CS229 Section: Probability Theory

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Content adapted from past CS229 teams, CS109 content

October 7, 2022

Outline

Note: Basics as Recap

- This review assumes basic background in probability (events, sample space, probability axioms etc.) and focuses on concepts useful to CS229 and to machine learning in general.

Definitions, Axioms, and Corollaries

- Performing an **experiment** $\rightarrow$ **outcome**
- **Sample Space** (S): set of all possible outcomes of an experiment
- **Event** (E): a subset of S ($E \subseteq S$)
- **Probability** (**Bayesian** definition)

  A number between 0 and 1 to which we ascribe meaning
  i.e. our belief that an event E occurs

- **Frequentist** definition of probability

$$P(E) = \lim_{n \to \infty} \frac{n(E)}{n}$$

Axiom 1: $0 \leq P(E) \leq 1$

Axiom 2: $P(S) = 1$

Axiom 3: If E and F are mutually exclusive ($E \cap F = \emptyset$), then $P(E) + P(F) = P(E \cup F)$

Corollary 1: $P(E^C) = 1 - P(E) \qquad (= P(S) - P(E))$

Corollary 2: $E \subseteq F$, then $P(E) \leq P(F)$

Corollary 3: $P(E \cup F) = P(E) + P(F) - P(EF)$ (Inclusion-Exclusion Principle)

General Inclusion-Exclusion Principle:

$$P\left(\bigcup_{i=1}^{n} E_i\right) = \sum_{r=1}^{n} (-1)^{r+1} \sum_{i_1 < \cdots < i_r} P(E_{i_1} E_{i_2} \ldots E_{i_r})$$

Equally Likely Outcomes: Define S as a sample space with equally likely outcomes. Then $P(E) = \frac{|E|}{|S|}$

Conditional Probability and Bayes' Rule

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Conditioned Bayes' Rule: given events A, B, C,

$$P(A \mid B, C) = \frac{P(B \mid A, C)P(A \mid C)}{P(B \mid C)}$$

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$$P(B_k \mid A) = \frac{P(B_k) P(A \mid B_k)}{P(A)} = \boxed{\frac{P(B_k) P(A \mid B_k)}{\sum_{i=1}^{n} P(A \mid B_i) P(B_i)}}$$

Law of Total Probability

Treasure chest **A** holds 100 gold coins. Treasure chest **B** holds 60 gold and 40 silver coins. Choose a treasure chest uniformly at random, and pick a coin from that chest uniformly at random. If the coin is gold, then what is the probability that you chose chest **A**? [1]

Solution:

[1] Question based on slides by Koochak & Irvin

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Solution:

$$\begin{aligned} P(A \mid G) &= \frac{P(A)P(G \mid A)}{P(A)P(G \mid A) + P(B)P(G \mid B)} \\ &= \frac{0.5 \times 1}{0.5 \times 1 + 0.5 \times 0.6} \\ &= \boxed{0.625} \end{aligned}$$

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Chain Rule

For any n events $A_1, ..., A_n$, the joint probability can be expressed as a product of conditionals:

$$P(A_1 \cap A_2 \cap ... \cap A_n)$$
$$= P(A_1)P(A_2 \mid A_1)P(A_3 \mid A_2 \cap A_1)...P(A_n \mid A_{n-1} \cap A_{n-2} \cap ... \cap A_1)$$

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In general: events $A_1, ..., A_n$ are **mutually independent** if

$$P(\bigcap_{i \in S} A_i) = \prod_{i \in S} P(A_i)$$

for any subset $S \subseteq \{1, ..., n\}$.

Outline

Random Variables

- A **random variable** X is a variable that probabilistically takes on different values. It maps outcomes to real values
- X takes on values in $Val(X) \subseteq \mathbb{R}$ or Support $\text{Sup}(X)$
- $X = k$ is the **event** that random variable X takes on value k

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Discrete RVs:

- $Val(X)$ is a set
- $P(X = k)$ can be nonzero

Continuous RVs:

- $Val(X)$ is a range
- $P(X = k) = 0$ for all k. $P(a \leq X \leq b)$ can be nonzero.

Probability Mass Function (PMF)

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For a valid PMF, $\sum_{x \in Val(x)} p_X(x) = 1$.

Cumulative Distribution Function (CDF)

A CDF maps a continuous RV to a probability (i.e. $\mathbb{R} \rightarrow [0, 1]$)

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A CDF must fulfill the following:

- $\lim_{x \to -\infty} F_X(x) = 0$
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Also note: $P(a \leq X \leq b) = F_X(b) - F_X(a)$.

