

CSE 417T

Introduction to Machine Learning

Lecture 8

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Logistics

- HW1: Due tomorrow
 - Reserve time if you have never used Gradescope
 - Make sure the submission is readable (if you scan your handwriting)
 - Assign pages to each problem
- HW2: Will be announce between this Friday and next Monday
- Exam1: **March 23 (Tue)**
 - Timed exam at the lecture time
 - Content: LFD Chapter 1 to 5
 - More logistical details to come within 1~2 weeks

Recap

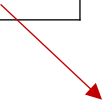
Linear Models

This is why it's called linear models



- H contains hypothesis $h(\vec{x})$ as **some function of $\vec{w}^T \vec{x}$**

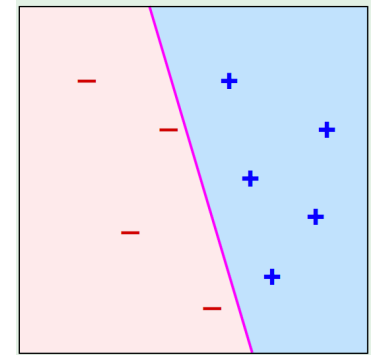
	Domain	Model	Credit Card Example
Linear Classification	$y \in \{-1, +1\}$	$H = \{h(\vec{x}) = \text{sign}(\vec{w}^T \vec{x})\}$	Approve or not
Linear Regression	$y \in \mathbb{R}$	$H = \{h(\vec{x}) = \vec{w}^T \vec{x}\}$	Credit line
Logistic Regression	$y \in [0,1]$	$H = \{h(\vec{x}) = \theta(\vec{w}^T \vec{x})\}$	Prob. of default


$$\theta(s) = \frac{e^s}{1 + e^s}$$

- Algorithm:
 - Focus on $g = \operatorname{argmin}_{h \in H} E_{in}(h)$

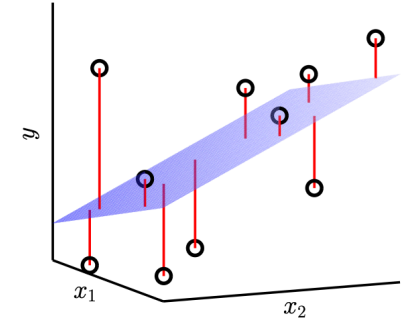
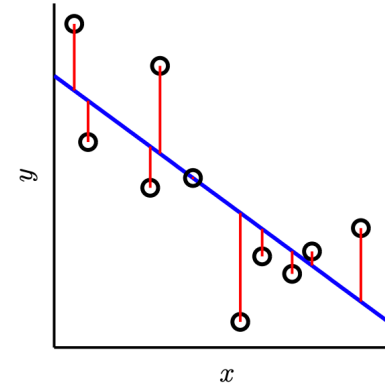
Linear Classification

- Formulation
 - Hypothesis set $H = \{h(\vec{x}) = \text{sign}(\vec{w}^T \vec{x})\}$
 - Error measure: binary error $e(h(\vec{x}), y) = \mathbb{I}[h(\vec{x}) \neq y]$
- Data is linearly separable
 - Run PLA $\Rightarrow E_{in} = 0 \Rightarrow$ Low E_{out}
- Data is not linearly separable
 - Minimizing E_{in} is NP hard
 - Pocket algorithm
 - Engineering the features (e.g., handwritten digits)
 - More discussion later in the semester



Linear Regression

- Formulation
 - Hypothesis set $H = \{h(\vec{x}) = \vec{w}^T \vec{x}\}$
 - Squared error $e(h(\vec{x}), y) = (h(\vec{x}) - y)^2$
- Given dataset $D = \{(\vec{x}_1, y_1), \dots, (\vec{x}_N, y_N)\}$
 - $E_{in}(\vec{w}) = \frac{1}{N} \sum_{n=1}^N (\vec{w}^T \vec{x}_n - y_n)^2$
- Goal: find $\vec{w}_{lin} = \operatorname{argmin}_{\vec{w}} E_{in}(\vec{w})$



Linear Regression “Algorithm”

- There is a closed-form solution for minimizing E_{in}
 - Closed-form solution for $\nabla_{\vec{w}} E_{in}(\vec{w}) = 0$
- One-step algorithm
 - Given $D = \{(\vec{x}_1, y_1), \dots, (\vec{x}_N, y_N)\}$

