Machine learning: lecture 17

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Topics

- Clustering cont'd
  - semi-supervised clustering
  - clustering by dynamics
- Structured probability models
  - hidden Markov models

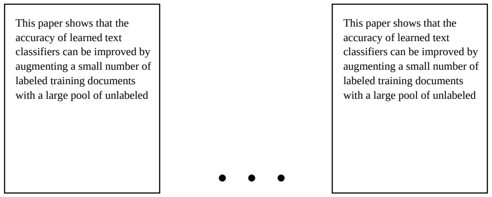
Overview of clustering methods

- Flat clustering methods
  - e.g., mixture models, k-means clustering
- Hierarchical clustering methods:
  - Top-down (splitting)
    - e.g., hierarchical mixture models
  - Bottom-up (merging)
    - e.g., hierarchical agglomerative clustering
- Spectral clustering
- Semi-supervised clustering
- Clustering by dynamics

Etc.

Semi-supervised clustering

- Let's assume we have some additional *relevance* information about the examples and we'd like clusters to preserve this information as much as possible.



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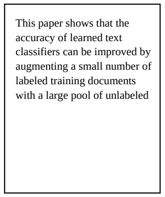

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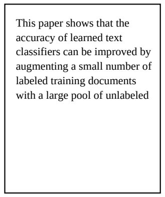

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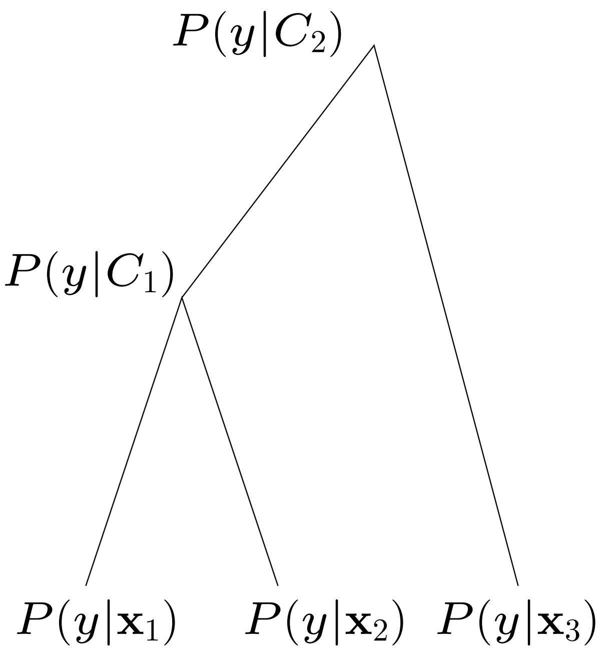
For example, by merging together documents we do not wish to loose information about the words they contain (word distributions).

$\mathbf{x}_i$	Training example (e.g., a text document)
y	Relevance variable (e.g., a word)
$P(y\|\mathbf{x}_i)$	Relevance information (e.g., word distribution)

Semi-supervised clustering cont'd

- We cluster documents $\{\mathbf{x}_i\}$ on the basis of their word distributions $\{P(y|\mathbf{x}_i)\}$
- The word distribution for a cluster is the average word distribution of documents in the cluster

$$P(y|C) = \frac{1}{|C|} \sum_{i \in C} P(y|\mathbf{x}_i)$$



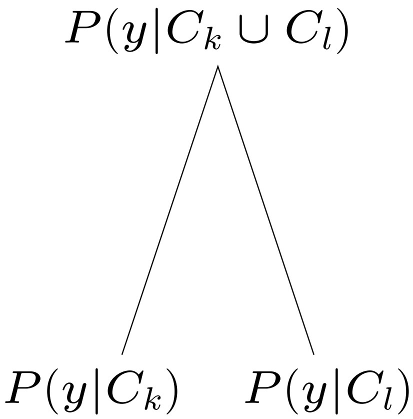
- When merging two clusters we need to take into account their sizes: for example, if $C_2 = C_1 \cup \mathbf{x}_3$ then

$$P(y|C_2) = \frac{1}{2+1}\big(2 \cdot P(y|C_1) + 1 \cdot P(y|\mathbf{x}_3)\big)$$

Semi-supervised clustering cont'd

- We still need to specify a distance metric to determine which clusters to merge and in what order.
- The distance should reflect how much relevance information we loose by merging the clusters

