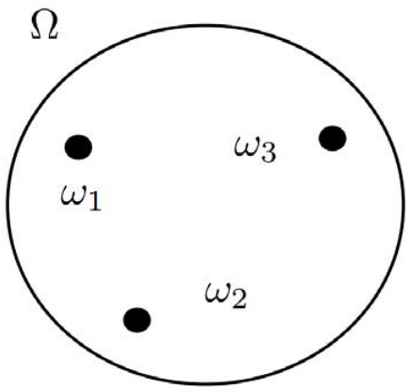
ENM 5310: Data-driven Modeling and Probabilistic Scientific Computing

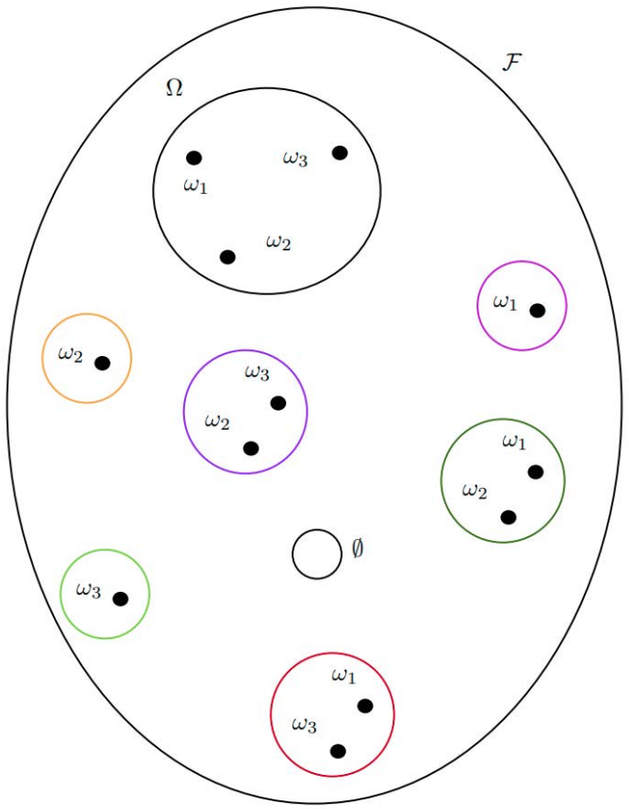
Lecture #2

Probability theory, statistics, and information theory fundamentals

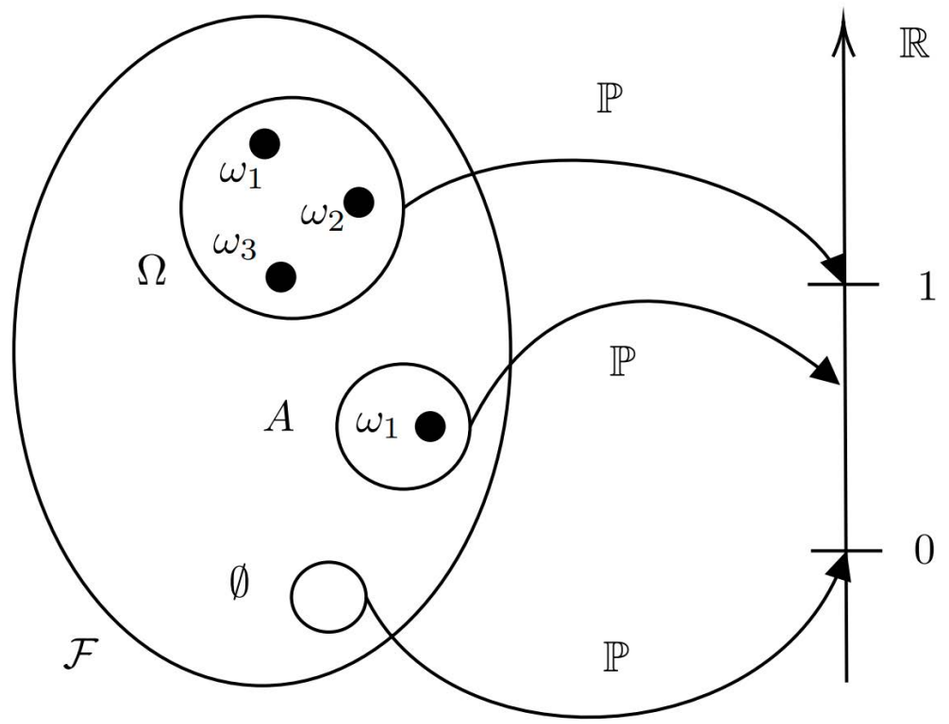
Probability spaces & random variables



Sample space



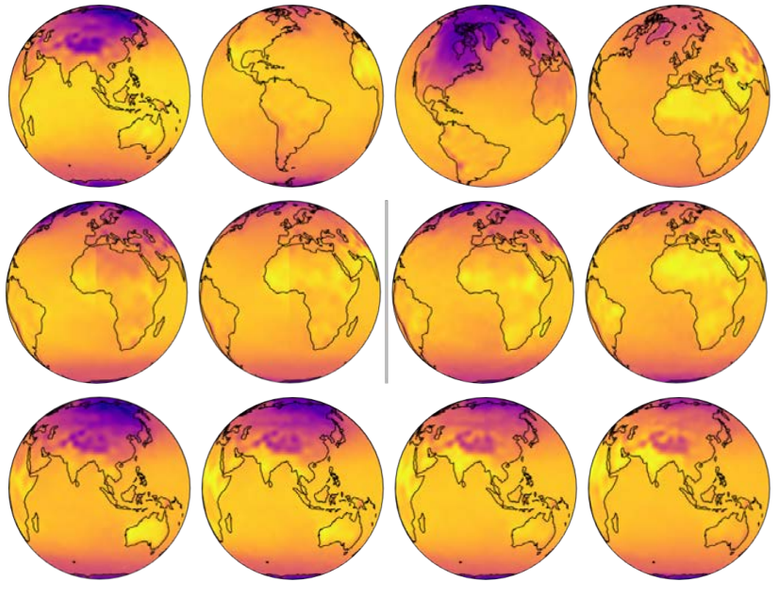
σ-algebra of events



Probability measure

vectors

matrices



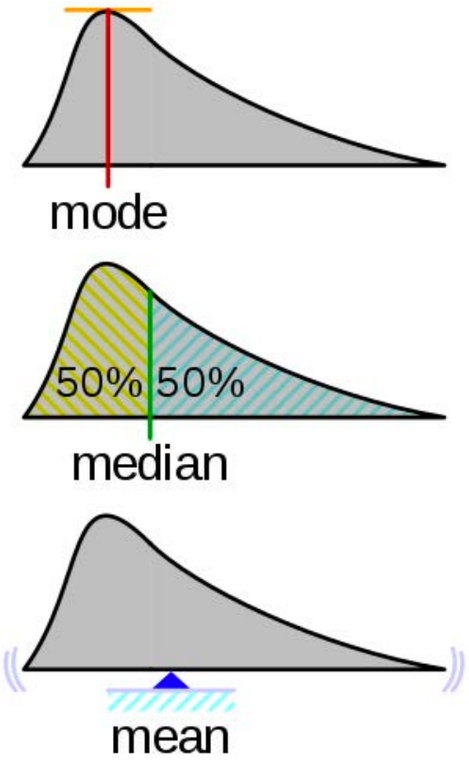
functions

Recap: Continuous random variables

- A ***continuous random variable*** is one which takes an infinite number of possible values. Continuous random variables are usually measurements. Examples include height, weight, the amount of sugar in an orange, the time required to run a mile.
