10-601 Recitation #4

Gaussian Naive Bayes and Logistic Regression

October 5th, 2011

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Office hours: Friday 3-4 PM

Agenda

- HW #2 due tomorrow 5 PM
  - Submit written copy and post code to Blackboard
- Gaussian Naive Bayes
- Logistic Regression
- Gradient Descent
- Discriminative vs. Generative classifiers
- Bias/Variance Tradeoff

Naive Bayes

- Features are conditionally independent given class

$$\mathbb{P}(X_1, ..., X_n | Y) = \prod_{i=1}^{n} \mathbb{P}(X_i | Y)$$

$$\mathbb{P}(X_i | Y) \sim Bernoulli(\theta_H)$$

- Assumed that all variables were binary (or discrete)
- What if we have continuous features?

Gaussian Naive Bayes

- Still assume features are conditionally independent given class

$$\mathbb{P}(X_1, ..., X_n | Y) = \prod_{i=1}^{n} \mathbb{P}(X_i | Y)$$

$$\mathbb{P}(X_i | Y) \sim N(\mu, \sigma^2)$$

- Generally assume Gaussian features (why?)
- Can use other distributions as well

Gaussian Distribution

- Also called normal distribution

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

$$\mathbb{E}(X) = \mu$$

$$\mathbb{V}(X) = \sigma^2$$

You will compute the MLE and MAP estimates in HW2

Why Gaussian?

- Many natural phenomenon are normally distributed
  - Biological functions (height, weight, etc.)
- Central Limit Theorem implies that sample means tend to a normal distribution
- Mathematically easy to work with

Working with Continuous Variables

- Discrete variables:

$$\mathbb{E}(X) = \sum_{x \in Val(X)} x \cdot \mathbb{P}(x)$$

$$\mathbb{V}(X) = \mathbb{E}(X - \mathbb{E}(X))^2 = \sum_{x \in Val(X)} (x - \mathbb{E}(X))^2 \cdot \mathbb{P}(x)$$

$$\mathbb{P}(a \leq X \leq b) = \sum_{x \in [a,b]} \mathbb{P}(X = x)$$

- Continuous variables:

$$\mathbb{E}(X) = \int_{-\infty}^{\infty} x \cdot f(x) dx$$

$$\mathbb{V}(X) = \mathbb{E}(X - \mathbb{E}(X))^2 = \int_{-\infty}^{\infty} (x - \mathbb{E}(X))^2 \cdot f(x) dx$$

$$\mathbb{P}(a \leq X \leq b) = \int_{a}^{b} f(x) dx$$

Generative vs. Discriminative Classifiers

- Generative classifiers learn P(X|Y)
- Use Bayes rule to calculate P(Y|X)
- Discriminative classifiers learn P(Y|X)
- Which type is Naive Bayes?

Generative vs. Discriminative Classifiers

- Discriminative classifiers are only good for classification
- Generative classifiers enable other tasks (e.g., data generation)
- Generally speaking, generative is more accurate with less data, discriminative with more data

Logistic Regression

- Example of a discriminative classifier

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

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

Logistic Regression

- Can handle arbitrarily many classes

Now $y \in \{y_1 \ldots y_R\}$: learn R-1 sets of weights

for $k<R$ $$P(Y = y_k|X) = \frac{\exp(w_{k0} + \sum_{i=1}^{n} w_{ki}X_i)}{1 + \sum_{j=1}^{R-1} \exp(w_{j0} + \sum_{i=1}^{n} w_{ji}X_i)}$$

for $k=R$ $$P(Y = y_R|X) = \frac{1}{1 + \sum_{j=1}^{R-1} \exp(w_{j0} + \sum_{i=1}^{n} w_{ji}X_i)}$$

Logistic Regression

Consider learning f: X → Y, where

- X is a vector of real-valued features, < X_1 … X_n >
- Y is boolean
- assume all X_i are conditionally independent given Y
- model $P(X_i \mid Y = y_k)$ as Gaussian $N(\mu_{ik},\sigma_i)$
- model P(Y) as Bernoulli (π)

$$\sum_i \left(\frac{\mu_{i0} - \mu_{i1}}{\sigma_i^2} X_i + \frac{\mu_{i1}^2 - \mu_{i0}^2)}{2\sigma_i^2} \right)$$

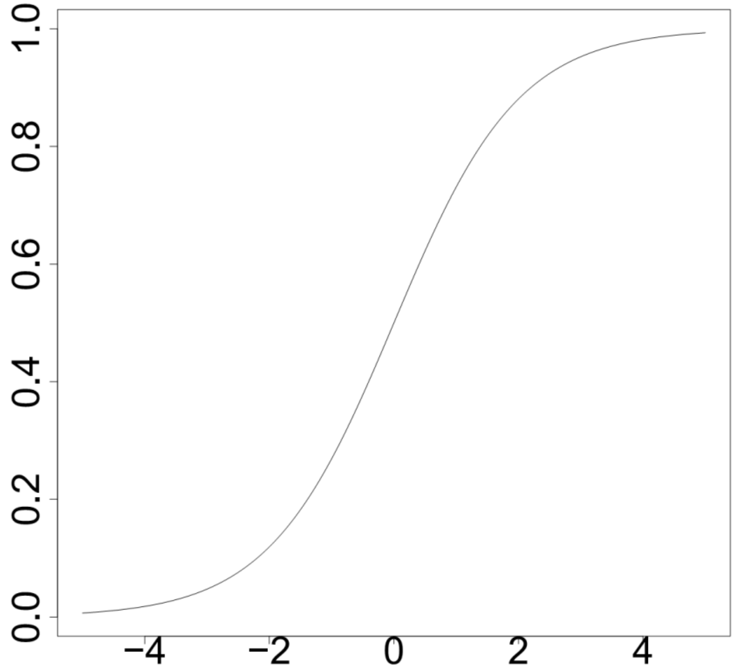
$$P(Y = 1|X) = \frac{1}{1 + \exp(w_0 + \sum_{i=1}^n w_i X_i)}$$

Finding the weights

- We were able to derive an analytic expression for the weights for the special Gaussian case

- How can we find the weights in the general case?

