Directed Graphical Models I

Definition and Basic Properties

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Recap

- We talked about reasonably weak assumption to facilitate the efficient representation of a probabilistic model
- Independence assumptions reduce the number of interacting variables, e.g.
  - $p(\mathbf{x}, \mathbf{y}, \mathbf{z}) = p(\mathbf{x})p(\mathbf{y})p(\mathbf{z})$
  - $p(x_1, \ldots, x_d) = p(x_1)p(x_2|x_1) \ldots p(x_d|x_{d-1})$
- Chain rule: $p(\mathbf{x}) = \prod_{i=1}^{d} p(x_i|\mathrm{pre}_i)$ where $\mathrm{pre}_i = \{x_1, \ldots, x_{i-1}\}$ are the predecessors of x_i in a given ordering of the variables.
- Parametric assumptions, e.g. on $p(x_i|\mathrm{pre}_i)$ in the chain rule, restrict the way the variables may interact.

Program

1. Visualising factorisations with directed acyclic graphs
2. Directed graphical models

Program

1. Visualising factorisations with directed acyclic graphs
   - Conditional independencies simplify factors in the chain rule
   - Visualisation as a directed acyclic graph
   - Graph concepts

2. Directed graphical models

Cond independencies simplify factors in the chain rule

- We can always express a pdf/pmf $p(\mathbf{x})$ in terms of the chain rule as

$$p(\mathbf{x}) = p(x_1)p(x_2|x_1)p(x_3|x_2, x_1)\dots p(x_d|x_1, \dots x_{d-1}) \quad (1)$$

$$= \prod_{i=1}^{d} p(x_i|\mathrm{pre}_i) \quad (2)$$

- Assume that, for each i, there is a minimal subset of variables $\mathrm{pa}_i \subseteq \mathrm{pre}_i$ (called the "parents" of x_i) such that $p(\mathbf{x})$ satisfies

$$x_i \perp\!\!\!\perp (\mathrm{pre}_i \setminus \mathrm{pa}_i) \mid \mathrm{pa}_i \quad \text{for all } i \quad (3)$$

- By conditional independence: $p(x_i|\mathrm{pre}_i) = p(x_i|\mathrm{pa}_i)$
- With the convention $\mathrm{pa}_1 = \varnothing$, we obtain the factorisation

$$p(x_1, \dots, x_d) = \prod_{i=1}^{d} p(x_i|\mathrm{pa}_i) \quad (4)$$

What can we do with it?

$$p(x_1, \ldots, x_d) = \prod_{i=1}^{d} p(x_i|\mathrm{pa}_i)$$

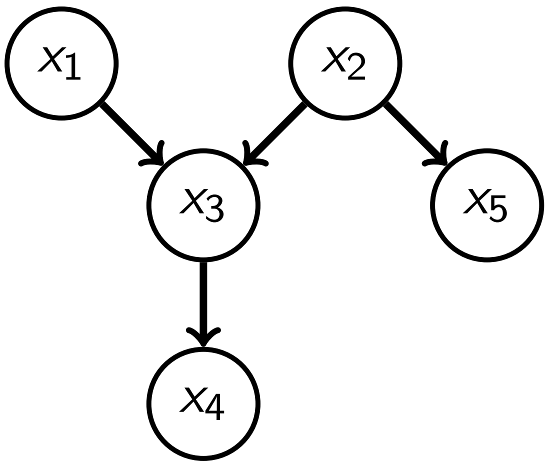
1. $p(x_i|\mathrm{pa}_i)$ involve fewer interacting variables than $p(x_i|\mathrm{pre}_i)$.
   - Makes them easier to model.
   - If specified as a table, fewer numbers are needed for their representation (computational advantage).
2. We can visualise the interactions between the variables with a graph.

Visualisation as a directed graph

Assume $p(\mathbf{x}) = \prod_{i=1}^{d} p(x_i|\mathrm{pa}_i)$ with $\mathrm{pa}_i \subseteq \mathrm{pre}_i$. We visualise the model as a graph with the random variables x_i as nodes, and directed edges that point from the $x_j \in \mathrm{pa}_i$ to the x_i. This results in a directed acyclic graph (DAG).

