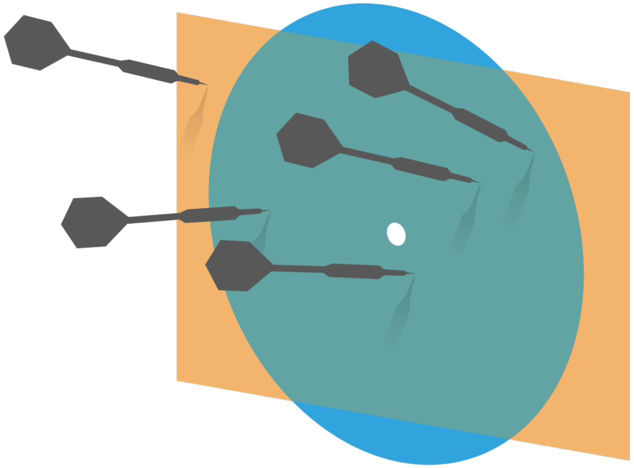
Probability and Statistics for Computer Science



Credit: wikipedia

"…many problems are naturally classification problems"---Prof. Forsyth

Hongye Liu, Teaching Assistant Prof, CS361, UIUC, 11.5.2021

Last time

- Decision tree (II)
- Random forest
- Support Vector Machine (I)

$a^T x + b = 0$

$\text{sign}(a^T x + b)$

Objectives

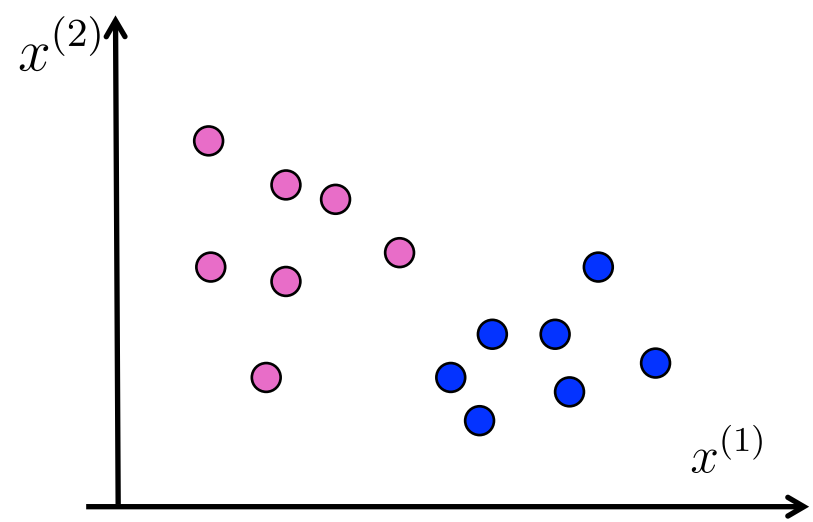
- Support Vector Machine (II)
  - * Hinge loss + Regularization
  - * Convex function, Gradient Descent
    Stochastic Gradient Descent
  - * Training & Validation
- Naïve Bayesian Classifier

Motivation for Studying Support Vector Machine

- When solving a classification problem, it is good to try several techniques.
- Criteria to consider in choosing the classifier include
  - Accuracy ✔
  - Training speed
  - Classification speed ✔
  - Performance with small training set
  - Interpretability ✔

SVM problem formulation

- At first we assume a binary classification problem
- The training set consists of N items
  - Feature vectors x_i of dimension d
  - Corresponding class labels $y_i \in \{\pm 1\}$
- We can picture the training data as a d-dimensional scatter plot with colored labels



Decision boundary of SVM

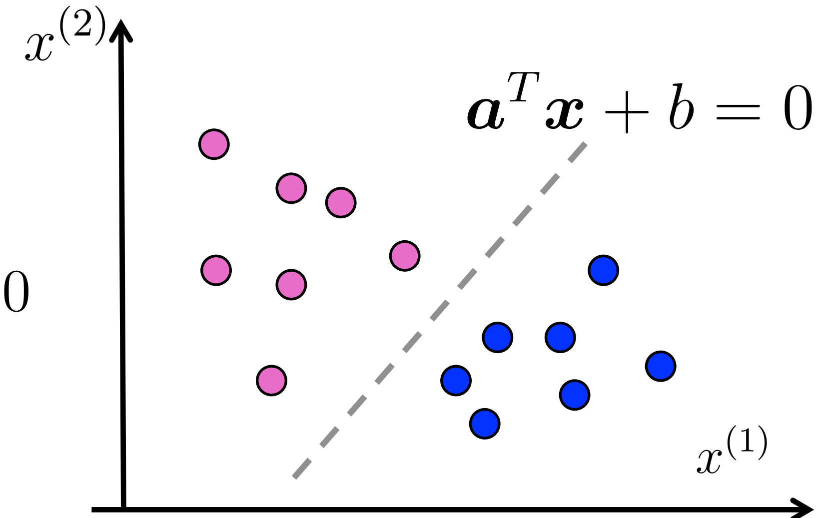
- SVM uses a hyperplane as its **decision boundary**
- The decision boundary is:

$$a_1x^{(1)} + a_2x^{(2)} + \ldots + a_dx^{(d)} + b = 0$$

- In vector notation, the hyperplane can be written as:

$$\boldsymbol{a}^T\boldsymbol{x} + b = 0$$

$[a, b]$



$a = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_d \end{bmatrix}$ $\quad x = \begin{bmatrix} x^{(1)} \\ x^{(2)} \\ \vdots \\ x^{(d)} \end{bmatrix}$

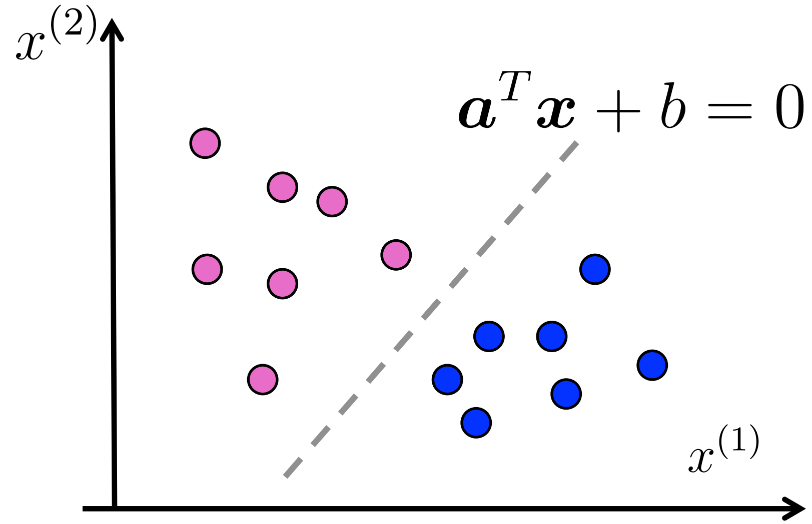
Classification function of SVM

- SVM assigns a class label to a feature vector according to the following rule:

