High-dimension Gaussians

Separating Gaussians

Fitting Spherical Gaussian to Data

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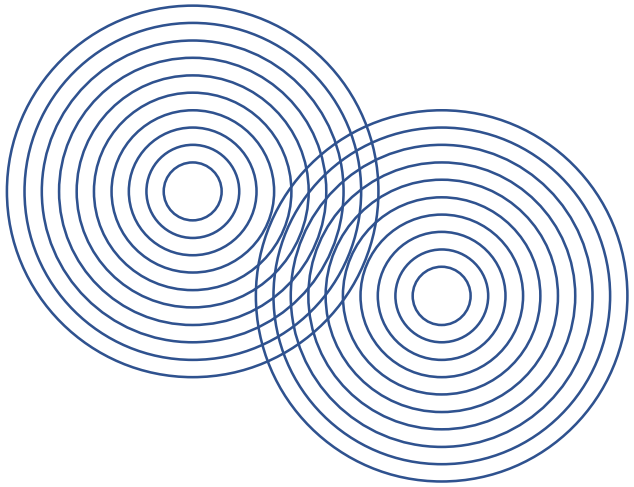
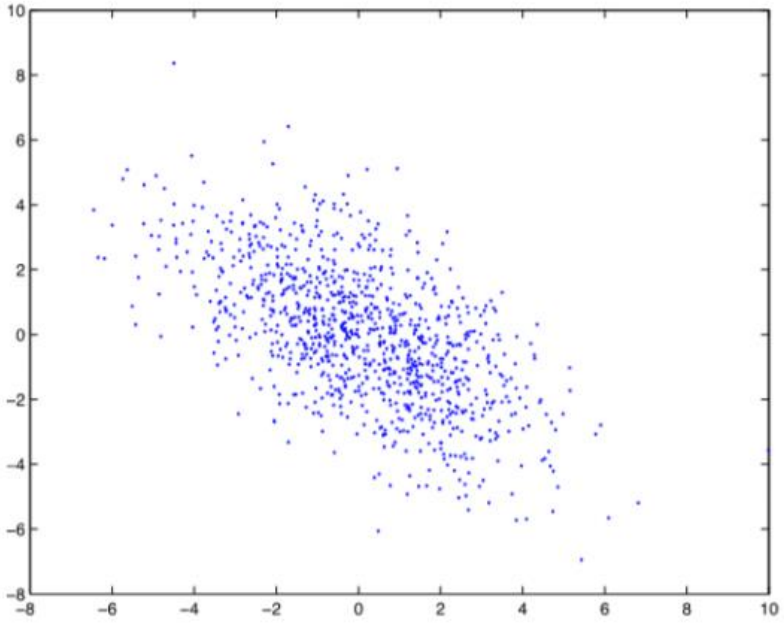
Separating Gaussians

- Heterogeneous data coming from multiple sources
- Gaussian mixture model $p(x) = w_1 p_1(x) + w_2 p_2(x)$
- Parameter estimation problem: given access to samples from the overall density p, reconstruct the parameters for the distribution (mean and variance for each distribution: $\mu_1, \mu_2, \sigma_1, \sigma_2$)
- Mixed-density function
  - Gaussian p_i has its own mean μ_i and variance σ_i
  - Defines the probability to sample Gaussian's p_i's distribution

MVN – Multivariant Normal Distribution

- Defined over vectors, not scalars
- Intuition: each coordinate in the random vector is sampled from a normal distribution



