# Basic Assumptions for Efficient Model Representation 

Chris Williams<br>(based on slides by Michael U. Gutmann)

Probabilistic Modelling and Reasoning (INFR11134)
School of Informatics, The University of Edinburgh

Spring Semester 2024

## Recap

$$
p\left(\mathbf{x} \mid \mathbf{y}_{o}\right)=\frac{\sum_{\mathbf{z}} p\left(\mathbf{x}, \mathbf{y}_{o}, \mathbf{z}\right)}{\sum_{\mathrm{x}, \mathrm{z}} p\left(\mathbf{x}, \mathbf{y}_{o}, \mathbf{z}\right)}
$$

Assume that $\mathbf{x}, \mathbf{y}, \mathbf{z}$ each are $d=500$ dimensional, and that each element of the vectors can take $K=10$ values.

- Issue 1: To specify $p(\mathbf{x}, \mathbf{y}, \mathbf{z})$, we need to specify $K^{3 d}-1=10^{1500}-1$ non-negative numbers, which is impossible.
Topic 1: Representation What reasonably weak assumptions can we make to efficiently represent $p(\mathbf{x}, \mathbf{y}, \mathbf{z})$ ?


## Two fundamental assumptions

Consider two assumptions:

1. only a limited number of variables may directly interact with each other (independence assumptions)
2. for any number of interacting variables, the form of interaction is limited or restricted (often: parametric family assumptions)

The two assumptions can be used together or separately.

## Program

1. Independence assumptions
2. Assumptions on form of interaction

## Program

1. Independence assumptions

- Definition and properties of statistical independence
- Factorisation of the pdf and reduction in the number of directly interacting variables

2. Assumptions on form of interaction

## Statistical independence

- Let $\mathbf{x}$ and $\mathbf{y}$ be two disjoint subsets of random variables. Then $\mathbf{x}$ and $\mathbf{y}$ are independent of each other if and only if (iff)

$$
p(\mathbf{x}, \mathbf{y})=p(\mathbf{x}) p(\mathbf{y})
$$

for all possible values of $\mathbf{x}$ and $\mathbf{y}$; otherwise they are said to be dependent.

- We say that the joint factorises into a product of $p(\mathbf{x})$ and $p(\mathbf{y})$.
- Equivalent definition by the product rule (or by definition of conditional probability)

$$
p(\mathbf{x} \mid \mathbf{y})=p(\mathbf{x})
$$

for all values of $\mathbf{x}$ and $\mathbf{y}$ where $p(\mathbf{y})>0$.

- Notation: $\mathbf{x} \Perp \mathbf{y}$
- Variables $\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}$ are independent iff

$$
p\left(\mathbf{x}_{1}, \ldots, \mathbf{x}_{n}\right)=\prod_{i=1}^{n} p\left(\mathbf{x}_{i}\right)
$$

## Conditional statistical independence

- The characterisation of statistical independence extends to conditional pdfs (pmfs) $p(\mathbf{x}, \mathbf{y} \mid \mathbf{z})$.
- The condition $p(\mathbf{x}, \mathbf{y})=p(\mathbf{x}) p(\mathbf{y})$ becomes $p(\mathbf{x}, \mathbf{y} \mid \mathbf{z})=p(\mathbf{x} \mid \mathbf{z}) p(\mathbf{y} \mid \mathbf{z})$
- The equivalent condition $p(\mathbf{x} \mid \mathbf{y})=p(\mathbf{x})$ becomes $p(\mathbf{x} \mid \mathbf{y}, \mathbf{z})=p(\mathbf{x} \mid \mathbf{z})$
- We say that $\mathbf{x}$ and $\mathbf{y}$ are conditionally independent given $\mathbf{z}$ iff, for all possible values of $\mathbf{x}, \mathbf{y}$, and $\mathbf{z}$ with $p(\mathbf{z})>0$ :

$$
\begin{gathered}
p(\mathbf{x}, \mathbf{y} \mid \mathbf{z})=p(\mathbf{x} \mid \mathbf{z}) p(\mathbf{y} \mid \mathbf{z}) \quad \text { or } \\
p(\mathbf{x} \mid \mathbf{y}, \mathbf{z})=p(\mathbf{x} \mid \mathbf{z}) \quad(\text { for } p(\mathbf{y}, \mathbf{z})>0)
\end{gathered}
$$

