Logistic Regression

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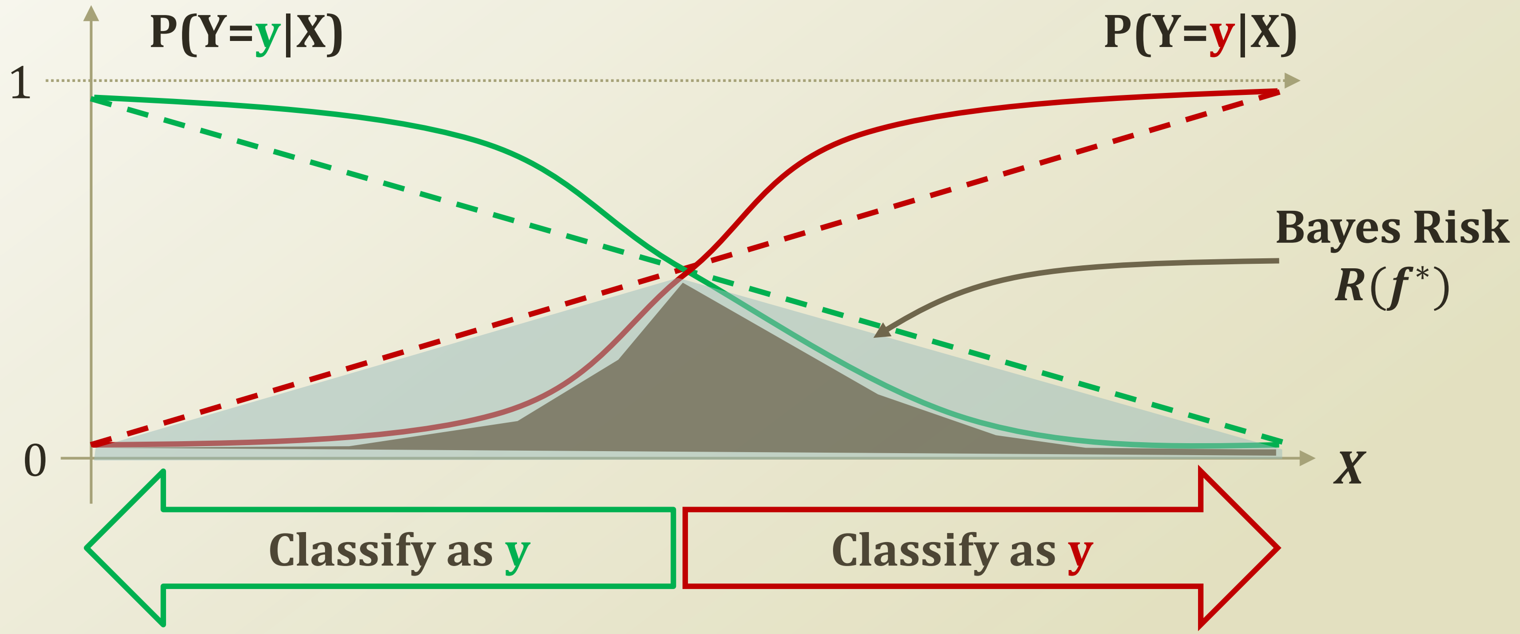
Weekly Objectives

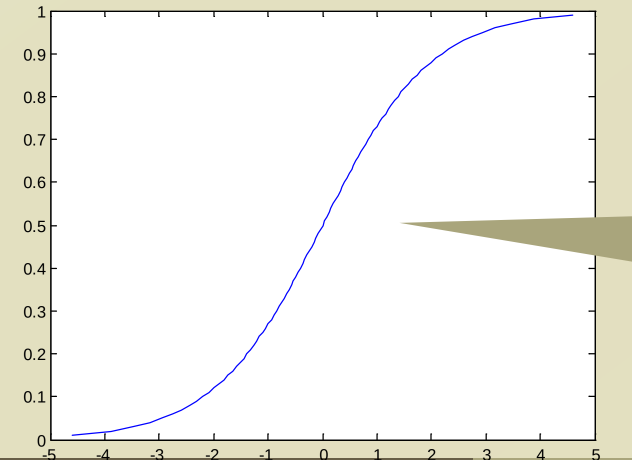
- Learn the logistic regression classifier
  - Understand why the logistic regression is better suited than the linear regression for classification tasks
  - Understand the logistic function
  - Understand the logistic regression classifier
  - Understand the approximation approach for the open form solutions
- Learn the gradient descent algorithm
  - Know the tailor expansion
  - Understand the gradient descent/ascent algorithm
- Learn the different between the naïve Bayes and the logistic regression
  - Understand the similarity of the two classifiers
  - Understand the differences of the two classifiers
  - Understand the performance differences

LOGISTIC REGRESSION

Optimal Classification and Bayes Risk



- Linear function vs. Non-linear function of P(Y|X)
  - Which is better?
- Problems of linear function
  - Range
  - Risk optimization
- Which function to use?
  - Need S-curve!

