


More on Multivariate Probability

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Recap: Multivariate probability

Let's say you are in a zoo that has infinite number of animals:

Ω : sample space



$X_1: \Omega \rightarrow \mathbb{R}$
"height of the animal in cm"

$$X_1(\text{chick}) = 9.6$$

$$X_1(\text{dog}) = 72.8$$

...

$X_2: \Omega \rightarrow \mathbb{R}$
"weight of the animal in kg"

$$X_2(\text{chick}) = 1.02$$

$$X_2(\text{dog}) = 17.4$$

...

$X_3: \Omega \rightarrow \mathbb{N}^+$
"fur colour of the animal"

$$X_3(\text{chick}) = 1$$

$$X_3(\text{dog}) = 3$$

...

(1: yellow, 2: blue, 3: orange, ...)

- Support: $\mathcal{A} = \{(x_1, x_2, x_3) : X_n(\omega) = x_n, \omega \in \Omega\}$
- Set $P(A) := \mathbb{P}(E)$ for the biggest event set $E \subset \Omega$ such that $(X_1, \dots, X_N)(E) := \{(X_1(\omega), \dots, X_N(\omega)) : \omega \in E\} \subset A$,
- PMF/PDF $p(x_1, x_2, x_3)$ satisfies:

$$\int_{(x_1, x_2, x_3) \in A} p(x_1, x_2, x_3) dx_1 dx_2 dx_3 = P(A), \quad \forall A \subset \mathcal{A}.$$

Conditional probability

Joint probability of events $E_A, E_B \subset \Omega$, $\mathcal{E} = 2^\Omega$:

$$\mathbb{P}(E_A \cap E_B)$$

Conditional probability: given that E_A occurs, what is the probability that E_B also occurs?

$$\mathbb{P}(E_B|E_A) := \frac{\mathbb{P}(E_A \cap E_B)}{\mathbb{P}(E_A)}$$

By symmetry:

$$\mathbb{P}(E_A|E_B) := \frac{\mathbb{P}(E_A \cap E_B)}{\mathbb{P}(E_B)}$$

We can write these expressions in random variable support space:
for $A, B \subset \mathcal{A}$,

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

Conditional probability

Conditional probability for $A, B \subset \mathcal{A}$,
 $\mathcal{A} = \{(x_1, x_2, \dots, x_N) : X_n(\omega) = x_n, \omega \in \Omega\},$

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

Specifically, we can define $P(X_2 \in A_2 | x_1 \in A_1)$ if we define:

$$A = \{(x_1, x_2, \dots, x_N) : X_n(\omega) = x_n, \omega \in \Omega, \mathbf{x_1 \in A_1}\}$$

$$B = \{(x_1, x_2, \dots, x_N) : X_n(\omega) = x_n, \omega \in \Omega, \mathbf{x_2 \in A_2}\}$$

Conditional PMF/PDF $p(X_2 = x_2 | x_1 \in A_1)$ can be defined similar to the joint PMF/PDF case: just need to ensure $\forall A_1 \subset V_{X_1}, A_2 \subset V_{X_2}$

$$\int_{A_2} p(X_2 = x_2 | X_1 \in A_1) dx_2 = P(X_2 \in A_2 | X_1 \in A_1).$$

Conditional probability

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(1: yellow, 2: blue, 3: orange, ...)

Joint probability $P(1.0 \leq X_2 \leq 10.0, 10.0 \leq X_1 \leq 50.0)$:

► Figure out the event sets

$$E_1 = \{\omega \in \Omega \mid 10.0 \leq X_1(\omega) \leq 50.0\}, \quad E_2 = \{\omega \in \Omega \mid 1.0 \leq X_2(\omega) \leq 10.0\}$$

$$\Rightarrow E_1 \cap E_2 = \{\omega \in \Omega \mid 10.0 \leq X_1(\omega) \leq 50.0, 1.0 \leq X_2(\omega) \leq 10.0\}$$

Conditional probability

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Joint probability $P(1.0 \leq X_2 \leq 10.0, 10.0 \leq X_1 \leq 50.0)$:

- Compute $P(1.0 \leq X_2 \leq 10.0, 10.0 \leq X_1 \leq 50.0)$ as

$$P(1.0 \leq X_2 \leq 10.0, 10.0 \leq X_1 \leq 50.0) = \mathbb{P}(E_1 \cap E_2)$$

Conditional probability

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Marginal probability $P(10.0 \leq X_1 \leq 50.0)$:

- Figure out the event $E_1 = \{\omega \in \Omega | 10.0 \leq X_1(\omega) \leq 50.0\}$, then

$$P(10.0 \leq X_1 \leq 50.0) = \mathbb{P}(E_1)$$

Conditional probability

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Conditional probability $P(1.0 \leq X_2 \leq 10.0 | 10.0 \leq X_1 \leq 50.0)$:

- Compute $P(1.0 \leq X_2 \leq 10.0 | 10.0 \leq X_1 \leq 50.0)$ as

$$P(1.0 \leq X_2 \leq 10.0 | 10.0 \leq X_1 \leq 50.0) = \frac{\mathbb{P}(E_1 \cap E_2)}{\mathbb{P}(E_1)}$$

Sum rule and product rule

By definition of the **conditional probability**:

$$P(X_2 \in A_2 | X_1 \in A_1) := \frac{P(X_2 \in A_2, X_1 \in A_1)}{P(X_1 \in A_1)}$$

Product rule:

$$P(X_2 \in A_2, X_1 \in A_1) = P(X_2 \in A_2 | X_1 \in A_1) \times P(X_1 \in A_1)$$

“Joint dist. = conditional dist. \times marginal dist.”

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“Joint dist. = conditional dist. \times marginal dist.”

Sum rule:

$$P(X_1 \in A_1) = \int_{V_{X_2}} p(X_1 \in A_1, X_2 = x_2) dx_2$$

“Marginal dist. = sum/integral of joint dist.”

Sum rule and product rule

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$$P(X_2 \in A_2 | X_1 \in A_1) := \frac{P(X_2 \in A_2, X_1 \in A_1)}{P(X_1 \in A_1)}$$

Product rule:

$$P(X_2 \in A_2, X_1 \in A_1) = P(X_2 \in A_2 | X_1 \in A_1) \times P(X_1 \in A_1)$$

“Joint dist. = conditional dist. \times marginal dist.”

Sum rule:

$$P(X_1 \in A_1) = \int_{V_{X_2}} p(X_1 \in A_1, X_2 = x_2) dx_2$$

“Marginal dist. = sum/integral of joint dist.”

Combining both:

$$P(X_1 \in A_1) = \int_{V_{X_2}} P(X_2 = x_2 | X_1 \in A_1) \times P(X_1 \in A_1) dx_2$$

Conditional independence

Independence of two random variables X_1, X_2 :

$$X_1 \perp\!\!\!\perp X_2 \quad \Leftrightarrow \quad p(X_1, X_2) = p(X_1)p(X_2)$$

Equivalently, using product rule:

$$X_1 \perp\!\!\!\perp X_2 \quad \Leftrightarrow \quad p(X_1|X_2) = p(X_1), p(X_2|X_1) = p(X_2)$$

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$$X_1 \perp\!\!\!\perp X_2 \quad \Leftrightarrow \quad p(X_1|X_2) = p(X_1), p(X_2|X_1) = p(X_2)$$

Conditional Independence of two random variables X_1, X_2 given X_3 :

$$X_1 \perp\!\!\!\perp X_2|X_3 \quad \Leftrightarrow \quad p(X_1, X_2|X_3) = p(X_1|X_3)p(X_2|X_3)$$

Equivalently, using product rule:

$$X_1 \perp\!\!\!\perp X_2|X_3 \quad \Leftrightarrow \quad p(X_1|X_2, X_3) = p(X_1|X_3), p(X_2|X_1, X_3) = p(X_2|X_3)$$

Conditional independence

Example: drawing 5 cards from a standard 52-card poker deck

Define the following random variables:

- X_1 : number of hearts ♥
- X_2 : number of diamonds ♦
- X_3 : number of clubs ♣
- X_4 : number of spades ♠

What is the joint distribution $p(X_1, X_2, X_3, X_4)$ for the card draws –

- with replacement?
- without replacement?

