Large Scale Machine Learning: SVMs

CS246: Mining Massive Datasets
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New Topic: ML!

High dim.

Locality sensitive hashing

Clustering

Dimensional ity reduction

Graph data

PageRank, SimRank

Community Detection

Spam Detection

Infinite data

Filtering data streams

Web advertising

Queries on streams

Machine learning

SVM

Decision Trees

Perceptron, kNN

Apps

Recommen der systems

Association Rules

Duplicate document detection

Machine Learning

Study of algorithms that...

- improve their <u>performance</u>
- at some task
- with experience

Given some data:

"Learn" a function to map from the input to the output

Given:

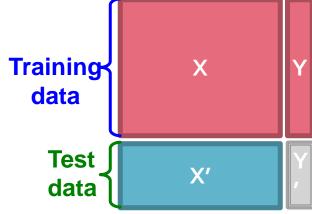
Training examples $(x_i, y = f(x_i))$ for some unknown function f

Find:

A good approximation to f

- Would like to do prediction:
 estimate a function f(x) so that y = f(x)
- Where y can be:
 - Real number: Regression
 - Categorical: Classification
 - Complex object:
 - Ranking of items, Parse tree, etc.
- Data is labeled:
 - Have many pairs {(x, y)}
 - x ... vector of binary, categorical, real valued features
 - **y** ... class ({+1, -1}, or a real number)

- Task: Given data (X,Y) build a model f() to predict Y' based on X'
- Strategy: Estimate y = f(x) on (X, Y).
 Hope that the same f(x) also works to predict unknown Y'

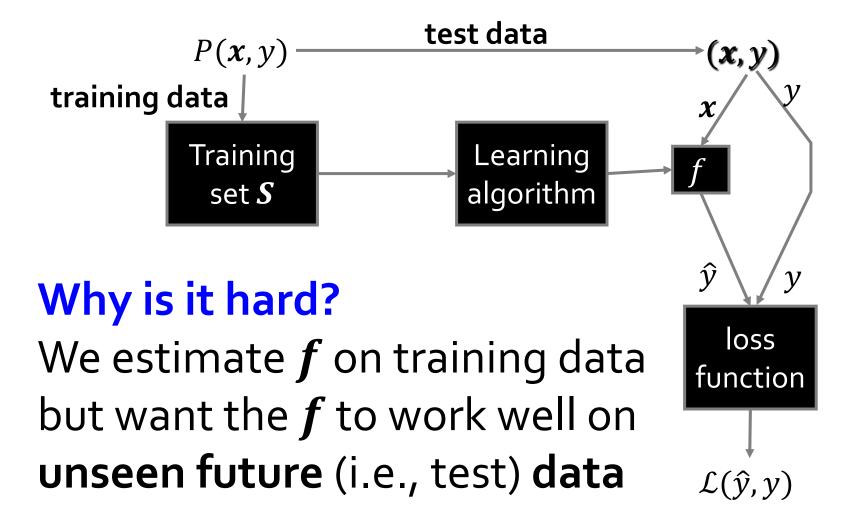


- The "hope" is called generalization
 - Overfitting: If f(x) predicts well Y but is unable to predict Y'
- We want to build a model that generalizes well to unseen data
 - But Jure, how can we well on data we have never seen before?!?

Formal Setting

- 1) Training data is drawn independently at random according to unknown probability distribution P(x, y)
- 2) The learning algorithm analyzes the examples and produces a classifier f
- Given **new** data (x, y) drawn from P, the classifier is given x and predicts $\hat{y} = f(x)$
- The loss $\mathcal{L}(\widehat{y}, y)$ is then measured
- Goal of the learning algorithm: Find f that minimizes expected loss $E_P[\mathcal{L}]$

Formal Setting



Minimizing the Loss

Goal: Minimize the expected loss

$$\min_{\mathbf{w}} \mathbb{E}_{\mathbf{P}}[\mathcal{L}]$$

But, we don't have access to P but only to training sample D:

$$\min_{\mathbf{w}} \mathbb{E}_{\mathbf{D}}[\mathcal{L}]$$

So, we minimize the average loss on the training data:

$$\min_{\mathbf{w}} J(\mathbf{w}) = \frac{1}{N} \sum_{i=1}^{N} \mathcal{L}(h(x), y_i)$$

Problem: Just memorizing the training data gives us a perfect model (with zero loss)

ML == Optimization

Given:

A set of N training examples

$$\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \dots, (x^{(n)}, y^{(n)})\}$$

A loss function £

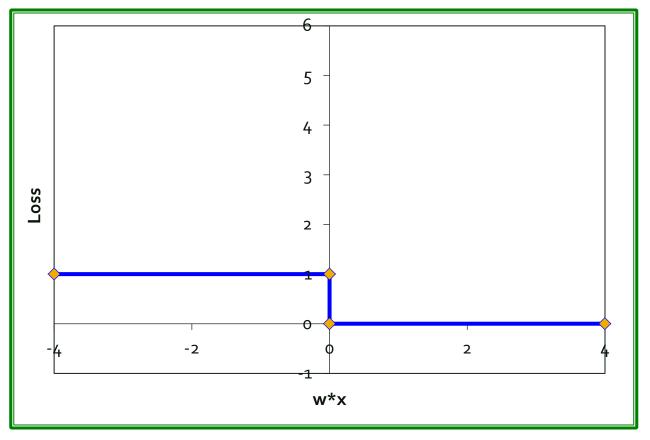
Find:

The weight vector w that minimizes the expected loss on the training data

$$J(\mathbf{w}) = \frac{1}{N} \sum_{i=1}^{N} \mathcal{L}(sgn(\mathbf{w}^{\mathsf{T}} \mathbf{x}_i), y_i)$$

Problem

Problem: Step-wise Constant Loss function



Derivative is either o or ∞

Approximating the Loss

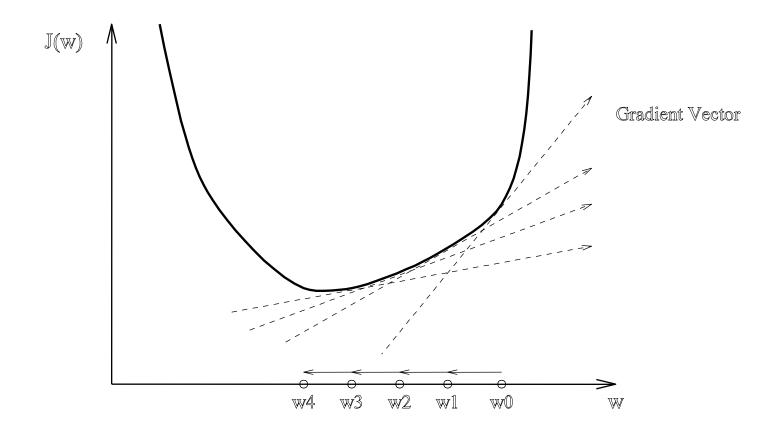
- Approximating the expected loss by a smooth function
 - Replace the original objective function by a surrogate loss function. E.g., hinge loss:

$$\tilde{J}(w) = \frac{1}{N} \sum_{i=1}^{N} \max(0, 1 - y^{(i)} w^{T} x^{(i)})$$
When $y = 1$:

Only Loss

When $y = 1$:

Gradient Descent



Gradient Descent

Minimize f by Gradient Descent

- Start with weight vector $\boldsymbol{w}^{(0)}$
- Compute gradient

$$\nabla J(\mathbf{w}^{(0)}) = \left(\frac{\partial J(\mathbf{w}^{(0)})}{\partial w_0}, \frac{\partial J(\mathbf{w}^{(0)})}{\partial w_1}, \dots, \frac{\partial J(\mathbf{w}^{(0)})}{\partial w_n}\right)$$

- Compute $\mathbf{w}^{(1)} = \mathbf{w}^{(0)} \eta \nabla J(\mathbf{w}^{(0)})$ where η is a "step size" parameter
- Repeat until convergence

Example: Spam Detection

Example: Spam filtering

	viagra	learning	the	dating	nigeria	spam?
$\vec{x}_1 = ($	1	0	1	0	0)	$y_1 = 1$
$\vec{x}_2 = ($	0	1	1	0	0)	$y_2 = -1$
$\vec{x}_3 = ($	0	0	0	0	1)	$y_3 = 1$

- Instance space $x \in X(|X| = n)$ data points)
 - Binary or real-valued feature vector x of word occurrences
 - d features (words + other things, d~100,000)
- Class y ∈ Y
 - y: Spam (+1), Ham (-1)

Spam Detection

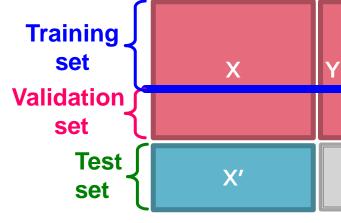
- P(x, y): distribution of email messages x and their true labels y ("spam", "ham")
- Training sample: a set of email messages that have been labeled by the user
- Learning algorithm: What we study!
- f: The classifier output by the learning alg.
- Test point: A new email x
 (with its true, but hidden, label y)
- Loss function $\mathcal{L}(\hat{y}, y)$:

predicted	true label y			
label \hat{y}	spam	ham		
spam	0	10		
not spam	1	0		

Idea: Pretend we do not know the data/labels we actually do know

Build the model f(x) on the training data (minimize J)

- See how well f(x) does on the validation data
 - If it does well, then apply it also to X'
- Refinement: Cross validation
 - Splitting into training/validation set is brutal
 - Let's split our data (X,Y) into 10-folds (buckets)
 - Take out 1-fold for validation, train on remaining 9
 - Repeat this 10 times, report average performance



Estimate y = f(x) on X, Y. Hope that the same f(x) also works on unseen X', Y'

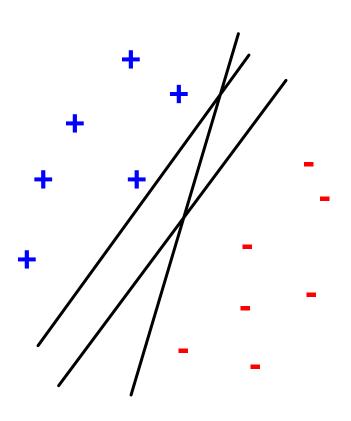
Large Scale Machine Learning

- We will talk about the following methods:
 - Support Vector Machines
 - Decision trees
- Main question:
 How to efficiently train
 (build a model/find model parameters)?

