# Density Estimation

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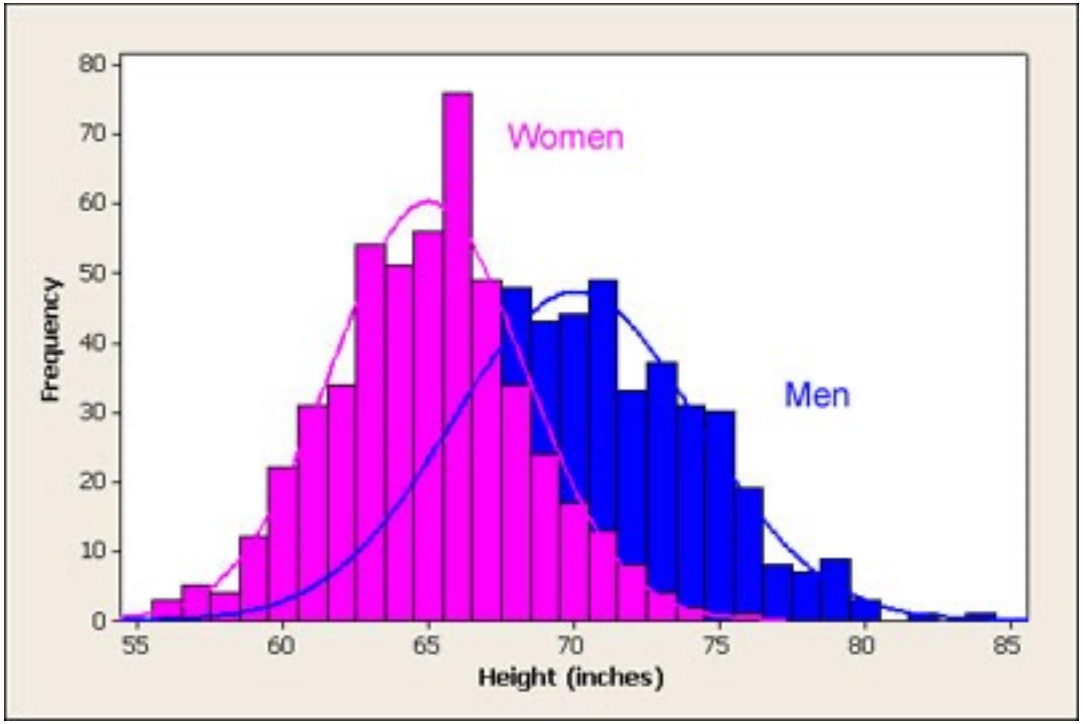
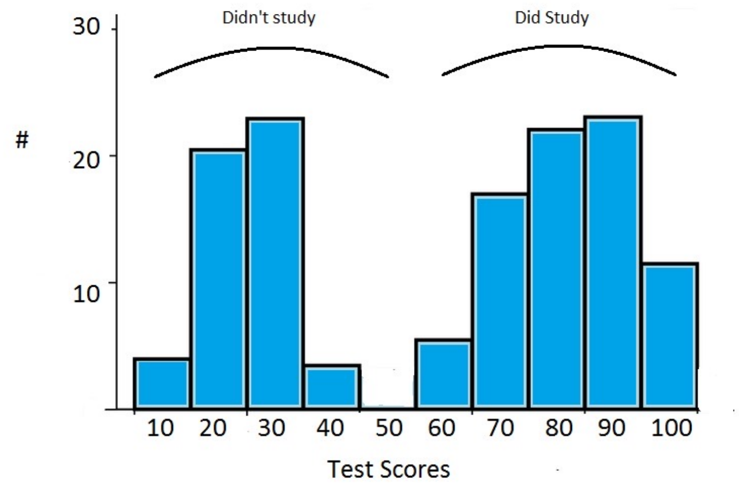
**Density estimation** finds a density (PDF/PMF) that represents the data (or empirical distribution) well

