6. Multivariate Distributions

Spring 2023

Matthew Blackwell

Gov 2002 (Harvard)

Where are we? Where are we going?

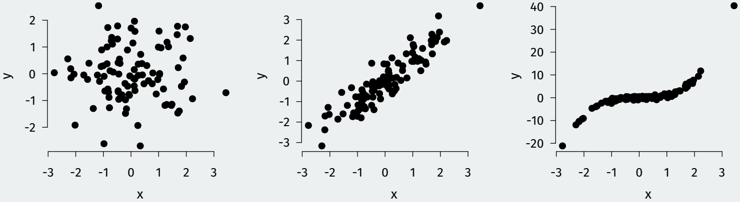
- Distributions of one variable: how to describe and summarize uncertainty about one variable.
- Today: **distributions of multiple variables** to describe relationships between variables.
- Later: use data to **learn** about probability distributions.

Why multiple random variables?

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

Discrete r.v.s

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:

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

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

Example: Gay marriage and gender

	Support Gay Marriage $Y = 1$	Oppose Gay Marriage $Y = 0$
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?

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

Marginal distributions

- 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 Marriage $Y = 1$	Oppose Gay Marriage $Y = 0$	Marginal
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!
  - $P(Y = y \mid X = x) \geq 0$ and $\sum_y \mathbb{P}(Y = y \mid X = x) = 1$
- Can define the **conditional expectation** of this p.m.f.:

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

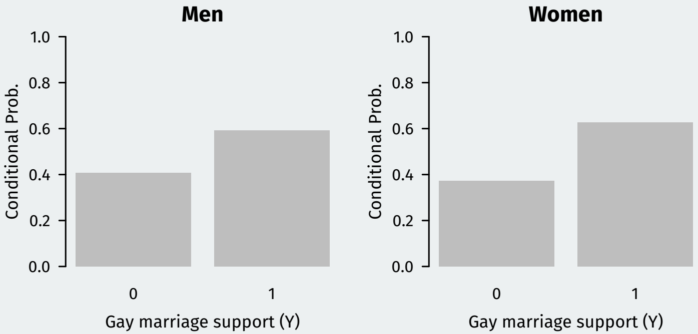
Example: conditionals for gay marriage

	Support Gay Marriage $Y = 1$	Oppose Gay Marriage $Y = 0$	Marginal
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 $X \rightsquigarrow$ two **univariate** conditional distributions of Y

Bayes and LTP

- 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:

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

Joint c.d.f.s

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,

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

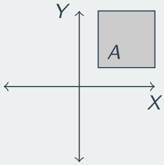
- Well-defined for discrete and continuous X and Y.
- For discrete we simply have:

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

Continuous r.v.s

- 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.



Continuous joint p.d.f.

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:

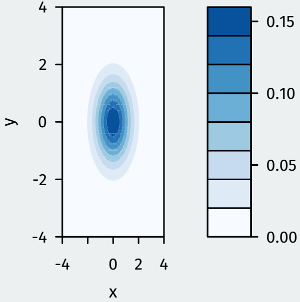
$$\mathbb{P}((X,Y) \in A) = \iint_{(x,y)\in A} f_{X,Y}(x,y)dxdy.$$

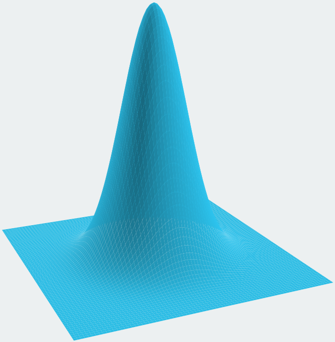
- $\{(x,y) : f_{X,Y}(x,y) > 0\}$ is called the **support** of the distribution.

Properties of the joint p.d.f.

- Joint p.d.f. must meet the following conditions:
  1. $f_{X,Y}(x, y) \geq 0$ 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.

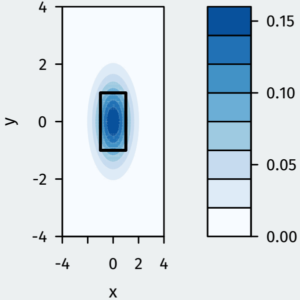
Joint densities are 3D

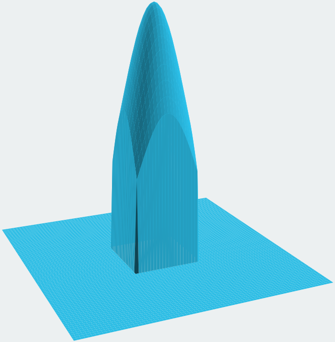




- X and Y axes are on the “floor,” height is the value of $f_{X,Y}(x, y)$.
- Remember $f_{X,Y}(x, y) \neq \mathbb{P}(X = x, Y = y)$.