Vector mean & covariance

Univariate case:

$$\text{mean: } \mathbb{E}[X] = \int x p_X(x) dx$$

$$\text{variance: } \mathbb{V}[X] = \mathbb{E}[(X - \mathbb{E}[X])] = \int (x - \mathbb{E}[X]) p_X(x) dx$$

Multivariate case: write $X = (X_1, \dots, X_N)^\top$

$$\text{mean: } \mathbb{E}[X] = (\mathbb{E}[X_1], \dots, \mathbb{E}[X_N])^\top$$

$$\text{covariance: } \mathbb{V}[X] = \Sigma, \quad \Sigma_{ij} = \mathbb{E}[(X_i - \mathbb{E}[X_i])(X_j - \mathbb{E}[X_j])]$$

Using **sum rule**: only need marginals

$$\mathbb{E}[X_i] = \int x_i p_X(\mathbf{x}) d\mathbf{x} = \int x_i p_X(X_i = x_i) dx_i$$

$$\begin{aligned} \Sigma_{ij} &= \int (x_i - \mathbb{E}[X_i])(x_j - \mathbb{E}[X_j]) p_X(\mathbf{x}) d\mathbf{x} \\ &= \int (x_i - \mathbb{E}[X_i])(x_j - \mathbb{E}[X_j]) p_X(X_i = x_i, X_j = x_j) dx_i dx_j \end{aligned}$$

Vector mean & covariance

Connecting univariate & multivariate cases:

$$\begin{aligned}\mathbb{E}[\mathbf{a}^\top X] &= \int \mathbf{a}^\top \mathbf{x} p_X(\mathbf{x}) d\mathbf{x} = \int \sum_i a_i x_i p(\mathbf{x}) d\mathbf{x} = \sum_i a_i \int x_i p(\mathbf{x}) d\mathbf{x} \\ &= \sum_i a_i \int x_i p(x_i) p(\{x_j\}_{j \neq i} | x_i) d\mathbf{x} \\ &= \sum_i a_i \int x_i p(x_i) dx_i \int p(\{x_j\}_{j \neq i} | x_i) d\mathbf{x}_{-i} \\ &= \mathbf{a}^\top (\mathbb{E}[X_1], \dots, \mathbb{E}[X_N])^\top = \mathbf{a}^\top \mathbb{E}[X]\end{aligned}$$

\implies mean vector is the mean of each marginal!

Vector mean & coariance

Connecting univariate & multivariate cases:

Write $\bar{x} := \mathbb{E}[X]$ and use sum rule

$$\begin{aligned}\mathbb{V}[\mathbf{a}^\top X] &= \int (\mathbf{a}^\top \mathbf{x} - \mathbf{a}^\top \bar{\mathbf{x}})^2 p_X(\mathbf{x}) d\mathbf{x} \\ &= \int \left(\sum_i a_i x_i - a_i \bar{x}_i \right) \left(\sum_j a_j x_j - a_j \bar{x}_j \right) p_X(\mathbf{x}) d\mathbf{x} \\ &= \sum_i \sum_j a_i a_j \int (x_i - \bar{x}_i)(x_j - \bar{x}_j) p_X(X_i = x_i, X_j = x_j) dx_i dx_j \\ &= \sum_i \sum_j a_i a_j \Sigma_{ij} = \mathbf{a}^\top \Sigma \mathbf{a}\end{aligned}$$

The covariance Σ allows us to find the scalar variance in any direction.

Conditional expectations

Expectation of a function $f(X)$ under distribution $p(X)$:

$$\mathbb{E}_{p(X)}[f(X)] = \int f(x)p(X = x)dx$$

Conditional expectation of a function $g(Y)$ given $X = x$ under conditional distribution $p(Y|X = x)$:

$$\mathbb{E}_{p(Y|X=x)}[g(Y)] = \int g(y)p(Y = y|X = x)dy$$

An equivalent notation: $\mathbb{E}[g(Y)|X = x] = \mathbb{E}_{p(Y|X=x)}[g(Y)]$

Conditional expectations

Conditional expectation of a function $g(Y)$ given $X = x$:

$$\mathbb{E}[g(Y)|X = x] = \mathbb{E}_{p(Y|X=x)}[g(Y)] = \int g(y)p(Y = y|X = x)dy$$

- $\mathbb{E}[g(Y)|X = x]$ is a function of x
- As X is a random variable, $\mathbb{E}[g(Y)|X]$ is also a random variable

Law of Total Expectation:

$$\mathbb{E}[Y] = \mathbb{E}[\mathbb{E}[Y|X]]$$

Conditional expectations

Conditional expectation of a function $g(Y)$ given $X = x$:

$$\mathbb{E}[g(Y)|X = x] = \mathbb{E}_{p(Y|X=x)}[g(Y)] = \int g(y)p(Y = y|X = x)dy$$

- $\mathbb{E}[g(Y)|X = x]$ is a function of x
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Law of Total Expectation:

$$\mathbb{E}_{p(Y)}[Y] = \mathbb{E}_{p(X)}[\mathbb{E}_{p(Y|X)}[Y]]$$

Conditional expectations

Conditional expectation of a function $g(Y)$ given $X = x$:

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- As X is a random variable, $\mathbb{E}[g(Y)|X]$ is also a random variable

Law of Total Expectation:

$$\begin{aligned}\mathbb{E}_{p(Y)}[Y] &= \mathbb{E}_{p(X)}[\mathbb{E}_{p(Y|X)}[Y]] \\ &= \int p(X = x)\mathbb{E}_{p(Y|X=x)}[Y]dx\end{aligned}$$

Conditional expectations

Conditional expectation of a function $g(Y)$ given $X = x$:

$$\mathbb{E}[g(Y)|X = x] = \mathbb{E}_{p(Y|X=x)}[g(Y)] = \int g(y)p(Y = y|X = x)dy$$

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$$\begin{aligned}\mathbb{E}_{p(Y)}[Y] &= \mathbb{E}_{p(X)}[\mathbb{E}_{p(Y|X)}[Y]] \\ &= \int p(X = x)p(Y = y|X = x)ydydx\end{aligned}$$

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- $\mathbb{E}[g(Y)|X = x]$ is a function of x
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Law of Total Expectation:

$$\begin{aligned}\mathbb{E}_{p(Y)}[Y] &= \mathbb{E}_{p(X)}[\mathbb{E}_{p(Y|X)}[Y]] \\ &= \int p(Y = y, X = x)ydydx \quad (\text{product rule})\end{aligned}$$

Conditional expectations

Conditional expectation of a function $g(Y)$ given $X = x$:

$$\mathbb{E}[g(Y)|X = x] = \mathbb{E}_{p(Y|X=x)}[g(Y)] = \int g(y)p(Y = y|X = x)dy$$

- $\mathbb{E}[g(Y)|X = x]$ is a function of x
- As X is a random variable, $\mathbb{E}[g(Y)|X]$ is also a random variable

Law of Total Expectation:

$$\begin{aligned}\mathbb{E}_{p(Y)}[Y] &= \mathbb{E}_{p(X)}[\mathbb{E}_{p(Y|X)}[Y]] \\ &= \int p(Y = y)ydy \quad (\text{sum rule})\end{aligned}$$

Conditional expectations

Conditional expectation of a function $g(Y)$ given $X = x$:

$$\mathbb{E}[g(Y)|X = x] = \mathbb{E}_{p(Y|X=x)}[g(Y)] = \int g(y)p(Y = y|X = x)dy$$

- ▶ $\mathbb{E}[g(Y)|X = x]$ is a function of x
- ▶ As X is a random variable, $\mathbb{E}[g(Y)|X]$ is also a random variable

Law of Total Expectation:

Extention to functions of Y :

$$\mathbb{E}[g(Y)] = \mathbb{E}[\mathbb{E}[g(Y)|X]]$$

Conditional expectations

Conditional variance of Y given $X = x$:

$$\begin{aligned}\mathbb{V}[Y|X = x] &:= \mathbb{V}_{p(Y|X=x)}[Y] \\ &= \mathbb{E}_{p(Y|X=x)}[(Y - \mathbb{E}_{p(Y|X=x)}[Y])^2] \\ &= \mathbb{E}[(Y - \mathbb{E}[Y|X = x])^2 | X = x]\end{aligned}$$

- $\mathbb{V}[Y|X = x]$ is a function of x
- As X is a random variable, $\mathbb{V}[Y|X]$ is also a random variable

Law of Total Variance:

$$\mathbb{V}[Y] = \mathbb{E}[\mathbb{V}[Y|X]] + \mathbb{V}[\mathbb{E}[Y|X]]$$

Summary

Topics we've covered about multivariate probability:

- Definitions and some examples
- Joint, marginal, and conditional distributions
- Sum rule and product rule
- Change-of-variables rule
- Computing mean/variance/expectations

Next lecture: Model selection via cross-validation

Appendix: math formula for deriving sum rule

Deriving **sum rule** using \mathbb{P} defined on sets:

Define for any $A_1 \subset V_{X_1}$, $A_2 \subset V_{X_2}$

$$\mathcal{A}(A_1) = \{(X_1(\omega), X_2(\omega), \dots, X_N(\omega)) : \mathbf{X}_1(\omega) \in A_1\}$$

$$\mathcal{A}(A_2) = \{(X_1(\omega), X_2(\omega), \dots, X_N(\omega)) : \mathbf{X}_2(\omega) \in A_2\}$$