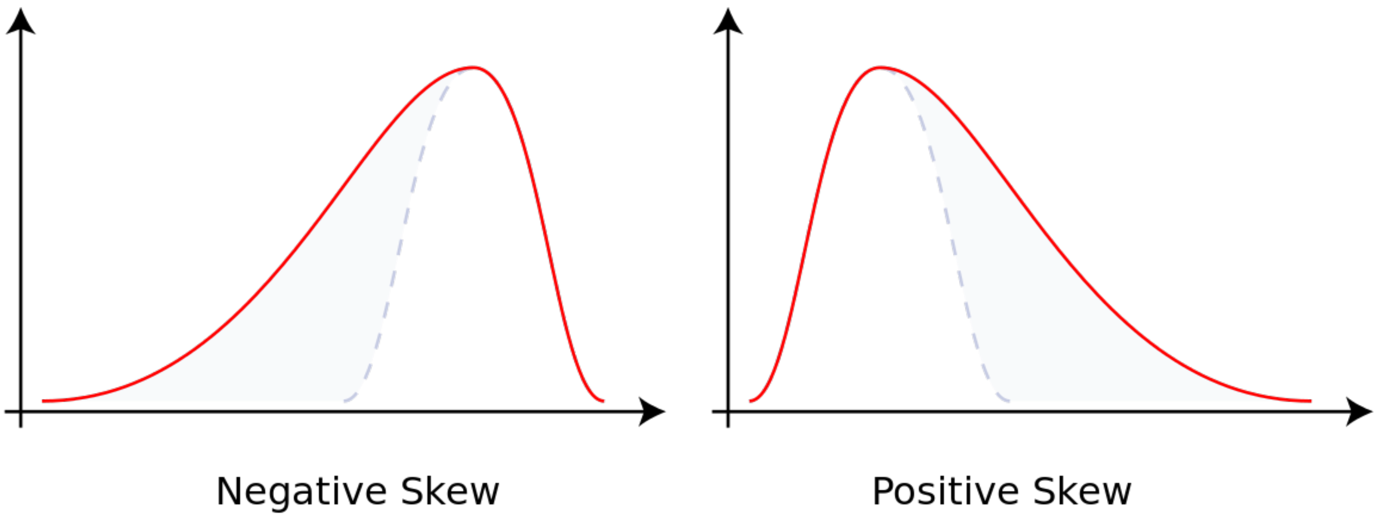


# Motivation: Density estimation can be used to uncover underlying structure

- Uncover multi-modal structure

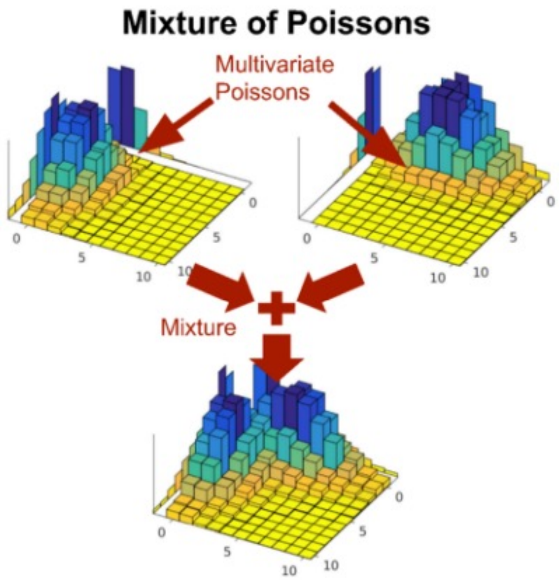


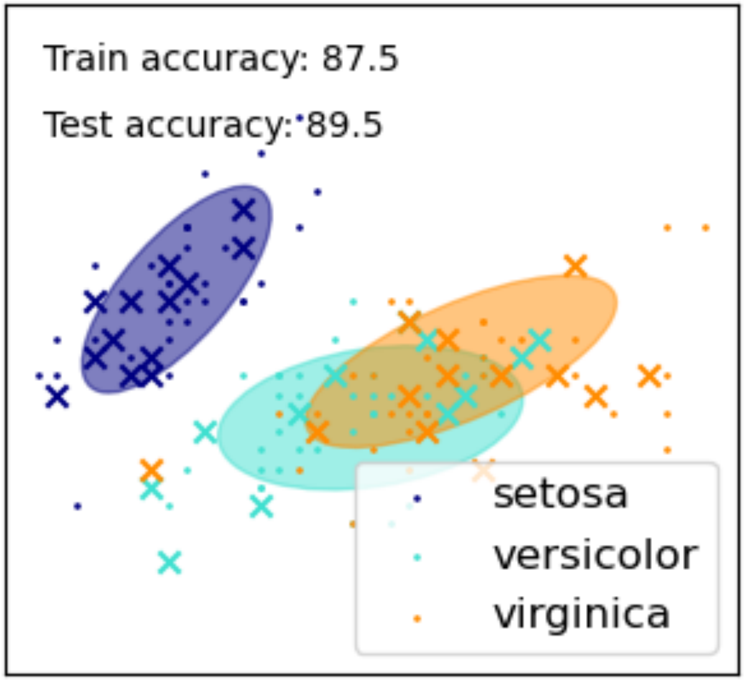

- Uncover skewness



# Motivation: Density estimation can be used to uncover underlying structure

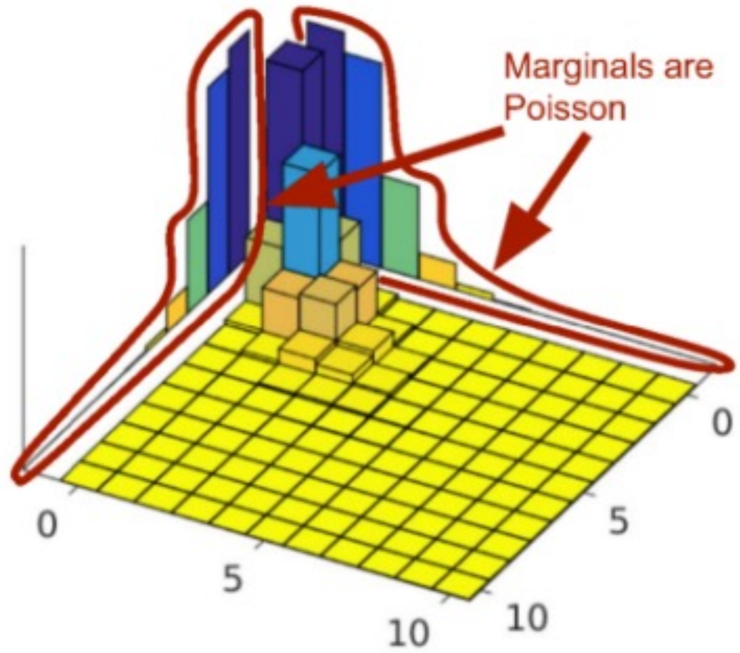
- Cluster structure
  - Gaussian mixture models
  - Poisson mixture models

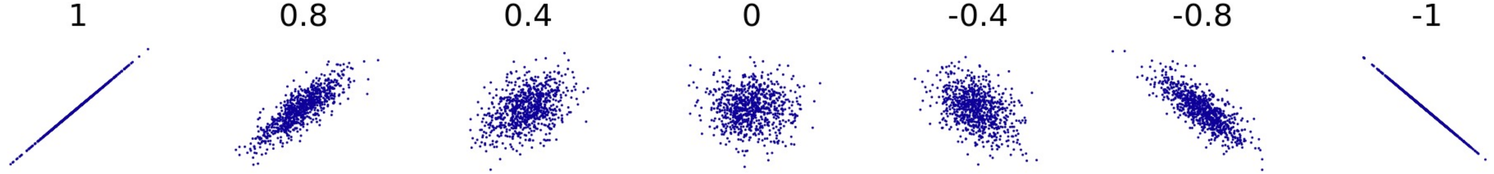


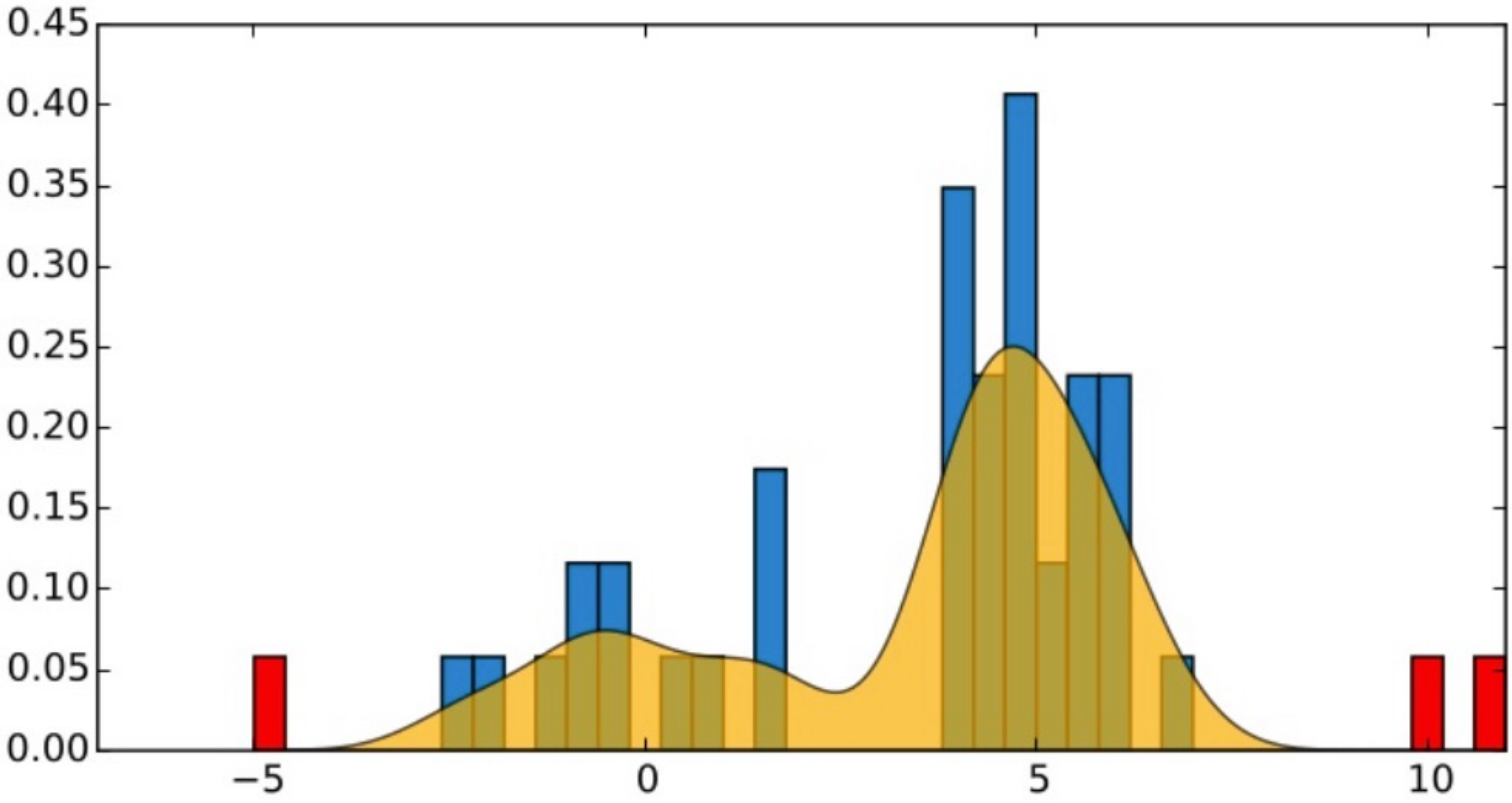
# Motivation: Density estimation can be used to uncover underlying structure

