EM Algorithm & High Dimensional Data

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Gaussian EM Algorithm

- For the Gaussian mixture model, we have
  - Expectation Step (E-Step):

$$\begin{aligned} h_{ij} &= P_{\mathbf{Z}|\mathbf{X}}(j|\mathbf{x}_i) \\ &= \frac{\mathcal{G}\left(\mathbf{x}_i, \mu_j, \sigma_j\right)\pi_j}{\sum_{k=1}^{C}\mathcal{G}\left(\mathbf{x}_i, \mu_k, \sigma_k\right)\pi_k} \end{aligned}$$

  - Maximization Step (M-Step):

$$\mu_j^{new} = \frac{\sum_i h_{ij}\mathbf{x}_i}{\sum_i h_{ij}} \qquad \pi_j^{new} = \frac{1}{n}\sum_i h_{ij}$$

$$\sigma_j^{2new} = \frac{\sum_i h_{ij}(\mathbf{x}_i - \mu_j)^2}{\sum_i h_{ij}}$$

EM versus K-means

EM | *k*-Means

Data Class Assignments

Soft Decisions:

$$h_{ij} = P_{\mathbf{Z}|\mathbf{X}}(j|\mathbf{x}_i)$$

Hard Decisions:

$$i^*(x_i) = \arg\max_j P_{Z|X}(j \mid x_i)$$

$$h_{ij} = \begin{cases} 1, & P_{Z|X}(j \mid x_i) > P_{Z|X}(k \mid x_i), k \neq j \\ 0, & \text{otherwise} \end{cases}$$

Parameter Updates

Soft Updates:

$$\mu_j^{new} = \frac{\sum_i h_{ij}\mathbf{x}_i}{\sum_i h_{ij}}$$

$$\pi_j^{new} = \frac{1}{n}\sum_i h_{ij}$$

$$\sigma_j^{2new} = \frac{\sum_i h_{ij}(\mathbf{x}_i - \mu_j)^2}{\sum_i h_{ij}}$$

Hard Updates:

$$\mu_i^{\text{new}} = \frac{1}{n}\sum_j x_j^{(i)}$$

Important Application of EM

- Recall, in Bayesian decision theory we have
  - World: States Y in {1, ..., M} and observations of X
  - Class-conditional densities $P_{X|Y}(x|y)$
  - Class (prior) probabilities $P_Y(i)$
  - Bayes decision rule (BDR)

$$i^* = \arg\max_i P_{X|Y}(x|i) P_Y(i)$$

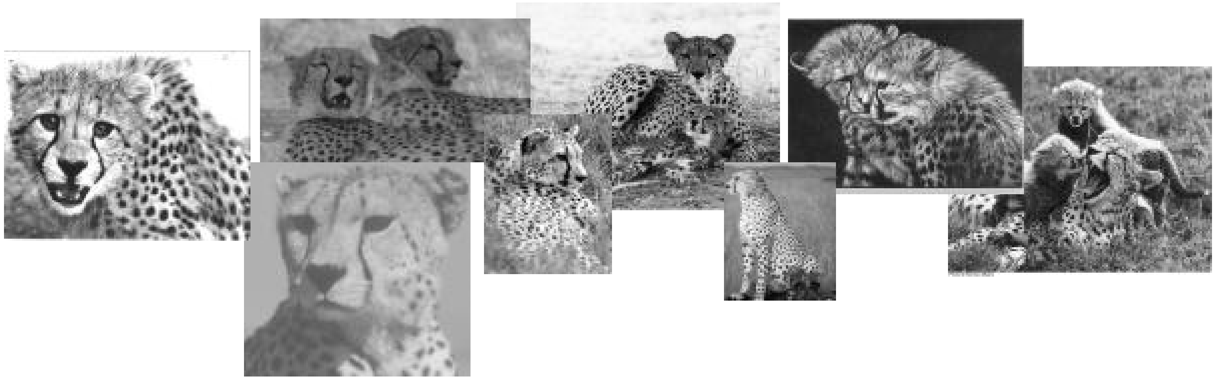
- We have seen that this is only optimal insofar as all probabilities involved are correctly estimated
- One of the important applications of EM is to more accurately learn the class-conditional densities

Example

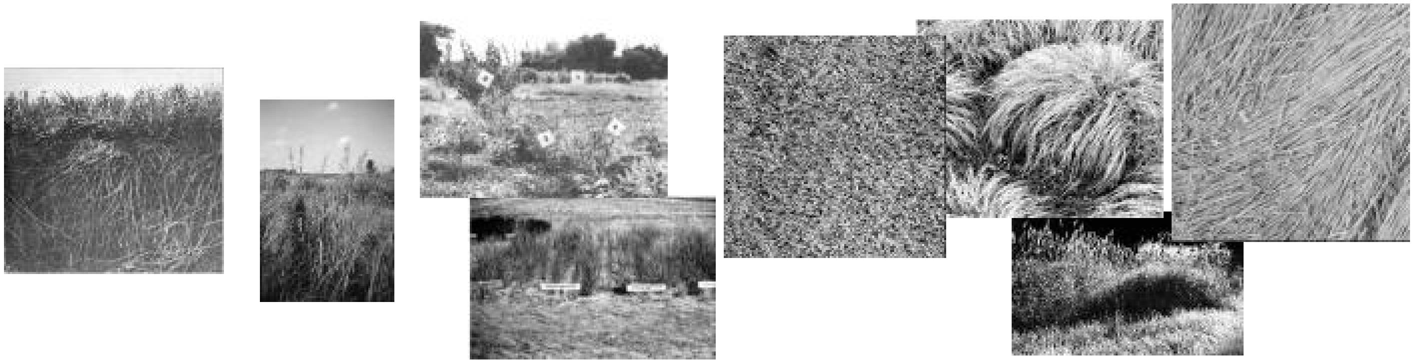
- Image segmentation:
  - Given this image, can we segment it into the cheetah and background classes?
  - Useful for many applications
    - Recognition: "this image has a cheetah"
    - Compression: code the cheetah with fewer bits
    - Graphics: plug in for photoshop would allow manipulating objects
- Since we have two classes (cheetah and grass), we should be able to do this with a Bayesian classifier