  +1 if $\boldsymbol{a}^T\boldsymbol{x}_i + b \geq 0$

  -1 if $\boldsymbol{a}^T\boldsymbol{x}_i + b < 0$

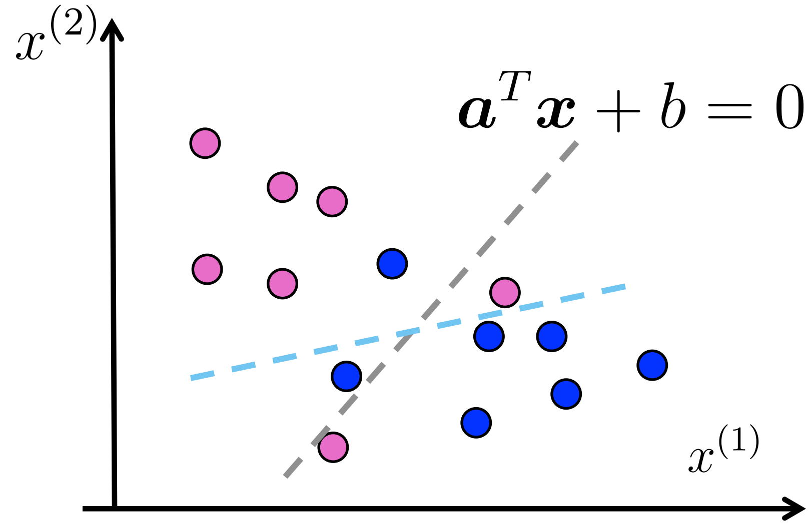
- In other words, the classification function is: $sign(\boldsymbol{a}^T\boldsymbol{x}_i + b)$



- Note that
  - If $\left|\boldsymbol{a}^T\boldsymbol{x}_i + b\right|$ is small, then $\boldsymbol{x}_i$ was close to the decision boundary
  - If $\left|\boldsymbol{a}^T\boldsymbol{x}_i + b\right|$ is large, then $\boldsymbol{x}_i$ was far from the decision boundary

What if there is no clean cut boundary?

- Some boundaries are better than others for the training data
- Some boundaries are likely more robust for run-time data
- We need to a quantitative measure to decide about the boundary
- The **loss function** can help decide if one boundary is better than others



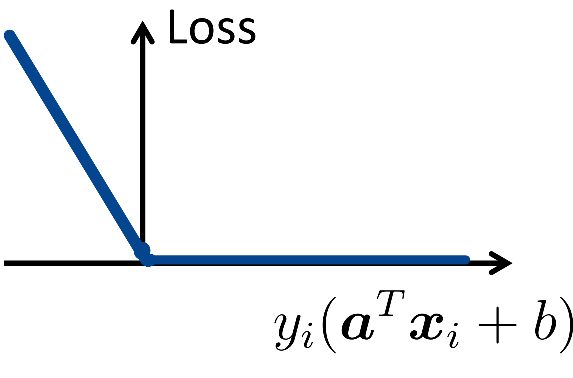
Loss function 1

- For any given feature vector $\boldsymbol{x}_i$ with class label $y_i \in \{\pm 1\}$, we want
  - Zero loss if $\boldsymbol{x}_i$ is classified correctly $sign(\boldsymbol{a}^T \boldsymbol{x}_i + b) = y_i$
  - Positive loss if $\boldsymbol{x}_i$ is misclassified $sign(\boldsymbol{a}^T \boldsymbol{x}_i + b) \neq y_i$
  - If $\boldsymbol{x}_i$ is misclassified, more loss is assigned if it's further away from the boundary

y_i is either -1 or $+1$

- This loss function 1 meets the criteria above:

$$max(0, -y_i(\boldsymbol{a}^T \boldsymbol{x}_i + b))$$



- Training error cost

$$S(\boldsymbol{a}, b) = \frac{1}{N} \sum_{i=1}^{N} max(0, -y_i(\boldsymbol{a}^T \boldsymbol{x}_i + b))$$

Q. What's the value of this function ?

$$max(0, -y_i(\boldsymbol{a}^T\boldsymbol{x}_i + b)) \quad \text{if} \quad sign(\boldsymbol{a}^T\boldsymbol{x}_i + b) = y_i$$

A. 0.
B. others.

Q. What's the value of this function ?

$$max(0, -y_i(\boldsymbol{a}^T\boldsymbol{x}_i + b)) \quad \text{if} \quad sign(\boldsymbol{a}^T\boldsymbol{x}_i + b) \neq y_i$$

A. 0.
$\boxed{\text{B.}}$ A value greater than or equal to 0.

Loss function 1

- For any given feature vector $\boldsymbol{x}_i$ with class label $y_i \in \{\pm 1\}$, we want
  - Zero loss if $\boldsymbol{x}_i$ is classified correctly $sign(\boldsymbol{a}^T \boldsymbol{x}_i + b) = y_i$
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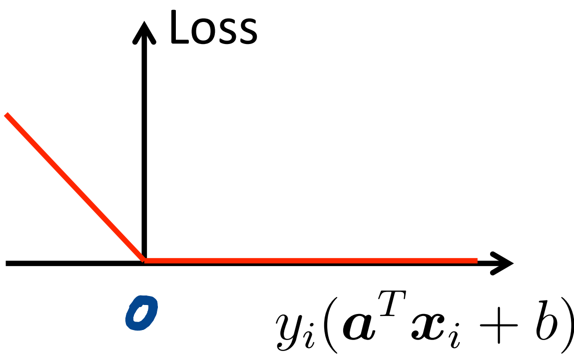


- Training error cost

$$S(\boldsymbol{a}, b) = \frac{1}{N} \sum_{i=1}^{N} max(0, -y_i(\boldsymbol{a}^T \boldsymbol{x}_i + b))$$

The problem with loss function 1

- Loss function1 does not distinguish between the following decision boundaries if they both classify $\boldsymbol{x}_i$ correctly.
  - One passes the two classes closely
  - One that passes with a wider margin

- But leaving a larger margin gives robustness for run-time data- **the large margin principle**

