CS685: Data Mining
Classification

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Tue, Wed, Fri 0900-1000 at CS101

Outline

1. Naïve Bayes classifiers
2. Bayesian networks
3. Support vector machines (SVM)

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2. Bayesian networks
3. Support vector machines (SVM)

Bayes' theorem

$$P(C|O) = \frac{P(O|C)P(C)}{P(O)}$$

- $P(C|O)$ is the probability of class C given object O – posterior probability
- $P(O|C)$ is the probability that O is from class C – likelihood probability
- $P(C)$ is the probability of class C – prior probability
- $P(O)$ is the probability of object O – evidence probability

$$posterior = \frac{likelihood \times prior}{evidence}$$

Naïve Bayes classifier

- Naïve Bayes classifier or simple Bayes classifier
- To classify a new object O_q, compute posterior probabilities $P(C_i|O_q)$ for all classes $C_i, i = 1, \ldots, k$

$$P(C_i|O_q) = \frac{P(O_q|C_i)P(C_i)}{P(O_q)}$$

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- $P(O_q)$ is constant for all classes and, therefore, can be removed
- Since it maximizes posterior probability, it is called maximum a posteriori (MAP) method
- If priors are unknown or same, this essentially maximizes the likelihood $P(O_q|C_i)$
- This is called maximum likelihood (ML) method

Computing likelihood

- In general, O_q has m features $O_{q_1}, \ldots, O_{q_m}$

$$
\begin{aligned}
P(O_q|C_i) &= P(O_{q_1}, O_{q_2}, \ldots, O_{q_m}|C_i) \\
&= P(O_{q_1}|C_i) \times P(O_{q_2}, \ldots, O_{q_m}|O_{q_1}, C_i) \\
&= P(O_{q_1}|C_i) \times P(O_{q_2}|O_{q_1}, C_i) \times P(O_{q_3}, \ldots, O_{q_m}|O_{q_1}, O_{q_2}, C_i)
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\therefore P(O_q|C_i) &= P(O_{q_1}, O_{q_2}, \dots, O_{q_m}|C_i) \\
&= \prod_{j=1}^{m} P(O_{q_j}|C_i)
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- If O_{q_j} is categorical, then empirical probabilities are the estimates

$$P(O_{q_j} = v|C_i) = \frac{|\{O_k \in C_i : O_{k_j} = v\}|}{|\{O_k \in C_i\}|}$$

- A particular discrete distribution can also be assumed

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- If O_{q_j} is numerical, then a certain continuous distribution is assumed
- Generally, Gaussian or normal distribution $N(\mu, \sigma)$
- μ and σ are estimated from training objects in C_i

$$P(O_{q_j} = v|C_i) = N(v; \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(v-\mu)^2}{2\sigma^2}}$$

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- $P(C_i)$ is just the empirical estimate $|C_i|/|D|$

Example: training

Class	Rank	Motivated	Exam marks
Successful (S)	2	Y	78.3
	99	Y	70.3
	5	N	88.5
	87	Y	75.1
Unsuccessful (U)	1	N	76.3
	90	N	66.2
	9	Y	68.1
	62	N	75.4

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Likelihoods

Class	Rank	Motivated	Exam marks
S	$\mu = 48.25$ $\sigma = 51.92$	$P(Y) = 0.75$ $P(N) = 0.25$	$\mu = 78.05$ $\sigma = 7.70$
U	$\mu = 40.50$ $\sigma = 42.68$	$P(Y) = 0.25$ $P(N) = 0.75$	$\mu = 71.50$ $\sigma = 5.10$

