# A Section 9: Support Vector Machines 

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CS109A Introduction to Data Science
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What do you get when you cross an elephant and a rhino?

Q: What does logistic regression think of LDA/QDA?

What do you get when you cross an elephant and a rhino?

Q: What does logistic regression think of LDA/QDA?

- LDA/QDA tell the complete story of how the data came to be
- Correspondingly, it makes heavy assumptions, and much can go wrong


## A: You're modelling too much

- Logistic doesn't care how the $X$ data came to be, it only tells the story of the Y data
- Since there are fewer assumptions, the math is more advanced and the method is slower


# SVM:Logistic Regression::Logistic Regression:QDA 

## Less is More

SVMs

- Only predict the final class, not the probability of each class
- Make no assumptions about the data
- Still work well with Iarge numbers of features



## Our Path

- I: Get comfy with the key expressions and concepts

Bundles, signed distance, class-based distance

- II: Extract the highlights of SVMs from the loss function

Only certain observations matter; effects of the C parameter

- III: Derivation of the primal and dual problems, fulfilling the promises from Part II
Lagrangian, Piramal/Dual games, KKT conditions as souped-up
"derivative=0"
- IV: Interpret the dual problem and see SVMs in a new way SVMs can be seen as an advanced neighbors-style algorithm

Part I
REVIEW
P

## Act I: Setting

- Like Logistic regression, SVMs set three parameters: a weight on each feature ( w 1 and w 2 ) and an intercept (b)
- This is MORE than we need to define a line
- So what are we really defining?


CS109A, PRotopapas, Rader

## Key Concept \#1

- Via $w^{T} x+b, w$ and $b$ define an output at each point of input space
- This is our first key quantity, and will

$$
w^{T} x+b=
$$ live in our 'reminder corner'

- $w^{T} x+b$ gives us:
- The rule to classify test points: if $w^{T} x+$ $b$ is + classify as +; if - classify as -
- A new measure of distance [from the decision boundary in units of $1 /\|w\|]$
- We [arbitrarily] define +1 and -1 as the
 margin for a given $w, b$ (bundle)


## DEMO:

In the notebook, we manipulate $\mathrm{w} 1, \mathrm{w} 2$, and b to see how they affect the bundle produced

Conclusions:

- $w 1$ and $w 2$ control the slope of the bundle, and the Iarger the norm, the more tightly packed the bundle is
- $b$ controls the height of the bundle, but its effect depends on the magnitude of $w 1$ and $w 2$
- The expression $y_{i}\left(w^{T} x_{i}+b\right)$ occurs a ton with SVMs
- It takes the signed distance function and multiplies it by an observation's class
- We're calling it "class-based distance"

$$
y_{i}\left(w^{T} x_{i}+b\right)=
$$

Example:
$y_{i}\left(w^{T} x_{i}+b\right)$

- is 0 on at the decision boundary
- is above 1 if you are safely beyond your margin
- is 1 (or less) if you are crowding the margin or misclassified
- is negative if you're really messing up



## A table of the key quantities at each point



| Point | Class | Signed <br> Distance | Class-based <br> distance | Loss |
| :--- | :--- | :--- | :--- | :--- |
| A | - | -3 | 3 | None |
| B | - | -1 | 1 | Marginal |
| C | + | 2 | 2 | None |
| D | - | 2 | -2 | Misclass |
| E | + | -1 | -1 | Misclass |

The same 'signed distance’ concepts apply to kernels, although:

1. The lines get wavy
2. The way we measure distance is less clear

Later on, we'll learn

- What kind distance is used for kernels

- Standard distance isn't what you think


## Recap:

- We're picking a best bundle (set of weights and b)
- The bundle implies a signed 'distance' $w^{T} x+b$ over the space, where 0 is the decision boundary
- Class-based distance $y_{i} w^{T} x_{i}+b$ is directly related to how sad we are about a training point
- Kernels put a wavy set of lines over the input space, instead of level ones

Part II
LOSS FUNCTIONS

We saw 1 was a critical value for $y_{i}\left(w^{T} x_{i}+\right.$ b)

- Above 1 means you're safely within your margin
- Below 1 means you're crowding the margin
- Below 0 means you're misclassified

Make it a loss function:

- Negate so bigger values are worse, not better,
- $\quad+1$ so points within their margin get loss 0 instead of -1
- If the loss would be negative, record 0 instead
- Which do you like best?