Example:

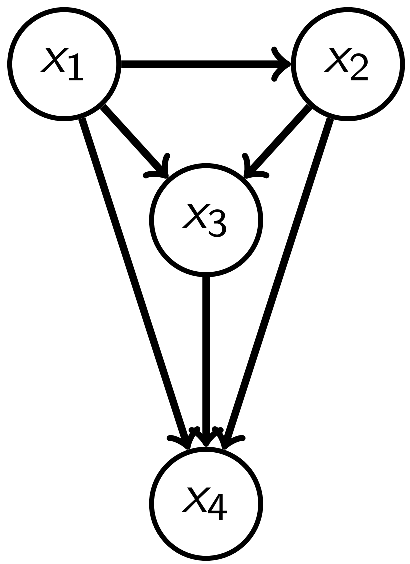
$$p(x_1, x_2, x_3, x_4, x_5) = p(x_1)p(x_2)p(x_3|x_1, x_2)p(x_4|x_3)p(x_5|x_2)$$



Visualisation as a directed graph

Example:

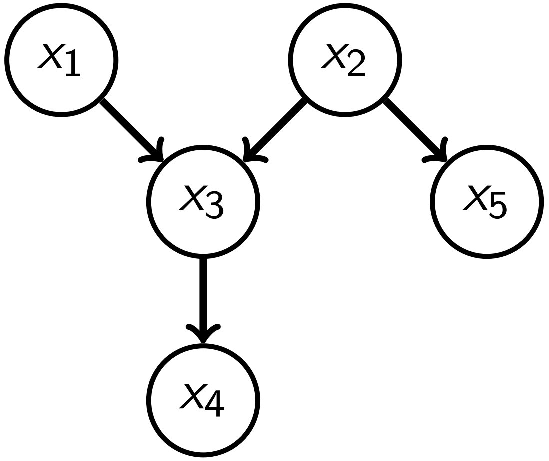
$$p(x_1, x_2, x_3, x_4) = p(x_1)p(x_2|x_1)p(x_3|x_1, x_2)p(x_4|x_1, x_2, x_3)$$



Factorisation obtained by chain rule $\equiv$ fully connected directed acyclic graph. Different orderings give different graphs.

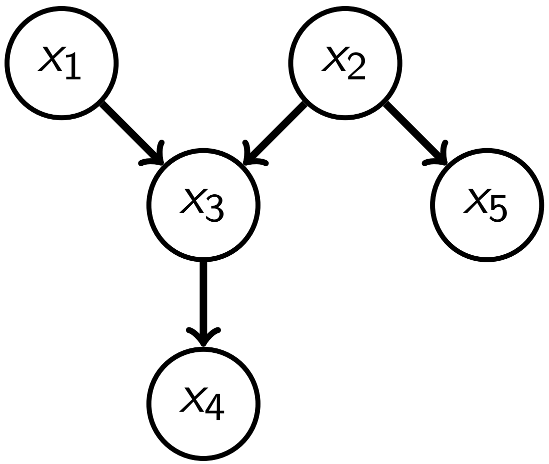
Graph concepts

- Directed graph: graph where all edges are directed
- Directed acyclic graph (DAG): by following the direction of the arrows you will never visit a node more than once
- x_i is a parent of x_j if there is a (directed) edge from x_i to x_j. The set of parents of x_i in the graph is denoted by $\mathrm{pa}(x_i) = \mathrm{pa}_i$, e.g. $\mathrm{pa}(x_3) = \mathrm{pa}_3 = \{x_1, x_2\}$.
- x_j is a child of x_i if $x_i \in \mathrm{pa}(x_j)$, e.g. x_3 and x_5 are children of x_2.