- A continuous random variable is not defined at specific values. Instead, it is defined over an *interval* of values, and is represented by the ***area under a curve*** (in advanced mathematics, this is known as an *integral*). The probability of observing any single value is equal to 0, since the number of values which may be assumed by the random variable is infinite.

Probability density functions

$$\Pr[a \leq X \leq b] = \int_a^b f_X(x)\,dx.$$



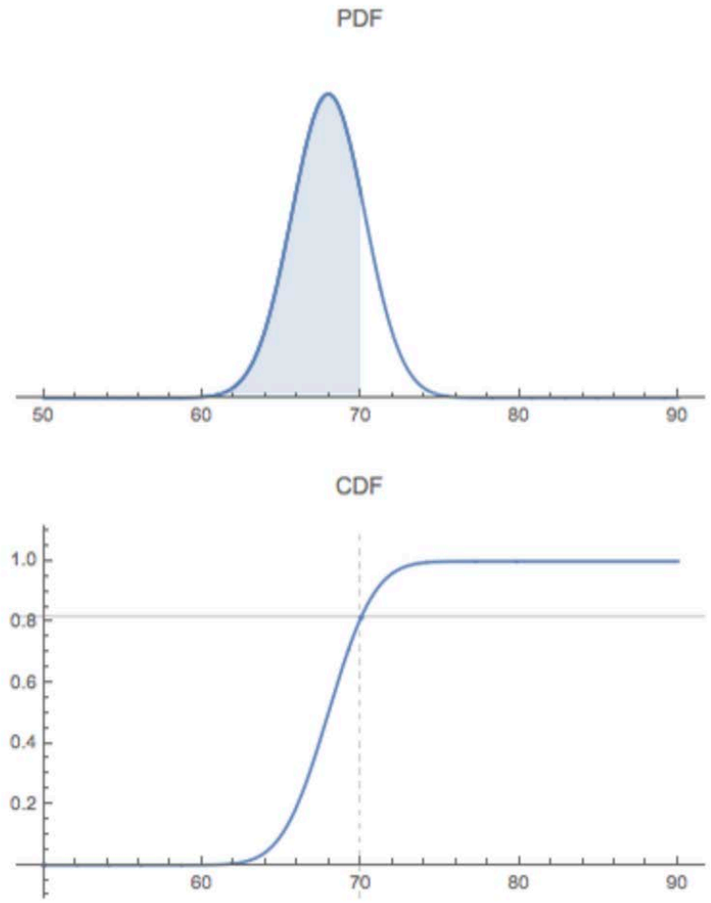
Hence, if F_X is the cumulative distribution function of X, then:

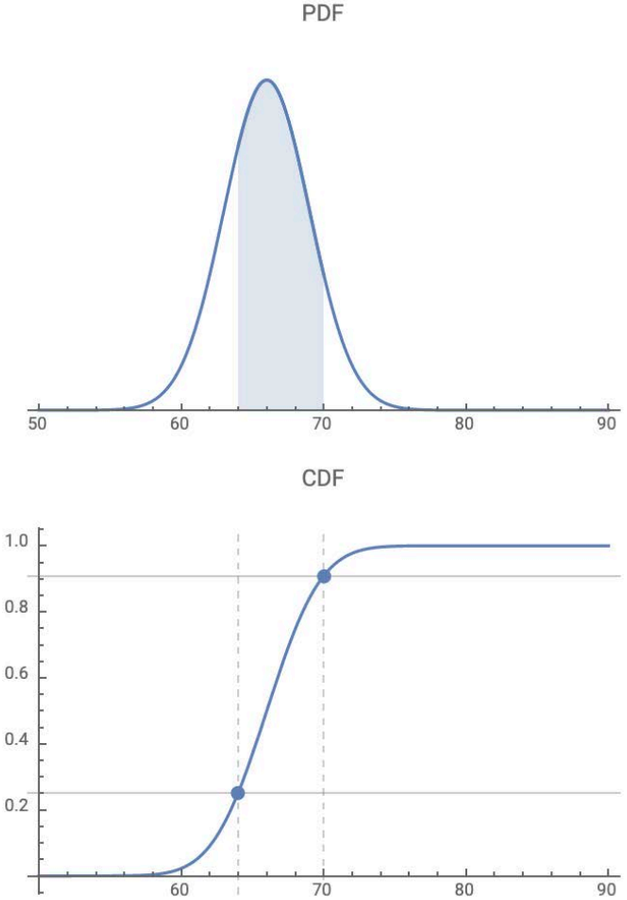
$$F_X(x) = \int_{-\infty}^{x} f_X(u)\,du,$$

and (if f_X is continuous at x)