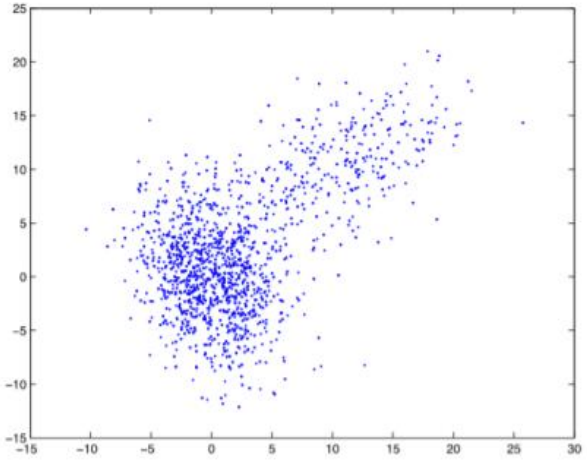


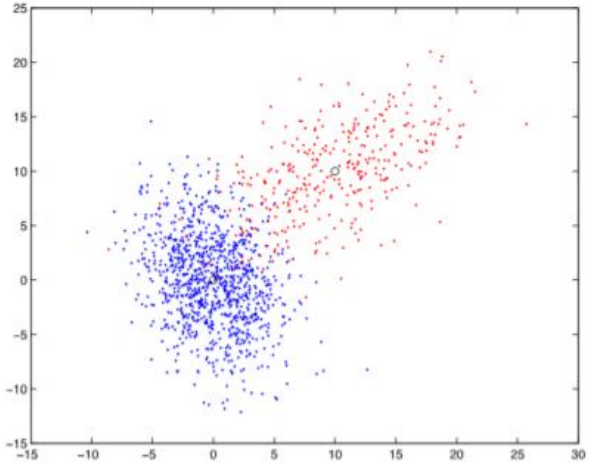
K-means

- We are given n vectors $x_1, \ldots, x_n$ and a number k
- We would like to partition the vectors into k sets, and with each set we associate a "center" μ_i
- The goal is to minimize the objective function
$$\min_{\mu_1,\ldots,\mu_k,S_1,\ldots,S_k} \sum_{j=1}^{k} \sum_{i \in S_j} \|x_i - \mu_i\|^2$$
- We assumed that each point has to be classified to a specific cluster.
  - This is a "hard" decision, since we need to decide for each point a single cluster.
  - We have to make some assumptions (distance between the means), in order to make this problem easier

GMM - Gaussian Mixture Model

- We have k Gaussian distributions, and a mixing distribution.
  - The mixing distribution gives a probability to each cluster
- To generate a point, we sample a Gaussian given the mixture distribution, and then sample the selected Gaussian to generate the point





GMM - Gaussian Mixture Model

- We have k unknown clusters $S_1, \dots, S_k$ where $S_i \sim N(\mu_i, \sigma_i^2)$
- Each point originates from cluster j with probability p_j
- The density function for cluster j is $f_j(x) = \frac{1}{\left(\sqrt{2\pi\sigma_j^2}\right)^d} \cdot e^{-\frac{\left(x-\mu_j\right)^2}{2\sigma_j^2}}$

Separating Gaussians

- Original objective: separate the samples into their original Gaussian distributions
- Women can be high, men can be low – and we might not be able to know for sure if a specific sample belongs to a male or a female.
  - We can't know for sure (with high probability) whether a point belongs to a specific Gaussian
- Alternative objective:
  - **More difficult**: mixture of two Gaussians in high-dimensions (d-dimension space), rather than 1-dimension
  - **Easier**: we assume the means are well-separated compared to the variances