Support Vector Machines

Support Vector Machines

Want to separate "+" from "-" using a line



Data:

- Training examples:
 - $(x_1, y_1) \dots (x_n, y_n)$
- Each example i:

$$x_i = (x_i^{(1)}, ..., x_i^{(d)})$$

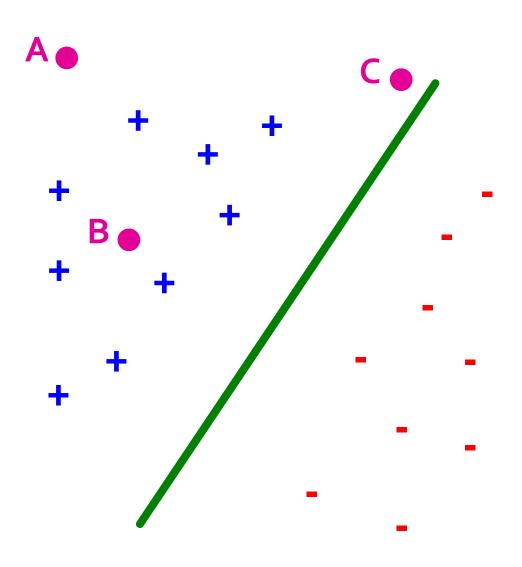
x_i(j) is real valued

Inner product:

$$\mathbf{w} \cdot \mathbf{x} = \sum_{j=1}^{d} w^{(j)} \cdot x^{(j)}$$

Which is best linear separator (defined by w)?

Largest Margin



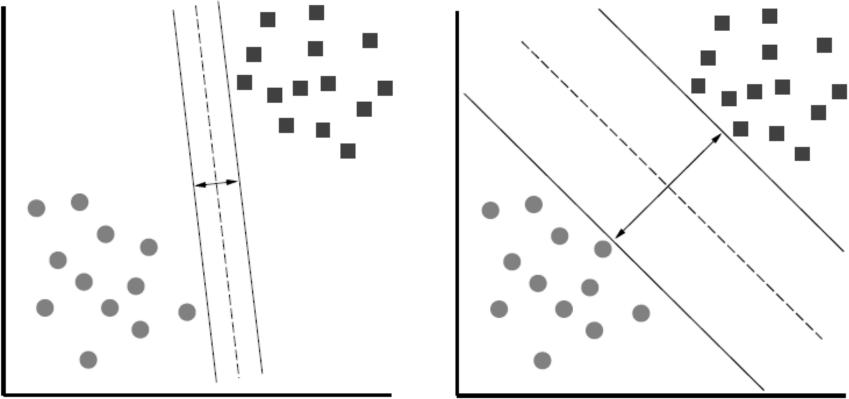
 Distance from the separating hyperplane corresponds to the "confidence" of prediction

Example:

We are more sure about the class of A and B than of C

Largest Margin

• Margin γ : Distance of closest example from the decision line/hyperplane

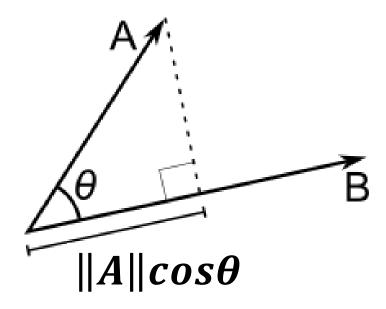


The reason we define margin this way is due to theoretical convenience and existence of generalization error bounds that depend on the value of margin.

Why maximizing γ a good idea?

Remember: the Dot product

$$A \cdot B = ||A|| \cdot ||B|| \cdot \cos \theta$$



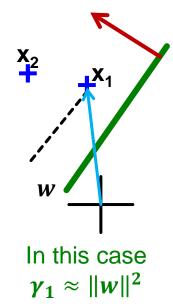
$$||A|| = \sqrt{\sum_{j=1}^{d} (A^{(j)})^2}$$

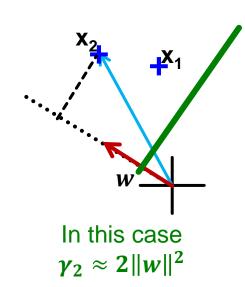
Why maximizing γ a good idea?

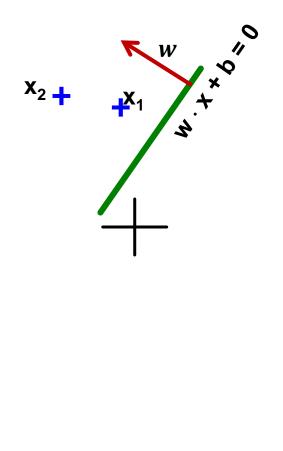
Dot product

$$A \cdot B = ||A|| ||B|| \cos \theta$$

• What is $w \cdot x_1$, $w \cdot x_2$?