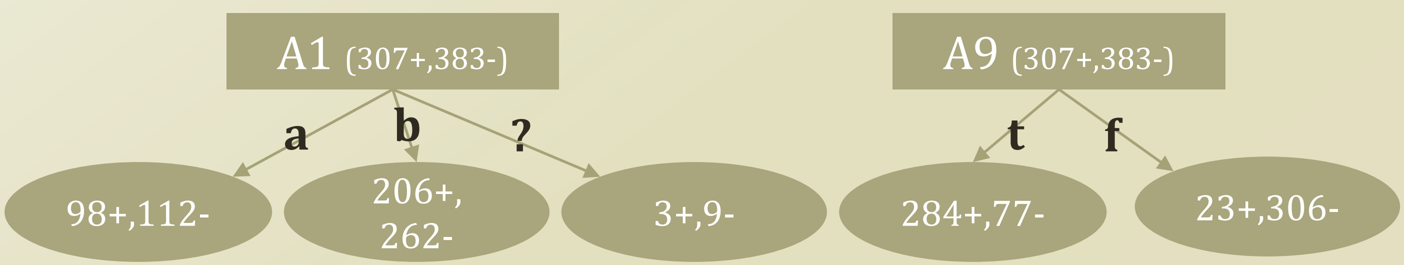


Detour: Credit Approval Dataset

- http://archive.ics.uci.edu/ml/datasets/Credit+Approval
- To protect the confidential information, the dataset is anonymized
  - Feature names and values, as well
- A1: b, a.
  A2: continuous.
  A3: continuous.
  A4: u, y, l, t.
  A5: g, p, gg.
  A6: c, d, cc, i, j, k, m, r, q, w, x, e, aa, ff.
  A7: v, h, bb, j, n, z, dd, ff, o.
  A8: continuous.
  A9: t, f.
  A10: t, f.
  A11: continuous.
  A12: t, f.
  A13: g, p, s.
  A14: continuous.
  A15: continuous.
  C: +,- (class attribute)

Some Counting Result

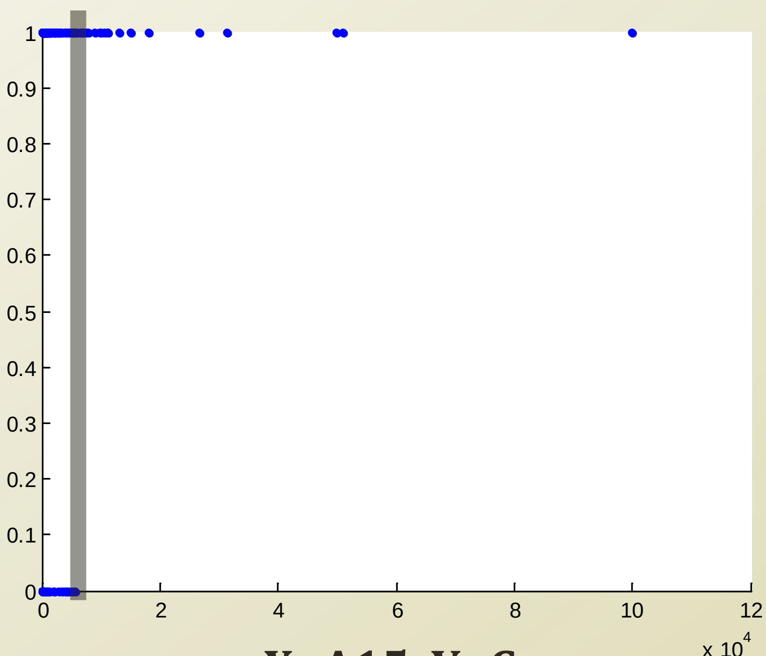
- 690 instances total
- 307 positive instances
- Considering A1
  - 98 positive when a
  - 112 negative when a
  - 206 positive when b
  - 262 negative when b
  - 3 positive when ?
  - 9 negative when ?
- Considering A9
  - 284 positive when t
  - 77 negative when t
  - 23 positive when f
  - 306 negative when f



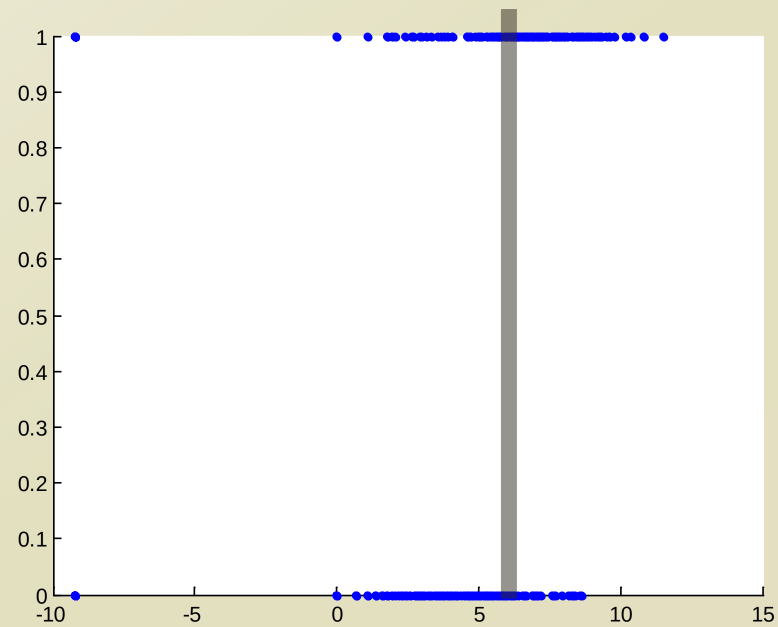
Which is a better attribute to include in the feature set of the hypothesis?

Classification with One Variable

- Let's predict the class, C, with an attribute, A15
  - Imagine that the Y axis shows P(Y|X)
  - There is a decision boundary
    - You can see it intuitively
- Then, How to find the boundary?