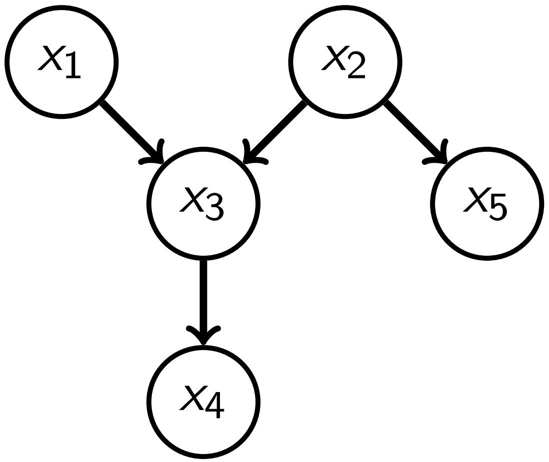
Graph concepts

- A path or trail from x_i to x_j is a sequence of distinct connected nodes starting at x_i and ending at x_j. The direction of the arrows does *not* matter. For example: x_5, x_2, x_3, x_1 is a trail.
- A directed path is a sequence of connected nodes where we follow the direction of the arrows. For example: x_1, x_3, x_4 is a directed path. But x_5, x_2, x_3, x_1 is not a directed path.



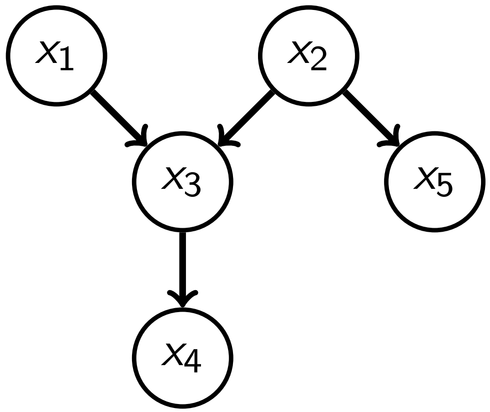
Graph concepts

- The ancestors $\mathrm{anc}(x_i)$ of x_i are all the nodes where a directed path leads to x_i. For example, $\mathrm{anc}(x_4) = \{x_1, x_3, x_2\}$.
- The descendants $\mathrm{desc}(x_i)$ of x_i are all the nodes that can be reached on a directed path from x_i. For example, $\mathrm{desc}(x_1) = \{x_3, x_4\}$.
  (Note: sometimes, x_i is included in the set of ancestors and descendants)
- The non-descendents of x_i are all the nodes in a graph except x_i and the descendants of x_i. For example, $\mathrm{nondesc}(x_3) = \{x_1, x_2, x_5\}$



Graph concepts

- Topological ordering: an ordering $(x_1, \ldots, x_d)$ of some variables x_i is topological relative to a graph if parents come before their children in the ordering.
  (whenever there is a directed edge from x_i to x_j, x_i occurs prior to x_j in the ordering.)
- Examples for the graph on the right: (non-exhaustive list)
  - x_1, x_2, x_3, x_4, x_5
  - x_2, x_5, x_1, x_3, x_4
  - x_2, x_1, x_3, x_5, x_4



- There is always at least one ordering that is topological relative to a DAG.

Program

1. Visualising factorisations with directed acyclic graphs
   - Conditional independencies simplify factors in the chain rule
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   - Graph concepts

2. Directed graphical models

Program

1. Visualising factorisations with directed acyclic graphs

2. Directed graphical models
   - Definition
   - Conditionals, marginals, and ancestral sampling
   - Examples

Directed graphical model (DGM)

- We started with a factorised pdf/pmf and associated a DAG with it.
- We can also go the other way around and start with a DAG.
- *Definition* A directed graphical model based on a DAG G with d nodes and associated random variables x_i is the set of pdfs/pmfs that factorise as

$$p(x_1, \ldots, x_d) = \prod_{i=1}^{d} k(x_i | \mathrm{pa}_i)$$

where the $k(x_i|\mathrm{pa}_i)$ are some conditional pdfs/pmfs. (They are sometimes called kernels or factors)
- A pdf/pmf $p(x_1, \ldots, x_d)$ that can be written as above is said to "factorise over the graph G". We say that it has property $F(G)$ ("F" for factorisation).

Why set of pdfs/pmfs?

- The directed graphical model corresponds to a set of probability distributions .
- This is because we did not specify any numerical values for the $k(x_i|\mathrm{pa}_i)$. We only specified which variables the conditionals take as input (namely x_i and pa_i).
- The set includes all those distributions that you get by looping, for all variables x_i, over all possible $k(x_i|\mathrm{pa}_i)$.
  (e.g. tables or parameter values in parametrised models)
- While a probability distribution corresponds to a probabilistic model, a set of probability distributions (probabilistic models) is often called a statistical model.
- Individual pdfs/pmf in the set are typically also called a directed graphical model.
- Other names for directed graphical models: belief network, Bayesian network, Bayes network.