Example

- Start by collecting a lot of examples of cheetahs



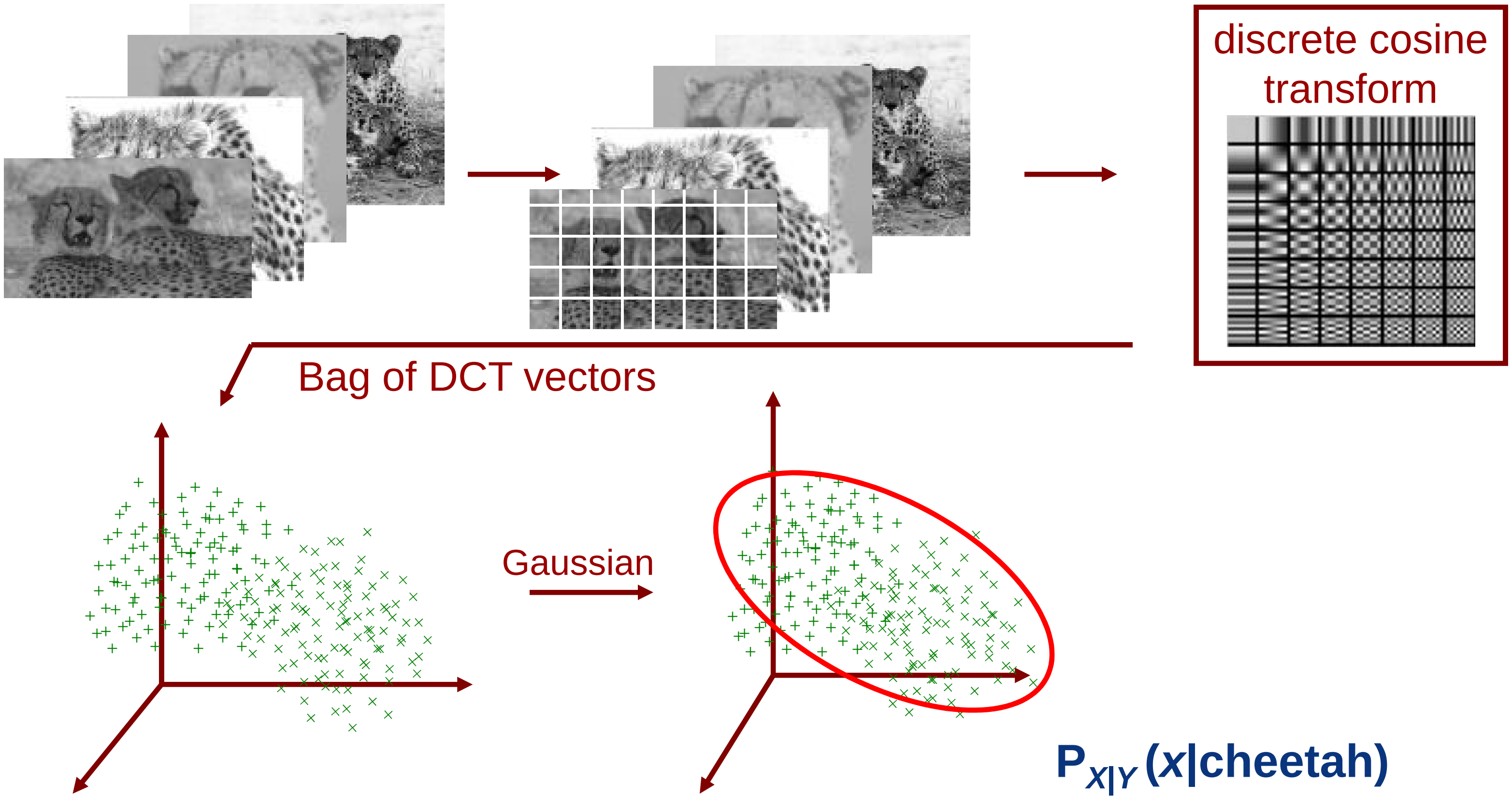
- and a lot of examples of grass



- One can get tons of such images via Google image search

Example

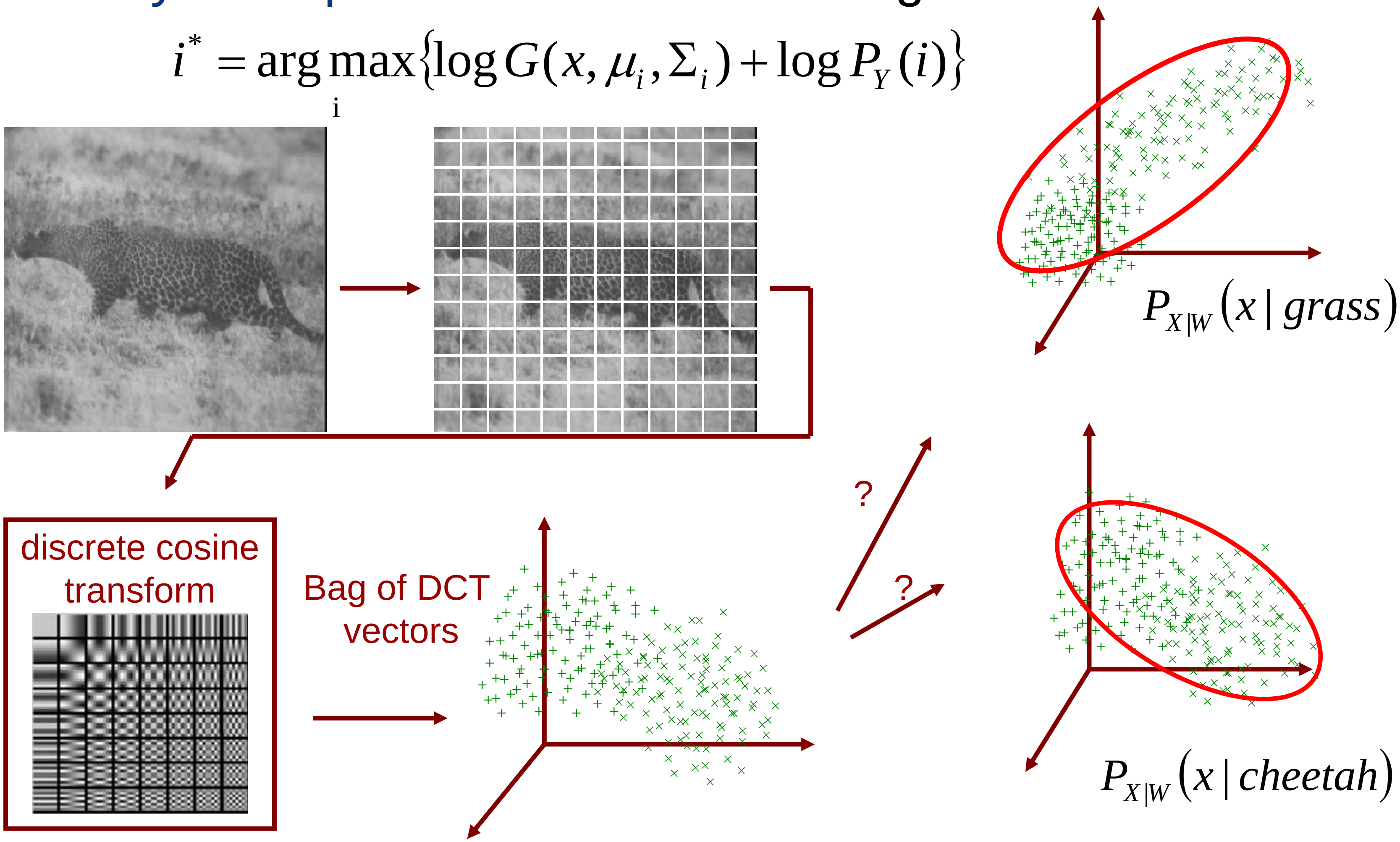