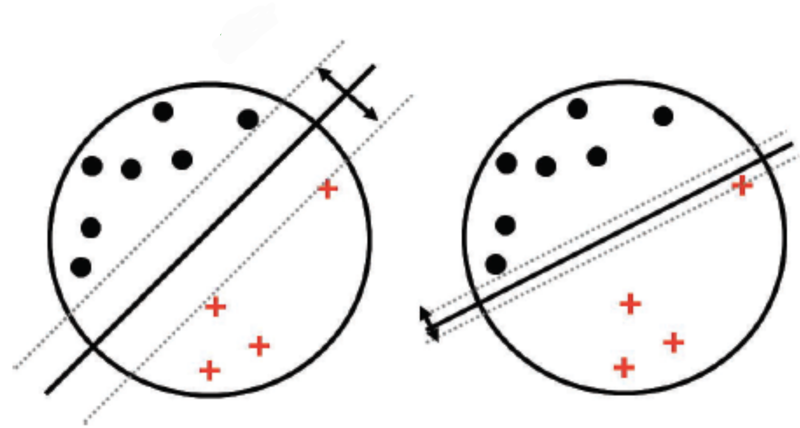


Figure 14.11 Illustration of the large margin principle. Left: a separating hyper-plane with large margin. Right: a separating hyper-plane with small margin.

Credit: Kelvin Murphy

Loss function 2: the hinge loss

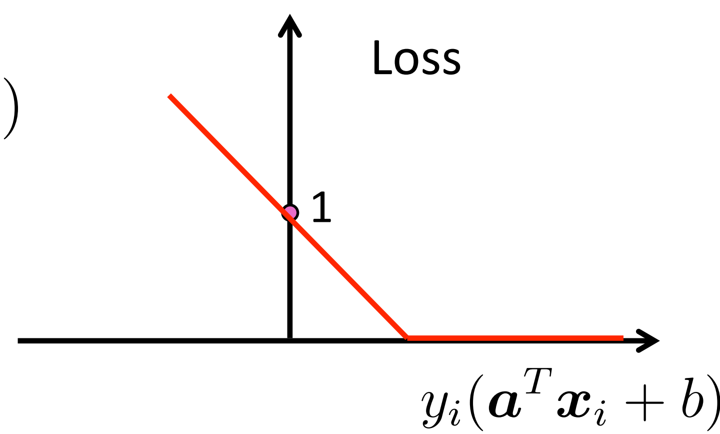
- We want to impose a small positive loss if $\boldsymbol{x}_i$ is correctly classified but close to the boundary

- The **hinge loss** function meets the criteria above:

$$max(0, 1 - y_i(\boldsymbol{a}^T\boldsymbol{x}_i + b))$$

- Training error cost

$$S(\boldsymbol{a}, b) = \frac{1}{N}\sum_{i=1}^{N} max(0, 1 - y_i(\boldsymbol{a}^T\boldsymbol{x}_i + b))$$



The problem with loss function 2

- Loss function 2 favors decision boundaries that have large $\|\boldsymbol{a}\|$ because increasing $\|\boldsymbol{a}\|$ can zero out the loss for a correctly classified $\boldsymbol{x}_i$ near the boundary.

- But large $\|\boldsymbol{a}\|$ makes the classification function $sign(\boldsymbol{a}^T\boldsymbol{x}_i + b)$ extremely sensitive to small changes in $\boldsymbol{x}_i$ and make it less robust to run-time data.

- So small $\|\boldsymbol{a}\|$ is better.

Hinge loss with regularization penalty

- We add a penalty on the square magnitude $\|\boldsymbol{a}\|^2 = \boldsymbol{a}^T\boldsymbol{a}$

$$a = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_d \end{bmatrix}$$

- Training error cost

$$S(\boldsymbol{a}, b) = \left[\frac{1}{N}\sum_{i=1}^{N} max(0, 1 - y_i(\boldsymbol{a}^T\boldsymbol{x}_i + b))\right] + \lambda(\frac{\boldsymbol{a}^T\boldsymbol{a}}{2})$$

- The **regularization parameter** λ trade off between these two objectives

Q. What does the penalty discourage?

$$S(\boldsymbol{a}, b) = \left[\frac{1}{N}\sum_{i=1}^{N} max(0, 1 - y_i(\boldsymbol{a}^T\boldsymbol{x}_i + b))\right] + \boxed{\lambda(\frac{\boldsymbol{a}^T\boldsymbol{a}}{2})}$$

$a_1 x^{(1)} + a_2 x^{(2)} + \cdots + b = 0$

$a^T x + b$

a_1
a_2
a_3
$\vdots$

$\boxed{\text{A.}}$ Too big a magnitude of the vector **a**

B. Too many data points in the training set

How to compute the decision boundary?

minimize Loss function $S(\vec{a}, b)$

$$(\vec{a}^*, b^*) = \operatorname{argmin}(S(\vec{a}, b))$$

$$\downarrow$$

$$\begin{bmatrix} a_1^* \\ a_2^* \\ \vdots \\ a_d^* \\ b^* \end{bmatrix}$$

Convex set and convex function

- If a set is convex, any line connecting two points in the set is completely included in the set

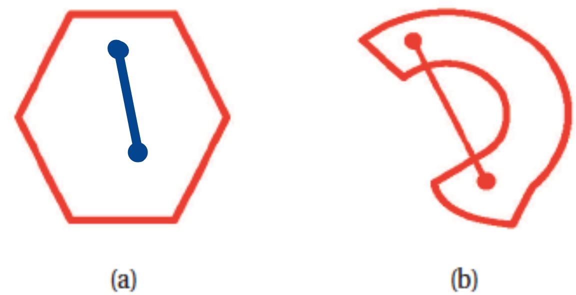
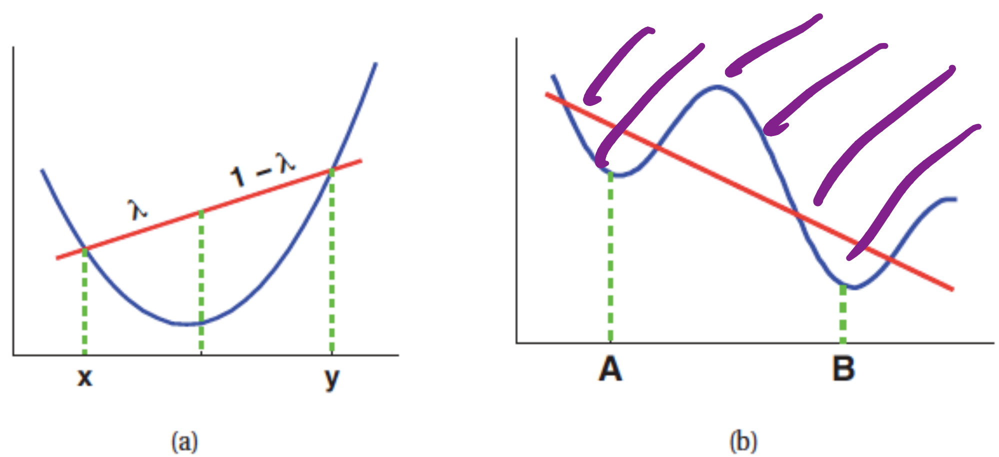


Figure 7.4 (a) Illustration of a convex set. (b) Illustration of a nonconvex set.