X=A15, Y=C

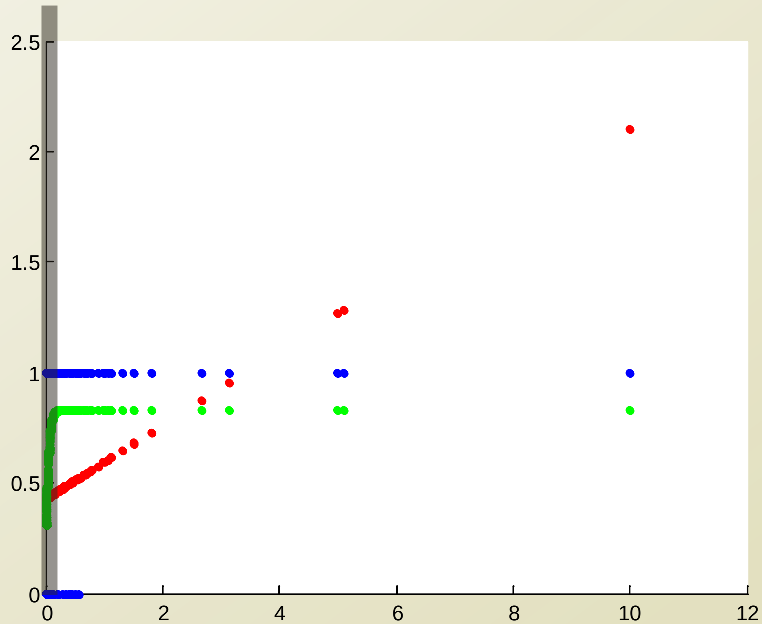


X=log(A15), Y=C

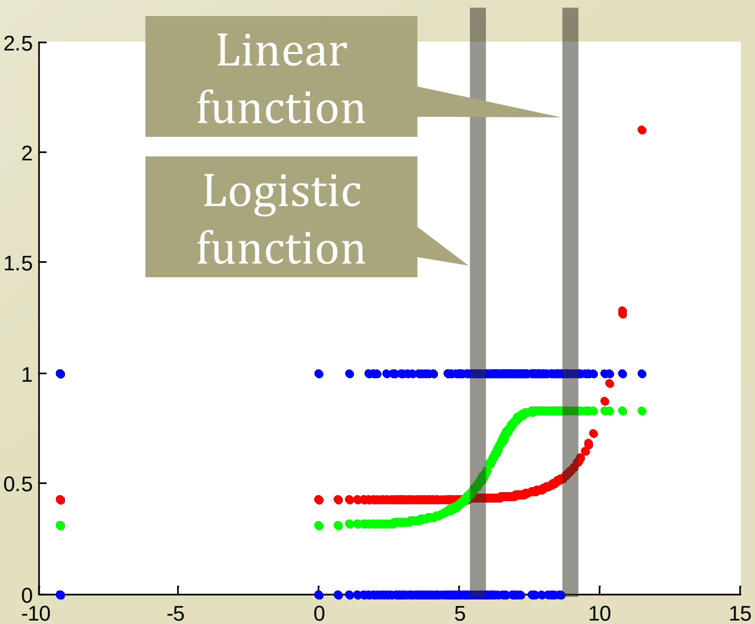
Linear Function vs. Non-Linear Function

- Problem of fitting to the linear function
  - Violate the probability axiom
  - Slow response to the examples
- Better to fit to the logistic function
  - Keep the probability axiom
  - Quick response around the decision boundary
- Which function to use?
  - Logistic fu

Blue = (X, Y_{true}), Red = $(X, P_{lin}(Y|X))$, Green=$(X, P_{log}(Y|X))$



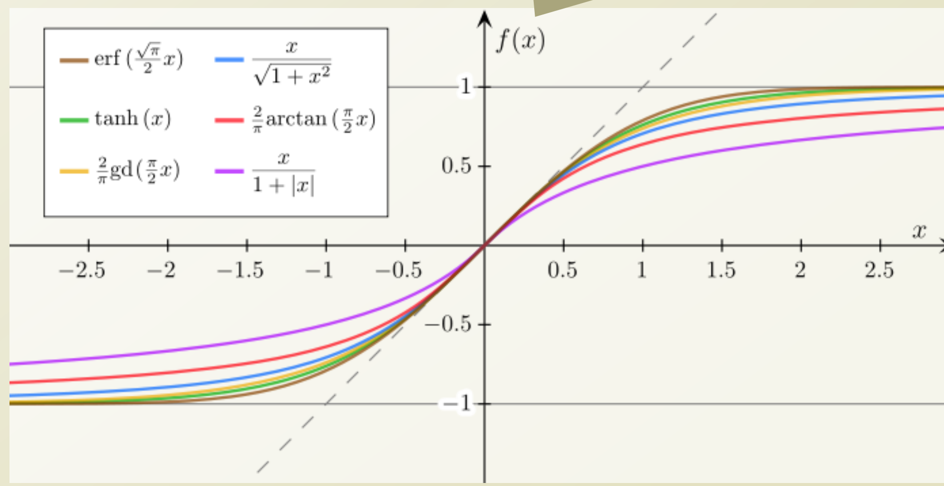
X=A15, Y=P(Y|X)



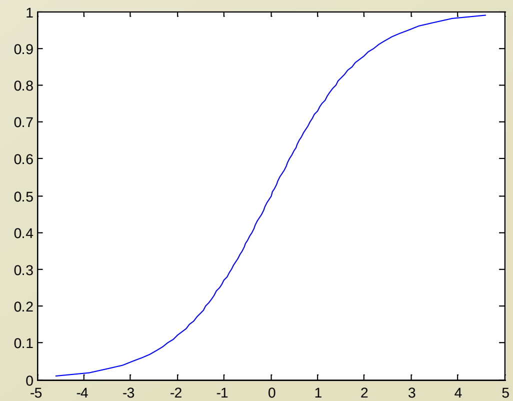
X=log(A15), Y=P(Y|X)