- Represent images as bags of little image patches
- We can fit a simple Gaussian to the transformed patches



Example

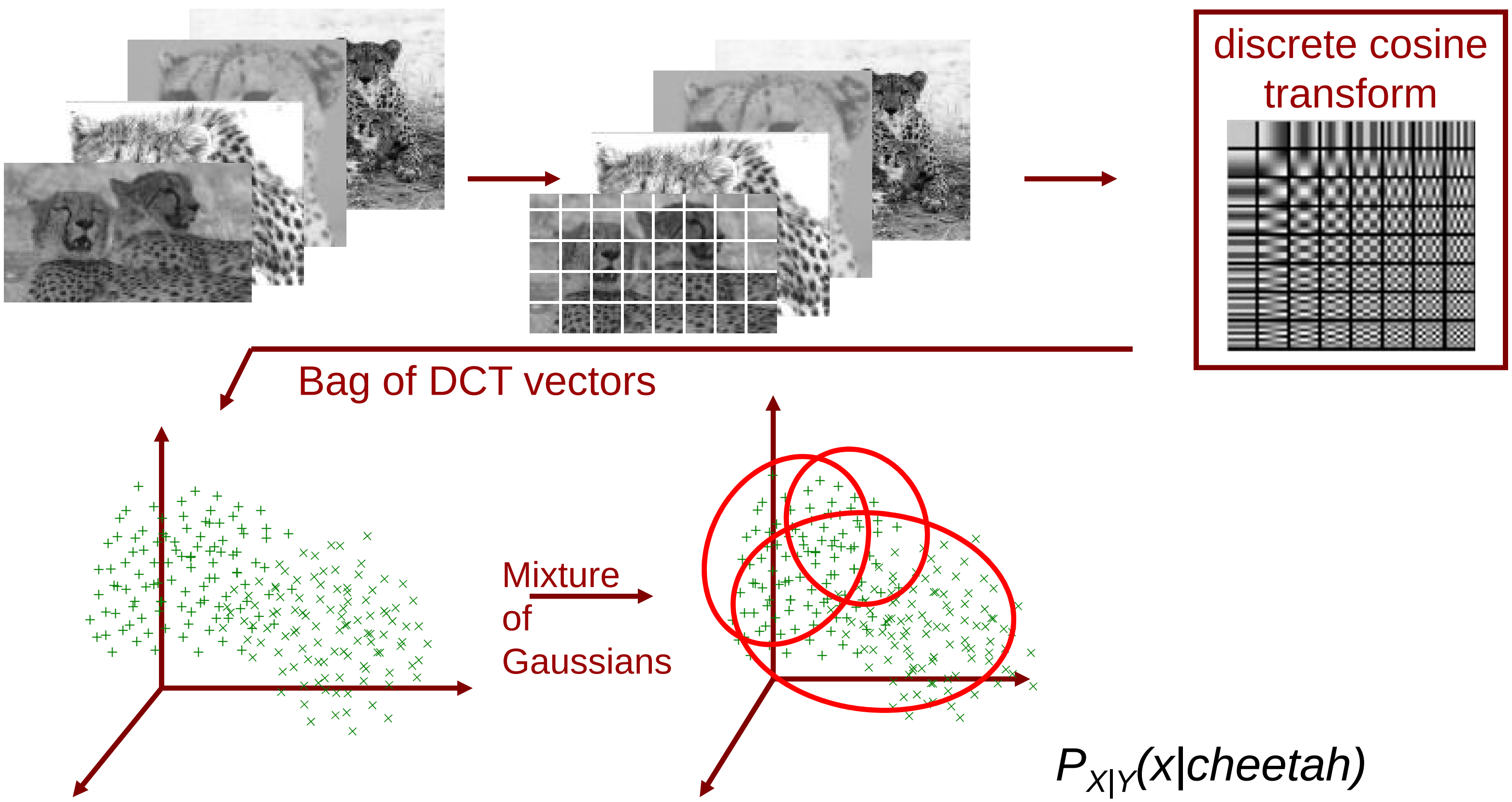
- Do the same for grass and apply BDR to each patch to classify each patch into “cheetah” or “grass”