## H|tL



- Which do you like best?

- Tradeoff exists between wanting wider margins and discomfort with points inside the margins

$$
\operatorname{Loss}(w, b, \text { train data })=\sum_{\text {train }} \max \left(1-y_{i}\left(w^{T} x_{i}+b\right), 0\right)+\lambda\|w\|^{2}
$$

- View A: minimize hinge loss, $L_{2}$ regularization

$$
\operatorname{Loss}(w, b, \text { train data })=\|w\|^{2}+C \sum_{\text {train }} \max \left(1-y_{i}\left(w^{T} x_{i}+b\right), 0\right)
$$

- View B: maximize the margin, but pay a price for points inside the margin (or misclassified)


## DEMO:

In the notebook, we manipulate $C$ and see how the solution found by SVM changes

## Conclusions:

- Big $C$ : we do anything to reduce invasion losses
- If seperable: finds separating plane
- If not: lumps non-separable points into margin, separates the rest
- Small $C$ : we stop caring about invasion (or even misclassification); just grow the margin

Observations from SVM loss:

1. Hinge loss zero for most points

- most points are behind the margin

2. Moving/deleting these points wouldn't change the solution
3. The outcome for a test point only depends on a handful of training points

- $\quad$ Should be able to write output value as combination of $(-2,1)$ and $(1,2)$
- Key question: HOW can we determine a test point's class using the few important training points?

- Leads to re-casting as a fancified neighbors algorithm

Our reward for sitting through the math:

1. A recipe for the most important training points
2. A way to make decisions while throwing out most of the training data
3. A new and more powerful view of what SVMs do

Like studying linear regression's loss minimization via calculus, but with a harder target and more advanced math

## Part III

## MATH

Ideas: http://cs229.stanford.edu/notes/cs229-notes3.pdf Soft-Margin derivation: http://www.ccs.neu.edu/home/vip/teach/MLcourse/6_SVM_kernels/lecture_notes/svm/svm.pdf

## Outline proof steps

1. Re-cast the loss function as a convex optimization
2. Re-write the one-player game into a two-player game (Primal)
3. Rewrite the two-player game into an equivalent game with opposite turn order (Dual)
4. Observe that assigning (mostly-zero) importance scores to each training point is equivalent to solving the original optimization (KKT)
5. Observe that our original SVM formulation was using a very counter-intuitive definition of distance, and we can do better

Our goal:

$$
\min _{\mathrm{w}, \mathrm{~b}}\|w\|^{2}+C \sum_{\text {train }} \max \left(1-y_{i}\left(w^{T} x_{i}+b\right), 0\right)
$$

First, re-write to an optimization problem with constraints:

$$
\min _{\mathrm{w}, \mathrm{~b}, \xi_{i}} \frac{1}{2}\|w\|^{2}+C \sum_{i=1}^{n} \xi_{i}
$$

Such that

$$
\xi_{i} \geq 1-y_{i}\left(w^{T} x_{i}+b\right), \xi_{i} \geq 0 \text { for all } i
$$

Basically, we delete loss and introduce some $\xi_{i}$ variables that you get to set Why is this the same problem?

- $\quad \xi_{i}$ must be at least as big as the loss: you'd be dumb to set them to anything bigger than the loss
- Now you're back to minimizing norm+loss
- You're trying to plan your week
- You have to choose how much time you allocate to study, work, etc.
 work-study sleep (Per week)
- CS109 maximum 1 day. No asec OH on Wednesday late • Job interview Thursday
- CS207 due by Thursday

Project meeting by Monday


- What if the constraints were flexible?
- You'd know what the cost of being each late day is
- And how about a reward for getting work done early!
- This brings us to the Lagrangian
- It takes all the mandatory requirements and attaches costs to them
- For $\xi_{i} \geq 1-y_{i}\left(w^{T} x_{i}+b\right)$ we attach a cost $\alpha_{i}$ for each unit that $1-y_{i}\left(w^{T} x_{i}+b\right)$ exceeds $\xi_{i}$
- Likewise for $\xi_{i} \geq 0$
- Overall, we get