Probability Density Function (PDF)

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Thus,

$$P(a \leq X \leq b) = F_X(b) - F_X(a) = \int_a^b f_X(x)dx$$

A valid PDF must be such that

- for all real numbers x, $f_X(x) \geq 0$.
- $\int_{-\infty}^{\infty} f_X(x)dx = 1$

Outline

Expectation

Let g be an arbitrary real-valued function.

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Intuitively, expectation is a weighted average of the values of $g(x)$, weighted by the probability of x.

Properties of Expectation

For any constant $a \in \mathbb{R}$ and arbitrary real function f:

- $\mathbb{E}[a] = a$
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Linearity of Expectation

Given n real-valued functions $f_1(X), ..., f_n(X)$,

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Law of Total Expectation

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N.B. $\mathbb{E}[X \mid Y] = \sum_{x \in Val(x)} x p_{X|Y}(x|y)$ is a function of Y.

Example of Law of Total Expectation

El Goog sources two batteries, A and B, for its phone. A phone with battery A runs on average 12 hours on a single charge, but only 8 hours on average with battery B. El Goog puts battery A in 80% of its phones and battery B in the rest. If you buy a phone from El Goog, how many hours do you expect it to run on a single charge?

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Solution: Let L be the time your phone runs on a single charge. We know the following:

- $p_X(A) = 0.8$, $p_X(B) = 0.2$,
- $\mathbb{E}[L \mid A] = 12$, $\mathbb{E}[L \mid B] = 8$.

Then, by Law of Total Expectation,

$$\begin{aligned}\mathbb{E}[L] = \mathbb{E}[\mathbb{E}[L \mid X]] &= \sum_{X \in \{A,B\}} \mathbb{E}[L \mid X] p_X(X) \\ &= \mathbb{E}[L \mid A] p_X(A) + \mathbb{E}[L \mid B] p_X(B) \\ &= 12 \times 0.8 + 8 \times 0.2 = \boxed{11.2}\end{aligned}$$

Variance

The **variance** of a RV X measures how concentrated the distribution of X is around its mean.

$$\begin{aligned} Var(X) &:= \mathbb{E}[(X - \mathbb{E}[X])^2] \\ &= \mathbb{E}[X^2] - \mathbb{E}[X]^2 \end{aligned}$$

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Properties: For any constant $a \in \mathbb{R}$, real-valued function $f(X)$

- $Var[a] = 0$
- $Var[af(X)] = a^2 Var[f(X)]$

Example Distributions

Distribution	PDF or PMF	Mean	Variance
$Bernoulli(p)$	$\begin{cases} p, & \text{if } x = 1 \\ 1-p, & \text{if } x = 0. \end{cases}$	p	$p(1-p)$
$Binomial(n, p)$	$\binom{n}{k} p^k (1-p)^{n-k}$ for $k = 0, 1, ..., n$	np	$np(1-p)$
$Geometric(p)$	$p(1-p)^{k-1}$ for $k = 1, 2, ...$	$\frac{1}{p}$	$\frac{1-p}{p^2}$
$Poisson(\lambda)$	$\frac{e^{-\lambda}\lambda^k}{k!}$ for $k = 0, 1, ...$	λ	λ
$Uniform(a, b)$	$\frac{1}{b-a}$ for all $x \in (a, b)$	$\frac{a+b}{2}$	$\frac{(b-a)^2}{12}$
$Gaussian(\mu, \sigma^2)$	$\frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$ for all $x \in (-\infty, \infty)$	μ	σ^2
$Exponential(\lambda)$	$\lambda e^{-\lambda x}$ for all $x \geq 0, \lambda \geq 0$	$\frac{1}{\lambda}$	$\frac{1}{\lambda^2}$

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- **Marginal PMF** of X, given joint PMF of X, Y:

$$p_X(x) = \sum_y p_{XY}(x,y)$$

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Joint and Marginal Distributions for Multiple RVs

- **Joint PMF** for discrete RV's $X_1, ..., X_n$:

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These definitions can be extended to multiple random variables in the same way as in the previous slide. For example, for n continuous RV's $X_1, .., X_n$ and function $g : \mathbb{R}^n \to \mathbb{R}$:

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$$\mathbb{E}[g(X)] = \int \int ... \int g(x_1, ..., x_n) f_{X_1,...,X_n}(x_1, ..., x_n) dx_1, ..., dx_n$$

Outline

Covariance

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$$\begin{aligned} Cov[X, Y] &:= \mathbb{E}\left[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])\right] \\ &= \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y] \end{aligned}$$

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$$= \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y]$$

- If $Cov[X, Y] < 0$, then X and Y are negatively correlated
- If $Cov[X, Y] > 0$, then X and Y are positively correlated
- If $Cov[X, Y] = 0$, then X and Y are uncorrelated

Properties Involving Covariance

- If $X \perp Y$, then $\mathbb{E}[XY] = \mathbb{E}[X]\mathbb{E}[Y]$. Thus,

$$Cov[X, Y] = \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y] = 0$$

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- **Variance of two variables:**

$$Var[X + Y] = Var[X] + Var[Y] + 2Cov[X, Y]$$

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  This is unidirectional! $Cov[X, Y] = 0$ **does not imply** $X \perp Y$

- **Variance of two variables:**

$$Var[X + Y] = Var[X] + Var[Y] + 2Cov[X, Y]$$

  i.e. if $X \perp Y$, $Var[X + Y] = Var[X] + Var[Y]$.

Properties Involving Covariance

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- **Special Case:**

$$Cov[X, X] = \mathbb{E}[XX] - \mathbb{E}[X]\mathbb{E}[X] = Var[X]$$

Outline

Conditional distributions for RVs

Works the same way with *RV*'s as with events:

- For discrete X, Y:

$$p_{Y|X}(y|x) = \frac{p_{XY}(x, y)}{p_X(x)}$$

- For continuous X, Y:

$$f_{Y|X}(y|x) = \frac{f_{XY}(x, y)}{f_X(x)}$$

- In general, for continuous $X_1, \ldots, X_n$:

$$f_{X_1|X_2,\ldots,X_n}(x_1|x_2, \ldots, x_n) = \frac{f_{X_1,X_2,\ldots,X_n}(x_1, x_2, \ldots, x_n)}{f_{X_2,\ldots,X_n}(x_2, \ldots, x_n)}$$

Bayes' Rule for RVs

Also works the same way for RV's as with events:

- For discrete X, Y:

$$p_{Y|X}(y|x) = \frac{p_{X|Y}(x|y)p_Y(y)}{\sum_{y' \in Val(Y)} p_{X|Y}(x|y')p_Y(y')}$$

- For continuous X, Y:

$$f_{Y|X}(y|x) = \frac{f_{X|Y}(x|y)f_Y(y)}{\int_{-\infty}^{\infty} f_{X|Y}(x|y')f_Y(y')dy'}$$

Chain Rule for RVs

Also works the same way as with events:

$$f(x_1, x_2, ..., x_n) = f(x_1)f(x_2|x_1)...f(x_n|x_1, x_2, ..., x_{n-1})$$
$$= f(x_1)\prod_{i=2}^{n} f(x_i|x_1, ..., x_{i-1})$$

Independence for RVs

- For $X \perp Y$ to hold, it must be that $F_{XY}(x, y) = F_X(x)F_Y(y)$ **FOR ALL VALUES** of x, y.

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- Since $f_{Y|X}(y|x) = f_Y(y)$ if $X \perp Y$, chain rule for mutually independent $X_1, ..., X_n$ is:

$$f(x_1, ..., x_n) = f(x_1)f(x_2)...f(x_n) = \prod_{i=1}^{n} f(x_i)$$

(very important assumption for a Naive Bayes classifier!)

Outline

Random Vectors

Given n RV's $X_1, ..., X_n$, we can define a random vector X s.t.

$$X = \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_n \end{bmatrix}$$

Note: all the notions of joint PDF/CDF will apply to X.

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Note: all the notions of joint PDF/CDF will apply to X.