Logistic function

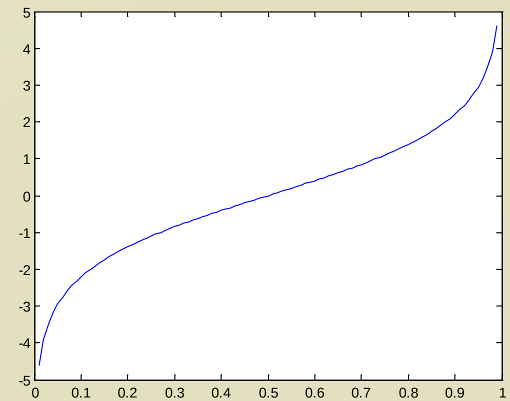
Many types of sigmoid functions



- Sigmoid function is
  - Bounded
  - Differentiable
  - Real function
  - Defined for all real inputs
  - With positive derivative
- Logistic function is
  - $f(x) = \frac{1}{1+e^{-x}}$
  - In relation to the population growth
  - Why is this good?
    - Sigmoid function
    - Particularly, easy to calculate the derivative…



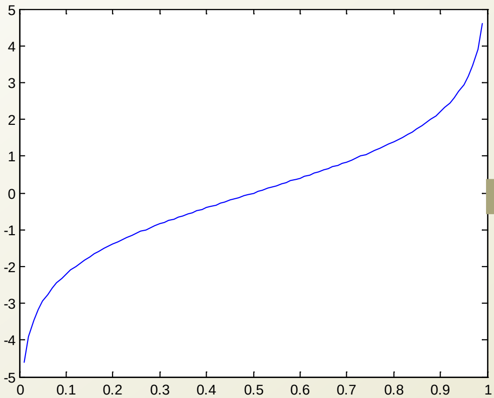
Logistic Function



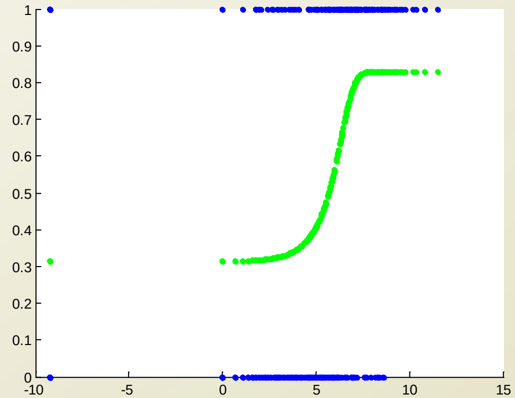
Logit Function

$$f(x) = \log\left(\frac{x}{1-x}\right)$$

Logistic Function Fitting



Logit Function



Logistic Fitting

Linear Regression:

$\hat{f} = X\theta \quad \theta = (X^TX)^{-1}X^TY$

Very similar to the linear regression.
Turning to the multivariate case

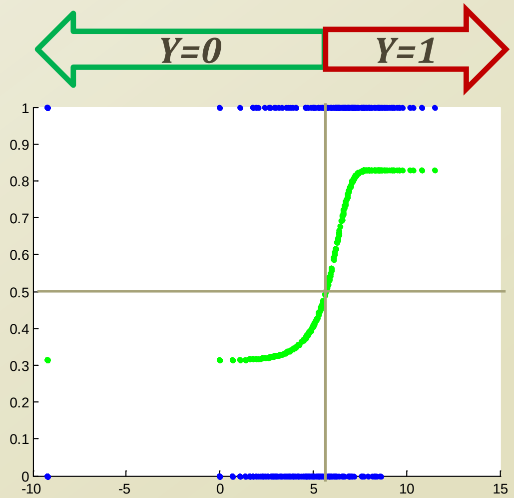
$$f(x) = \log\left(\frac{x}{1-x}\right) \rightarrow x = \log\left(\frac{p}{1-p}\right) \rightarrow ax + b = \log\left(\frac{p}{1-p}\right) \rightarrow X\theta = \log\left(\frac{p}{1-p}\right)$$

Logit→Logistic
Inverse of X and Y
X in Logit is the probability

Linear shift for a better function fitting

- When we are fitting the linear regression to approximate P(Y|X)
  - $X\theta = P(Y|X)$
  - Though, this is not going to keep the probability axiom
- Now we are fitting to the logistic function to approximate P(Y|X)
  - $X\theta = \log\left(\frac{P(Y|X)}{1-P(Y|X)}\right)$
  - From linear to logistic

Logistic Regression



- Logistic regression is a probabilistic classifier to predict the binomial or the multinomial outcome
  - by fitting the conditional probability to the logistic function.
- You can see the problem from the different view.
  - This way is actually closer to the formal definition.
- Given the Bernoulli experiment
  - $P(y|x) = \mu(x)^y(1-\mu(x))^{1-y}$
  - $\mu(x) = \frac{1}{1+e^{-\dot{\theta}^T x}} = P(y=1|x)$
  - Here, $\mu(x)$ is the logistic function
- From the previous slide,
  - $X\theta = \log\left(\frac{P(Y|X)}{1-P(Y|X)}\right) \rightarrow P(Y|X) = \frac{e^{X\theta}}{1+e^{X\theta}}$

Logistic Function

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

The goal, finally, becomes finding out $\boldsymbol{\theta}$, again

$$P(y=1|x)=\mu(x)=\frac{1}{1+e^{-\dot{\theta}^T x}}=\frac{e^{X\theta}}{1+e^{X\theta}}$$