The factors $k(x_i|\mathrm{pa}_i)$ equal the conditionals $p(x_i|\mathrm{pa}_i)$

- When we decomposed a given distribution $p(\mathbf{x})$ with the chain rule and inserted conditional independencies, we obtained

$$p(\mathbf{x}) = \prod_i p(x_i|\mathrm{pa}_i)$$

  with $p(x_i|\mathrm{pa}_i)$ equal to the conditionals of x_i given pa_i.
- We now show that the $k(x_i|\mathrm{pa}_i)$ in the definition of the DGM are equal to the conditionals $p(x_i|\mathrm{pa}_i)$ wrt $p(\mathbf{x})$, as above.
- First step is to label the variables such that the ordering $x_1, \ldots, x_d$ is topological relative to the DAG G.
- In a topological ordering, the parents come before the children. Hence $\mathrm{pa}_i \subseteq \mathrm{pre}_i = (x_1, \ldots, x_{i-1})$

The factors $k(x_i|\mathrm{pa}_i)$ equal the conditionals $p(x_i|\mathrm{pa}_i)$

$$p(x_1, \ldots, x_d) = \prod_{i=1}^d k(x_i|\mathrm{pa}_i)$$

- We next compute $p(x_1, \ldots, x_{d-1})$ using the sum rule:

$$\begin{aligned}
p(x_1, \ldots, x_{d-1}) &= \int p(x_1, \ldots, x_d)\mathrm{d}x_d \\
&= \int \prod_{i=1}^{d} k(x_i|\mathrm{pa}_i)\mathrm{d}x_d \\
&= \int \prod_{i=1}^{d-1} k(x_i|\mathrm{pa}_i)k(x_d|\mathrm{pa}_d)\mathrm{d}x_d \quad (x_d \notin \mathrm{pa}_i, i < d) \\
&= \prod_{i=1}^{d-1} k(x_i|\mathrm{pa}_i) \int k(x_d|\mathrm{pa}_d)\mathrm{d}x_d \\
&= \prod_{i=1}^{d-1} k(x_i|\mathrm{pa}_i)
\end{aligned}$$

The factors $k(x_i|\mathrm{pa}_i)$ equal the conditionals $p(x_i|\mathrm{pa}_i)$

Hence:

$$p(x_d|x_1,\ldots,x_{d-1}) = \frac{p(x_1,\ldots,x_d)}{p(x_1,\ldots,x_{d-1})} = \frac{\prod_{i=1}^{d} k(x_i|\mathrm{pa}_i)}{\prod_{i=1}^{d-1} k(x_i|\mathrm{pa}_i)}$$
$$= k(x_d|\mathrm{pa}_d)$$

Split $(x_1,\ldots,x_{d-1}) = \mathrm{pre}_d$ into non-overlapping sets pa_d and $\tilde{\mathbf{x}}_d = \mathrm{pre}_d \setminus \mathrm{pa}_d$ so that $p(x_d|x_1,\ldots,x_{d-1}) = p(x_d|\tilde{\mathbf{x}}_d,\mathrm{pa}_d)$.
By the product rule, we have

$$p(x_d,\tilde{\mathbf{x}}_d|\mathrm{pa}_d) = p(x_d|\tilde{\mathbf{x}}_d,\mathrm{pa}_d)p(\tilde{\mathbf{x}}_d|\mathrm{pa}_d)$$
$$= k(x_d|\mathrm{pa}_d)p(\tilde{\mathbf{x}}_d|\mathrm{pa}_d)$$

Next sum out $\tilde{\mathbf{x}}_d$ to obtain

$$p(x_d|\mathrm{pa}_d) = \int p(x_d,\tilde{\mathbf{x}}_d|\mathrm{pa}_d)\mathrm{d}\tilde{\mathbf{x}}_d = k(x_d|\mathrm{pa}_d)\int p(\tilde{\mathbf{x}}_d|\mathrm{pa}_d)\mathrm{d}\tilde{\mathbf{x}}_d$$
$$= k(x_d|\mathrm{pa}_d)$$

where we have used that x_d and pa_d are not part of $\tilde{\mathbf{x}}_d$.