- Dependence structure of random variables (e.g., correlation)



# Motivation: Density estimation can be used for anomaly detection




https://www.slideshare.net/agramfort/anomalynovelty-detection-with-scikitlearn

# <u>Parametric</u> density estimation assumes a <u>density model class</u> parameterized by $\theta$

- Assumption: Bernoulli density

$$\theta = [p], \qquad p \in [0,1]$$

- Assumption: Exponential density

$$\theta = [\lambda], \qquad \lambda \in \mathbb{R}_{++}$$

- Assumption: Gaussian density

$$\theta = [\mu, \sigma^2], \qquad \mu \in \mathbb{R}, \sigma^2 \in \mathbb{R}_{++}$$

- Assumption: DNN-based model

$$\theta = [\text{“}\mathit{all\ neural\ network\ parameters}\text{”}]$$

# How do we determine which model in the model class is the best?

- Classically, people have turned to information theoretic quantities
  - Entropy
  - Kullback Liebler (KL) Divergence
  - Maximum likelihood estimation (MLE)

# Informally, **entropy** measures the “amount of randomness/disorder” of a distribution

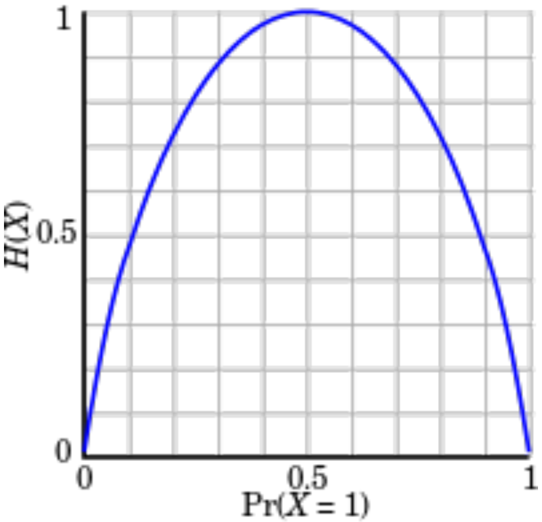
- Formally, **entropy** for discrete variables

$$H\big(P(\cdot)\big) = \mathbb{E}[-\log P(x)] = \sum_x -P(x)\log P(x)$$

- Formally, **differential entropy** for continuous variables

$$H\big(p(\cdot)\big) = \mathbb{E}[-\log p(x)] = \int_x -p(x)\log p(x)\,dx$$

- Consider fair coin vs coin where both sides are heads



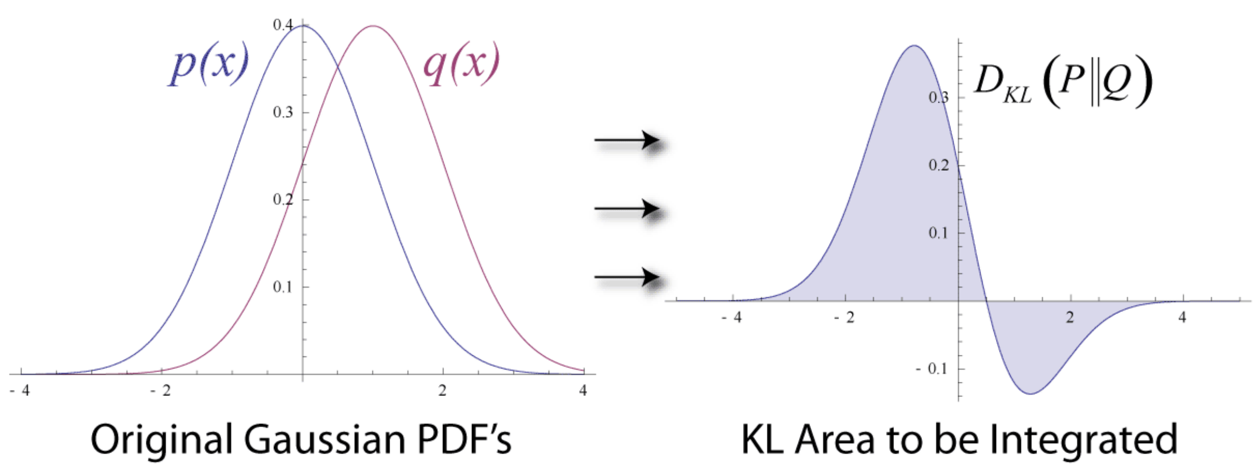
# Informally, Kullback-Leibler Divergence (KL) measures the distance between distributions

- Formally, **KL divergence** for discrete variables

$$KL(P(\cdot), Q(\cdot)) = \mathbb{E}_{x\sim P}\left[\log\frac{P(x)}{Q(x)}\right] = \sum_x P(x)\log\frac{P(x)}{Q(x)}$$

- Formally, **KL divergence** for continuous variables

$$KL(p(\cdot), q(\cdot)) = \mathbb{E}_{X\sim p}\left[\log\frac{p(x)}{q(x)}\right] = \int_x p(x)\log\frac{p(x)}{q(x)}\,dx$$



# Informally, Kullback-Leibler Divergence (KL) measures the distance between distributions

$$KL(p(\cdot), q(\cdot)) = \mathbb{E}_{X\sim p}\left[\log \frac{p(x)}{q(x)}\right] = \int_x p(x) \log \frac{p(x)}{q(x)} dx$$

- Not symmetric!

$$KL\big(p(\cdot), q(\cdot)\big) \neq KL\big(q(\cdot), p(\cdot)\big)$$

- Non-negative property

$$KL\big(p(\cdot), q(\cdot)\big) \geq 0$$

- Equal distribution property:

$$KL\big(p(\cdot), q(\cdot)\big) = 0 \Leftrightarrow p(\cdot) = q(\cdot)$$

# One use of KL divergence is to estimate distribution parameters only from samples

- Let $p(x)$ denote the **real/true** distribution of the data
  - $p(x)$ is ***unknown***
  - We only have samples $\{x_i\}_{i=1}^n$ from $p(x)$
- Let $\hat{q}(x;\theta)$ denote an **estimate** of the true distribution
  - Parametrized by $\theta$
- We want to find $\hat{q}(x;\theta)$ that is closest to $p(x)$

$$\theta^* = \arg\min_\theta \mathrm{KL}(p(\cdot), \hat{q}(\cdot;\theta))$$

# One use of KL divergence is to estimate distribution parameters only from samples

- We want to find $\hat{q}(x;\theta)$ that is closest to $p(x)$

$$\theta^* = \arg\min_\theta \mathrm{KL}(p(\cdot), \hat{q}(\cdot;\theta))$$

- Wait, but we don't know $p(x)$, how do we do this?