Separating Gaussians

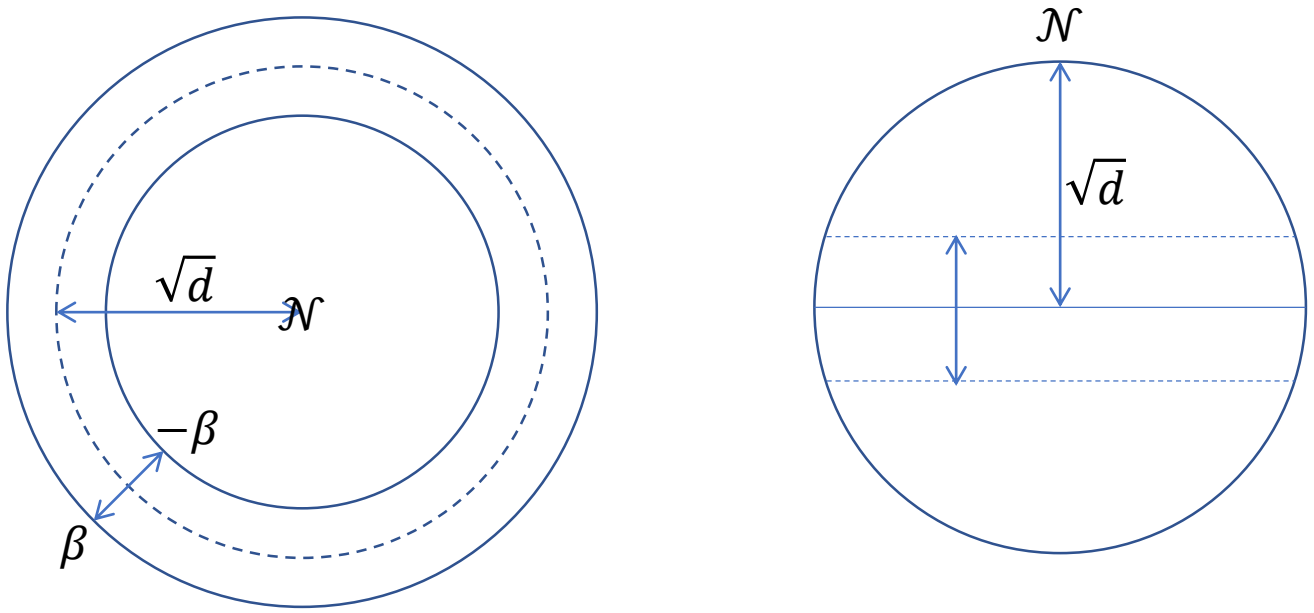
- We will focus on a mixture of two spherical unit-variance Gaussians whose means are separated by a distance $\Omega\left(d^{\frac{1}{4}}\right)$
  - Goal: Prove that using those assumptions, we can know with high confidence the origin of a given sample. This is k-means with $k = 2$.
- Simple solution: Calculate the distance between all pairs of points.
  - Points whose distance apart is smaller are from the same Gaussian
  - Points whose distance is larger are from different Gaussians

Sample distances – one Gaussian

- Reminder: Gaussian Annulus Theorem
  - For a d-dimensional spherical Gaussian with unit variance in each direction, for any $\beta \leq \sqrt{d}$, all but at most $3e^{-c_1\beta^2}$ of the probability mass lies within the annulus $\sqrt{d} - \beta \leq |x| \leq \sqrt{d} + \beta$, where c is a fixed positive constant
  - A fixed value for β is good for fixed number of sampled points
- Reminder: Volume near the equator
  - For any unit-length vector v defining "north", most of the volume of the unit ball lies in the thin slab of points whose dot-product with v has magnitude $O\left(\frac{1}{\sqrt{d}}\right)$
    - At least $1 - \frac{2}{c}e^{-\frac{c^2}{2}}$ fraction of the volume of the d-dimensional unit ball, has $|x_1| \leq \frac{c}{\sqrt{d-1}} \leq O(1)$

Sample distances – one Gaussian

- Most of the Gaussian's probability mass lies on an annulus of width $O(\beta)$ at radius $\sqrt{d}$ from the origin
- Most of its probability mass lies in a $O\left(\frac{1}{\sqrt{d}}\right)$-width slab on the equator
  - For simplicity – assume it is a constant, $O(1)$



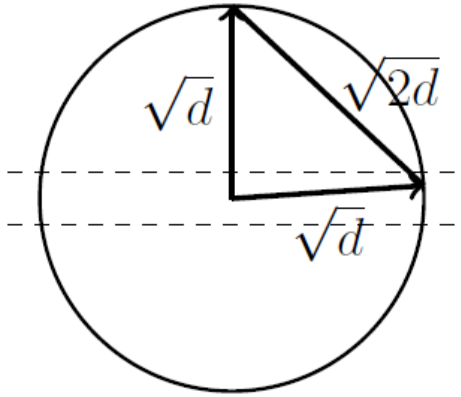
Sample distances – one Gaussian

- Consider one spherical unit-variance Gaussian centered at the origin
  - $\mu = (0, \ldots, 0)$
  - $\sigma^2 = 1$
  - Density function is $f(x) = \frac{1}{\sqrt{2\pi}^d} \cdot e^{-\frac{x^2}{2}}$ (for $e^{-\frac{x^2}{2}} = \prod_i e^{-\frac{x_i^2}{2}}$)
- Almost all of the mass is within the slab $\{x | -\text{const} \leq x_1 \leq \text{const}\}$

