Naïve Bayes, Support Vector Machines

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https://www.ischool.utexas.edu/~dannag/Courses/IntroToMachineLearning/CourseContent.html

Review

- Last week:
 - Multiclass classification applications and evaluating models
 - Motivation for new era: need non-linear models
 - Nearest neighbor classification
 - Decision tree classification
 - Parametric versus non-parametric models
- Assignments (Canvas)
 - Problem set 3 due yesterday
 - Problem set 4 due next week
 - Lab assignment 2 out and due in two weeks
- Questions?

Today's Topics

- Evaluating Machine Learning Models Using Cross-Validation
- Naïve Bayes
- Support Vector Machines
- Lab

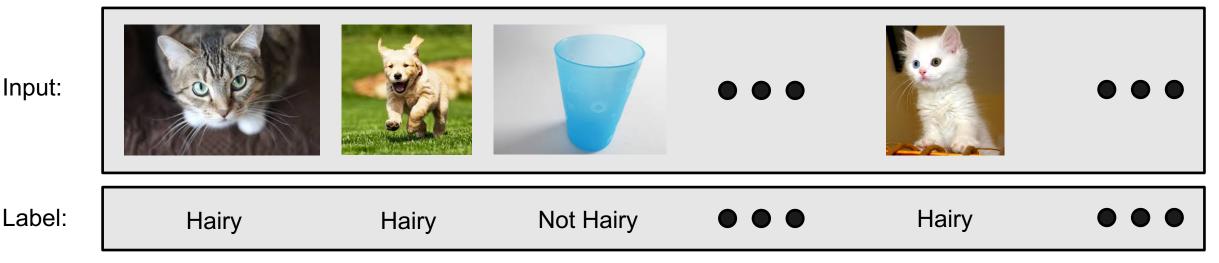
Today's Topics

• Evaluating Machine Learning Models Using Cross-Validation

• Naïve Bayes

- Support Vector Machines
- Lab

Goal: Design Models that Generalize Well to New, Previously Unseen Examples



Input:

Goal: Design Models that **Generalize** Well to New, Previously Unseen Examples



Classifier **predicts well** when test data **matches** training data. Lucky?

Goal: Design Models that **Generalize** Well to New, Previously Unseen Examples

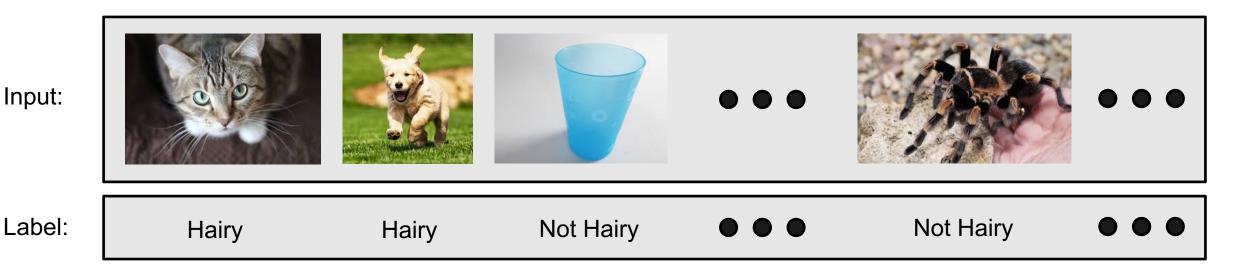


Classifier **predicts poorly** when test data **does not match** training data. Unlucky?

Goal: Design Models that **Generalize** Well to New, Previously Unseen Examples

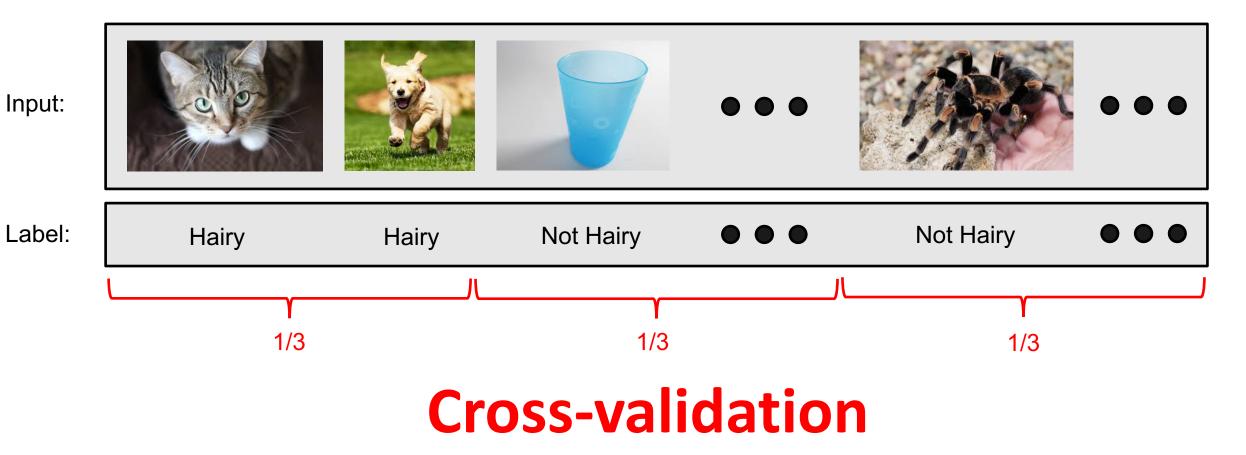


How to know if good/bad evaluation scores happen from good/bad luck?



Cross-validation: limit influence of chosen dataset split

e.g., 3-fold cross-validation



Fold 1:

Fold 2:

Fold 3:

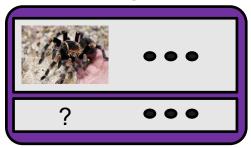
e.g., 3-fold cross-validation

Input: - train on k-1 partitions - test on k partitions Hairy Hairy Not Hairy Label: ? 000 **Testing Data** Input: - train on k-1 partitions - test on k partitions Hairy Hairy Hairy . . . Label: ? **Testing Data** Input: - train on k-1 partitions Label: Hairy ? ? Not Hairy - test on k partitions 000

