6. Multivariate Distributions

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Where are we? Where are we going?

- Distributions of one variable: how to describe and summarize uncertainty about one variable.
- Today: **distributions of multiple variables** to describe relationships between variables.
- Later: use data to **learn** about probability distributions.

- 1. How to measure the relationship between two variables X and Y?
- 2. What if we have many observations of the same variable, X_1, X_2, \dots, X_n ?

1/ Distributions of Multiple Random Variables

Joint distributions



- The **joint distribution** of two r.v.s, *X* and *Y*, describes what pairs of observations, (*x*, *y*) are more likely than others.
- Shape of the joint distribution \rightsquigarrow the relationship between X and Y

Definition

The **joint probability mass function (p.m.f.)** of a pair of discrete r.v.s, (X, Y) describes the probability of any pair of values:

$$p_{X,Y}(x,y) = \mathbb{P}(X = x, Y = y)$$

- Properties of a joint p.m.f.:
 - $p_{X,Y}(x,y) \ge 0$ (probabilities can't be negative)
 - $\sum_{x} \sum_{y} p_{X,Y}(x,y) = 1$ (something must happen)
 - \sum_{x} is shorthand for sum over all possible values of X

Example: Gay marriage and gender

	Support Gay	Oppose Gay
	Marriage	Marriage
	Y = 1	Y = 0
Female $X = 1$	0.32	0.19
Male $X = 0$	0.29	0.20

- Joint p.m.f. can be summarized in a cross-tab:
 - Each is the probability of that combination, $p_{X,Y}(x,y)$
- Probability that we randomly select a woman who supports gay marriage?

$$p_{X,Y}(1,1) = \mathbb{P}(X = 1, Y = 1) = 0.32$$

- Can we get the distribution of just one of the r.v.s alone?
 - Called the **marginal distribution** in this context.
- Computing marginal p.m.f. from the joint p.m.f.:

$$\mathbb{P}(Y = y) = \sum_{x} \mathbb{P}(X = x, Y = y)$$

- Intuition: sum over the probability that Y = y and X = x for all possible values of x
 - Called marginalizing out X.
 - Works because values of X are disjoint.

Example: marginals for gay marriage

	Support Gay	Oppose Gay	
	Marriage	Marriage	Marginal
	Y = 1	Y = 0	
Female $X = 1$	0.32	0.19	0.51
Male $X = 0$	0.29	0.20	0.49
Marginal	0.61	0.39	

• What's
$$\mathbb{P}(Y = 1)$$
?

• Probability that a man supports gay marriage plus the probability that a woman supports gay marriage.

$$\mathbb{P}(Y = 1) = \mathbb{P}(X = 1, Y = 1) + \mathbb{P}(X = 0, Y = 1) = 0.32 + 0.29 = 0.61$$

• Works for all marginals.

Conditional p.m.f.

Definition

The **conditional probability mass function** or conditional p.m.f. of *Y* conditional on *X* is

$$\mathbb{P}(Y = y \mid X = x) = \frac{\mathbb{P}(X = x, Y = y)}{\mathbb{P}(X = x)}$$

for all values x s.t. $\mathbb{P}(X = x) > 0$.

• This is a valid univariate probability distribution!

•
$$P(Y = y \mid X = x) \ge 0$$
 and $\sum_{y} \mathbb{P}(Y = y \mid X = x) = 1$

• Can define the **conditional expectation** of this p.m.f.:

$$E[Y \mid X = x] = \sum_{y} y \mathbb{P}(Y = y \mid X = x)$$

Example: conditionals for gay marriage

	Support Gay	Oppose Gay	
	Marriage	Marriage	Marginal
	Y = 1	Y = 0	
Female $X = 1$	0.32	0.19	0.51
Male $X = 0$	0.29	0.20	0.49
Marginal	0.61	0.39	

• Probability of favoring gay marriage conditional on male?