- Two main ideas for simplification
  - Constants with respect to (w.r.t.) $\theta$ can be ignored
  - Full expectation replaced by empirical expectation

# Derivation of minimum KL divergence with samples

- $\arg\min_{\theta} \mathrm{KL}(p(\cdot), \hat{q}(\cdot;\theta))$
- $= \arg\min_{\theta} \mathbb{E}_{X\sim p}\left[\log \frac{p(x)}{\hat{q}(x;\theta)}\right]$
- $= \arg\min_{\theta} -\mathbb{E}_{X\sim p}[\log \hat{q}(x;\theta)] + \mathbb{E}_{X\sim p}[\log p(x)]$
- $= \arg\min_{\theta} -\mathbb{E}_{X\sim p}[\log \hat{q}(x;\theta)] + C$
- $\approx \arg\min_{\theta} -\hat{\mathbb{E}}_{X\sim p}[\log \hat{q}(x;\theta)]$
- $= \arg\min_{\theta} -\frac{1}{n}\sum_{i=1}^{n} \log \hat{q}(x_i;\theta)$

# Maximum likelihood estimation (MLE) is another way to estimate distribution parameters from samples

- **Likelihood function** how likely (or probable) a dataset $\mathcal{D} = \{x_i\}_{i=1}^n$ is under a distribution with parameters $\theta$
$$\mathcal{L}(\theta; \mathcal{D}) = \hat{q}(x_1, x_2, \dots, x_n; \theta)$$
- If we ***assume*** samples (or observations) of dataset are **independent and identically distributed (iid)**, then

$$\mathcal{L}(\theta; \mathcal{D}) = \prod_{i=1}^{n} \hat{q}(x_i; \theta)$$

- Often simplified to the **log-likelihood function**

$$\ell(\theta; \mathcal{D}) = \log \mathcal{L}(\theta; \mathcal{D}) = \sum_{i=1}^n \log \hat{q}(x_i; \theta)$$

# Maximum likelihood (MLE) is another way to estimate distribution parameters from samples

- Optimize the following

$$\theta^* = \arg\max_\theta \ell(\theta;\mathcal{D}) = \arg\max_\theta \sum_{i=1}^{n} \log \hat{q}(x_i;\theta)$$

- Equivalent to

$$\theta^* = \arg\min_\theta -\frac{1}{n}\sum_{i=1}^{n} \log \hat{q}(x_i;\theta)$$

- Wait, doesn't that look familiar?
- **MLE equivalent to minimum KL divergence!**

# The most ubiquitous multivariate distribution is the **multivariate Gaussian/normal distribution**

- Compare univariate to multivariate:
  - $\mu$ is mean and $\Sigma$ is covariance

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

$$p(x_1, \dots, x_d) = \frac{1}{\left(\sqrt{2\pi}\right)^d \sqrt{\det \Sigma}} \exp\left\{-\frac{1}{2}(x-\mu)^T \Sigma^{-1} (x-\mu)\right\}$$

- $\Theta = \Sigma^{-1}$ is called the **precision matrix** (or **inverse covariance**)
- $\Sigma$ (and $\Theta$) must be positive definite $\Sigma > 0$
- (Suppose $\Sigma = I$, suppose $\mu = 0$)

# MLE of multivariate Gaussian can be computed via empirical mean and covariance matrix

- The MLE estimate (or equivalently minimum KL divergence) is simply the empirical mean and covariance matrix

$$\hat{\mu}_{\mathrm{MLE}} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

$$\hat{\Sigma}_{\mathrm{MLE}} = \frac{1}{n}\sum_{i=1}^{n} (x_i - \hat{\mu}_{\mathrm{MLE}})(x_i - \hat{\mu}_{\mathrm{MLE}})^T$$

- Derivation for $\hat{\Sigma}_{\mathrm{MLE}}$ is at the end

# Why are multivariate Gaussian distributions so ubiquitous?

- Reason from nature
  - The sum of independent random variables approaches a Gaussian distribution.
  - Central limit theorem!

- Math reason
  - Closed-form marginal and conditionals!
    *(Usually, very difficult to compute because sum/integral!)*
  - Affine/linear transformations of Gaussians are Gaussians

# Marginal and conditional distributions are Gaussian and can be computed in closed-form

- 2D case:

$$\boldsymbol{x} = [x_1, x_2] \sim \mathcal{N}\left(\mu = [\mu_1, \mu_2], \Sigma = \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{21} & \sigma_2^2 \end{bmatrix}\right)$$

- Marginal distributions:

$$x_1 \sim \mathcal{N}(\mu = \mu_1, \sigma^2 = \sigma_1^2)$$
$$x_2 \sim \mathcal{N}(\mu = \mu_2, \sigma^2 = \sigma_2^2)$$

- Conditional distributions:

$$x_1 | x_2 = a$$
$$\sim \mathcal{N}\left(\mu = \mu_1 + \frac{\sigma_{12}}{\sigma_2^2}(\mathrm{a} - \mu_2), \sigma^2 = \sigma_1^2 - \frac{\sigma_{21}^2}{\sigma_2^2}\right)$$