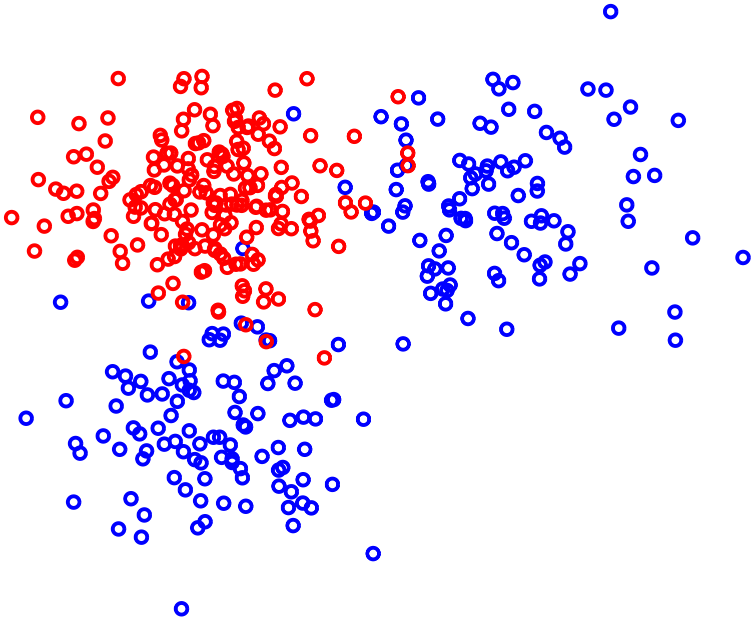
$$
\begin{aligned}
d(C_k, C_l) &= \big(|C_k| + |C_l|\big) \cdot I(y; \text{cluster identity}) \\
&= |C_k| \sum_y P(y|C_k) \log \frac{P(y|C_k)}{P(y|C_k \cup C_k)} \\
&\quad + |C_l| \sum_y P(y|C_l) \log \frac{P(y|C_l)}{P(y|C_k \cup C_k)}
\end{aligned}
$$



Semi-supervised clustering: example

- Suppose we have a set of labeled examples $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)$ and we take the label as the relevance variable:

$$P(y|\mathbf{x}_i) = \begin{cases} 1, & \text{if } y = y_i \\ 0, & \text{otherwise} \end{cases}$$



Clustering by dynamics

- We may wish to cluster time course signals not by direct comparison but in terms of dynamics that governs the signals
  - system behavior monitoring (anomaly detection)
  - biosequencies, processes

    etc.

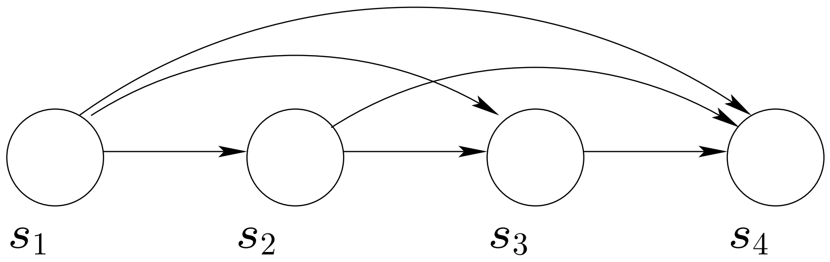
```
1.  0010011001000101000001000011101101010100
2.  0101111110100110101000001000000101011001
3.  1101011000000110110010001101111101011101
4.  1101010111101011110111101101101101000101
```

- We will use *Markov models* to capture the dynamics. The distance metric for clustering is based on similarity of models.

Modeling time course signals

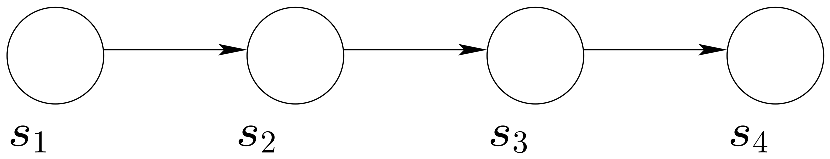
- Full probability model

$$P(s_1, \ldots, s_t) = P(s_1)P(s_2|s_1)P(s_3|s_2, s_1)P(s_4|s_3, s_2, s_1)\cdots$$