- Construct $X = \begin{bmatrix} \vec{x}_1^T \\ \vdots \\ \vec{x}_N^T \end{bmatrix} = \begin{bmatrix} x_{1,0} & x_{1,1} & \cdots & x_{1,d} \\ x_{2,0} & x_{2,1} & \cdots & x_{2,d} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N,0} & x_{N,1} & \cdots & x_{N,d} \end{bmatrix}$ and $\vec{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$

- Output $\vec{w}_{lin} = (X^T X)^{-1} X^T \vec{y}$ (Assume $X^T X$ is invertible)

Today's Lecture

The notes are not intended to be comprehensive. They should be accompanied by lectures and/or textbook.
Let me know if you spot errors.

Logistic Regression

Logistic Regression: Predicting a Probability

- Will this patient have a heart attack within the next year?

age	62 years
gender	male
blood sugar	120 mg/dL40,000
HDL	50
LDL	120
Mass	190 lbs
Height	5' 10''
...	...

Classification: Yes/No

Logistic regression: Probability of Yes

- A hypothesis $h(\vec{x})$ output a value in $[0,1]$
 - Interpreting it as the probability of yes

Logistic Regression

- Hypothesis set $H = \{h(\vec{x}) = \theta(\vec{w}^T \vec{x})\}$
 - Want θ to map from $(-\infty, \infty)$ to $[0,1]$

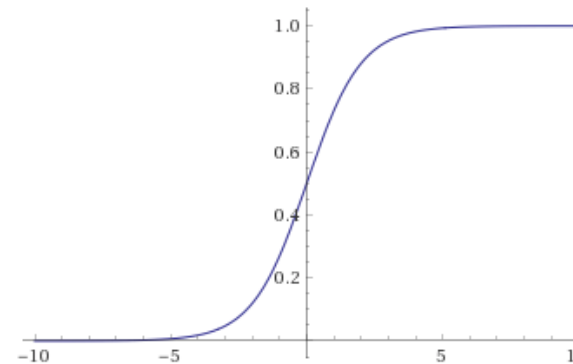
- $\theta(s) = \frac{e^s}{1+e^s} = \frac{1}{1+e^{-s}}$

- A sigmoid function ("S"-shaped function)

- $\theta(s) = \begin{cases} 1 & \text{when } s \rightarrow \infty \\ 0.5 & \text{when } s = 0 \\ 0 & \text{when } s \rightarrow -\infty \end{cases}$

- Useful property

- $1 - \theta(s) = \frac{1+e^s}{1+e^s} - \frac{e^s}{1+e^s} = \frac{1}{1+e^s} = \theta(-s)$



What kind of Dataset do We Get?

- Dataset $D = \{(\vec{x}_1, y_1), \dots, (\vec{x}_N, y_N)\}$

$\vec{x} =$

age	62 years
gender	male
blood sugar	120 mg/dL40,000
HDL	50
LDL	120
Mass	190 lbs
Height	5' 10"
...	...

- What are the values of y_n ?
 - Ideally, we want to have y_n to be the probability value
 - In practice, we **cannot measure a probability**
 - We can only see the occurrence of an event and infer the probability
 - (We often only observe whether the person had heart attack, we don't observe the "probability")
- Need to address the case when $y_n \in \{-1, +1\}$ in the given dataset D

Error Measure: Quantifying $g \approx f$

Side note:

You probably can guess why the property $1 - \theta(s) = \theta(-s)$ might be helpful

- Target function $f(\vec{x}) = \Pr(y = +1|\vec{x})$

- Another way to write it: $\Pr(y|\vec{x}) = \begin{cases} f(\vec{x}) & \text{for } y = +1 \\ 1 - f(\vec{x}) & \text{for } y = -1 \end{cases}$

- How do we define the error measure to quantify $g \approx f$
 - Ideally, we want it to be **meaningful**
 - Binary error for classification: tell us the number of mistakes we make
 - Squared error for regression: the error minimizer is the "mean (average)"
 - We also want it to be **easy to optimize**

Cross Entropy Error

$$E_{in}(\vec{w}) = \frac{1}{N} \sum_{n=1}^N \ln(1 + e^{-y_n \vec{w}^T \vec{x}_n})$$