# <u>Marginal</u> and <u>conditional</u> distributions are **Gaussian** and can be computed in **closed-form**

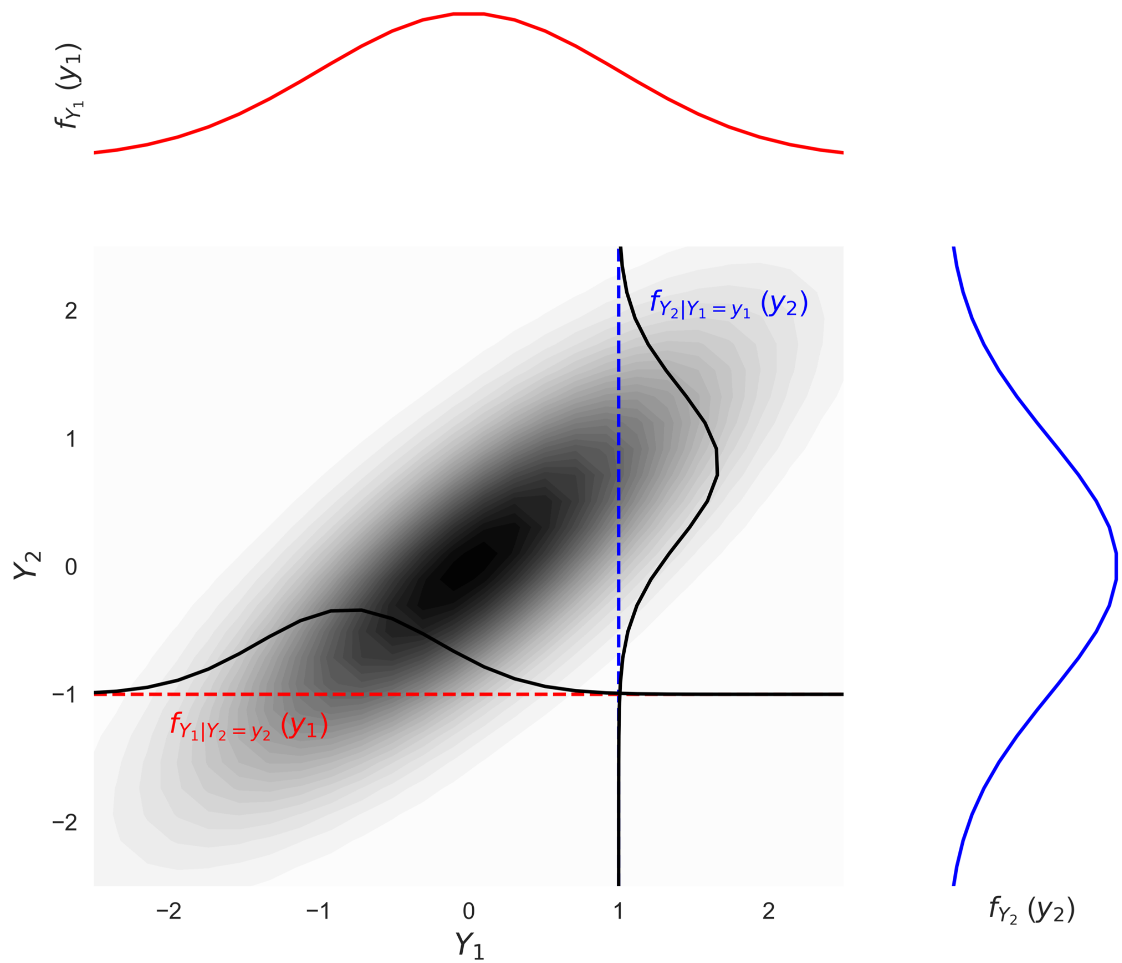
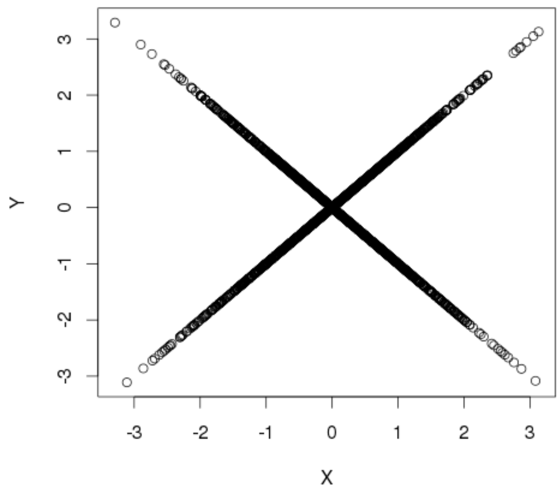
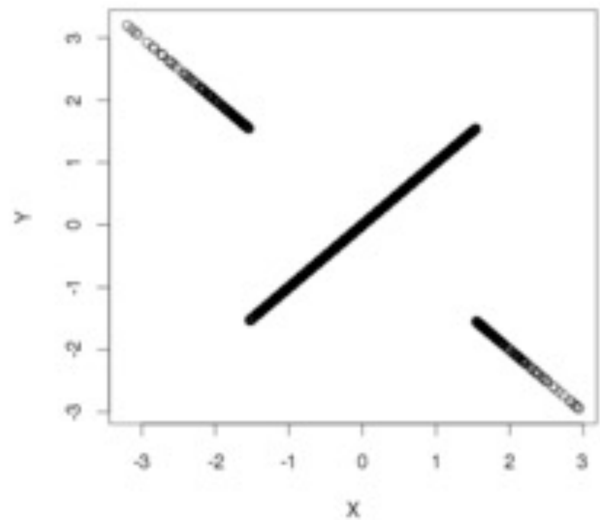
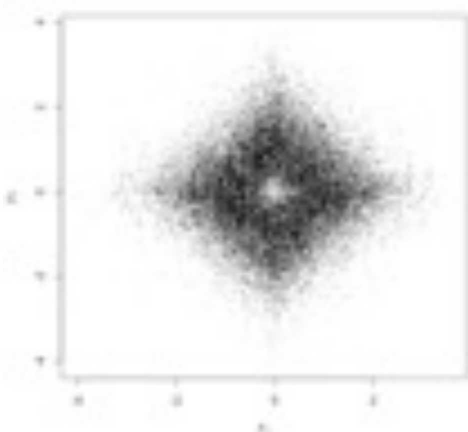


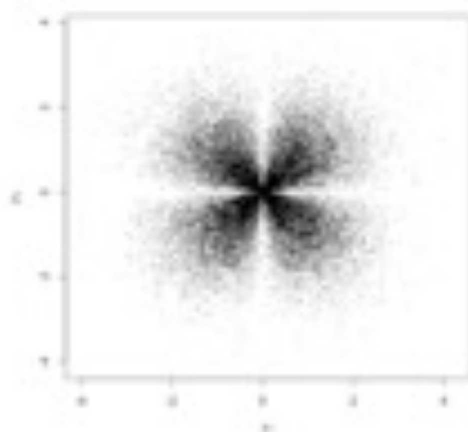

Image from https://geostatisticslessons.com/lessons/multigaussian

# Gaussian marginals does <u>NOT</u> imply jointly multivariate Gaussian (converse <u>NOT</u> generally true)





# <u>Affine transformations</u> of multivariate Gaussian vector are also multivariate Gaussian

- If $x \sim \mathcal{N}(\mu, \Sigma)$ and $y = Ax + b$, then
$$y \sim \mathcal{N}\left(A\mu + b, A\Sigma \mathrm{A}^{\mathrm{T}}\right).$$
- Special case: Marginal distribution when $A$ is:
$$A_i = \begin{cases} 1, & \text{if } i = k \\ 0, & \text{otherwise} \end{cases}$$
$$\text{then } y = x_k \sim p(x_k).$$
- Key point: Marginals, conditionals and affine functions known in **<u>closed-form</u>**.
- Consequence 1: Easy to manipulate.
- Consequence 2: Gaussians and linear ideas play nicely with each other.