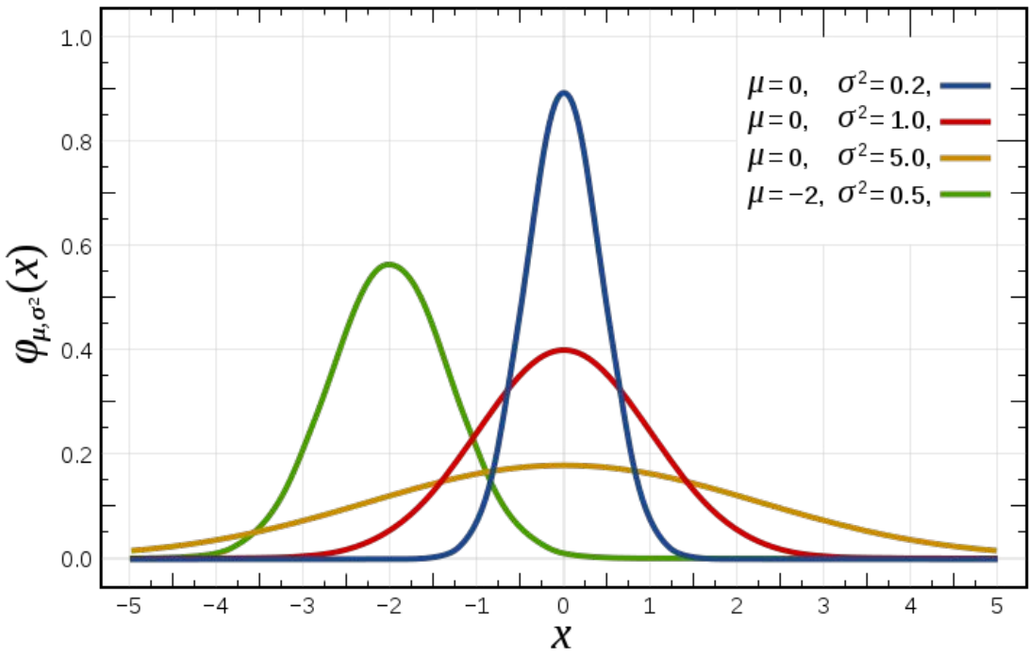
$$f_X(x) = \frac{d}{dx} F_X(x).$$

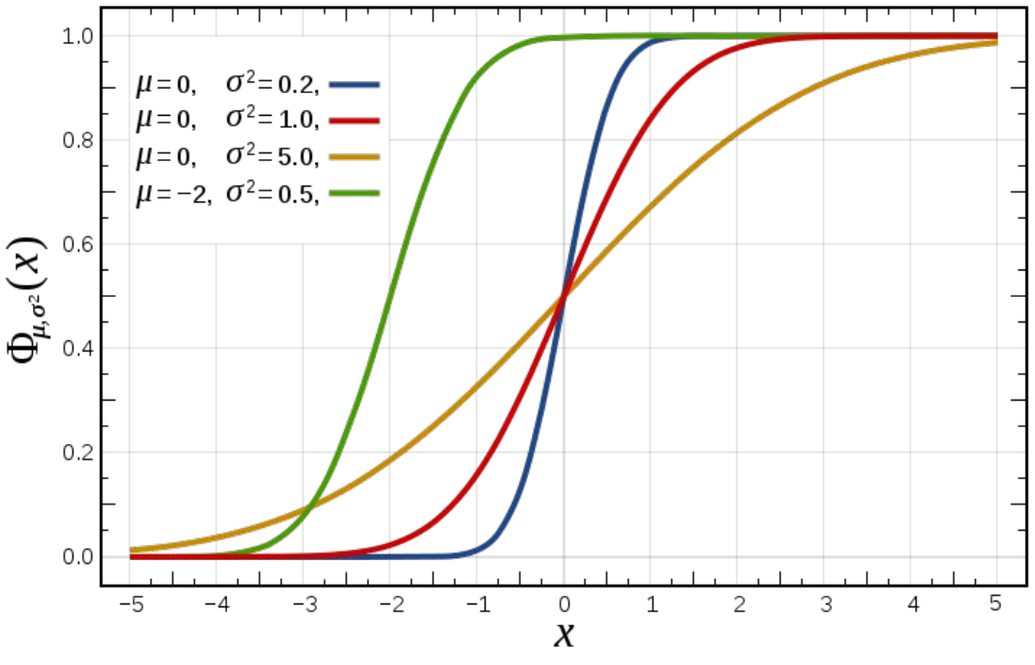
Intuitively, one can think of $f_X(x)\,dx$ as being the probability of X falling within the infinitesimal interval $[x, x + dx]$.