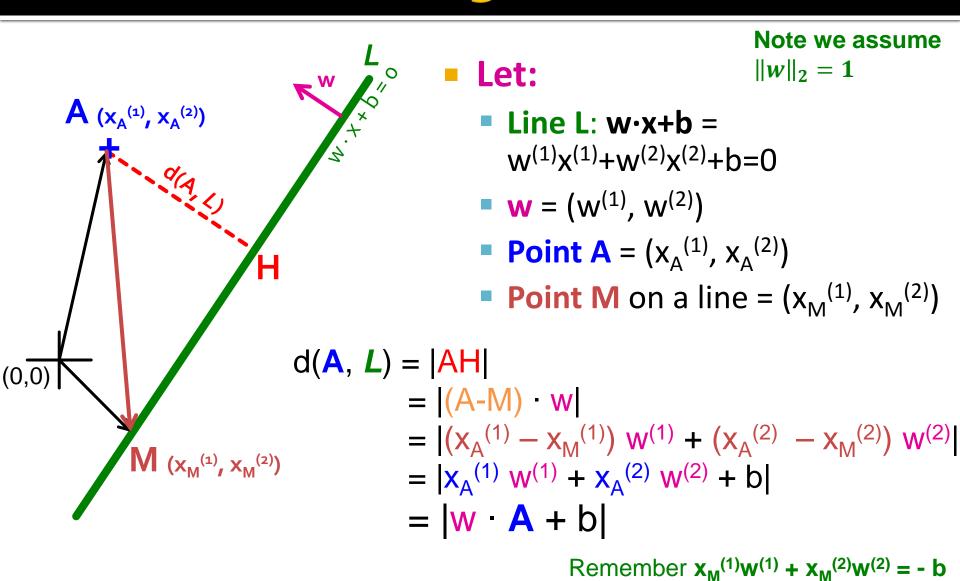






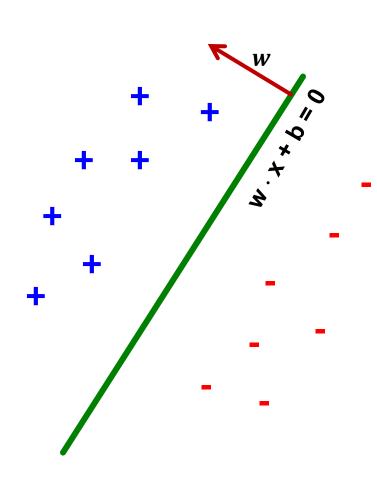
- So, γ roughly corresponds to the margin
 - **Bottom line:** Bigger γ bigger the separation

What is the margin?



since **M** belongs to line **L**

Largest Margin



- Prediction = sign(w x + b)
- "Confidence" = $(w \cdot x + b) y$
- For i-th datapoint:

$$\gamma_i = (w \cdot x_i + b) y_i$$

Want to solve:

$$\max_{w} \min_{i} \gamma_{i}$$

Can rewrite as

$$\max_{w,\gamma} \gamma$$

$$s.t. \forall i, y_i(w \cdot x_i + b) \ge \gamma$$

Support Vector Machine

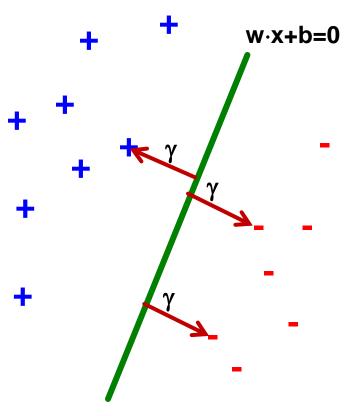
• Maximize the margin:

 Good according to intuition, theory (c.f. "VC dimension") and practice

$$\max_{w,\gamma} \gamma$$

$$s.t. \forall i, y_i (w \cdot x_i + b) \ge \gamma$$

γ is margin ... distance from the separating hyperplane

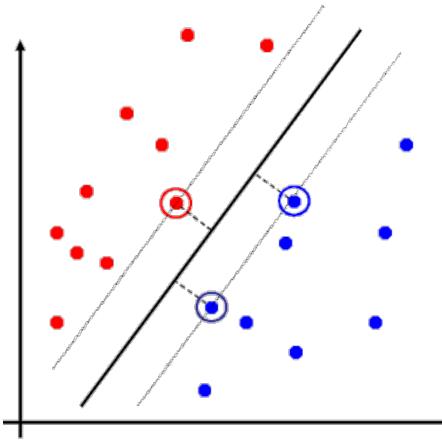


Maximizing the margin

Support Vector Machines: Deriving the margin

Support Vector Machines

- Separating hyperplane is defined by the support vectors
 - Points on +/- planes from the solution
 - If you knew these points, you could ignore the rest
 - Generally,
 d+1 support vectors (for d dim. data)



Canonical Hyperplane: Problem

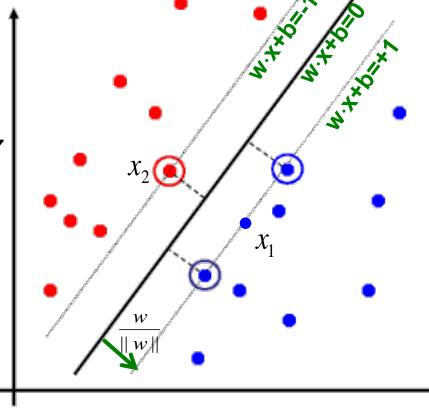
Problem:

- Let $(w \cdot x + b)y = \gamma$ then $(2w \cdot x + 2b)y = 2\gamma$
 - Scaling w increases margin!