Good weights



$$a = \frac{1}{1 + \exp(-b)}$$

$$P(Y = 1|X) = \frac{1}{1 + \exp(w_0 + \sum_{i=1}^{n} w_i X_i)}$$

Maximum Conditional Likelihood Estimate

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

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

$$D = \{\langle X^1, Y^1\rangle, \ldots \langle X^L, Y^L\rangle\}$$

Data conditional likelihood = $\prod_l P(Y^l|X^l, W)$

$$W_{MCLE} = \arg\max_W \prod_l P(Y^l|W, X^l)$$

Maximum Conditional Likelihood Estimate

$$l(W) \equiv \ln \prod_l P(Y^l|X^l, W) = \sum_l \ln P(Y^l|X^l, W)$$

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

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

$$\begin{aligned} l(W) &= \sum_l Y^l \ln P(Y^l = 1|X^l, W) + (1 - Y^l) \ln P(Y^l = 0|X^l, W) \\ &= \sum_l Y^l \ln \frac{P(Y^l = 1|X^l, W)}{P(Y^l = 0|X^l, W)} + \ln P(Y^l = 0|X^l, W) \\ &= \sum_l Y^l (w_0 + \sum_i^n w_i X_i^l) - \ln(1 + exp(w_0 + \sum_i^n w_i X_i^l)) \end{aligned}$$

Maximizing l(w)

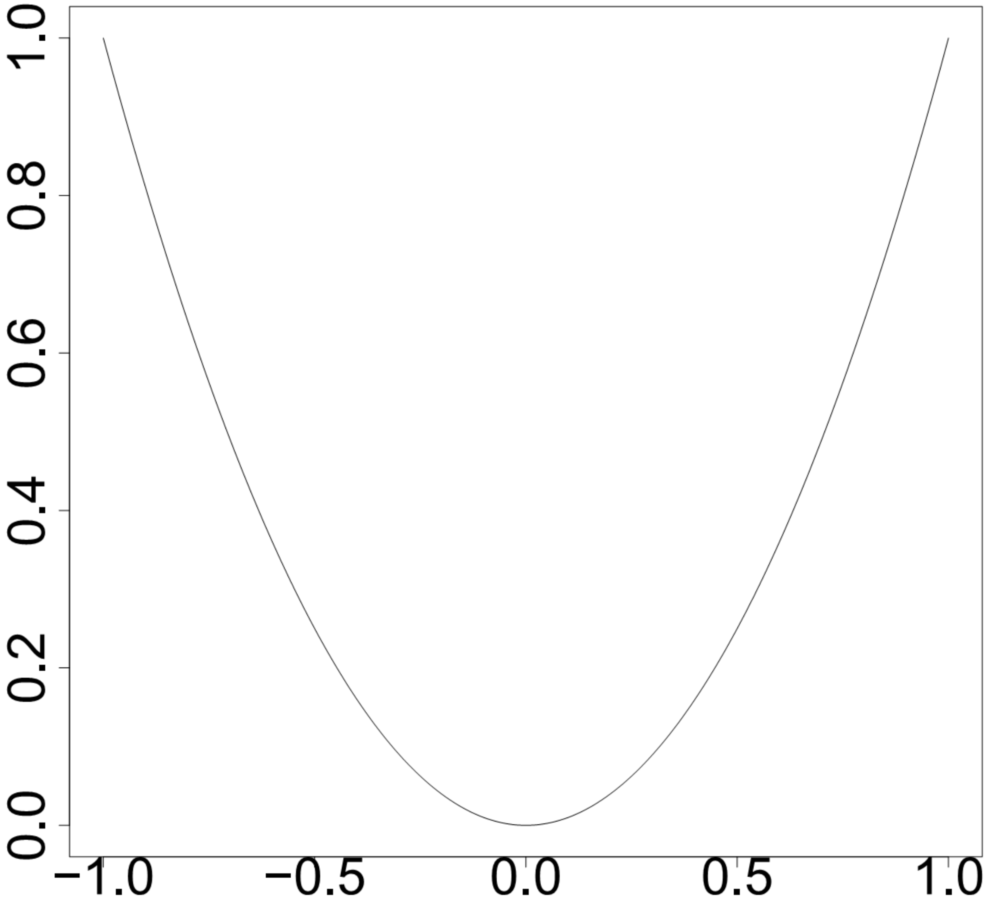
$$
\begin{aligned}
l(W) &\equiv \ln \prod_l P(Y^l | X^l, W) \\
&= \sum_l Y^l (w_0 + \sum_i^n w_i X_i^l) - \ln(1 + exp(w_0 + \sum_i^n w_i X_i^l))
\end{aligned}
$$

- No closed form for the maximum
- So how do we find the MCLE?