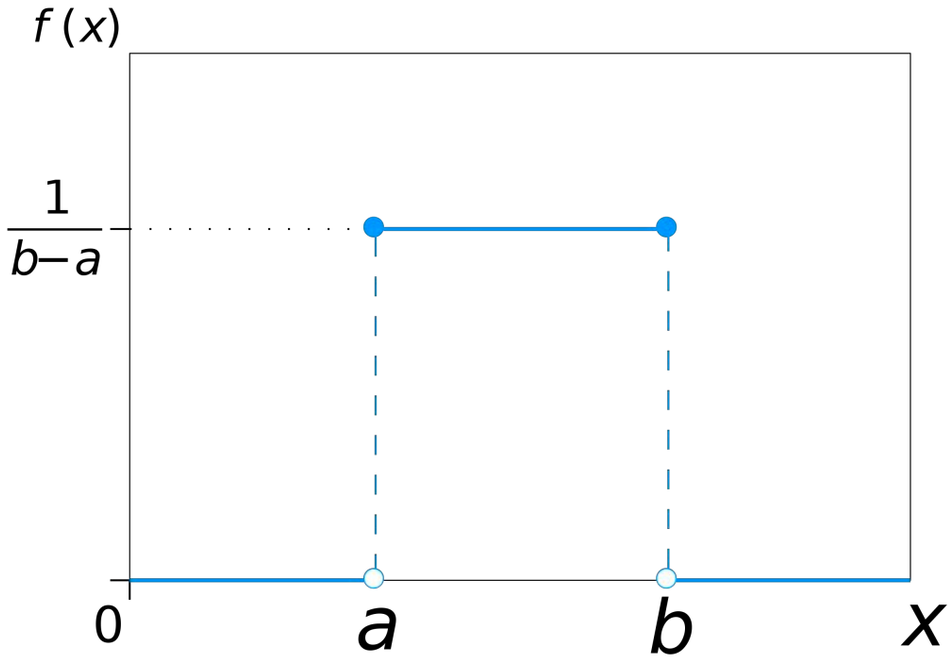
Recap: Univariate Gaussian distribution

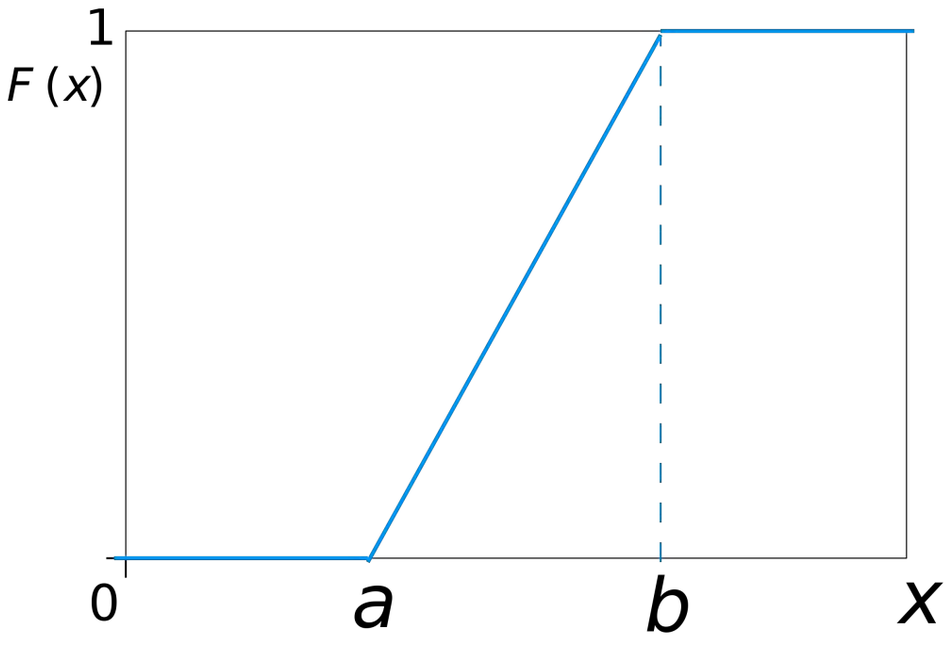




Notation	$\mathcal{N}(\mu, \sigma^2)$
Parameters	$\mu \in \mathbb{R}$ = mean (location) $\sigma^2 > 0$ = variance (squared scale)
Support	$x \in \mathbb{R}$
PDF	$\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$
CDF	$\frac{1}{2}\left[1 + \operatorname{erf}\left(\frac{x-\mu}{\sigma\sqrt{2}}\right)\right]$
Quantile	$\mu + \sigma\sqrt{2}\,\operatorname{erf}^{-1}(2F-1)$
Mean	μ
Median	μ
Mode	μ
Variance	σ^2
Skewness	0
Ex. kurtosis	0
Entropy	$\frac{1}{2}\log(2\pi e\sigma^2)$
MGF	$\exp(\mu t + \sigma^2 t^2/2)$
CF	$\exp(i\mu t - \sigma^2 t^2/2)$
Fisher information	$\mathcal{I}(\mu,\sigma) = \begin{pmatrix} 1/\sigma^2 & 0 \\ 0 & 2/\sigma^2 \end{pmatrix}$ $\mathcal{I}(\mu,\sigma^2) = \begin{pmatrix} 1/\sigma^2 & 0 \\ 0 & 1/(2\sigma^4) \end{pmatrix}$
Kullback-Leibler divergence	$D_{\mathrm{KL}}(\mathcal{N}_0 \parallel \mathcal{N}_1) = \frac{1}{2}\{(\sigma_0/\sigma_1)^2 + \frac{(\mu_1-\mu_0)^2}{\sigma_1^2} - 1 + 2\ln\frac{\sigma_1}{\sigma_0}\}$

