

From Regression to Classification with Logistic Regression

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Machine Learning
CS 600.475



Classification

- Data $\{(x_i, y_i)\}_{i=1}^N$ $x_i \in \mathcal{X}^M$ $y_i \in \mathcal{Y}$
- Learn: a mapping from x to discrete value y
 - $f(x) = y$
- Examples
 - Spam classification
 - Document topic classification
 - Identifying faces in images

Binary Classification

- We'll focus on binary classification
 - $y_i \in \{0, 1\}$
- Usually easy to generalize to multi-class classification

Different Definition

Fitting a function to data

- Fitting: Optimization, what parameters can we change?
- **Function: Model, loss function**
- Data: Data/model assumptions? How we use data?
- ML Algorithms: minimize a function on some data

Evaluation

- Accuracy

$$\frac{\text{number of correct predictions}}{\text{total number of predictions}}$$

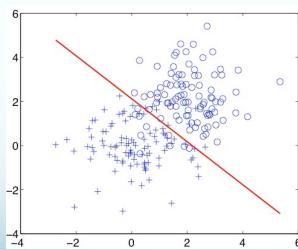
- Other measurements appropriate for some tasks
 - Ex. we care more about certain types of mistakes

Regression

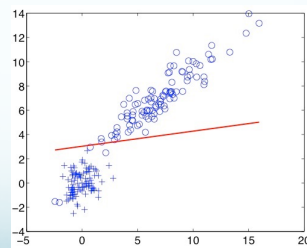
- Least squares regression
 - Outputs real number for each example
- It seems that classification should be easier!
- Let's use regression for classification
 - Learn least squares regression model $f_w(x)=y$
 - $f_w(x)=w^T x$
 - If $y>0$, predict "True (1)"
 - If $y\leq 0$ predict "False (0)"

Regression for Classification

- $f_w(x)=0$ partitions the input space into two class specific regions
 - Linear decision boundary



Good



Bad

Figures by Tommi Jaakkola

Regression for Classification

- Mismatch between regression loss and classification
 - Classification: accuracy
 - We don't care about large vs. small values of output
- Outliers problematic
 - Prediction of 42 for example is fine for classification, bad for regression
- We need output to be either 1 or 0

Machine Learning

Fitting a function to data

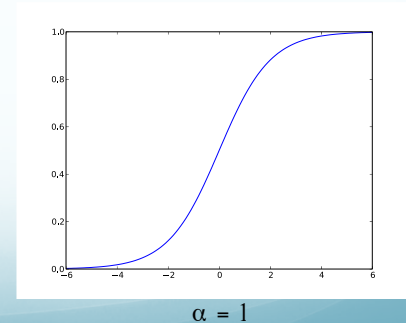
- Fitting: Solve for w given y and x
- Function: Regression uses squared loss
 - Bad match for our task!
- Data: assume dependent variable linear combination of independent variables
- Our loss function doesn't match classification goals

Logistic Function

- Quick fix: apply a function to the output of regression that gives desired value
- Logistic function

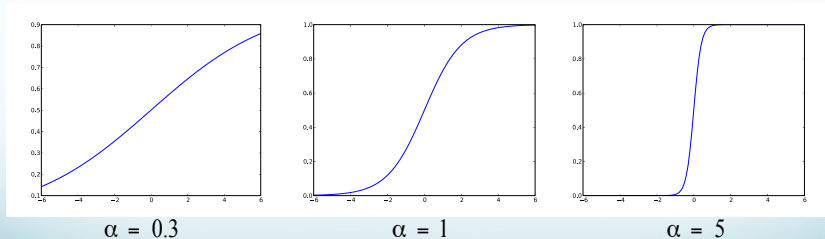
- Outputs between 0 and 1
- Scaling parameter α
- Most outputs are close to 1 or 0

$$g_{\alpha}(x) = \frac{1}{1 + e^{-\alpha x}}$$



Logistic Function

$$g_{\alpha}(x) = \frac{1}{1 + e^{-\alpha x}}$$



Logistic Regression

- We can combine the logistic function and our regression model

$$g(w^T \cdot x_i) = \frac{1}{1 + e^{-w^T \cdot x_i}}$$

- Notice: as $w^T \cdot x_i$ becomes:
 - Large- output closer to 1
 - Small- output closer to 0

Probabilistic View

- In regression we modeled probability of the output
- Probability of the example and classification?
 - $p(x,y)$?
 - $p(x,y) = p(x|y) p(y)$
 - Since we know x , we want to maximize y
 - $p(x|y)p(y) = p(y|x)p(x)$
 - Since $p(x)$ is fixed:
 - $\arg\max_{y=0,1} p(x|y) p(y) = \arg\max_{y=0,1} p(y|x)$

Why?