Gradient Descent

- Iterative optimization algorithm
- Basic idea:
  - Find the direction of greatest decrease
  - Take a small step in that direction
  - Repeat these two steps until we are satisfied
  - Usually stop when change is very small
- Guaranteed to find optimal point in some cases

1-D Gradient Descent



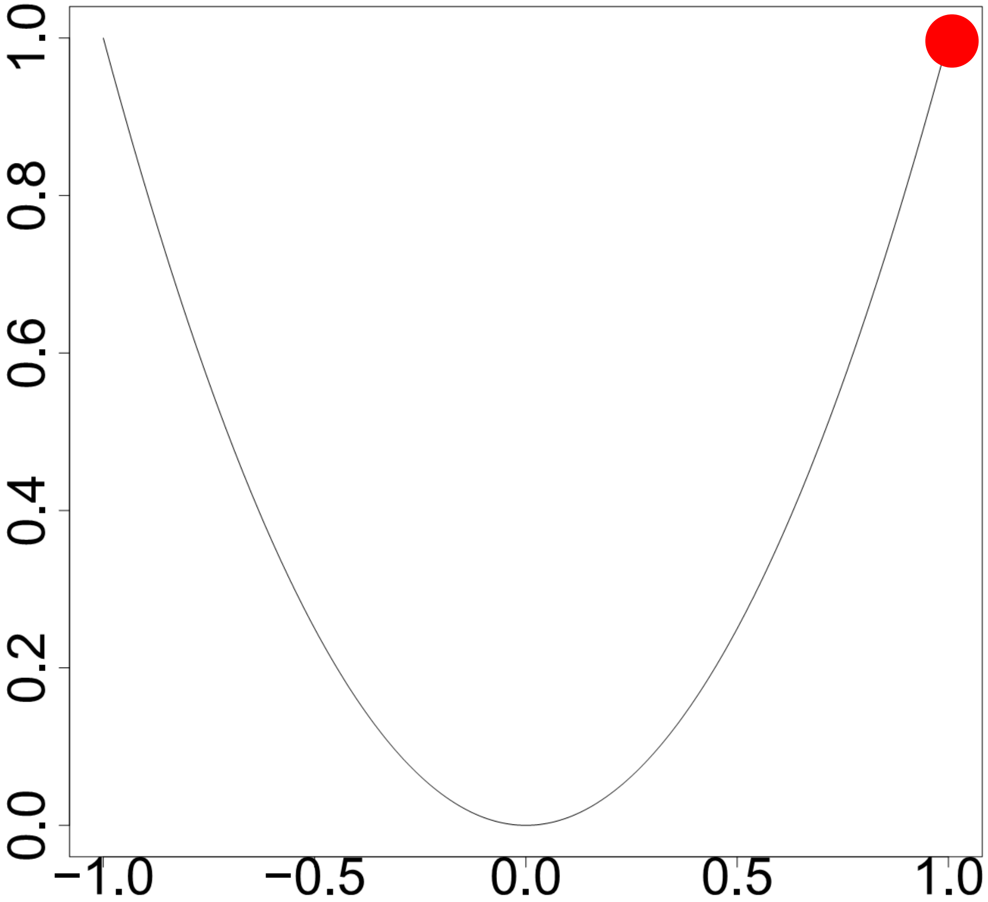
$$y = f(x) = x^2$$

$$\frac{dy}{dx} = 2x$$

$$\eta = 0.1$$

- 1-D gradient is the derivative

1-D Gradient Descent



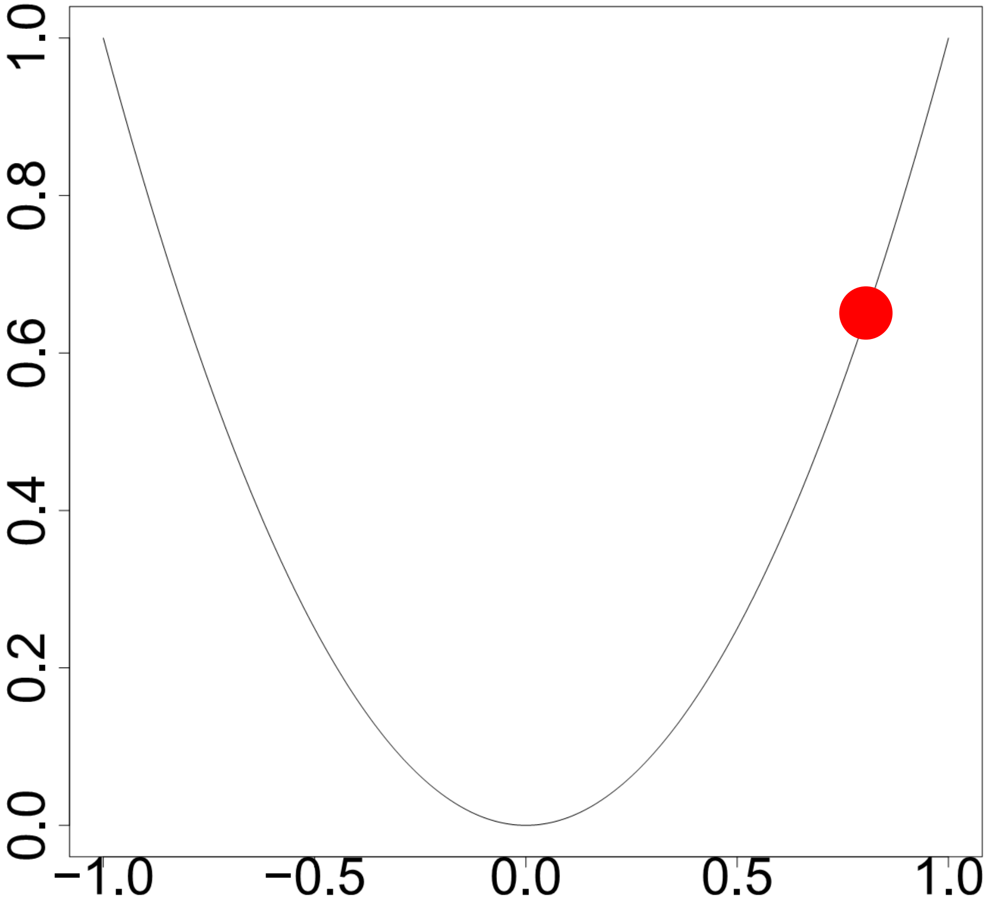
$$y = f(x) = x^2$$

$$\frac{dy}{dx} = 2x$$

$$\eta = 0.1$$

- Start at a random point (1, 1)