Example: testing

- $O_q = (70, Y, 67.3)$

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\begin{aligned}
P(O_q|S) &= P(70|S) \times P(Y|S) \times P(67.3|S) \times P(S) \\
&= N(70; 48.25, 51.92) \times 0.75 \times N(67.3; 78.05, 7.70) \times 0.5 \\
&= 0.00704 \times 0.75 \times 0.0195 \times 0.5 \\
&= 5.16 \times 10^{-5} \\
P(O_q|U) &= P(70|U) \times P(Y|U) \times P(67.3|U) \times P(U) \\
&= N(70; 40.50, 42.68) \times 0.25 \times N(67.3; 71.50, 5.10) \times 0.5 \\
&= 0.00736 \times 0.25 \times 0.0597 \times 0.5 \\
&= 5.49 \times 10^{-5}
\end{aligned}
$$

- Therefore, O_q is from class U

Discussion

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  - Robust to noise as probability of noise is low
  - Robust to irrelevant attributes as their probability tends to be uniform across classes
- Disadvantages
  - Treats attributes as independent and ignores any correlation information

Outline

Bayesian networks

- Bayesian networks or Bayesian belief networks or Bayes nets or belief nets
- Takes into account the correlations of attributes by modeling them as conditional probabilities
- Forms a directed acyclic graph (DAG)
- Edges model the *dependencies*
- Parent is the *cause* and children are the *effects*

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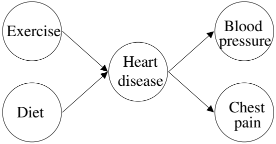
- Forms a directed acyclic graph (DAG)
- Edges model the *dependencies*
- Parent is the *cause* and children are the *effects*
- A node is conditionally independent of all its non-descendants given its parents
- For every node, there is a conditional probability table (CPT) that describes its values given its parents' values
- CPT for node X is of the form $P(X|parents(X))$

Example



- CPTs: rows are values; columns are parents (i.e., conditionals)
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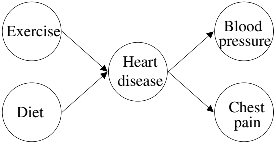

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Exercise (E)	Φ
regular (r)	0.70
irregular (i)	0.30

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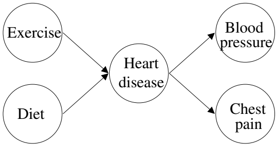

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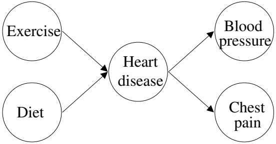

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no (n)	0.75	0.60	0.45	0.20

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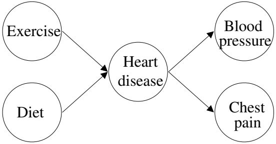

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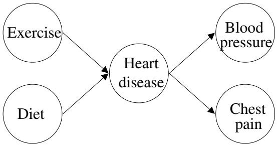

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Chest pain (C)	H=y	H=n
normal (m)	0.70	0.45
pain (p)	0.30	0.55

Classification using Bayesian networks

- Given no prior information, is a person suffering from heart disease?
- Essentially, a yes/no classification problem with some information
- Note that no other information (e.g., chest pain, etc.) are known
- Compute $P(H = y)$; if it is greater than $P(H = n)$, then predict "heart disease"

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P(H = y) &= \sum_{\alpha,\beta} [P(H = y | E = \alpha, D = \beta).P(E = \alpha, D = \beta)] \\
&= \sum_{\alpha,\beta} [P(H = y | E = \alpha, D = \beta).P(E = \alpha).P(D = \beta)] \\
&= 0.25 \times 0.70 \times 0.25 + 0.40 \times 0.70 \times 0.75 \\
&\quad\quad + 0.55 \times 0.30 \times 0.25 + 0.80 \times 0.30 \times 0.75 \\
&= 0.475
\end{aligned}
$$

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&= \frac{P(B = g|H = y).P(H = y)}{\sum_\alpha [P(B = g|H = \alpha).P(H = \alpha)]} \\
&= \frac{0.85 \times 0.475}{0.85 \times 0.475 + 0.20 \times 0.525} \\
&= 0.794
\end{aligned}
$$

Classification using Bayesian networks (contd.)