The factors $k(x_i|\mathrm{pa}_i)$ equal the conditionals $p(x_i|\mathrm{pa}_i)$

Hence:

$$p(x_d|x_1, \ldots, x_{d-1}) = k(x_d|\mathrm{pa}_d) = p(x_d|\mathrm{pa}_d)$$

Next, note that $p(x_1, \ldots, x_{d-1})$ has the same form as $p(x_1, \ldots, x_d)$: apply the same procedure to all $p(x_1, \ldots, x_k)$, for smaller and smaller $k \leq d-1$

Proves that for DGMs, the factors $k(x_i|\mathrm{pa}_i)$ are equal to the conditionals $p(x_i|\mathrm{pa}_i)$ of $p(\mathbf{x})$.

In what follows, we will thus use $p(x_i|\mathrm{pa}_i)$ instead of $k(x_i|\mathrm{pa}_i)$ when we work with DGMs.

Some independences satisfied by DGMs

- When we started from the chain rule $p(\mathbf{x}) = \prod_i p(x_i|\mathrm{pre}_i)$, we inserted the conditional independencies

$$x_i \perp\!\!\!\perp (\mathrm{pre}_i \setminus \mathrm{pa}_i) \mid \mathrm{pa}_i \quad \text{for all } i \tag{5}$$

  to obtain $p(\mathbf{x}) = \prod_i p(x_i|\mathrm{pa}_i)$.
- For directed graphical models, we started with the factorisation $p(\mathbf{x}) = \prod_i p(x_i|\mathrm{pa}_i)$. Does it imply the above conditional independences?
- In the proof above, we found that for all i,

$$p(x_i|x_1, \ldots, x_{i-1}) = p(x_i|\mathrm{pa}_i), \tag{6}$$

  which means that $x_i \perp\!\!\!\perp (\mathrm{pre}_i \setminus \mathrm{pa}_i) \mid \mathrm{pa}_i$ for all i in the chosen topological ordering.
- Chosen topological ordering was not special: holds for all orderings that are topological relative to the DAG.
- Factorisation $p(\mathbf{x}) = \prod_i p(x_i|\mathrm{pa}_i)$ implies the independences and vice versa.

Some marginals

- In the proof, we also found that (for the chosen topological ordering)

$$p(x_1, \ldots, x_k) = \prod_{i=1}^{k} p(x_i | \mathrm{pa}_i) \tag{7}$$

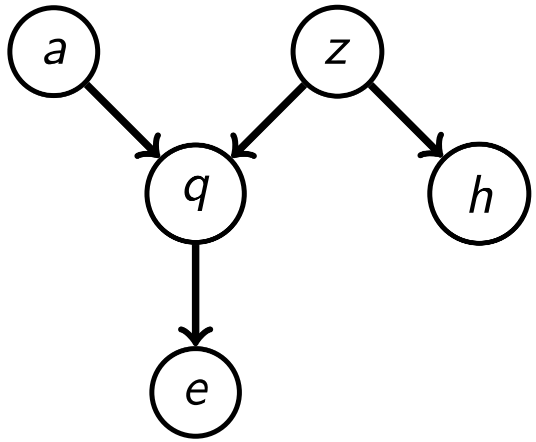
- The marginal joint distribution of the first k variables in the chosen topological ordering is given by the product of the corresponding factors $p(x_i | \mathrm{pa}_i)$.
- Chosen topological ordering was not special: holds for all orderings that are topological relative to the DAG.
- While marginalisation can be very expensive (see later), the above marginals are available for free for DGMs.

Ancestral sampling

- The DAG not only specifies the joint distribution $p(\mathbf{x}) = \prod_{i=1}^{d} p(x_i | \mathrm{pa}_i)$ but also a sampling/data generating process.
- To generate data from $p(\mathbf{x})$:
  1. Pick an ordering $x_1, \ldots, x_d$ of the random variables that is topological to G.
  2. x_1 does not have any parents, i.e. set $\mathrm{pa}_1 = \varnothing$ and $p(x_1 | \varnothing) = p(x_1)$.
  3. Following the topological ordering, sample from $p(x_i | \mathrm{pa}_i)$, $i = 1, \ldots, d$.
- It's called ancestral sampling because we sample the parents before the children, following the arrows in the DAG.
- The DAG visualises the data generating process, which can be used as modelling tool.

