Computational Data Analysis

Machine Learning

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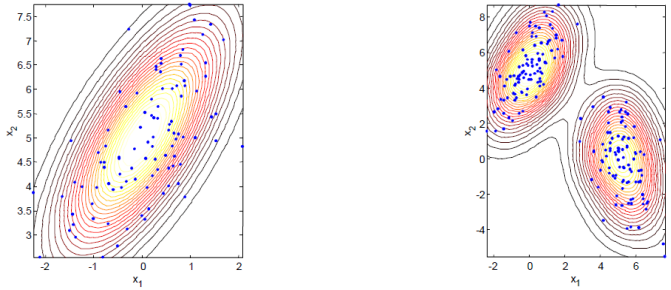
Density Estimation

Why do we need density estimation?

- Learn more about the “shape” of the data cloud

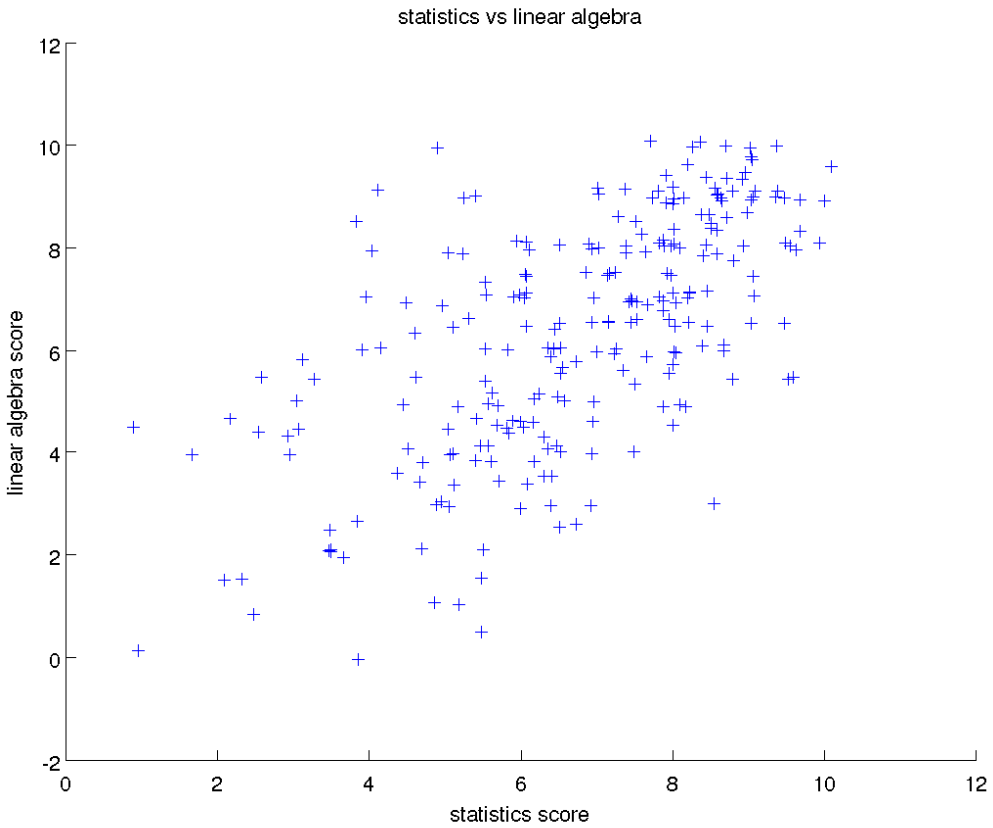


- Assess the likelihood of seeing a particular data point
  - Is this a typical data point? (high density value)
  - Is this an abnormal data point / outlier? (low density value)

- Building block for more sophisticated learning algorithms
  - Classification, regression, graphical models …
  - A simple recommendation system

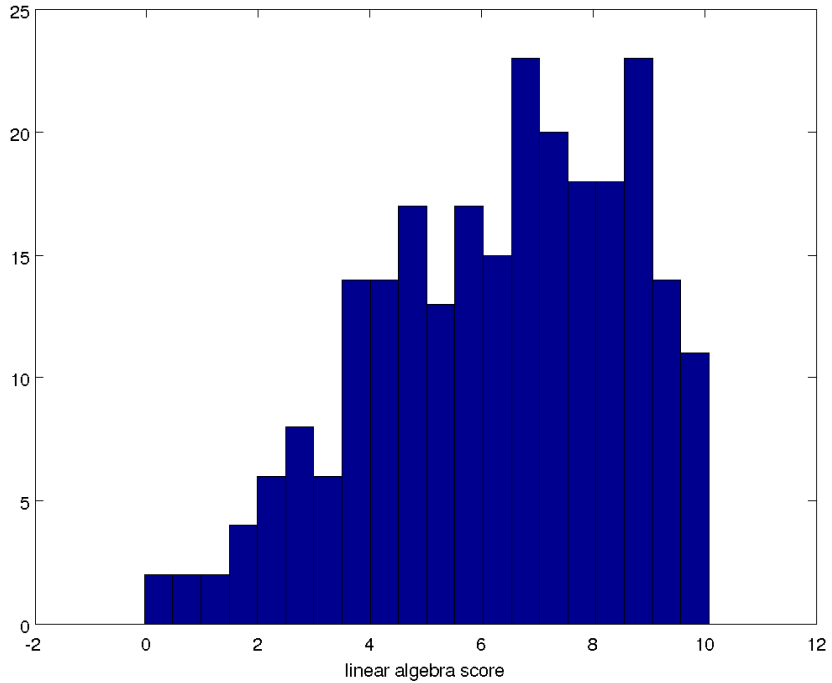
http://www.datawrangling.org/python-montage-code-for-displaying-arrays/

