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Center for Data Science

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#### Competition results

# Speed

As some of you noticed, a slightly more efficient way to compute the variance is to notice that:

$$\mathbb{V}[X] := \mathbb{E}\left[ (X - \mathbb{E}[X])^2 \right] = \mathbb{E}[X^2] - (\mathbb{E}[X])^2.$$

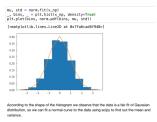
As a general rule, try using numpy functions and numpy broadcasting as much possible. To compute  $\mathbb{E}[X^2]$ , we have 2 efficient solutions : np.dot and @ (same as np.matmul). For 1D vector dot product, it is recommended to use np.dot, while for 2D matrix product you should use @.

- ► Tina Wan : Using np.dot
- $\triangleright$  Yirong Bian and Hanyuan Zhang : Computing using X.T@X(note that it is equivalent to X@X for 1D array)
- Yuhao Zheng: Naive variance computation using numba's njit decorator

#### Competition results

# Originality

Jiayun Wang: Fitting a normal distribution on this particular dataset



- Ken Zeng: Defining the mean as argmin  $\mathbb{E}[(X-\theta)^2]$  and minimizing this cost via gradient descent on a linear layer.
- Boyu Hu and Mingxuan Wu: Online mean computation

Probability terminology 00000000

- Probability terminology

#### Introduction

Probability terminology

- Experiment : Repeatable operation carried out under controlled conditions, with well defined outcomes.
- Sample space : Set of possible outcomes, often denoted  $\Omega$  Rolling a dice :  $\Omega = \{1, 2, 3, 4, 5, 6\}$ .
- Event : A subset of the sample space Event of obtaining a number greater than  $4 = \{5, 6\}$ .
- ▶ Random variable : Mapping from the possible outcomes in the sample space to a measurable space (often a real number) X = "The number rolled, mod 2"  $\in \{0,1\}$
- Probability : How likely an event is to occur. We often denote  $p(x) = \mathbb{P}(X = x)$ .

### Independence

# Independence

Two random variables A, B are said to be independent if any of the following is satisfied :

#### Mutual independence

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### Mutual independence

Let I an ensemble and  $(A_i)_{i \in I}$  a set of events. The  $(A_i)_{i \in I}$  are said to be mutually independent iif

$$\forall J \in \mathcal{P}(I), \quad \mathbb{P}\left(\bigcap_{j \in J} A_j\right) = \prod_{j \in J} \mathbb{P}(A_j).$$

A set of events is said to be mutually independent if the probability of each event in the set is the same no matter which of the other events has occurred.

# 000000000 A remark

In particular when I = J:

$$\mathbb{P}\left(\bigcap_{i\in I}A_i\right)=\prod_{i\in I}\mathbb{P}(A_i).$$

This formula is NOT equivalent to mutual independence.

# Counter example

Assume we are doing coin flips.

A: The first flip is T

B: At most one T in the first 3 flips

C : Same as B

We have  $\mathbb{P}(A \cap B \cap C) = \frac{1}{8} = \mathbb{P}(A)\mathbb{P}(B)\mathbb{P}(C)$  but the events are clearly not mutually independent!

### Computing a probability

There a 3 fundamental theorems for computing probabilities :

Law of total probability (aka marginalization or sum rule)

$$\mathbb{P}(A) = \sum_{b \in B} \mathbb{P}(A|B=b)$$

Chain rule (aka product rule)

$$\mathbb{P}(A \cap B \cap C) = \mathbb{P}(A)\mathbb{P}(B|A)\mathbb{P}(C|A,B)$$

► Bayes' theorem

$$\mathbb{P}(A \cap B) = \frac{\mathbb{P}(B \cap A)\mathbb{P}(A)}{\mathbb{P}(B)}$$

#### Law of total probability

Probability terminology 00000000

Marginalization or process of "forgetting irrelevant information".