- First order Markov model

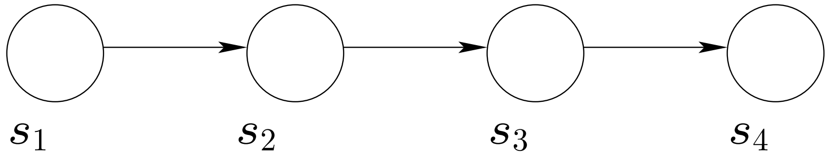
$$P(s_1, \ldots, s_t) = P(s_1)P(s_2|s_1)P(s_3|s_2)P(s_4|s_3)\cdots$$



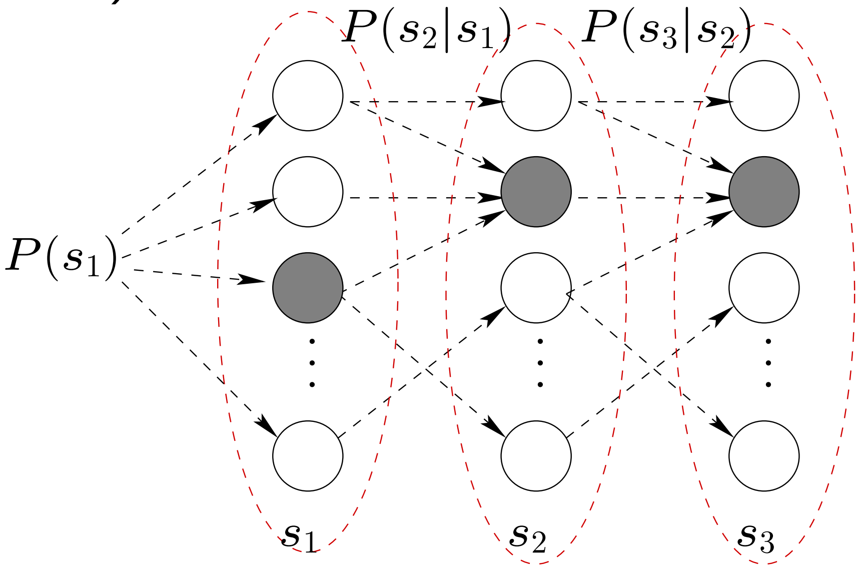
Discrete Markov models

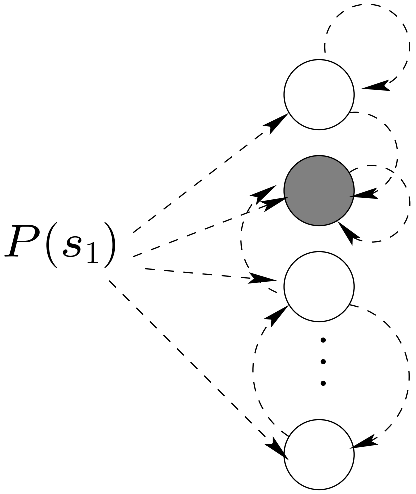
- Representation in terms of variables and dependencies (a graphical model):

$$P(s_1, \ldots, s_t) = P(s_1)P(s_2|s_1)P(s_3|s_2)P(s_4|s_3)\cdots$$



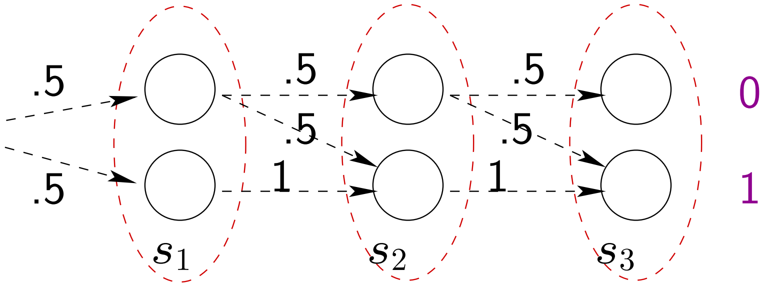
- Representation in terms of state transitions (transition diagram)





Discrete Markov models: properties

- The values of each s_t are known as *states*



$$P(\cdot): \quad \begin{array}{c} 0.5 \\ 0.5 \end{array}$$

$$P_1(\cdot|\cdot): \quad \begin{array}{cc} 0.5 & 0.5 \\ 0.0 & 1.0 \end{array}$$

- When successive state transitions are governed by the same (one-step) transition probability matrix $P_1(s_t|s_{t-1})$, the Markov model is *homogeneous*

