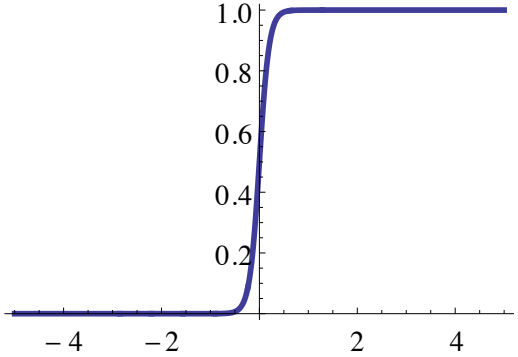
$$\frac{1}{1+e^{-ax}}$$



a=1



a=5



a=10

- Maximum likelihood solution: prefers higher weights
  - higher likelihood of (properly classified) examples close to decision boundary
  - larger influence of corresponding features on decision
  - *can cause overfitting!!!*
- Regularization: penalize high weights

Why small weights correspond to simpler solution/function?

- Remember the Occam's razor?
- What does it mean by simple functions?
- Image a linear classifier:

$$a = \left[\sum_{d=1}^{D} w_d x_d\right] + b$$

- Large w_d might changes a a lot when x_d only changes a little, so high variance
- Simple functions mean small variance
- High variance has higher chance to overfit (the bias and variance tradeoff)

Weight Regularization

Q: How do we prevent overfitting for parametric models?

A: Adjust our inductive bias with a **regularization function** which penalizes large weights (or anything else we wish to avoid).

Regularized loss function:

$$\min_{\boldsymbol{w},b} \quad \sum_n \ell(y_n, \boldsymbol{w} \cdot \boldsymbol{x}_n + b) + \lambda R(\boldsymbol{w}, b)$$

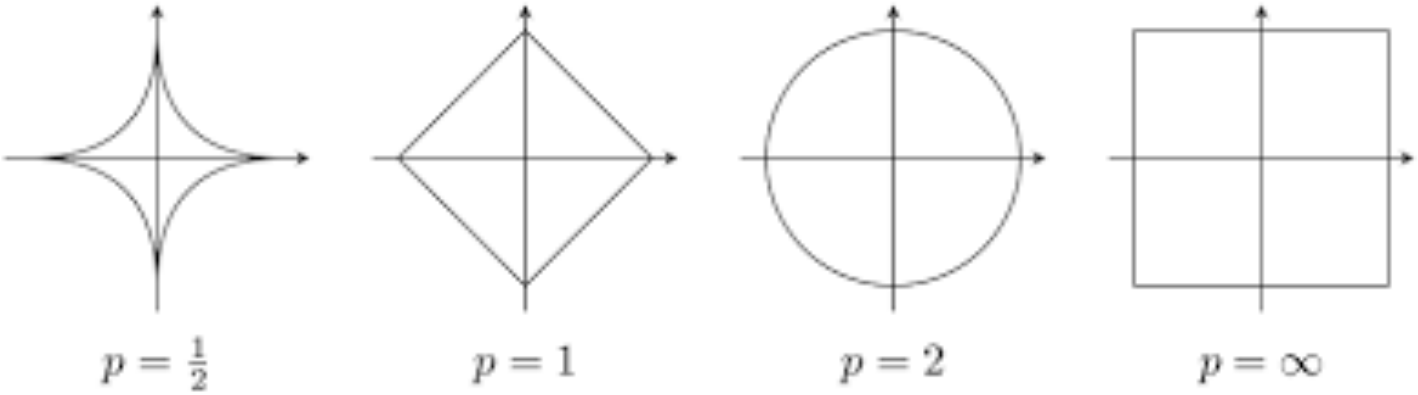
P-Norms

- Common loss functions:
  - L_2 norm of weight vector (square root of sum of squared weights)
  - L_1 norm of weight vector (sum of absolute weights)
- Generalizing these:

$$||\boldsymbol{w}||_p = \left(\sum_d |w_d|^p \right)^{\frac{1}{p}}$$

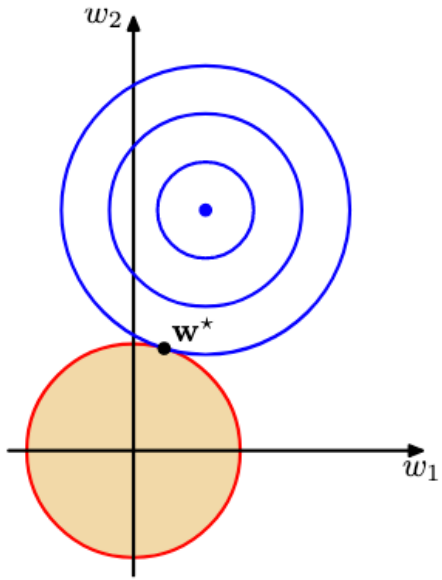
What if $p = 0$?

P-Norms



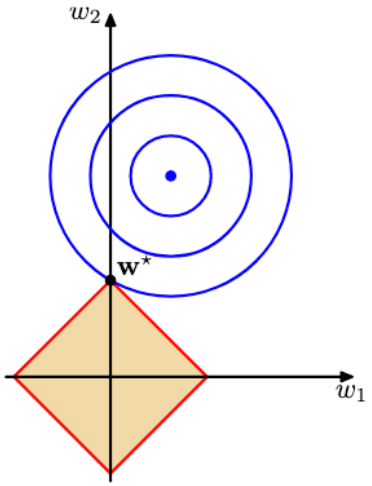
Isosurfaces: $||w||_p = \text{const}$

L2 Regularization (Ridge Regression)



- If λ is at a "good" value, regularization helps to avoid overfitting
- Choosing λ may be hard: cross-validation is often used
- If there are irrelevant features in the input (i.e. features that do not affect the output), L_2 will give them small, but non-zero weights.
- Ideally, irrelevant input should have weights exactly equal to 0.

L1 Regularization (Lasso)



- If λ is big enough, the circle is very likely to intersect the diamond at one of the corners
- This makes L_1 regularization much more likely to make some weights *exactly* 0

- If there are irrelevant input features, Lasso is likely to make their weights 0, while L_2 is likely to just make all weights small
- Lasso is biased towards providing *sparse solutions* in general
- Lasso optimization is computationally more expensive than L_2
- More efficient solution methods have to be used for large numbers of inputs (e.g. least-angle regression, 2003).

The p in Lp norm: a trade-off between convexity and sparsity

Justify L1 and L2 with Bayes Learning

$$h_{MAP} = \arg\max_{h \in \mathcal{H}} P(D|h)P(h)$$

- We assume all the hypothesis are equally likely to obtain the maximum likelihood principal with Bayes Learning
- If we impose some priors over $P(h)$, the solution will be different.

Maximum A Posteriori

$$h_{MAP} = \arg\max_{h \in \mathcal{H}} P(D|h)P(h)$$

- Common priors on **w**
  - Normal distribution, zero mean, diagonal covariance

$$p(\mathbf{w}) = \prod_i \frac{1}{\kappa\sqrt{2\pi}} \; e^{\frac{-w_i^2}{2\kappa^2}}$$

  - Laplace distribution

$$p(w) = \frac{1}{2}\prod_i e^{-|w_i|}$$

- Normal Distribution: $\log p(w) = \frac{-w^2}{2\kappa^2}$ + constants = L2 regularizer
- Laplace distribution: $\log p(w) = -|w|$ + constants = L1 regularizer.