Solution:

Work with normalized w:

$$\boldsymbol{\gamma} = \left(\frac{w}{\|w\|} \cdot \boldsymbol{x} + \boldsymbol{b}\right) \boldsymbol{y}$$



Let's also require support vectors x_j to be on the plane defined by:

$$\boldsymbol{w}\cdot\boldsymbol{x_j}+\boldsymbol{b}=\pm\mathbf{1}$$

$$||w|| = \sqrt{\sum_{j=1}^{d} (w^{(j)})^2}$$

Canonical Hyperplane: Solution

- Want to maximize margin $\gamma!$
- What is the relation between x₁ and x₂?

$$x_1 = x_2 + 2\gamma \frac{w}{||w||}$$

We also know:

$$w \cdot x_1 + b = +1$$

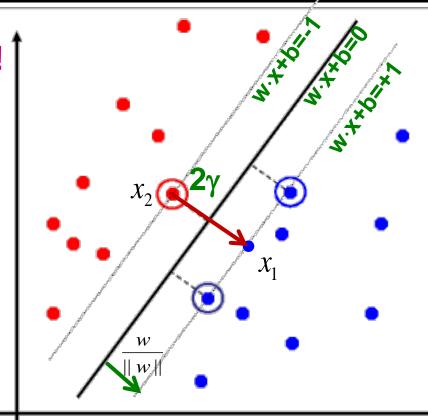
$$w \cdot x_2 + b = -1$$

So:

•
$$w \cdot x_1 + b = +1$$

$$w\left(x_2+2\gamma\frac{w}{||w||}\right)+b=+1$$

$$\underbrace{w \cdot x_2 + b + 2\gamma \frac{w \cdot w}{||w||}}_{1} = +1$$



$$\Rightarrow \gamma = \frac{\|w\|}{w \cdot w} = \frac{1}{\|w\|}$$

Note: $\mathbf{w} \cdot \mathbf{w} = \|\mathbf{w}\|^2$

Maximizing the Margin

We started with

$$\max_{w,\gamma} \gamma$$

$$s.t. \forall i, y_i(w \cdot x_i + b) \ge \gamma$$

But w can be arbitrarily large!

We normalized and...

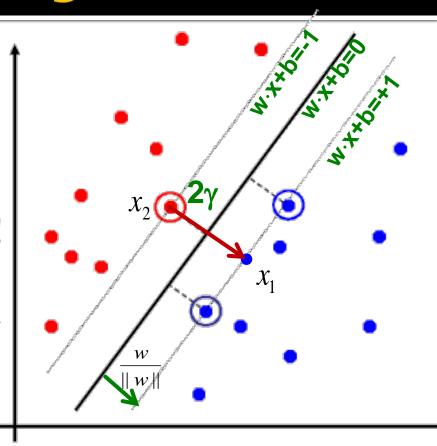
$$\arg\max\gamma = \arg\max\frac{1}{\|w\|} = \arg\min\|w\| = \arg\min\frac{1}{2}\|w\|^2$$

Then:

$$\min_{w} \frac{1}{2} ||w||^2$$

$$s.t. \forall i, y_i(w \cdot x_i + b) \ge 1$$

This is called SVM with "hard" constraints



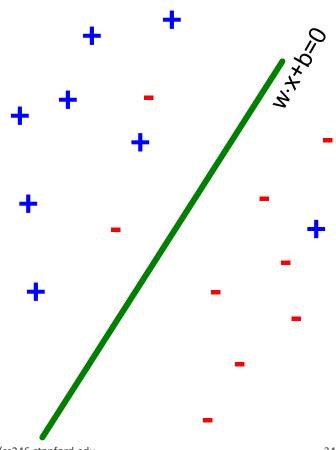
Non-linearly Separable Data

If data is not separable introduce penalty:

$$\min_{w} \frac{1}{2} ||w||^2 + \mathbf{C} \cdot (\text{# number of mistakes})$$

$$s.t. \forall i, y_i(w \cdot x_i + b) \ge 1$$

- Minimize $||w||^2$ plus the number of training mistakes
- Set C using cross validation
- How to penalize mistakes?
 - All mistakes are not equally bad!



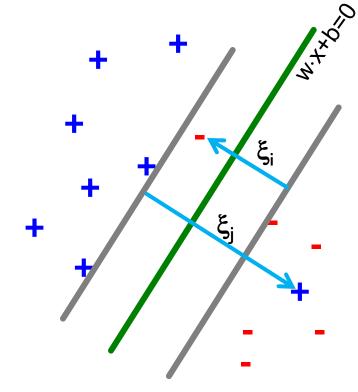
Support Vector Machines

Introduce slack variables ξ_i

$$\min_{w,b,\xi_i \ge 0} \ \frac{1}{2} \|w\|^2 + C \cdot \sum_{i=1}^n \xi_i$$

$$s.t. \forall i, y_i(w \cdot x_i + b) \ge 1 - \xi_i$$

If point x_i is on the wrong side of the margin then get penalty ξ_i



For each data point:

If margin ≥ 1, don't care
If margin < 1, pay linear penalty

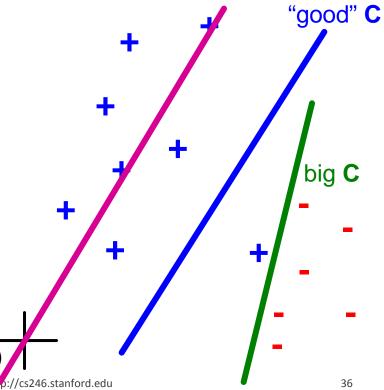
Slack Penalty C

$$\min_{w} \frac{1}{2} ||w||^2 + \mathbf{C} \cdot (\text{# number of mistakes})$$

$$s.t. \forall i, y_i (w \cdot x_i + b) \ge 1$$

What is the role of slack penalty C:

- C=∞: Only want to w, b that separate the data
- C=0: Can set ξ_i to anything, then w=0 (basically ignores the data)



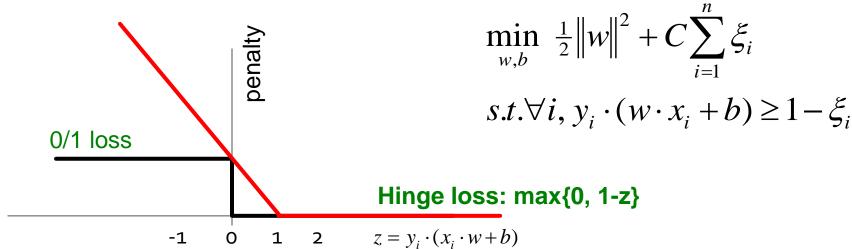
small C

Support Vector Machines

SVM in the "natural" form

$$\underset{w,b}{\operatorname{arg\,min}} \quad \frac{1}{2} \underbrace{w \cdot w + C} \cdot \sum_{i=1}^{n} \max\{0, 1 - y_i(w \cdot x_i + b)\}$$
Regularization parameter Empirical loss L (how well we fit training data)

SVM uses "Hinge Loss":



Support Vector Machines: How to compute the margin?

$$\min_{w,b} \frac{1}{2} w \cdot w + C \cdot \sum_{i=1}^{n} \xi_{i}$$

$$s.t. \forall i, y_{i} \cdot (x_{i} \cdot w + b) \ge 1 - \xi_{i}$$

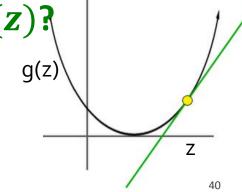
- Want to estimate w and b!
 - Standard way: Use a solver!
 - Solver: software for finding solutions to "common" optimization problems
- Use a quadratic solver:
 - Minimize quadratic function
 - Subject to linear constraints
- Problem: Solvers are inefficient for big data!

- Want to estimate w, b!
- Alternative approach:
 - Want to minimize J(w,b):

$$\min_{w,b} \ \frac{1}{2} w \cdot w + C \sum_{i=1}^{n} \xi_i$$

$$s.t. \forall i, y_i \cdot (x_i \cdot w + b) \ge 1 - \xi_i$$

- $J(w,b) = \frac{1}{2}w \cdot w + C \cdot \sum_{i=1}^{n} \max \left\{ 0, 1 y_i \left(\sum_{j=1}^{d} w^{(j)} x_i^{(j)} + b \right) \right\}$
- Side note:
 - How to minimize convex functions g(z)?
 - Use gradient descent: min_z g(z)
 - Iterate: $\mathbf{z}_{\mathsf{t+1}} \leftarrow \mathbf{z}_{\mathsf{t}} \eta \ \nabla \mathbf{g}(\mathbf{z}_{\mathsf{t}})$



Want to minimize J(w,b):

$$J(w,b) = \frac{1}{2} \sum_{j=1}^{d} (w^{(j)})^2 + C \sum_{i=1}^{n} \max \left\{ 0, 1 - y_i (\sum_{j=1}^{d} w^{(j)} x_i^{(j)} + b) \right\}$$

Empirical loss $L(x_i y_i)$

Compute the gradient \nabla(j) w.r.t. $w^{(j)}$

$$\nabla J^{(j)} = \frac{\partial L(w,b)}{\partial w^{(j)}} = w^{(j)} + C \sum_{i=1}^{n} \frac{\partial L(x_i, y_i)}{\partial w^{(j)}}$$

$$\frac{\partial L(x_i, y_i)}{\partial w^{(j)}} = 0 \quad \text{if } y_i(\mathbf{w} \cdot x_i + b) \ge 1$$
$$= -y_i x_i^{(j)} \quad \text{else}$$

Gradient descent:

Iterate until convergence:

• For $j = 1 \dots d$ • Evaluate: $\nabla J^{(j)} = \frac{\partial f(w,b)}{\partial w^{(j)}} = w^{(j)} + C \sum_{i=1}^{n} \frac{\partial L(x_i, y_i)}{\partial w^{(j)}}$

Update:

 $\mathbf{w}^{(j)} \leftarrow \mathbf{w}^{(j)} - \eta \nabla \mathbf{J}^{(j)}$

η...learning rate parameterC... regularization parameter

Problem:

- Computing $\nabla J^{(j)}$ takes O(n) time!
 - **n** ... size of the training dataset

We just had:

Stochastic Gradient Descent

$$\nabla J^{(j)} = w^{(j)} + C \sum_{i=1}^{n} \frac{\partial L(x_i, y_i)}{\partial w^{(j)}}$$