Probability = volume





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

Continuous marginal distributions

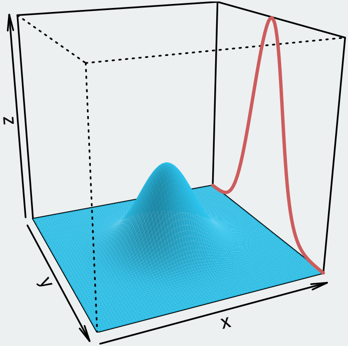
- We can recover the marginal PDF of one of the variables by integrating over the distribution of the other variable:

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

- 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. $f_X(x) > 0$.

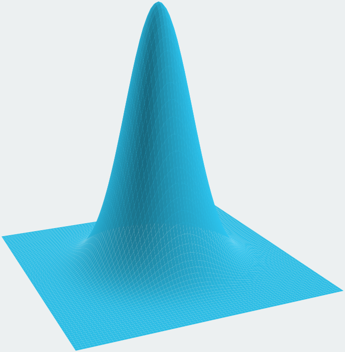
- Implies

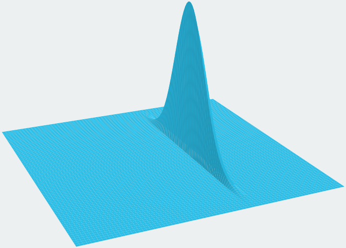
$$\mathbb{P}(a < Y < b|X = x) = \int_a^b f_{Y|X}(y|x)dy$$

- 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 $X \perp\!\!\!\perp Y$) 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:
    - $f_{X,Y}(x, y) = f_X(x)f_Y(y)$ (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

Properties 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:

$$\mathbb{E}[g(X, Y)] = \sum_x \sum_y g(x, y)\ f_{X,Y}(x, y)$$

- 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:

$$\mathbb{E}[Y] = \sum_x \sum_y y\ f_{X,Y}(x, y)$$

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:

$$\begin{aligned}
\mathbb{E}[XY] &= \sum_x \sum_y xy\ f_{X,Y}(x,y) \\
&= \sum_x \sum_y xy\ f_X(x) f_Y(y) \\
&= \left(\sum_x x\ f_X(x)\right)\left(\sum_y y\ f_Y(y)\right) \\
&= \mathbb{E}[X]\mathbb{E}[Y]
\end{aligned}$$

3/ Covariance and Correlation

Why (in)dependence?

- 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.?

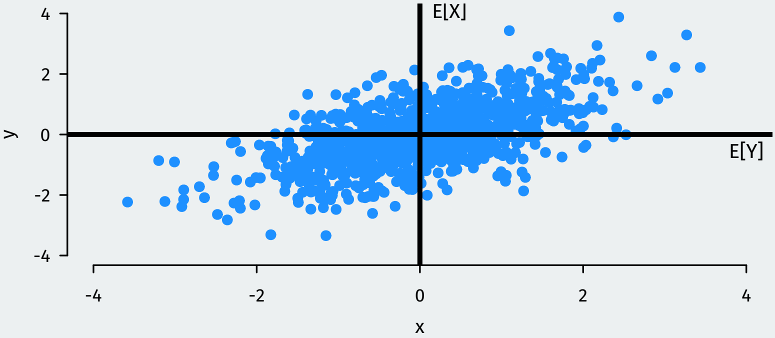
Covariance

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

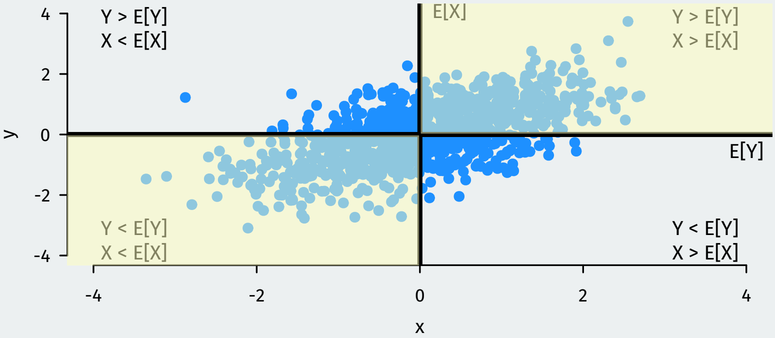
$$\text{Cov}[X, Y] = \mathbb{E}\Big[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])\Big]$$