$$\mathbb{P}(Y = 1 \mid X = 0) = \frac{\mathbb{P}(X = 0, Y = 1)}{\mathbb{P}(X = 0)} = \frac{0.29}{0.29 + 0.20} = 0.592$$

Example: conditionals for gay marriage



• Two values of X \log two **univariate** conditional distributions of Y

• Bayes' rule for r.v.s:

$$\mathbb{P}(Y = y \mid X = x) = \frac{\mathbb{P}(X = x \mid Y = y)\mathbb{P}(Y = y)}{\mathbb{P}(X = x)}$$

• Law of total probability for r.v.s:

$$\mathbb{P}(X = x) = \sum_{y} \mathbb{P}(X = x \mid Y = y)\mathbb{P}(Y = y)$$

Definition

For two r.v.s X and Y, the **joint cumulative distribution function** or joint c.d.f. $F_{X,Y}(x, y)$ is a function such that for finite values x and y,

$$F_{X,Y}(x,y) = \mathbb{P}(X \le x, Y \le y)$$

- Well-defined for discrete and continuous X and Y.
- For discrete we simply have:

$$F_{X,Y}(x,y) = \sum_{i \le x} \sum_{j \le y} \mathbb{P}(X = i, Y = j)$$

• One continuous r.v.: prob. of being in a subset of the real line.



• Two continuous r.v.s: probability of being in some subset of the 2-dimensional plane.



Definition

If two continuous r.v.s X and Y with joint c.d.f. $F_{X,Y}$, their **joint p.d.f.** $f_{X,Y}(x, y)$ is the derivative of $F_{X,Y}$ with respect to x and y,

$$f_{X,Y}(x,y) = \frac{\partial^2}{\partial x \partial y} F_{X,Y}(x,y)$$

• Integrate over both dimensions to get the probability of a region:

$$\mathbb{P}((X,Y)\in A) = \iint_{(x,y)\in A} f_{X,Y}(x,y)dxdy.$$

+ $\{(x, y) : f_{X,Y}(x, y) > 0\}$ is called the **support** of the distribution.

- Joint p.d.f. must meet the following conditions:
 - 1. $f_{X,Y}(x,y) \ge 0$ for all values of (x,y), (nonnegative)
 - 2. $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f_{X,Y}(x,y) dx dy = 1$, (probabilities "sum" to 1)
- $\mathbb{P}(X = x, Y = y) = 0$ for similar reasons as with single r.v.s.

Joint densities are 3D



- X and Y axes are on the "floor," height is the value of $f_{X,Y}(x,y)$.
- Remember $f_{X,Y}(x,y) \neq \mathbb{P}(X = x, Y = y)$.

Probability = volume



- $\mathbb{P}((X, Y) \in A) = \iint_{(x,y)\in A} f_{X,Y}(x,y) dx dy$
- Probability = volume above a specific region.

• We can recover the marginal PDF of one of the variables by integrating over the distribution of the other variable:

$$f_Y(y) = \int_{-\infty}^{\infty} f_{X,Y}(x,y) dx$$

• Works for either variable:

$$f_X(x) = \int_{-\infty}^{\infty} f_{X,Y}(x,y) dy$$

Visualizing continuous marginals



• Marginal integrates (sums, basically) over other r.v.:

$$f_{Y}(y) = \int_{-\infty}^{\infty} f_{X,Y}(x,y) dx$$

• Pile up/flatten all of the joint density onto a single dimension.

Continuous conditional distributions

Definition

The conditional p.d.f. of a continuous random variable is

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

for all values x s.t. $f_X(x) > 0$.

• Implies

$$\mathbb{P}(\mathbf{a} < \mathbf{Y} < \mathbf{b} | \mathbf{X} = \mathbf{x}) = \int_{\mathbf{a}}^{\mathbf{b}} f_{\mathbf{Y} | \mathbf{X}}(\mathbf{y} | \mathbf{x}) d\mathbf{y}$$

• Based on the definition of the conditional p.m.f./p.d.f., we have the following factorization:

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

Conditional distributions as slices



- $f_{Y|X}(y|x_0)$ is the conditional p.d.f. of Y when $X = x_0$
- $f_{Y|X}(y|x_0)$ is proportional to joint p.d.f. along x_0 : $f_{X,Y}(y,x_0)$
- Normalize by dividing by $f_X(x_0)$ to ensure proper p.d.f.