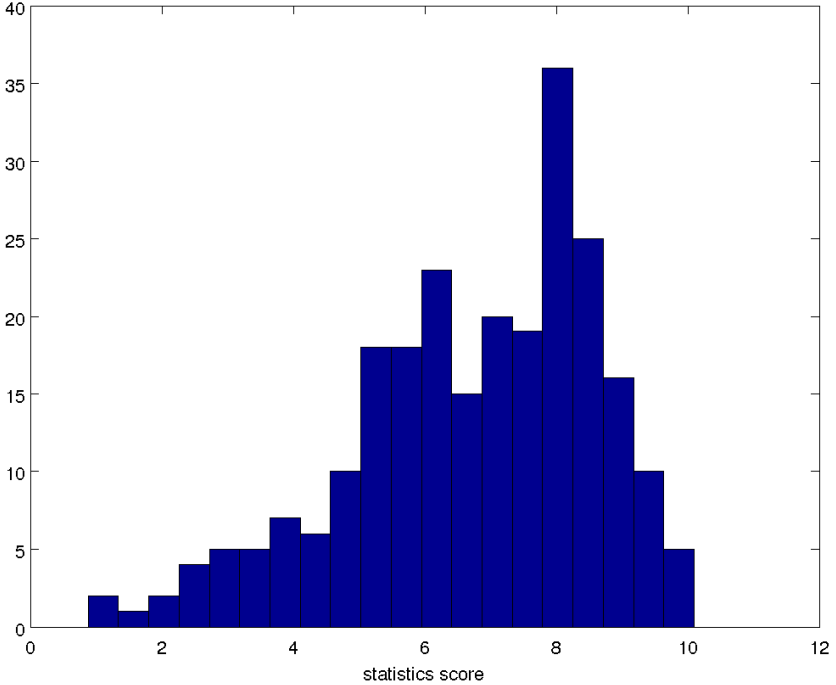
Example: background test scores



Example: background test scores

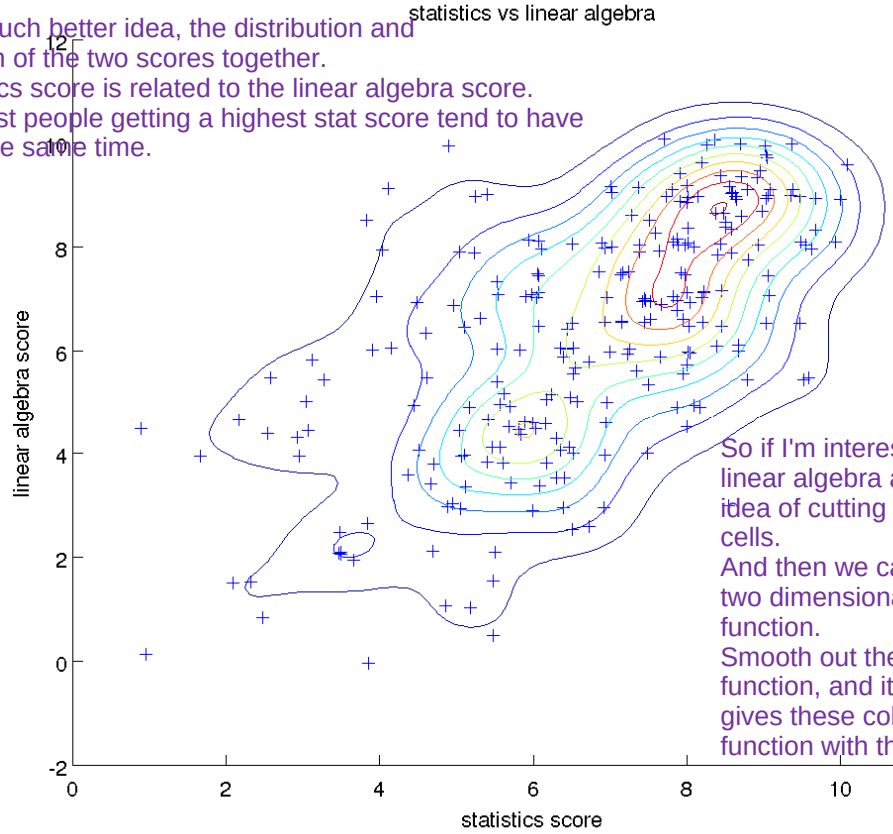
And you can see this captures the density for each of the variables, but not necessarily jointly.





Example: background test scores (cont.)

As you can see, this gives us a much better idea, the distribution and the density, the jointed distribution of the two scores together.
You can see how people's statistics score is related to the linear algebra score.
You can see a mode here, so most people getting a highest stat score tend to have a higher linear algebra score at the same time.



So if I'm interested in capturing both the statistic and linear algebra at the same time, and you can actually use the idea of cutting the space, the two dimensional space into small cells.
And then we can try to count a number of cells like if they're the two dimensional histogram. And I try to smooth out this density function.
Smooth out the two dimensional histogram that gives the density function, and it plot out the contour of my density function that gives these colored curves. Each curve representing the density function with the same value.

Parametric models

So talking about density estimation, there are two major approaches. One is so-called parametric approach.

- Models which can be described by a fixed number of parameters

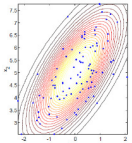
- Discrete case: eg. Bernoulli distribution

$$P(x|\theta) = \theta^x(1-\theta)^{1-x}$$

one parameter, $\theta \in [0,1]$, which generate a family of models, $\mathcal{F} = \{P(x|\theta) \mid \theta \in [0,1]\}$,

- Continuous case: eg. Gaussian distribution in R^n

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



Two sets of parameters $\{\mu, \Sigma\}$, which again generate a family of models, $\mathcal{F} = \{p(x|\mu,\Sigma) \mid \mu \in R^n, \Sigma \in R^{n\times n} \text{ and } PSD\}$,

The mu representing the main parameter is going to be a vector, and the sigma representing the covariance matrix, it is a matrix parameter.

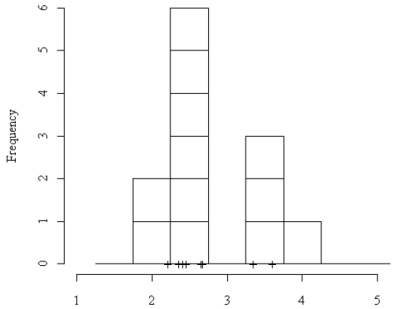
Nonparametric models

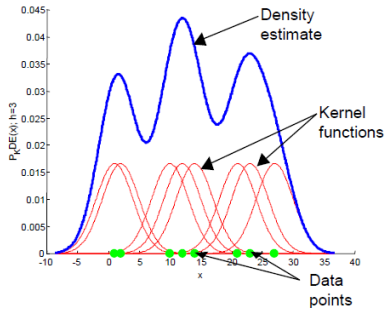
And so the nonparametric model means we do not assume a particular form of the distribution, so there is no parameter. But we try to describe the data using some shapes

- What are nonparametric models?
  - "nonparametric" does not mean there are no parameters
  - can not be described by a fixed number of parameters
  - one can think of there are many many parameters
- Eg. Histogram

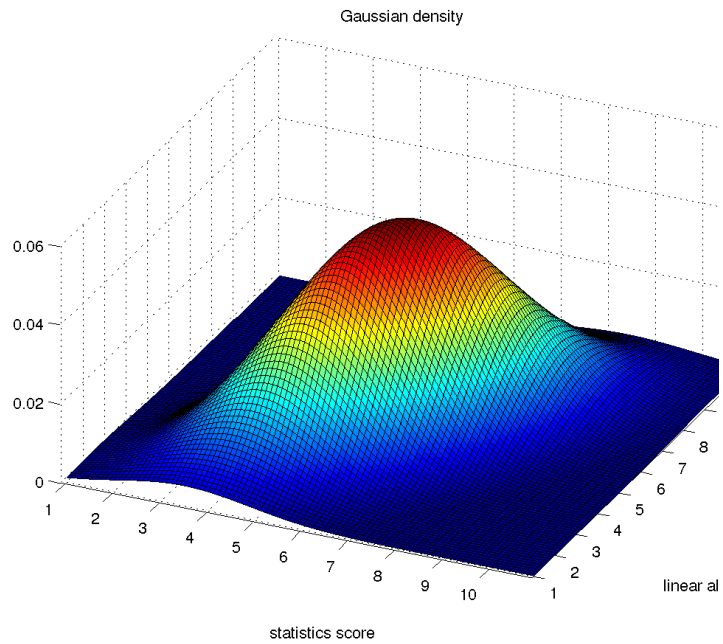
And you can also think about this as a problem of having no parameter, meaning there's no parameter for the model.
But also has many many parameters, and these parameters are actually the height of the kernel function you're gonna use to represent your distribution.

