Support Vector Machines

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CSCI 5622
2021 Fall

Course Logistics

- Project Pitch Feedback – Did you get your Projects to Review?
- Exam 1 – October ~~20th~~ 21st
- Problem Set 3 – Due ~~October 25th~~ Early Nov
  - It still has~~n't yet~~ been released, so the due date ~~will need to be~~ is adjusted
  - This ~~will~~ impacted the project milestone 3 deadline (which is *tiny*, but still don't want a 0 - 3 day gap)
  - This will probably only minorly impact "Problem Set 4"
    - It's going to be a very different kind of activity

Classification – Weeks 1 – 7*

- K Nearest Neighbors
  - Manhattan, Euclidian Distance
- Naïve Bayes
  - Class-Conditional, Prior, Evidence
- Trees & Ensemble Methods
  - Splitting, Pruning
  - Random Forests
  - AdaBoost
- Logistic Regression
  - Idea, Proof, Implementation
    - Gradient Descent
    - Stochastic & Mini-Batch Gradient Descent
- SVM
  - Idea, Proof, Implementation
    - Sequential Minimal Optimizer
    - Kernel Trick

Regression

- Linear Regression
  - Idea, Proof, Implementation
    - Minimizing MSE / LSS

Dimensionality Reduction

- Select-K-Best / Best Subset
- Stepwise selection
- Stagewise Selection

- Lasso & Ridge Regression
    - Idea, Proof, Implementation
        - Within Linear Regression

Skills

- Evaluation
  - Accuracy
  - Types of Errors & Confusion Matrix
  - ROC Curves
  - R^2
- Training
  - Train, Test, Validation (Hold-Out)
  - Cross-Fold Validation
- Multi-Class
  - One vs. All
  - All-Pairs (One vs. Another)
- Data Transformation
  - Encoding, Binning, Smoothing, Binarization / One-Hot Encoding, etc.
- Scaling & Normalization
  - Min-Max, Mean & Std. Dev

Concerns

- Impact of Errors
    - False Positive vs. False Negative
- Overfitting
    - High Variance
- Underfitting
    - High Bias
- Curse of Dimensionality

?

- When to use what classifiers?

Exam 1 – Logistics

- Delivered via Canvas
- Open on Oct. 2~~0~~1, Approximately all day
    - (Probably not 12:01AM to 11:59PM, but *well* beyond the class period, including morning through evening times)
- It will be *Timed* to only allow you 75 ~~50~~ minutes to complete
    - Those with 1.5X dispensation, etc. will be accommodated via Canvas.
- Exam *support* will be provided in-lecture and via Zoom *during lecture time*.
    - A slightly longer window of support (i.e. to accommodate extra time students) will be via Zoom, timing TBD.

Exam 1 – Format

- It is considered “open-resources”, but “individual”
  - Previous work, notes, Piazza discussions, textbook, etc. are all fair game
  - (Piazza will be in “read-only” mode for the day, so don’t be scared someone will post solutions there)
  - In general, follow the same plagiarism and honor code policies as any other assignment
- Conceptual Questions
  - Closed-ended (multiple choice, matching, word bank, etc.)
  - Open-ended short answer with clear guidance (name one reason we would choose X over Y)
- Problem Solving
  - Can be done with a 4-function calculator and some paper in a ~~50~~ 75-minute exam
  - No coding or code analysis

Continued Milestone 2 Videos

- 19
- 20
- 21
- 22
- 23
- 24
- 26
- 27
- 0
- 10

Best Decision Boundary

$\text{argmax}_{w,\,b}\ (1 / ||w||)$ such that $y_i(w^T x_i + b) >= 1$ for $i = \{1,2,...,m\}$

Optimize to find w, b

Best Decision Boundary

$\text{argmax}_{w,\,b}\ (1 / ||w||)$ such that $y_i(w^T x_i + b) >= 1$ for $i = \{1,2,...,m\}$

Optimize to find w, b

But it's not differentiable! (i.e. we can't find a gradient vector)

Best Decision Boundary

$\mathrm{argmax}_{w,\, b}\ (1\ /\ ||w||)$ such that $y_i(w^T x_i + b) >= 1$ for $i = \{1,2,...,m\}$

Not Differentiable

$\mathrm{argmin}_{w,\, b}\ (||w||)$ such that $y_i(w^T x_i + b) >= 1$ for $i = \{1,2,...,m\}$

Best Decision Boundary

$\text{argmax}_{w,\,b}\ (1\ /\ ||w||)$ such that $y_i(w^Tx_i + b) >= 1$ for $i = \{1,2,...,m\}$

Not Differentiable

$\text{argmin}_{w,\,b}\ (||w||)$ such that $y_i(w^Tx_i + b) >= 1$ for $i = \{1,2,...,m\}$

Not Differentiable

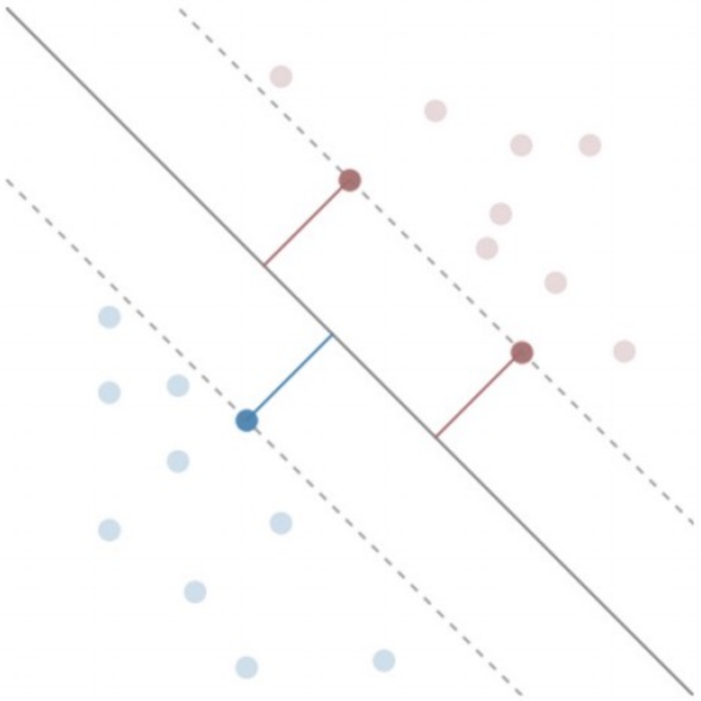
Best Decision Boundary

Support Vectors

$$w^T x + b = \pm 1$$

DB is unaffected by scale

$$(2w)^T x + 2b = 0$$



Best Decision Boundary

END

$\text{argmax}_{w,\,b}\ (1 / ||w||)$ such that $y_i(w^T x_i + b) >= 1$ for $i = \{1,2,\dots,m\}$

Not Differentiable

$\text{argmin}_{w,\,b}\ (||w||)$ such that $y_i(w^T x_i + b) >= 1$ for $i = \{1,2,\dots,m\}$

Not Differentiable

$\text{argmin}_{w,\,b}\ (||w||^2)$ such that $y_i(w^T x_i + b) >= 1$ for $i = \{1,2,\dots,m\}$

Convex + Differentiable

Requires a Convex quadratic program

Underlying Math – Finding our Maximum Margin

Generalizing – adding Lagrange Multipliers

$\min_w f(w)$ such that $g_i(w) <= 0$ for $i = \{1,2,\ldots,m\}$

Generalizing – adding Lagrange Multipliers

$\min_w f(w)$

such that $g_i(w) <= 0$ for $i = \{1,2,\ldots,m\}$

The Lagrangian of this function

$L(w, \alpha) = f(w) + \Sigma_{i=1\ldots m} (\alpha_i g_i(w))$

such that $\alpha_i >= 0$

Generalizing – adding Lagrange Multipliers

$\min_w f(w)$

such that $g_i(w) <= 0$ for $i = \{1,2,\ldots,m\}$

The Lagrangian of this function

$L(w, \alpha) = f(w) + \Sigma_{i=1\ldots m} (\alpha_i g_i(w))$

such that $\alpha_i >= 0$

$\mathrm{Max}_\alpha\, L(w, \alpha) = f(w)^*$

* Holds if f(w) is feasible, otherwise it goes to infinity

Generalizing – adding Lagrange Multipliers

$\min_w \max_\alpha \mathcal{L}(w, \alpha) = \min_w \max_\alpha f(w) + \Sigma_{i=1\ldots m} (\alpha_i g_i(w))$

such that $\alpha_i >= 0$

Problem is convex

Global minimum means

$\nabla_w \mathcal{L}(w, \alpha) = 0$ and $\nabla_\alpha \mathcal{L}(w, \alpha) = 0$

Generalizing – adding Lagrange Multipliers

$\min_w \max_\alpha L(w, \alpha) = \min_w \max_\alpha f(w) + \Sigma_{i=1...m} (\alpha_i g_i(w))$

such that $\alpha_i >= 0$

Problem is convex

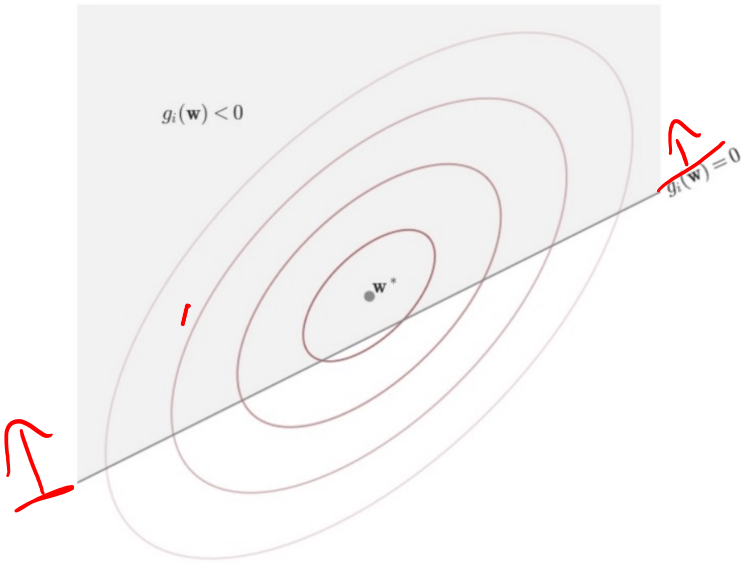
Global minimum means

$\nabla_w L(w, \alpha) = 0$ and $\nabla_\alpha L(w, \alpha) = 0$

$\min_w f(w)$

such that $g_i(w) <= 0$ for $i = \{1,2,...,m\}$

Visualizing f(x) and g(x)