- We can now write the distribution as
$$p_w(y=1|x) = \frac{1}{1 + e^{-w^T \cdot x}}$$
- Which implies that
$$p_w(y=0|x) = \frac{e^{-w^T \cdot x}}{1 + e^{-w^T \cdot x}}$$
- The odds of the event is then $\frac{p_w(y=1|x)}{p_w(y=0|x)} = \exp(-w^T \cdot x)$
- And the log-odds are
$$\log \frac{p_w(y=1|x)}{p_w(y=0|x)} = -w^T \cdot x$$

Generalized Linear Models

- Decision boundary/surface
 - An $n-1$ dimensional hyper-plane that separates the data into two groups
 - These are linear functions of x , even though logistic is not linear
- Generalized linear models
 - A linear model whose output is passed through non-linear function
- Hypothesis class
 - Linear decision boundaries

Logistic Regression Decisions

- Given parameters w , how do we make predictions?

$$p_w(y=1|x) = \frac{1}{1 + e^{-w^T \cdot x}}$$

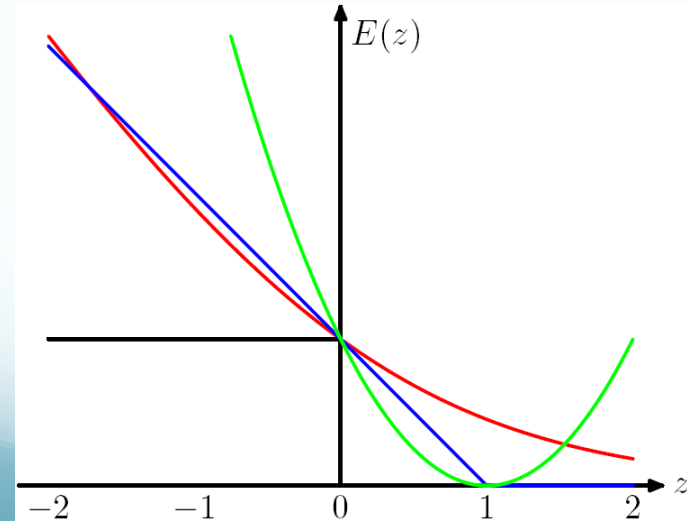
- If output $> .5$, predict 1, else predict 0
- In addition to prediction, we have confidence in prediction
 - Confidence is the probability of the prediction

Logistic Regression

Fitting a function to data

- Fitting: Solve for w given y and x
- Function: Generalized linear function: logistic over regression
- Data: assume dependent variable linear combination of independent variables

Logistic Loss



Objective Function: Likelihood

- Conditional data likelihood

$$p(Y|X, w) = \prod_{i=1}^n p(y_i | x_i, w)$$

Conditional Log Likelihood

$$p(Y|X, w) = \prod_{i=1}^n p(y_i | x_i, w)$$

$$\ell(Y, X, w) = \log p(Y|X, w) = \sum_{i=1}^n \log p(y_i | x_i, w)$$

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

Logistic Regression

Fitting a function to data

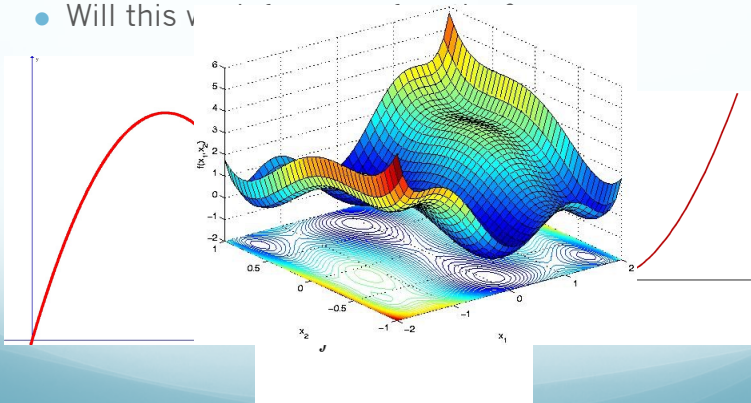
- **Fitting: Solve for w given y and x**
- Function: Generalized linear function: logistic over regression: conditional log likelihood
- Data: assume dependent variable linear combination of independent variables