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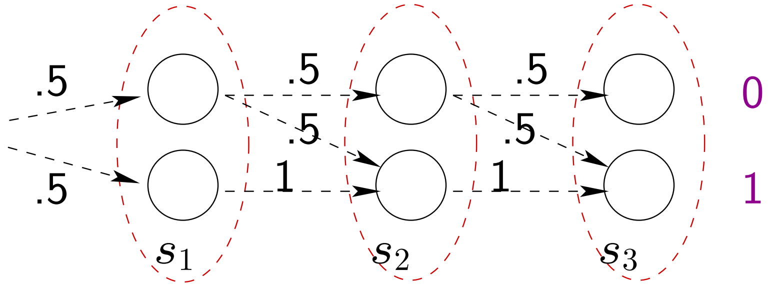

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- Example: a language model

$$\text{This} \rightarrow \text{is} \rightarrow \text{a} \rightarrow \text{boring} \rightarrow \ldots$$

Is a homogeneous Markov model appropriate in this case?

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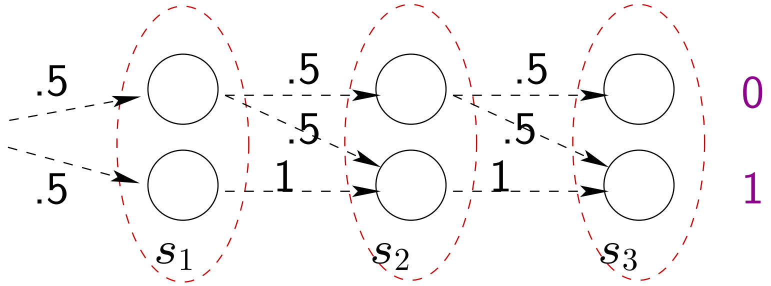

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- If after k transitions we can get from any state i to any other state j, the markov chain is *ergodic*.

  More precisely, the multi-step transition probabilities must satisfy $P_k(s|r) > 0$ for all r, s, and some fixed k

Discrete Markov models: ML estimation

$$S^{(1)} : \texttt{0010011001000101000001000011101101010100}$$
$$S^{(2)} : \texttt{0101111110100110101000001000000101011001}$$

$$l(S^{(1)}, S^{(2)}) = \sum_{i=1,2} \left[\log P(s_1^{(i)}) + \sum_{t=2}^{40} \log P_1(s_t^{(i)} | s_{t-1}^{(i)}) \right]$$

- ML estimates of the parameters (initial state and transition probabilities) are based on simple counts:

$$\begin{aligned}
\hat{n}(s) &= \# \text{ of times } s_1 = s \\
\hat{n}(r, s) &= \# \text{ number of times } r \rightarrow s \\
\hat{P}(s) &= \frac{\hat{n}(s)}{\sum_{s'} \hat{n}(s')} \\
\hat{P}_1(s|r) &= \frac{\hat{n}(r, s)}{\sum_{s'} \hat{n}(r, s')}
\end{aligned}$$

Simple clustering example cont'd

- Four binary sequences of length 40:

```
1.   0010011001000101000001000011101101010100
2.   0101111110100110101000001000000101011001
3.   1101011000000110110010001101111101011101
4.   1101010111101011110111101101101101000101
```

- We can estimate a Markov model based on any subset of the sequences
- We still need to derive the clustering metric based on the resulting transitition probabilities (dynamics)

Clustering metric

- To determine a distance between two arbitrary sequences

$$S^{(1)} = \{s_1^{(1)}, \ldots, s_{n_1}^{(1)}\} \text{ and } S^{(2)} = \{s_1^{(2)}, \ldots, s_{n_2}^{(2)}\},$$

we measure how well a Markov model would capture the sequences separately or jointly.

$$\begin{aligned} l(S^{(1)}) &= \log P(S^{(1)}|\hat{\theta}_1) \\ l(S^{(2)}) &= \log P(S^{(2)}|\hat{\theta}_2) \\ l(S^{(1)}, S^{(2)}) &= \log P(S^{(2)}|\hat{\theta}) + \log P(S^{(2)}|\hat{\theta}) \end{aligned}$$