Finding the Parameter, θ

$$X\theta=\log\left(\frac{P(Y|X)}{1-P(Y|X)}\right)$$

- **Maximum Likelihood Estimation (MLE) of $\boldsymbol{\theta}$**
  - Choose θ that maximizes the probability of observed data

$$\boldsymbol{\hat{\theta}=argmax_{\theta}P(D|\theta)}$$

- **This is Maximum Conditional Likelihood Estimation (MCLE)**
- $\hat{\theta}=argmax_{\theta}P(D|\theta)=argmax_{\theta}\prod_{1\le i\le N}P(Y_i|X_i;\theta)$

$$=argmax_{\theta}log(\prod_{1\le i\le N}P(Y_i|X_i;\theta))=argmax_{\theta}\sum_{1\le i\le N}log(P(Y_i|X_i;\theta))$$

- $P(Y_i|X_i;\theta)=\mu(X_i)^{Y_i}(1-\mu(X_i))^{1-Y_i}$
- $log\left(P(Y_i|X_i;\theta)\right)=Y_i\log\left(\mu(X_i)\right)+(1-Y_i)\log\left(1-\mu(X_i)\right)$

$$=Y_i\{\log\left(\mu(X_i)\right)-\log\left(1-\mu(X_i)\right)\}+\log\left(1-\mu(X_i)\right)$$

$$=Y_i\log\left(\frac{\mu(X_i)}{1-\mu(X_i)}\right)+\log\left(1-\mu(X_i)\right)$$

$$=Y_iX_i\theta+\log\left(1-\mu(X_i)\right)=Y_iX_i\theta-\log\left(1+e^{X_i\theta}\right)$$

Finding the Parameter, θ, contd.

Linear Regression (Closed Form):

$\hat{f} = X\theta$ $\quad \nabla_\theta(\theta^T X^T X\theta - 2\theta^T X^T Y)=0$

$2X^T X\theta - 2X^T Y = 0$

$\theta = (X^T X)^{-1} X^T Y$

- $\hat{\theta} = argmax_\theta \sum_{1\le i\le N} log(P(Y_i|X_i;\theta))$
- $= argmax_\theta \sum_{1\le i\le N}\{Y_i X_i\theta - \log(1+e^{X_i\theta})\}$
- Partial derivative to find a certain element in θ
- $\frac{\partial}{\partial\theta_j}\{\sum_{1\le i\le N} Y_i X_i\theta - \log(1+e^{X_i\theta})\}$

$$P(y=1|x) = \frac{e^{X\theta}}{1+e^{X\theta}}$$

$$= \left\{\sum_{1\le i\le N} Y_i X_{i,j}\right\} + \left\{\sum_{1\le i\le N} -\frac{1}{1+e^{X_i\theta}} \times e^{X_i\theta} \times X_{i,j}\right\}$$

$$= \sum_{1\le i\le N} X_{i,j}\left(Y_i - \frac{e^{X_i\theta}}{1+e^{X_i\theta}}\right) = \sum_{1\le i\le N} X_{i,j}(Y_i - P(Y_i=1|X_i;\theta)) = 0$$

- There is no way to derive further
  - There is no closed form solution!
  - Open form solution → approximate!

Cannot be easily solved in the closed form because of the logistic function

GRADIENT METHOD

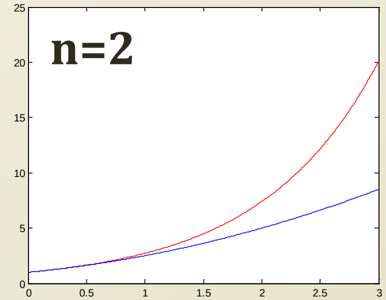
Taylor Expansion

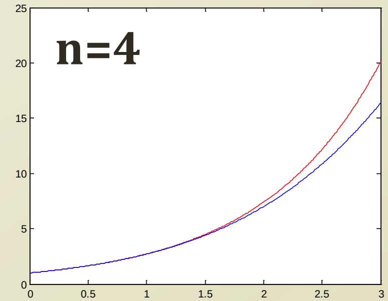
- Taylor series is a representation of a function
  - as a infinite sum of terms calculated from the values of the function's derivatives at a fixed point.
  - $f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \cdots$

    $$= \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!}(x-a)^n$$
  - a = a constant value
- Taylor series is possible when
  - Infinitely differentiable at a real or complex number of a
- Taylor expansion is a process of generating the Taylor series

$when\ a = 0,$

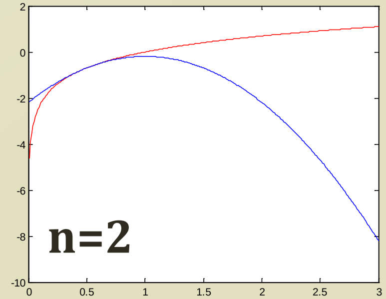
$$e^x = 1 + \frac{e^0}{1!}(x-0)^1 + \frac{e^0}{2!}(x-0)^2 + \cdots$$

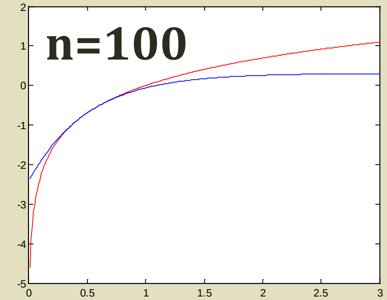




$when\ a = 0.5,$

$$logx = \log(0.5) + \frac{\frac{1}{0.5}}{1!}(x-0.5)^1 + \frac{\frac{1}{0.5^2}}{2!}(x-0.5)^2 + \cdots$$