Testing Data

e.g., 3-fold cross-validation

Testing Data

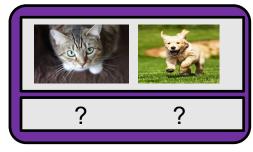


Classifier accuracy: prediction accuracy across all folds of test data

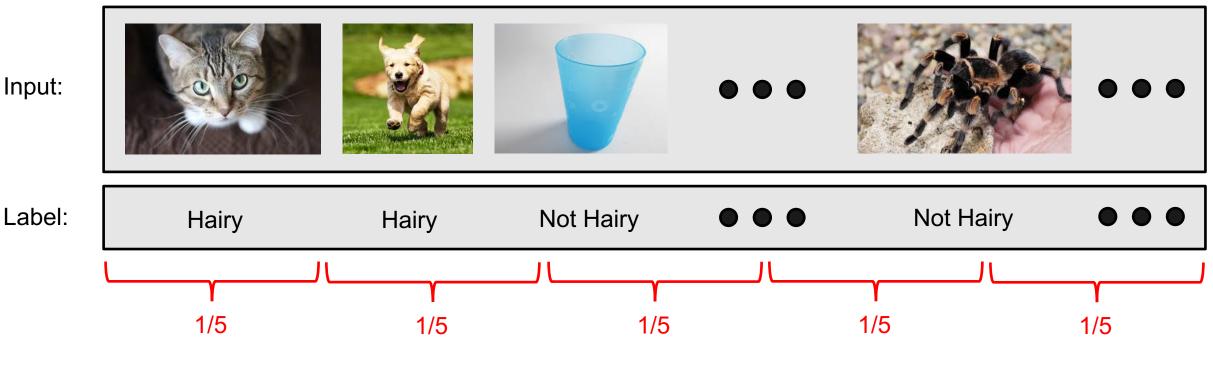
Testing Data



Testing Data

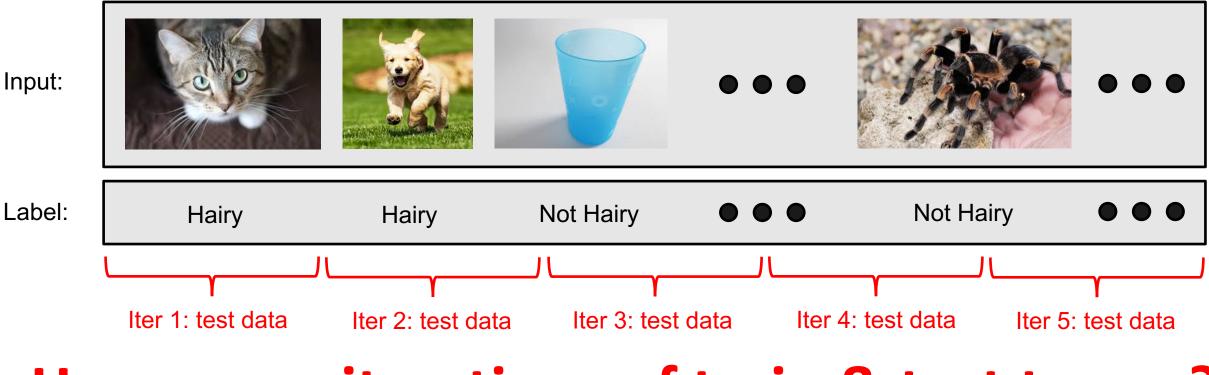


e.g., 5-fold cross-validation



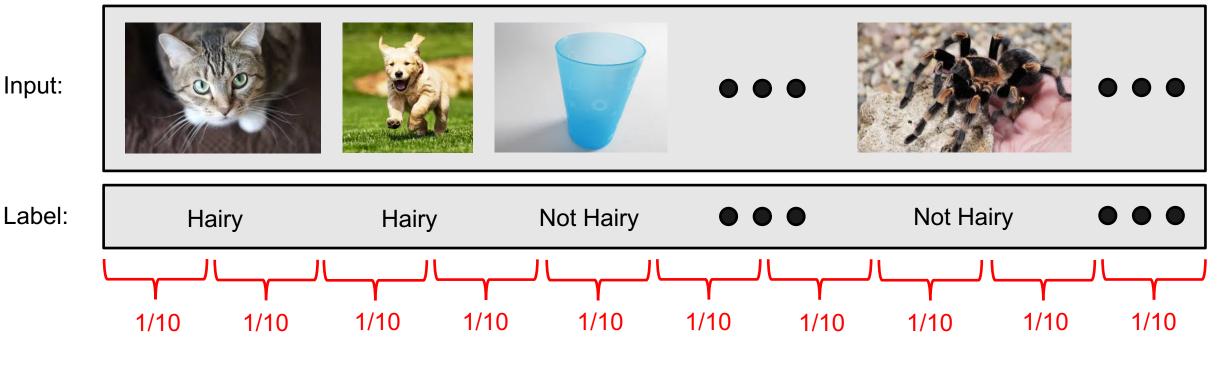
How many partitions of the data to create?

e.g., 5-fold cross-validation



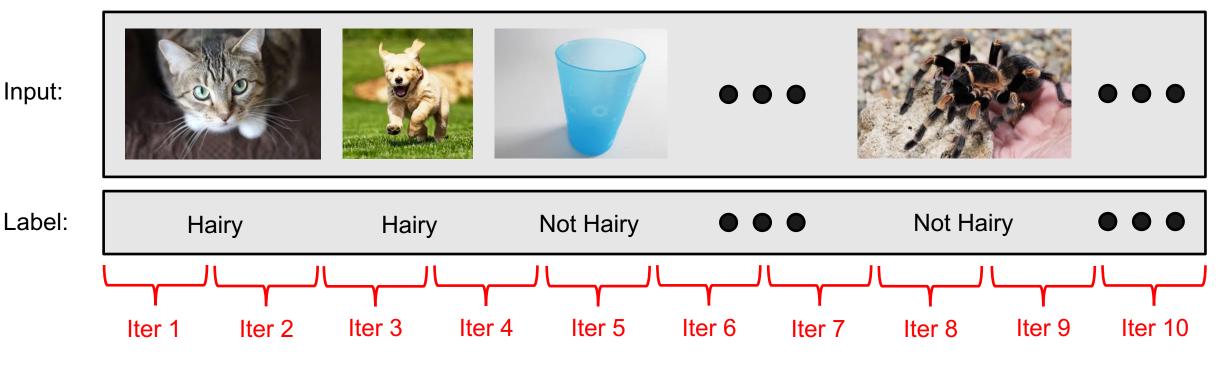
How many iterations of train & test to run?

e.g., 10-fold cross-validation



How many partitions of the data to create?

e.g., 10-fold cross-validation



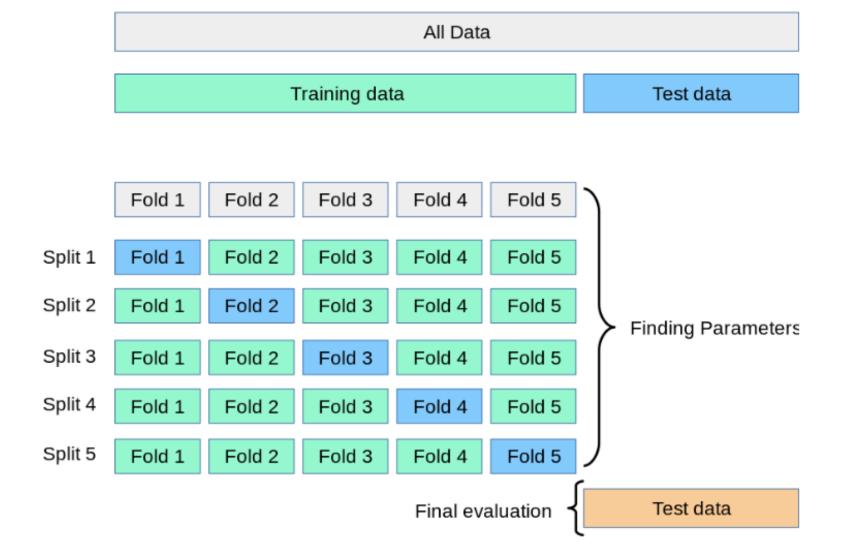
How many iterations of train & test to run?

e.g., k-fold cross-validation



What are the (dis)advantages of using larger values for "k"?

Summary: K-Fold Cross Validation



https://kevinzakka.github.io/2016/07/13/k-nearest-neighbor/

K-Fold Cross-Validation: How to Partition Data?

• e.g., 3-fold cross validation?