- A convex function: the area above the curve is convex

$$f(\lambda x + (1-\lambda)y) < \lambda f(x) + (1-\lambda) f(y)$$

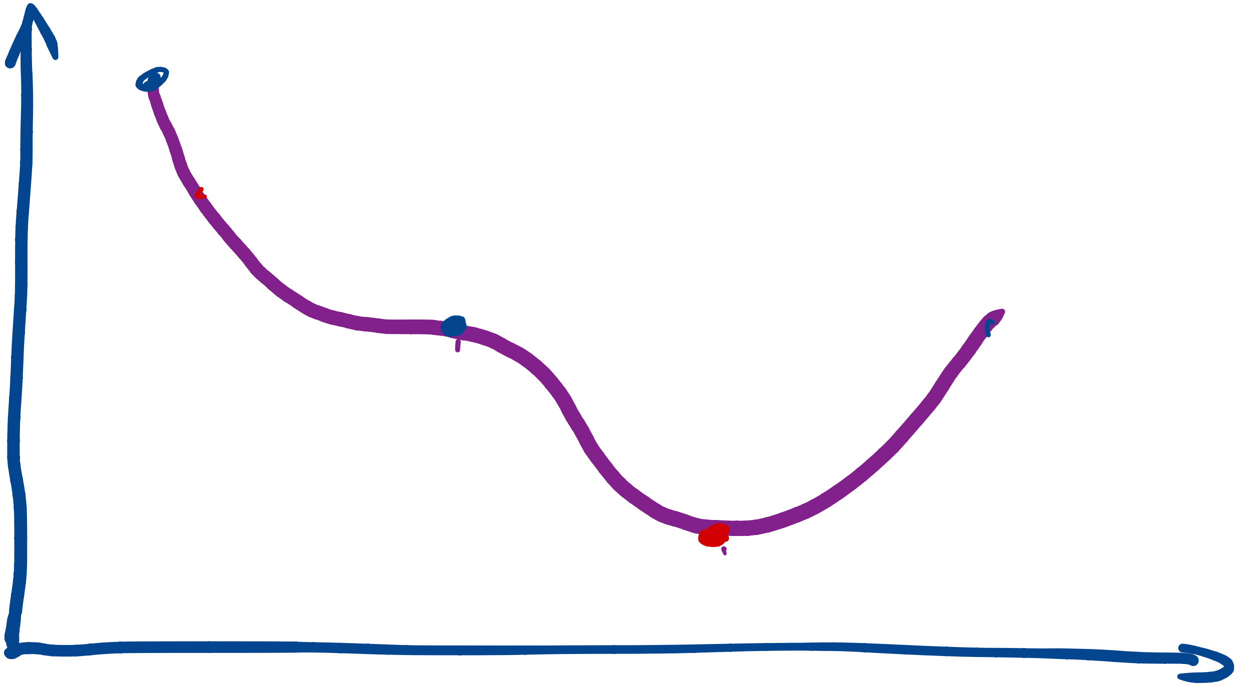


Credit: Dr. Kelvin Murphy

Q. Is this curve a convex curve?

A. YES

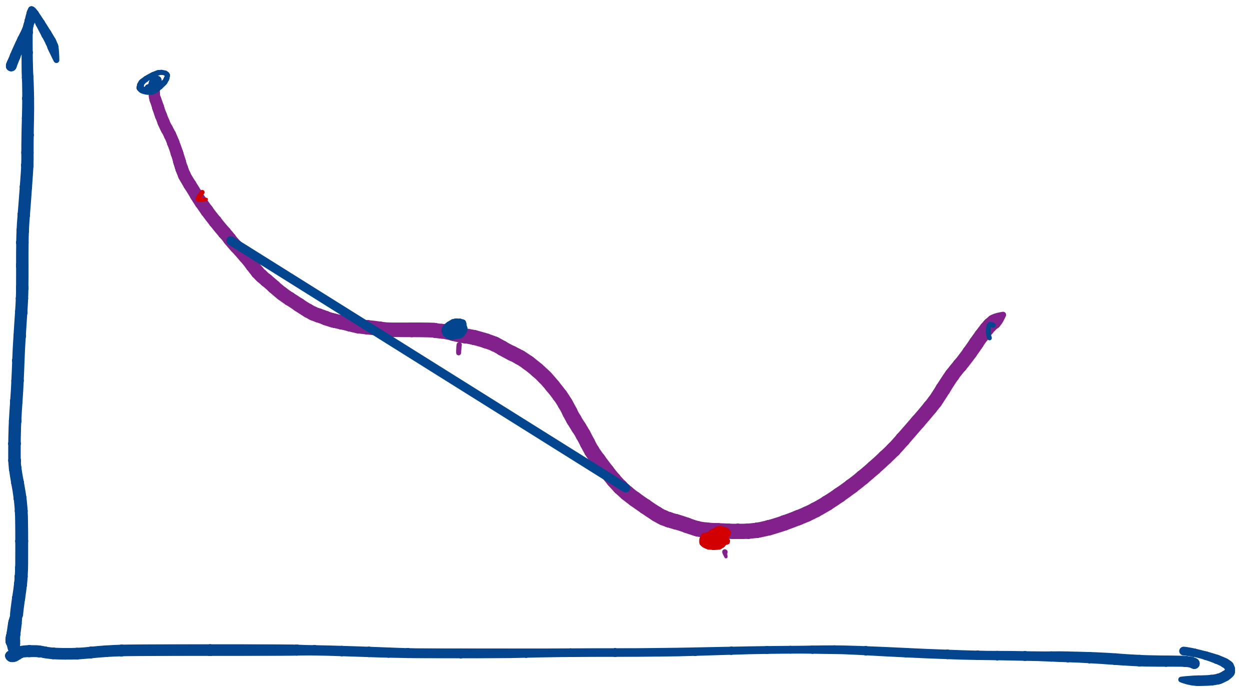
B. NO



Q. Is this curve a convex curve?

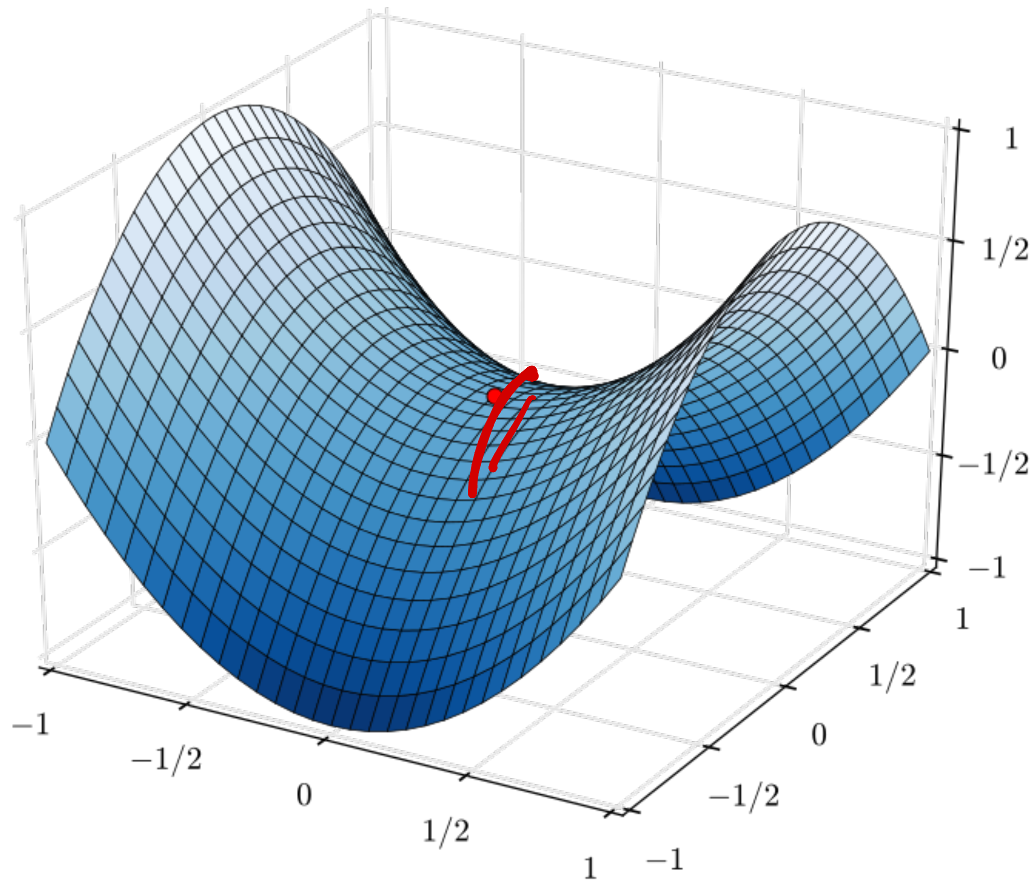
A. YES

B. NO



Q. Is this surface convex?

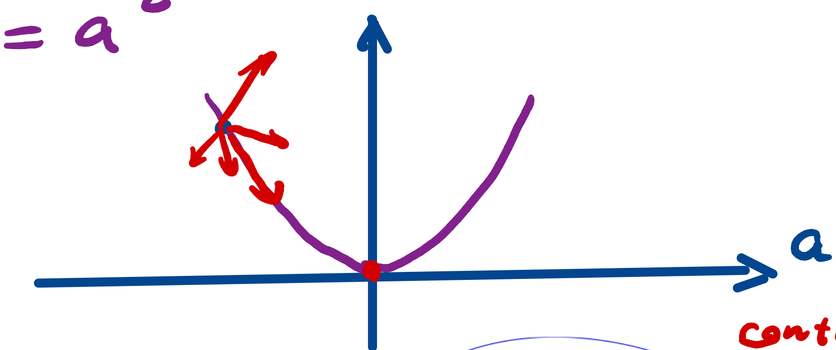
A. YES
B. NO



Source: wikipedia

Iterative minimization by gradient descent

- For a function such as $f(a) = a^2$

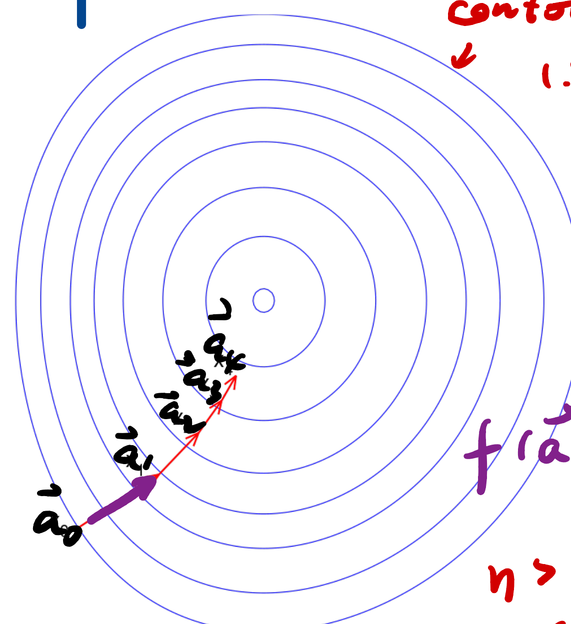


- A convex surface $f(\vec{a})$ $= \text{height}(\vec{a})$

$\vec{a}_1 = \vec{a}_0 + \eta_0 \vec{p}$

$\vec{p} = -\nabla f$

f is scalar



$f(\vec{a}_i) \downarrow$

$\eta > 0$

$\eta \ll 1$

Source: wikipedia

Gradient Descent

$\vec{a} = [a_1 \; a_2 \; \cdots \; a_d]^T$ let's omit b for now

$\vec{a}_n \sim \vec{a}^*$

Loss function: $f = f(\vec{a})$

$\vec{a}^*$ minimizes $f(\vec{a})$

$$\nabla f = \begin{pmatrix} \frac{\partial f}{\partial a_1} \\ \frac{\partial f}{\partial a_2} \\ \vdots \\ \frac{\partial f}{\partial a_d} \end{pmatrix}$$

$\vec{a}_0, \vec{a}_1, \cdots \vec{a}_n$

$f(\vec{a}_0) > \cdots > f(\vec{a}_n)$

$\vec{a}_{n+1} = \vec{a}_n + \eta \vec{p}_n$

Taylor expansion

$$f(\vec{a}_{n+1}) = f(\vec{a}_n + \eta_n \vec{p}_n) = f(\vec{a}_n) + \eta_n (\nabla f)^T \vec{p}_n + O(\eta_n^2)$$