$$\mathbb{P}(A) = \sum_{b \in B} \mathbb{P}(A|B = b).$$

More generally, let  $(B_i)_{i \in I}$  a collectively exhaustive family of events, i.e.  $\sum_{i\in I} \mathbb{P}(B_i) = 1$ ,

$$\mathbb{P}(A) = \sum_{i \in I} \mathbb{P}(A|B_i).$$

# Chain rule

# Conditional probability

$$\mathbb{P}(A \cap B) = \mathbb{P}(A)\mathbb{P}(B|A).$$

#### Chain rule

By proceeding recursively, we can expand the formula. Let  $(A_i)_{i \in [\![1,n]\!]}$  a set of random variables, s.t.  $\mathbb{P}(\bigcap_{i=1}^n A_i) \neq 0$ 

$$\mathbb{P}\left(\bigcap_{i=1}^n A_i\right) = \mathbb{P}(A_1) \prod_{i=2}^n \mathbb{P}\left(A_i \bigg| \bigcap_{j=1}^{i-1} A_j\right).$$

#### Bayes Theorem

Bayes theorem derives directly from the definition of conditional probabilities.

### Bayes Theorem

Let A, B two events such as  $\mathbb{P}(A) > 0$  and  $\mathbb{P}(B) > 0$ . Then,

$$\mathbb{P}(A|B) = rac{\mathbb{P}(B|A)\mathbb{P}(A)}{\mathbb{P}(B)}$$
 $ext{posterior} = rac{ ext{likelihood} imes ext{prior}}{ ext{evidence}}$ 

As we use it to estimate parameters, we sometimes drop the evidence:

$$p(\theta|\mathcal{D}) \propto p(\mathcal{D}|\theta)p(\theta).$$

#### **Table of Contents**

- Probability terminology
- 2 Bayesian networks
- Gaussian properties
- 4 Exercise

- We can use these three theorems to take advantage of structure in models to make computations cheaper and inference easier
- Probabilistic models with any sort of conditional structure can be described as Bayesian networks
- Formally:

# Bayesian network

A probabilistic graphical model representing the joint probability of a set of random variables, capturing conditional dependencies via a Directed Acyclic Graph (DAG).

# **Conditioning**: 3 fundamental patterns



Figure 1: Three fundamental patterns

$$p(B, C, D) = p(B)p(C|B)p(D|B)$$
  
$$p(C, D|B) = p(C|B)p(D|B)$$

# **Conditioning**: 3 fundamental patterns

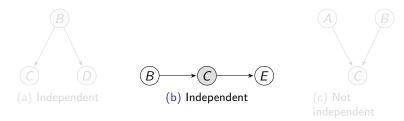


Figure 1: Three fundamental patterns

$$p(B, C, E) = p(B)p(C|B)p(E|C)$$

$$= p(B)\frac{p(B|C)p(C)}{p(B)}p(E|C)$$

$$p(B, E|C) = p(B|C)p(E|C)$$

#### **Conditioning**: 3 fundamental patterns

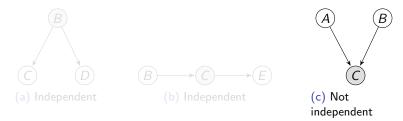


Figure 1: Three fundamental patterns

$$p(A, B, C) = p(A)p(B)p(C|A, B)$$

$$= \frac{p(C)^{2}p(A|C)p(B|C)}{p(C|A)p(C|B)}p(C|A, B)$$

$$p(A, B|C) = p(A|C)p(B|C)\frac{p(C)p(C|A, B)}{p(C|A)p(C|B)}$$

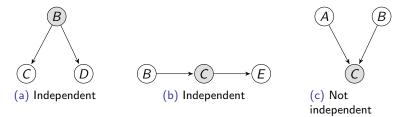


Figure 1: Three fundamental patterns

The **Markov blanket** for an ensemble *X* consists in the **children**, **parents** and the **co-parents**.