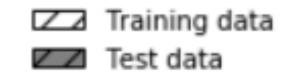
In [4]: iris.target Ο, Ο, 1, 1, 2, 2, 2. 2. 2. 2. 2. 2. 2. 2. 2. 2. 2. 2. 1)

Stratified k-fold Cross Validation

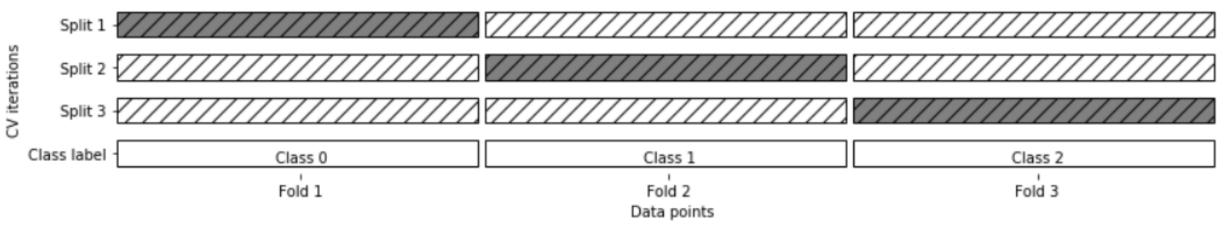
• e.g., 3-fold cross validation? Preserve class proportions in each fold to represent proportions in the whole dataset

In [4]: iris.target Ο, Ο, 1, 1, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2]

Stratified k-fold Cross Validation

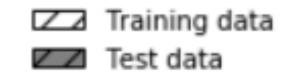


Standard cross-validation with sorted class labels

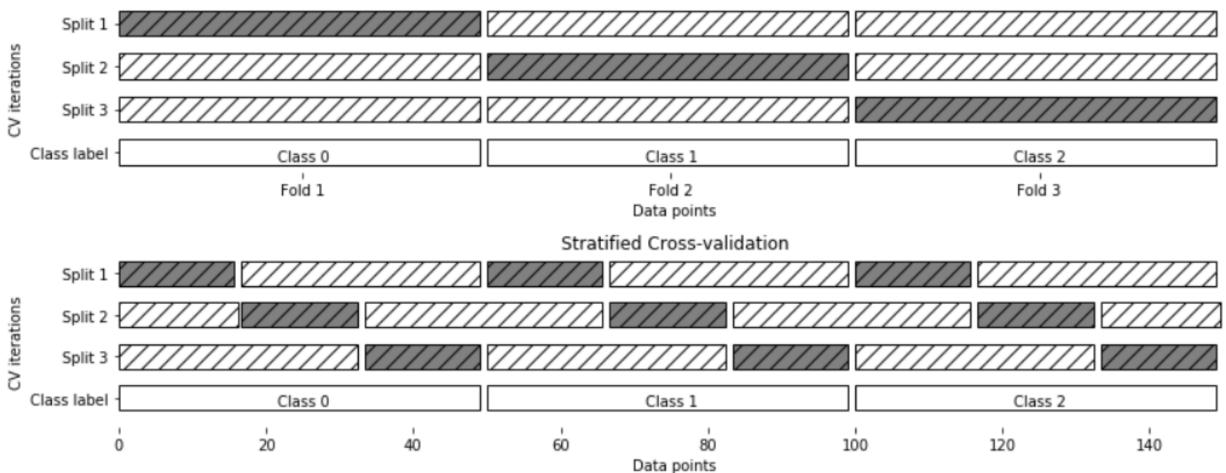


https://github.com/amueller/introduction_to_ml_with_python/blob/master/05-model-evaluation-and-improvement.ipynb

Stratified k-fold Cross Validation



Standard cross-validation with sorted class labels



https://github.com/amueller/introduction_to_ml_with_python/blob/master/05-model-evaluation-and-improvement.ipynb

Group Discussion: Cross Validation

- Why would you choose cross validation over percentage split?
- Why would you choose percentage split over cross validation?
- What does high variance of test accuracy between different folds tell you?
- Each student should submit a response in a Google Form (tracks attendance)
 - Question: Does cross validation build a model that you would apply to new data?

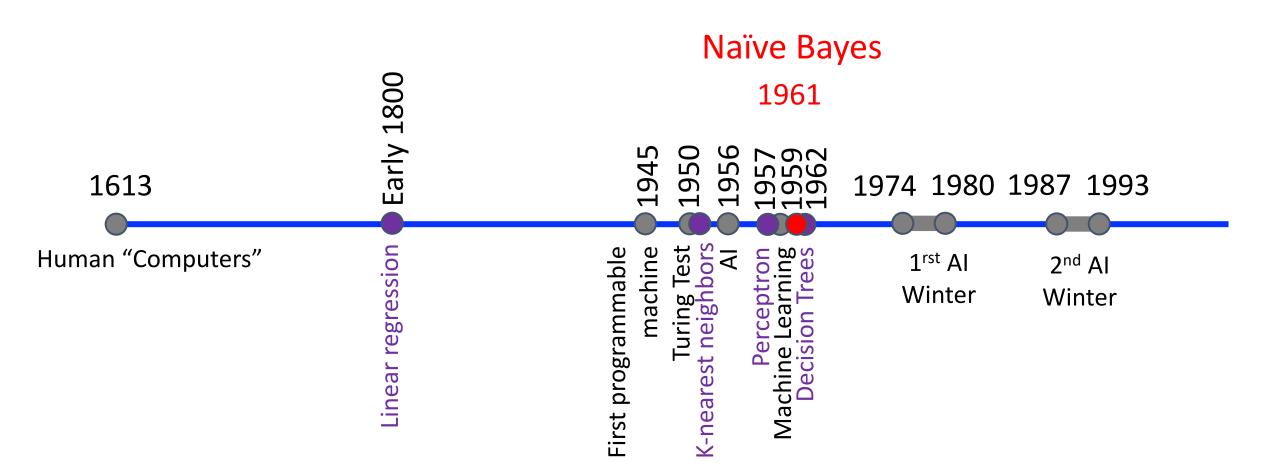
Today's Topics

• Evaluating Machine Learning Models Using Cross-Validation

• Naïve Bayes

- Support Vector Machines
- Lab

Historical Context of ML Models

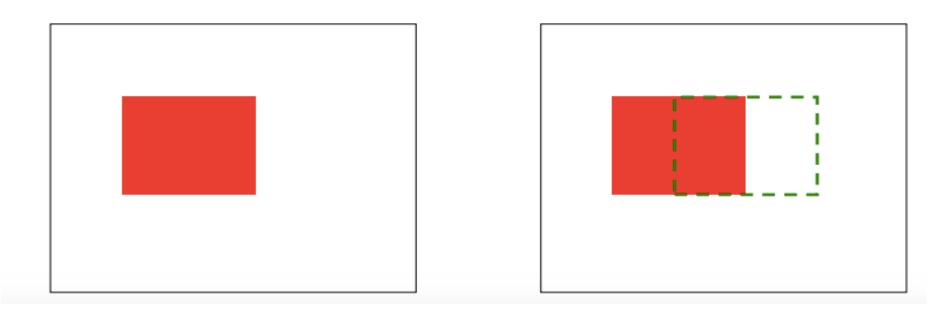


M. E. Maron. Automatic Indexing: An Experimental Inquiry. Journal of the ACM. 1961

Background: Conditional Probability

• P(A = 1 | B = 1): fraction of cases where A is true if B is true

P(A = 0.2) P(A|B = 0.5)



Background: Conditional Probability

- Knowledge of additional random variables can improve our prior belief of another random variable
- P(Slept in movie) = ?
 - 0.5
- P(Slept in movie | Like Movie) = ?
 1/4
- (Didn't sleep in movie | Like Movie) = ?
 - 3/4

Slept	Liked
1	0
0	1
1	1
1	0
0	0
1	0
0	1
0	1

Background: Joint Distribution

• P(A, B): probability a set of random variables will take a specific value

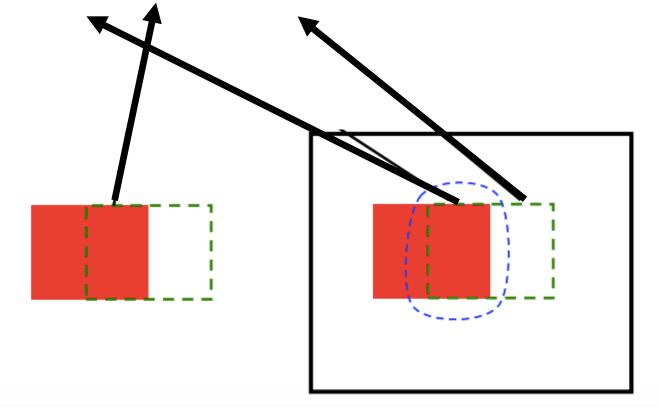
If we assume independence then

P(A,B)=P(A)P(B)