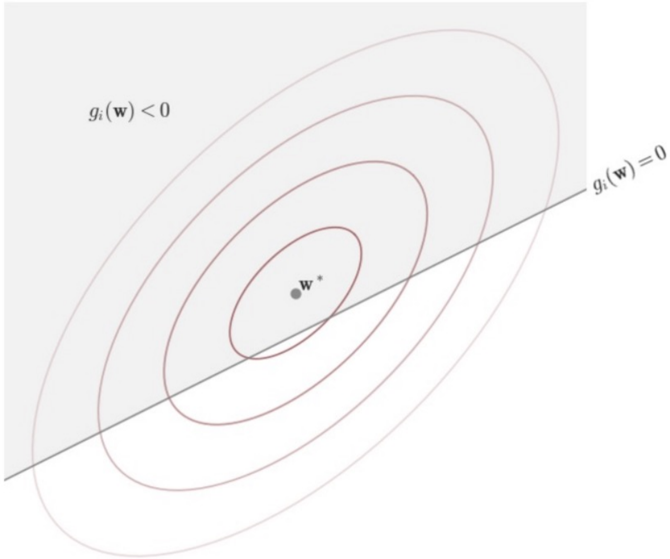


Visualizing f(x) and g(x)

f(x) is minimized within the $g_i(x)$ constraint, $g_i(x)$ is *inactive*

we can "ignore" our α, $\alpha_i = 0$

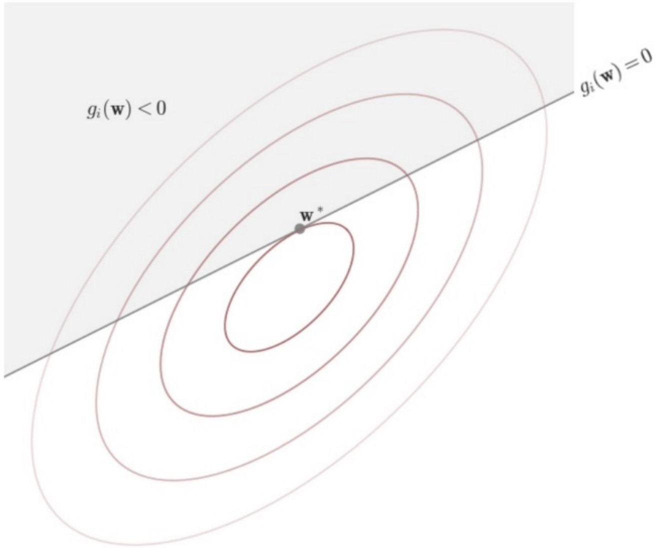
$\nabla_w f(w) = 0$



Visualizing f(x) and g(x)

$f(x)$ is not minimized within the $g_i(x)$ constraint, $g_i(x)$ is *active*

$\alpha_i > 0$



Complementary Slackness

$\alpha_i g_i(w^*) = 0$ for $I = \{1,2,\ldots,m\}$

if $\alpha_i = 0$ if we are not on the boundary of g_i

else $\alpha_i > 0$

The Dual Formulation

$\min_w \max_\alpha L(w, \alpha)$

such that $\alpha_i g_i(w) = 0$

and $\alpha_i >= 0$

$\max_\alpha \min_w L(w, \alpha) <= \min_w \max_\alpha L(w, \alpha)$

DUAL **PRIMAL**

Our New Formulation

$\text{argmin}_{w,\,b}\ (||w||^2)$ such that $y_i(w^T x_i + b) >= 1$ for $i = \{1,2,\ldots,m\}$

$\min_w \max_\alpha \mathcal{L}(w, \alpha) = \min_w \max_\alpha f(w) + \Sigma_{i=1\ldots m}\ (\alpha_i g_i(w))$ - PRIMAL

Becomes

$L_D = \max_\alpha \min_{w,b} (\overbrace{\tfrac{1}{2}||w||^2} + \overbrace{\Sigma_{i=1\ldots m}\ (\alpha_i\,(1 - y_i(w^T x_i + b)))})$

DUAL

Lagragian Form of Maximizing the Margin

$L_D = \max_\alpha \underbrace{\min_{w,b} \left(\tfrac{1}{2}||w||^2 + \Sigma_{i=1\ldots m} (\alpha_i (1 - y_i(w^T x_i + b)))\right)}$

We want the derivative of w & b to be 0

Now that $min_{w,b}$ is the inner optimization, we can do this!

$w = \Sigma_i \alpha_i y_i x_i$

$0 = \Sigma_i \alpha_i y_i$

Lagragian Form of Maximizing the Margin

$L_D = \max_\alpha \min_{w,b} (½||w||^2 + \Sigma_{i=1...m} (\alpha_i (1 - y_i(w^T x_i + b))))$

Apply complementary slackness & set derivative w, b to 0

Karush-Kuhn-Tucker Conditions

$\max_\alpha (L_D) = \max_\alpha (\Sigma_i \alpha_i - ½ \Sigma_{i,j} \alpha_i \alpha_j y_i y_j x_i \cdot x_j)$

$\alpha_i > 0 \text{ if } y_i(w^T x_i + b) = 1$

$\alpha_i = 0 \text{ if } y_i(w^T x_i + b) < 1$

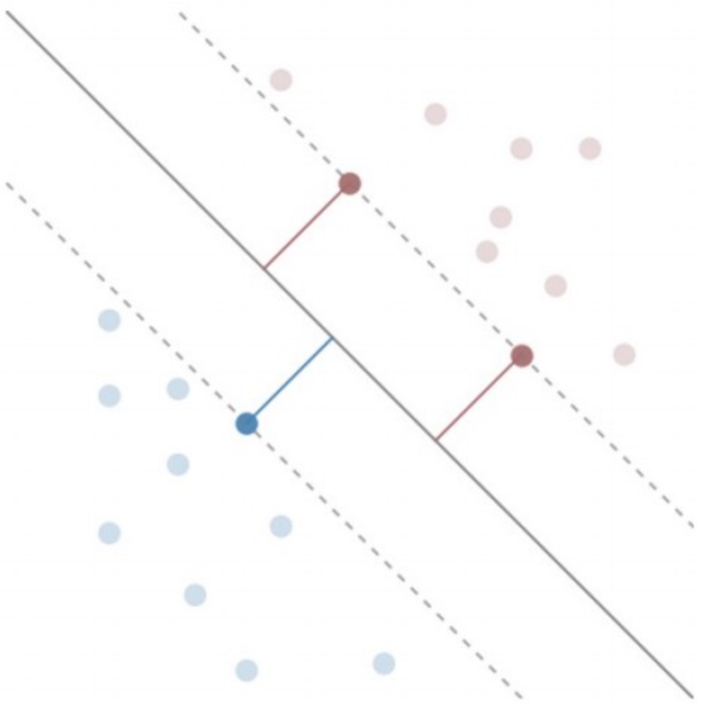
Maximizing our Margin

END

$$\max_\alpha \left(\Sigma_i \alpha_i - \tfrac{1}{2} \Sigma_{i,j} \alpha_i \alpha_j y_i y_j x_i \cdot x_j\right)$$

$$\alpha_i > 0 \text{ if } y_i(w^T x_i + b) = 1$$

$$\alpha_i = 0 \text{ if } y_i(w^T x_i + b) < 1$$



Thursday

Course Logistics

- ~~Project Pitch Feedback – Did you get your Projects to Review?~~
- Exam 1 – October 21st
  - Just released a "Practice Exam" that should show off the formatting, etc.
- Problem Set 3 – Due November 2

Participation: Exam 1 Review Poll

Best Decision Boundary

END

$\text{argmax}_{w,\,b}\ (1\ /\ ||w||)$ such that $y_i(w^Tx_i + b) >= 1$ for $i = \{1,2,...,m\}$

Not Differentiable

$\text{argmin}_{w,\,b}\ (||w||)$ such that $y_i(w^Tx_i + b) >= 1$ for $i = \{1,2,...,m\}$

Not Differentiable

$\text{argmin}_{w,\,b}\ (||w||^2)$ such that $y_i(w^Tx_i + b) >= 1$ for $i = \{1,2,...,m\}$