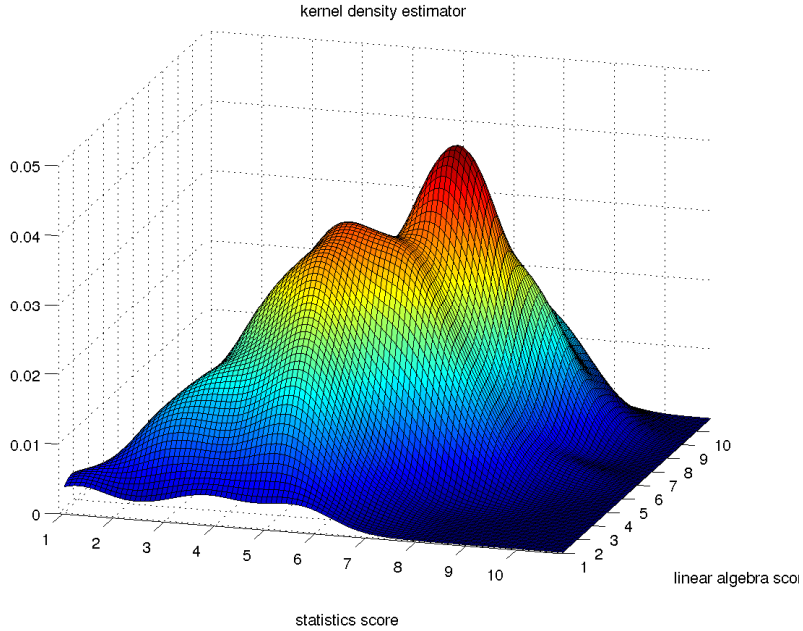
- Eg. Kernel density estimator





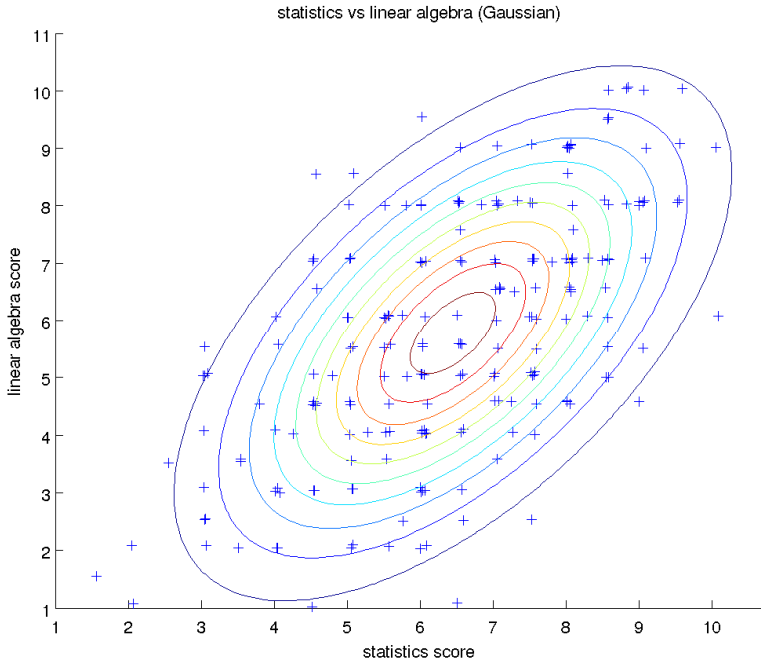
Parametric vs. nonparametric

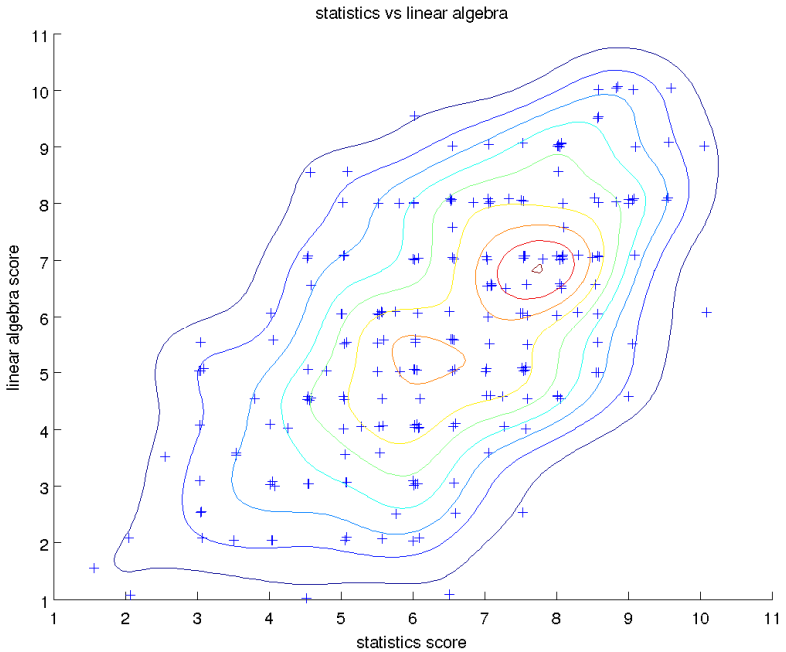




In general, if you believe you have a pretty good model, and you can make such an assumption of your data, then it's better to use the parametric approach and incorporate the model knowledge.
But if you think it's not very easy to build a model and the better to let the data to represent themselves, and if you have lots of data at the same time, the non parametric model might be a better fit, okay?

Parametric vs. nonparametric





On the left hand side is a Gaussian density.
You try to fit a one multi-variate Gaussian distribution to the statistics versus the algebra,
you have very concentrated the ellipse-shaped contours.
And versus in the right hand side the KDE gives you two modes and
then it's going to be a littlebit noisy here.

Estimation of parametric models

- A very popular estimator is the maximum likelihood estimator (MLE), which is simple and has good statistical properties

- Assume that m data points $\mathcal{D} = \{x^1, x^2, \ldots x^m\}$ drawn independently and identically (iid) from some distribution $P^*(x)$

- Want to fit the data with a model $P(x|\theta)$ with parameter θ

$$\theta = argmax_\theta \ \log P(\mathcal{D}|\theta) = argmax_\theta \ \log \prod_{i=1}^{m} P(x^i|\theta)$$

Example problem

- Estimate the probability θ of landing in heads using a biased coin

- Given a sequence of m independently and identically distributed (iid) flips
  - Eg.,$\mathcal{D} = \{x^1, x^2, \ldots x^m\} = \{1,0,1, \ldots, 0\}, x^i \in \{0,1\}$

- Model: $P(x|\theta) = \theta^x(1-\theta)^{1-x}$
  - $P(x|\theta) = \begin{cases} 1-\theta, for\ x = 0 \\ \theta, \quad for\ x = 1 \end{cases}$

- Likelihood of a single observation x_i ?
  - $P(x^i|\theta) = \theta^{x^i}(1-\theta)^{1-x^i}$

compact form.

MLE for Biased Coin

- Objective function, log likelihood

$$l(\theta;\mathcal{D}) = \log P(\mathcal{D}|\theta) = \log \theta^{n_h}(1-\theta)^{n_t}$$
$$= n_h \log\theta + (m - n_h)\log(1-\theta)$$

n_h: number of heads, n_t: number of tails

- Maximize $l(\theta;\mathcal{D})$ w.r.t. θ

- Take derivatives w.r.t. θ

$$\frac{\partial l}{\partial \theta} = \frac{n_h}{\theta} - \frac{(m - n_h)}{1-\theta} = 0$$

$$\Rightarrow \hat{\theta}_{MLE} = \frac{n_h}{m} \text{ or } \hat{\theta}_{MLE} = \frac{1}{m}\sum_i x^i$$

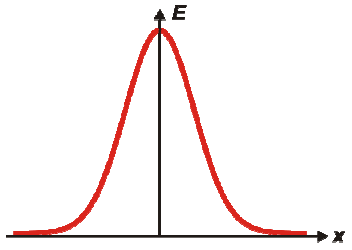
Estimating Gaussian distribution

Another example is to estimating Gaussian distribution.