However, in many cases such an assumption maybe too strong (more later in the class)

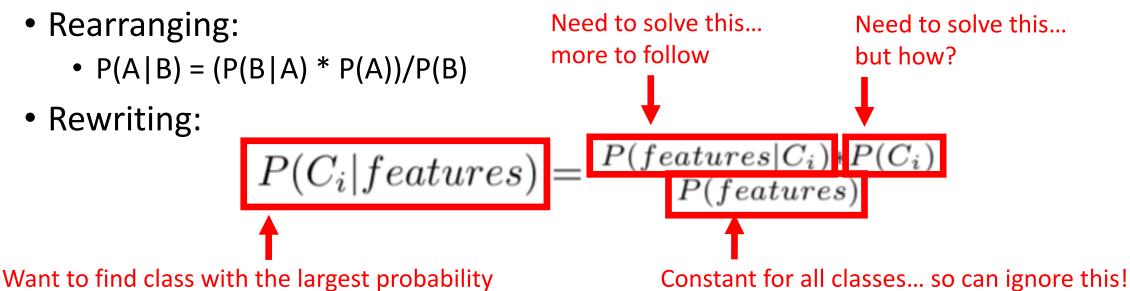
Background: Chain Rule

- Joint probability can be represented with conditional probability
- P(A, B) = P(A|B)*P(B)



Bayes' Theorem: Derivation of Formula

- Recall Chain Rule:
 - P(A, B) = P(A|B) * P(B)
 - P(A, B) = P(B|A) * P(A)
- Therefore:
 - P(A|B) * P(B) = P(B|A) * P(A)
- Rearranging:
 - P(A|B) = (P(B|A) * P(A))/P(B)
- Rewriting:



Naïve Bayes

• Learns a model of the joint probability of the input features and each class, and then picks the most probable class

Naïve Bayes: Naively Assumes Features Are Class Conditionally Independent

• Recall:

$$P(C_i | features) = P(features | C_i) * P(C_i)$$

If we assume independence then

P(A,B)=P(A)P(B)

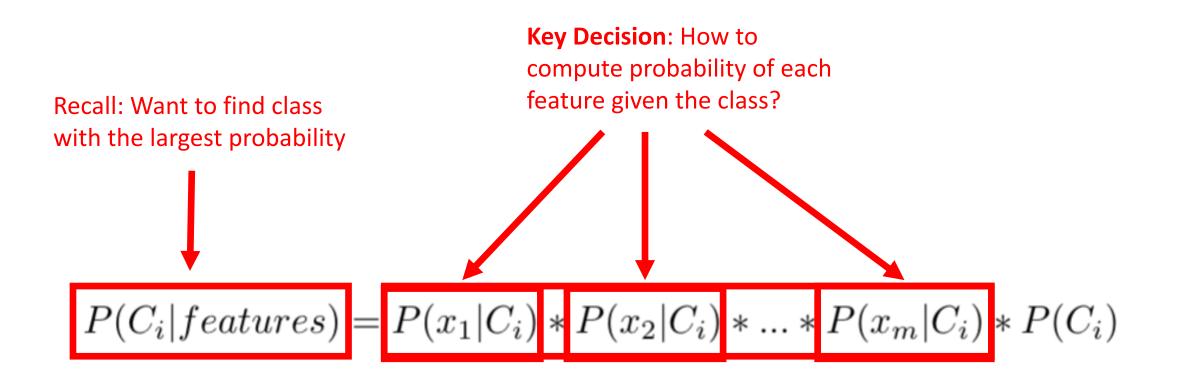
However, in many cases such an assumption maybe too strong (more later in the class)

 $P(features|C_i) = \prod_{j=1}^m P(x_j|C_i)$

 $P(features|C_i) = P(x_1|C_i) * P(x_2|C_i) * ... * P(x_m|C_i)$

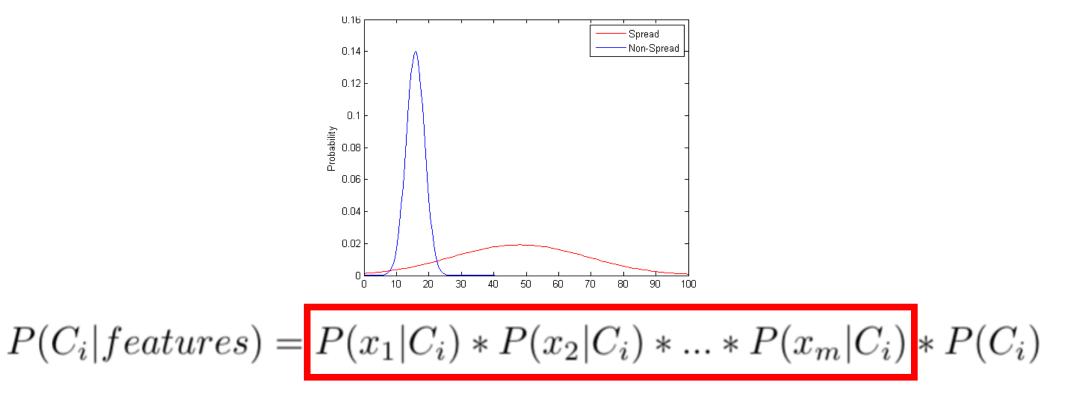
 $P(C_i | features) = P(x_1 | C_i) * P(x_2 | C_i) * \dots * P(x_m | C_i) * P(C_i)$

Naïve Bayes: Different Generative Models Can Yield the Observed Features



Naïve Bayes: Different Generative Models Can Yield the Observed Features

- Gaussian Naïve Bayes (typically used for "continuous"-valued features)
 - Assume data drawn from a Gaussian distribution: mean + standard deviation



Naïve Bayes: Different Generative Models Can Yield the Observed Features

- Multinomial Naïve Bayes (typically used for "discrete"-valued features)
 - Assume count data and computes fraction of entries belonging to the category

e.g.,	Movie	Type	Length	Liked?
	m1	Comedy	Short	Yes
	m2	Drama	Medium	Yes
	m3	Comedy	Medium	No
	m4	Drama	Long	No
	m5	Drama	Medium	Yes
	m6	Drama	Short	No
	m7	Comedy	Short	Yes
	m8	Drama	Medium	Yes

 $P(C_i | features) = P(x_1 | C_i) * P(x_2 | C_i) * \dots * P(x_m | C_i) * P(C_i)$

Gaussian Naïve Bayes: Example

 x_1

e.g.,	IMD	Ob Rating	Liked?
		7.2	Yes
		9.3	Yes
	'	5.1	No
		6.9	No
		8.3	Yes
		4.5	No
		8.0	Yes
		7.5	Yes

P(Liked) = ?
5/8 = 0.625

 $P(C_i | features) = P(x_1 | C_i) * P(C_i)$

Gaussian Naïve Bayes: Example

 x_1

e.g.,	IMDb Rating	Liked?
	7.2	Yes
	9.3	Yes
	5.1	No
	6.9	No
	8.3	Yes
	4.5	No
	8.0	Yes
	7.5	Yes

- P(Liked) = ?
 - 5/8 = 0.625
- P(Not Liked) = ?
 - 3/8 = 0.375

 $P(C_i | features) = P(x_1 | C_i) * P(C_i)$

Gaussian Naïve Bayes: Example

 x_1

e.g.,	IMI	Db Rating	Liked?
		7.2	Yes
		9.3	Yes
		5.1	No
		6.9	No
		8.3	Yes
		4.5	No
		8.0	Yes
		7.5	Yes