Gradient Descent/Ascent

- Gradient descent/ascent method is
  - Given a differentiable function of *f(x)* and an initial parameter of x_1
  - Iteratively moving the parameter to the lower/higher value of *f(x)*
  - By taking the direction of the negative/positive gradient of *f(x)*
- Why this works?
  - $f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + O(||x-a||^2)$

    Useful Big-Oh Notation
    - Assume $a=x_1$ and $x=x_1+h\mathbf{u}$, $\mathbf{u}$ is the unit direction vector for the partial deriv.
    - $f(x_1 + h\mathbf{u}) = f(x_1) + hf'(x_1)\mathbf{u} + h^2 O(1)$
    - $f(x_1 + h\mathbf{u}) - f(x_1) \approx hf'(x_1)\mathbf{u}$

      Always???
    - $\mathbf{u}^* = argmin_{\mathbf{u}}\{f(x_1 + h\mathbf{u}) - f(x_1)\} = argmin_{\mathbf{u}} hf'(x_1)\mathbf{u} = -\frac{f'(x_1)}{|f'(x_1)|}$
    - $\because f(x_1 + h\mathbf{u}) \le f(x_1), \vec{a} \cdot \vec{b} = |\vec{a}||\vec{b}|cos\alpha$

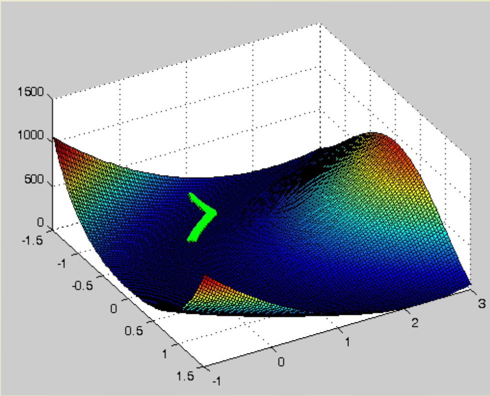
      Gradient Descent
  - $x_{t+1} \leftarrow x_t + h\mathbf{u}^* = x_t - h\frac{f'(x_t)}{|f'(x_t)|}$
- Perfectly applicable to $\hat{\theta} = argmax_{\theta} \sum_{1 \le i \le N} log(P(Y_i|X_i;\theta))$

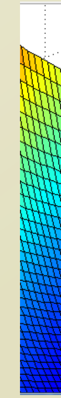
  Gradient Ascent
  - $f(\theta) = \sum_{1 \le i \le N} log(P(Y_i|X_i;\theta))$
  - Setup an initial parameter of θ_1
  - Iteratively moving θ_t to the higher value of $f(\theta_t)$
  - By taking the direction of the ***positive*** gradient of $f(\theta_t)$

How Gradient Descent Works

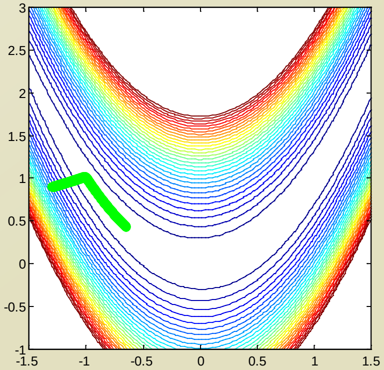
- Example function: Rosenbrock function
  - $f(x_1, x_2) = (1 - x_1)^2 + 100(x_2 - x_1^2)^2$
  - $\frac{\partial}{\partial x_1} f(x_1, x_2) = -2(1 - x_1) - 400x_1(x_2 - x_1^2)$
  - $\frac{\partial}{\partial x_2} f(x_1, x_2) = 200(x_2 - x_1^2)$
- Assume the initial point
  - $\mathbf{x}^0 = (x_1^0, x_2^0) = (-1.3, 0.9)$

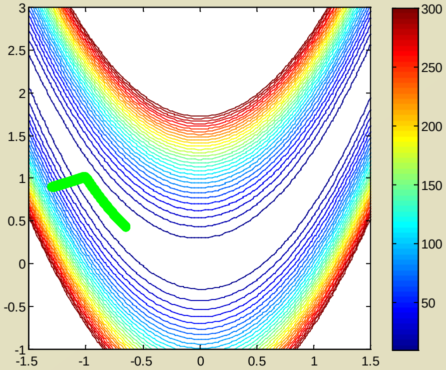
Global Minimum=0 at (1,1)





- Partial derivative vector at the point
  - $\boldsymbol{f}'(\mathbf{x}^0) = \left(\frac{\partial}{\partial x_1} f(x_1, x_2), \frac{\partial}{\partial x_2} f(x_1, x_2)\right) = (-415.4, -158)$
- Update the point with the negative partial derivative in a small scale, h=0.001
  - $\mathbf{x}^1 \leftarrow \mathbf{x}^0 - h \frac{f'(\mathbf{x}^0)}{|f'(\mathbf{x}^0)|}$
  - $\mathbf{x}^1 = \begin{pmatrix} -1.3 - 0.001 \times -415.4/444.4335, \\ 0.9 - 0.001 \times -158/444.4335 \end{pmatrix}$
  - $= (-1.2991, 0.9004)$
- Repeat the update until converges