 Instead of evaluating gradient over all examples evaluate it for each individual training example

$$\nabla J^{(j)}(x_i) = w^{(j)} + C \cdot \frac{\partial L(x_i, y_i)}{\partial w^{(j)}}$$

Notice: no summation over *i* anymore

Stochastic gradient descent:

Iterate until convergence:

- For i = 1 ... n
 - For j = 1 ... d
 - Compute: ∇J^(j)(x_i)
 - Update: $\mathbf{w}^{(j)} \leftarrow \mathbf{w}^{(j)} \eta \nabla \mathbf{J}^{(j)}(\mathbf{x}_i)$

Support Vector Machines: Example

Example: Text categorization

- Example by Leon Bottou:
 - Reuters RCV1 document corpus
 - Predict a category of a document
 - One vs. the rest classification
 - \blacksquare n = 781,000 training examples (documents)
 - 23,000 test examples
 - d = 50,000 features
 - One feature per word
 - Remove stop-words
 - Remove low frequency words

Example: Text categorization

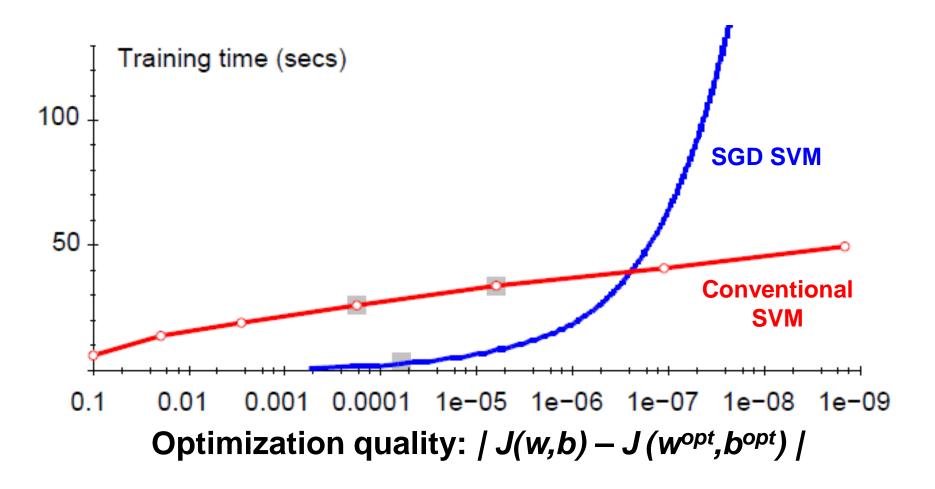
• Questions:

- (1) Is SGD successful at minimizing J(w,b)?
- (2) How quickly does **SGD** find the min of *J(w,b)*?
- (3) What is the error on a test set?

	Training time	Value of J(w,b)	Test error
Standard SVM	23,642 secs	0.2275	6.02%
"Fast SVM"	66 secs	0.2278	6.03%
SGD-SVM	1.4 secs	0.2275	6.02%

- (1) SGD-SVM is successful at minimizing the value of *J(w,b)*
- (2) SGD-SVM is super fast
- (3) SGD-SVM test set error is comparable

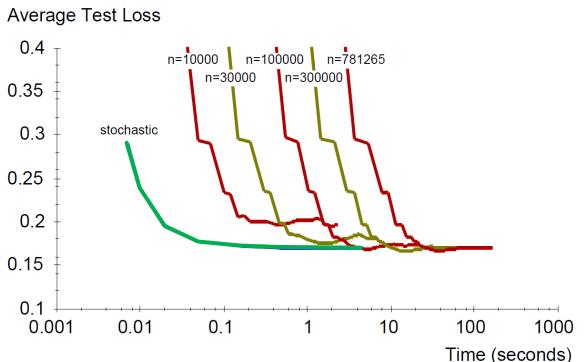
Optimization "Accuracy"



For optimizing J(w,b) within reasonable quality SGD-SVM is super fast

SGD vs. Batch Conjugate Gradient

 SGD on full dataset vs. Conjugate Gradient on a sample of n training examples



Bottom line: Doing a simple (but fast) SGD update many times is better than doing a complicated (but slow) CG update a few times

Theory says: Gradient descent converges in linear time k. Conjugate gradient converges in \sqrt{k} .

k... condition number

Practical Considerations

Sparse Linear SVM:

- Feature vector x_i is sparse (contains many zeros)
 - Do not do: $\mathbf{x}_i = [0,0,0,1,0,0,0,0,5,0,0,0,0,0,0,0]$
 - But represent x_i as a sparse vector $x_i = [(4,1), (9,5), ...]$
- Can we do the SGD update more efficiently?

$$w \leftarrow w - \eta \left(w + C \frac{\partial L(x_i, y_i)}{\partial w} \right)$$

Approximated in 2 steps:

$$w \leftarrow w - \eta C \frac{\partial L(x_i, y_i)}{\partial w}$$

$$w \leftarrow w(1-\eta)$$

 $w \leftarrow w - \eta C \frac{\partial L(x_i, y_i)}{\partial w}$ cheap: x_i is sparse and so few coordinates j of w will be updated

expensive: w is not sparse, all coordinates need to be updated

Practical Considerations

- Solution 1: $w = s \cdot v$
 - Represent vector w as the product of scalar s and vector v
 - Then the update procedure is:

• (1)
$$v = v - \eta C \frac{\partial L(x_i, y_i)}{\partial w}$$

• (2) $s = s(1 - \eta)$

Solution 2:

- Perform only step (1) for each training example
- Perform step (2) with lower frequency and higher η

Two step update procedure:

(1)
$$w \leftarrow w - \eta C \frac{\partial L(x_i, y_i)}{\partial w}$$

(2)
$$w \leftarrow w(1-\eta)$$

Practical Considerations

Stopping criteria:

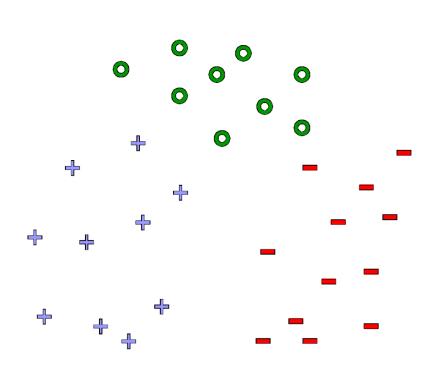
How many iterations of SGD?

- Early stopping with cross validation
 - Create a validation set
 - Monitor cost function on the validation set
 - Stop when loss stops decreasing

Early stopping

- Extract two (very) small sets of training data A and B
- Train on A, stop by validating on B
- Number of training epochs on A is an estimate of k
- Train for k epochs on the full dataset

What about multiple classes?



Idea 1:

One against all

Learn 3 classifiers

Obtain:

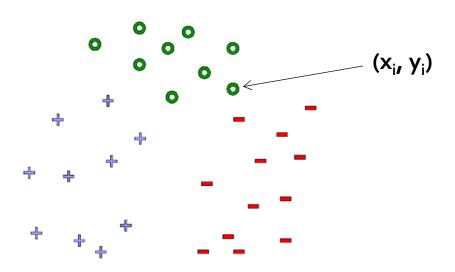
$$\mathbf{w}_{+} \mathbf{b}_{+}, \mathbf{w}_{-} \mathbf{b}_{-}, \mathbf{w}_{0} \mathbf{b}_{0}$$

- How to classify?
- Return class c $arg max_c w_c x + b_c$

Learn 1 classifier: Multiclass SVM

- Idea 2: Learn 3 sets of weights simoultaneously!
 - For each class c estimate w_c , b_c
 - Want the correct class y_i to have highest margin:

$$\mathbf{w}_{\mathbf{y}_i} \mathbf{x}_i + \mathbf{b}_{\mathbf{y}_i} \ge 1 + \mathbf{w}_{\mathbf{c}} \mathbf{x}_i + \mathbf{b}_{\mathbf{c}} \quad \forall \mathbf{c} \ne \mathbf{y}_i , \forall i$$



Multiclass SVM

Optimization problem:

$$\min_{w,b} \frac{1}{2} \sum_{c} ||w_{c}||^{2} + C \sum_{i=1}^{n} \xi_{i}
w_{y_{i}} \cdot x_{i} + b_{y_{i}} \ge w_{c} \cdot x_{i} + b_{c} + 1 - \xi_{i} \xi_{i} \ge 0, \forall i$$

- To obtain parameters \mathbf{w}_c , \mathbf{b}_c (for each class \mathbf{c}) we can use similar techniques as for 2 class **SVM**
- SVM is widely perceived a very powerful learning algorithm

Support Vector Machines: Example

Online Learning

New setting: Online Learning

- Allows for modeling problems where we have a continuous stream of data
- We want an algorithm to learn from it and slowly adapt to the changes in data
- Idea: Do slow updates to the model
 - SGD-SVM makes updates if misclassifying a datapoint
 - So: First train the classifier on training data.
 Then for every example from the stream, if we misclassify, update the model (using a small learning rate)

Example: Shipping Service

Protocol:

- User comes and tell us origin and destination
- We offer to ship the package for some money (\$10 -\$50)
- Based on the price we offer, sometimes the user uses our service (y = 1), sometimes they don't (y = -1)
- Task: Build an algorithm to optimize what price we offer to the users
- Features x capture:
 - Information about user
 - Origin and destination
- Problem: Will user accept the price?

Example: Shipping Service

Model whether user will accept our price:

$$y = f(x; w)$$

- Accept: y =1, Not accept: y=-1
- Build this model with say Perceptron or SVM
- The website that runs continuously
- Online learning algorithm would do something like
 - User comes
 - User is represented as an (x,y) pair where
 - x: Feature vector including price we offer, origin, destination
 - y: If they chose to use our service or not
 - The algorithm updates w using just the (x,y) pair
 - Basically, we update the w parameters every time we get some new data

Example: Shipping Service

- We discard this idea of a data "set"
- Instead we have a continuous stream of data
- Further comments:
 - For a major website where you have a massive stream of data then this kind of algorithm is pretty reasonable
 - Don't need to deal with all the training data
 - If you had a small number of users you could save their data and then run a normal algorithm on the full dataset
 - Doing multiple passes over the data

Online Algorithms

- An online algorithm can adapt to changing user preferences
- For example, over time users may become more price sensitive
- The algorithm adapts and learns this
- So the system is dynamic