- P(Liked) = 5/8 = 0.625
- P(Not Liked) = 3/8 = 0.375
- P(IMDb Rating | Liked): Mean and Standard Deviation?
 - Mean = 8.06
 - Standard Deviation = 0.81

$$P(C_i | features) = P(x_1 | C_i) * P(C_i)$$

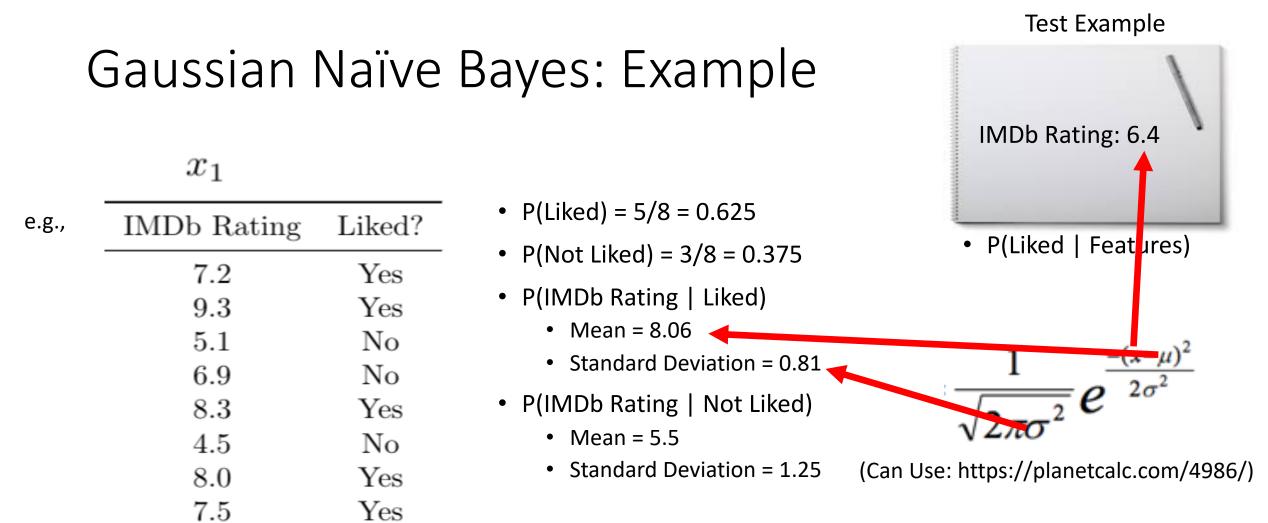
Gaussian Naïve Bayes: Example

 x_1

e.g.,	IMDb Rating	Liked?
	7.2	Yes
	9.3	Yes
	5.1	No
	6.9	No
	8.3	Yes
	4.5	No
	8.0	Yes
	7.5	Yes

- P(Liked) = 5/8 = 0.625
- P(Not Liked) = 3/8 = 0.375
- P(IMDb Rating | Liked)
 - Mean = 8.06
 - Standard Deviation = 0.81
- P(IMDb Rating | Not Liked): Mean and Standard Deviation?
 - Mean = 5.5
 - Standard Deviation = 1.25

$$P(C_i | features) = P(x_1 | C_i) * P(C_i)$$



$$P(C_i | features) = P(x_1 | C_i) * P(C_i)$$

Test Example

Gaussian Naïve Bayes: Example

x_1

e

.g.,	IMDb Rating	Liked?
	7.2	Yes
	9.3	Yes
	5.1	No
	6.9	No
	8.3	Yes
	4.5	No
	8.0	Yes
	7.5	Yes

- P(Liked) = 5/8 = 0.625
- P(Not Liked) = 3/8 = 0.375
- P(IMDb Rating | Liked)
 - Mean = 8.06
 - Standard Deviation = 0.81
- P(IMDb Rating | Not Liked)
 - Mean = 5.5
 - Standard Deviation = 1.25

 $P(C_i | features) = P(x_1 | C_i) * P(C_i)$



- P(Liked | Features)
 - = 0.06 * 0.625

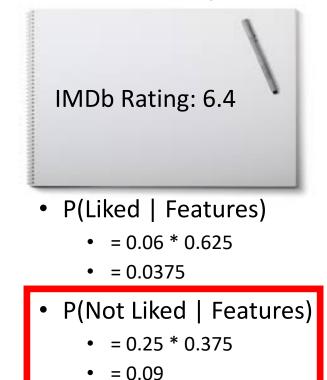
Test Example

Gaussian Naïve Bayes: Example

x_1

IMDb Rating	Liked?
7.2	Yes
9.3	Yes
5.1	No
6.9	No
8.3	Yes
4.5	No
8.0	Yes
7.5	Yes
	7.2 9.3 5.1 6.9 8.3 4.5 8.0

- P(Liked) = 5/8 = 0.625
- P(Not Liked) = 3/8 = 0.375
- P(IMDb Rating | Liked)
 - Mean = 8.06
 - Standard Deviation = 0.81
- P(IMDb Rating | Not Liked)
 - Mean = 5.5
 - Standard Deviation = 1.25



Which class is the most probable?

 $P(C_i | features) = P(x_1 | C_i) * P(C_i)$

Multinomial Naïve Bayes: Example

	x_1	x_2	
Movie	Type	Length	Liked?
m1	Comedy	Short	Yes
m2	Drama	Medium	Yes
m3	Comedy	Medium	No
m4	Drama	Long	No
m5	Drama	Medium	Yes
m6	Drama	Short	No
m7	Comedy	Short	Yes
m8	Drama	Medium	Yes

- P(Liked) = 5/8 = 0.625
- P(Not Liked) = 3/8 = 0.375
- P(Comedy | Liked) = ?
 2/5 = 0.4
- P(Comedy | Not Liked) = ?
 1/3 = 0.333
- P(Drama | Liked) = ?

• 3/5 = 0.6

- P(Drama | Not Liked) =
 - 2/3 = 0.666

 $P(C_i | features) = P(x_1 | C_i) * P(x_2 | C_i) * P(C_i)$

Multinomial Naïve Bayes: Example

	x_1	x_2	
Movie	Type	Length	Liked?
m1	Comedy	Short	Yes
m2	Drama	Medium	Yes
m3	Comedy	Medium	No
m4	Drama	Long	No
m5	Drama	Medium	Yes
m6	Drama	Short	No
m7	Comedy	Short	Yes
m8	Drama	Medium	Yes

• P(Short | Liked) = ?

• 2/5 = 0.4

- P(Short | Not Liked) = ?
 - 1/3 = 0.333
- P(Medium | Liked) = ?

• 3/5 = 0.6

- P(Medium | Not Liked) = ?
 1/3 = 0.333
- P(Long | Liked) = ?
 - 0/5 = 0
- P(Long | Not Liked) = ?
 - 1/3 = 0.333

 $P(C_i | features) = P(x_1 | C_i) * P(x_2 | C_i) * P(C_i)$

Test Example



Which class is the most probable?

- P(Short | Liked) = 0.4
- P(Short | Not Liked) = 0.33
- P(Medium | Liked) = 0.6
- P(Medium | Not Liked) = 0.33
- P(Long | Liked) = 0
- P(Long | Not Liked) = 0.33

 $P(C_i | features) = P(x_1 | C_i) * P(x_2 | C_i) * P(C_i)$

 $P(Liked | Features) = 0.4 \times 0.6 \times 0.63 = 0.15$

 $P(Not Liked | Features) = 0.33 \times 0.33 \times 0.38 = 0.04$

Multinomial Naïve Bayes: Example

• P(Liked) = 0.63

• P(Not Liked) = 0.38

• P(Comedy | Liked) = 0.4

• P(Drama | Liked) = 0.6

• P(Comedy | Not Liked) = 0.33

P(Drama | Not Liked) = 0.67

	x_1	x_2	_
Movie	Type	Length	Liked?
m1	Comedy	Short	Yes
m2	Drama	Medium	Yes
m3	Comedy	Medium	No
m4	Drama	Long	No
m5	Drama	Medium	Yes
m6	Drama	Short	No
m7	Comedy	Short	Yes
m8	Drama	Medium	Yes

Test Example



Which class is the most probable?