Sample distances – one Gaussian

- Pick a random point x from the Gaussian
- Rotate the coordinate system to make the first axis align with x
- Pick an independent sample y
  - y is located on the equator, with high probability, considering x as the north pole
  - y's component along x's direction, is $O(1)$ with high probability

Sample distances – one Gaussian



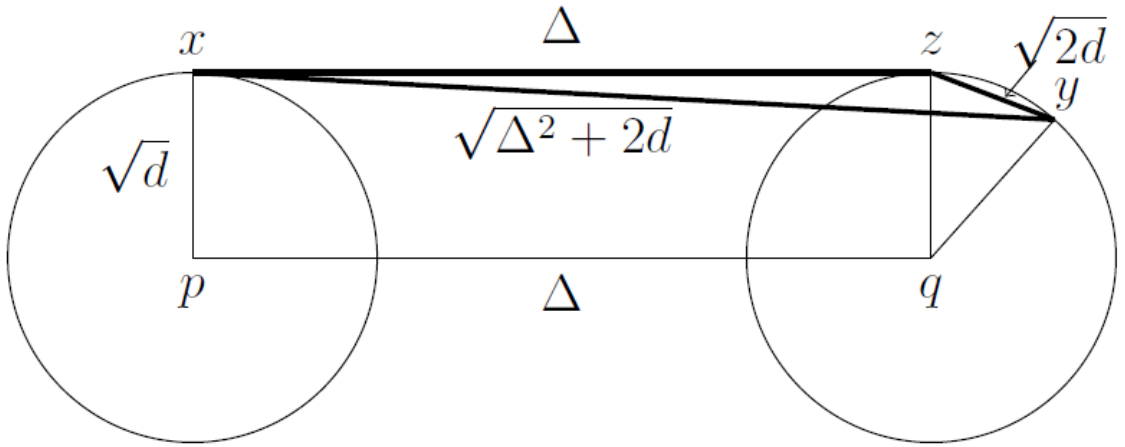
- y is nearly-perpendicular to x
  - $|x-y|^2 \approx |x|^2 + |y|^2$
- x is considered as the "north pole"
  - $x = \left(\sqrt{d} \pm O(\beta), 0, 0, \ldots, 0\right)$
- y is nearly on the equator, we can further rotate the coordinate system so that the component of y that is perpendicular to the axis of the "north pole", is in the second coordinate
  - $y = \left(O(1), \sqrt{d} \pm O(\beta), 0, 0, \ldots, 0\right)$
- $|x-y|^2 = 2d \pm O\left(\beta\sqrt{d}\right)$ with high probability

Sample distances – two Gaussians

- Consider two spherical unit-variance Gaussians with centers p, q separated by a distance Δ
- We want to prove that every two random points, each selected from a different Gaussian, will have significant distance between them
  - $\approx \sqrt{\Delta^2 + 2d \pm O(\beta\sqrt{d})}$
- Pick x from the 1st Gaussian and rotate the coordinate system so x will be the north pole
  - Let z be the north pole of the 2nd spherical Gaussian, using the same coordinate system
- Pick y from the 2nd Gaussian
  - Most of the 2nd Gaussian's mass is within $O(1)$ of the equator perpendicular to $q - z$
  - Most of the 2nd Gaussian's mass is within $O(1)$ of the equator perpendicular to $q - p$

Sample distances – two Gaussians

- The distance $|z - y|$ is $O(\sqrt{2d})$
  - Two samples from the same Gaussian
- High-dimension Pythagorean Theorem
- $|x - y|^2 \approx \Delta^2 + |z - q|^2 + |q - y|^2 \approx \Delta^2 + 2d \pm O(\beta\sqrt{d})$
  - $|z - q|^2 \approx |q - y|^2 \approx \left(\sqrt{d} \pm O(\beta)\right)^2 \approx d \pm O(\beta\sqrt{d}) + \beta^2$