Convex + Differentiable

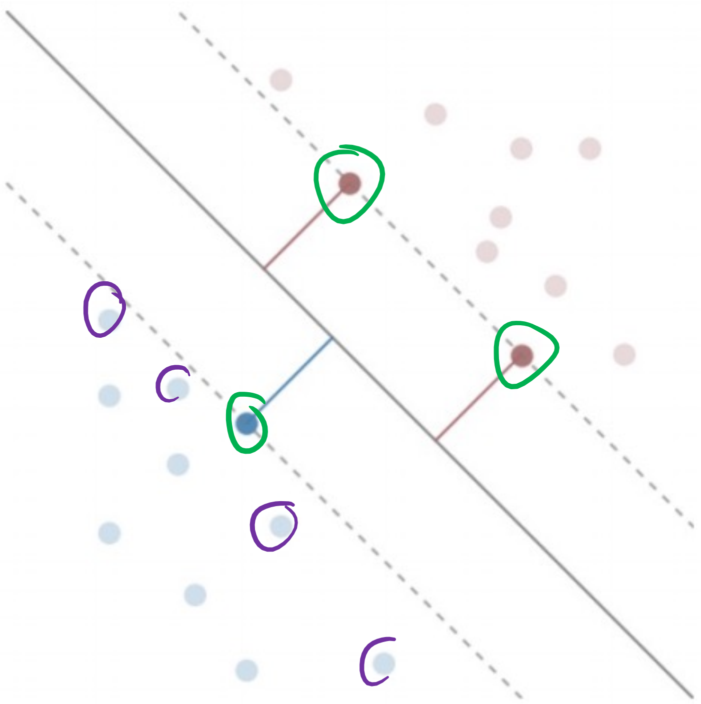
Requires a Convex quadratic program

END

Maximizing our Margin

$$\max_{\alpha}\left(\sum_i \alpha_i - \tfrac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j x_i \cdot x_j\right)$$

$$\begin{cases} \alpha_i > 0 \text{ if } y_i(w^T x_i + b) = 1 \\ \alpha_i = 0 \text{ if } y_i(w^T x_i + b) < 1 \end{cases}$$



Maximizing our Margin

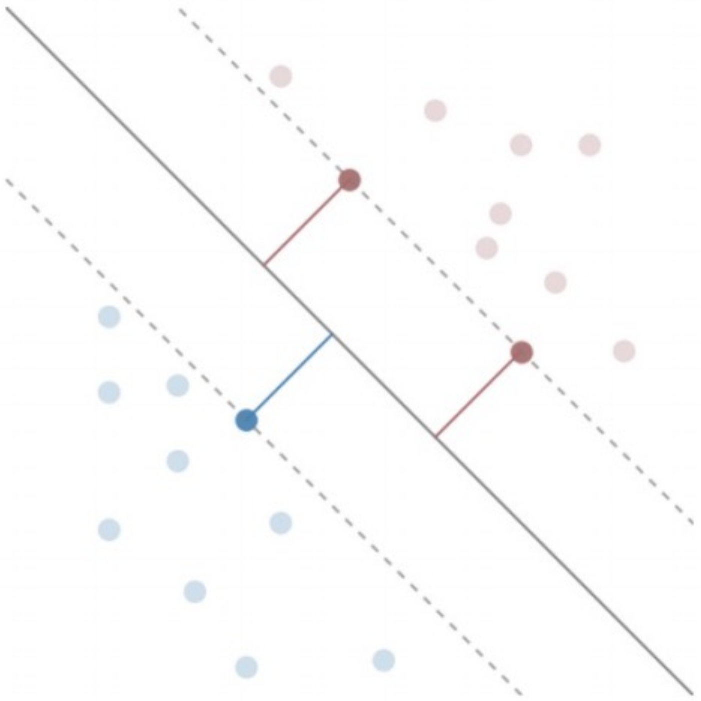
$$\max_\alpha \left(\Sigma_i \alpha_i - \tfrac{1}{2} \Sigma_{i,j} \alpha_i \alpha_j y_i y_j x_i \cdot x_j\right)$$

$$\alpha_i > 0 \text{ if } y_i(w^T x_i + b) = 1$$

$$\alpha_i = 0 \text{ if } y_i(w^T x_i + b) < 1$$

Most of these points (all the greyed out ones) Are 0!

- *They have no impact on what we are maximizing...*

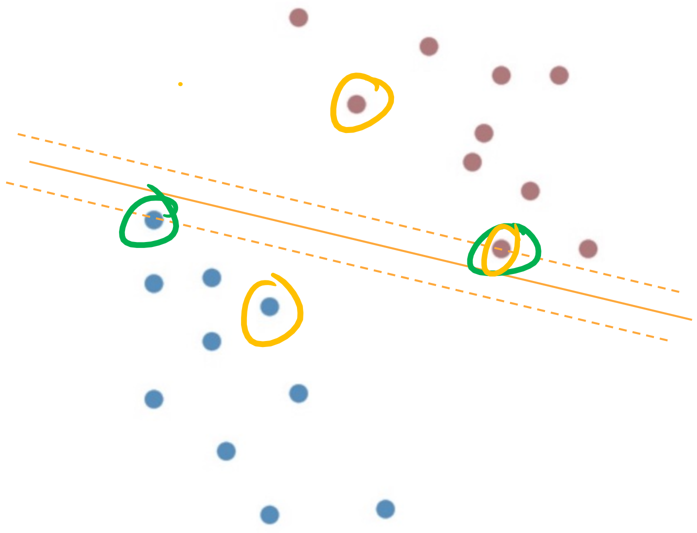


A Less Good Margin

$$\max_\alpha \left(\Sigma_i\, \alpha_i - \tfrac{1}{2}\, \Sigma_{i,j}\, \alpha_i\, \alpha_j\, y_i\, y_j\, x_i \cdot x_j\right)$$

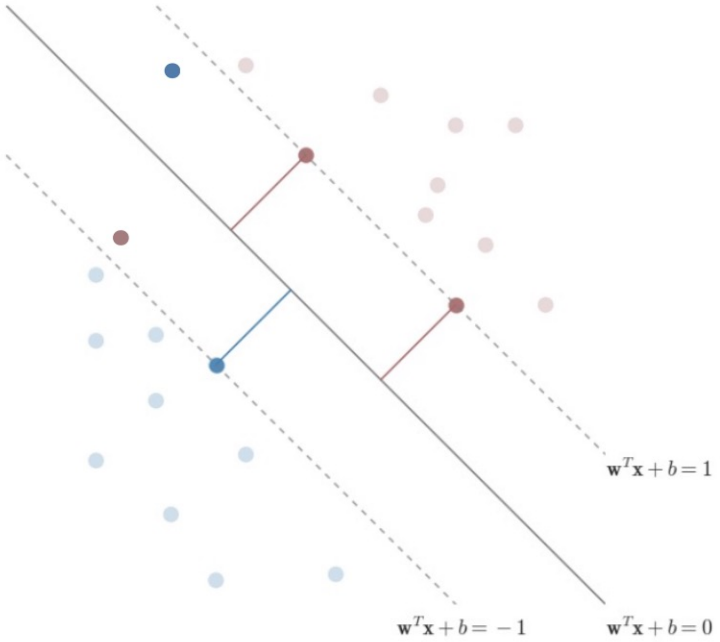
$$\alpha_i > 0 \text{ if } y_i(w^T x_i + b) = 1$$

$$\alpha_i = 0 \text{ if } y_i(w^T x_i + b) < 1$$



Shortcomings of Hard-Margin SVM

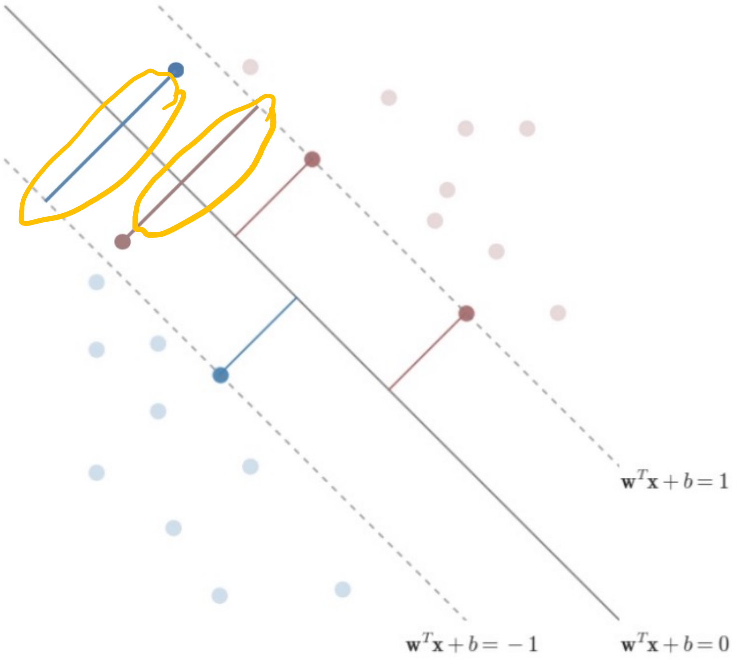
What if Linear Separability does not apply?



Interlude - Soft-Margin SVMs

Overcoming Linear Separability Problem

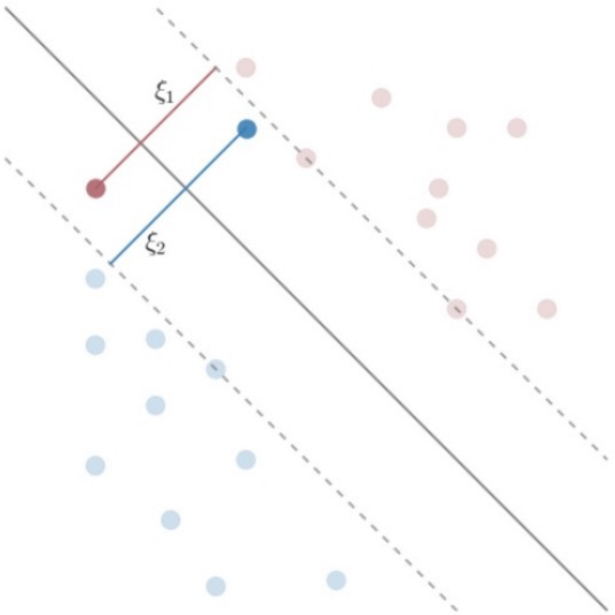
Add some wiggle room to our problem space



Adding a slack term ξ

Add a slack term ξ to every example

(for most examples the ξ is 0)



Adding a slack term ξ – Objective Function

$\text{argmin}_{w,\, b}\,(\tfrac{1}{2}\|w\|^2) \rightarrow \qquad \text{argmin}_{w,\, b}\,(\tfrac{1}{2}\|w\|^2) + C\,\Sigma_{i=1\rightarrow m}\,\xi_i^{\,p}$