- P(Short | Liked) = 0.4
- P(Short | Not Liked) = 0.33
- P(Medium | Liked) = 0.6
- P(Medium | Not Liked) = 0.33
 - P(Long | Liked) = 0

 $\frac{m8}{P(Long | Not Liked)} = 0.33$ To avoid zero, assume training data is so large that adding one to each count makes a negligible difference $P(C_i | features) = P(x_1 | C_i) * P(x_2 | C_i) * P(C_i)$

• P(Liked) = 0.63

• P(Not Liked) = 0.38

• P(Comedy | Liked) = 0.4

• P(Drama | Liked) = 0.6

• P(Comedy | Not Liked) = 0.33

Multinomial Naïve Bayes: Example

Liked?

Yes

Yes

No

No

Yes

No

Yes

 x_1

Type

Comedy

Drama

Comedy

Drama

Drama

Drama

Comedy

Movie

m1

 m^2

 m_{3}

m4

 m_{5}

 m_{6}

m7

 x_2

Length

Short

Medium

Medium

Long

Medium

Short

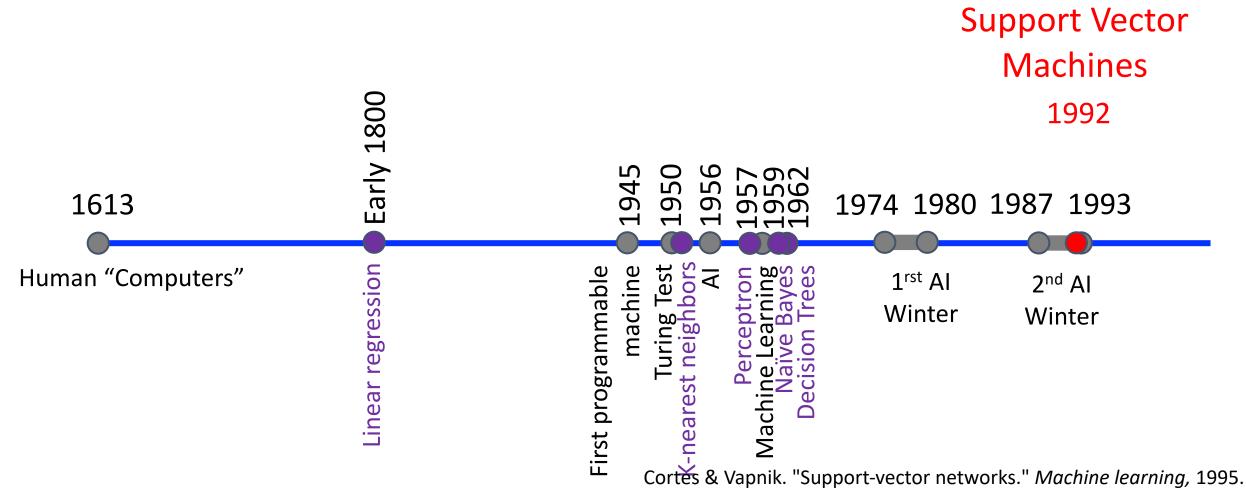
Short

Today's Topics

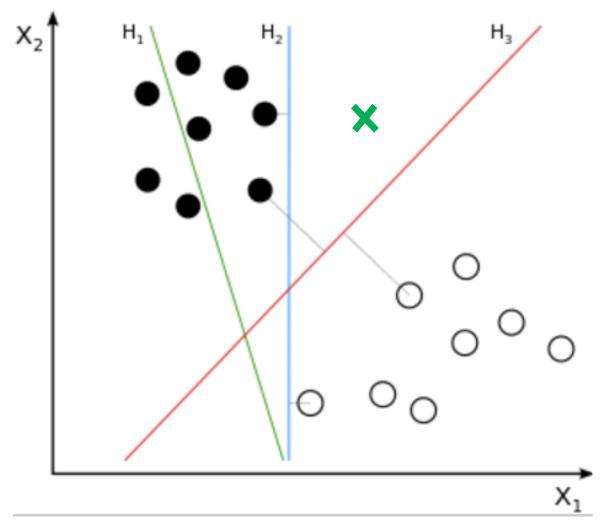
- Evaluating Machine Learning Models Using Cross-Validation
- Naïve Bayes
- Support Vector Machines

• Lab

Historical Context of ML Models

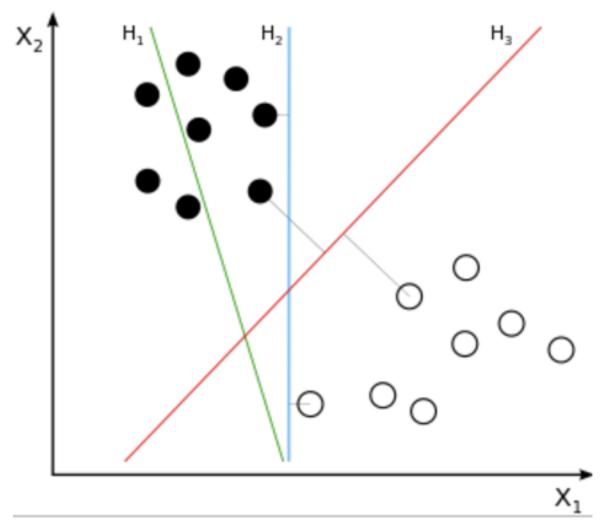


Boser, Guyon, & Vapnik. "A training algorithm for optimal margin classifiers." Workshop on Computational learning theory, 1992.



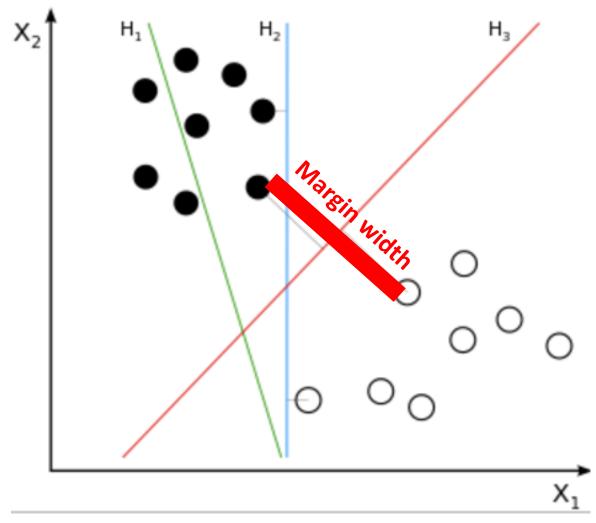
To which class would each decision boundary assign the new data point?

https://en.wikipedia.org/wiki/Linear_separability



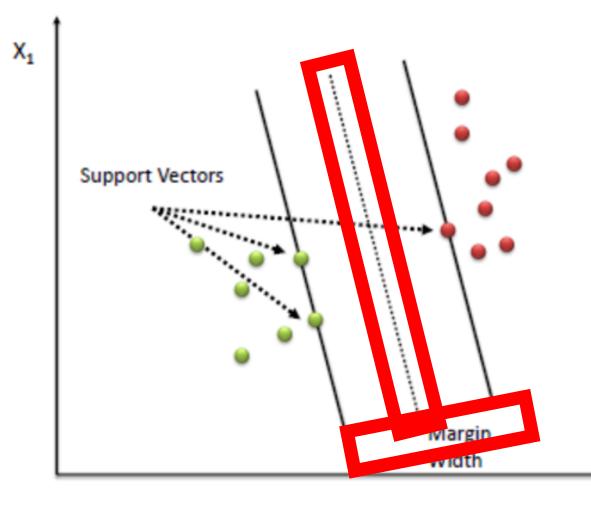
Which decision boundary would you choose to separate data?

https://en.wikipedia.org/wiki/Linear_separability



Idea: choose hyperplane that maximizes the margin width.