- Notation: $\mathbf{x} \Perp \mathbf{y} \mid \mathbf{z}$


## The impact of independence assumptions

- The key is that the independence assumption leads to a partial factorisation of the pdf/pmf with factors that involve fewer variables.
- Reduces the number of directly interacting variables.
- For example, if $\mathbf{x}, \mathbf{y}, \mathbf{z}$ are independent of each other, then

$$
p(\mathbf{x}, \mathbf{y}, \mathbf{z})=p(\mathbf{x}) p(\mathbf{y}) p(\mathbf{z})
$$

- Independence assumption forces $p(\mathbf{x}, \mathbf{y}, \mathbf{z})$ to take on a particular form.


## The impact of independence assumptions

Assume $p(\mathbf{x}, \mathbf{y}, \mathbf{z})=p(\mathbf{x}) p(\mathbf{y}) p(\mathbf{z})$

- If $\operatorname{dim}(\mathbf{x})=\operatorname{dim}(\mathbf{y})=\operatorname{dim}(\mathbf{z})=d$, and each element of the vectors can take $K$ values, factorisation reduces the numbers that need to be specified ("parameters") from $K^{3 d}-1$ to $3\left(K^{d}-1\right)$.
- If all variables were independent: $3 d(K-1)$ numbers needed.

For example: $10^{1500}-1$ vs. $3\left(10^{500}-1\right)$ vs. $1500(10-1)=13500$

- But full independence (factorisation) assumption is often too strong and does not hold.


## The impact of independence assumptions

- Conditional independence assumptions are a powerful middle-ground.
- For $p(\mathbf{x})=p\left(x_{1}, \ldots, x_{d}\right)$, we have by the product rule:

$$
p(\mathbf{x})=p\left(x_{d} \mid x_{1}, \ldots x_{d-1}\right) p\left(x_{1}, \ldots, x_{d-1}\right)
$$

- If, for example, $x_{d} \Perp x_{1}, \ldots, x_{d-4} \mid x_{d-3}, x_{d-2}, x_{d-1}$, we have

$$
p\left(x_{d} \mid x_{1}, \ldots, x_{d-1}\right)=p\left(x_{d} \mid x_{d-3}, x_{d-2}, x_{d-1}\right)
$$

- If the $x_{i}$ can take $K$ different values:
$p\left(x_{d} \mid x_{1}, \ldots, x_{d-1}\right)$ specified by $K^{d-1} \cdot(K-1)$ numbers $p\left(x_{d} \mid x_{d-3}, x_{d-2}, x_{d-1}\right)$ specified by $K^{3} \cdot(K-1)$ numbers

For $d=500, K=10: 10^{499} \cdot 9 \approx 10^{500}$ vs $9000 \approx 10^{4}$.

## Program

1. Independence assumptions
2. Assumptions on form of interaction

- Parametric model to restrict how a given number of variables may interact


## Assumption 2: limiting the form of the interaction

- The (conditional) independence assumption limits the number of variables that may directly interact with each other, e.g. $x_{d}$ only directly interacted with $x_{d-3}, x_{d-2}, x_{d-1}$.
- How $x_{d}$ interacts with the three variables, however, was not restricted.
- Assumption 2: We restrict how a given number of variables may interact with each other.
- For example, for $x_{i} \in\{0,1\}$, we may assume that $p\left(x_{d} \mid x_{1}, \ldots, x_{d-1}\right)$ is specified as

$$
p\left(x_{d}=1 \mid x_{1}, \ldots, x_{d-1}\right)=\frac{1}{1+\exp \left(-w_{0}-\sum_{i=1}^{d-1} w_{i} x_{i}\right)}
$$

with $d$ free numbers ("parameters") $w_{0}, \ldots, w_{d-1}$.