- Given a person has high blood pressure, unhealthy diet and irregular exercise, is she suffering from heart disease?
- Essentially, a yes/no classification problem with some information
- Note that not all information (e.g., chest pain, etc.) are known
- Compute $P(H = y|B = g, D = u, E = i)$; if it is greater than $P(H = n|B = g, D = u, E = i)$, then predict "heart disease"

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\begin{aligned}
& P(H = y|B = g, D = u, E = i) \\
& \quad = \frac{P(B = g|H = y, D = u, E = i).P(H = y|D = u, E = i)}{P(B = g|D = u, E = i)} \\
& \quad = \frac{P(B = g|H = y).P(H = y|D = u, E = i)}{\sum_\alpha [P(B = g|H = \alpha).P(H = \alpha|D = u, E = i)]} \\
& \quad = \frac{0.85 \times 0.80}{0.85 \times 0.80 + 0.20 \times 0.20} \\
& \quad = 0.944
\end{aligned}
$$

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- First, learning the network topology
  - Which edges are present?

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Training

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- First, learning the network topology
  - Which edges are present?
  - Domain knowledge from human experts
- Second, learning the CPTs
  - Same method as naïve Bayes
  - Empirical probabilities
  - If not categorical, use Gaussian

Discussion

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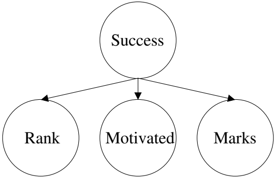
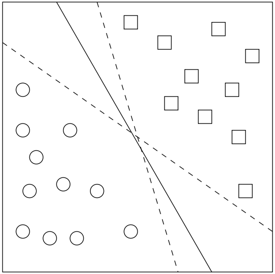
    - Class is boring and not paying attention
- Topology of network is very important
- For large CPTs, require lots of training data
- Naïve Bayes is a special case
    - Class is parent and attributes are children



Outline

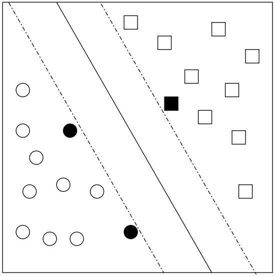
Support vector machines

- Support vector machine or SVM is a maximal margin classifier
- Binary classifier, i.e., two classes only
- It finds a hyperplane (called decision boundary) that separates the two classes
- Of multiple such hyperplanes, it finds the one whose distance or margin from the two classes is maximal
- Assumption is that classes are linearly separable



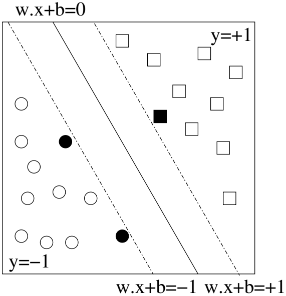
Support vectors

- Objects that are closest to the decision boundary on either side are called support vectors
- Optimal decision boundary and margin depend only on support vectors
- Support vectors are the most important objects
  - Optimal decision boundary will not change unless support vectors are changed
  - Other objects do not influence the decision boundary



Decision boundary

- Each object is represented as $\vec{x_i}$ with its corresponding class y_i
- For convenience, y_i is considered $+1$ or -1
- Decision boundary hyperplane is represented by $w.x + b = 0$
  - $\vec{w}$ essentially acts as weights on dimensions of $\vec{x}$
- *Support vectors* have $w.x + b = \pm 1$
  - w can always be scaled to achieve this
- For every object, $y_i(w.x_i + b) \geq 1$
  - Objects in class $y_i = +1$ have $w.x + b \geq +1$
  - Objects in class $y_i = -1$ have $w.x + b \leq -1$