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

Covariance intuition

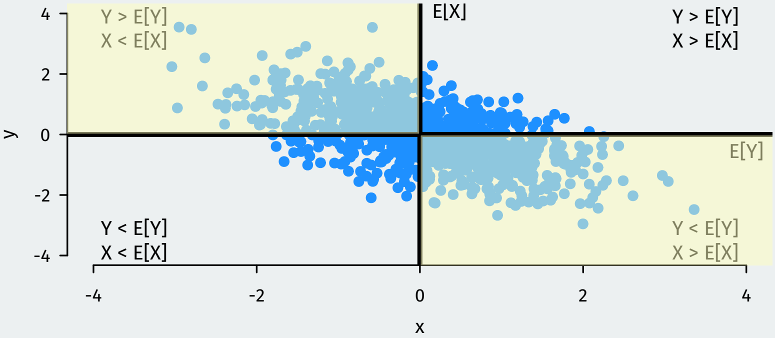


Covariance intuition



- 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

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

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

Covariances and variances

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

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

- More generally for n r.v.s $X_1, \ldots, X_n$:

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

- 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 $X \perp\!\!\!\perp Y \rightsquigarrow \text{Cov}[X, Y] = 0$.
- Does $\text{Cov}[X, Y] = 0$ imply that $X \perp\!\!\!\perp Y$? **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

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

Definition

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

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

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

4/ Random vectors

Multivariate random vectors

- When we have many r.v.s, we sometimes group them into **random vectors** $X = (X_1, \dots, X_m)^T$
    - X is a function from the sample space to $\mathbb{R}^m$
    - x is now a length-m vector and potential value of X
    - Generalizes all ideas from 2 variables to m
- Joint distribution function: $F(x) = \mathbb{P}(X \leq x) = \mathbb{P}(X_1 \leq x_1, \dots, X_m \leq x_m)$.
    - Discrete: joint p.m.f. $\mathbb{P}(X = x)$.
    - Continuous: joint p.d.f.

$$f(x) = \frac{\partial^m}{\partial x_1 \cdots \partial x_m} F(x)$$

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

$$\mathbb{E}[X] = (\mathbb{E}[X_1], \mathbb{E}[X_2], \dots, \mathbb{E}[X_m])^T$$

Covariance matrices

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

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

- We usually write $\mathbb{V}[X] = \Sigma$ and it is a $m \times m$ **symmetric** matrix:

$$\Sigma = \begin{pmatrix} \sigma_1^2 & \sigma_{12} & \cdots & \sigma_{1m} \\ \sigma_{21} & \sigma_2^2 & \cdots & \sigma_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{m1} & \sigma_{m2} & \cdots & \sigma_m^2 \end{pmatrix}$$

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

- Symmetric ($\Sigma = \Sigma^T$) because $\text{Cov}(X_i, X_j) = \text{Cov}(X_j, X_i)$.

Linear transformations of random vectors

Theorem

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

Multivariate random vectors

- Can group r.v.s into **random vectors** $\mathbf{X} = (X_1, \dots, X_k)'$
  - $\mathbf{X}$ is a function from the sample space to $\mathbb{R}^k$
  - $\mathbf{x}$ is now a length-k vector and potential value of $\mathbf{X}$
  - 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. $\mathbb{P}(\mathbf{X} = \mathbf{x})$.
  - 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:

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

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:

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

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

- Symmetric ($\mathbf{\Sigma} = \mathbf{\Sigma}'$) because $\text{Cov}(X_i, X_j) = \text{Cov}(X_j, X_i)$.

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 $\mathbb{V}[\mathbf{Z}] = \mathbf{I}_k$.
    - $\mathbf{I}_k$ is the k by k identity matrix because $\mathbb{V}[Z_j] = 1$ and $\text{Cov}(Z_i, Z_j) = 0$.

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 $\mathbf{AX}$ is a random vector with mean $\mathbf{A}\boldsymbol{\mu}$ and covariance matrix $\mathbf{A}\boldsymbol{\Sigma}\mathbf{A}'$.

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

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 $\text{Cov}(X, Y) = 0$, then X and Y are independent.