- Gaussian distribution in R

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

- Need to estimate two sets of parameters μ, σ



- Given m iid samples

$$\mathcal{D} = \{x^1, x^2, \dots x^m\}, x^i \in R$$

- Likelihood of one data point:

$$p(x^i|\mu,\sigma) \propto exp\left(-\frac{1}{2\sigma^2}(x^i-\mu)^2\right)$$

MLE for Gaussian distribution

- Objective function, log likelihood

$$l(\mu, \sigma; \mathcal{D}) = \log \prod_{i=1}^{m} \frac{1}{(2\pi)^{\frac{1}{2}}\sigma} exp\left(-\frac{1}{2\sigma^2}\left(x^i - \mu\right)^2\right)$$

$$= -\frac{m}{2}\log 2\pi - \frac{m}{2}\log \sigma^2 \; - \sum_{i=1}^{m} \frac{\left(x^i - \mu\right)^2}{2\sigma^2}$$

- Maximize $l(\mu, \sigma; \mathcal{D})$ with respect to μ, σ

- Take derivatives w.r.t. μ, σ^2

$$\frac{\partial l}{\partial \mu} = 0$$

$$\frac{\partial l}{\partial \sigma^2} = 0$$

Gaussian

$$l(\mu, \sigma; \mathcal{D}) = -\frac{m}{2}\log 2\pi - \frac{m}{2}\log \sigma^2 \; - \sum_{i=1}^{m} \frac{\left(x^i - \mu\right)^2}{2\sigma^2}$$

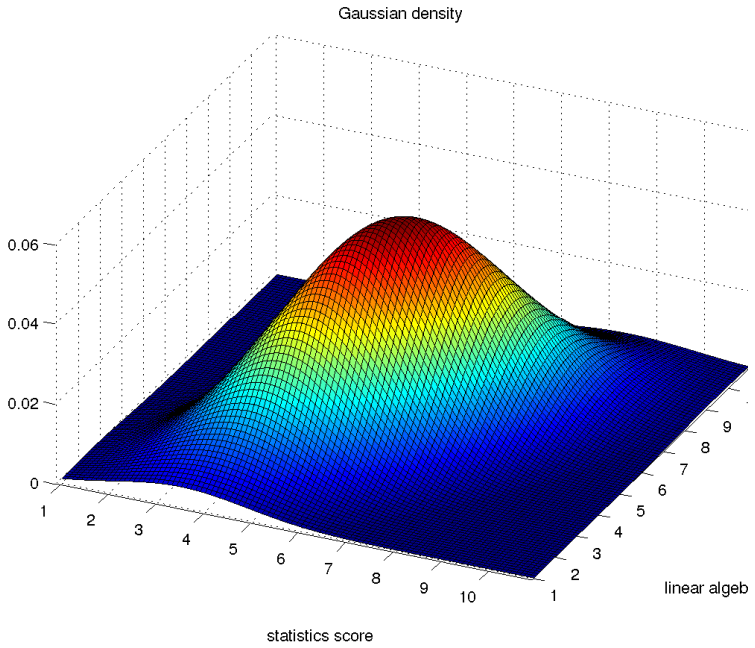
$$\frac{\partial l}{\partial \mu} = \frac{1}{\sigma^2}\sum_{i=1}^{m}(x^i - \mu) = 0$$

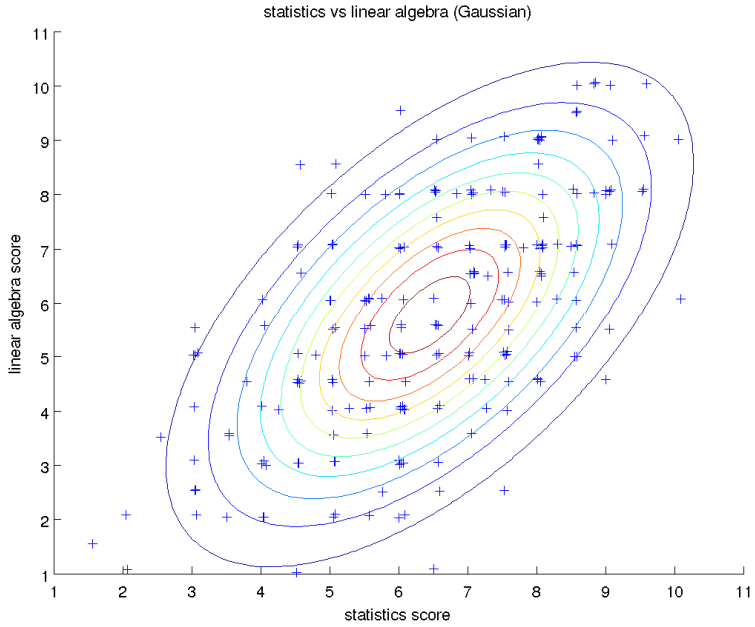
$$\Rightarrow \sum_{i}^{m} x^i = m\mu \Rightarrow \mu = \frac{1}{m}\sum_{i=1}^{m} x^i$$

$$\frac{\partial l}{\partial \sigma^2} = -\frac{m}{2\sigma^2} + \frac{1}{2\sigma^4}\sum_{i}^{m}\left(x^i - \mu\right)^2 = 0$$

$$\Rightarrow \sum_{i}^{m}\left(x^i - \mu\right)^2 = m\sigma^2 \Rightarrow \frac{1}{m}\sum_{i=1}^{m}\left(x^i - \mu\right)^2$$

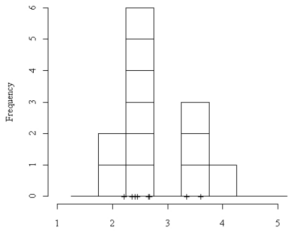
Density example





1-D Histogram

- One the simplest nonparametric density estimator
- Given m iid samples $\mathcal{D} = \{x^1, x^2, \dots x^m\}, x^i \in [0,1)$



- Split $[0,1)$ into n bins

$$B_1 = \left[0, \frac{1}{n}\right), B_2 = \left[\frac{1}{n}, \frac{2}{n}\right), \dots B_n = \left[\frac{n-1}{n}, 1\right)$$

- Count the number of points, c_1 within B_1, c_2 within B_2…
- For a new test point x

$$p(x) = \sum_{j=1}^{n} \frac{nc_j}{m} I(x \in B_j)$$

So this multiplication by n is a little bit mysterious but
I can tell you this is because we want to normalize it to one.
So if I perform an integration of the p(x) from zero to 1,
I want this integral of the p(x) to be 1, so that it's a PDF,
it's a probability density function.
So this n factor here is essentially due to the fact that each of the bin is
size m over and n.
So it's gonna compensate this result and
give you the integrate of p(x) is going to be 1

Why is histogram valid?