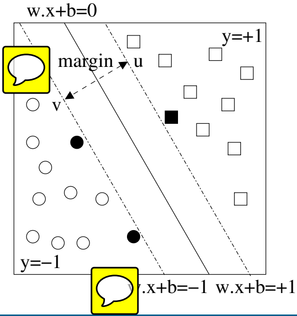


Margin

- Direction of $\vec{w}$ is perpendicular to decision boundary
- Margin is defined as the distance between the two hyperplanes $w.x + b = +1$ and $w.x + b = -1$
- Consider two points u and v on the two hyperplanes
- Margin d is distance between u and v

$$\vec{w}.(\vec{u} - \vec{v}) = 2$$

$$\therefore \; d = ||\vec{u} - \vec{v}|| = 2/||\vec{w}||$$



SVM problem specification

- SVM tries to maximize the margin d
- Constraints are on the objects
- Maximizing d is equivalent to minimizing $||w||$ or $||w||^2/2$

$$\min \frac{||w||^2}{2}$$
$$\text{s.t. } \forall i,\ y_i(w.x_i + b) \geq 1$$

- Convex (quadratic) optimization problem
- Lagrange multipliers λ_i for each object
- Karush-Kuhn-Tucker (KKT) conditions

SVM solution

- Essentially finds all λ_i and b
- Margin can then be expressed in terms of λ_i

$$\vec{w} = \sum_{\forall i} \lambda_i y_i \vec{x_i}$$

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- Only for objects that are *support vectors*, $\lambda_i > 0$
- For all other objects, $\lambda_i = 0$
- Thus, complexity of testing is only the number of support vectors
- Complexity of training is enormous though

Dual problem specification

- Minimization problem can be converted to maximization by primal-dual transformation
- Dual formulation becomes

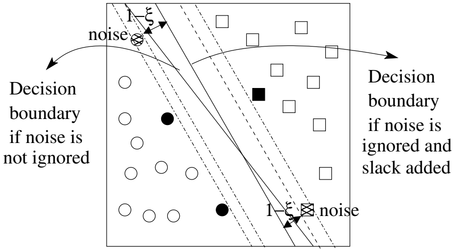
$$\max \sum_{\forall i} \lambda_i - \frac{1}{2} \sum_{\forall i} \sum_{\forall j} \lambda_i \lambda_j y_i y_j \vec{x_i} . \vec{x_j}$$

$$\text{s.t. } \forall i,\ \lambda_i \geq 0,\ \sum_{\forall i} \lambda_i y_i = 0$$

- Dual problem has only dot products of vectors

Handling noise

- SVM builds a classifier that is correct for *all* training objects
- If noise is present, decision boundary changes
- To handle noise, slack variables ξ_i are modeled
- For positive class, $w.x_i + b \geq +(1 - \xi_i)$
- For negative class, $w.x_i + b \leq -(1 - \xi_i)$
- Together, for every object, $y_i(w.x_i + b) \geq 1 - \xi_i$



SVM problem with slack

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- However, $||w||^2/2||$ cannot be simply minimized any more
- SVM may find a decision boundary with too many objects modeled as noise
- In other words, too much slack can be added
- Hence, slack needs to be factored in the minimization as well

$$\min \frac{||w||^2}{2} + C.\sum_{\forall i} f(\xi_i)$$

$$\text{s.t. } \forall i,\ y_i(w.x_i + b) \geq 1 - \xi_i$$

- $f(\xi_i)$ is a monotonic function and can be simply ξ_i itself
- Solution yields Lagrange multipliers λ_i and slack variables ξ_i for each object

Non-linearly separable data

- Data may not be linearly separable
- Find a transformation ϕ from x space to $\phi(x)$ space
- Data *becomes* linearly separable in $\phi(x)$ space