C = Tuning Parameter

p = scaling of wrongness

p = 1 is often used

Adding a slack term ξ – Constraints

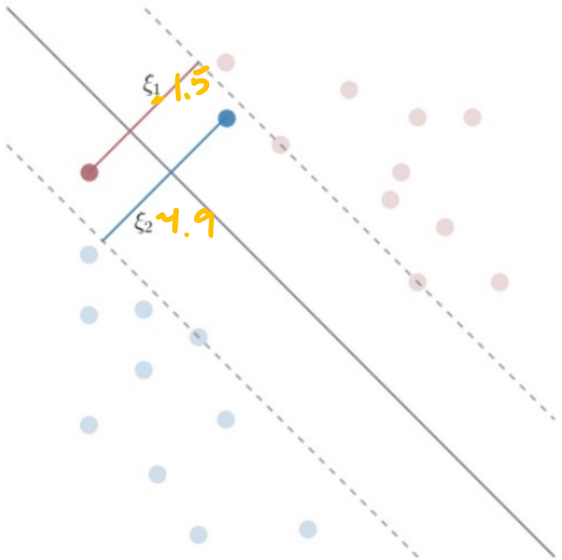
$y_i(w^T x_i + b) >= 1$ → $y_i(w^T x_i + b) >= 1 - \xi_i$

ξ_i relates to distance from the correct margin

ξ_i = 0 when we are on the correct side (or on the boundary) of our *margin*

ξ_i = ½ when we are halfway between margin and decision boundary

ξ_i = 2 when we are 1 margin on the wrong side of the decision boundary



Adding a slack term ξ – Lagrangian

$L(w,b,\alpha) = (½||w||^2 + \Sigma_{i=1...m} (\alpha_i (1 - y_i(w^T x_i + b))))$ →

$L(w,b,\alpha,\xi) = (½||w||^2 - \Sigma_{i=1...m} (\alpha_i (y_i(w^T x_i + b) - 1 + \xi_i))) - \Sigma_{i=1...m} \beta_i \xi_i$

Add ξ as a term to minimize...

Adding a slack term ξ – Lagrangian

$L(w,b,\alpha) = (\frac{1}{2}||w||^2 + \Sigma_{i=1\ldots m} (\alpha_i (1 - y_i(w^T x_i + b))))$ →

$L(w,b,\alpha,\xi)=(\frac{1}{2}||w||^2 - \Sigma_{i=1\ldots m} (\alpha_i (y_i(w^T x_i + b) - 1 + \xi_i))) - \Sigma_{i=1\ldots m} \beta_i \xi_i$

Add ξ as a term to minimize...

------------------------------------ *Magic Happens* --

$\max_\alpha (\Sigma_i \alpha_i - \frac{1}{2} \Sigma_{i,j} \alpha_i \alpha_j y_i y_j x_i \cdot x_j)$ – *unchanged*

New constraint: $0 <= \alpha <= C$

Adding a slack term ξ – Final Form

$\max_\alpha (L_D) = \max_\alpha \left(\Sigma_i \alpha_i - \frac{1}{2} \Sigma_{i,j} \alpha_i \alpha_j y_i y_j x_i \cdot x_j\right)$

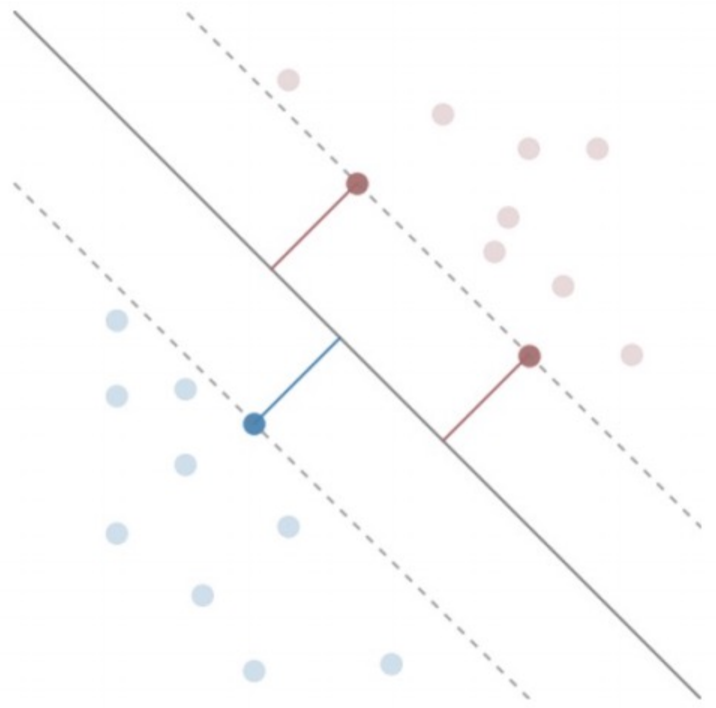
$\alpha_i = C$	if	$y_i(w^T x_i + b) < 1$
$C > \alpha_i > 0$	if	$y_i(w^T x_i + b) = 1$
$\alpha_i = 0$	if	$y_i(w^T x_i + b) > 1$

Maximizing our Margin

$$\max_\alpha \left(\Sigma_i\, \alpha_i - \tfrac{1}{2}\, \Sigma_{i,j}\, \alpha_i\, \alpha_j\, y_i\, y_j\, x_i \cdot x_j\right)$$

$$\alpha_i > 0 \text{ if } y_i(w^T x_i + b) = 1$$

$$\alpha_i = 0 \text{ if } y_i(w^T x_i + b) < 1$$



(Finally) Calculating our Maximum

Coordinate Ascent

$L(\alpha_{i=1\rightarrow m}) = (\Sigma_i \alpha_i - ½ \Sigma_{i,j} \alpha_i \alpha_j y_i y_j x_i \cdot x_j)$

Change α_i to make $L(\alpha)$ as big as possible

```
In [ ]: while not converged:
            for ii in [1,...,m]:
                alpha[ii] = argmax_ahat L(alpha[1], ..., ahat, ..., alpha[m])
```

Coordinate Ascent

$L(\alpha_{i=1\rightarrow m}) = (\Sigma_i \alpha_i - ½ \Sigma_{i,j} \alpha_i \alpha_j y_i y_j x_i \cdot x_j)$

Change α_i to make $L(\alpha)$ as big as possible

In [ ]:
```
while not converged:
    for ii in [1,...,m]:
        alpha[ii] = argmax_ahat L(alpha[1], ..., ahat, ..., alpha[m])
```

$0 = \Sigma_{i=1\rightarrow m} \alpha_i y_i$

We can't change α_i one at a time!

Sequential Minimal Optimizer

$L(\alpha_{i=1\rightarrow m}) = (\Sigma_i \alpha_i - ½ \Sigma_{i,j} \alpha_i \alpha_j y_i y_j x_i \cdot x_j)$

Change α_i, α_j to make $L(\alpha)$ as big as possible

In [ ]:
```
while not converged:
    for ii in [1,...,m]:
        select jj != ii at random (or via heuristic)
        update alpha[ii] and alpha[jj] to maximize L(alpha)
    if KKT conditions satisfied:
        exit
```

$0 = \Sigma_{i=1\rightarrow m} \alpha_i y_i$

Sequential Minimal Optimizer

Change α_i, α_j to make $L(\alpha)$ as big as possible

$0 = \Sigma_{i=1 \rightarrow m} \alpha_i y_i$

$0 = \alpha_1 y_1 + \alpha_2 y_2 + \Sigma_{k=3 \rightarrow m} \alpha_k y_k$

Sequential Minimal Optimizer

Change α_i, α_j to make $L(\alpha)$ as big as possible

$0 = \Sigma_{i=1 \rightarrow m} \alpha_i y_i$

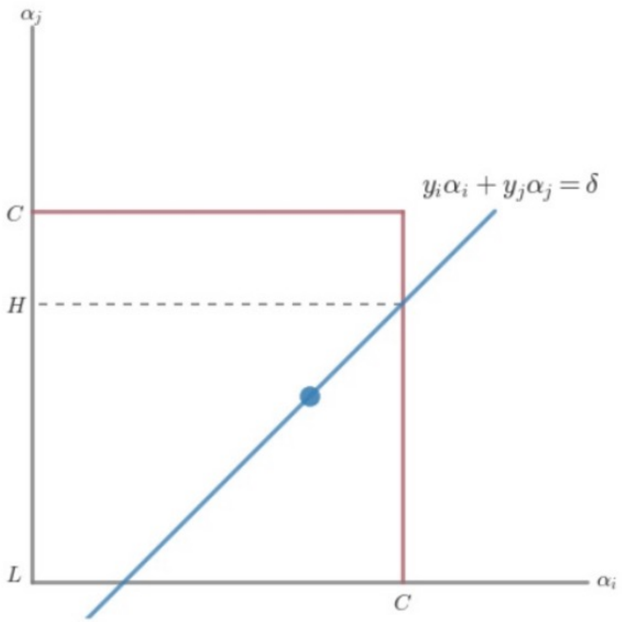
$0 = \alpha_1 y_1 + \alpha_2 y_2 + \Sigma_{k=3 \rightarrow m} \alpha_k y_k$

