MATH 829: Introduction to Data Mining and Analysis
Graphical Models I

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University of Delaware

May 2, 2016
We begin with a classical example (Whittaker, 1990):

- We study the examination marks of 88 students in five subjects: mechanics, vectors, algebra, analysis, statistics (Mardia, Kent, and Bibby, 1979).
- Mechanics and vectors were closed books.
- All the remaining exams were open books.
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We can examine the results using a stem and leaf plot.

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Note: Data appears to be normally distributed.
We compute the correlation between the grades of the students:

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We observe that the grades are positively correlated between subjects (performance of a student across subjects (good or bad) is consistent).

We now examine the inverse correlation matrix:

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Interpreting the inverse correlation matrix:

Diagonal entries $\frac{1}{1 - R^2}$ are related to the proportion of variance explained by regressing the variable on the other variables.

O-diagonal entries: proportional to the correlation of pairs of variables, given the rest of the variables.

For example, $R^2_{\text{mech}} = (1 - 0.60 - 1) / 1.60 = 37.5\%$.

For the o-diagonal entries, we first scale the inverse correlation matrix $\Omega = (\omega_{ij})$ by computing $\omega_{ij} \sqrt{\omega_{ii} \omega_{jj}}$:

\[
\begin{array}{cccc}
\text{mech} & \text{vect} & \text{alg} & \text{anal} & \text{stat} \\
1.0 & -0.33 & 1.0 & -0.23 & -0.08 \\
& & -0.28 & 1.0 & -0.43 \\
& & & & 1.0 \\
\end{array}
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The o-diagonal entries of the scaled inverse correlation matrix are the negative of the conditional correlation coefficients (i.e., the correlation coefficients after conditioning on the rest of the variables).
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\[ \begin{pmatrix}
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Notation:

We denote the fact that two random variables $X$ and $Y$ are independent by $X \perp \perp Y$. We write $X \perp \perp Y | \{Z_1, \ldots, Z_n\}$ when $X$ and $Y$ are independent given $Z_1, \ldots, Z_n$.

When the context is clear (i.e. when working with a fixed collection of random variables $\{X_1, \ldots, X_n\}$), we write $X_i \perp \perp X_j | \text{rest}$ instead of $X_i \perp \perp X_j | \{X_k : 1 \leq k \leq n, k \neq i, j\}$.

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1. anal \perp mech | rest.
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We put no edge between two variables iff they are conditionally independent (given the rest of the variables).
Graphical models (a.k.a. Markov random fields) are multivariate probability models whose independence structure is characterized by a graph.
Independence and factorizations

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Recall: Independence of random vectors is characterized by a factorization of their joint density:
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- **Independent variables:** For two random vectors $X, Y$:

  \[ X \perp Y \iff f_{X,Y}(x, y) = g(x)h(y) \quad \forall x, y \]

  for some functions $g, h$. 

- **Conditionally independent variables:** Similarly, for three random vectors $X, Y, Z$:

  \[ X \perp Y \mid Z \iff f_{X,Y,Z}(x, y, z) = g(x, z)h(y, z) \quad \forall x, y, z \text{ for which } f_Z(z) > 0 \]
Independence and factorizations

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- The **conditional independence graph** of $X$ is the graph $G = (V, E)$ where $V = \{1, \ldots, p\}$ and

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- A subset $S \subset V$ is said to separate $A \subset V$ from $B \subset V$ if every path from $A$ to $B$ contains a vertex in $S$. 

**Theorem:** (the separation theorem) Suppose the density of $X$ is positive and continuous. Let $V = A \cup S \cup B$ be a partition of $V$ such that $S$ separates $A$ from $B$. Then $X_A \independent X_B \mid X_S$. 

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Independence graphs

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Notation: If \( X = (X_1, \ldots, X_p) \) and \( A \subset \{1, \ldots, p\} \), then \( X_A := (X_i : i \in A) \).
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Let $X = (X_1, \ldots, X_p)$ be a random vector and let $G$ be a graph on \{1, \ldots, p\}. The vector is said to satisfy:

1. The \textit{pairwise Markov property} if $X_i \perp \perp X_j \mid \text{rest}$ whenever $(i,j) \not\in E$.
2. The \textit{local Markov property} if for every vertex $i \in V$, $X_i \perp \perp X_{V \setminus \text{cl}(i)} \mid X_{\text{ne}(i)}$, where $\text{ne}(i) = \{j \in V : (i,j) \in E, j \neq i\}$ and $\text{cl}(i) = \{i\} \cup \text{ne}(i)$.
3. The \textit{global Markov property} if for every disjoint subsets $A, S, B \subset V$ such that $S$ separates $A$ from $B$ in $G$, we have $X_A \perp \perp X_B \mid X_S$.

Clearly, global $\Rightarrow$ local $\Rightarrow$ pairwise. When $X$ has a positive and continuous density, by the separation theorem, pairwise $\Rightarrow$ global and so all three properties are equivalent.
Markov properties

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Markov properties

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Example: the local Markov property

Illustration of the local Markov property:
An **undirected graphical model** (a.k.a. Markov random field) is a set of random variables satisfying a Markov property.

The Hammersley–Clifford theorem

Let $X$ be a random vector with a positive and continuous density $f$. Then $X$ satisfies the pairwise Markov property with respect to a graph $G$ if and only if $f(x) = \prod_{C \in C} \psi_C(x)$, where $C$ is the set of (maximal) cliques (complete subgraphs) of $G$. 

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The Hammersley–Clifford theorem

- An **undirected graphical model** (a.k.a. Markov random field) is a set of random variables satisfying a Markov property.
- Independence and conditional independence correspond to a factorization of the joint density.

**Theorem:** (Hammersley–Clifford) Let \( X \) be a random vector with a positive and continuous density \( f \). Then \( X \) satisfies the pairwise Markov property with respect to a graph \( G \) if and only if
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- The Hammersley–Clifford theorem provides a necessary and sufficient condition for a random vector to have a Markov random field structure.

**Theorem:** (Hammersley–Clifford) Let $X$ be a random vector with a positive and continuous density $f$. Then $X$ satisfies the *pairwise Markov property* with respect to a graph $G$ if and only if

$$f(x) = \prod_{C \in \mathcal{C}} \psi_C(x_C),$$

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