$$P(y=1|x) = \frac{e^{X\theta}}{1+e^{X\theta}}$$

Finding θ with Gradient Ascent

- $\hat{\theta} = argmax_\theta \sum_{1\le i\le N} log(\, P(Y_i|X_i;\theta))$
  - $f(\theta) = \sum_{1\le i\le N} log(\, P(Y_i|X_i;\theta))$
  - $\frac{\partial f(\theta)}{\partial \theta_j} = \frac{\partial}{\partial \theta_j}\{\sum_{1\le i\le N} log(\, P(Y_i|X_i;\theta))\} = \sum_{1\le i\le N} X_{i,j}(Y_i - P(y=1|x;\theta))$
- To utilize the gradient method
  - We need to know *f'(x)* which are above
    - Case of ascent: $x_{t+1} \leftarrow x_t + h\mathbf{u}^* = x_t + h\frac{f'(x_t)}{|f'(x_t)|}$
  - Then, how to iteratively update the parameter, $\boldsymbol{\theta}$
  - $\theta_j^{t+1} \leftarrow \theta_j^t + h\frac{\partial f(\theta^t)}{\partial \theta_j^t} = \theta_j^t + h\{\sum_{1\le i\le N} X_{i,j}\big(Y_i - P(Y=1|X_i;\theta^t)\big)\}$

$$= \theta_j^t + \frac{h}{C}\{\sum_{1\le i\le N} X_{i,j}\left(Y_i - \frac{e^{X_i\theta^t}}{1+e^{X_i\theta^t}}\right)\}$$

C=Normalization to the unit vector

  - θ_j^0 can be arbitrarily chosen.

Logistic Regression Matlab Exercise

- Let's do some coding…

Linear Regression Revisited

- Previously,
  - $\hat{\theta} = argmin_\theta (f - \hat{f})^2 = argmin_\theta (Y - X\theta)^2$
    $= argmin_\theta (Y - X\theta)^T (Y - X\theta) = argmin_\theta (Y - X\theta)^T (Y - X\theta)$
    $= argmin_\theta (\theta^T X^T X\theta - 2\theta^T X^T Y + Y^T Y) = argmin_\theta (\theta^T X^T X\theta - 2\theta^T X^T Y)$
  - $\nabla_\theta (\theta^T X^T X\theta - 2\theta^T X^T Y)$=0
    - $2X^T X\theta - 2X^T Y = 0$
  - $\theta = (X^T X)^{-1} X^T Y$
- Any problem???
- Gradient descent can be a solution
  - $\hat{\theta} = argmin_\theta (f - \hat{f})^2 = argmin_\theta (Y - X\theta)^2 =$
    $argmin_\theta \sum_{1 \le i \le N} (Y^i - \sum_{1 \le j \le d} X_j^i \theta_j)^2$
  - $\frac{\partial}{\partial \theta_k} \sum_{1 \le i \le N} (Y^i - \sum_{1 \le j \le d} X_j^i \theta_j)^2 = -\sum_{1 \le i \le N} 2(Y^i - \sum_{1 \le j \le d} X_j^i \theta_j) X_k^i$
  - $\theta_k^{t+1} \leftarrow \theta_k^t - h \frac{\partial f(\theta^t)}{\partial \theta_k^t} = \theta_k^t + h \sum_{1 \le i \le N} 2(Y^i - \sum_{1 \le j \le d} X_j^i \theta_j) X_k^i$

NAÏVE BAYES
VS. LOGISTIC REGRESSION

Gaussian Naïve Bayes

- We want to compare the performance of the two classifiers
  - Logistic regression handles the continuous features
  - Why not naïve Bayes?
- Naïve Bayes Classifier Function
  - $f_{NB}(x) = argmax_{Y=y} P(Y = y) \prod_{1 \le i \le d} P(X_i = x_i | Y = y)$
- What-if the feature is a continuous random variable?
  - We can assume that the variable follows the Gaussian distribution with the mean of μ and the variance of σ^2
    - $P(X_i | Y, \mu, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(X_i - \mu)^2}{2\sigma^2}}$
  - In addition, let's use more shortened terms
    - $P(Y = y) = \pi_1$
  - $P(Y) \prod_{1 \le i \le d} P(X_i | Y) = \pi_k \prod_{1 \le i \le d} \frac{1}{\sigma_k^i C} \exp(-\frac{1}{2}\left(\frac{X_i - \mu_k^i}{\sigma_k^i}\right)^2)$

Derivation to Logistic Regression (1)

- Derivation from the naïve Bayes to the logistic regression
  - $P(Y)\prod_{1\le i\le d} P(X_i|Y) = \pi_k \prod_{1\le i\le d} \frac{1}{\sigma_k^i C} \exp(-\frac{1}{2}\left(\frac{X_i-\mu_k^i}{\sigma_k^i}\right)^2)$
- With naïve Bayes assumption
  - $P(Y=y|X) = \frac{P(X|Y=y)P(Y=y)}{P(X)} = \frac{P(X|Y=y)P(Y=y)}{P(X|Y=y)P(Y=y)+P(X|Y=n)P(Y=n)}$

$$= \frac{P(Y=y)\prod_{1\le i\le d} P(X_i|Y=y)}{P(Y=y)\prod_{1\le i\le d} P(X_i|Y=y) + P(Y=n)\prod_{1\le i\le d} P(X_i|Y=n)}$$

  - $P(Y=y|X) = \frac{\pi_1 \prod_{1\le i\le d} \frac{1}{\sigma_1^i C} \exp(-\frac{1}{2}\left(\frac{X_i-\mu_1^i}{\sigma_1^i}\right)^2)}{\pi_1 \prod_{1\le i\le d} \frac{1}{\sigma_1^i C} \exp(-\frac{1}{2}\left(\frac{X_i-\mu_1^i}{\sigma_1^i}\right)^2) + \pi_2 \prod_{1\le i\le d} \frac{1}{\sigma_2^i C} \exp(-\frac{1}{2}\left(\frac{X_i-\mu_2^i}{\sigma_2^i}\right)^2)}$

$$= \frac{1}{1 + \frac{\pi_2 \prod_{1\le i\le d} \frac{1}{\sigma_2^i C} \exp(-\frac{1}{2}\left(\frac{X_i-\mu_2^i}{\sigma_2^i}\right)^2)}{\pi_1 \prod_{1\le i\le d} \frac{1}{\sigma_1^i C} \exp(-\frac{1}{2}\left(\frac{X_i-\mu_1^i}{\sigma_1^i}\right)^2)}}$$