- It looks complicated, but
 - It has nice interpretations (min error => max likelihood)
 - It is easy to optimize (continuous, differentiable, convex)

Minimizing Cross Entropy Error



Maximizing Likelihood

Maximum Likelihood Estimation

- Likelihood $\Pr(D|h)$
 - The probability of seeing dataset D if D is generated according to h
 - $\Pr(D|h) = \Pr((\vec{x}_1, y_1), \dots, (\vec{x}_N, y_N)|h)$
 - Maximum likelihood estimation (MLE)
 - $g = \operatorname{argmax}_{h \in H} \Pr(D|h)$
- Sidenote: Two different concepts in ML
 - Likelihood: $\Pr(D|h)$ [Focus of this course]
 - Posterior: $\Pr(h|D)$ [Focus of Bayesian machine learning: More in 515T]
- Connection: $\Pr(h|D) = \frac{\Pr(h)\Pr(D|h)}{\Pr(D)}$
 - Prior $\Pr(h)$: the additional assumption Bayesian ML makes

Write Down the Likelihood

- How are $D = \{(\vec{x}_1, y_1), \dots, (\vec{x}_N, y_N)\}$ generated?
 - $(\vec{x}_1, \dots, \vec{x}_N)$ are i.i.d. drawn from a distribution
 - (y_1, \dots, y_N) are labeled according to target function $f(\vec{x})$

- Likelihood $\Pr(D|h)$

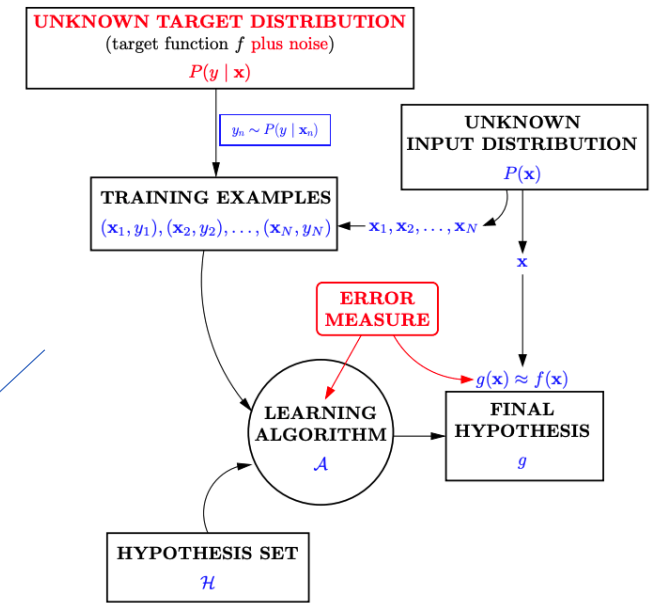
- The probability of seeing dataset D if D is generated according to h

- $\Pr(D|h) = \Pr((\vec{x}_1, y_1), \dots, (\vec{x}_N, y_N)|h)$

$$= \Pr(\vec{x}_1, \dots, \vec{x}_N) \Pr((y_1, \dots, y_N)|(\vec{x}_1, \dots, \vec{x}_N), h)$$

$$= \prod_{n=1}^N \Pr(\vec{x}_n) \prod_{n=1}^N \Pr(y_n|\vec{x}_n, h)$$

(Assumption of independent data)



Maximum Likelihood

- Choosing the hypothesis that maximizes the likelihood

- $g = \operatorname{argmax}_{h \in H} \Pr(D|h)$
 $= \operatorname{argmax}_{h \in H} \prod_{n=1}^N \Pr(\vec{x}_n) \prod_{n=1}^N \Pr(y_n|\vec{x}_n, h)$
 $= \operatorname{argmax}_{h \in H} \prod_{n=1}^N \Pr(y_n|\vec{x}_n, h)$

$\prod_{n=1}^N \Pr(\vec{x}_n)$ doesn't depend on h

- We interpret $h(\vec{x})$ as the probability of $y = +1$

- $\Pr(y|\vec{x}, h) = \begin{cases} h(\vec{x}) = \theta(\vec{w}^T \vec{x}) & \text{for } y = +1 \\ 1 - h(\vec{x}) = 1 - \theta(\vec{w}^T \vec{x}) & \text{for } y = -1 \end{cases}$