1-D Gradient Descent



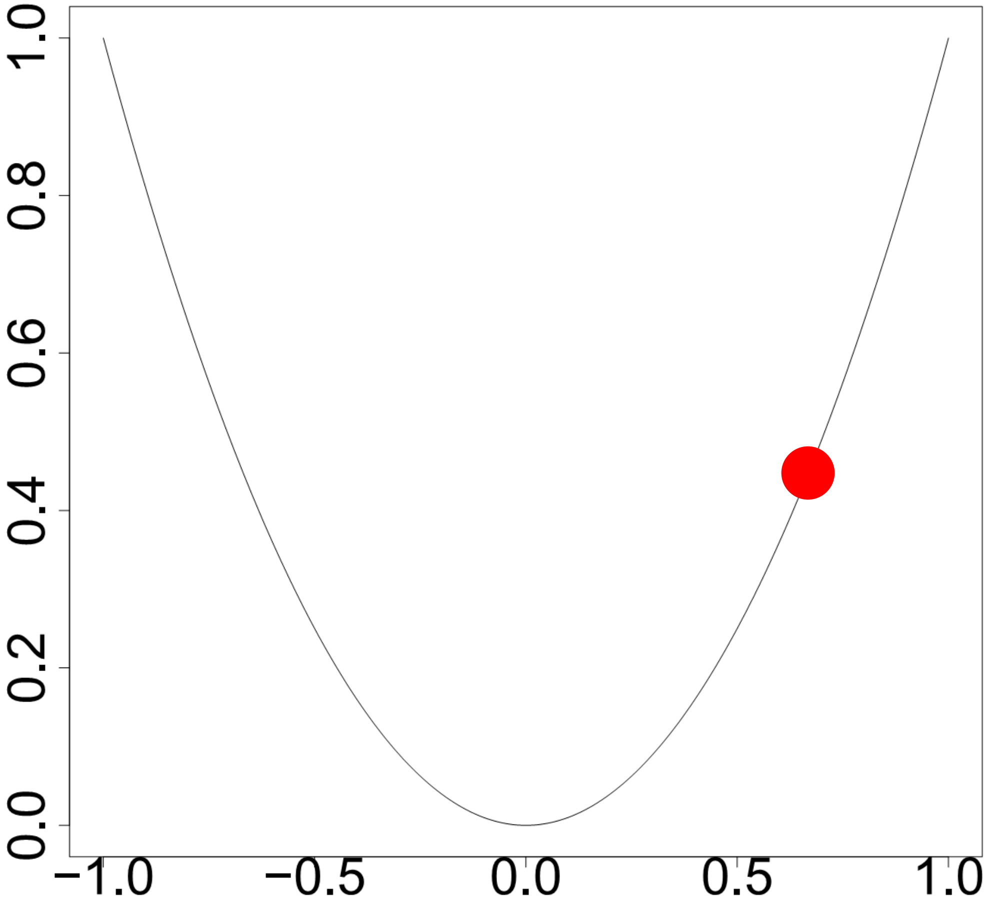
$$y = f(x) = x^2$$

$$\frac{dy}{dx} = 2x$$

$$\eta = 0.1$$

- Take a step in the negative gradient direction

1-D Gradient Descent



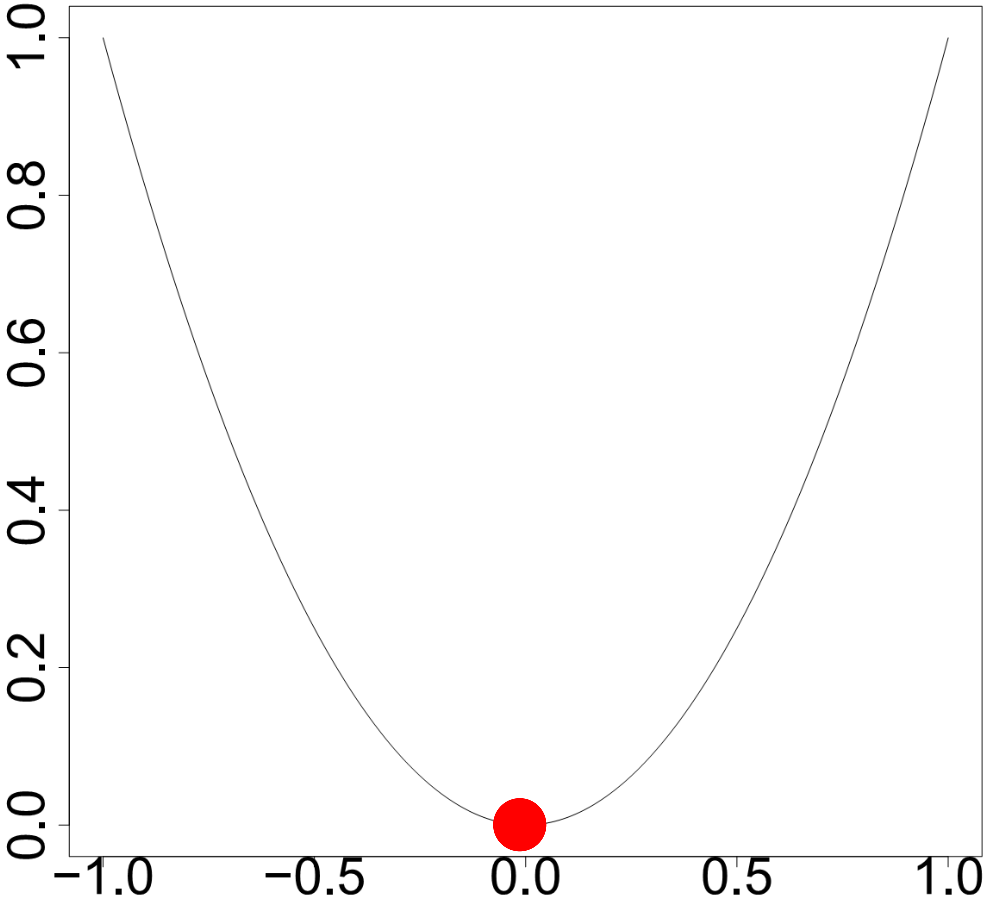
$$y = f(x) = x^2$$

$$\frac{dy}{dx} = 2x$$

$$\eta = 0.1$$

- Repeat the process

1-D Gradient Descent