Original objective

Cost (or benefit) from $\xi_{i} \geq 1$ $y_{i}\left(w^{T} x_{i}+b\right)$ "objective"

Cost (or benefit) from $\xi_{i} \geq 0$ "objective"

- But there aren't actually penalties for each day late, or rewards for being early...
- What you neeals a demon
- The demon takes any plan you make and manipulates the $\alpha_{i}$ and $\beta_{i}$ costs
- So you better present a plan


You shall not pass that actually meets the constraints

We have a two-player game (you and demon) equivalent to the original hard-constraint problem:

You choose the parameters

$$
\varlimsup_{w, b, \xi_{i}}^{\min _{\alpha_{i} \geq 0}} \max _{\alpha^{2}} \frac{1}{2}\|w\|^{2}+C \sum_{i=1}^{n} \xi_{i}+\sum_{i=1}^{n} \alpha_{i}\left[1-y_{i}\left(w^{T} x_{i}+b\right)-\xi_{i}\right]+\sum_{i=1}^{n}-\beta_{i} \xi_{i}
$$

Then the demon chooses the costs

- The demon will try to screw you, so you'll only propose points that meet all constraints
- And you'll try to minimize the original objective
- Level one complete: we wrote the "Primal Problem"
- Now, like Gandalf and the Balrog, there's a Duel
- Still pondering how to set your schedule, an Econ 101 student walks by

- "The free market solves everything"
- "What about companies polluting?"
- "Well, charge them for each ton of carbon they emit
- If you get prices right, they'll stop"
- Could you set the costs/rewards yourself and let the free market minimize the objective?
- Can you set costs that guide them to the same solution as the original?

Reversing the turn order (the min and max), we get

You set the costs/rewards

$$
\max _{\alpha \geq 0} \underbrace{\min _{w, b, \xi_{i}}} \frac{1}{2}\|w\|^{2}+C \sum_{i=1}^{n} \xi_{i}+\sum_{i=1}^{n} \alpha_{i}\left[1-y_{i}\left(w^{T} x_{i}+b\right)-\xi_{i}\right]+\sum_{i=1}^{n}-\beta_{i} \xi_{i}
$$

The market tries to minimize the objective, including any costs/subsidies you offer

- No guarantee there are prices that force the free market to obey constraints and give the same solution as the original
- However, because ...
- 1) the objective is convex and 2) the constraints are convex and 3) there is some solution that fits the constraints (pick $\xi$ large)]:
- ...there are such prices, even if they're hard to write down

IF the dual can be rigged to give the same solution as the original
THEN we get helpful facts about the solution called the KKT conditions

- KKT can be used to check a candidate solution, or derive facts of the eventual solution

1. Derivative of Lagrangian (wrt any parameter) is 0
2. Derivative of Lagrangian (wrt cost of violating an equality) is 0
3. Constraint function $\leq 0$ (i.e. constraints are satisfied)
4. Cost*constraint $=0$ (only binding constraints get non-zero costs)

## Let's recap

- Wrote our optimization problem (minimize loss)
- Massaged into a convex optimization problem
- Horary for hinge loss and convexity
- Applied Lagrangian to make progress on the constrained optimization
- Costs instead of mandates, but a demon controls costs
- Convexity let us study the dual problem instead
- We control costs, but it's not always possible to set them well
- KKT gave us a bunch of useful properties we're about to apply

Let's recap

- Wrote our optimization problem /ninimize loss)
- Massaged into a convex optimiz cion prolen

- Convexity let us study the dul pron instead
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- KKT gave us a bunch of useful properties we're about to apply

Part III: Part II
THE LAST MATH

Rule 1 (for w) says that

$$
\nabla_{w} \frac{1}{2}\|w\|^{2}+C \sum_{i=1}^{n} \xi_{i}+\sum_{i=1}^{n} \alpha_{i}\left[1-y_{i}\left(w^{T} x_{i}+b\right)\right]-\xi_{i}+\sum_{i=1}^{n}-\beta_{i} \xi_{i}=0
$$