Given $g : \mathbb{R}^n \to \mathbb{R}^m$, we have:

$$g(x) = \begin{bmatrix} g_1(x) \\ g_2(x) \\ \vdots \\ g_m(x) \end{bmatrix}, \mathbb{E}[g(X)] = \begin{bmatrix} \mathbb{E}[g_1(X)] \\ \mathbb{E}[g_2(X)] \\ \vdots \\ \mathbb{E}[g_m(X)] \end{bmatrix}$$

Covariance Matrices

For a random vector $X \in \mathbb{R}^n$, we define its **covariance matrix** Σ as the $n \times n$ matrix whose ij-th entry contains the covariance between X_i and X_j.

$$\Sigma = \begin{bmatrix} Cov[X_1, X_1] & \dots & Cov[X_1, X_n] \\ \vdots & \ddots & \vdots \\ Cov[X_n, X_1] & \dots & Cov[X_n, X_n] \end{bmatrix}$$

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$$\Sigma = \mathbb{E}[(X - \mathbb{E}[X])(X - \mathbb{E}[X])^T]$$

Properties:

- Σ is symmetric and PSD
- If $X_i \perp X_j$ for all i, j, then $\Sigma = diag(Var[X_1], ..., Var[X_n])$

Outline

Multivariate Gaussian

The multivariate Gaussian $X \sim \mathcal{N}(\mu, \Sigma)$, $X \in \mathbb{R}^n$:

$$p(x; \mu, \Sigma) = \frac{1}{det(\Sigma)^{\frac{1}{2}}(2\pi)^{\frac{n}{2}}} \exp\left(-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right)$$

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$$p(x; \mu, \sigma^2) = \frac{1}{\sigma(2\pi)^{\frac{1}{2}}} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)$$

Notice that if $\Sigma \in \mathbb{R}^{1\times 1}$, then $\Sigma = Var[X_1] = \sigma^2$, and so
$\Sigma^{-1} = \frac{1}{\sigma^2}$ and $det(\Sigma)^{\frac{1}{2}} = \sigma$

Some Nice Properties of MV Gaussians

- Marginals and conditionals of a joint Gaussian are Gaussian

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- A d-dimensional Gaussian $X \in \mathcal{N}(\mu, \Sigma = diag(\sigma_1^2, ..., \sigma_n^2))$ is equivalent to a collection of d **independent** Gaussians $X_i \in \mathcal{N}(\mu_i, \sigma_i^2)$. This results in isocontours aligned with the coordinate axes.

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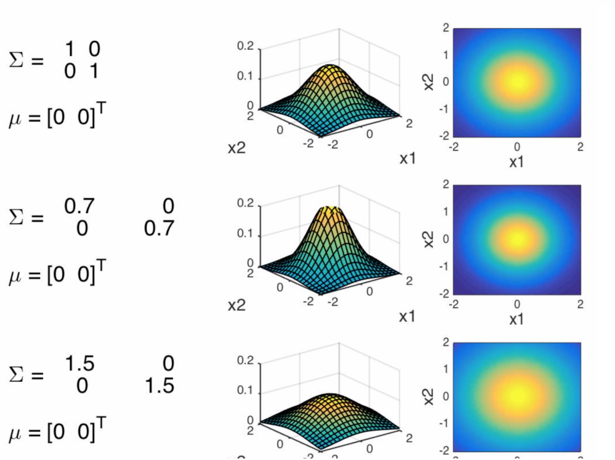
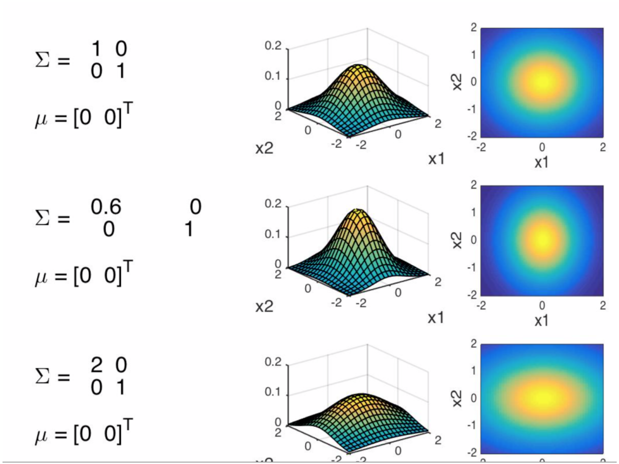
- A d-dimensional Gaussian $X \in \mathcal{N}(\mu, \Sigma = diag(\sigma_1^2, ..., \sigma_n^2))$ is equivalent to a collection of d **independent** Gaussians $X_i \in \mathcal{N}(\mu_i, \sigma_i^2)$. This results in isocontours aligned with the coordinate axes.
- In general, the isocontours of a MV Gaussian are n-dimensional ellipsoids with principal axes in the directions of the eigenvectors of covariance matrix Σ (remember, Σ is PSD, so all n eigenvectors are non-negative). The axes' relative lengths depend on the eigenvalues of Σ.