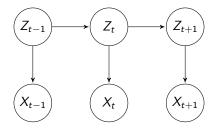
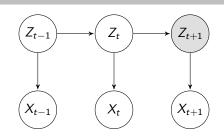
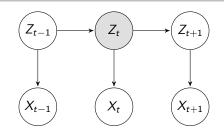


Figure 2: Bayesian Network

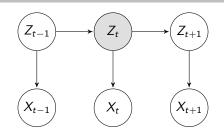
#### **Fact**

Each variable is conditionally independent of all its nondescendants in the graph given the value of all its parents.

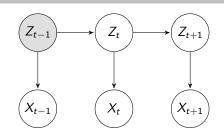


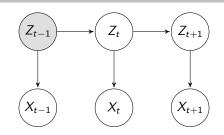


$$egin{array}{lll} X_{t+1} \perp \!\!\! \perp Z_{t-1}, X_{t-1}, Z_t, X_t & | Z_{t+1} \ X_t \quad \perp Z_{t-1}, X_{t-1}, Z_{t+1}, X_{t+1} & | Z_t \ Z_{t+1} \perp \!\!\! \perp Z_{t-1}, X_{t-1}, X_t & | Z_t \ X_{t-1} \perp \!\!\! \perp Z_t, X_t, Z_{t+1}, X_{t+1} & | Z_{t-1} \ Z_t \quad \perp X_{t-1} & | Z_{t-1} \ \end{array}$$



$$egin{array}{lll} X_{t+1} \perp \!\!\! \perp Z_{t-1}, X_{t-1}, Z_t, X_t & | Z_{t+1} \ X_t \quad \perp Z_{t-1}, X_{t-1}, Z_{t+1}, X_{t+1} & | Z_t \ Z_{t+1} \perp \!\!\! \perp Z_{t-1}, X_{t-1}, X_t & | Z_t \ X_{t-1} \perp \!\!\! \perp Z_t, X_t, Z_{t+1}, X_{t+1} & | Z_{t-1} \ Z_t \quad \perp X_{t-1} & | Z_{t-1} \ \end{array}$$





Bayesian networks

#### Computational costs in Bayesian networks

- ▶ We can take advantage of the structure in Bayesian networks to simplify calculations and reduce the computational cost.
- ▶ The probability  $p(X_{t+1}, X_t, X_{t-1})$  (the evidence) is often one of interest.

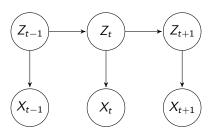
$$p(X_{t+1}, X_t, X_{t-1}) = \sum_{Z_{t+1}} \sum_{Z_t} \sum_{Z_{t-1}} p(X_{t+1}, X_t, X_{t-1}, Z_{t+1}, Z_t, Z_{t-1})$$

Assuming Z can take one of 3 values, and not using the conditional structure of the model, this has a computational cost of  $3^3$ 

# Using the conditional structure of Bayesian networks

Using the conditional structure, we can rewrite the  $p(X_{t+1}, X_t, X_{t-1}, Z_{t+1}, Z_t, Z_{t-1})$  as the product of conditionals:

$$p(X_{t+1}|Z_{t+1})p(Z_{t+1}|Z_t)p(X_t|Z_t)p(Z_t|Z_{t-1})p(X_{t-1}|Z_{t-1})p(Z_{t-1})$$



▶ Using the conditional structure, we can rewrite the  $p(X_{t+1}, X_t, X_{t-1}, Z_{t+1}, Z_t, Z_{t-1})$  as the product of conditionals:

$$p(X_{t+1}|Z_{t+1})p(Z_{t+1}|Z_t)p(X_t|Z_t)p(Z_t|Z_{t-1})p(X_{t-1}|Z_{t-1})p(Z_{t-1})$$