$$i^* = \arg\max_i \left\{ \log G(x, \mu_i, \Sigma_i) + \log P_Y(i) \right\}$$



Example

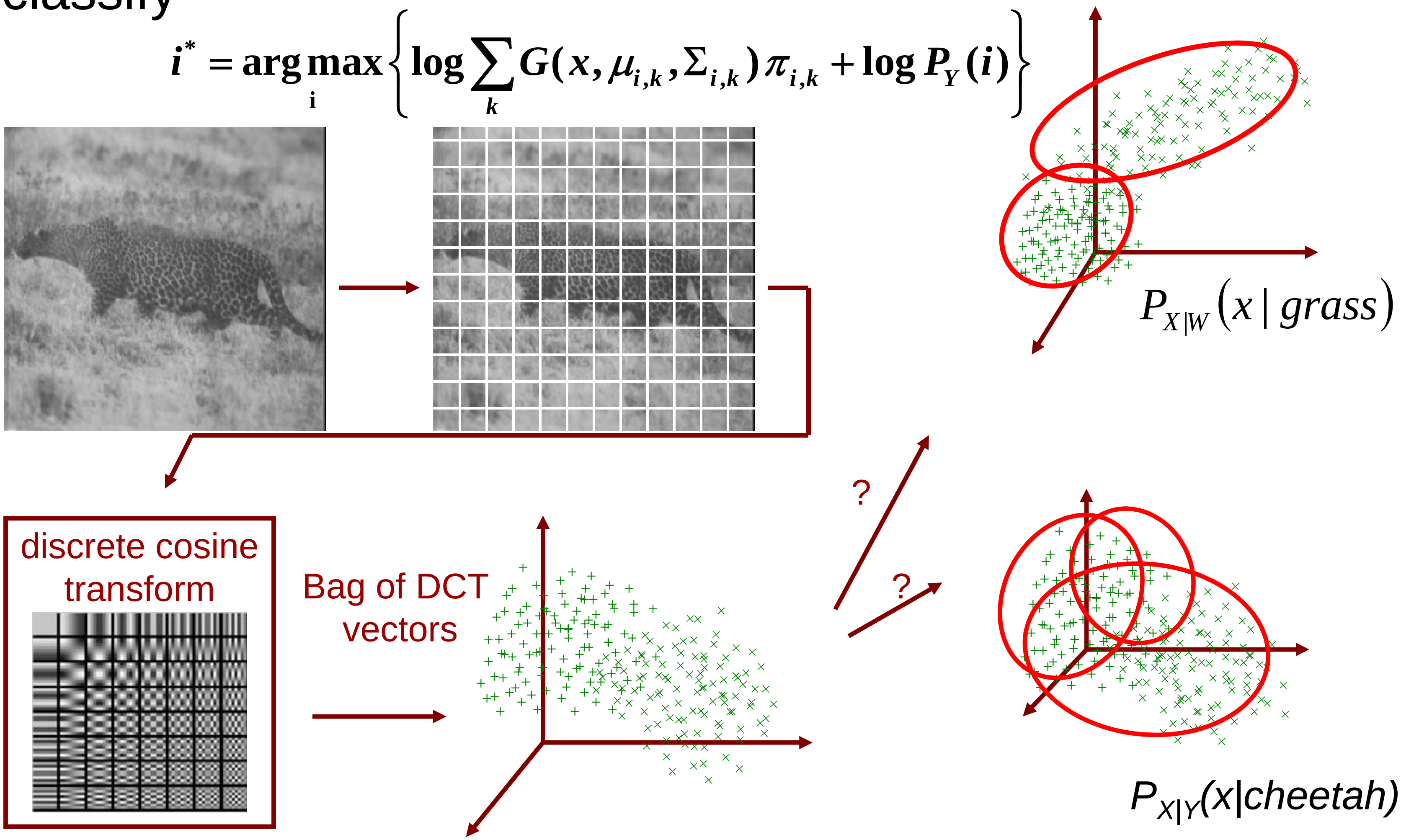
- Better performance is achieved by modeling the cheetah class distribution as a mixture of Gaussians



Example

- Do the same for grass and apply BDR to each patch to classify

$$i^* = \arg\max_i \left\{ \log \sum_k G(x, \mu_{i,k}, \Sigma_{i,k}) \pi_{i,k} + \log P_Y(i) \right\}$$