Example

DAG:



Random variables: a, z, q, e, h

Parent sets: $\mathrm{pa}_a = \mathrm{pa}_z = \varnothing, \mathrm{pa}_q = \{a, z\}, \mathrm{pa}_e = \{q\}, \mathrm{pa}_h = \{z\}$.

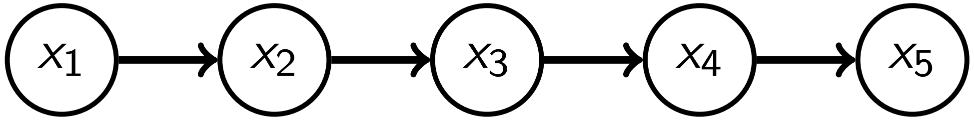
Directed graphical model: set of pdfs/pmfs $p(a, z, q, e, h)$ that factorise as:

$$p(a, z, q, e, h) = p(a)p(z)p(q|a, z)p(e|q)p(h|z)$$

Data generating process: For topological ordering a, z, q, e, h:
$a \sim p(a), z \sim p(z), q \sim p(q|a, z), e \sim p(e|q), h \sim p(h|z)$

Example: Markov chain

DAG:



Random variables: x_1, x_2, x_3, x_4, x_5

Parent sets:
$\mathrm{pa}_1 = \varnothing, \mathrm{pa}_2 = \{x_1\}, \mathrm{pa}_3 = \{x_2\}, \mathrm{pa}_4 = \{x_3\}, \mathrm{pa}_5 = \{x_4\}.$

Directed graphical model: set of pdfs/pmfs $p(x_1, \ldots, x_5)$ that factorise as:

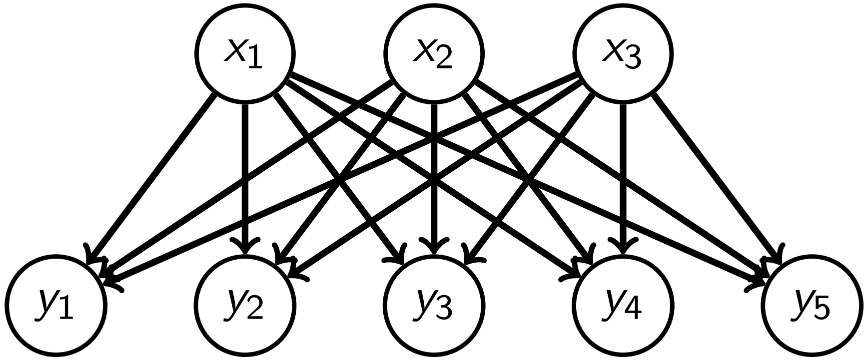
$$p(\mathbf{x}) = p(x_1)p(x_2|x_1)p(x_3|x_2)p(x_4|x_3)p(x_5|x_4)$$

Data generating process: For topological ordering $x_1, \ldots, x_5$:
$x_1 \sim p(x_1), x_2 \sim p(x_2|x_1), x_3 \sim p(x_3|x_2), x_4 \sim p(x_4|x_3), x_5 \sim p(x_5|x_4)$

Example: Probabilistic PCA, factor analysis, ICA, VAEs

(PCA/ICA: principal/independent component analysis; VAE: var autoencoders)

DAG:



Random variables: $x_1, x_2, x_3, y_1, \ldots, y_5$

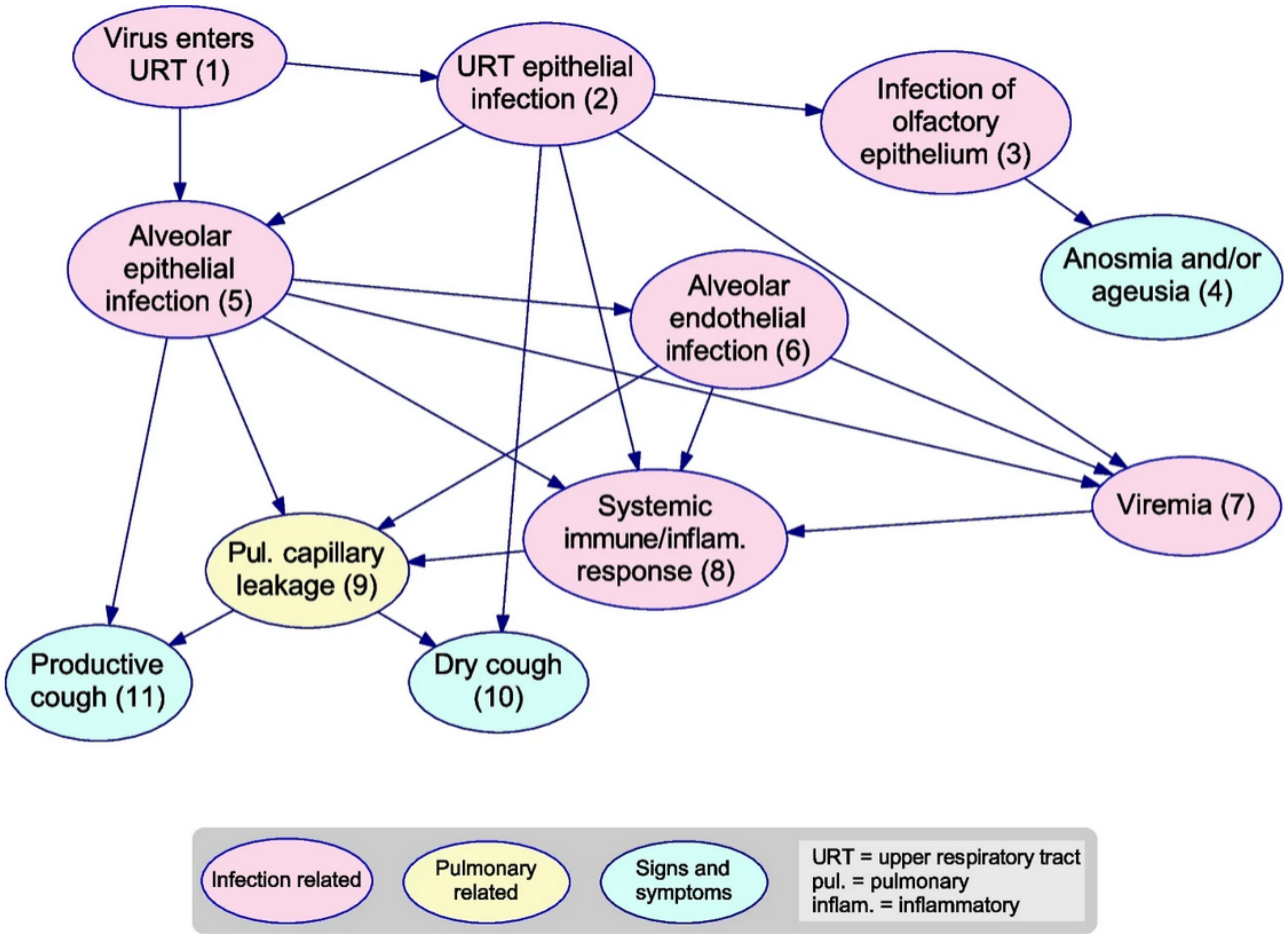
Parent sets: $\mathrm{pa}(x_i) = \emptyset, \mathrm{pa}(y_i) = \{x_1, x_2, x_3\}$ for all i.

Directed graphical model: set of pdfs/pmfs $p(x_1, x_2, x_3, y_1, \ldots, y_5)$ that factorise as:

$$p(x_1, x_2, x_3, y_1, \ldots, y_5) = p(x_1)p(x_2)p(x_3)p(y_1|x_1, x_2, x_3) \\ p(y_2|x_1, x_2, x_3) \ldots p(y_5|x_1, x_2, x_3)$$

Data generating process: topological ordering $x_1, x_2, x_3, y_1, \ldots, y_4$
$x_i \sim p(x_i), y_i \sim p(y_i|x_1, x_2, x_3)$

Example: Modeling COVID-19 disease processes



BMC Med Res Methodol, 2023. `https://doi.org/10.1186/s12874-023-01856-1`

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