Function Optimization

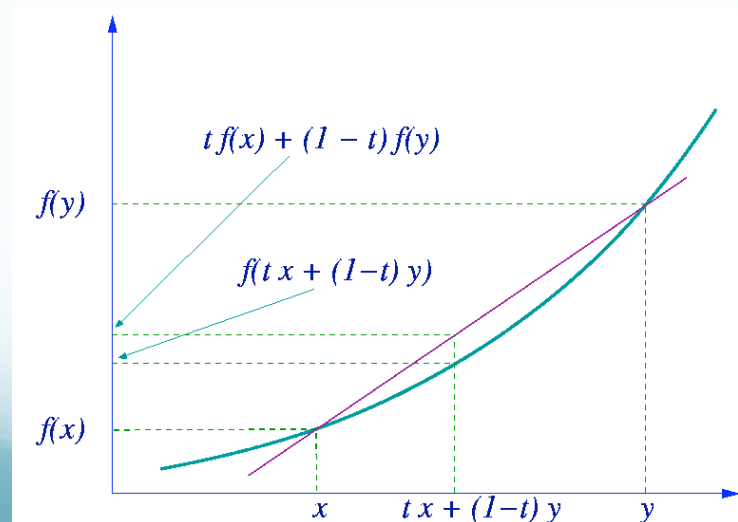
- We have a function and want to maximize/minimize it
- How do we find the point at which the function reaches its max/min?

Function Optimization

- Take the derivative, set it equal to 0, solve!
- Will this v



Convex Functions



Maximum Likelihood Estimation

- MLE: Find the value at which the likelihood is maximized
 - We'll talk about other options later in the semester
- Given the conditional log likelihood
 - Take the derivatives for parameters w
 - Set each derivative to 0
 - M equations and M variables
 - Solve for w
- Problem
 - No closed form (analytical) solution for w

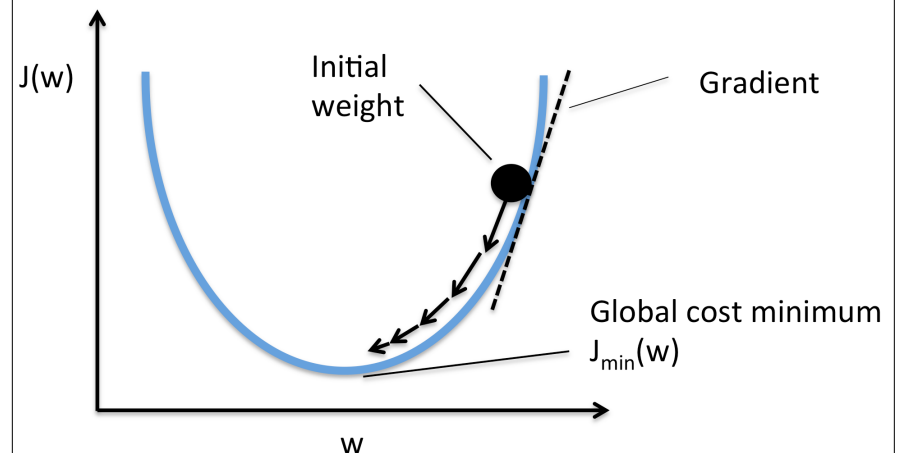
Convex Optimization

- The conditional maximum likelihood is concave
 - There is a single maximal solution
- We can maximize using convex optimization techniques
 - Its easy to optimize convex functions
 - There are **many** convex optimization algorithms

Gradient Descent

- First order method: needs first order derivatives
- Assuming $F(x)$ is defined and differentiable, then $F(x)$ decreases fastest if we go from x in the direction of the gradient of F
 - $-\nabla F(x)$ - vector of partial derivatives of F
 - $x' = x - \gamma \nabla F(x)$ - Update
- For sufficiently small values of γ , the value of the function will get smaller

Gradient Descent



Derivatives

$$\frac{\partial \ell(Y, X, w)}{\partial w} = \sum_{i=1}^n (y_i - p(y_i = 1 | x_i, w)) x_i = 0$$

- The derivative is 0 when $y_i = p(y_i = 1 | x_i, w)$
 - Minimize the prediction error

Gradient Descent Solution

$$w^{(t+1)} = w^t + \gamma \frac{\partial \ell(Y, X, w)}{\partial w}$$
$$\frac{\partial \ell(Y, X, w)}{\partial w} = \sum_{i=1}^n (y_i - p(y_i = 1 | x_i, w)) x_i = 0$$
$$w^{(t+1)} = w^t + \gamma \sum_{i=1}^n (y_i - p(y_i = 1 | x_i, w)) x_i$$