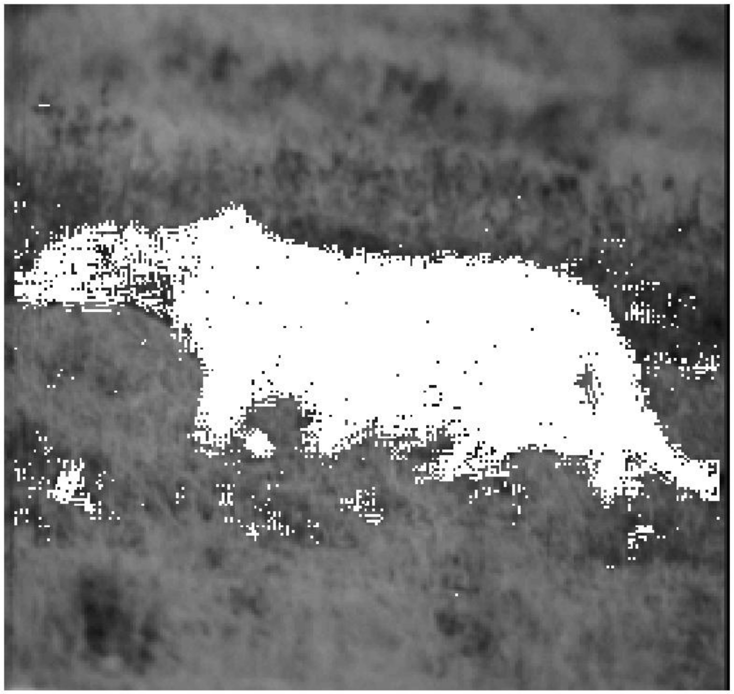
Classification

- The use of more sophisticated probability models, e.g. mixtures, *usually* improves performance
- However, it is not a magic solution
- Earlier on in the course we talked about features
- Typically, you have to start from a good feature set
- It turns out that even with a good feature set, you must be careful
- Consider the following example, from our image classification problem

Example

- Cheetah Gaussian classifier, DCT space

8 first DCT features



Prob. of error: 4%

all 64 features

8%

- Interesting observation: more features = higher error!

Comments on the Example

- The first reason why this happens is that things are not always what we think they are in high dimensions
- One could say that high dimensional spaces are STRANGE!!!
- In practice, we invariable have to do some form of dimensionality reduction
- We will see that eigenvalues play a major role in this
- One of the major dimensionality reduction techniques is principal component analysis (PCA)
- But let’s start by discussing the problems of high dimensions

High Dimensional Spaces

- Are strange!
- First thing to know:

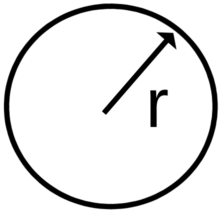
  "Never fully trust your intuition in high dimensions!"

- More often than not you will be wrong!
  - There are many examples of this
  - We will do a couple here, skipping most of the math
  - These examples are both fun and instructive

The Hypersphere

- Consider the ball of radius *r* in a space of dimension *d*

$$\mathcal{S} = \left\{ \mathbf{x} \middle| \sum_{i=1}^{d} x_i^2 \leq r^2 \right\}$$



The surface of this ball is a (*d*-*1*)-dimensional hypersphere.

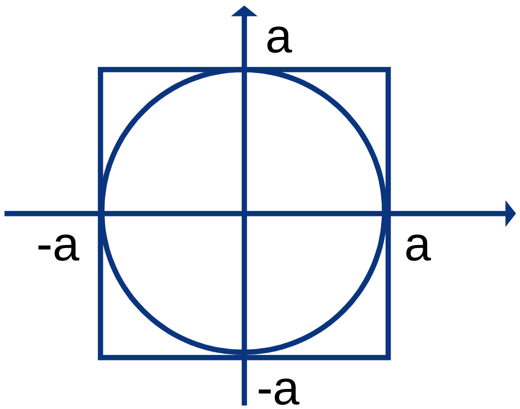
- The ball has volume $V_d(r) = \dfrac{r^d \pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}+1\right)}$

where Γ(n) is the gamma function $\Gamma(n) = \int_0^\infty e^{-x} x^{n-1} dx$

- When we talk of the “volume of a hypersphere”, we will actually mean the volume of the ball it contains.
- Similarly, for “the volume of a hypercube”, etc.

Hypercube versus Hypersphere

- Consider the hypercube $[-a,a]^d$ and an inscribe hypersphere:



- **Q:** what does your intuition tell you about the relative sizes of these two volumes?
  1. volume of sphere $\approx$ volume of cube?
  2. volume of sphere **>>** volume of cube?
  3. volume of sphere **<<** volume of cube?

Answer

- To find the answer, we can compute the relative volumes:

$$f_d = \frac{Vol(sphere)}{Vol(cube)} = \frac{\frac{a^d \pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}+1\right)}}{(2a)^d} = \frac{\pi^{\frac{d}{2}}}{2^d \Gamma\left(\frac{d}{2}+1\right)}$$

- This is a sequence that does ***not*** depend on the radius ***a***, just on the dimension ***d*** !

d	1	2	3	4	5	6	7
f_d	1	.785	.524	.308	.164	.08	.037

- The relative volume goes to zero, and goes to zero fast!