Independence

Independence

Two r.v.s *Y* and *X* are **independent** (which we write *X* \perp *Y*) if for all sets *A* and *B*:

$$\mathbb{P}(X \in A, Y \in B) = \mathbb{P}(X \in A)\mathbb{P}(Y \in B)$$

- Knowing the value of X gives us no information about the value of Y.
- If X and Y are independent, then:
 - $f_{X,Y}(x,y) = f_X(x)f_Y(y)$ and $p_{X,Y}(x,y) = p_X(x)p_Y(y)$ (joint is the product of marginals)
 - $F_{X,Y}(x,y) = F_X(x)F_Y(y)$
 - $f_{Y|X}(y|x) = f_Y(y)$ (conditional is the marginal)
- · Conditional independence implies similar to conditional distributions:

$$\mathbb{P}(X \in A, Y \in B \mid Z) = \mathbb{P}(X \in A \mid Z)\mathbb{P}(Y \in B \mid Z)$$

2/ Expectations of Joint Distributions

- Single r.v.: summarized $f_X(x)$ with $\mathbb{E}[X]$ and $\mathbb{V}[X]$
- With 2 r.v.s: how strong is the dependence is between X and Y?
- First: **expectations** over joint distributions.

Expectations over multiple r.v.s

- 2-d LOTUS: take expectations over the joint distribution.
- With discrete X and Y:

$$\mathbb{E}[g(X,Y)] = \sum_{x} \sum_{y} g(x,y) \ p_{X,Y}(x,y)$$

• With continuous *X* and *Y*:

$$\mathbb{E}[g(X,Y)] = \int_{X} \int_{Y} g(x,y) f_{X,Y}(x,y) dx dy$$

• Marginal expectations:

$$\mathbb{E}[Y] = \sum_{x} \sum_{y} y \ p_{X,Y}(x,y)$$

Applying 2D LOTUS

Theorem

If X and Y are independent r.v.s, then

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

• Proof for discrete X and Y:

F

$$\begin{split} [XY] &= \sum_{x} \sum_{y} xy \ f_{X,Y}(x,y) \\ &= \sum_{x} \sum_{y} xy \ f_{X}(x) f_{Y}(y) \\ &= \left(\sum_{x} x \ f_{X}(x) \right) \left(\sum_{y} y \ f_{Y}(y) \right) \\ &= \mathbb{E}[X] \mathbb{E}[Y] \end{split}$$

3/ Covariance and Correlation

- Independence assumptions are **everywhere** in statistics.
 - Each response in a poll is considered **independent** of all other responses.
 - In a randomized control trial, treatment assignment is **independent** of background characteristics.
- Lack of independence is a blessing or a curse:
 - Two variables not independent \rightsquigarrow potentially interesting relationship.
 - In observational studies, treatment assignment is usually not independent of background characteristics.

Defining covariance

• How do we measure the strength of the dependence between two r.v.?

Covariance

The **covariance** between two r.v.s, X and Y is defined as:

$$\operatorname{Cov}[X, Y] = \mathbb{E}\Big[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])\Big]$$

- How often do high values of X occur with high values of Y?
- Properties of covariances:
 - $\operatorname{Cov}[X, Y] = \mathbb{E}[XY] \mathbb{E}[X]\mathbb{E}[Y]$
 - If $X \perp Y$, then Cov[X, Y] = 0

Covariance intuition



Covariance intuition



• Large values of X tend to occur with large values of Y:

* $(X - \mathbb{E}[X])(Y - \mathbb{E}[Y]) = (\text{pos. num.}) \times (\text{pos. num}) = +$

• Small values of X tend to occur with small values of Y:

• $(X - \mathbb{E}[X])(Y - \mathbb{E}[Y]) = (\text{neg. num.}) \times (\text{neg. num}) = +$

- If these dominate \rightsquigarrow positive covariance.