- Requirement for density $p(x)$
- $p(x) \geq 0, \int_{\Omega} p(x)dx = 1$

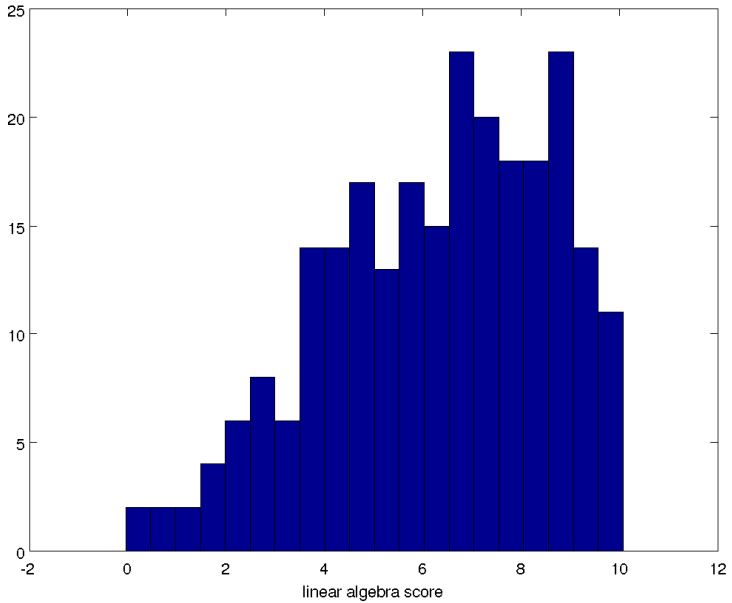
- For histogram,

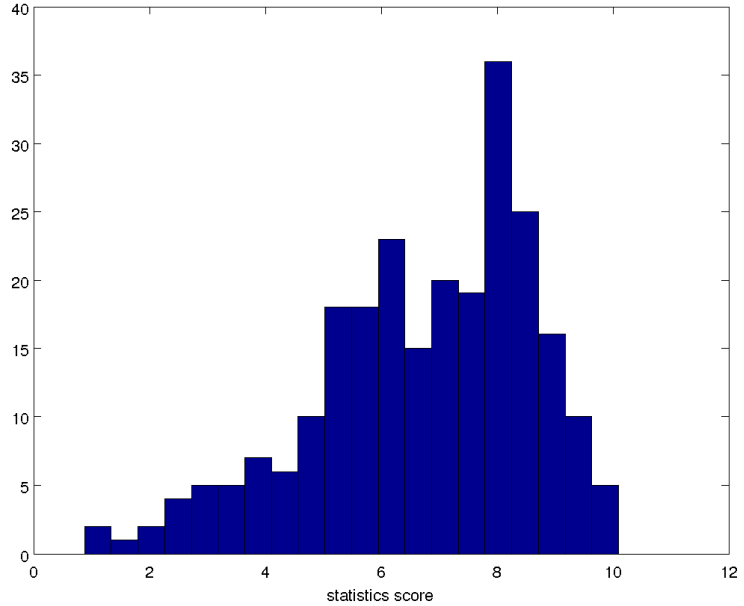
$$\int_{[0,1)} p(x)dx = \int_{[0,1)} \sum_{j=1}^{n} \frac{nc_j}{m} I\left(x \in B_j\right)dx$$

$$= \sum_{j=1}^{n} \int_{\left[\frac{j-1}{n}, \frac{j}{n}\right)} \frac{nc_j}{m} dx$$

$$= \sum_{j=1}^{n} \frac{c_j}{m} = 1$$

Example: background test scores





Higher dimensional histogram

- Given m iid samples $\mathcal{D} = \{x^1, x^2, \dots x^m\}, x^i \in [0,1)^d$
- Split $[0,1)^d$ evenly into n^d bins

$$B_1 = \left[0, \frac{1}{n}\right) \times \left[0, \frac{1}{n}\right) \dots \times \left[0, \frac{1}{n}\right),$$

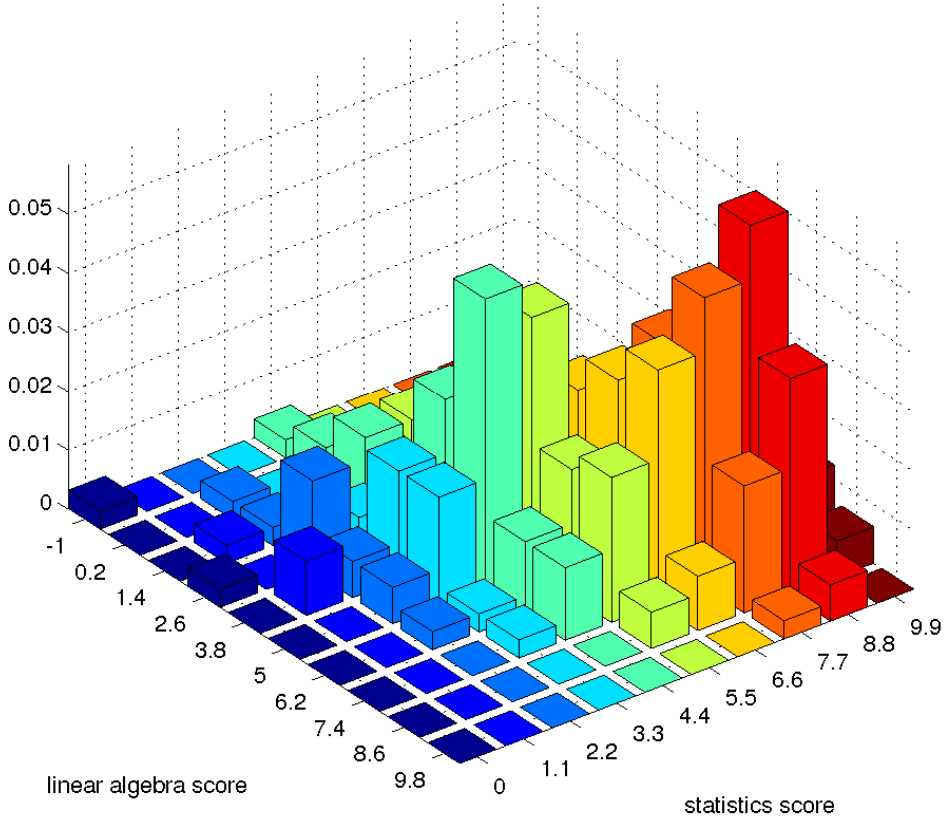
$$B_2 = \left[\frac{1}{n}, \frac{2}{n}\right) \times \left[0, \frac{1}{n}\right) \dots \times \left[0, \frac{1}{n}\right),$$

$$\dots$$

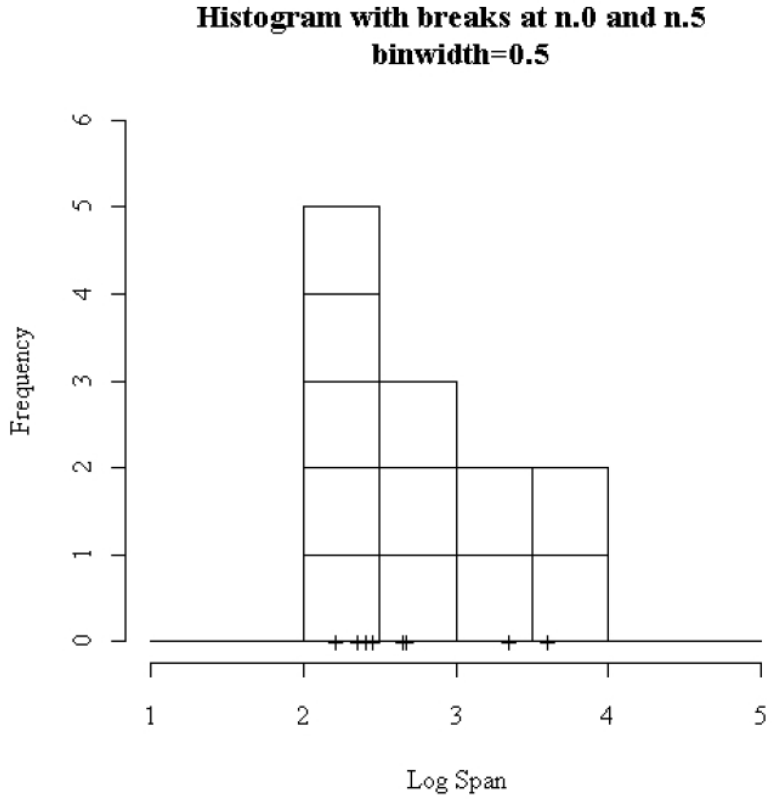
$$B_{n^d} = \left[\frac{n-1}{n}, 1\right) \times \left[\frac{n-1}{n}, 1\right) \dots \times \left[\frac{n-1}{n}, 1\right)$$