Hypercube vs Hypersphere

- This means that:

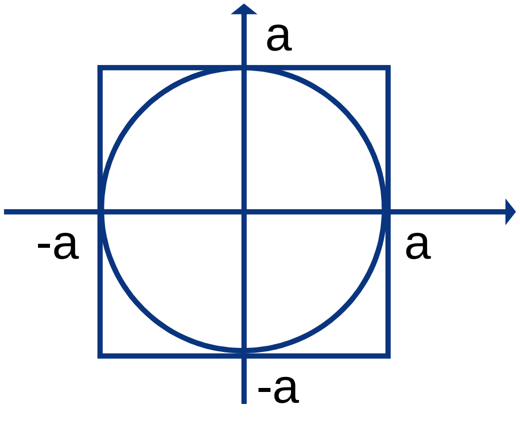
  "As the dimension of the space increases, the volume of the sphere is much smaller (infinitesimally so) than that of the cube!"

- Is this *really* going against intuition?
- It is actually not very surprising, if we think about it. we can see it even in low dimensions:

1. d = 1

volume is the same

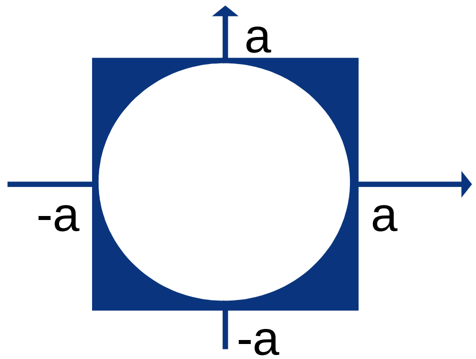
2. d = 2



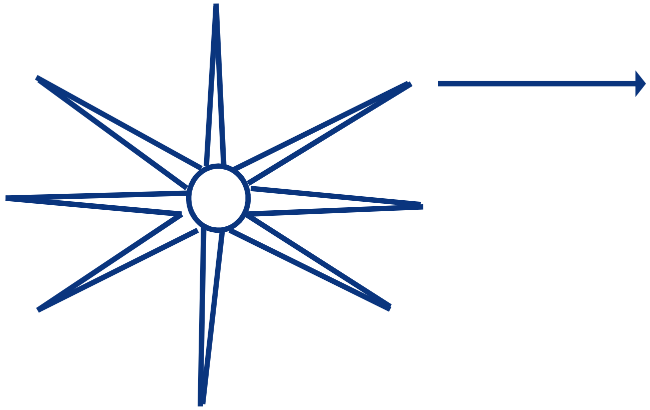
volume of sphere is already smaller

Hypercube vs Hypersphere

- As the dimension increases, the volume of the shaded corners becomes larger.



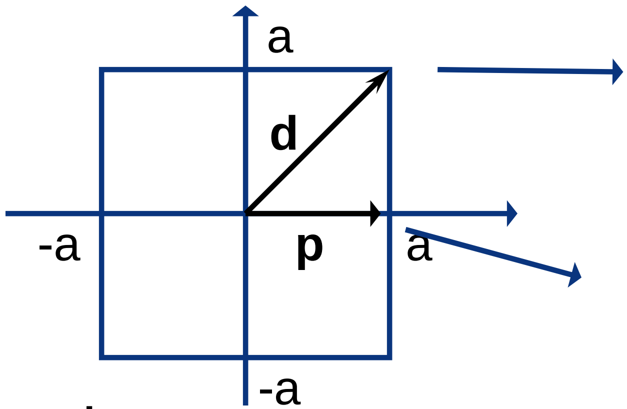
- In high dimensions the picture you should imagine is:



All the volume of the cube is in the "spikes" (corners)!

Believe it or Not …

… we can actually check this mathematically: Consider ***d*** and ***p***



$$\mathbf{d} = (a, a, \ldots, a) \in \mathcal{R}^d$$

$$\mathbf{p} = (a, 0, \ldots, 0) \in \mathcal{R}^d$$

- note that

$$\begin{aligned} cos\theta &= \frac{\mathbf{d}^T\mathbf{p}}{\sqrt{||d||^2||p||^2}} \\ &= \frac{a^2}{\sqrt{da^2a^2}} = \frac{1}{\sqrt{d}} \to 0 \end{aligned}$$

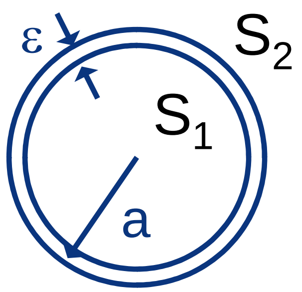
$$\frac{||d||^2}{||p||^2} = \frac{da^2}{a^2} = d \to \infty$$

- *d* becomes orthogonal to *p* as *d* increases,

  and infinitely larger!!!

But there is even more …

- Consider the crust of unit sphere of thickness ε
- We can compute the volume of the crust:



$$Vol(crust) = \left[1 - \frac{Vol(S_1)}{Vol(S_2)}\right] Vol(S_2)$$

$$\frac{Vol(S_1)}{Vol(S_2)} = \frac{\frac{(a-\epsilon)^d \pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}+1\right)}}{\frac{a^d \pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}+1\right)}} = \frac{a^d\left(1-\frac{\epsilon}{a}\right)^d}{a^d} = \left(1-\frac{\epsilon}{a}\right)^d$$

- No matter how small ε is, ratio goes to zero as *d* increases
- I.e. "all the volume is in the crust!"