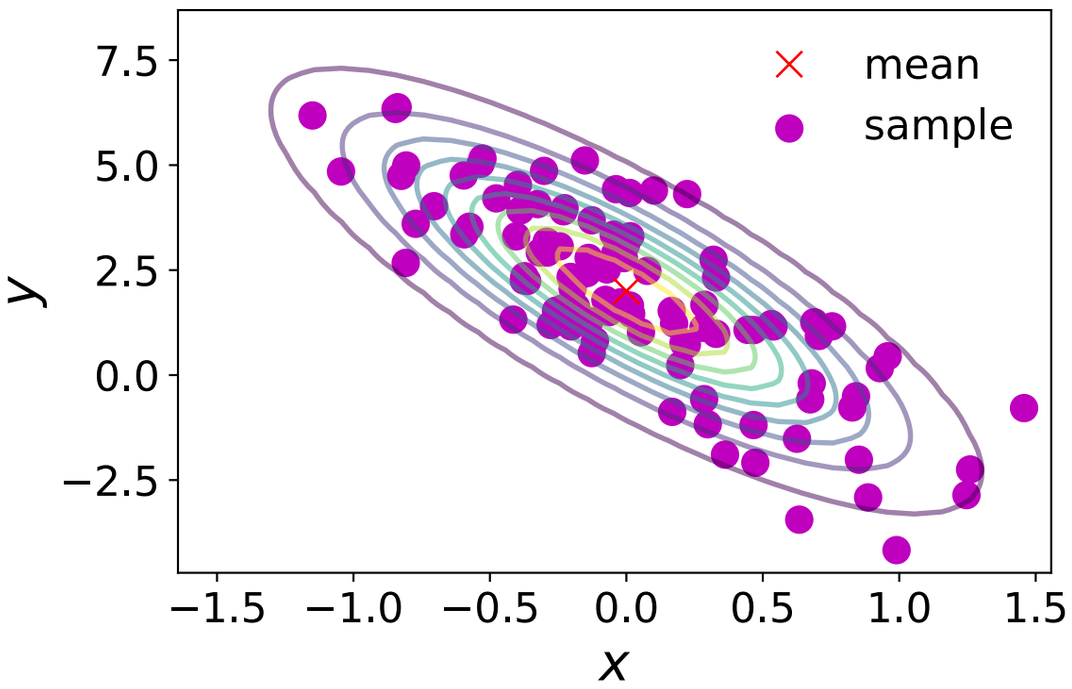
Recap: Uniform distribution

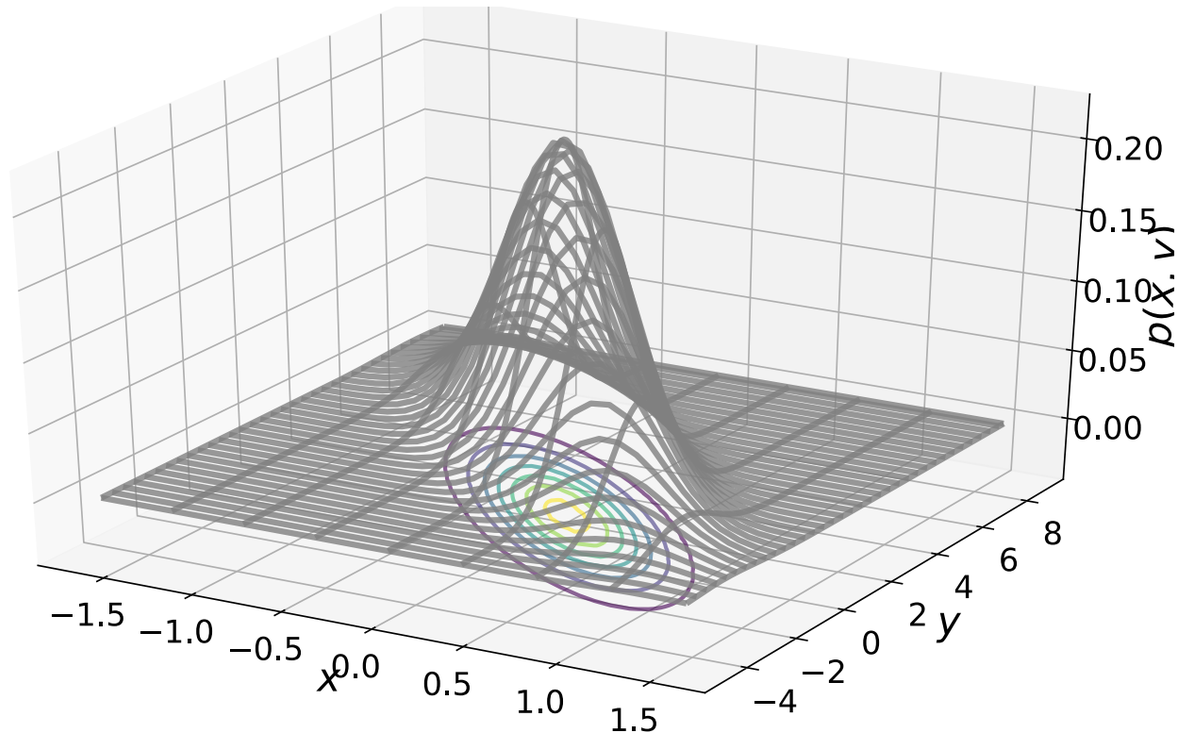




Notation	$\mathcal{U}(a,b)$ or $\operatorname{unif}(a,b)$
Parameters	$-\infty < a < b < \infty$
Support	$x \in [a,b]$
PDF	$\begin{cases} \frac{1}{b-a} & \text{for } x \in [a,b] \\ 0 & \text{otherwise} \end{cases}$
CDF	$\begin{cases} 0 & \text{for } x < a \\ \frac{x-a}{b-a} & \text{for } x \in [a,b) \\ 1 & \text{for } x \geq b \end{cases}$
Mean	$\frac{1}{2}(a+b)$
Median	$\frac{1}{2}(a+b)$
Mode	any value in (a,b)
Variance	$\frac{1}{12}(b-a)^2$
Skewness	0
Ex. kurtosis	$-\frac{6}{5}$
Entropy	$\ln(b-a)$
MGF	$\begin{cases} \frac{e^{tb}-e^{ta}}{t(b-a)} & \text{for } t \neq 0 \\ 1 & \text{for } t = 0 \end{cases}$
CF	$\begin{cases} \frac{e^{itb}-e^{ita}}{it(b-a)} & \text{for } t \neq 0 \\ 1 & \text{for } t = 0 \end{cases}$