Now we can define a “split” of X_2 value space V_{X_2} :

$$V_{X_2} = \cup_{k=1}^K A_2^k, \quad A_2^k \neq \emptyset, \quad A_2^i \cap A_2^j = \emptyset, \forall i \neq j$$

$$\begin{aligned} \Rightarrow \quad \cup_{k=1}^K (\mathcal{A}(A_1) \cap \mathcal{A}(A_2^k)) &= \mathcal{A}(A_1) \cap (\cup_{k=1}^K \mathcal{A}(A_2^k)) \\ &= \mathcal{A}(A_1) \cap \mathcal{A}(V_{X_2}) \\ &= \mathcal{A}(A_1) \cap \mathcal{A} = \mathcal{A}(A_1) \end{aligned}$$

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$$\begin{aligned} \Rightarrow \quad P(\cup_{k=1}^K (\mathcal{A}(A_1) \cap \mathcal{A}(A_2^k))) &= P(\mathcal{A}(A_1) \cap (\cup_{k=1}^K \mathcal{A}(A_2^k))) \\ &= P(\mathcal{A}(A_1) \cap \mathcal{A}(V_{X_2})) \\ &= P(\mathcal{A}(A_1) \cap \mathcal{A}) = P(\mathcal{A}(A_1)) \end{aligned}$$

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$$\text{As } A_2^i \cap A_2^j = \emptyset \quad \Rightarrow \quad (\mathcal{A}(A_1) \cap \mathcal{A}(A_2^k)) \cap (\mathcal{A}(A_1) \cap \mathcal{A}(A_2^j)) = \emptyset$$

$$\Rightarrow P(\mathcal{A}(A_1)) = P(\cup_{k=1}^K (\mathcal{A}(A_1) \cap \mathcal{A}(A_2^k))) = \sum_{k=1}^K P(\mathcal{A}(A_1) \cap \mathcal{A}(A_2^k))$$

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$$\Rightarrow \quad P(X_1 \in A_1) = \sum_{k=1}^K P(X_1 \in A_1, X_2 \in A_2^k)$$

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Now we can define a “split” of X_2 value space V_{X_2} :

$$V_{X_2} = \cup_{k=1}^K A_2^k, \quad A_2^k \neq \emptyset, \quad A_2^i \cap A_2^j = \emptyset, \forall i \neq j$$

$$\text{As } A_2^i \cap A_2^j = \emptyset \Rightarrow (\mathcal{A}(A_1) \cap \mathcal{A}(A_2^k)) \cap (\mathcal{A}(A_1) \cap \mathcal{A}(A_2^j)) = \emptyset$$

$$\begin{aligned} \Rightarrow P(X_1 \in A_1) &= \sum_{k=1}^K P(X_1 \in A_1, X_2 \in A_2^k) \\ &= \sum_{k=1}^K \int_{A_2^k} p(X_1 \in A_1, X_2 = x_2) dx_2 \end{aligned}$$

Appendix: math formula for deriving sum rule

Deriving **sum rule** using \mathbb{P} defined on sets:

Define for any $A_1 \subset V_{X_1}, A_2 \subset V_{X_2}$

$$\mathcal{A}(A_1) = \{(X_1(\omega), X_2(\omega), \dots, X_N(\omega)) : \mathbf{X}_1(\omega) \in A_1\}$$

$$\mathcal{A}(A_2) = \{(X_1(\omega), X_2(\omega), \dots, X_N(\omega)) : \mathbf{X}_2(\omega) \in A_2\}$$

Now we can define a “split” of X_2 value space V_{X_2} :

$$V_{X_2} = \cup_{k=1}^K A_2^k, \quad A_2^k \neq \emptyset, \quad A_2^i \cap A_2^j = \emptyset, \forall i \neq j$$

$$\text{As } A_2^i \cap A_2^j = \emptyset \Rightarrow (\mathcal{A}(A_1) \cap \mathcal{A}(A_2^k)) \cap (\mathcal{A}(A_1) \cap \mathcal{A}(A_2^j)) = \emptyset$$

$$\begin{aligned} \Rightarrow P(X_1 \in A_1) &= \sum_{k=1}^K P(X_1 \in A_1, X_2 \in A_2^k) \\ &= \int_{V_{X_2}} p(X_1 \in A_1, X_2 = x_2) dx_2 \quad (\text{sum rule}) \end{aligned}$$