$\alpha_i y_i + \alpha_j y_j = - \Sigma_{k!=i,j} \alpha_k y_k = \delta$

Sequential Minimal Optimizer

$\alpha_i\, y_i + \alpha_j\, y_j = - \Sigma_{k!=i,j}\, \alpha_k\, y_k = \delta$

$0 <= \alpha_i <= C$



Sequential Minimal Optimizer

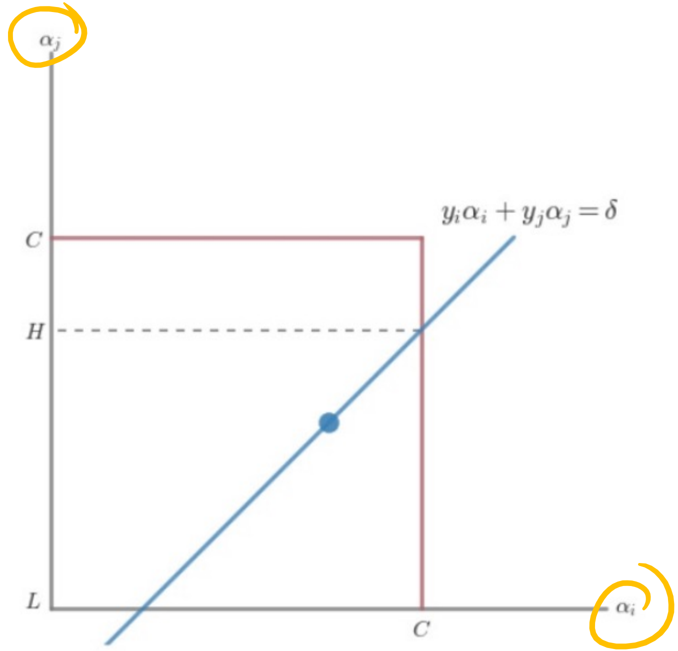
$\alpha_i y_i + \alpha_j y_j = - \Sigma_{k!=i,j} \alpha_k y_k = \delta$

$0 <= \alpha_i <= C$

$y_i = -1$

$y_j = +1$

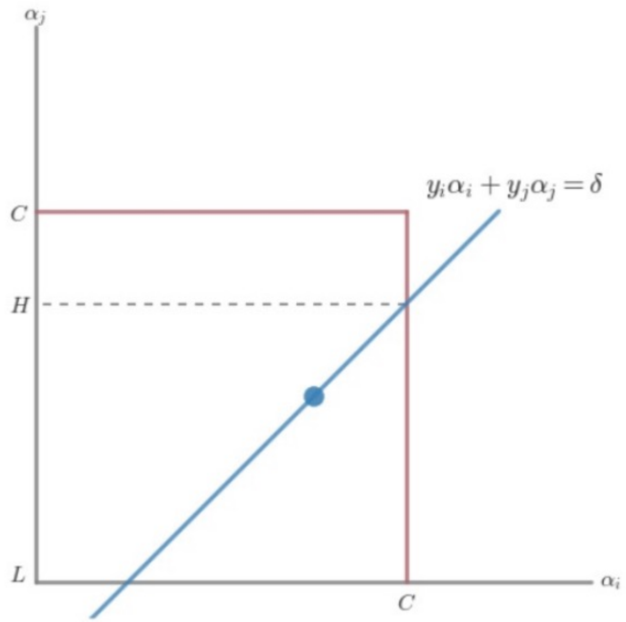
	$y_i != y_j$		$y_i = y_j$
$L = \max(0, \alpha_j - \alpha_i)$	or		$\max(0, \alpha_j + \alpha_i - C)$
$H = \min(C, C + \alpha_j - \alpha_i)$	or		$\min(C, \alpha_j + \alpha_i)$



Sequential Minimal Optimizer

$$\alpha_j = \begin{cases} H \text{ if } \alpha_j > H \\ \alpha_j \text{ if } L <= \alpha_j <= H \\ L \text{ if } \alpha_j < L \end{cases}$$

α_i such that $\alpha_i\, y_i + \alpha_j\, y_j = - \Sigma_{k!=i,j}\, \alpha_k\, y_k = \delta$



Sequential Minimal Optimizer

$$\alpha_j = \begin{cases} H \text{ if } \alpha_j > H \\ \alpha_j \text{ if } L <= \alpha_j <= H \\ L \text{ if } \alpha_j < L \end{cases}$$

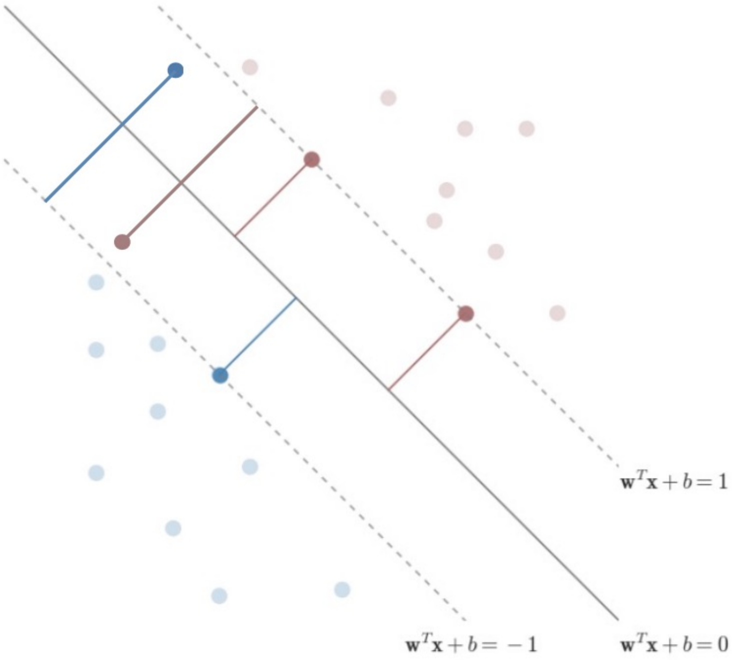
α_i such that $\alpha_i y_i + \alpha_j y_j = - \Sigma_{k!=i,j} \alpha_k y_k = \delta$

In [ ]:

```
while not converged:
    for ii in [1,...,m]:
        select jj != ii at random (or via heuristic)
        update alpha[ii] and alpha[jj] to maximize L(alpha)
    if KKT conditions satisfied:
        exit
```

Shortcomings of Soft-Margin SVM

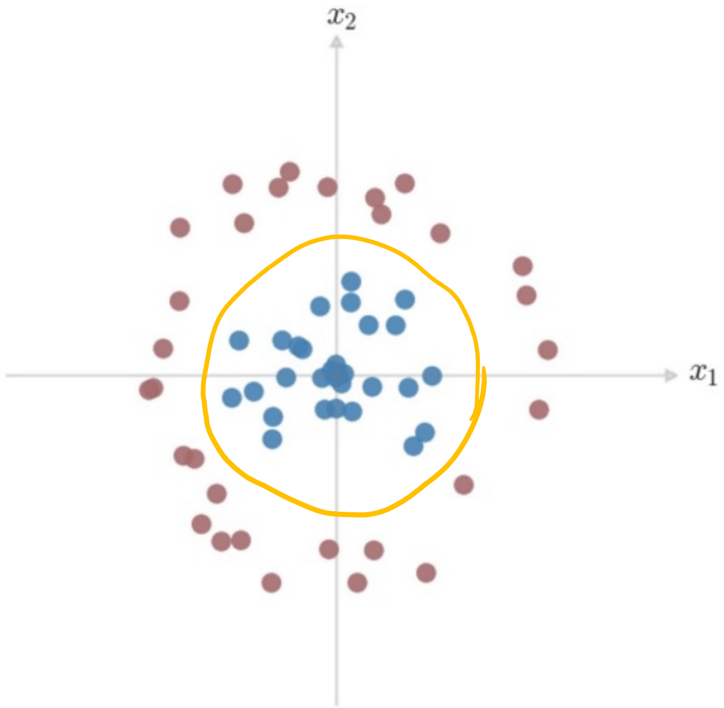
We added some wiggle room



Shortcomings of Soft-Margin SVM

We added some wiggle room

But what if it's not linearly separable?



Linear Inseparability – 1D Case

Linear Inseparability – 1D Case

Your arterial blood's pH should be between 7.35 and 7.45

Otherwise, you're unhealthy (for some reason), we should run further tests.

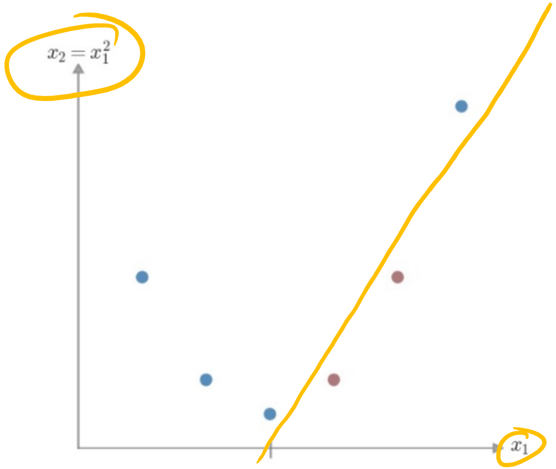
https://www.maximumfun.org/sawbones/sawbones-alkaline-water
https://opentextbc.ca/anatomyandphysiology/chapter/26-5-disorders-of-acid-base-balance/

Linear Inseparability – 1D Case

What can we do to capture this idea?

Linear Inseparability – 1D Case

Project our data into a higher dimensional space



Linear Inseparability – Dimension Projection

Start with our initial feature vector $x = [x_1]$

Create an augmented feature vector $\varphi(x) = [x_1, x_1^2]$

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Replace x with $\varphi(x)$ in our optimization problem!