$$y = f(x) = x^2$$

$$\frac{dy}{dx} = 2x$$

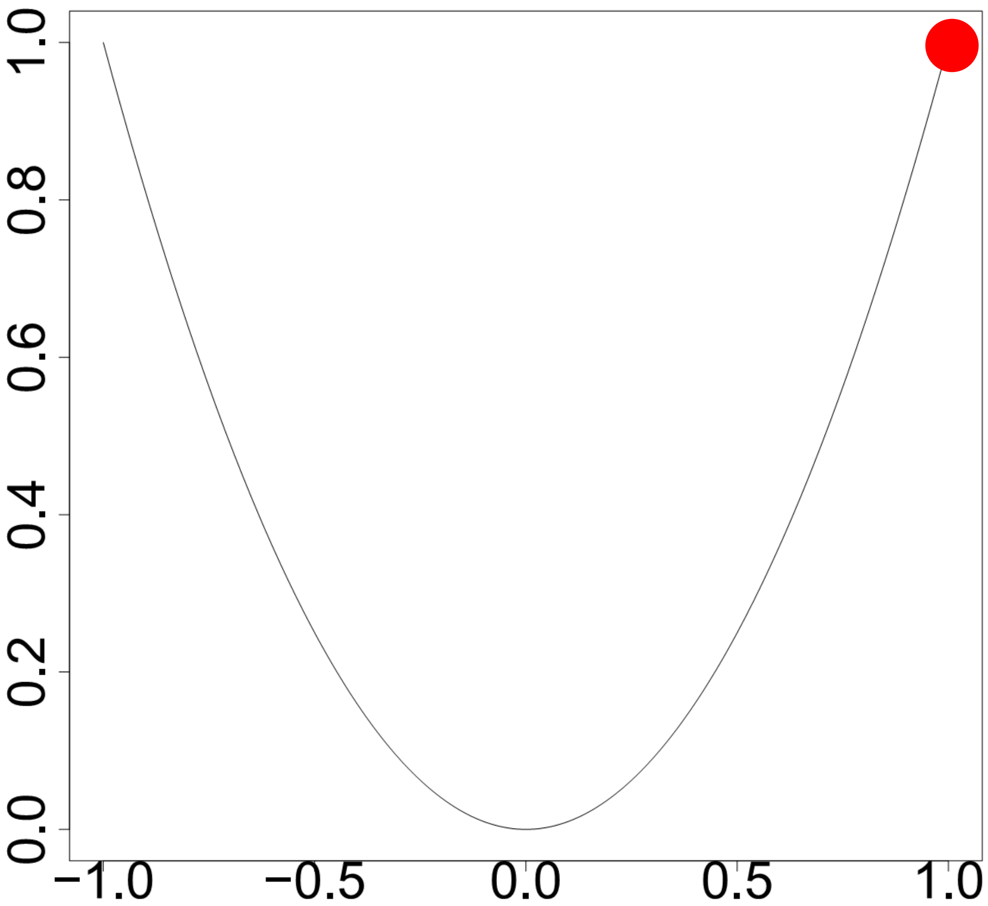
$$\eta = 0.1$$

- Eventually converge to the optimum point

Problems with Gradient Descent

- If step-size is too big, can end up going back and forth between two values
- If the function is not convex/concave, we may end up in a local optima