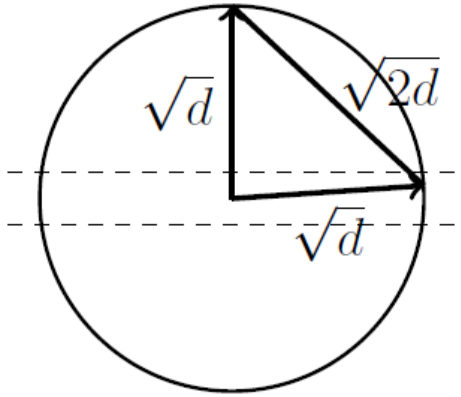
Sample distances - assumptions

- We have to ensure that the distance between two points picked from the same Gaussian are closer to each other, than two points picked from different Gaussians
  - The upper limit of the distance between a pair of points from the same Gaussian is at most the lower limit of the distance between points from different Gaussians
- Squared-distance between two points picked from the same Gaussian
  - $2d \pm O\left(\beta\sqrt{d}\right)$
- Squared-distance between two points picked from different Gaussians
  - $\Delta^2 + 2d \pm O\left(\beta\sqrt{d}\right)$
- $2d \pm O\left(\beta\sqrt{d}\right) \leq \Delta^2 + 2d \pm O\left(\beta\sqrt{d}\right)$ holds for $\Delta \in \omega\left(d^{\frac{1}{4}}\right)$, as needed

Separating Gaussians - algorithm

- Calculate all pairwise distances between points
- The cluster of smallest pairwise distances must come from a single Gaussian
  - Remove these points
- The remaining points come from the second Gaussian
- We used a constant β. What happens if we take n samples?
  - Any fixed β will not be good enough. β has to be dependent on n
  - $\beta = O\left(\sqrt{\ln n}\right)$ is a good value for the annulus-theorem equation
    - The probability to sample the annulus is $1 - 3e^{-c_1\beta^2} = 1 - \frac{3}{n^{c_1}} = 1 - \frac{1}{poly(n)}$

Sample distances – one Gaussian, $\boldsymbol{n}$ samples



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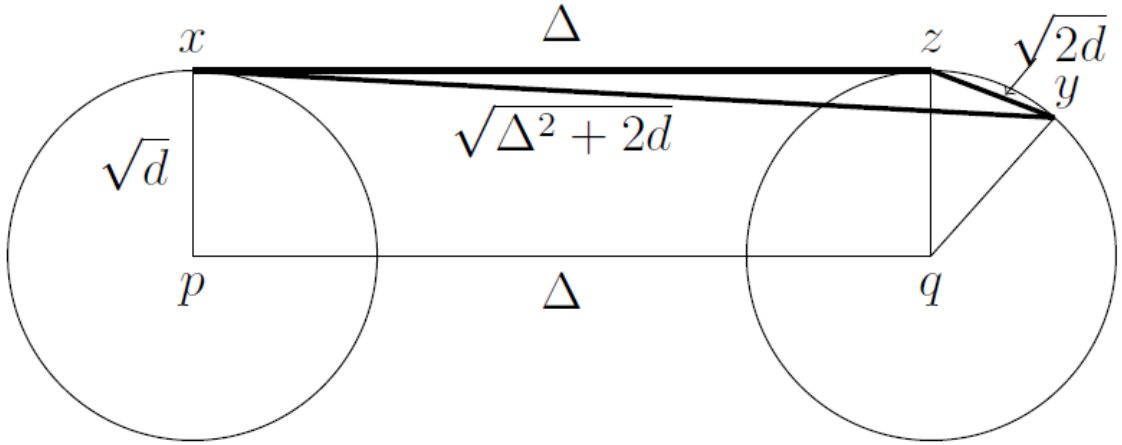
- x is considered as the "north pole"
  - $x = \left(\sqrt{d} \pm O\left(\sqrt{\boldsymbol{\ln n}}\right), 0, 0, \ldots, 0\right)$
- y is nearly on the equator, we can further rotate the coordinate system so that the component of y that is perpendicular to the axis of the "north pole", is in the second coordinate
  - $y = \left(O(1), \sqrt{d} \pm O\left(\sqrt{\boldsymbol{ln\, n}}\right), 0, 0, \ldots, 0\right)$
- $|x-y|^2 = 2d \pm O\left(\sqrt{\boldsymbol{ln\, n}}\sqrt{d}\right)$ with high probability