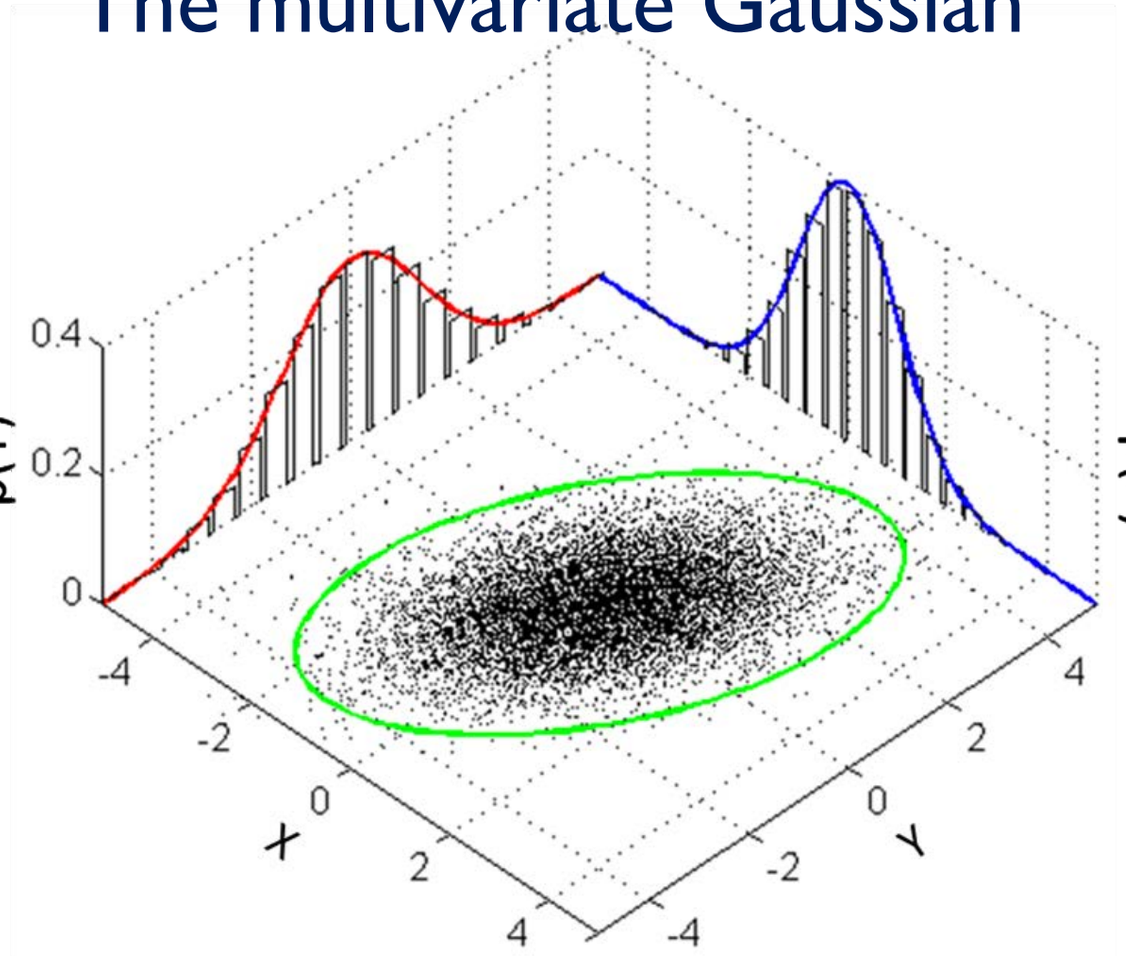
The multivariate Gaussian





$$p(\boldsymbol{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = (2\pi)^{-\frac{D}{2}} |\boldsymbol{\Sigma}|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} - \boldsymbol{\mu}) \right)$$

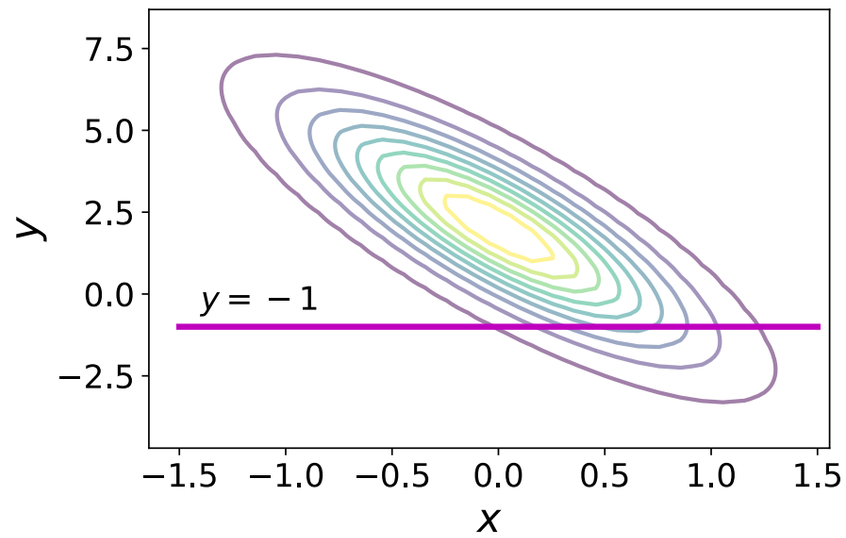
The multivariate Gaussian



Notation	$\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$
Parameters	$\boldsymbol{\mu} \in \mathbf{R}^k$ — location $\boldsymbol{\Sigma} \in \mathbf{R}^{k \times k}$ — covariance (positive semi-definite matrix)
Support	$\boldsymbol{x} \in \boldsymbol{\mu} + \operatorname{span}(\boldsymbol{\Sigma}) \subseteq \mathbf{R}^k$
PDF	$\det(2\pi\boldsymbol{\Sigma})^{-\frac{1}{2}}\, e^{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})'\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})}$, exists only when $\boldsymbol{\Sigma}$ is positive-definite
Mean	$\boldsymbol{\mu}$
Mode	$\boldsymbol{\mu}$
Variance	$\boldsymbol{\Sigma}$

Marginals and conditionals of a Gaussian

$$p(\boldsymbol{x}, \boldsymbol{y}) = \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\mu}_x \\ \boldsymbol{\mu}_y \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{xx} & \boldsymbol{\Sigma}_{xy} \\ \boldsymbol{\Sigma}_{yx} & \boldsymbol{\Sigma}_{yy} \end{bmatrix} \right)$$



Conditional distribution

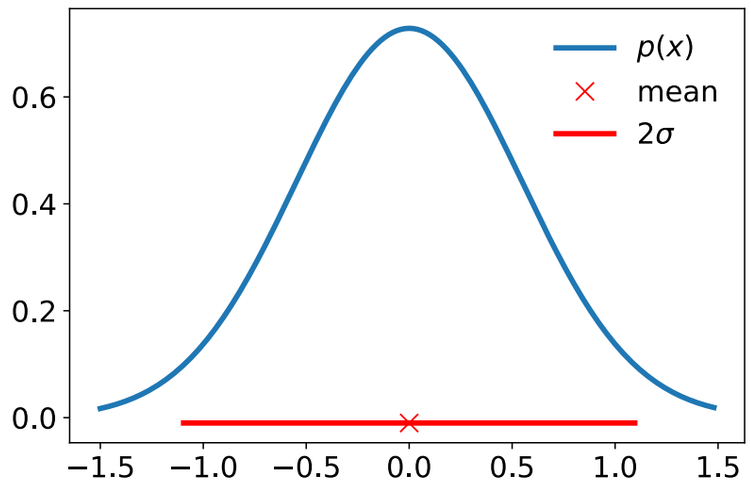
$$p(\boldsymbol{x} \mid \boldsymbol{y}) = \mathcal{N}\left(\boldsymbol{\mu}_{x \mid y}, \boldsymbol{\Sigma}_{x \mid y}\right)$$