Bad Step-Size



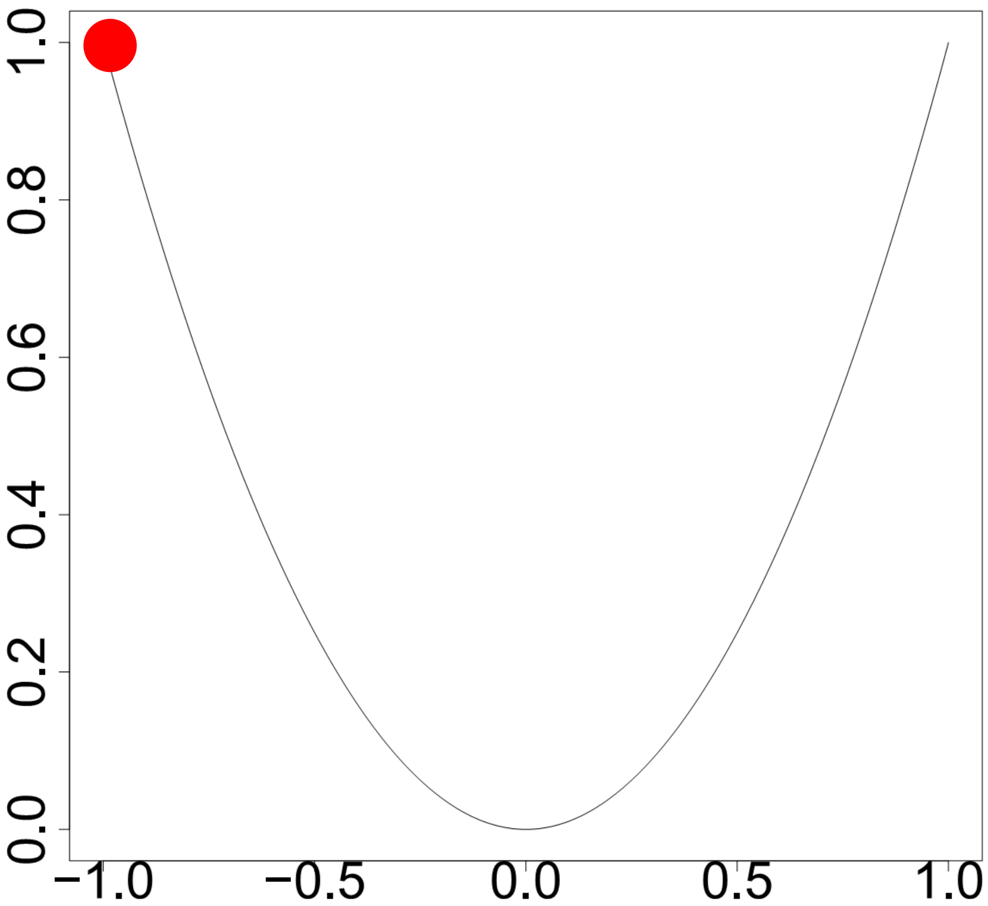
$$y = f(x) = x^2$$

$$\frac{dy}{dx} = 2x$$

$$\eta = 1.0$$

- Start at (1, 1)

Bad Step-Size



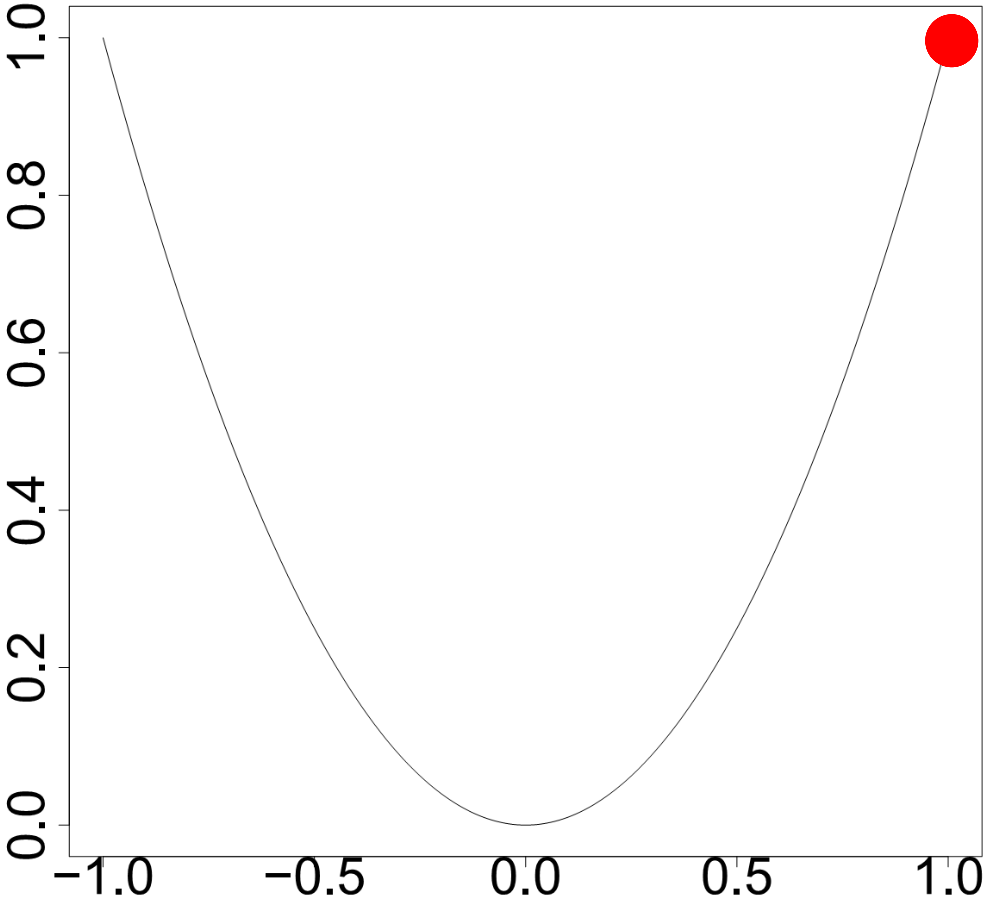
$$y = f(x) = x^2$$

$$\frac{dy}{dx} = 2x$$

$$\eta = 1.0$$

- Step to (-1, 1)