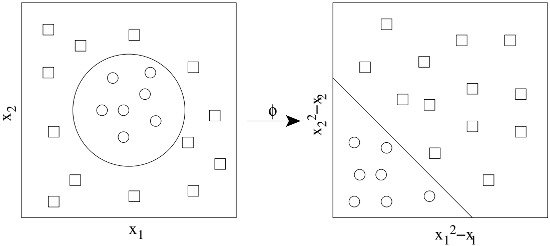
Example

- Suppose the decision boundary is a circle
- Centre is $0.5, 0.5$ and radius is 1
- Class is $+1$ if outside the circle, -1 otherwise
- Equation of decision boundary becomes

$$\sqrt{(x_1 - 0.5)^2 + (x_2 - 0.5)^2} = 1$$

$$\text{or, } x_1^2 - x_1 + x_2^2 - x_2 - 0.5 = 0$$

- In $(x_1^2 - x_1, x_2^2 - x_2)$ space, data becomes linearly separable



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- Even if such a transformation exists, the transformed objects may reside in a very high-dimensional or *infinite* dimensional space
- How to use an SVM then?
- Use the famous kernel trick
- A kernel is a function that computes the similarity between two vectors

Kernel trick

- Note that testing an object does not require value of w
- All it requires is an ability to compute *dot product* with the support vectors
- Same is true for training when dual of optimization problem is used
- Hence, testing can be simply written as

$$sign(w.\phi(x_q) + b) = sign\left(\sum_{\forall i} \lambda_i y_i \phi(\vec{x_i}).\phi(\vec{x_q}) + b\right)$$

- Use a kernel K that computes the dot product directly without transformation

$$K(x_i, x_j) = \phi(x_i).\phi(x_j)$$

Example of a kernel

- Vectors $\vec{u}$ and $\vec{v}$ are of dimensionality n
- Transformations $\phi(\vec{\cdot})$ are circles

$$\phi(\vec{u}) = \langle u_1 u_1, u_1 u_2, \ldots, u_n u_n, \sqrt{2} u_1, \ldots, \sqrt{2} u_n, 1 \rangle$$
$$\phi(\vec{v}) = \langle v_1 v_1, v_1 v_2, \ldots, v_n v_n, \sqrt{2} v_1, \ldots, \sqrt{2} v_n, 1 \rangle$$

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$$\text{Dot product } \phi(\vec{u}).\phi(\vec{v}) = \sum_{i=1}^{n} \sum_{j=1}^{n} u_i u_j v_i v_j + \sum_{i=1}^{n} \sqrt{2}u_i \sqrt{2}v_i + 1$$
$$= (\vec{u}.\vec{v} + 1)^2$$

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$$\begin{aligned}\text{Dot product } \phi(\vec{u}).\phi(\vec{v}) &= \sum_{i=1}^{n}\sum_{j=1}^{n} u_i u_j v_i v_j + \sum_{i=1}^{n} \sqrt{2}u_i \sqrt{2}v_i + 1 \\ &= (\vec{u}.\vec{v} + 1)^2\end{aligned}$$

$$\therefore K(\vec{u}, \vec{v}) = (\vec{u}.\vec{v} + 1)^2$$

- Dimensionality of $\phi(\cdot)$ is $n^2 + n + 1$
- Computation of kernel $K(\cdot, \cdot)$ requires only $O(n)$ computations

Example of kernels used

- Three kernels are most frequently used
- Polynomial kernel

$$K(u, v) = (u.v + 1)^h$$

- Gaussian radial basis kernel

$$K(u, v) = e^{-\frac{||u-v||^2}{2\sigma^2}}$$

- Sigmoid kernel

$$K(u, v) = tanh(\kappa u.v - \delta)$$

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- One-against-one
  - Every class is compared against every other
  - For m classes, $m(m-1)/2 = O(m^2)$ classifiers
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  - Every class is compared against every other
  - For m classes, $m(m-1)/2 = O(m^2)$ classifiers
  - Majority voting to determine final class
- One-against-others
  - For every class, belonging to class versus not in class
  - For m classes, m classifiers
  - Final class is one with highest value of $w.x + b$
  - Farthest away from margin

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