Visualizations of MV Gaussians



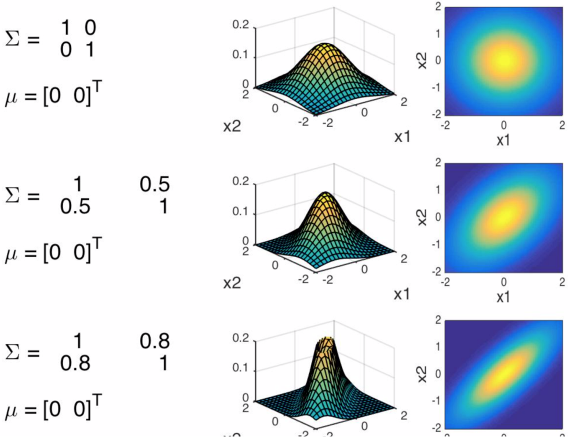
Effect of changing variance

Visualizations of MV Gaussians



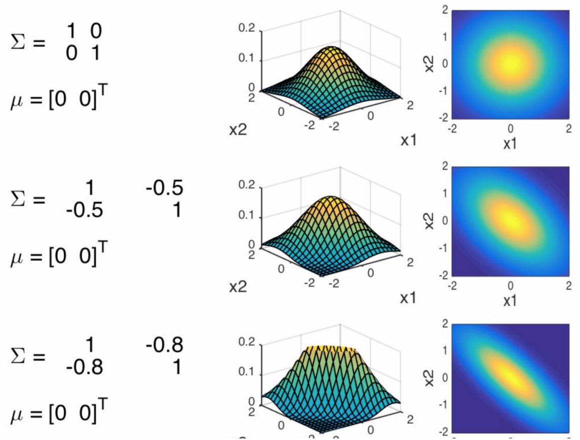
If $Var[X_1] \neq Var[X_2]$:

Visualizations of MV Gaussians



If X_1 and X_2 are positively correlated:

Visualizations of MV Gaussians



If X_1 and X_2 are negatively correlated:

Thank you and good luck!

For further reference, consult the following CS229 handouts

- Probability Theory Review
- The MV Gaussian Distribution
- More on Gaussian Distribution

For a comprehensive treatment, see

- Sheldon Ross: **A First Course in Probability**

Appendix: More on Total Expectation

Why is $\mathbb{E}[X|Y]$ a function of Y? Consider the following:

- $\mathbb{E}[X|Y=y]$ is a scalar that only depends on y.
- Thus, $\mathbb{E}[X|Y]$ is a random variable that only depends on Y. Specifically, $\mathbb{E}[X|Y]$ is a function of Y mapping $Val(Y)$ to the real numbers.

An example: Consider RV X such that

$$X = Y^2 + \epsilon$$

such that $\epsilon \sim \mathcal{N}(0,1)$ is a standard Gaussian. Then,

- $\mathbb{E}[X|Y] = Y^2$
- $\mathbb{E}[X|Y=y] = y^2$

Appendix: More on Total Expectation

A derivation of Law of Total Expectation for discrete X, Y:

$$\mathbb{E}[\mathbb{E}[X|Y]] = \mathbb{E}[\sum_x xP(X = x \mid Y)] = \sum_y \sum_x xP(X = x \mid Y)P(Y = y) \quad (1)$$

$$= \sum_y \sum_x xP(X = x, Y = y) \quad (2)$$

$$= \sum_x x \sum_y P(X = x, Y = y) \quad (3)$$

$$= \sum_x xP(X = x) = \boxed{\mathbb{E}[X]} \quad (4)$$

where (1) and (4) result from the definition of expectation, (2) results from the definition of cond. prob., and (3) results from marginalizing out Y.

Appendix: A proof of Conditioned Bayes Rule

Repeatedly applying the definition of conditional probability, we have:

$$\begin{aligned}
\frac{P(b|a,c)P(a|c)}{P(b|c)} &= \frac{P(b,a,c)}{P(a,c)} \cdot \frac{P(a|c)}{P(b|c)} \\
&= \frac{P(b,a,c)}{P(a,c)} \cdot \frac{P(a,c)}{P(b|c)P(c)} \\
&= \frac{P(b,a,c)}{P(b|c)P(c)} \\
&= \frac{P(b,a,c)}{P(b,c)} \\
&= P(a|b,c)
\end{aligned}$$