Bad Step-Size



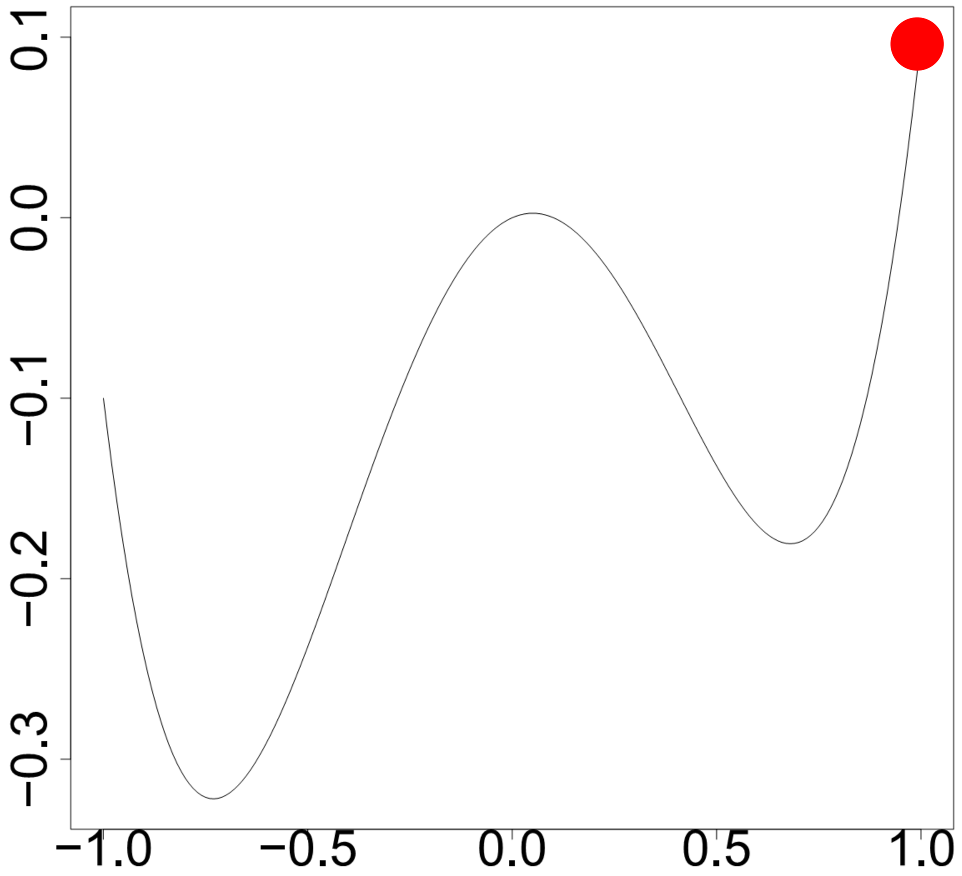
$$y = f(x) = x^2$$

$$\frac{dy}{dx} = 2x$$

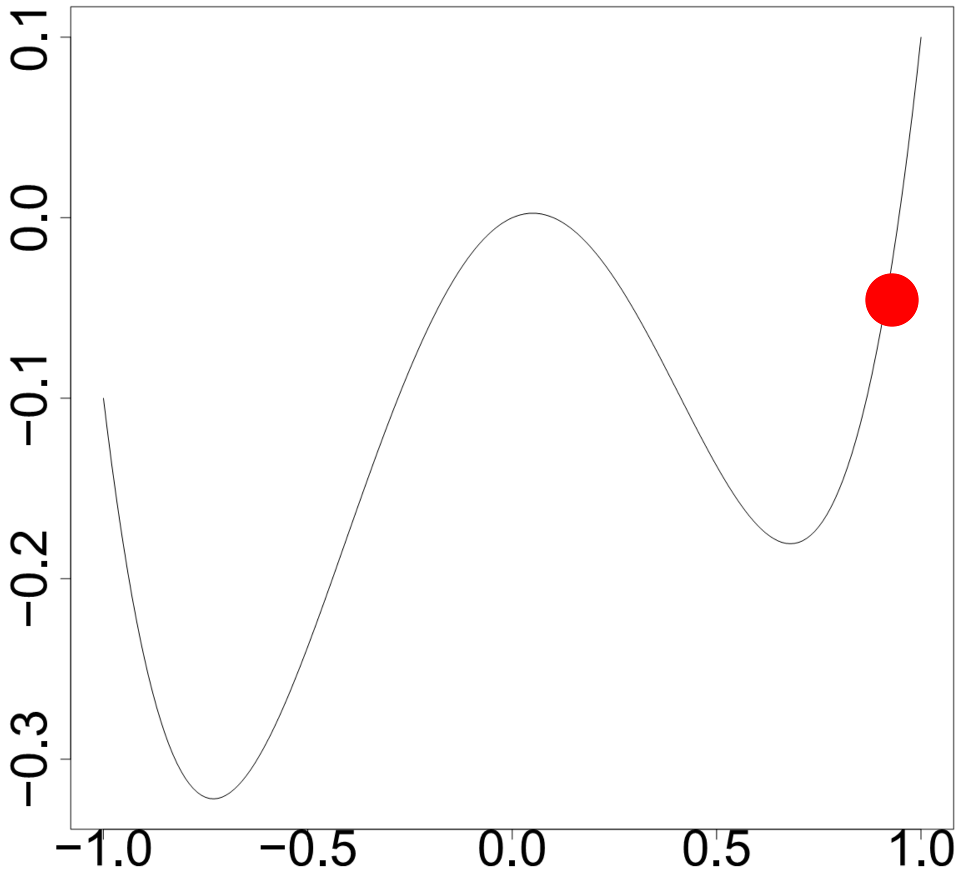
$$\eta = 1.0$$

- Step back to (1, 1)