- Since $1 - \theta(s) = \theta(-s)$

- $\Pr(y|\vec{x}, h) = \theta(y \vec{w}^T \vec{x})$

Maximum Likelihood

- Choosing the hypothesis that maximizes the likelihood

- $g = \operatorname{argmax}_{h \in H} \Pr(D|h)$
 $= \operatorname{argmax}_{h \in H} \prod_{n=1}^N \Pr(y_n | \vec{x}_n, h)$

- $\vec{w}^* = \operatorname{argmax}_{\vec{w}} \prod_{n=1}^N \theta(y_n \vec{w}^T \vec{x}_n)$
 $= \operatorname{argmax}_{\vec{w}} \ln(\prod_{n=1}^N \theta(y_n \vec{w}^T \vec{x}_n))$
 $= \operatorname{argmax}_{\vec{w}} \sum_{n=1}^N \ln(\theta(y_n \vec{w}^T \vec{x}_n))$
 $= \operatorname{argmin}_{\vec{w}} - \sum_{n=1}^N \ln(\theta(y_n \vec{w}^T \vec{x}_n))$
 $= \operatorname{argmin}_{\vec{w}} \sum_{n=1}^N \ln \frac{1}{\theta(y_n \vec{w}^T \vec{x}_n)}$
 $= \operatorname{argmin}_{\vec{w}} \sum_{n=1}^N \ln(1 + e^{-y_n \vec{w}^T \vec{x}_n})$
 $= \operatorname{argmin}_{\vec{w}} \frac{1}{N} \sum_{n=1}^N \ln(1 + e^{-y_n \vec{w}^T \vec{x}_n})$

$$\theta(s) = \frac{e^s}{1+e^s} = \frac{1}{1+e^{-s}}$$

$$E_{in}(\vec{w}) = \frac{1}{N} \sum_{n=1}^N \ln(1 + e^{-y_n \vec{w}^T \vec{x}_n})$$

Cross Entropy Error

$$E_{in}(\vec{w}) = \frac{1}{N} \sum_{n=1}^N \ln(1 + e^{-y_n \vec{w}^T \vec{x}_n})$$

- Minimizing $E_{in}(\vec{w})$ is the same as maximizing likelihood
- Next question: How to solve $\vec{w}^* = \operatorname{argmin}_{\vec{w}} E_{in}(\vec{w})$
 - Answer: Solve for $\nabla_{\vec{w}} E_{in}(\vec{w}) = 0$
 - No single-step solution like we have in linear regression

Break and Discussion

- Using logistic regression for classification
 - Let \vec{w}^* or g be the learned logistic regression model, can we make classification predictions using \vec{w}^* ?
- Discuss potential ways to do this
 - Conditions on $g(\vec{x})$?
 - Conditions on $\vec{w}^{*T} \vec{x}$?

Break and Discussion

- Using logistic regression for classification
 - Let \vec{w}^* or g be the learned logistic regression model, can we make classification predictions using \vec{w}^* ?
- Yes
 - Set a cutoff probability $C\%$ (e.g., 50%).
 - Classify +1 if $g(\vec{x}) = \theta(\vec{w}^{*T} \vec{x}) > C\%$
 - Classify -1 if $g(\vec{x}) = \theta(\vec{w}^{*T} \vec{x}) < C\%$
 - When C is 50 (a common choice)
 - $\theta(\vec{w}^{*T} \vec{x}) > 50\% \Rightarrow \vec{w}^{*T} \vec{x} > 0$
 - Equivalent to using \vec{w}^* as the linear classification hypothesis, i.e., $g(\vec{x}) = \text{sign}(\vec{w}^{*T} \vec{x})$