Our Optimization Problem

$(\Sigma_i \alpha_i - ½ \Sigma_{i,j} \alpha_i \alpha_j y_i y_j x_i \cdot x_j)$

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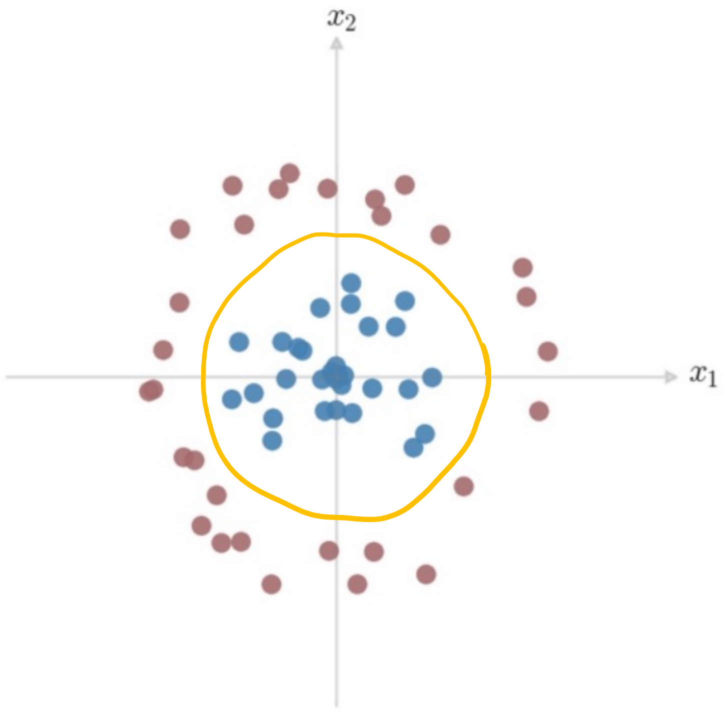
$(\Sigma_i \alpha_i - ½ \Sigma_{i,j} \alpha_i \alpha_j y_i y_j \varphi(x)_i \cdot \varphi(x)_j)$

Dimension Projection

How would we separate these classes?

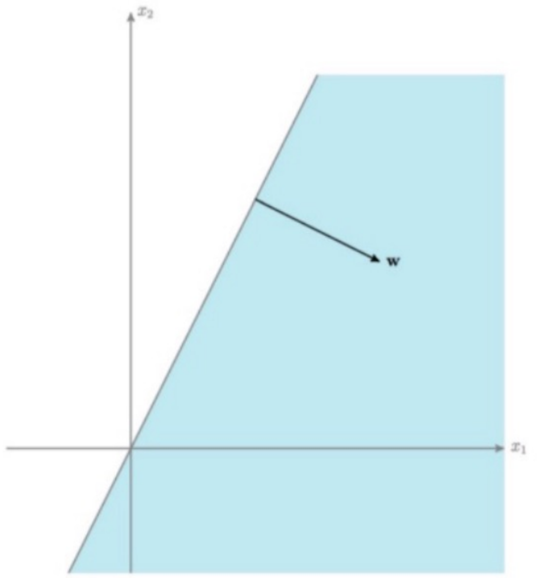
$x_1^2 + x_2^2$



Dimension Projection - Circle

How would we separate these classes?

We think in terms of sides of a boundary...

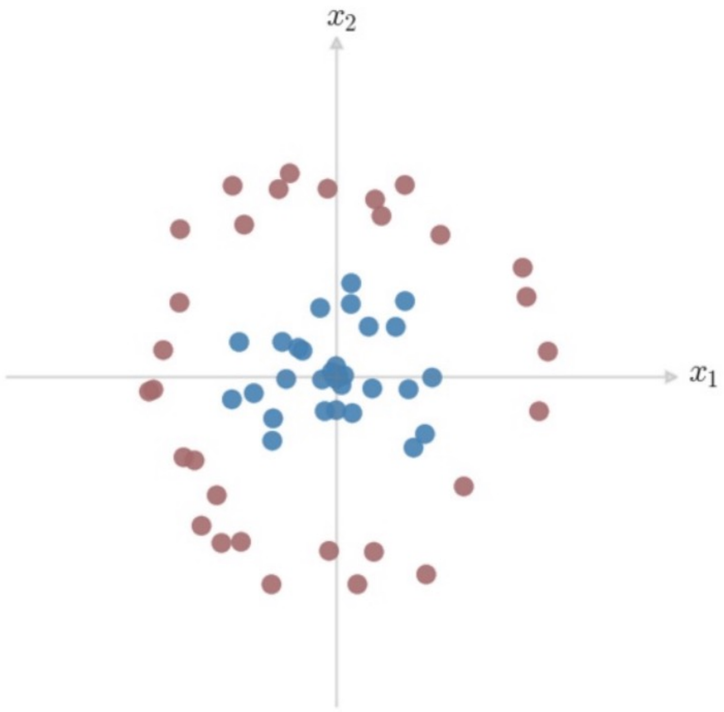


Dimension Projection

How would we separate these classes?

What kind of boundary can we give this space?

Can we express that boundary in terms of our given features?



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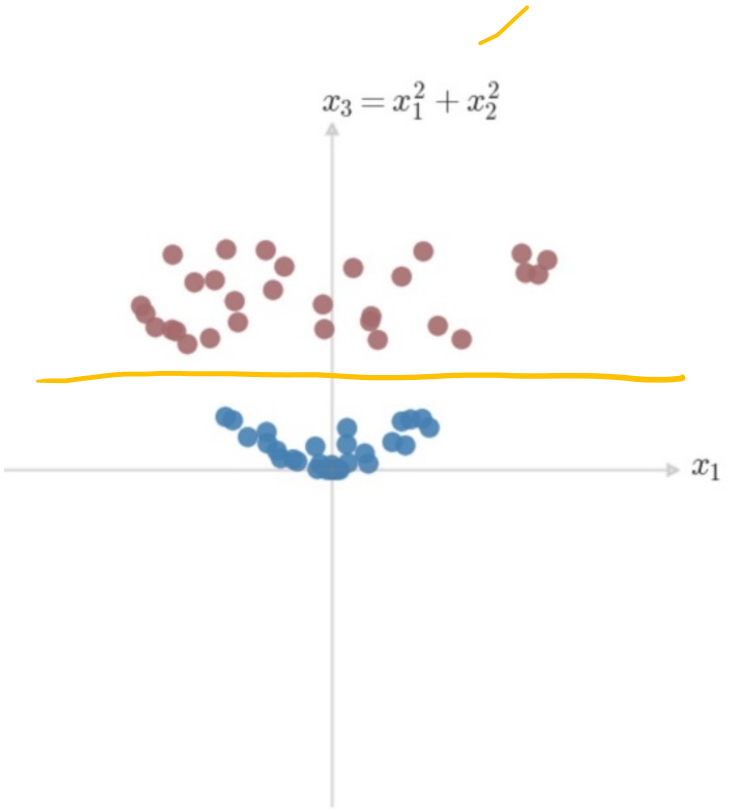
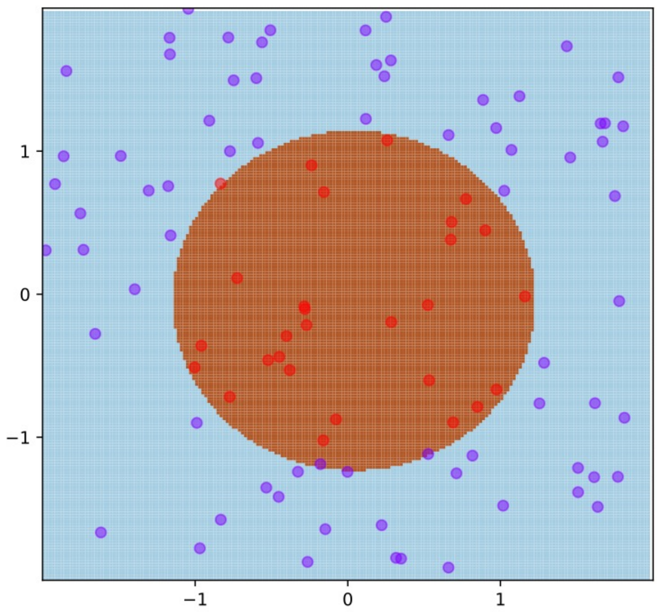
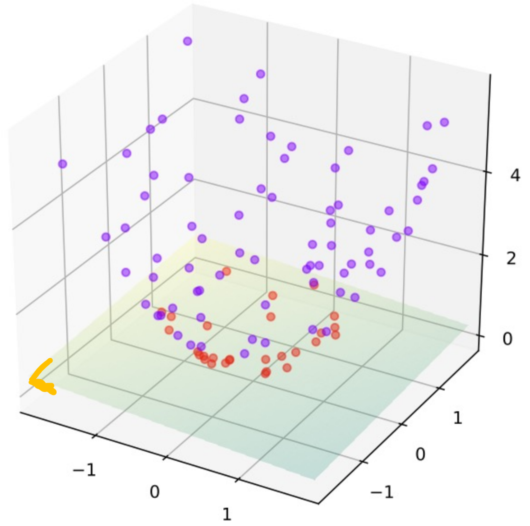


Dimension Projection - Circle





Linear Inseparability – Dimension Projection

Start with our initial feature vector $x = [x_1, x_2]$

Create an augmented feature vector $\varphi(x) = [x_1, x_2, x_1^2 + x_2^2]$

Replace x with $\varphi(x)$ in our optimization problem!