- $d$ vs $2^{d-1}$ parameters (for $d=500: 500$ vs. $2^{499} \approx 10^{150}$ )


## Gaussian parametric assumption for real-valued variables

- Multivariate Gaussian $N(\boldsymbol{\mu}, \Sigma)$
- Has mean $\mu$ and covariance $\Sigma$
- $\Sigma_{i j}=\Sigma_{j i}=\mathbb{E}\left[\left(X_{i}-\mu_{i}\right)\left(X_{j}-\mu_{j}\right)\right]$
- Probability density $p(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^{d}$

$$
p(\mathbf{x})=\frac{1}{(2 \pi)^{d / 2}|\Sigma|^{1 / 2}} \exp \left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{T} \Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}
$$



## Exact inference for Gaussian RVs

Exact inference is possible for the multivariate Gaussian $N(\mu, \Sigma)$. Basic rules:

- Partition variables into two groups, $\mathbf{X}_{1}$ and $\mathbf{X}_{2}$

$$
\begin{aligned}
\mu & =\binom{\mu_{1}}{\mu_{2}} \\
\Sigma & =\left(\begin{array}{ll}
\Sigma_{11} & \Sigma_{12} \\
\Sigma_{21} & \Sigma_{22}
\end{array}\right)
\end{aligned}
$$

- Marginal distribution: $\mathbf{x}_{1} \sim N\left(\mu_{1}, \Sigma_{11}\right)$
- Conditional distribution

$$
\begin{aligned}
& \mu_{1 \mid 2}^{c}=\boldsymbol{\mu}_{1}+\Sigma_{12} \Sigma_{22}^{-1}\left(\mathbf{x}_{2}-\boldsymbol{\mu}_{2}\right) \\
& \Sigma_{1 \mid 2}^{c}=\Sigma_{11}-\Sigma_{12} \Sigma_{22}^{-1} \Sigma_{21}
\end{aligned}
$$

- For proof see sec. 2.3.1 of Bishop (2006) (not examinable)
- We have joint Gaussian for $p(\mathbf{x}, \mathbf{y}, \mathbf{z})$, and want $p\left(\mathbf{x} \mid \mathbf{y}_{0}\right)$
- z can be marginalized out trivially (just ignore the $\mathbf{z}$ parts of the mean and covariance)
- Use the conditional distribution rule to obtain $\mathbf{x} \mid \mathbf{y}_{o} \sim N\left(\mu_{\mathrm{x} \mid \mathrm{y}_{0}}^{c}, \Sigma_{\mathrm{x} \mid \mathbf{y}_{0}}^{c}\right)$ with

$$
\begin{aligned}
& \mu_{\mathrm{x} \mid \mathrm{y}}^{c}=\mu_{\mathrm{x}}+\Sigma_{\mathrm{xy}} \Sigma_{\mathrm{yy}}^{-1}\left(\mathrm{y}_{o}-\mu_{\mathrm{y}}\right) \\
& \Sigma_{\mathrm{x} \mid \mathrm{y}}^{c}=\Sigma_{\mathrm{xx}}-\Sigma_{\mathrm{xy}} \Sigma_{\mathrm{yy}}^{-1} \Sigma_{\mathrm{yx}}
\end{aligned}
$$

- Assume that $\mathbf{x}, \mathbf{y}, \mathbf{z}$ each are each $d$ dimensional,
- Complexity is dominated by inversion of $\Sigma_{\mathrm{yy}}$ in $O\left(d^{3}\right)$ time
- If all variables are discretized into $K$ bins, complexity for computing $p\left(\mathbf{x} \mid \mathbf{y}_{o}\right)$ is $O\left(K^{d}\right)$, even for approximate inference

- Conditional distribution of $x_{2}$ given $x_{1}=2$ shown in red


## Program recap

We asked: What reasonably weak assumptions can we make to efficiently represent a probabilistic model?

1. Independence assumptions

- Definition and properties of statistical independence
- Factorisation of the pdf and reduction in the number of directly interacting variables

2. Assumptions on form of interaction

- Parametric model to restrict how a given number of variables may interact


## Credits

These slides are modified from ones produced by Michael Gutmann, made available under Creative Commons licence CC BY 4.0.
©Michael Gutmann and Chris Williams, The University of Edinburgh 2018-2024 CC BY 4.0 ©(i).