High Dimensional Gaussian

- For a Gaussian, it can be shown that if

$$\mathbf{X} \sim N(\mathbf{0}, \mathbf{I}), \quad \mathbf{x} \in \mathcal{R}^n$$

and one considers the region outside of the hypersphere where the probability density drops to 1% of peak value

$$S_{0.01}(\mathbf{x}) = \left\{ \mathbf{x} \,\middle|\, \frac{G(\mathbf{x}, \mathbf{0}, \mathbf{I})}{G(\mathbf{0}, \mathbf{0}, \mathbf{I})} \leq 0.01 \right\}$$

then the probability mass in this region is

$$P_n = P[\chi^2(n) \geq 9.21]$$

where $\chi^2(n)$ is a chi-squared random variable with ***n*** degrees of freedom

High-Dimensional Gaussian

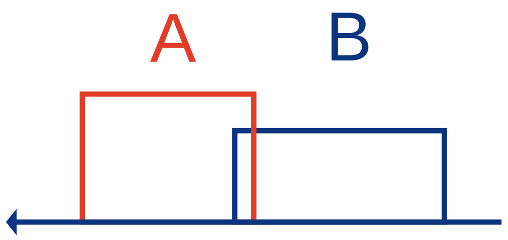
- If you evaluate this, you'll find out that

n	1	2	3	4	5	6	10	15	20
$1-P_n$	.998	.99	.97	.94	.89	.83	.48	.134	.02

- As the dimension increases, virtually all the probability mass is in the tails
- Yet, the point of maximum density is still the mean
- This is really strange: in high-dimensions the Gaussian is a very heavy-tailed distribution
- Take-home message:
  - "In high dimensions never trust your low-dimensional intuition!"

The Curse of Dimensionality

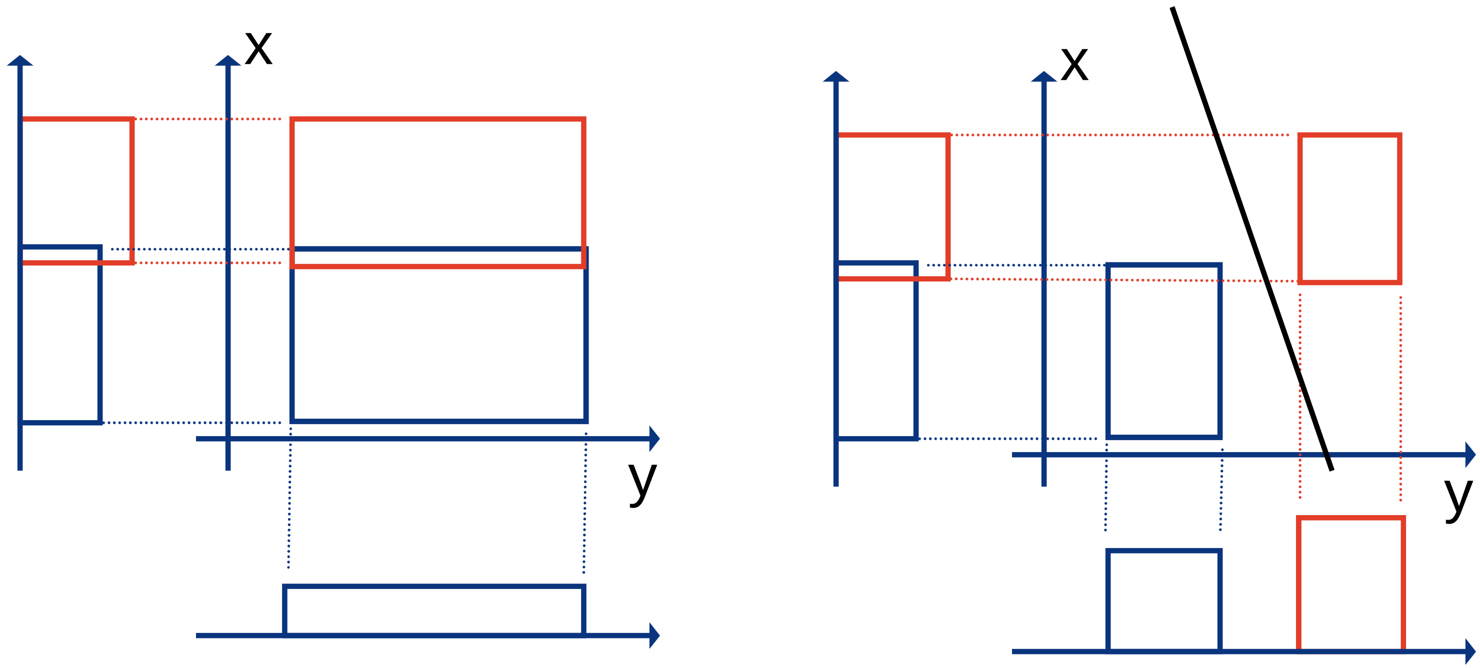
- Typical observation in Bayes decision theory:
  - Error increases when number of features is large
- This is unintuitive since theoretically:
  - If I have a problem in *n* dimensions I can always generate a problem in *n+1* dimensions without increasing the probability of error, and even often decreasing the probability of error.
- E.g. two uniform classes in 1-D



can be transformed into a 2-D problem with the same error

- Just add a non-informative variable (extra dimension) y.