Decision Boundary is a plane in 3D Space

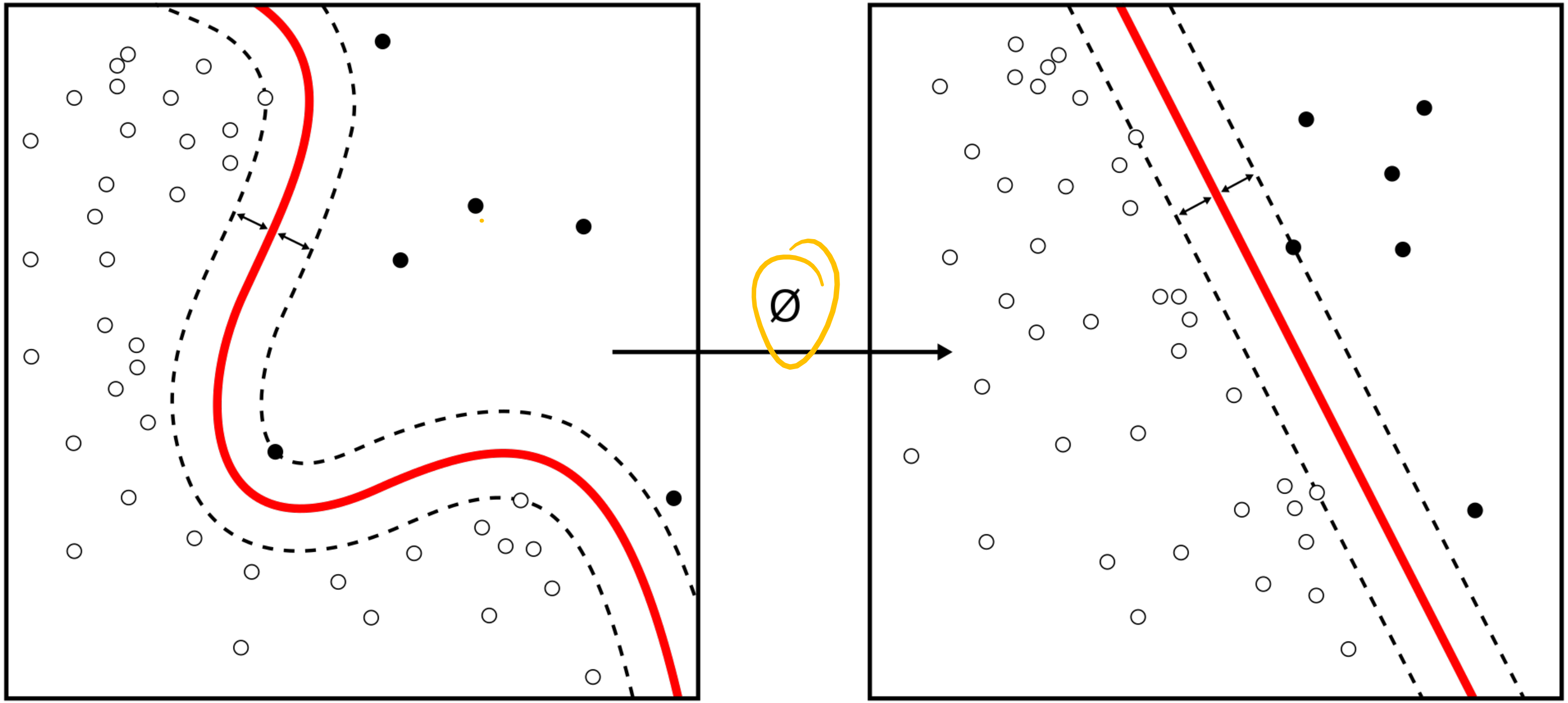
$$x_1^2 + x_2^2 = \textit{constant}$$

Our Optimization Problem

$$(\Sigma_i \alpha_i - ½ \Sigma_{i,j} \alpha_i \alpha_j y_i y_j x_i \cdot x_j)$$

$$(\Sigma_i \alpha_i - ½ \Sigma_{i,j} \alpha_i \alpha_j y_i y_j \varphi(x)_i \cdot \varphi(x)_j)$$

Generalizing our Optimization



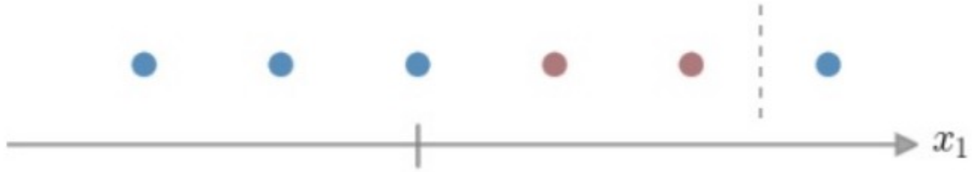
Our Optimization Problem – In Practice

For a 3-Dimensional Case…

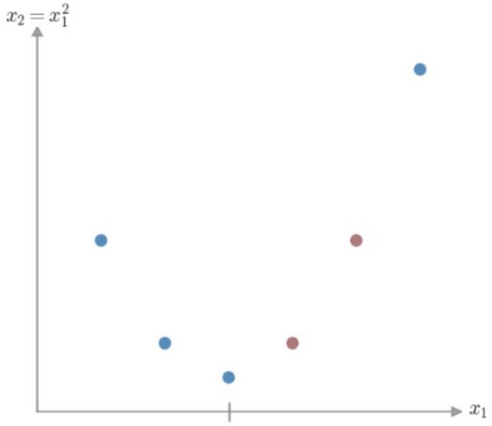
$X = [x_1, x_2, x_3]$

$\varphi(x) = (x_i^T x_j)^2$

Linear Inseparability – 1D Case



Project our data into a higher dimensional space



Our Optimization Problem – In Practice

For a 3-Dimensional Case...

$X = [x_1, x_2, x_3]$

$\varphi(x) = (x_i^T x_j)^2$

3^2

$\varphi[X] = [x_1\, x_1,\ x_1\, x_2,\ x_1\, x_3,\ x_2\, x_1,\ x_2\, x_2,\ x_2\, x_3,\ x_3\, x_1,\ x_3\, x_2,\ x_3\, x_3]$

Generalizing our Optimization – Curse of Dimensionality

Take a 64-feature vector

Transform it using $\varphi(x) = (x_i^T x_j)^4$

How many dimensions do I have?

64^2

Generalizing our Optimization – Curse of Dimensionality

Take a 64-feature vector

Transform it using $\varphi(x) = (x_i^T x_j)^2$

How many dimension do I have?

64^2 = 4096

Our Optimization Problem

$(\Sigma_i \alpha_i - \frac{1}{2} \Sigma_{i,j} \alpha_i \alpha_j y_i y_j \underbrace{x_i \cdot x_j})$

$(\Sigma_i \alpha_i - \frac{1}{2} \Sigma_{i,j} \alpha_i \alpha_j y_i y_j \underbrace{\varphi(x)_i \cdot \varphi(x)_j})$

Redefine $\varphi(x)_i \cdot \varphi(x)_j$ as $K(x, z)$ (x_i becomes x, x_j becomes z)*

*there are restrictions on this mapping – we'll get there!

Our Optimization Problem – In Practice

x, z are vectors of real numbers in N-Dimensional Space

$K(x, z) = (x^T z)^2$

Our Optimization Problem – In Practice

x, z are vectors of real numbers in N-Dimensional Space

$K(x, z) = (x^T z)^2$

$K(x, z) = (\Sigma_{i=1 \rightarrow n} (x_i z_i)) (\Sigma_{j=1 \rightarrow n} (x_j z_j))$

Our Optimization Problem – In Practice

x, z are vectors of real numbers in N-Dimensional Space

$K(x, z) = (x^T z)^2$

$K(x, z) = (\Sigma_{i=1 \rightarrow n} (x_i z_i)) (\Sigma_{j=1 \rightarrow n} (x_j z_j))$

$= \Sigma_{i=1 \rightarrow n} \Sigma_{j=1 \rightarrow n} (x_i z_i x_j z_j)$

$= \Sigma_{i,j=1 \rightarrow n} (x_i z_i x_j z_j)$

$(\Sigma_i \alpha_i - ½ \Sigma_{i,j} \alpha_i \alpha_j y_i y_j (x_i z_i x_j z_j))$

Kernels Save Time!

Computing $\varphi(x) = (x_i^T x_j)^2$ takes $O(n^2)$

Computing $K(x,z)$ takes $O(n)$

Boundaries of Valid Kernels

For any set of points (x_m), you can store $K(x_i,x_j)$ in an *m* by *m* matrix K

Boundaries of Valid Kernels – Symmetry

For any set of points (x_m), you can store $K(x_i,x_j)$ in an *m* by *m* matrix K

$K_{ij} = K(x^i) , x^j) = \varphi(x^i))^T \varphi(x^j) = \varphi(x^j)^T \varphi(x^i) = K(x^j , x^i) = K_{ji}$

K must be symmetric

Boundaries of Valid Kernels – Positive Semi-Definite

For any set of points (x_m), you can store $K(x_i, x_j)$ in an m by m matrix K

$z^T K z \geq 0$

Boundaries of Valid Kernels – Mercer's Theorem

Theorem (Mercer). Let $K : R^n \times R^n \longrightarrow \mathbb{R}$ be given. Then for K to be a valid (Mercer) kernel, it is necessary and sufficient that for any $\{x^1, \ldots, x^m\}$, $(m < \infty)$, the corresponding kernel matrix is symmetric positive semi-definite.

Kernels Intuition

Dot product $x \cdot y$ tells you about the similarity between x and y

If both vectors are positive along a dimension, dot product will grow
If one vector is 0 along a dimension, dot product does not grow
If vectors are opposite signs along a dimension, dot product will shrink

Kernels just add dimension combinations to dot product!