Sample distances – two Gaussians, $\boldsymbol{n}$ samples

- The distance $|z-y|$ is $O(\sqrt{2d})$
  - Two samples from the same Gaussian
- High-dimension Pythagorean Theorem
- $|x-y|^2 \approx \Delta^2 + |z-q|^2 + |q-y|^2 \approx \Delta^2 + 2d \pm O\left(\sqrt{\boldsymbol{\ln n}}\sqrt{d}\right) + \boldsymbol{O(\ln n)}$
  - $|z-q|^2 \approx |q-y|^2 \approx \left(\sqrt{d} \pm O\left(\sqrt{\boldsymbol{\ln n}}\right)\right)^2 \approx d \pm O\left(\sqrt{\boldsymbol{\ln n}}\sqrt{d}\right) + \boldsymbol{O(\ln n)}$



Sample distances – assumptions, $\boldsymbol{n}$ samples

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- Squared-distance between two points picked from different Gaussians
  - $\Delta^2 + 2d \pm O\left(\sqrt{\ln \boldsymbol{n}}\sqrt{d}\right)$
- $2d \pm O\left(\sqrt{\ln \boldsymbol{n}}\sqrt{d}\right) \leq \Delta^2 + 2d \pm O\left(\sqrt{\ln \boldsymbol{n}}\sqrt{d}\right)$ holds for $\Delta \in \omega\left((d \cdot \ln n)^{\frac{1}{4}}\right)$

Fitting a Spherical Gaussian to Data

- Given d-dimensional sample points $x_1, \ldots, x_n$, our objective is to find a spherical Gaussian that best fits those points
  - Find the distributions' mean μ and variance σ^2
- Let f be a Gaussian with mean μ and variance σ^2
  - μ is a d-dimensional vector, containing the mean values for each dimension

Fitting a Spherical Gaussian to Data

- f's density function is $f(x) = \frac{1}{\left(\sqrt{2\pi\sigma^2}\right)^d} \cdot e^{-\frac{(x-\mu)^2}{2\sigma^2}}$ (remember: x, μ are vectors)
- Definition: MLE (Maximal Likelihood Estimator) of a set samples $x_1, \dots, x_n$ is the density function f that maximizes the above probability density
- We want the Gaussian which gives us the highest probability to get the data $x_1, \dots x_n$ under its density function $f(x)$.
  - The density function becomes a function of μ, σ instead of x, because we want to maximize the likelihood
  - $F(\mu, \sigma) = f(x_1, \dots, x_n) = \frac{1}{(2\pi\sigma^2)^{\frac{dn}{2}}} \cdot \prod_{i=1}^{n} \left[e^{-\frac{(x_i-\mu)^2}{2\sigma^2}} \right]$ where $x_1, \dots, x_n$ are vectors

MLE– mean value μ

- Let $x_1, \ldots, x_n$ be samples in d-dimensional space. We will prove that $(x_1 - \mu)^2 + \cdots + (x_n - \mu)^2$ is minimized when μ is the centroid of $x_1, \ldots, x_n$
  - Why minimize? $F(\mu, \sigma) = c \cdot e^{-\frac{(x_1-\mu)^2+\cdots+(x_n-\mu)^2}{2\sigma^2}}$, so maximizing F's value is minimizing $(x_1 - \mu)^2 + \cdots + (x_n - \mu)^2$
- Proof: We would like to find the minimal point of the sum, by finding its derivative
  - Note that every part of the sum is a vector, its first coordinate is the derivative by μ_1.
    - Each row is a different derivative, and we have d derivatives in total
  - $-2(x_1 - \mu) - \cdots - 2(x_n - \mu) = 0$
  - Solving for μ gives $\mu = \frac{1}{n}(x_1 + \cdots + x_n)$

MLE – variance σ^2

- We would like to find the MLE of σ^2 for f
- Let μ be the real centroid.
- Let $\upsilon = \frac{1}{2\sigma^2}$ and $a = \sum_{i=1}^{n}(x_i - \mu)^2$ (for simplicity)
- The density function is now $f(x) = \left[\frac{\upsilon}{\pi}\right]^{\frac{dn}{2}} \cdot e^{-a\upsilon}$
  - To find its maximal value, we will find the derivative of $\ln f(x)$
  - $\frac{dn}{2\upsilon} - a = 0$
  - $\sigma = \frac{\sqrt{a}}{\sqrt{nd}}$
- σ is the square root of the average coordinate distance squared of the samples to their mean (the definition of standard deviation!)