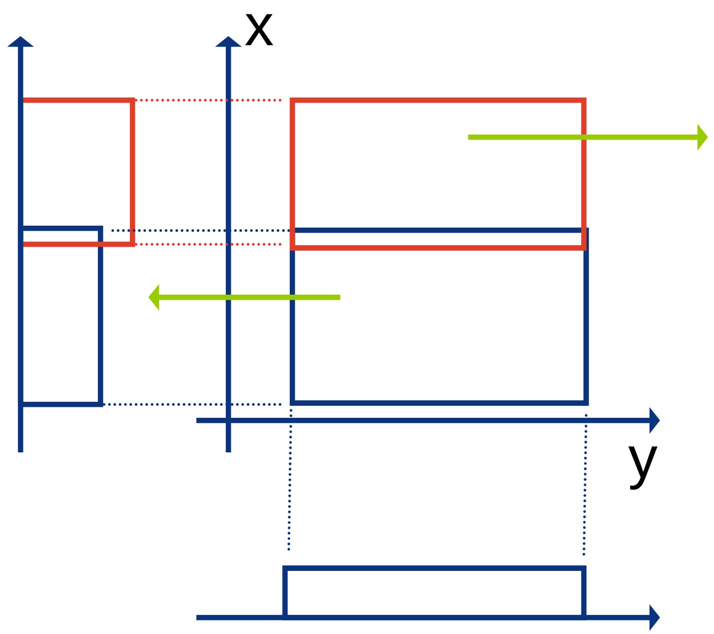
Curse of Dimensionality



- Sometimes it **<u>is</u>** possible to reduce the error by adding a second variable which **<u>is</u>** informative
  - On the left there is no decision boundary that will achieve zero error
  - On the right, the decision boundary shown has zero error

Curse of Dimensionality

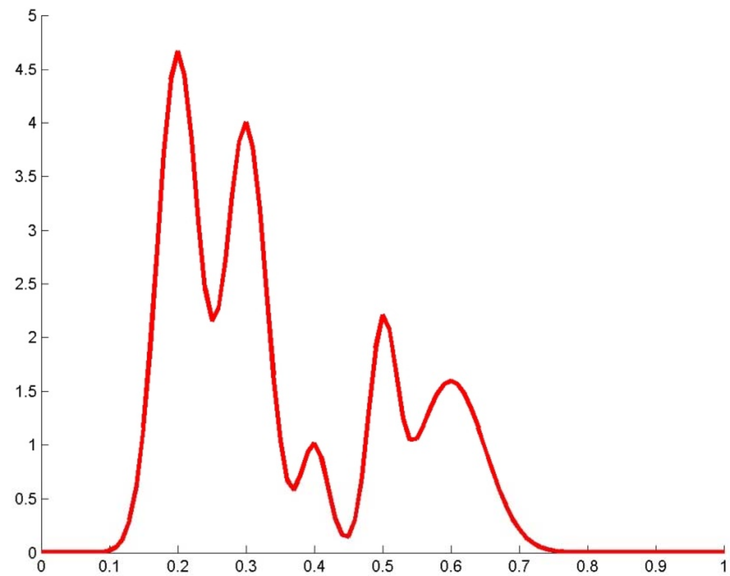
- In fact, it is *theoretically impossible* to do worse in 2-D than 1-D:



If we move the classes along the lines shown in green the error can only go down, since there will be less overlap

Curse of Dimensionality

- So why do we observe this "curse of dimensionality"?
- The problem is the quality of the density estimates
- All we have seen so far, assumes perfect estimation of the BDR
- We discussed various reasons why this is not easy
  - Most densities are not simply a Gaussian, exponential, etc
  - Typically densities are, at best, a mixture of several components.
  - There are many unknowns (# of components, what type), the likelihood has local minima, etc.
  - Even with algorithms like EM, it is difficult to get this right



Curse of Dimensionality

- But the problem goes much deeper than this
- Even for simple models (e.g. Gaussian) we need a large number of examples *n* to have good estimates
- Q: What does "large" mean? This depends on the dimension of the space
- The best way to see this is to think of an histogram:
  - Suppose you have 100 points and you need at least 10 bins per axis in order to get a reasonable quantization
  - For uniform data you get, on average:

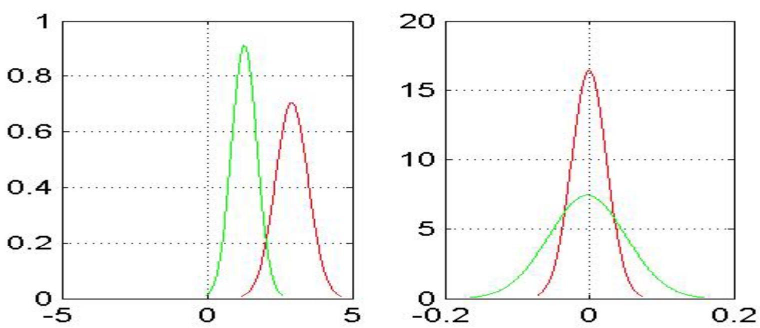
dimension	1	2	3
points/bin	10	1	0.1

  - This is decent in1-D; bad in 2-D; terrible in 3-D (9 out of each10 bins empty)

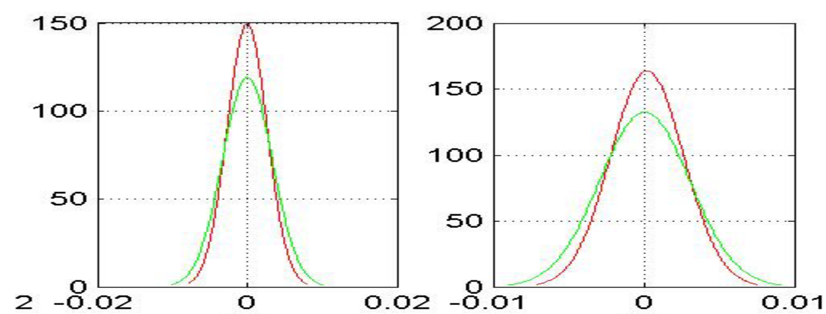
Dimensionality Reduction

- We see that it can quickly become impossible to fill up a high dimensional space with a sufficient number of data points.
  - What do we do about this? We avoid unnecessary dimensions!
- Unnecessary can be measured in two ways:
  1. Features are non-discriminant (insufficiently discriminating)
  2. Features are not independent
- Non-discriminant means that they don't separate classes well

Discriminant Feature



Non-Discriminant Feature



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