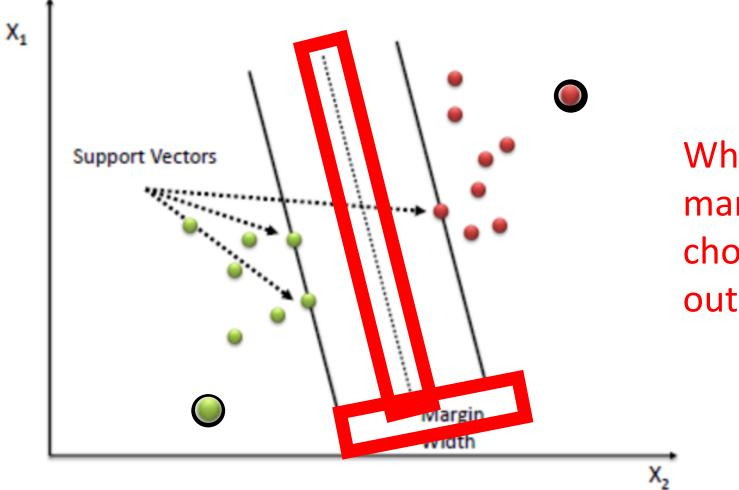
https://en.wikipedia.org/wiki/Linear_separability



Idea: choose hyperplane that maximizes the "margin" width.

Margin: distance between the separating hyperplane (decision boundary) and training samples ("support vectors") closest to the hyperplane.

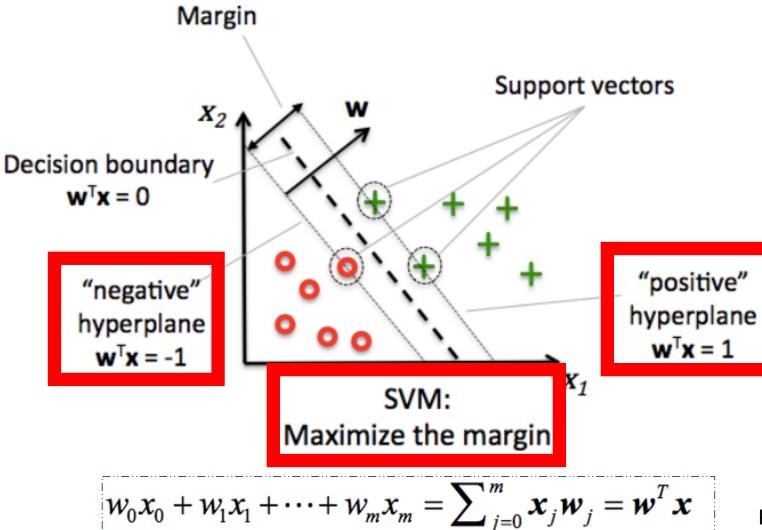
http://chem-eng.utoronto.ca/~datamining/dmc/support_vector_machine.htm



When trying to maximize the margin, what happens to the choice of line when you add outliers to the dataset?

http://chem-eng.utoronto.ca/~datamining/dmc/support_vector_machine.htm

Support Vector Machine (SVM): Formalizing Definition



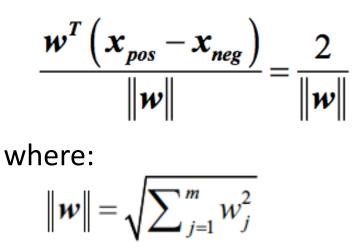
Distance Between Parallel Lines Tutorial: http://web.mit.edu/zoya/www/SVM.pdf

Derivation of Margin Length

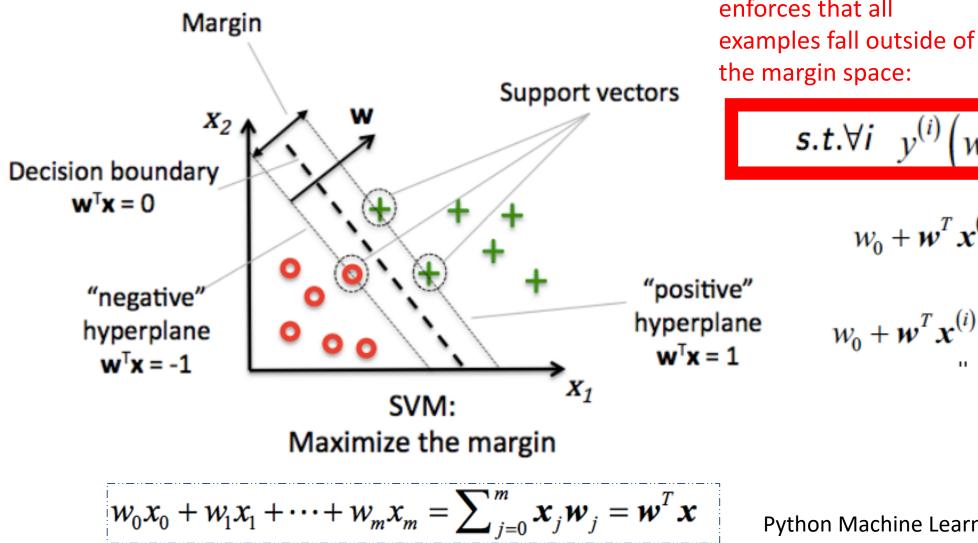
 Subtract two equations from each other:

$$\boldsymbol{w}^{T}\left(\boldsymbol{x}_{pos}-\boldsymbol{x}_{neg}\right)=2$$

 Normalize by length of w to compute margin length:



Support Vector Machine (SVM): Formalizing Definition Constraint that



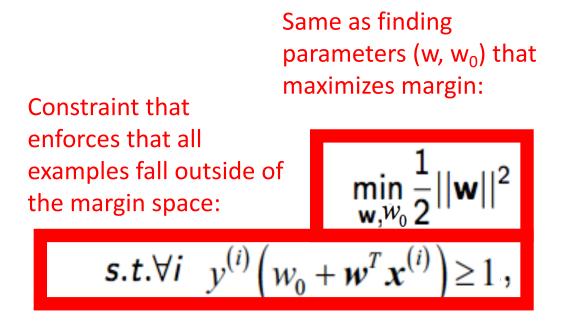
Same as finding parameters (w, w_o) that maximizes margin:

margin space: $\min_{\mathbf{w}, w_0} \frac{1}{2} ||\mathbf{w}||^2$ $s.t. \forall i \quad y^{(i)} \left(w_0 + \mathbf{w}^T \mathbf{x}^{(i)} \right) \ge 1$,

$$w_0 + w^T x^{(i)} \ge 1 \ if \ y^{(i)} = 1$$

 $w_0 + w^T x^{(i)} < -1$ if $y^{(i)} = -1$

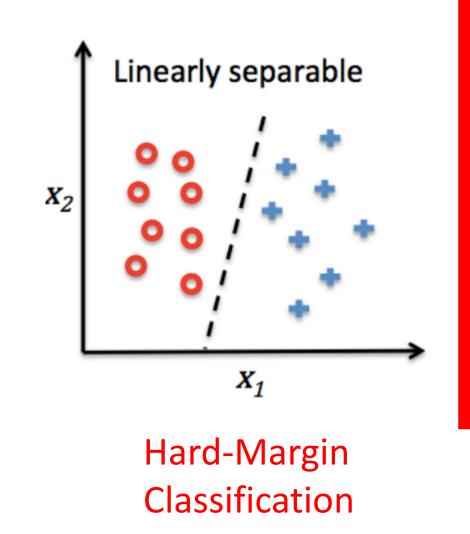
Support Vector Machine (SVM): Training a Classifier

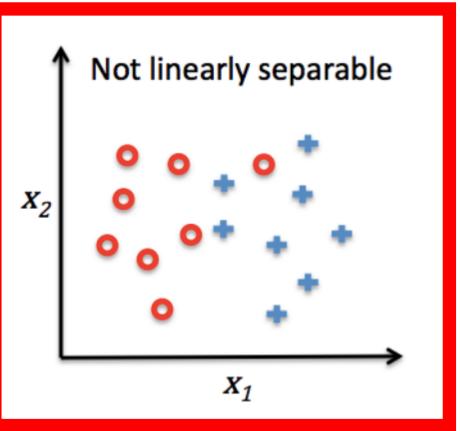


Can be solved with a quadratic programming solver... learn more about this at:

- "The Nature of Statistical Learning and Theory, by Vladimir Vapnik
- A Tutorial on Support Vector Machines for Pattern Recognition by Chris J. C. Burges'

What if the Decision Boundary is Not Linear?