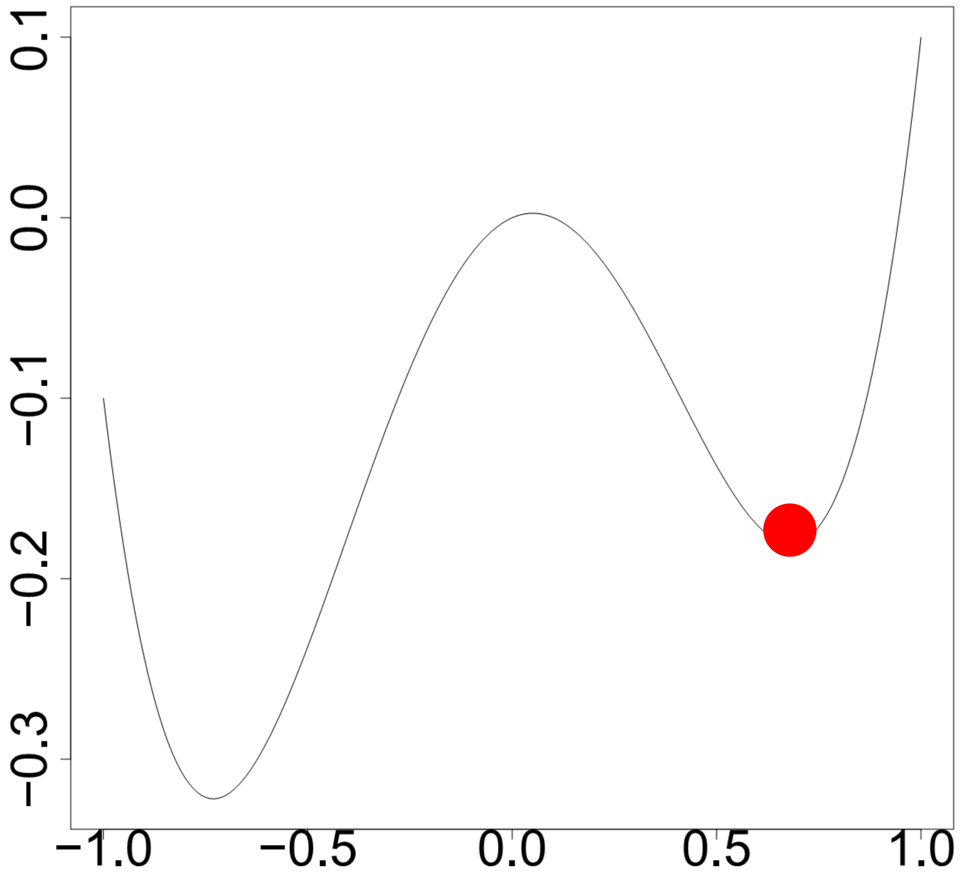
Non-convexity



Non-convexity



Non-convexity



Gradient Descent

- Generally have to shrink your step size as you continue to iterate
- Try to stick to convex/concave functions
- Do random restarts if you must use a non-convex/non-concave objective

n-dimensional Gradient Descent

- Use partial derivatives to compute the gradient
- Partial derivatives:

$$f(x, y, z) = xyz - 3xln(z)$$
$$\frac{\partial f}{\partial x} = yz - 3ln(z)$$
$$\frac{\partial f}{\partial z} = xy - \frac{3x}{z}$$

n-dimensional Gradient Descent

- Gradient is n-dimensional vector
- Gradient direction is the direction of greatest increase
- First-order (i.e., linear) approximation
- Second-order Newton methods

Logistic Regression and Gradient Descent

$$
\begin{aligned}
l(W) &\equiv \ln \prod_l P(Y^l|X^l, W) \\
&= \sum_l Y^l(w_0 + \sum_i^n w_i X_i^l) - \ln(1 + exp(w_0 + \sum_i^n w_i X_i^l))
\end{aligned}
$$

$$
\frac{\partial l(W)}{\partial w_i} = \sum_l X_i^l (Y^l - \hat{P}(Y^l = 1|X^l, W))
$$

- Objective function is concave!

MAP and Logistic Regression

Maximum a posteriori estimate with prior W~N(0,σI)

$$W \leftarrow \arg\max_W \ \ln[P(W) \prod_l P(Y^l|X^l, W)]$$

$$w_i \leftarrow w_i - \eta\lambda w_i + \eta \sum_l X_i^l (Y^l - \hat{P}(Y^l = 1|X^l, W))$$

MAP and Logistic Regression

- Use a MAP estimate to avoid overfitting (just like Naive Bayes)
- What can happen to weights without regularization term?
- What does the regularization term help do?

Other Forms of Regularization

- Can apply a Lasso or Ridge penalty to weights
- Lasso makes many weights zero
- Ridge shrinks all of the weights

$$l(W) = \sum_l Y^l (w_0 + \sum_i^n w_i X_i^l) - ln(1 + exp(w_0 + \sum_i^n w_i X_i^l)) - \lambda ||w||_1$$

$$l(W) = \sum_l Y^l (w_0 + \sum_i^n w_i X_i^l) - ln(1 + exp(w_0 + \sum_i^n w_i X_i^l)) - \lambda ||w||_2^2$$

Bias/Variance Tradeoff

- Simpler models are more biased because they make more assumptions
- More complex models are more variable, since they depend on the particulars of the data provided
- Have to trade the two off to get the best classifier possible

Extra Slides

Correlated Features

- Worst case scenario: duplicated features
- What will Naive Bayes do with duplicated features?
- What will Logistic Regression do with duplicated features?
- What if there is just correlation?

Estimating Some Features Jointly

- What if we are not willing to assume that all features are conditionally independent?
- How can we do Naive Bayes?
- What is the price we pay for not assuming conditional independence?

Estimating Some Features Jointly

- Graphical models are a formalization of this idea
- Can do things like Tree-Augmented Naive Bayes (TAN)
- More general framework for an arbitrary set of conditional independence assumptions

Neural Network Preview

- One sigmoid function is good (Logistic Regression), so more must be better
- Can chain them so that the output of one are the inputs to the next
- “Mimics” the brain (kind of), so such systems are termed Neural Networks

Numerical Gradient Descent

- What if we can only evaluate the function but cannot evaluate its derivative?
- Can take tiny steps in each direction to determine gradient
- Generally a lot more expensive because of all the function evaluations