Covariance intuition



• Large values of X tend to occur with small values of Y:

* $(X - \mathbb{E}[X])(Y - \mathbb{E}[Y]) = (\text{pos. num.}) \times (\text{neg. num}) = -$

• Small values of X tend to occur with large values of Y:

• $(X - \mathbb{E}[X])(Y - \mathbb{E}[Y]) = (\text{neg. num.}) \times (\text{pos. num}) = -$

- If these dominate \rightsquigarrow negative covariance.

Properties of variances and covariances

 $\operatorname{Cov}[X,Y] = \mathbb{E}[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])] = \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y]$

- Properties of covariances:
 - 1. $\operatorname{Cov}[X, X] = \mathbb{V}[X]$
 - 2. Cov[X, Y] = Cov[Y, X]
 - 3. Cov[X, c] = 0 for any constant c
 - 4. $\operatorname{Cov}[aX, Y] = a\operatorname{Cov}[X, Y]$.
 - 5. Cov[X + Y, Z] = Cov[X, Z] + Cov[Y, Z]
 - 6. Cov[X + Y, Z + W] = Cov[X, Z] + Cov[Y, Z] + Cov[X, W] + Cov[Y, W]

Covariances and variances

- Can now state a few more properties of variances.
- Variance of a sum:

$$\mathbb{V}[X+Y] = \mathbb{V}[X] + \mathbb{V}[Y] + 2\mathsf{Cov}[X,Y]$$

• More generally for *n* r.v.s X_1, \ldots, X_n :

$$\mathbb{V}[X_1 + \dots + X_n] = \mathbb{V}[X_1] + \dots + \mathbb{V}[X_n] + 2\sum_{i < j} \operatorname{Cov}(X_i, X_j)$$

- If X and Y independent, $\mathbb{V}[X + Y] = \mathbb{V}[X] + \mathbb{V}[Y]$.
 - Beware: $\mathbb{V}[X Y] = \mathbb{V}[X] + \mathbb{V}[Y]$ as well.

Zero covariance doesn't imply independence

- We saw that $X \perp \!\!\!\perp Y \rightsquigarrow \operatorname{Cov}[X, Y] = 0$.
- Does Cov[X, Y] = 0 imply that $X \perp Y$? No!
- **Counterexample:** $X \in \{-1, 0, 1\}$ with equal probability and $Y = X^2$.
- Covariance is a measure of **linear dependence**, so it can miss non-linear dependence.

• Correlation is a scale-free measure of linear dependence.

Definition

The **correlation** between two r.v.s X and Y is defined as:

$$\rho = \rho(X, Y) = \frac{\mathsf{Cov}[X, Y]}{\sqrt{\mathbb{V}[X]\mathbb{V}[Y]}} = \mathsf{Cov}\left(\frac{X - \mathbb{E}[X]}{SD[X]}, \frac{Y - \mathbb{E}[Y]}{SD[Y]}\right)$$

- Covariance after dividing out the scales of the respective variables.
- Correlation properties:
 - $-1 \le \rho \le 1$
 - $|\rho(X, Y)| = 1$ if and only if X and Y are perfectly correlated with a deterministic linear relationship: Y = a + bX.