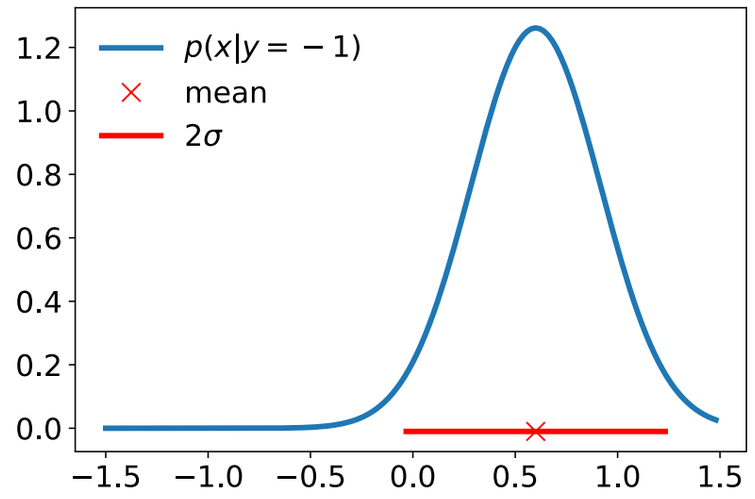
$$\boldsymbol{\mu}_{x \mid y} = \boldsymbol{\mu}_x + \boldsymbol{\Sigma}_{xy}\boldsymbol{\Sigma}_{yy}^{-1}(\boldsymbol{y} - \boldsymbol{\mu}_y)$$

$$\boldsymbol{\Sigma}_{x \mid y} = \boldsymbol{\Sigma}_{xx} - \boldsymbol{\Sigma}_{xy}\boldsymbol{\Sigma}_{yy}^{-1}\boldsymbol{\Sigma}_{yx} \,.$$

Marginal distribution

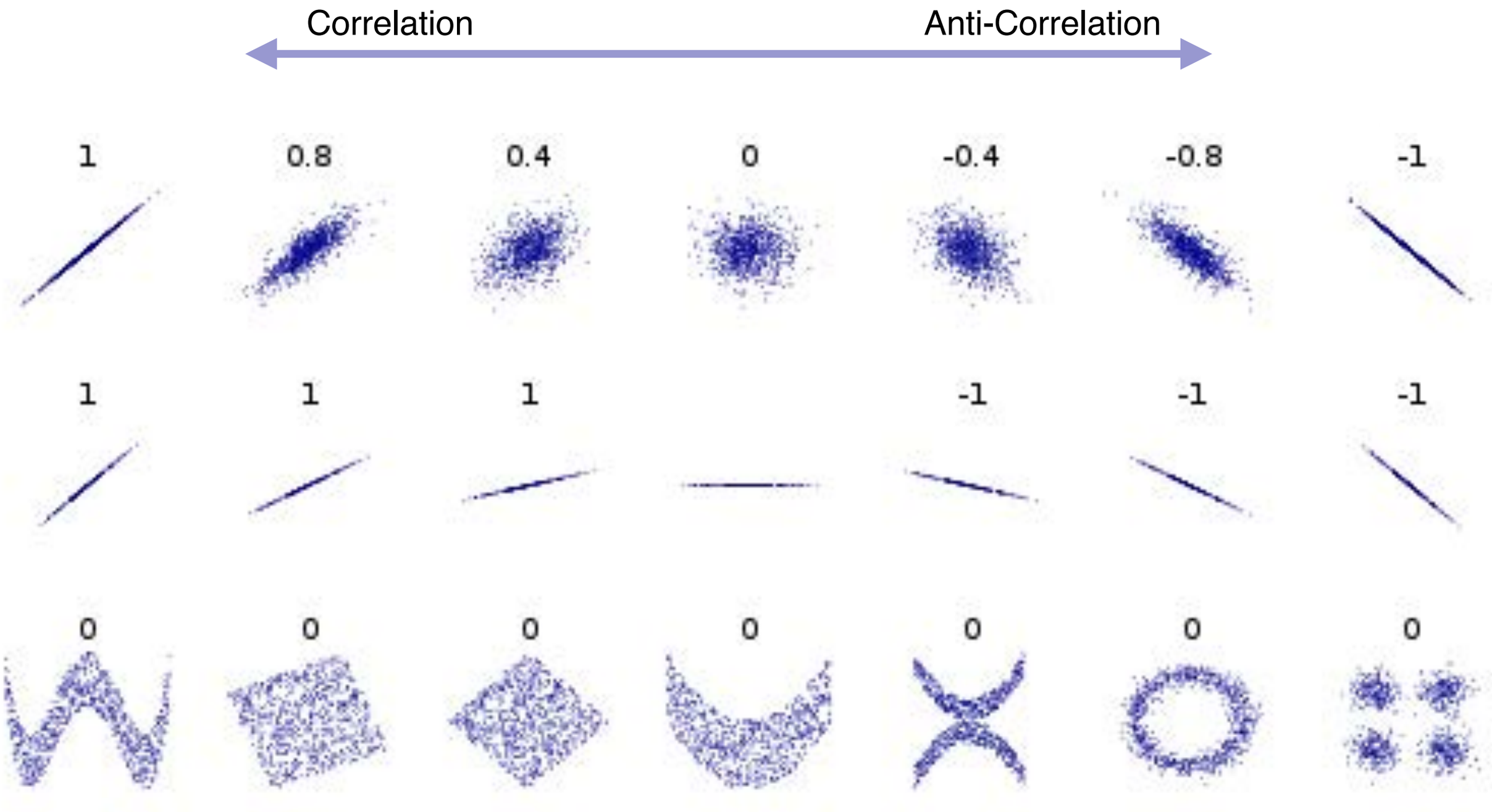
$$p(\boldsymbol{x}) = \int p(\boldsymbol{x}, \boldsymbol{y}) d\boldsymbol{y} = \mathcal{N}\left(\boldsymbol{x} \mid \boldsymbol{\mu}_x, \boldsymbol{\Sigma}_{xx}\right)$$





These are unique properties that make the Gaussian distribution very simple and attractive to compute with! It is essentially our main building block for computing under uncertainty.