$\eta_n > 0$

$\eta_n < 1$

if $\vec{p}_n = -\nabla f(\vec{a}_n)$

$$f(\vec{a}_{n+1}) = f(\vec{a}_n) - \eta_n (\nabla f)^T \nabla f$$

$$= f(\vec{a}_n) - \eta_n \|\nabla f\|^2$$

learning rate or stepsize

$$f(x) = f(\overset{0}{\cancel{x_0}}) + f'(\overset{0}{\cancel{x_0}})\,x + \cdots \frac{f^{(n)}\,x^{n}}{n!}$$

Stochastic gradient descent

if $f(\vec{a}) = \frac{1}{K} \sum_{j=1}^{K} Q(\vec{a}, j)$

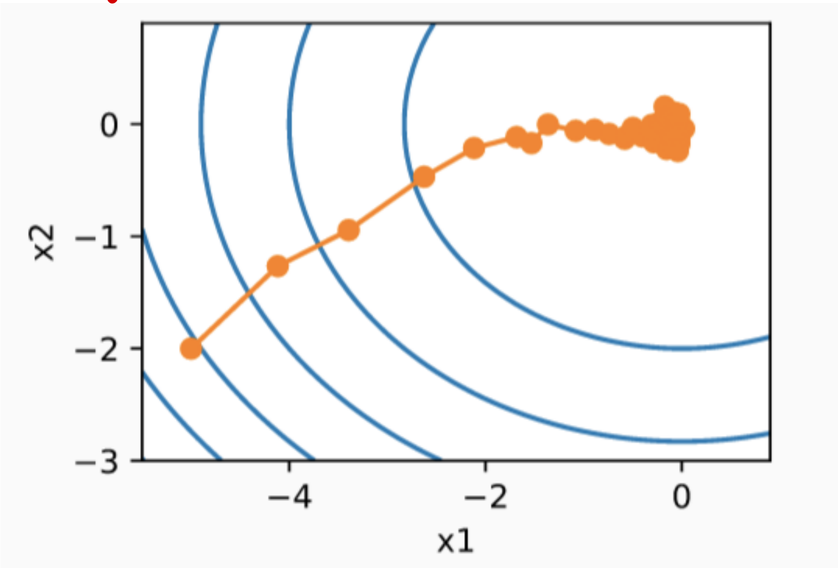
$K \rightarrow$ # of data in training set

Stochastic gradient descent approximates $f(\vec{a}) \doteq g(\vec{a}) = \frac{1}{m} \sum_{i=1}^{m} Q(\vec{a}, i)$

$\boldsymbol{x}_k \in \{\boldsymbol{x}_i\}$

i is RV. uniform in $[1, K]$

We often choose $m = 1$



The difference btw GD and SGD

GD

Loss:

$$f(\vec{a}) = \frac{1}{K}\sum_{j=1}^{K} Q(\vec{a}, j) \text{ +penalty}$$

$$Q = \max(0, 1 - y_j(a^T x_j + b))$$

$$\vec{a}_{n+1} = \vec{a}_n - \eta \nabla f(\vec{a}_n)$$

$$\lim_{n\to\infty} \vec{a}_n = \underset{\vec{a}}{\operatorname{argmin}}(f(\vec{a}))$$

if f is convex

SGD

Loss:

$$g(\vec{a}) = \frac{1}{m}\sum_{i=1}^{m} Q(\vec{a}, i) \text{ + penalty}$$

$$g(\vec{a}) = f(\vec{a}) + \underset{\text{noise}}{z}$$

$$\vec{a}_{n+1} = \vec{a}_n - \eta \nabla g(\vec{a}_n)$$

$$\lim_{n\to\infty} E[(\vec{a}_n - \vec{a}^*)^2] = 0$$

not always

given convex Loss and other conditions

Update parameters of the hyperplane during the stochastic gradient descent

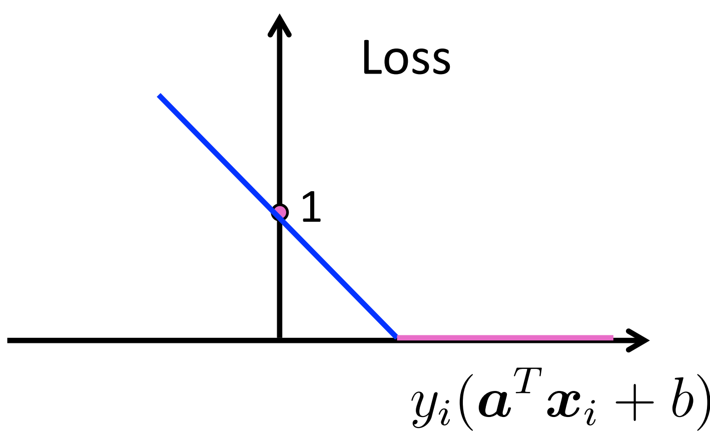
- Since $S_k(\boldsymbol{a}, b) = max(0, 1 - y_k(\boldsymbol{a}^T\boldsymbol{x}_k + b))$ and $S_0(\boldsymbol{a}, b) = \lambda(\frac{\boldsymbol{a}^T\boldsymbol{a}}{2})$

  We have the following updating equations:

$S(a, b) = S_k + S_0$ if $m=1$

If $y_k(\boldsymbol{a}^T\boldsymbol{x}_k + b) \geq 1$	If $y_k(\boldsymbol{a}^T\boldsymbol{x}_k + b) < 1$
$\boldsymbol{a} \leftarrow \boldsymbol{a} - \eta(\lambda\boldsymbol{a})$ $b \leftarrow b$	$\boldsymbol{a} \leftarrow \boldsymbol{a} - \eta(\lambda\boldsymbol{a} - y_k\boldsymbol{x}_k)$ $b \leftarrow b - \eta(-y_k)$

We often set $\eta_n = \frac{1}{n}$



Training procedure-minimizing the cost function

- The training error cost $S(\boldsymbol{a}, b)$ is a function of decision boundary parameters $(\boldsymbol{a}, b)$, so it can help us find the best decision boundary.
- Fix λ and set some initial values for $(\boldsymbol{a}, b)$
- Search iteratively for $(\boldsymbol{a}, b)$
- Repeat the previous steps for several values of λ and choose the one that gives the decision boundary with best accuracy on a validation data set.

Validation/testing of SVM model

- Split the labeled data into **training**, **validation** and **test** sets.
- For each choice of **λ**, run stochastic gradient descent to find the best decision boundary parameters (**a**, b) using the training set.
- Choose the best **λ** based on accuracy on the validation set.
- Finally evaluate the SVM's accuracy on the **test** set.
- This process avoids overfitting the data.