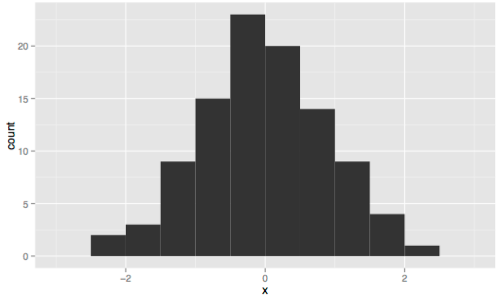
# Non-parametric density estimation

# <u>Non-parametric</u> density estimation

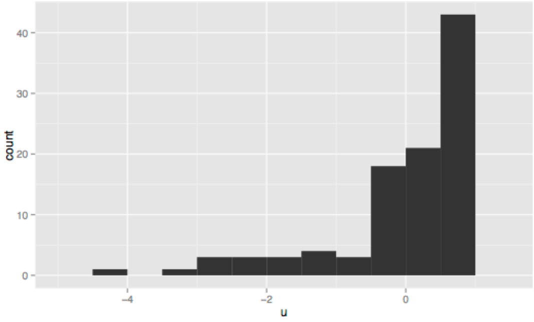
- Motivation
- Histograms
  - Choosing k
  - Choosing bin edges
- Kernel density
  - Choosing bandwidth
  - Curse of dimensionality again

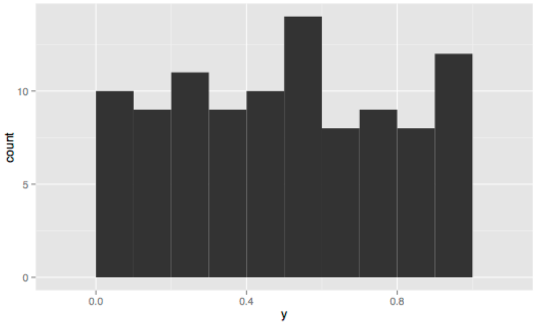
# Why non-parametric density estimates?

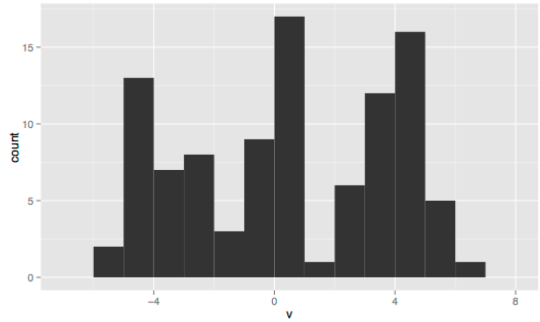
- Parametric densities are excellent if the assumptions are correct (e.g., Gaussian)

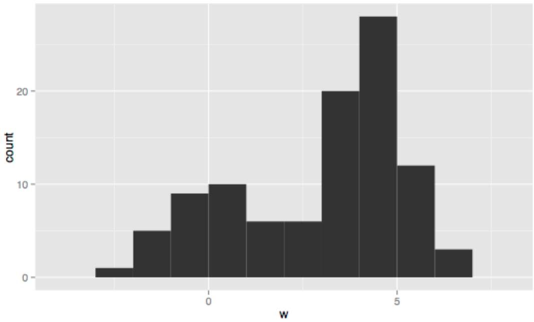



- However, the distributions may not align with the assumptions



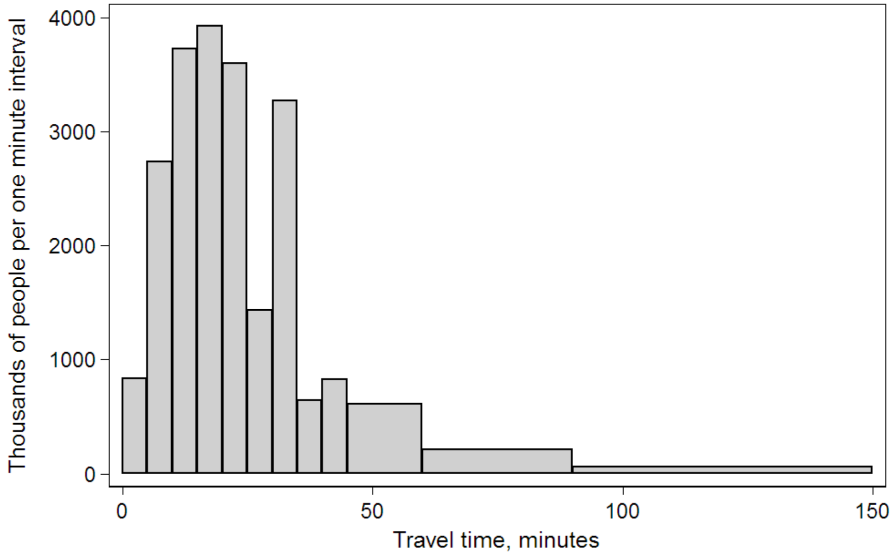



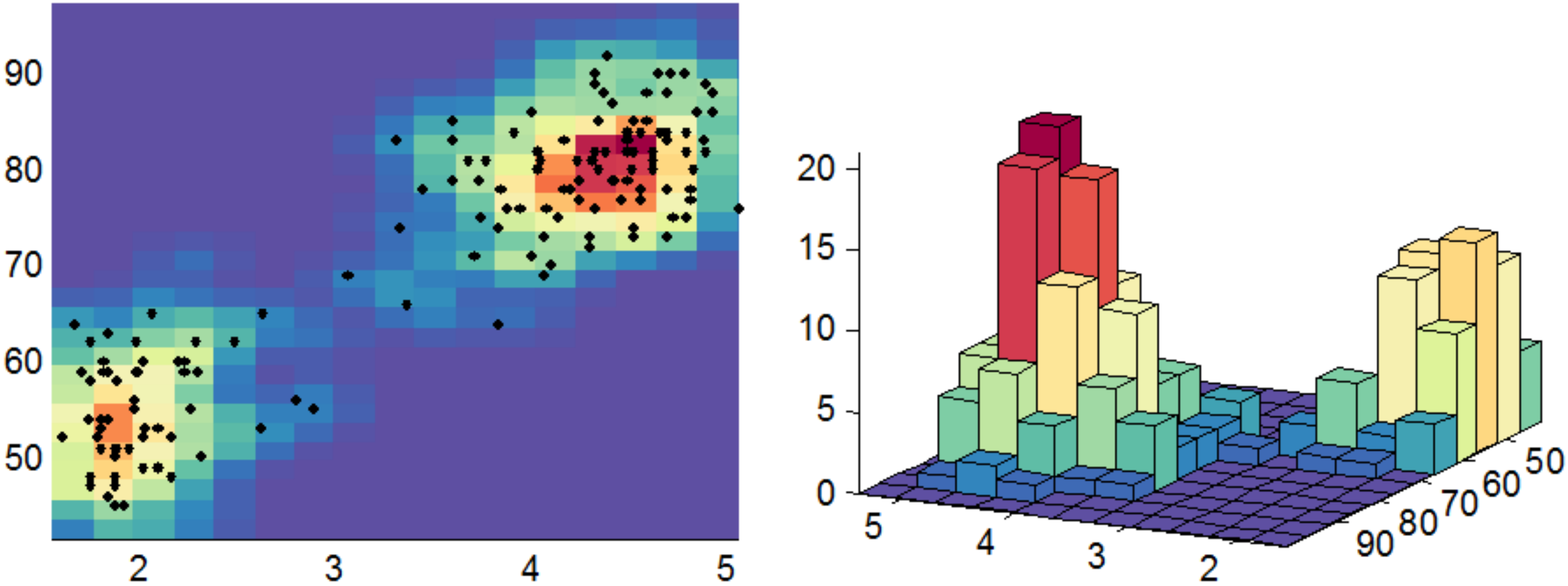



# Histograms are the simplest density estimators

- Setup bin locations
- Count number of samples that fall in each bin
- Normalize to be a density