- Bin size is $h = \frac{1}{n}$

Class scores



Output depends on where you put the bins



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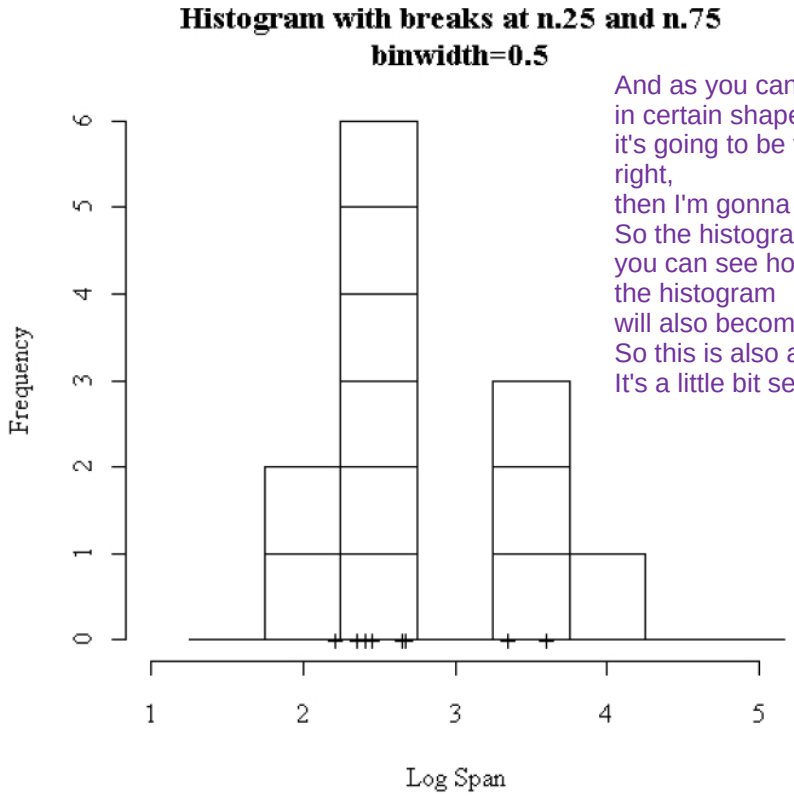
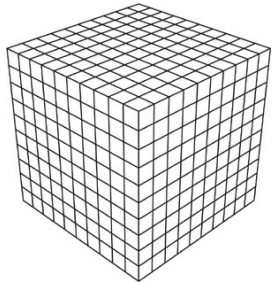


And as you can see in this example here, we come to bin two in certain shape and
it's going to be this, versus if I move my bins a little bit to the right,
then I'm gonna see a slightly different shape, okay?
So the histogram will in the end be sensitive to how the,
you can see how if I shifted my bins a little bit then the shape of the histogram
will also become different.
So this is also a problem with constructing the histogram.
It's a little bit sensitive to how you choose your bins.

Computation and statistical considerations

- Problem I: too many bin! Not good for high dimensional data
  - If n^d is larger than m, most bins are empty
  - Eg. $n = 10, d = 6$, need ~1 million data points



- Problem II: statistically histogram is not the best
  - Integrated risk:

$$r(\hat{p}, p) \coloneqq \int_R \mathbb{E}_X \left[\left(\hat{p}(x) - p(x) \right)^2 \right] dx$$

  - Histogram (with bin size $h \sim m^{-1/3}$)

$$r(\hat{p}, p) \sim \frac{C}{m^{2/3}}$$

  - Kernel density estimator (with bandwidth $h \sim m^{-1/5}$)

$$r(\hat{p}, p) \sim \frac{C}{m^{4/5}}$$

  - Difference even bigger for higher dimensional data

So this means that the histogram seems to have a lot of issue.
And it needs a lot of data to have a consistent estimator and statistically is not the best.
And so that's why people think about something better,
which is based on Kernel density estimator.

KDE here is going to be a lot smaller than the risk of the histogram.
So KDE is going to be better than the histogram in the sense

Kernel density estimation

It's not going to be sensitive to the choice of the bins because we don't have to decide the bins.
And also, the requirement to have number of the examples for Kernel density estimation is going to be a lot smaller.

- Kernel density estimator

$$p(x) = \frac{1}{m}\sum_{i}^{m}\frac{1}{h}K\left(\frac{x^i - x}{h}\right)$$

And question, how do I choose my k?
So here are some of the requirement.
First my k has to be a non negative because my p(x) has to be non negative.
And k will integrate to 1.
And another thing is the mean of my Kernel is 0 so
it's going to be somehow symmetrical.
And then I want the second order variance to be less infinity, so it's not blowing.
One commonly used Kernel, is going to be the Gaussian kernel.
So it's now very simple, it's like centered at zero and
then decays as u becomes large exponentially fast

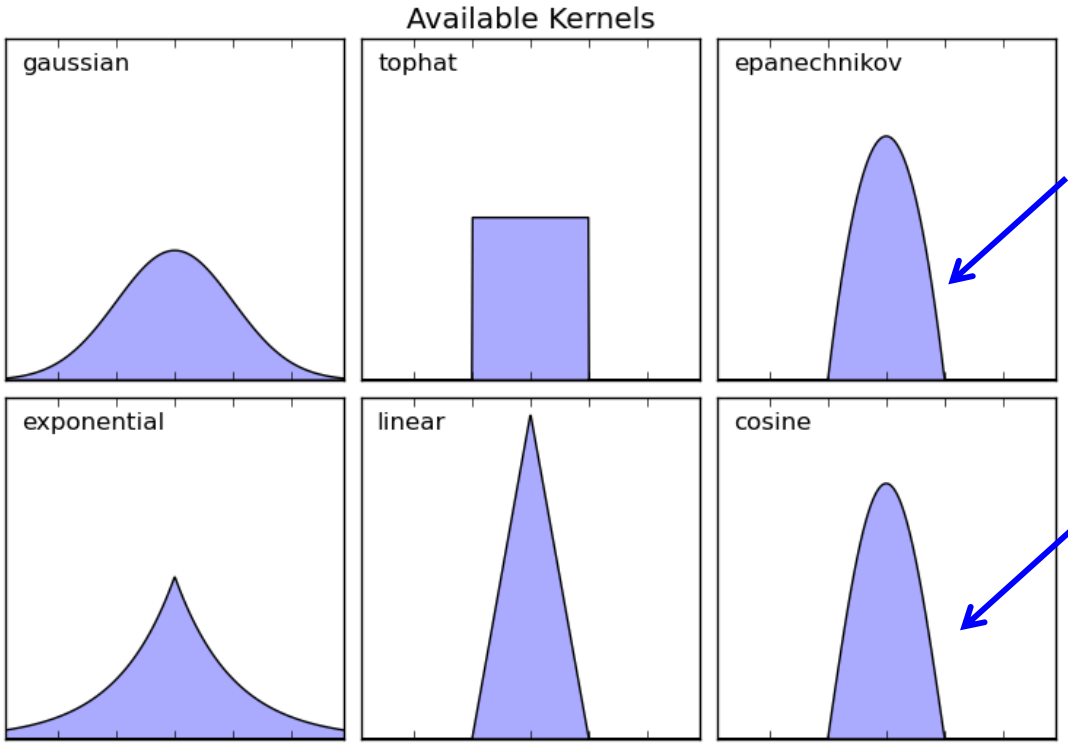
- Smoothing kernel function
  - $K(u) \geq 0,$
  - $\int K(u)du = 1,$
  - $\int uK(u) = 0,$
  - $\int u^2K(u)du \leq \infty$

So you measure the distance of x from each of data points and then you scale it by the h.
You can see now that h is not really the size of the bin because there is no bin.
But this h is like the scaling factor that measures how the influence of the highest point from the current xd case over distance.
So this h contains the sticking factor.
And then wrist 1 times 1 over h and then you sum this together for all the sample points.