Extension to multiclass classification

- All vs. all
  - Train a separate binary classifier for each pair of classes.
  - To classify, run all classifiers and see which class it will be labeled most with.
  - Computational complexity is quadratic to the number of classes.

1 2 3

1 2

1 3

2 3

$c \rightarrow \binom{c}{2}$

- One vs. all
  - Train a separate binary classifier for each class against all else.
  - To classify, run all classifiers and see which label gets the highest score
  - Computational complexity scales linearly.

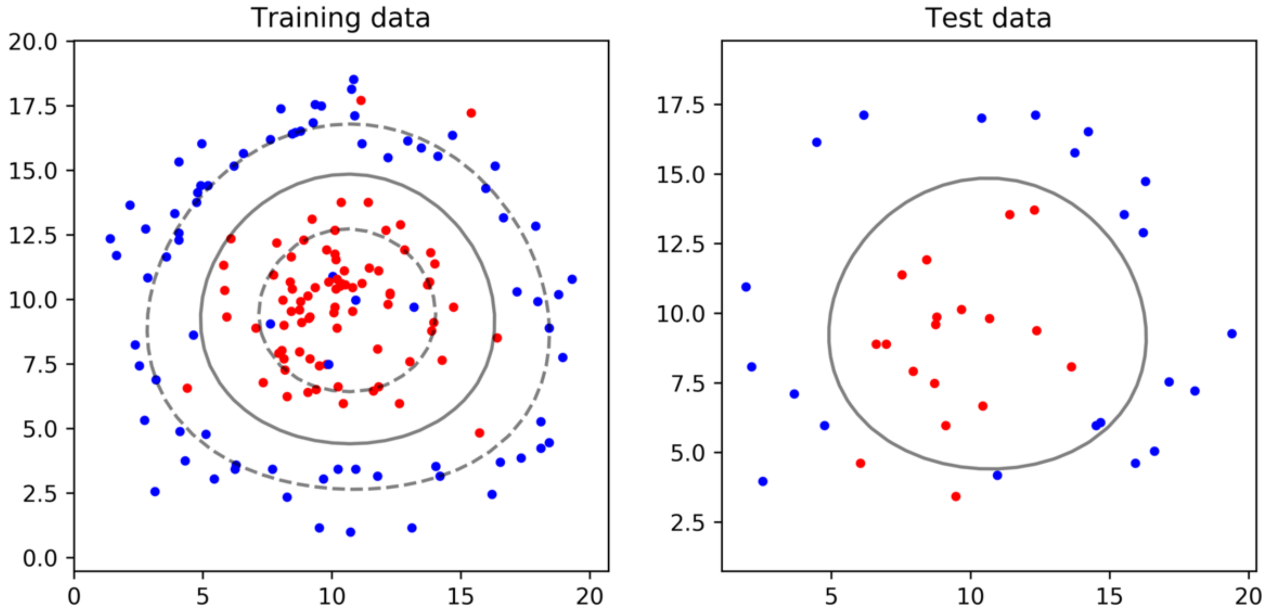
1 vs not 1

2 vs not 2

3 vs not 3

What if the data is inseparable linearly?

- There is a chance the data is inseparable
- Use the non-linear **SVM with kernels!**
- Decision boundary is curved



Naïve Bayes classifier

- Training
  - Use the training data $\{(\mathbf{x}_i, y_i)\}$ to estimate a probability model $P(y|\boldsymbol{x})$

    θ *

    $\boldsymbol{x} = [x^{(1)}\ x^{(2)}\ \dots\ x^{(d)}]^T$

    ie. petal length, petal width ...

    ↑ label/parameter
  - Assume that the features of $\{\boldsymbol{x}\}$ are conditionally independent given the class label y

    $P(D|\theta)$

$$P(\boldsymbol{x}|y) = \prod_{j=1}^{d} P(\boldsymbol{x}^{(j)}|y)$$

↑ Data

$$P(\theta|D) = \frac{L(\theta)\,P(\theta)}{P(D)}$$

- Classification
  - Assign the label $\underset{y}{argmax}\ P(y|\boldsymbol{x})$ to a feature vector $\boldsymbol{x}$

$$P(X|D \cap Y|D \cap Z|D) = P(X|D)\,P(Y|D)\,P(Z|D)$$

Naïve Bayes Model

- MAP estimator of class variable y given the data $\boldsymbol{x}$

$$\underset{y}{argmax}\ P(y|\boldsymbol{x})$$

$$=$$

Naïve Bayes Model

- MAP estimator of class variable y given the data $\boldsymbol{x}$

$$\underset{y}{argmax}\; P(y|\boldsymbol{x})$$

$$= \underset{y}{argmax}\; \frac{P(\boldsymbol{x}|y)P(y)}{P(\boldsymbol{x})}$$

Naïve Bayes Model

- MAP estimator of class variable y given the data $\boldsymbol{x}$

$$
\begin{aligned}
& \underset{y}{argmax}\ P(y|\boldsymbol{x}) \\
= & \underset{y}{argmax}\ \frac{P(\boldsymbol{x}|y)P(y)}{P(\boldsymbol{x})} \\
= & \underset{y}{argmax}\ P(\boldsymbol{x}|y)P(y)
\end{aligned}
$$

Because P(x) doesn't depend on y

Naïve Bayes Model

- MAP estimator of class variable y given the data $\boldsymbol{x}$

$\boldsymbol{x} = [x^{(1)} \; x^{(2)} \; \dots \; x^{(d)}]^T$

ie. petal length, petal width ...

$$
\begin{aligned}
&\underset{y}{argmax} \; P(y|\boldsymbol{x}) \\
&= \underset{y}{argmax} \; \frac{P(\boldsymbol{x}|y)P(y)}{P(\boldsymbol{x})} \\
&= \underset{y}{argmax} \; P(\boldsymbol{x}|y)P(y) \\
&= \underset{y}{argmax} \; \left[\prod_{j=1}^{d} P(\boldsymbol{x}^{(j)}|y) \right] P(y)
\end{aligned}
$$

"Naïve" assumption of conditional independence of features

Naïve Bayes Model

- MAP estimator of class variable y given the data $\boldsymbol{x}$

$$\underset{y}{argmax}\ P(y|\boldsymbol{x})$$

$$= \underset{y}{argmax}\ \frac{P(\boldsymbol{x}|y)P(y)}{P(\boldsymbol{x})}$$

$$= \underset{y}{argmax}\ P(\boldsymbol{x}|y)P(y)$$

$$= \underset{y}{argmax}\ \left[\prod_{j=1}^{d} P(\boldsymbol{x}^{(j)}|y)\right] P(y)$$