The derivative is practically trivial:

$$
\begin{gathered}
w+\sum_{i=1}^{n} \alpha_{i}\left[-y_{i} x_{i}\right]=0 \\
w=\sum_{i=1}^{n} \alpha_{i}\left[y_{i} x_{i}\right]
\end{gathered}
$$

Conclusions

- The w are just a weighted sum of the training points

If we know $\alpha_{i}$, we can make classification decisions using only the x and y data

Rule 1 (for b) says that

$$
\nabla_{b} \frac{1}{2}\|w\|^{2}+C \sum_{i=1}^{n} \xi_{i}+\sum_{i=1}^{n} \alpha_{i}\left[1-y_{i}\left(w^{T} x_{i}+b\right)-\xi_{i}\right]+\sum_{i=1}^{n}-\beta_{i} \xi_{i}=0
$$

The derivative is again trivial:

$$
\begin{gathered}
\sum_{i=1}^{n} \alpha_{i}\left[-y_{i}\right]=0 \\
\sum_{i=1}^{n} \alpha_{i} y_{i}=0
\end{gathered}
$$

Conclusions

- The $\alpha_{i}$ assigned to the positive class cancel with the $\alpha_{i}$ assigned to the negative class
- Not very insightful, but allows a simplification later

Rule 1 (for $\xi_{j}$ ) says that

$$
\text { 2) } \sum_{i=1}^{n} \alpha_{i} y_{i}=0
$$

$$
\nabla_{\xi_{i}} \frac{1}{2}\|w\|^{2}+C \sum_{i=1}^{n} \xi_{i}+\sum_{i=1}^{n} \alpha_{i}\left[1-y_{i}\left(w^{T} x_{i}+b\right)-\xi_{i}\right]+\sum_{i=1}^{n}-\beta_{i} \xi_{i}=0
$$

$$
\text { 3) } C=\alpha_{j}+\beta_{j}
$$

The derivative is again trivial:

$$
\begin{array}{ll}
C-\alpha_{j}-\beta_{j}=0 \\
\\
C=\alpha_{j}+\beta_{j}, & \text { for all } j
\end{array}
$$

Conclusions

- The cost of setting $\xi_{i}$ above the loss and the cost of setting $\xi_{i}$ below 0 add up to the total cost associated with $\xi_{i}$
- Again, not terribly informative, but useful on the next slide


## That's all the facts we need. Let's simplify the dual.

2) $\sum_{i=1}^{n} \alpha_{i} y_{i}=0$
3) $C=\alpha_{j}+\beta_{j}$

## Starting from the Lagrangian

1) $w=\sum_{i=1}^{n} \alpha_{i}\left[y_{i} x_{i}\right]$

$$
\frac{1}{2} w^{T} w+C \sum_{i=1}^{n} \xi_{i}+\sum_{i=1}^{n} \alpha_{i}\left[1-y_{i}\left(w^{T} x_{i}+b\right)-\xi_{i}\right]+\sum_{i=1}^{n}-\beta_{i} \xi_{i}
$$

Fact 3 ( $C-\alpha_{j}-\beta_{j}=0$ for all $j$ ) to kill C
Rearrange

$$
\frac{1}{2} w^{T} w+\sum_{i=1}^{n} C \xi_{i}+\sum_{i=1}^{n}-\beta_{i} \xi_{i}+\sum_{i=1}^{n}-\alpha_{i} \xi_{i} \sum_{i=1}^{n} \alpha_{i}\left[1-y_{i}\left(w^{T} x_{i}+b\right)\right]
$$

Apply the fact

$$
\frac{1}{2} w^{T} w+\sum_{i=1}^{n} \alpha_{i}\left[1-y_{i}\left(w^{T} x_{i}+b\right)\right]
$$