- An example: Gaussian kernel $K(u) = \frac{1}{\sqrt{2\pi}}e^{-u^2/2}$

Smoothing kernel functions

- An example: Gaussian kernel $K(u) = \frac{1}{\sqrt{2\pi}} e^{-u^2/2}$

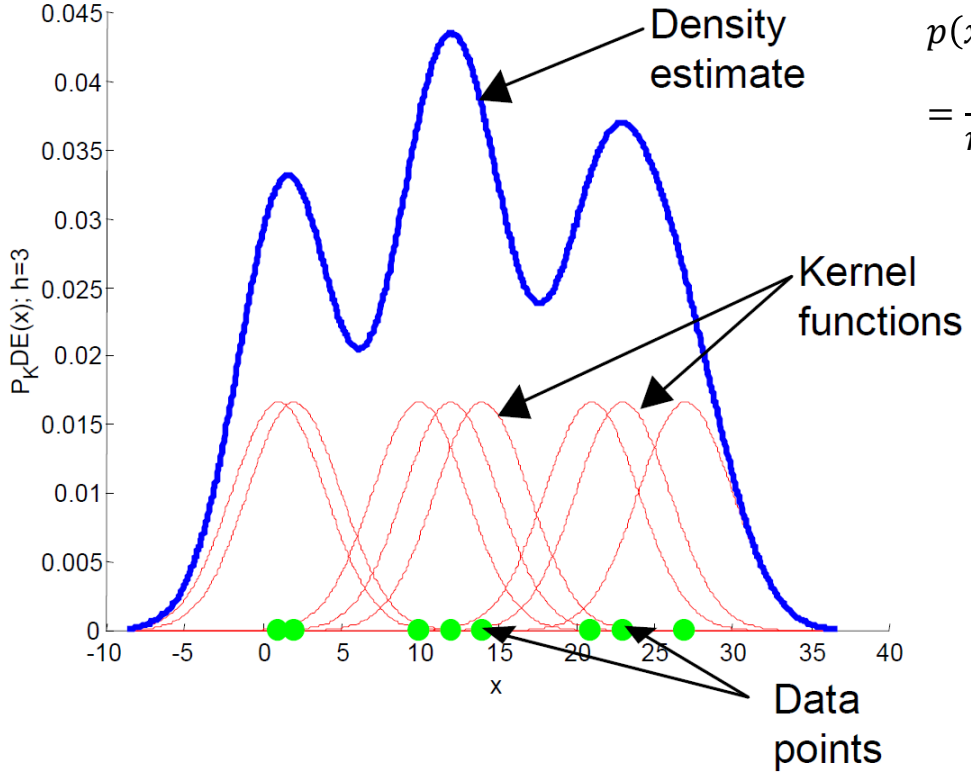


$$K(u) = \frac{3}{4}(1-u^2)I(|u| \leq 1)$$

$$K(u) = \frac{\pi}{4}\cos\left(\frac{\pi}{2}u\right)I(|u| \leq 1)$$

And these are all pretty commonly used of the kernel especially the Gaussian kernel and the cosine kernels.