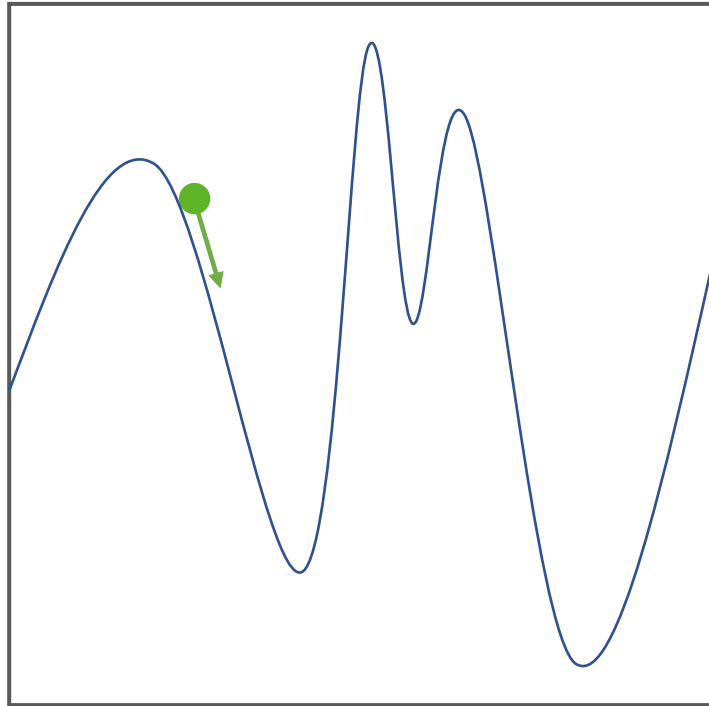
$$\theta(s) = \begin{cases} 1 & \text{when } s \rightarrow \infty \\ 0.5 & \text{when } s = 0 \\ 0 & \text{when } s \rightarrow -\infty \end{cases}$$

Gradient Descent

A general optimization technique

Gradient Descent

- A technique for optimizing functions that **gradients exist everywhere**.



- An iterative method that converges to local optimum.
- Converge to global optimum if the function is convex (since there is only one local optimum).

Gradient Descent: Minimizing $E_{in}(\vec{w})$

- An iterative method of the form:

$$\vec{w}(t + 1) \leftarrow \vec{w}(t) + \eta_t \vec{v}_t$$

- \vec{v}_t : a unit vector, determining the direction of the update
- η_t : a scalar, determining how much to update
- How to choose \vec{v}_t and η_t ?

Choosing \vec{v}_t in $\vec{w}(t+1) \leftarrow \vec{w}(t) + \eta_t \vec{v}_t$

- Intuition: Choose \vec{v}_t that moves towards the “steepest” direction
 - Approaching the minimum faster

- Taylor’s approximation:

- $E_{in}(\vec{w}(t) + \eta_t \vec{v}_t) = E_{in}(\vec{w}(t)) + \eta_t \nabla_{\vec{w}} E_{in}(\vec{w}(t))^T \vec{v}_t + O(\eta_t^2)$

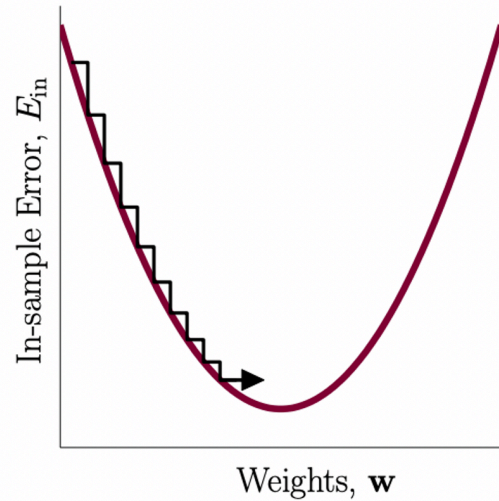
- $E_{in}(\vec{w}(t+1)) - E_{in}(\vec{w}(t)) \approx \eta_t \nabla_{\vec{w}} E_{in}(\vec{w}(t))^T \vec{v}_t$

η_t is usually small, so ignoring this term

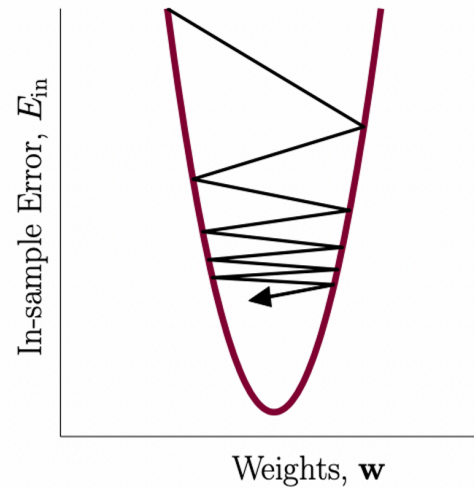
- Choose unit vector \vec{v}_t that minimizes $\nabla_{\vec{w}} E_{in}(\vec{w}(t))^T \vec{v}_t$
 - \vec{v}_t should be in the opposite direction of $\nabla_{\vec{w}} E_{in}(\vec{w}(t))$
 - $\vec{v}_t = \frac{-\nabla_{\vec{w}} E_{in}(\vec{w}(t))}{\|\nabla_{\vec{w}} E_{in}(\vec{w}(t))\|}$