Copy over from slide above

1) $w=\sum_{i=1}^{n} \alpha_{i}\left[y_{i} x_{i}\right]$
2) $\sum_{i=1}^{n} \alpha_{i} y_{i}=0$

$$
\frac{1}{2} w^{T} w+\sum_{i=1}^{n} \alpha_{i}\left[1-y_{i}\left(w^{T} x_{i}+b\right)\right]
$$

Fact $2\left(\sum_{i=1}^{n} \alpha_{i} y_{i}=0\right)$ to kill $b$
Rearrange

$$
\frac{1}{2} w^{T} w+\sum_{i=1}^{n} \alpha_{i}\left[1-y_{i}\left(w^{T} x_{i}\right)\right]+\sum_{i=1}^{n} \alpha_{i} y_{i} b
$$

Apply the fact

$$
\frac{1}{2} w^{T} w+\sum_{i=1}^{n} \alpha_{i}\left[1-y_{i}\left(w^{T} x_{i}\right)\right]
$$

Copy over from slide above

$$
\frac{1}{2} w^{T} w+\sum_{i=1}^{n} \alpha_{i}\left[1-y_{i}\left(w^{T} x_{i}\right)\right]
$$

Fact 1 ( $w=\sum_{j=1}^{n} \alpha_{j}\left[y_{j} x_{j}\right]$ ) to kill w
Rearrange

$$
\frac{1}{2} w^{T} w-\sum_{i=1}^{n} \alpha_{i} y_{i}\left(w^{T} x_{i}\right)+\sum_{i=1}^{n} \alpha_{i}
$$

Apply the fact

$$
\frac{1}{2} \sum_{i=1}^{n} \alpha_{i}\left[y_{i} x_{i}^{T}\right] \sum_{j=1}^{n} \alpha_{j}\left[y_{j} x_{j}\right]-\sum_{i=1}^{n} \alpha_{i} y_{i}\left(\sum_{j=1}^{n} \alpha_{j}\left[y_{j} x_{j}^{T}\right] x_{i}\right)+\sum_{i=1}^{n} \alpha_{i}
$$

Copy

$$
\frac{1}{2} \sum_{i=1}^{n} \alpha_{i}\left[y_{i} x_{i}^{T}\right] \sum_{j=1}^{n} \alpha_{j}\left[y_{j} x_{j}\right]-\sum_{i=1}^{n} \alpha_{i} y_{i}\left(\sum_{j=1}^{n} \alpha_{j}\left[y_{j} x_{j}^{T}\right] x_{i}\right)+\sum_{i=1}^{n} \alpha_{i}
$$

Simplify

$$
\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{j} \alpha_{i} y_{j} y_{i} x_{i}^{T} x_{j}-\sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{j} \alpha_{i} y_{j} y_{i} x_{i}^{T} x_{j}+\sum_{i=1}^{n} \alpha_{i}
$$

Final form:

$$
\max _{\alpha} \sum_{i=1}^{n} \alpha_{i}-\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{j} \alpha_{i} y_{j} y_{i} x_{i}^{T} x_{j}
$$

Such that $0 \leq \alpha_{i} \leq C$ for all $i$ and $\sum_{i=1}^{n} \alpha_{i} y_{i}=0$

Part IV
WHAT IT MEANS


$$
\begin{gathered}
\max _{\alpha} \sum_{i=1}^{n} \alpha_{i}-\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{j} \alpha_{i} y_{j} y_{i} x_{i}^{T} x_{j} \\
\text { Such that } 0 \leq \alpha_{i} \leq C \text { for all } i \text { and } \sum_{i=1}^{n} \alpha_{i} y_{i}=0
\end{gathered}
$$

Interpretation time: what the heck are the $\alpha_{i}$ ?