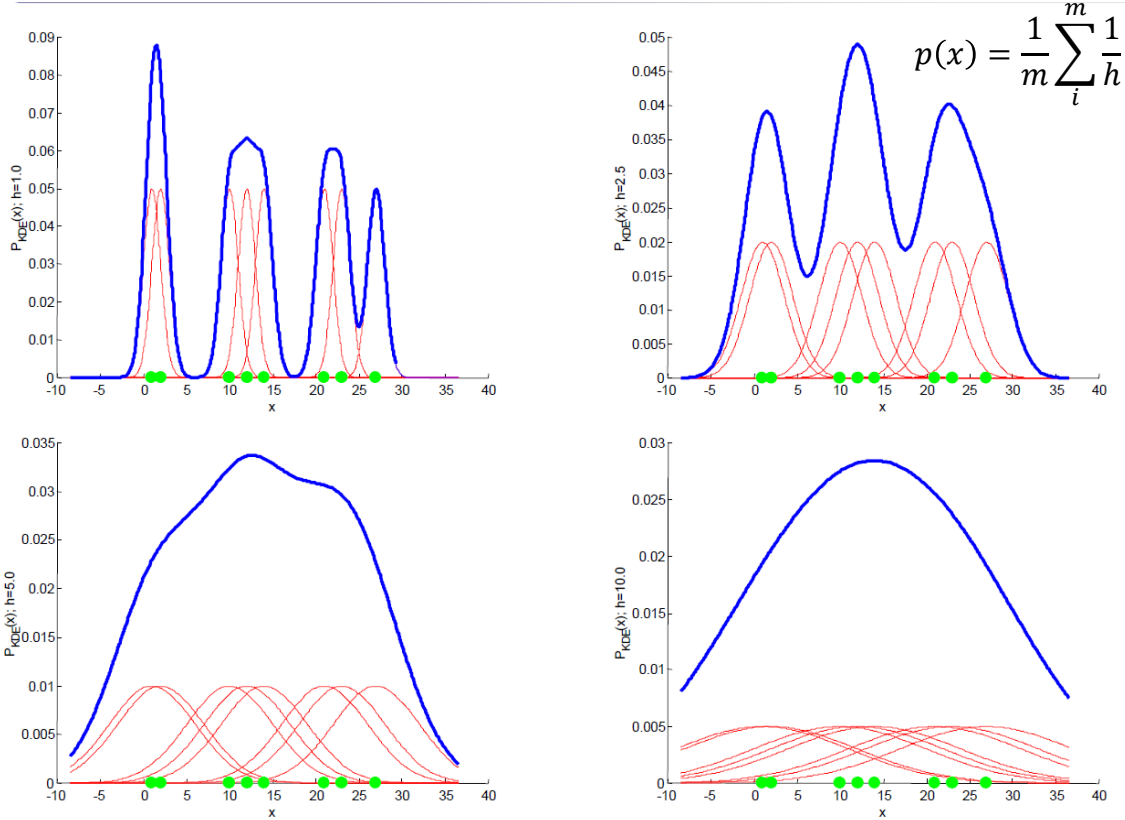
Example



$$p(x) = \frac{1}{m}\sum_{i}^{m}\frac{1}{h}K\left(\frac{x^i - x}{h}\right)$$

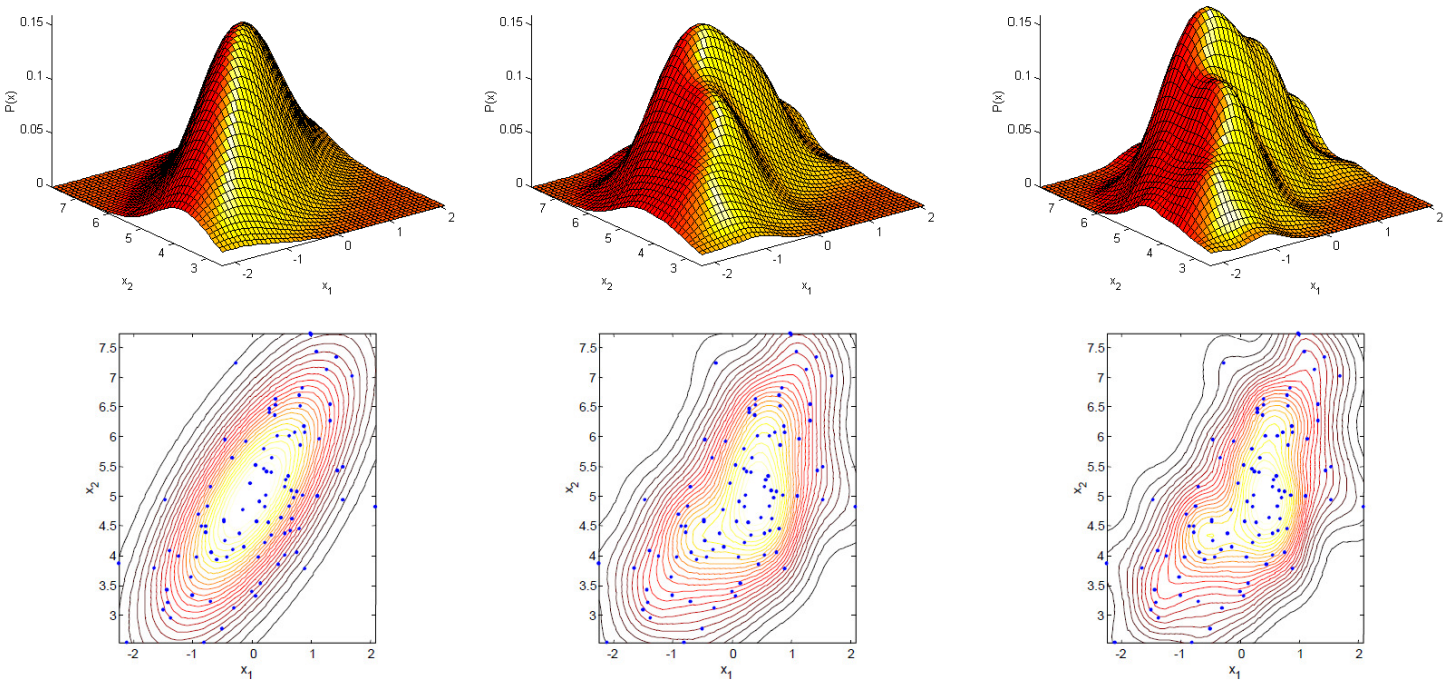
Effect of the kernel bandwidth h

$$p(x) = \frac{1}{m}\sum_{i}^{m}\frac{1}{h}K\left(\frac{x^i - x}{h}\right)$$



So you want to find an effective kernel with.
That is not too large or not to small.

Two-dimensional example



So, here's where the two dimensions example you can see when I choose my kernel there was to be very large versus very small.
When it's very small I have very noisy result.
When it's large, you have very smooth sound result that you started losing some features of your data distribution.
And in general, how dimensions may age, usually it's a, you can tune as age and to have a desired result.

Wine data example

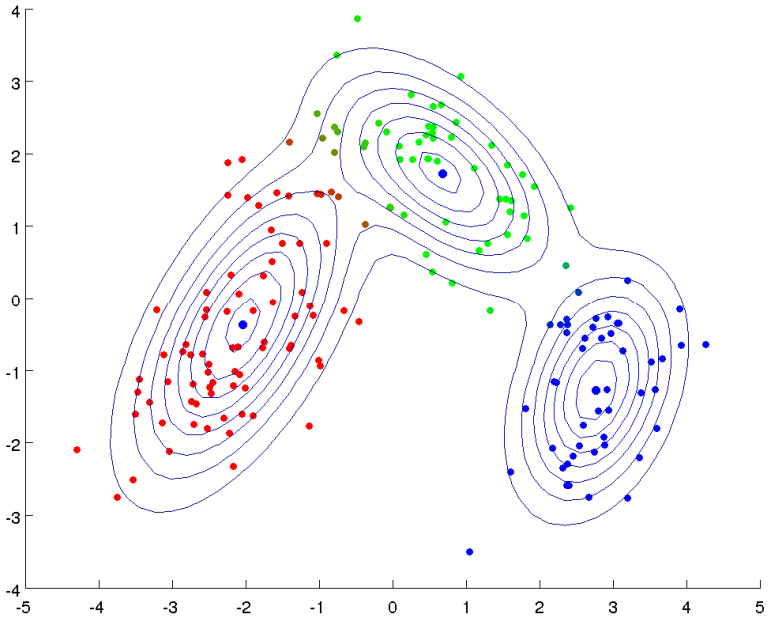
- The wine data set was introduced by Forina et al. (1986).
- It originally included the results of 27 chemical measurements on 178 wines made in the same region in Italy but derived from three different cultivars: Barolo, Grignolino and Barbera.
- We extract the first two principle components of the data, and aim to fit a density distribution

Wine data set (http://archive.ics.uci.edu/ml/datasets/Wine+Quality)

- These data are the results of a chemical analysis of wines grown in the same region in Italy but derived from three different cultivars. Feature include
  - 1) Alcohol
  - 2) Malic acid
  - 3) Ash
  - 4) Alcalinity of ash
  - 5) Magnesium
  - 6) Total phenols
  - 7) Flavanoids
  - 8) Nonflavanoid phenols
  - 9) Proanthocyanins
  - 10)Color intensity
  - 11)Hue
  - 12)OD280/OD315 of diluted wines
  - 13)Proline

Demo: test_wine.m

- Chemical analysis of wines grown in three different places
- Clear cluster structure, can we fit 3 Gaussians?



What is the best kernel bandwidth?

- Silverman's rule of thumb: If using the Gaussian kernel, a good choice for is

$$h \approx 1.06\,\hat{\sigma}\,m^{-1/5}$$

where is the standard deviation of the samples

- A better but more computational intensive approach:
  - Randomly split the data into two sets
  - Obtain a kernel density estimate for the first
  - Measure the likelihood of the second set
  - Repeat over many random splits and average

Parametric vs. nonparametric

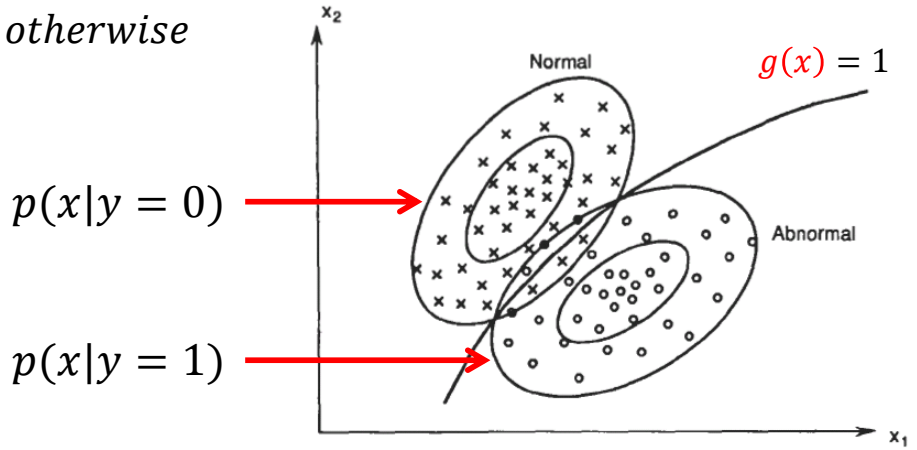
- Data $x \in R^d$ with fixed dimension d
- Given m training data points $\{x^1, x^2 \ldots, x^m\}$
- Partition n bin in each dimension

Aspects	Gaussian	Histogram	KDE
Flexible	Not	Yes	Yes
Assumption	Strong	Not	Not
Parameter number	Fixed	Increase with n	Increase with m
Memory requirement	$d + d^2$	n^d	md
Training computation	Closed form	Binning and Counting	nothing
Test computation	Plug in formula	Find the bin	Evaluate m functions
Statistical guarantee	only Gaussian case	Arbitrary (worse)	Arbitrary (better)

Classification using density estimation

- Simple binary classifier for input $x^i \in R^d$ and label $y^i \in \{0,1\}$
  - Step I: use label to estimate $p(y=0)$ and $p(y=1)$
  - Step II: divide your data according to the value of y, and estimate
    $$p(x|y=0) \text{ and } p(x|y=1)$$
  - Step III: Classify a new test point x as

$$\begin{cases} 1, & g(x) := \dfrac{p(x|y=1)p(y=1)}{p(x|y=0)p(y=0)} > 1 \\ 0, & otherwise \end{cases}$$




SUMMARY