where the parameters are ML estimates. Our distance is now defined as

$$d_M(S^{(1)}, S^{(2)}) = l(S^{(1)}) + l(S^{(2)}) - l(S^{(1)}, S^{(2)})$$

Simple example cont'd

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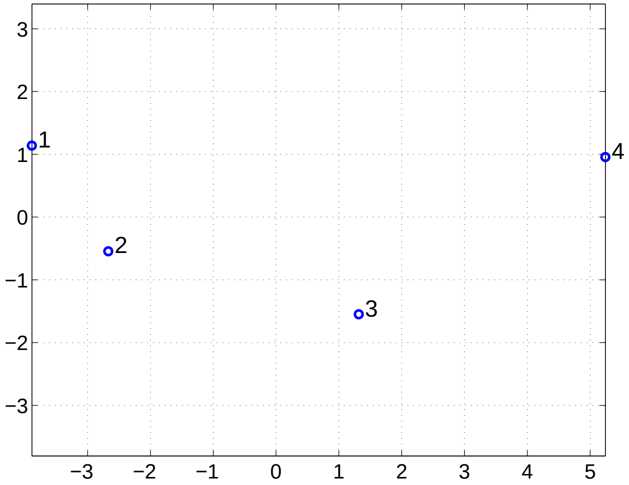
```

- The resulting pairwise distance matrix:

	1	2	3	4
1	0	0.4155	2.8010	5.8505
2	0.4155	0	1.6849	4.1799
3	2.8010	1.6849	0	1.7682
4	5.8505	4.1799	1.7682	0



(distances need to be recomputed after merging)

Clustering metrics, equivalence

- We have seen two different ways of inducing a metric, one based on information theory, the other through defining a model. These are closely related ideas.

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  Suppose we transform each observed binary sequence 0010011001000. . . into a bag of pairs $\{$00, 01, 10, ...$\}$.

  Let's use a variable y to refer to the possible pairs (4 of them). For example, $y = 1$ would mean 00.

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  Let's use a variable y to refer to the possible pairs (4 of them). For example, $y = 1$ would mean 00.

  We model each sequence with a distribution over pairs $P(y|S^{(1)})$ whose ML estimate is obtained by counting

$$\hat{P}(y|S^{(1)}) \quad = \quad \frac{n(y)}{n}$$

Clustering metrics, equivalence cont'd

The maximum value of the log-likelihood is given by

$$\begin{aligned} l(S^{(1)}) &= \sum_t \log \hat{P}(y_t|S^{(1)}) = \sum_y n(y) \log \hat{P}(y|S^{(1)}) \\ &= n \sum_y \frac{n(y)}{n} \log \hat{P}(y|S^{(1)}) \\ &= n \sum_y \hat{P}(y|S^{(1)}) \log \hat{P}(y|S^{(1)}) \end{aligned}$$

Similarly, if we merge two sequences

$$\begin{aligned} l(S^{(1)}, S^{(2)}) &= n \sum_y \hat{P}(y|S^{(1)}) \log \hat{P}(y|S^{(1)} \cup S^{(2)}) \\ & \quad + n \sum_y \hat{P}(y|S^{(2)}) \log \hat{P}(y|S^{(1)} \cup S^{(2)}) \end{aligned}$$

Clustering metrics, equivalence cont'd

- The model based metric is now given by

$$
\begin{aligned}
d_M(S^{(1)}, S^{(2)}) &= l(S^{(1)}) + l(S^{(2)}) - l(S^{(1)}, S^{(2)}) \\
&= n \sum_y \hat{P}(y|S^{(1)}) \log \frac{\hat{P}(y|S^{(1)})}{\hat{P}(y|S^{(1)} \cup S^{(2)})} \\
&\quad + n \sum_y \hat{P}(y|S^{(2)}) \log \frac{\hat{P}(y|S^{(2)})}{\hat{P}(y|S^{(1)} \cup S^{(2)})} \\
&= n \cdot I(y; \text{seq identity})
\end{aligned}
$$

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  - clustering by dynamics
- Structured probability models
  - hidden Markov models

Beyond Markov models

- How can we model

    1. 0101010101010101010101010101010101010101...

Beyond Markov models

- How can we model

  1. `0101010101010101010101010101010101010101...`
  2. `0010010010010010010010010010010010010010...`

Beyond Markov models

- How can we model

  1. 0101010101010101010101010101010101010101...
  2. 0010010010010010010010010010010010010010...
  3. 0100100010000101001000100001010010001000...

Beyond Markov models

- How can we model

  1. 0101010101010101010101010101010101010101...
  2. 0010010010010010010010010010010010010010...
  3. 0100100010000101001000100001010010001000...

- What about