Derivation to Logistic Regression (2)

- Assuming the same variable of the two classes, $\sigma_2^i = \sigma_1^i$
  - $P(Y=y|X) = \dfrac{1}{1+\dfrac{\pi_2 \prod_{1\le i\le d} \frac{1}{\sigma_2^i C} \exp\left(-\frac{1}{2}\left(\frac{X_i-\mu_2^i}{\sigma_2^i}\right)^2\right)}{\pi_1 \prod_{1\le i\le d} \frac{1}{\sigma_1^i C} \exp\left(-\frac{1}{2}\left(\frac{X_i-\mu_1^i}{\sigma_1^i}\right)^2\right)}} = \dfrac{1}{1+\dfrac{\pi_2 \prod_{1\le i\le d} \exp\left(-\frac{1}{2}\left(\frac{X_i-\mu_2^i}{\sigma_2^i}\right)^2\right)}{\pi_1 \prod_{1\le i\le d} \exp\left(-\frac{1}{2}\left(\frac{X_i-\mu_1^i}{\sigma_1^i}\right)^2\right)}}$

$$= \frac{1}{1+\dfrac{\pi_2 \exp\left(-\sum_{1\le i\le d}\left\{\frac{1}{2}\left(\frac{X_i-\mu_2^i}{\sigma_2^i}\right)^2\right\}\right)}{\pi_1 \exp\left(-\sum_{1\le i\le d}\left\{\frac{1}{2}\left(\frac{X_i-\mu_1^i}{\sigma_1^i}\right)^2\right\}\right)}} = \frac{1}{1+\dfrac{\exp\left(-\sum_{1\le i\le d}\left\{\frac{1}{2}\left(\frac{X_i-\mu_2^i}{\sigma_2^i}\right)^2\right\}+log\pi_2\right)}{\exp\left(-\sum_{1\le i\le d}\left\{\frac{1}{2}\left(\frac{X_i-\mu_1^i}{\sigma_1^i}\right)^2\right\}+log\pi_1\right)}}$$

$$= \frac{1}{1+\exp\left(-\sum_{1\le i\le d}\left\{\frac{1}{2}\left(\frac{X_i-\mu_2^i}{\sigma_2^i}\right)^2\right\}+log\pi_2+\sum_{1\le i\le d}\left\{\frac{1}{2}\left(\frac{X_i-\mu_1^i}{\sigma_1^i}\right)^2\right\}-log\pi_1\right)}$$

$$= \frac{1}{1+\exp\left(\sum_{1\le i\le d} -\frac{1}{2\left(\sigma_1^i\right)^2}\left(\left\{\left(X_i-\mu_1^i\right)^2-\left(X_i-\mu_2^i\right)^2\right\}+log\pi_2-log\pi_1\right)\right)}$$

$$= \frac{1}{1+\exp\left(\sum_{1\le i\le d} -\frac{1}{2\left(\sigma_1^i\right)^2}\left(\left\{2\left(\mu_2^i-\mu_1^i\right)X_i+{\mu_2^i}^2-{\mu_2^i}^2\right\}++log\pi_2-log\pi_1\right)\right)}$$

Naïve Bayes vs. Logistic Regression

- Naïve Bayes classifier
  - $P(Y|X) = \frac{1}{1+\exp(-\frac{1}{2(\sigma_1^i)^2}\sum_{1\le i\le d}\left\{2(\mu_2^i-\mu_1^i)X_i+{\mu_2^i}^2-{\mu_2^i}^2\right\}+log\pi_2-log\pi_1)}$
  - Assumption to get this formula
    - Naïve Bayes assumption, Same variance assumption between classes
    - Gaussian distribution for P(X|Y)
    - Bernoulli distribution for P(Y)
  - # of parameters to estimate = 2*2*d+1=4d+1
    - With the different variances between classes
- Logistic Regression
  - $P(Y|X) = \frac{1}{1+e^{-\dot{\theta}^T x}}$
  - Assumption to get this formula
    - Fitting to the logistic function
  - # of parameters to estimate = d+1
- Who is the winner?
  - Really??? There is no winner… Why?

Together, modeling joint prob.

Generative-Discriminative Pair

- Generative model, $P(Y|X)=P(X,Y)/P(X)=P(X|Y)P(Y)/P(X)$
  - Full probabilistic model of all variables
    - Estimate the parameters of $P(X|Y)$, $P(Y)$ from the data
  - Characteristics: Bayesian, Prior, Modeling the joint probability
  - Naïve Bayes Classifier
- Discriminative model, $P(Y|X)$
  - Do not need to model the distribution of the observed variables
    - Estimate the parameters of $P(Y|X)$ from the data
  - Characteristics: Modeling the conditional probability
  - Logistic Regression
- Pros and Cons [Ng & Jordan, 2002]
  - Logistic regression is less biased
  - Probably approximately correct learning: Naïve Bayes learns faster

Acknowledgement

- This slideset is greatly influenced
  - By Prof. Carlos Guestrin at CMU
  - By Prof. Eric Xing at CMU
  - By Prof. Tom Mitchell at CMU

Further Readings

- Bishop Chapter 4.3, 5.2.1-5.2.4