▶ Moving the terms that don't appear out of each sum, we can simplify the computation

$$p(X_{t+1}, X_t, X_{t-1}) = \sum_{Z_{t+1}} \left( p(X_{t+1}|Z_{t+1}) \right.$$

$$\sum_{Z_t} \left( p(Z_{t+1}|Z_t) p(X_t|Z_t) \right.$$

$$\sum_{Z_{t-1}} p(Z_t|Z_{t-1}) p(X_{t-1}|Z_{t-1}) p(Z_{t-1}) \right)$$

▶ To compute the inner most sum, we must create a table of  $Z_{t-1}$  and  $Z_t$  values, and sum over  $Z_t$ , this has a cost of  $3^2$ 

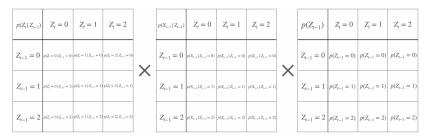


Figure 3: Product of inner sum

▶ To compute the inner most sum, we must create a table of  $Z_{t-1}$  and  $Z_t$  values, and sum over  $Z_t$ , this has a cost of  $3^2$ 

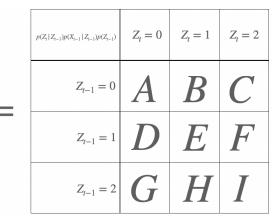


Figure 4: Result of product

▶ To compute the inner most sum, we must create a table of  $Z_{t-1}$  and  $Z_t$  values, and sum over  $Z_t$ , this has a cost of  $3^2$ 

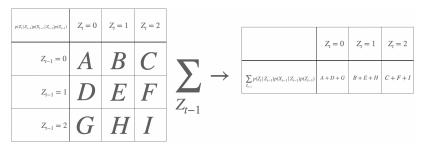


Figure 5: Summing  $Z_{t-1}$ 

Now do the same thing for the second sum, where the sum we computed on the previous slide is equal to  $p(X_{t-1}, Z_t)$ . The cost is again  $3^2$ .

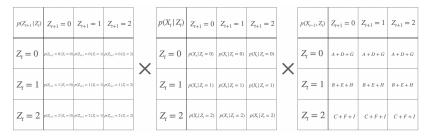


Figure 6: Product of second sum

Bayesian networks

Now do the same thing for the second sum, where the sum computed two slides ago is equal to  $p(X_{t-1}, Z_t)$ . The cost is again  $3^2$ .

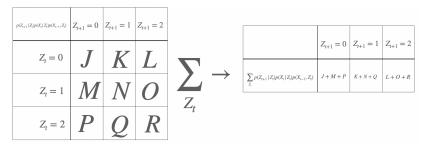


Figure 7: Summing  $Z_t$ 

For the final sum, we only have two tables with only one row (for  $Z_{t+1}$ ), so the cost for this will only be  $3^1$ . The sum on the previous slide is now  $p(X_t, X_{t-1}, Z_{t+1})$ 



Figure 8: Product of final sum

- As a the final result, we get that  $\sum_{Z_{t+1}} p(X_{t+1}|Z_{t+1}) p(X_t, X_{t-1}, Z_{t+1}) = S + T + U = p(X_{t+1}, X_t, X_{t-1})$
- ▶ The total cost of this computation is  $2 \times 3^2 + 3^1$

# Generalizing the model

- ▶ If instead of only having  $\{Z_i, X_i | i \in \{t-1, t, t+1\}\}$ , we extend the model to  $\{Z_i, X_i | i \in \{1, \dots, T\}\}$  and we allow the dimensionality of  $Z_i$  to be generalized to d, we find that the computational cost is  $T \times d^2 + d^1$
- ▶ The cost of computing the evidence naively is  $d^T$
- ▶ We have thus reduced the cost from being exponential in time (where time is defined as the value of T) and polynomial in dimension (d) to linear in time and quadratic in dimension