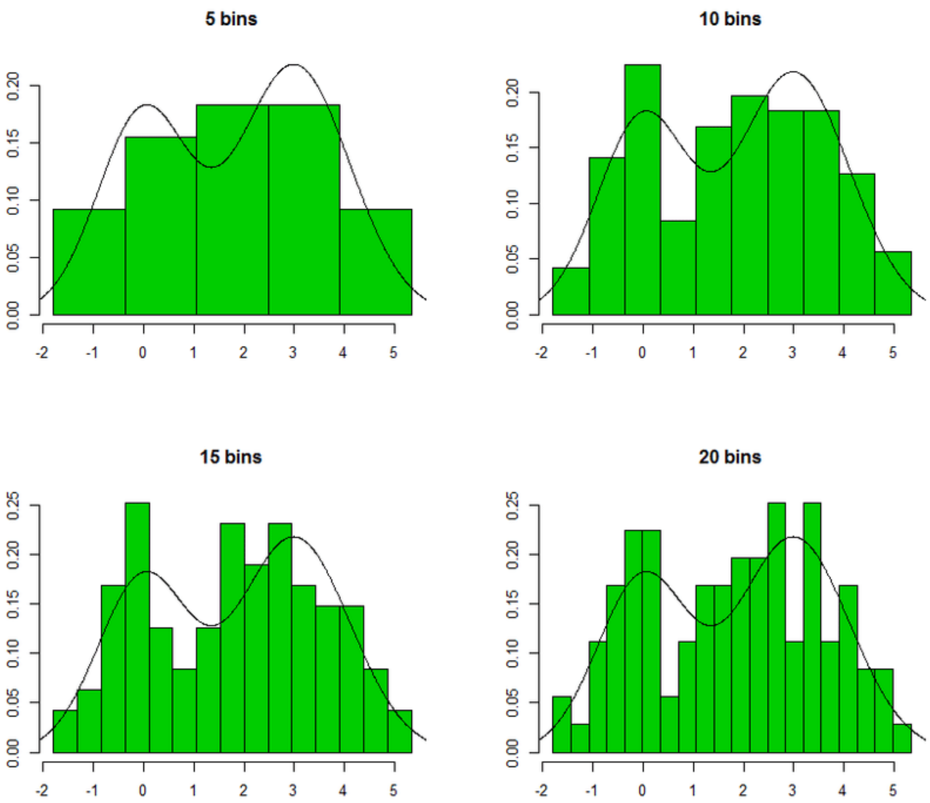


# 2D Histograms can be created

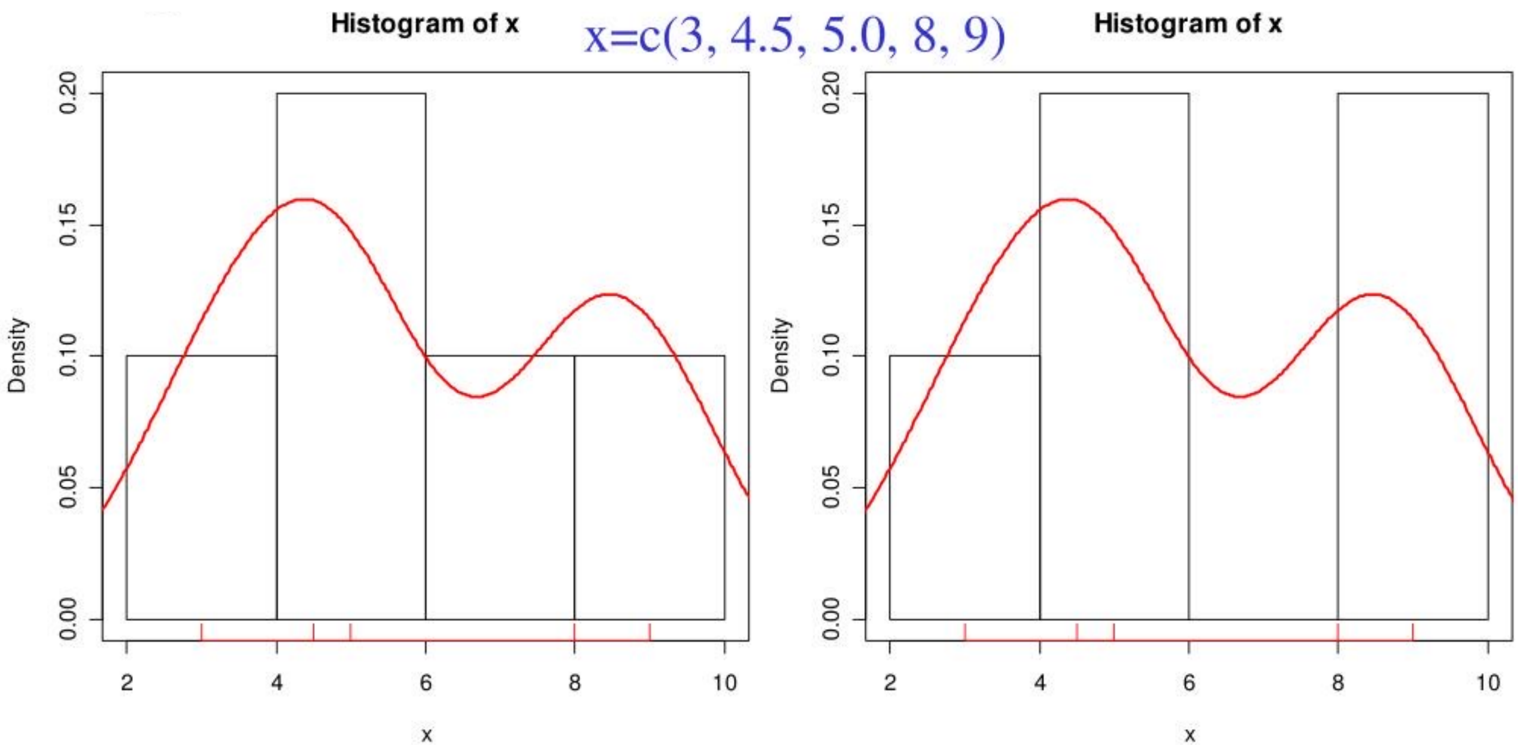


# How to select the number of bins (usually denoted $k$)?

- Too few bins will underfit
- Too many bins will overfit
- ML approach: <u>**CV/Test**</u> log likelihood



# Drawbacks: Histograms can depend on bin edges and are not smooth




- hist(x,right=**T**,freq=F), R-default
- (a,b] right closed (left-open)

- hist(x,right=**F**,freq=F)
- [a,b) left closed (right-open)