"Naïve" assumption of conditional independence of features

$$= \underset{y}{argmax}\ \left[\sum_{j=1}^{d} log P(\boldsymbol{x}^{(j)}|y) + log\ P(y)\right]$$

Modeling the prior and the likelihoods

- Model the prior based on the frequency of y in the training set
  - For a binary classifier, this model is a Bernoulli random variable

- Model each likelihood $P(\boldsymbol{x}^{(j)}|y)$ by:
  - Selecting an appropriate family of distributions
    - Normal for real-valued numerical data
    - Poisson for counts in fixed intervals
    - Etc.
  - Fitting the parameters of the distribution using MLE

An example of Naive Bayes training

Training data

$X^{(1)}$	$X^{(2)}$	y
3.5	10	1
1.0	8	1
0.0	10	-1
-3.0	14	-1

Dataframe format for illustration

Modeling $P(\boldsymbol{x}^{(1)}|y)$ as normal

$$P(\boldsymbol{x}^{(1)}|y=1)$$

$$\mu_{MLE} = \frac{3.5+1.0}{2} = 2.25$$

$$\sigma_{MLE} = 1.25$$

$$P(\boldsymbol{x}^{(1)}|y=-1)$$

$$\mu_{MLE} = -1.5$$

$$\sigma_{MLE} = 1.5$$

Modeling $P(\boldsymbol{x}^{(2)}|y)$ as Poisson

$$P(\boldsymbol{x}^{(2)}|y=1)$$

$$\lambda_{MLE} = \frac{10+8}{2} = 9$$

$$P(\boldsymbol{x}^{(2)}|y=-1)$$

$$\lambda_{MLE} = 12$$

Modeling $P(y)$ as Bernoulli

$$P(y=1) = \frac{2}{4} = 0.5$$

$$P(y=-1) = 0.5$$

Classification example:

For a new feature vector x = [x1,x2,...], ie x = [3,9] in the example

$$\underset{y}{argmax} \left[\sum_{j=1}^{d} log P(\boldsymbol{x}^{(j)}|y) + log \ P(y) \right]$$

Classification example:

For a new feature vector x = [x1,x2,...], ie x = [3,9] in the example

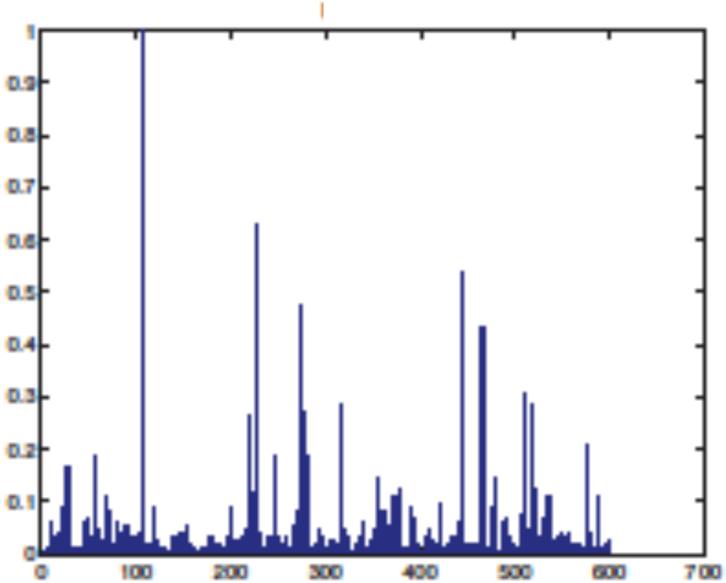
$$\underset{y}{argmax} \left[\sum_{j=1}^{d} logP(\boldsymbol{x}^{(j)}|y) + log\ P(y) \right]$$

$$g(y) = \begin{cases} \log \dfrac{e^{-\frac{(3-2.5)^2}{2\times 1.25^2}}}{\sqrt{2\pi}\cdot 1.25} + \log \dfrac{e^{-9}\, 9^9}{9!} + \log \frac{1}{2} & \text{if } y=1 \\ \log \dfrac{e^{-\frac{(3-(-1.5))^2}{2\times 1.5^2}}}{\sqrt{2\pi}\cdot 1.5} + \log \dfrac{e^{-12}\, 12^9}{9!} + \log \frac{1}{2} & \text{if } y=-1 \end{cases}$$

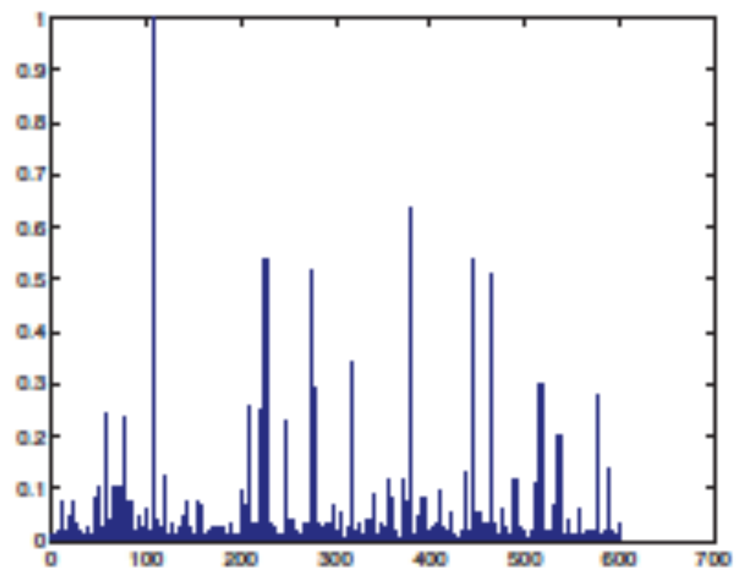
if $\dfrac{g(y=1)}{g(y=-1)} > 1$ then label for x is 1

Example of Naïve Bayesian Model

"Bag of words" Naive Bayesian models for document class



(a)



(b)

X-windows

document (represented as a bag-of-words bit vector), each column is a word

MS-windows

credit: K. Murphy

What about the decision boundary?

- Not explicit as in the case of decision tree
- This method is parametric, generative
  - The model was specified with parameters to generate label for test data

Pros and Cons of Naïve Bayesian Classifier

- Pros:
  - Simple approach
  - Good accuracy
  - Good for high dimensional data
- Cons:
  - The assumption of conditional independence of features
  - No explicit decision boundary
  - Sometimes has numerical issues

Assignments

- Finish Chapter 11 of the textbook
- Next time: Linear regression

Additional References

- Robert V. Hogg, Elliot A. Tanis and Dale L. Zimmerman. “Probability and Statistical Inference”
- Kelvin Murphy, “Machine learning, A Probabilistic perspective”

See you next time

See You!