#### **Table of Contents**

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#### Gaussian identities

- ► Gaussians are the preferred distributions data scientists work with due to their nice properties
- ► The two most important identities are that the sum and product of two Gaussians is another Gaussian
- ► These give rise to the fact that the marginal of a Gaussian over two variables is another Gaussian
- This means inference can be done exactly with analytical solutions since the normalization constants can be computed exactly.
- https://cs.nyu.edu/ $\sim$ roweis/notes/gaussid.pdf (replace the  $\sim$  with the one from your keyboard for link to work)

letz:

$$\mathbf{z} = \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} \sim \mathcal{N} \left( \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix}, \begin{bmatrix} \mathbf{A} & \mathbf{C} \\ \mathbf{C}^\top & \mathbf{B} \end{bmatrix} \right).$$

Then

$$\begin{split} \textbf{x}|\textbf{y} &\sim \mathcal{N}\left(\textbf{a} + \textbf{C}\textbf{B}^{-1}(\textbf{y} - \textbf{b}), \textbf{A} - \textbf{C}\textbf{B}^{-1}\textbf{C}^{\top}\right) \\ \textbf{y}|\textbf{x} &\sim \mathcal{N}\left(\textbf{b} + \textbf{C}^{\top}\textbf{A}^{-1}(\textbf{x} - \textbf{a}), \textbf{B} - \textbf{C}^{\top}\textbf{A}^{-1}\textbf{C}\right) \end{split}$$

# Two important identities (2/2)

Let x, y:

$$egin{aligned} 
ho(\mathbf{x}) &= \mathcal{N}(\mathbf{x}|\mathbf{\Lambda}^{-1}) \ 
ho(\mathbf{y}|\mathbf{x}) &= \mathcal{N}(\mathbf{y}|\mathbf{A}\mathbf{x}+\mathbf{b},\mathbf{L}^{-1}). \end{aligned}$$

Then,

$$\begin{split} & \rho(\mathbf{y}) = \mathcal{N}(\mathbf{y}|\mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{L}^{-1} + \mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^{\top}) \\ & \rho(\mathbf{x}|\mathbf{y}) = \mathcal{N}(\mathbf{x}|\mathbf{\Sigma}\left[\mathbf{A}^{\top}\mathbf{L}(\mathbf{y} - \mathbf{b}) + \boldsymbol{\Lambda}\boldsymbol{\mu}\right], \boldsymbol{\Sigma}), \end{split}$$

where

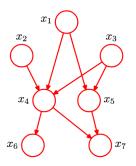
$$oldsymbol{\Sigma} = \left(oldsymbol{\Lambda} = oldsymbol{A}^{ op} oldsymbol{\mathsf{L}} oldsymbol{\mathsf{A}} 
ight)^{-1}.$$

#### **Table of Contents**

- Probability terminology

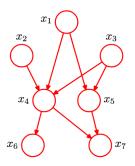
- Exercise

# From Bishop (Chapter 8)



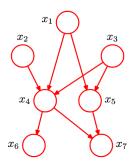
- Markov blanket of  $x_5$ ?
- Joint distribution?

# From Bishop (Chapter 8)

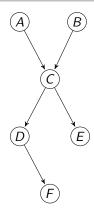


- **1** Markov blanket of  $x_5$ ?  $\{x_7, x_1, x_3, x_4\}$
- Joint distribution?

# From Bishop (Chapter 8)



- Markov blanket of  $x_5$ ?  $\{x_7, x_1, x_3, x_4\}$
- Joint distribution?  $p(x_1)p(x_2)p(x_3)p(x_4|x_1,x_2,x_3)p(x_5|x_1,x_3)p(x_6|x_4)p(x_7|x_4,x_5)$



- Are A and B conditionally independent given D and F?
- Are D and E conditionally independent given C?
- Are D and E conditionally independent given A and B?
- $P(D|CEF) \stackrel{?}{=} P(D|C)$

Are A and B conditionally independent given D and F? **No.** 