Choosing η_t in $\vec{w}(t+1) \leftarrow \vec{w}(t) + \eta_t \vec{v}_t$

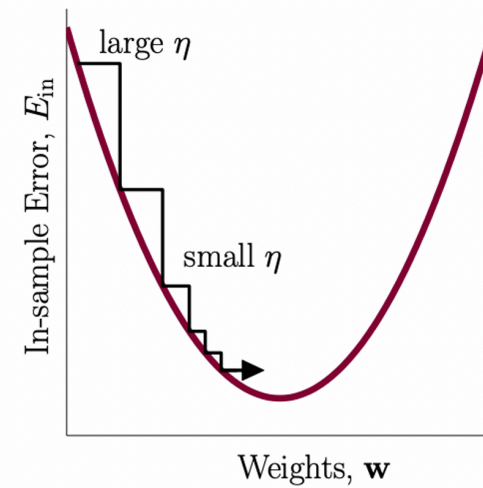
η too small



η too large

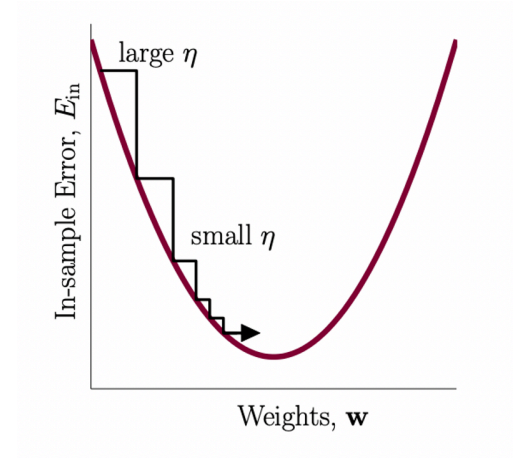


variable η_t – just right



Choosing η_t in $\vec{w}(t + 1) \leftarrow \vec{w}(t) + \eta_t \vec{v}_t$

- Intuition (for convex E_{in})
 - When E_{in} is closer to the minimum,
 - $\nabla_{\vec{w}} E_{in}(\vec{w}(t))$ is smaller
 - We should set η_t smaller
- Therefore, set $\eta_t = \eta \|\nabla_{\vec{w}} E_{in}(\vec{w}(t))\|$



Putting Them Together

- Iterative update rule: $\vec{w}(t + 1) \leftarrow \vec{w}(t) + \eta_t \vec{v}_t$

- $\vec{w}(t + 1) \leftarrow \vec{w}(t) - \eta \nabla_{\vec{w}} E_{in}(\vec{w}(t))$

$$\vec{v}_t = \frac{-\nabla_{\vec{w}} E_{in}(\vec{w}(t))}{\|\nabla_{\vec{w}} E_{in}(\vec{w}(t))\|}$$

$$\eta_t = \eta \|\nabla_{\vec{w}} E_{in}(\vec{w}(t))\|$$

- Gradient calculations

- $E_{in}(\vec{w}) = \frac{1}{N} \sum_{n=1}^N \ln(1 + e^{-y_n \vec{w}^T \vec{x}_n})$

- $\nabla_{\vec{w}} E_{in}(\vec{w}) = \frac{1}{N} \sum_{n=1}^N \frac{-y_n \vec{x}_n e^{-y_n \vec{w}^T \vec{x}_n}}{1 + e^{-y_n \vec{w}^T \vec{x}_n}} = -\frac{1}{N} \sum_{n=1}^N \frac{y_n \vec{x}_n}{1 + e^{y_n \vec{w}^T \vec{x}_n}}$

Gradient Descent for Logistic Regression

- Initialize $\vec{w}(0)$
- For $t = 0, \dots$
 - Compute $\nabla_{\vec{w}} E_{in}(\vec{w}(t)) = -\frac{1}{N} \sum_{n=1}^N \frac{y_n \vec{x}_n}{1 + e^{y_n \vec{w}(t)^T \vec{x}_n}}$
 - $\vec{w}(t + 1) \leftarrow \vec{w}(t) - \eta \nabla_{\vec{w}} E_{in}(\vec{w}(t))$
 - Terminate if the **stop conditions** are met
- Return the final weights

η : learning rate.
A parameter the learner can choose.