Correlation and linear dependence



Entropy and Mutual Information

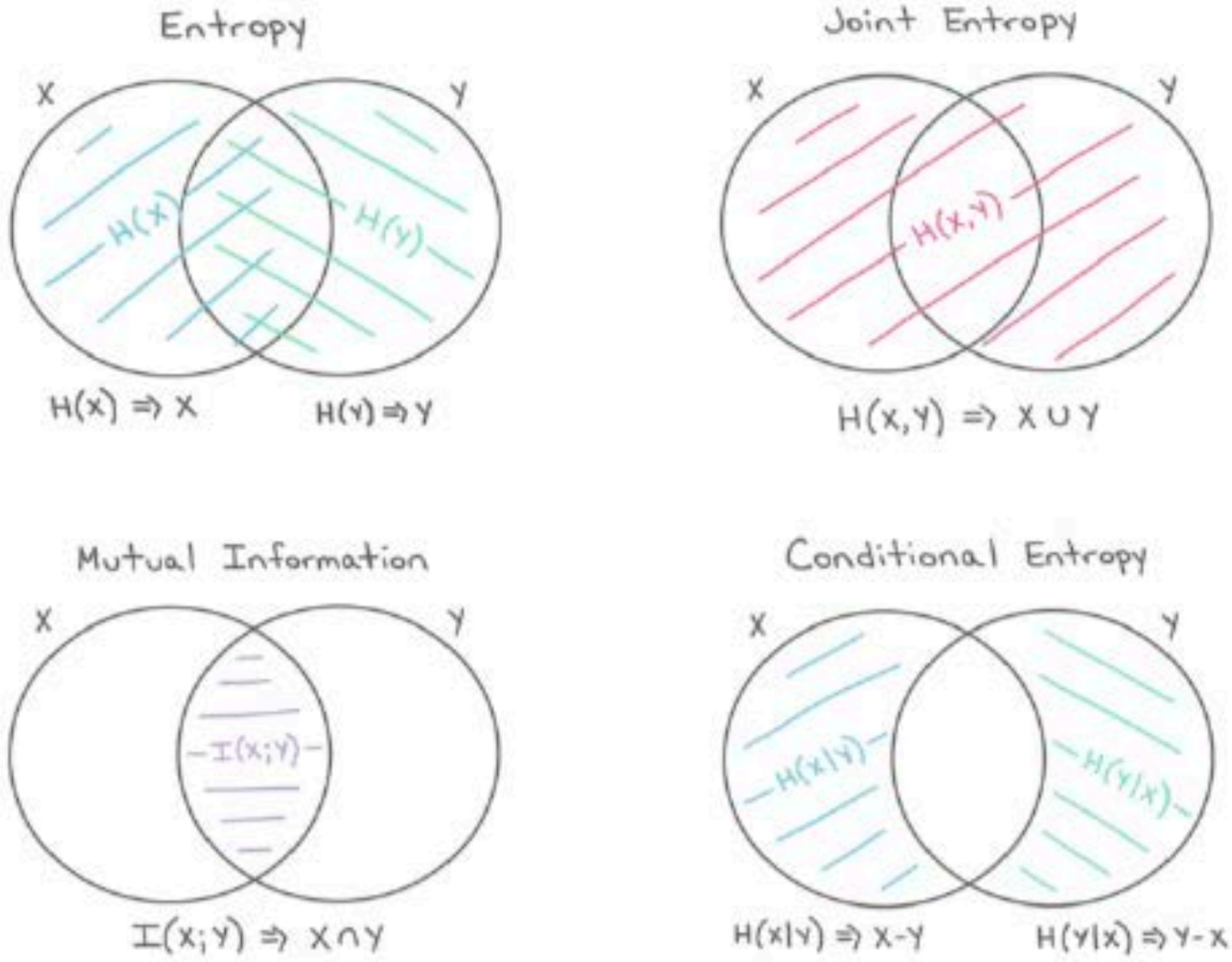
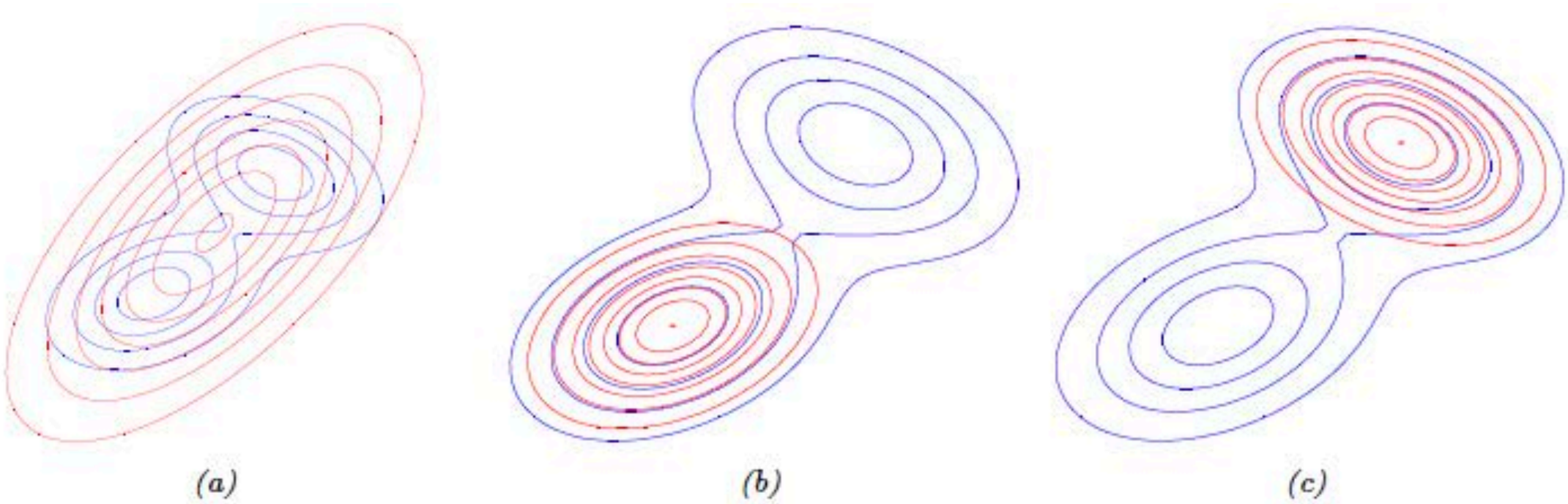


Figure 6.4: The marginal entropy, joint entropy, conditional entropy and mutual information represented as information diagrams. Used with kind permission of Katie Everett.

Forward vs Reverse KL



(a) (b) (c)

Figure 6.3: Illustrating forwards vs reverse KL on a bimodal distribution. The blue curves are the contours of the true distribution p. The red curves are the contours of the unimodal approximation q. (a) Minimizing forwards KL, $D_{\mathrm{KL}}(p \| q)$, wrt q causes q to "cover" p. (b-c) Minimizing reverse KL, $D_{\mathrm{KL}}(q \| p)$ wrt q causes q to "lock onto" one of the two modes of p. Adapted from Figure 10.3 of [Bis06]. Generated by KLfwdReverseMixGauss.ipynb.

Covariance vs Mutual Information