Algorithm: Logistic Regression

- Train: given data X and Y
 - Initialize w to starting value
 - Repeat until convergence
 - Compute the value of the derivative for X, Y and w
 - Update w by taking a gradient step
- Predict: given an example x
 - Using the learned w , compute $p(y|x, w)$

$$p(y=1 | x, w) = \frac{1}{1 + e^{-w^T \cdot x}}$$

- Note: many other optimization routines available

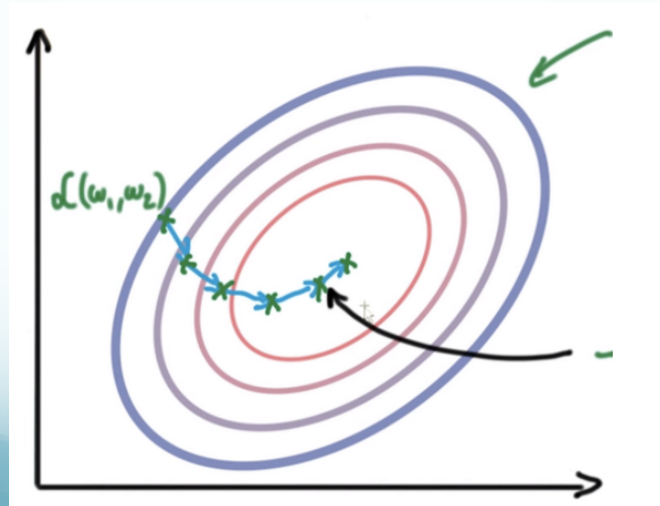
Gradient Based Optimization

- Multiple methods available for optimizing the same objective function
 - First order methods
 - Second order methods
 - Adaptive methods
 - ...

Alternate Methods

- Batch gradient descent
 - Utilize the gradient of all the data
 - Slow: need to consider all the data before making a single update

Gradient Descent



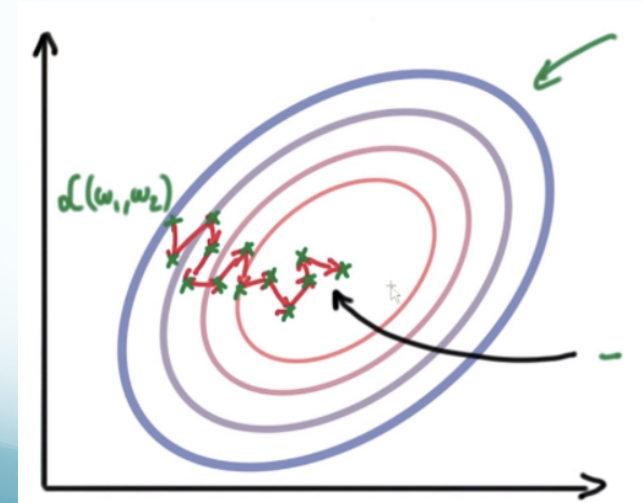
Stochastic Updates

- Compute the gradient on a single example at a time

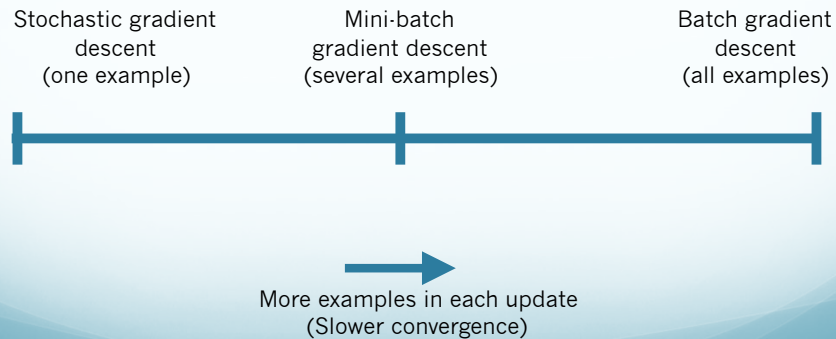
$$w^{(t+1)} = w^t + \gamma \sum_{i=1}^n \{y_i - p(y_i = 1|x_i, w)\}x_i$$

$$w^t + \gamma\{y_1 - p(y_1 = 1|x_1, w)\}x_1 + \gamma\{y_2 - p(y_2 = 1|x_2, w)\}x_2 \dots$$

Gradient Descent



Update Frequency



Regularization

- Same over-fitting problems as least squares
- Add regularization term to objective to favor different considerations
- Similar options
 - Quadratic regularization (L2)
 - L1 regularization (sparse solutions)
- For each regularization optimize new objective function

Summary

- Logistic regression
 - Learn $p(y|x)$ directly with functional form of distribution
 - Maximize the data conditional log-likelihood
 - Equivalent to linear prediction
 - Decision rule is a hyper-plane
 - Regularization to prevent over-fitting