1. Lagrangian view: the cost associated with each point; how much the objective would improve if we got to move that point
2. New view: the raw importance of each point

Explanation:

- The first goal is to maximize the alphas, but there's a second term punishing big alphas


## What Support Looks Like

$\sum_{j=1}^{n} \alpha_{j} y_{j} x_{j}^{T} x+\mathrm{b}:$ Signed distance Simplified Dual: $\max _{\alpha} \sum_{i=1}^{n} \alpha_{i}-\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{j} \alpha_{i} y_{j} y_{i} x_{i}^{T} x_{j}$

$$
\max _{\alpha} \sum_{i=1}^{n} \alpha_{i}-\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{j} \alpha_{i} y_{j} y_{i} x_{i}^{T} x_{j}
$$

Large $\alpha_{i}$ hurt us when they're associated with observations that are

1) From the same class
2) Pointing in the same direction

Large $\alpha_{i}$ help us when they're associated with observations that are

1) From different classes
2) Pointing in the same direction


Insight into inner products, graphically: 2 very very similar $x_{i}, x_{j}$ vectors that predict difft classes tend to maximize the margin width


Further, our predictions depend on the $\alpha_{i}$

$$
\text { Decision }=w^{T} x+b=\sum_{j=1}^{n} \alpha_{j} y_{j} x_{j}^{T} x+\mathrm{b}
$$

- We make our decision by
- Measuring the test point $x$ 's similarity to each training point $x_{j}$
- Weighting by the training point's overall importance ( $\alpha_{j}$ )
- Summing over all training points, comparing the + score against the - score (set by $y_{j}$ )
-     - SVMs are an intelligent form of nearest neighbors!!!
- We consider how similar our new point is to each training point
- In addition, each training point has a raw importance score
- (What does KNN think about SVMs?)

Example: classify $0=(1,0)$

$$
\sum_{j=1}^{n} \alpha_{j} y_{j} x_{j}^{T} x+\mathrm{b}
$$

Contributions:
$-(.03)(-1)(-2)=.06$
$-(.1)(-1)(-2)=.2$
$-(.1)(1)(1)=.1$
$-(.03)(1)(2)=.06$

- b =. 16


Total: . 58 -> classify as +

There's something weird about our calculation

- Our vector $(1,0)$ is as similar toz $(2,0)$ as it is to $(2,20)$
- Is there a more meaningful measure of similarity?



Part IV: Part II
KERNELS

Maximum margin view:

- Kernels map to a larger space where the classes can be separated by a plane
- Want to pick the plane with most margin

Neighbors view:

- Kernels define a measure of similarity between observations
- Classify based on test point's similarity to training points, and importance of training points


## Example kernel: RBF

## RBF kernel:

$$
r b f(x, y)=e^{-\left(\frac{\|x-y\|}{\gamma}\right)^{2}}
$$

- Based on actual distance between points
- Similarity decreases rapidly because of $e^{- \text {dist }}$
- $\quad \gamma$ determines a 'cliff' because of the ( $)^{2}$ - if $x$ and $y$ are within $\gamma$, fraction <1
- $\rightarrow$ they are more similar than you think
- It’s like a fishbowl lens



## RBF kernel has a geographic character to

it:
it uses literal Euclidean distance

Other kernels (similarity measures) exist for:Documents

- Geostatistics
- Points in graphs
- Images
- Randomly adding • Sound polynomial terms • Many more

http://crsouza.com/2010/03/17/kernel-functions-for-machine-learning-applications/

What makes a valid kernel?
a) Think of a set of features and compute the inner product post-transformation
b) Find a function so that no matter what points $x$ you feed in, the matrix you build is Positive Semi-Definite (all eigenvalues $\geq 0$ )
a) This is a Reproducing Kernel Hilbert Space
b) Don't ask.
...Or take ES 201 : )

## Practical kernel advice:

- Consider domain-specific kernels
- If more features than observations, you probably want linear
- If more observations than features, try RBF, but it may be slow

Other practical advice:

- SKlearn points out that its kernel implementation is too slow for >5-10K observations / features
- LinearSVC scales to millions, though no kernels allowed

REVIEW
P

In toto, here's what should stick:

- SVMs define bundles, not boundaries
- Convex optimization (here) is a better version of derivative = 0
- Lagrangian, Primal, Dual;
- Costs, Demons, Capitalism
- SVMs are BOTH
- Drawing maximum margin plane
- Measuring similarity to and importance of neighbors
- Kernels are how we define custom
 similarity


# Q: What does logistic regression think of LDA/QDA? 

A: What does KNN think of SVMs?