Soft-Margin Classification

Soft-Margin Classification

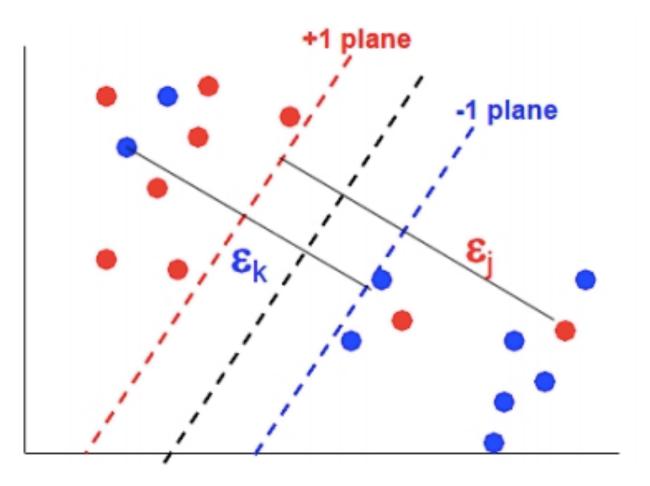
$$\min \frac{1}{2} ||\mathbf{w}||^2 + \lambda \sum_{i=1}^{N} \xi_i$$

s.t $\xi_i \ge 0$; $\forall i \ t^{(i)}(\mathbf{w}^T \mathbf{x}^{(i)}) \ge 1 - \xi_i = 0$

Introduce "slack" variable:

$$w^T x^{(i)} \ge 1 - \xi^{(i)} f y^{(i)} = 1$$

 $w^T x^{(i)} \le -1 + \xi^{(i)} f y^{(i)} = -1$



Soft-Margin Classification

$$\min \frac{1}{2} ||\mathbf{w}||^2 - \lambda \sum_{i=1}^{N} \xi_i$$

s.t $\xi_i \ge 0$; $\forall i \ t^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)}) \ge 1 - \xi_i = 0$

(Increases priority placed on minimizing error so margin is smaller)

 X_1

Which plot shows when the slack variable is **larger**?

 X_2

Python Machine Learning; Raschkka & Mirjalili

*X*₂

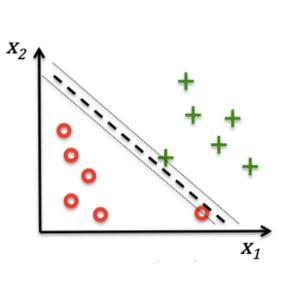
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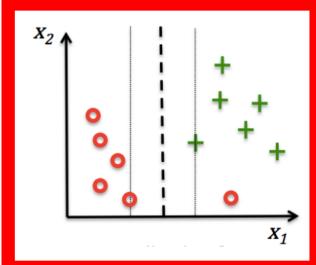
 X_1

Soft-Margin Classification

$$\min \frac{1}{2} ||\mathbf{w}||^2 - \lambda \sum_{i=1}^{N} \xi_i$$

s.t $\xi_i \ge 0$; $\forall i \ t^{(i)}(\mathbf{w}^T \mathbf{x}^{(i)}) \ge 1 - \xi_i = 0$

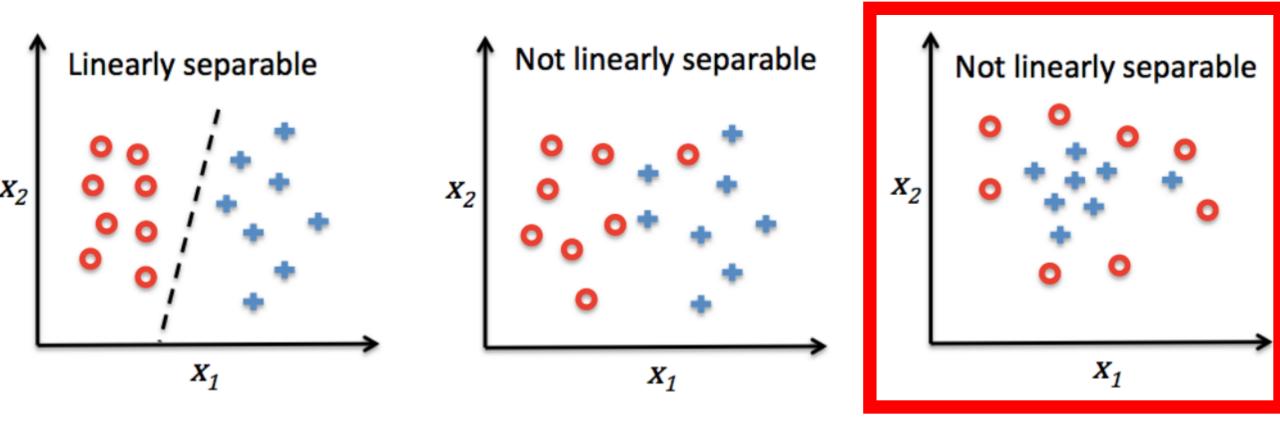




(Increases priority placed on maximizing margin so error is larger)

Which plot shows when the slack variable is **smaller**?

What if the Decision Boundary is Not Linear?

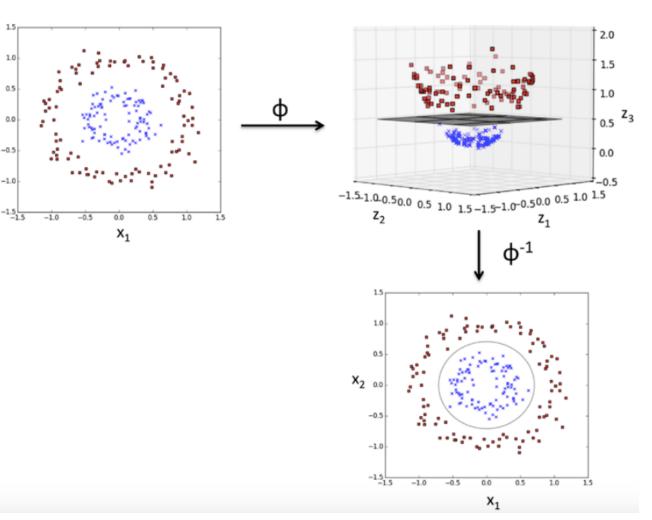


Hard-Margin Classification Soft-Margin Classification

Kernelized Support Vector Machines

 X_2

- Recall polynomial regression?
 - Project features to higher order space
- Kernels efficiently project features to higher order spaces
- What conversion to use? e.g.,
 - Polynomial kernel
 - Gaussian Radial Basis Function kernel



What are SVM's Strengths

- Insensitive to outliers (only relies on support vectors to choose dividing line)
- Once trained, prediction is fast
- Requires little memory (rely on a few support vectors)
- Work well with high-dimensional data

What are SVM's Weaknesses

- Prohibitive computational costs for large datasets
- Performance heavily dependent on soft margin value for non-linear classification
- Does not have a direct probabilistic interpretation

Today's Topics

- Evaluating Machine Learning Models Using Cross-Validation
- Naïve Bayes
- Support Vector Machines
- Lab