Popular Kernels

Linear Kernel: $K(x, z) = (x^T z)$

Popular Kernels

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Polynomial Kernel: $K(x, z) = (x^T z + c)^p$

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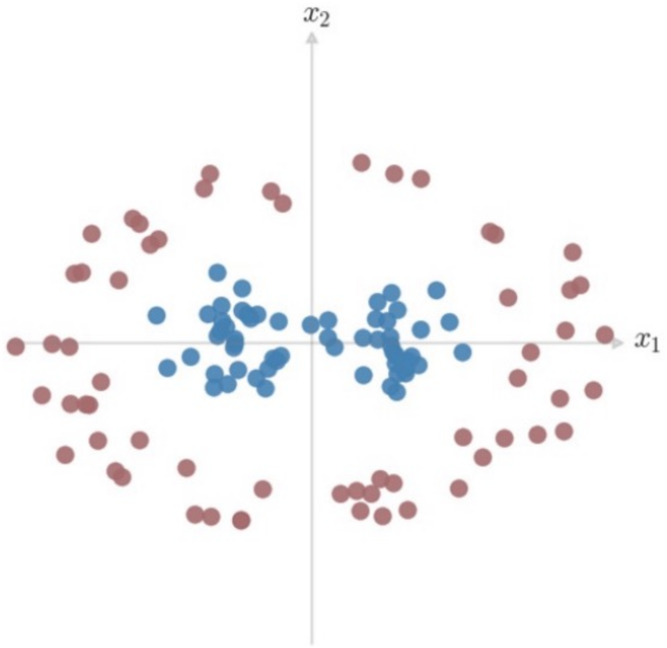
Radial Basis Function(RBF) Kernel: $K(x, z) = \exp(-\gamma ||x - z||^2)$

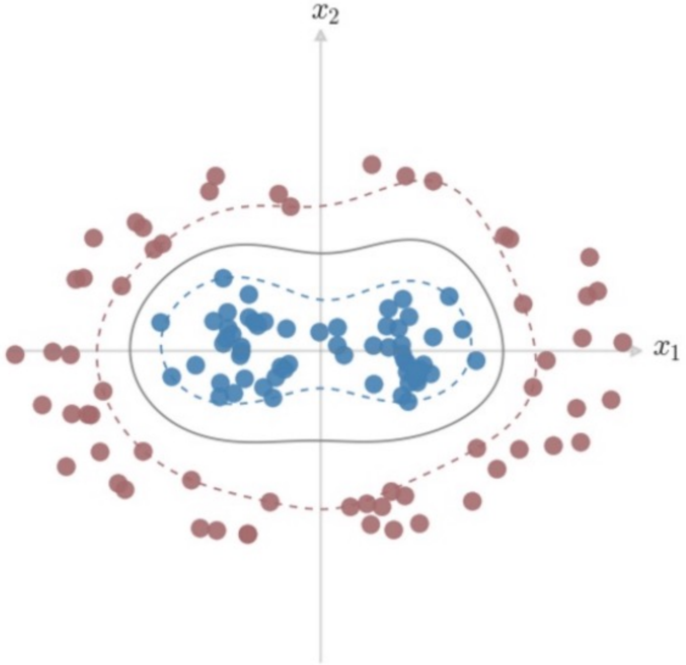
RBF Kernel for SVM



RBF Kernel for SVM

$\gamma = 3$

$C = 5$



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Gaussian RBF Kernel: $K(x, z) = \exp((-\ ||x - z||^2) / 2\sigma^2)$

SVM + Kernels

Pros

Works great “out-of-the-box”

Maintains convex objective function – guaranteed optimal solution

Solutions are *sparse* thanks to Kernels

Flexibly map to arbitrary decision boundary

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Pros

Works great “out-of-the-box”

Maintains convex objective function – guaranteed optimal solution

Solutions are *sparse* thanks to Kernels

Flexibly map to arbitrary decision boundary

Cons

Optimization can be slow

Choosing a Kernel is manual

Perceptrons

Linear Classification Task

$w^T x + b \rightarrow \pm 1$

If $w^T x + b > 0$, $y = 1$

If $w^T x + b < 0$, $y = -1$

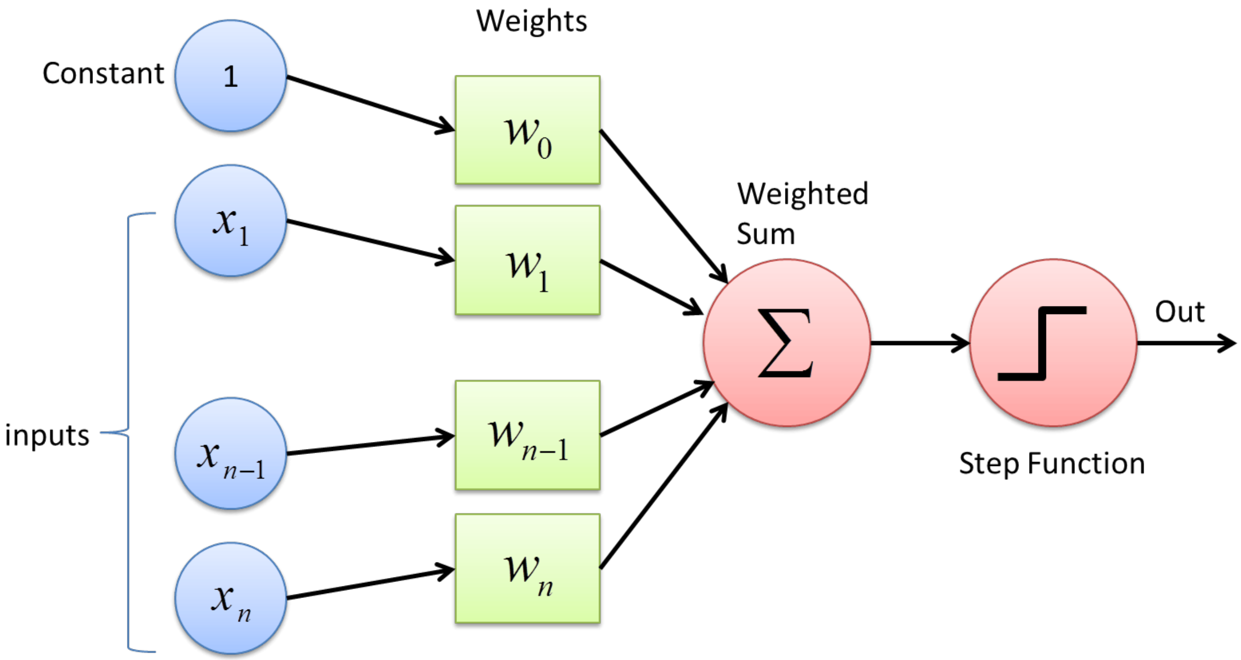
$w^T x + b = 0$ is an edge case

Visualizing Classification – The Perceptron

$w^T x + b \rightarrow \pm 1$

If $w^T x + b > 0, y = 1$

If $w^T x + b < 0, y = -1$



Training a Perceptron – "Online" Learning

Initialize w to an all-zero vector.

For some fixed number of iterations, or until some stopping criterion is met:

For each training example x_i with ground truth label $y_i \in \{-1, 1\}$:

Let $\hat{y} = \text{sign}(w^T x_i)$.

If $\hat{y} \neq y_i$, update $w \leftarrow w + y_i x_i$.

Kernel Perceptron

Perform our Kernel transformation of our data, then generate our perceptron!

Kernel Perceptron

Create the matrix of our Kernel representation of our data

Linear Kernel: $K(x, z) = (x^T z)$

Polynomial Kernel: $K(x, z) = (x^T z + c)^p$

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Training our Perceptron (Fit)

We no longer have “weights” to train on…

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We no longer have “weights” to train on...

But we can use our Dual Expression of the problem!

$$\Sigma_{i=1 \rightarrow n} \alpha_i y_i K(x_i, x_j)$$

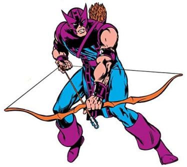
And use the same perceptron update as before, but increment our α by 1 each time.

If an example incremented α, then it’s a *support vector*

Interlude: Pros and Cons

When to use what classifiers

K-Nearest Neighbors



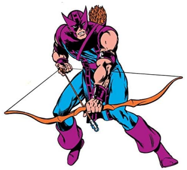
Pro

- Easy
- "train"?
- Non linear

Con

- Store whole data set for fitted model
- Not the best usually...

K-Nearest Neighbors



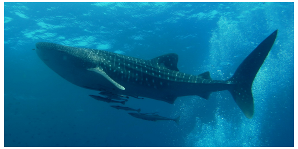
Pro

- Works with small N
- Works for non-binary cases
- Can be run without training

Con (Ex)

- Doesn't give much of a description of results beyond "similar to A, B, C..."
- Has trouble with features at differing scales

Naïve Bayes




Pro

Interpretable

Easy to Implement → Fast(ish)

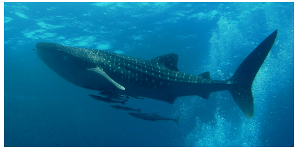
Probability or Score

Con

Assume Independence

Naïve Bayes

Pro

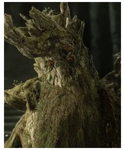


Con

- Works for non-binary cases
- Can be run without training

- Hard to implement for non-categorical data (without binning)

Decision Tree



Pro

Con (Ex)

Interpretable

Pruning

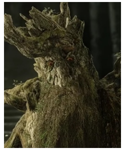
underfit

overfit

Nonlinear

Nonlinear

Decision Tree



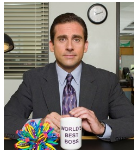
Pro

- Easy to implement
- Easy to follow
- Easy(ish) to interpret

Con (Ex)

- Prone to overfitting

Decision Forest / Adaboost



Pro

Deal w/ overfit/underfit

pretty effective

pseudo-feature selection

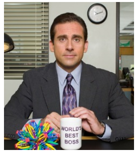
Con

Time to train

Depend on weak learner

Decision Forest / Adaboost

Pro



Con (Ex)

- Adaptive to difficult-to-classify cases

- Difficult to interpret

Logistic Regression

Pro

Con

Logistic Regression

Pro

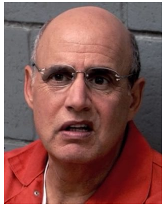
- Linear decision boundary

Con

- Binary only

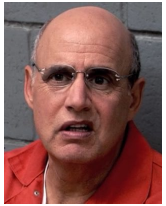
Support Vector Machines

Pro



Con

Support Vector Machines



Pro

- Linear decision boundary

Con (Ex)

- Binary only

slow

Next time...

Neural Networks!