4/ Random vectors

Multivariate random vectors

- Can group r.v.s into **random vectors X** = $(X_1, \dots, X_k)'$
 - **X** is a function from the sample space to \mathbb{R}^k
 - x is now a length-k vector and potential value of X
 - Generalizes all ideas from 2 variables to k
- Joint distribution function: $F(\mathbf{x}) = \mathbb{P}(\mathbf{X} \leq \mathbf{x}) = \mathbb{P}(X_1 \leq x_1, \dots, X_k \leq x_k).$
 - Discrete: joint p.m.f. $\mathbb{P}(\boldsymbol{X}=\boldsymbol{x}).$
 - Continuous: joint p.d.f.

$$f(\mathbf{x}) = \frac{\partial^k}{\partial x_1 \cdots \partial x_k} F(\mathbf{x})$$

• Expectation of a random vector is just the vector of expectations:

$$\mathbb{E}[\mathbf{X}] = \left(\mathbb{E}[X_1], \mathbb{E}[X_2], \dots, \mathbb{E}[X_k]\right)'$$

Covariance matrices

• Covariance matrix generalizes (co)variance to this setting:

$$\mathbb{V}[\mathbf{X}] = \mathbb{E}\left[(\mathbf{X} - \mathbb{E}[\mathbf{X}])(\mathbf{X} - \mathbb{E}[\mathbf{X}])'\right]$$

• We usually write $\mathbb{V}[\mathbf{X}] = \mathbf{\Sigma}$ and it is a $k \times k$ symmetric matrix:

$$\boldsymbol{\Sigma} = \begin{pmatrix} \sigma_1^2 & \sigma_{12} & \cdots & \sigma_{1k} \\ \sigma_{21} & \sigma_2^2 & \cdots & \sigma_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{k1} & \sigma_{k2} & \cdots & \sigma_k^2 \end{pmatrix}$$

where, $\sigma_j^2 = \mathbb{V}[X_j]$ and $\sigma_{ij} = \text{Cov}(X_i, X_j)$.

• Symmetric ($\Sigma = \Sigma'$) because $Cov(X_i, X_j) = Cov(X_j, X_i)$.

Multivariate standard normal distribution

- Let $\mathbf{Z} = (Z_1, Z_2, \dots, Z_k)$ be i.i.d. $\mathcal{N}(0, 1)$. What is their joint distribution?
- For vector of values $\mathbf{z} = (z_1, z_2, \dots, z_k)^T$

$$f(\mathbf{z}) = \frac{1}{(2\pi)^{k/2}} \exp\left(-\frac{\mathbf{z}'\mathbf{z}}{2}\right)$$

- Easy to see the mean/variance: $\mathbb{E}[\mathbf{Z}] = 0$ and $\mathbb{V}[\mathbf{Z}] = \mathbf{I}_k$.
 - I_k is the k by k identity matrix because $\mathbb{V}[Z_j] = 1$ and $Cov(Z_i, Z_j) = 0$.

Linear transformations of random vectors

Theorem

If $\mathbf{X} \in \mathbb{R}^k$ with $k \times 1$ expectation $\boldsymbol{\mu}$ and $k \times k$ covariance matrix $\boldsymbol{\Sigma}$, and \mathbf{A} is a $q \times k$ matrix, then $\mathbf{A}\mathbf{X}$ is a random vector with mean $\mathbf{A}\boldsymbol{\mu}$ and covariance matrix $\mathbf{A}\boldsymbol{\Sigma}\mathbf{A}'$.

- Let $Z \sim \mathcal{N}(0, I_k)$ and $X = \mu + BZ$, where B is $q \times k$ then $X \sim \mathcal{N}(\mu, BB')$
 - $\boldsymbol{\mu}$: $q \times 1$ mean vector $\mathbb{E}[\mathbf{X}] = \boldsymbol{\mu}$
 - $\mathbb{V}[\mathbf{X}] = \mathbf{B}\mathbf{B}'$: $q \times q$ covariance matrix.
- More generally, if $X \sim \mathcal{N}(\mu, \Sigma)$ then $Y = a + BX \sim \mathcal{N}(a + B\mu, B\Sigma B')$

Properties of the multivariate normal

- If (X_1, X_2, X_3) are MVN, then (X_1, X_2) is also MVN.
- If (X, Y) are multivariate normal with Cov(X, Y) = 0, then X and Y are independent.