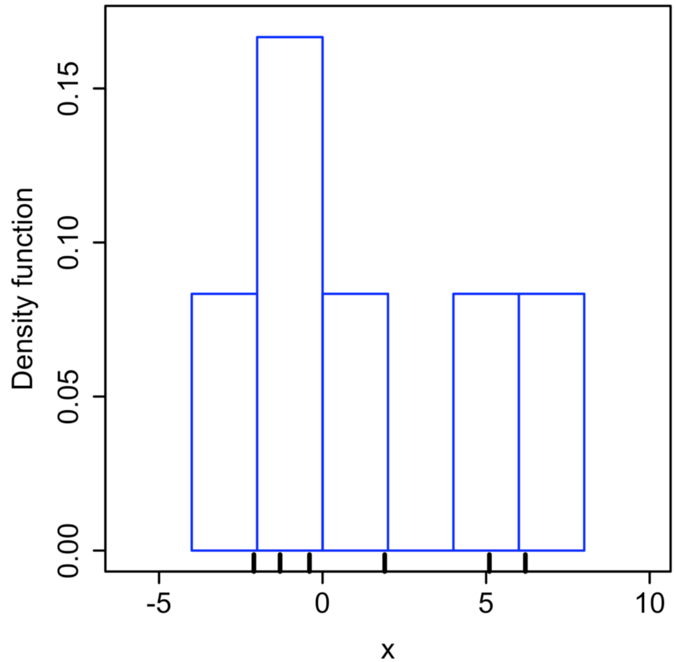
Area=1

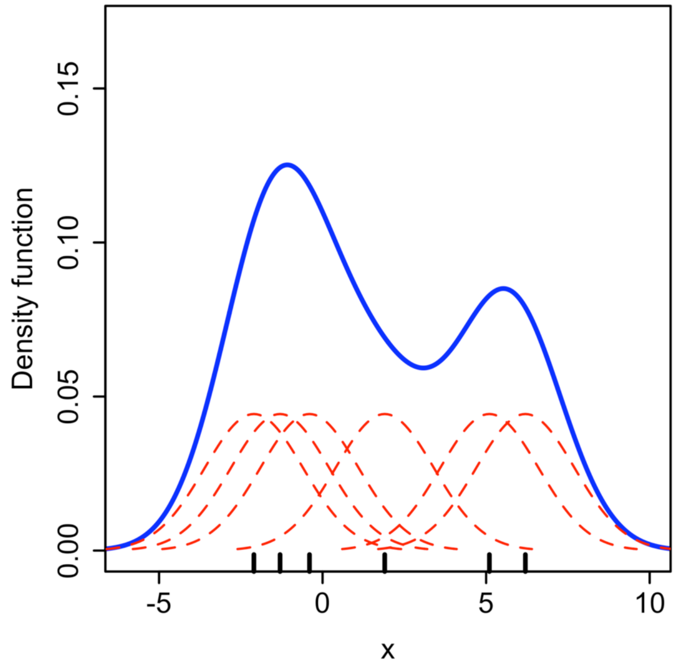
https://www.slideserve.com/geona/introduction-to-non-parametric-statistics-kernel-density-estimation

# <u>Kernel densities</u> overcome this drawback by placing a Gaussian density at each point

- Kernel density has the following form:

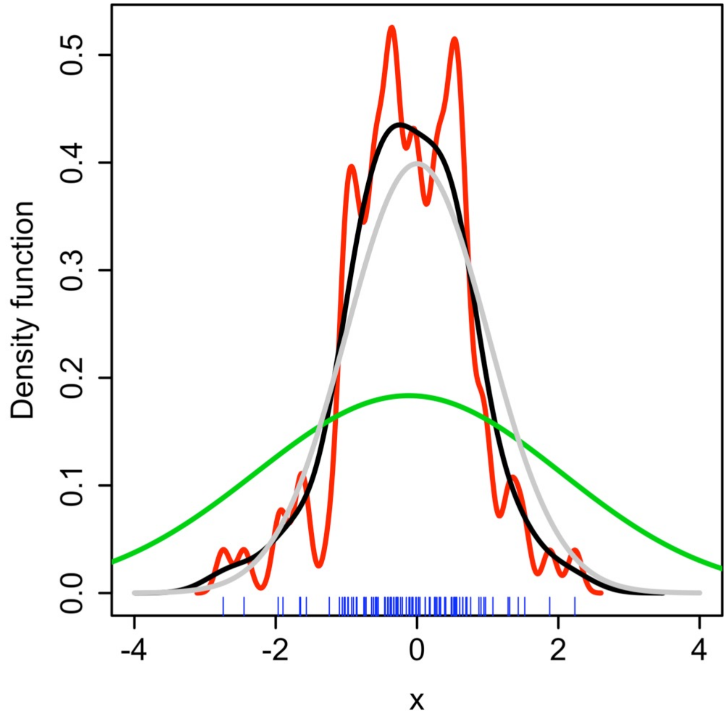
$$p(x) = \frac{1}{n}\sum_{i=1}^{n} p_{\text{base}}(x - x_i) = \frac{1}{n}\sum_{i=1}^{n} \mathcal{N}(x - x_i, \sigma)$$



Similar to number of bins, the key parameter for kernel densities is the "bandwidth" or $\sigma$ parameter

- Bandwidth can be selected via CV/Test log likelihood (similar to number of histogram bins)



# Derivations (optional)

# MLE of multivariate Gaussian derivation as minimum of negative log likelihood

- Log-likelihood of multivariate Gaussian ($\mu = 0$)

$$-\frac{1}{2}\log|\Sigma| - \frac{1}{2n}\sum_{i=1}^{n} x_i^T \Sigma^{-1} x_i + const$$

- Three main identities:
  - $\frac{\partial \log|\mathrm{A}|}{\partial \mathrm{A}} = A^{-T}$
  - $\mathrm{Tr}(x^T A x) = \mathrm{Tr}(A x x^T)$
  - $\frac{\partial \mathrm{Tr}(AX)}{\partial \mathrm{X}} = A$
- Hint: Do derivative with respect to $\Sigma^{-1}$

# Simplification and derivation of MLE for multivariate Gaussian

- $L(\Sigma; \mathcal{D}) = -\frac{1}{2}\log|\Sigma| - \frac{1}{2n}\sum_{i=1}^{n} x_i^T \Sigma^{-1} x_i$
- $= \frac{n}{2}\log|\Sigma^{-1}| - \frac{1}{2}\sum_{i=1}^{n} \mathrm{Tr}(x_i^T \Sigma^{-1} x_i)$
- $= \frac{n}{2}\log|\Sigma^{-1}| - \frac{1}{2}\mathrm{Tr}\left(\Sigma^{-1}\left(\sum_i x_i x_i^T\right)\right)$
- $\frac{\partial L}{\partial \Sigma^{-1}}$
- $= \frac{n}{2}\Sigma - \frac{1}{2}\sum_i x_i x_i^T = 0$
- $\Sigma = \frac{1}{n}\sum_i x_i x_i^T$

$$\frac{\partial \log|\mathrm{A}|}{\partial \mathrm{A}} = A^{-T}$$

$$\frac{\partial \mathrm{Tr}(AX)}{\partial \mathrm{X}} = A$$