Gradient Descent for Logistic Regression

- Initialization
 - Random initialization is a good idea and common approach
- Stop conditions (a mix of the following criteria)
 - When the **number of iteration** exceeds the pre-set threshold
 - When the **improvement on E_{in}** (e.g., check $\nabla_{\vec{w}} E_{in}$) is too small
 - When **E_{in} is small** enough

Computation of Gradient Descent

- Gradient Descent for Logistic Regression

- Initialize $\vec{w}(0)$

- For $t = 0, \dots$

- Compute $\nabla_{\vec{w}} E_{in}(\vec{w}(t)) = -\frac{1}{N} \sum_{n=1}^N \frac{y_n \vec{x}_n}{1 + e^{y_n \vec{w}(t)^T \vec{x}_n}}$

- $\vec{w}(t+1) \leftarrow \vec{w}(t) - \eta \nabla_{\vec{w}} E_{in}(\vec{w}(t))$

- Terminate if the **stop conditions** are met

- Return the final weights

- Which step requires the most computation?

- Calculate $\nabla_{\vec{w}} E_{in}(\vec{w}) = -\frac{1}{N} \sum_{n=1}^N \frac{y_n \vec{x}_n}{1 + e^{y_n \vec{w}^T \vec{x}_n}}$

- The time complexity is $O(N)$

- N is large for big datasets

Stochastic Gradient Descent

Deal with Heavy Computation of $\nabla_{\vec{w}} E_{in}(\vec{w})$

- Speed up the implementation of $\nabla_{\vec{w}} E_{in}(\vec{w}) = -\frac{1}{N} \sum_{n=1}^N \frac{y_n \vec{x}_n}{1 + e^{y_n \vec{w}^T \vec{x}_n}}$
 - E.g., check vectorization
- Solve $\nabla_{\vec{w}} E_{in}(\vec{w})$ "in expectation"
 - Define $e_n(\vec{w}) = \ln(1 + e^{-y_n \vec{w}^T \vec{x}_n})$, the point-wise error caused by (\vec{x}_n, y_n)
 - Observe that
 - $E_{in}(\vec{w}) = \frac{1}{N} \sum_{n=1}^N e_n(\vec{w})$
 - $\nabla_{\vec{w}} E_{in}(\vec{w}) = \frac{1}{N} \sum_{n=1}^N \nabla_{\vec{w}} e_n(\vec{w})$
 - Draw a point \vec{x}_n from $\{\vec{x}_1, \dots, \vec{x}_N\}$ uniformly at random
 - $E_{\vec{x}_n}[\nabla_{\vec{w}} e_n(\vec{w})] = \nabla_{\vec{w}} E_{in}(\vec{w})$

Stochastic Gradient Descent (SGD)

- Algorithm
 - Initialize $\vec{w}(0)$
 - For $t = 0, \dots$
 - Randomly choose n from $\{1, \dots, N\}$
 - $\vec{w}(t + 1) \leftarrow \vec{w}(t) - \eta \nabla_{\vec{w}} e_n(\vec{w}(t))$
 - Terminate if the stop conditions are met
 - Return the final weights
- $\mathbb{E}[\nabla_{\vec{w}} e_n(\vec{w})] = \nabla_{\vec{w}} E_{in}(\vec{w})$
 - SGD is doing the same thing as GD **in expectation**
 - More efficient (scale to large dataset), suitable for online data, helps escaping local min, etc.
 - Noisier, harder to define stop criteria

Mini-Batch Gradient Descent

- GD: Computationally heavy, stable updates
- SGD: Computationally light, noisy updates
- Middle ground: Mini-Batch Gradient Descent
 - In each iteration, randomly choose k points $\{n(1), \dots, n(k)\}$
 - Update rule
 - $\vec{w}(t + 1) \leftarrow \vec{w}(t) - \eta \frac{1}{k} \sum_{i=1}^k \nabla_{\vec{w}} e_{n(i)}(\vec{w}(t))$
- Side-note about HW2
 - Please report your results on GD (non-stochastic version)
 - You should feel free to play around with SGD or mini-batch on your own