An Introduction to Machine Learning

L2: Instance Based Estimation

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Overview

L1: Machine learning and probability theory
Introduction to pattern recognition, classification, regression, novelty detection, probability theory, Bayes rule, inference

L2: Density estimation and Parzen windows
Nearest Neighbor, Kernels density estimation, Silverman's rule, Watson Nadaraya estimator, crossvalidation

L3: Perceptron and Kernels
Hebb's rule, perceptron algorithm, convergence, feature maps, kernels

L4: Support Vector estimation
Geometrical view, dual problem, convex optimization, kernels

L5: Support Vector estimation
Regression, Quantile regression, Novelty detection, ν-trick

L6: Structured Estimation
Sequence annotation, web page ranking, path planning, implementation and optimization

L2 Instance Based Methods

Nearest Neighbor Rules

Density estimation

- empirical frequency, bin counting
- priors and Laplace rule

Parzen windows

- Smoothing out the estimates
- Examples

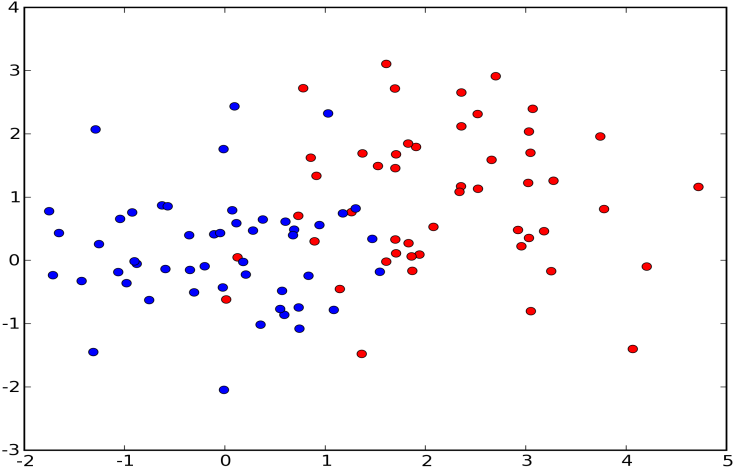
Adjusting parameters

- Cross validation
- Silverman's rule

Classification and regression with Parzen windows

- Watson-Nadaraya estimator

Binary Classification



Nearest Neighbor Rule

Goal

Given some data x_i, want to classify using class label y_i.

Solution

Use the label of the nearest neighbor.

Modified Solution (classification)

Use the label of the majority of the k nearest neighbors.

Modified Solution (regression)

Use the value of the average of the k nearest neighbors.

Key Benefits

- Basic algorithm is **very simple**.
- Can use arbitrary similarity measures
- Will eventually converge to the best possible result.

Problems

- Slow and inefficient when we have lots of data.
- Not very smooth estimates.

Python Pseudocode

Nearest Neighbor Classifier

```
from pylab import *
from numpy import *

...  load data ...

xnorm = sum(x**2)
xtestnorm = sum(xtest**2)

dists = (-2.0*dot(x.transpose(), xtest) + xtestnorm).transpose() + xnorm

labelindex = dists.argmin(axis=1)
```

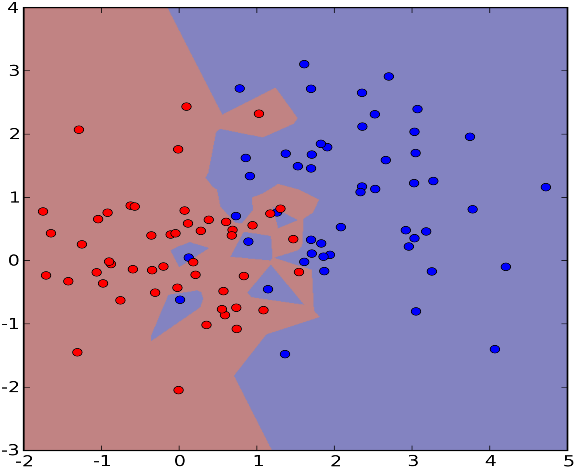
k-Nearest Neighbor Classifier

```
sortargs = dists.argsort(axis=1)
k = 7
ytest = sign(mean(y[sortargs[:,0:k]], axis=1))
```

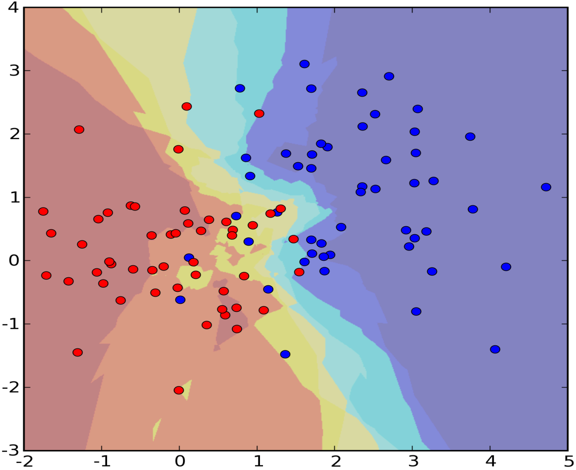
Nearest Neighbor Regression

just drop `sign(...)`

Nearest Neighbor



7 Nearest Neighbors



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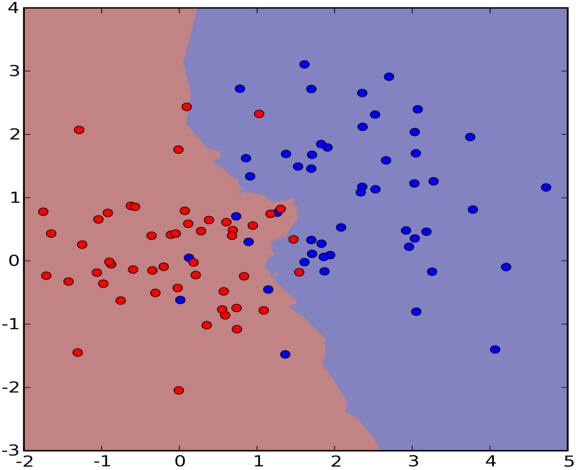
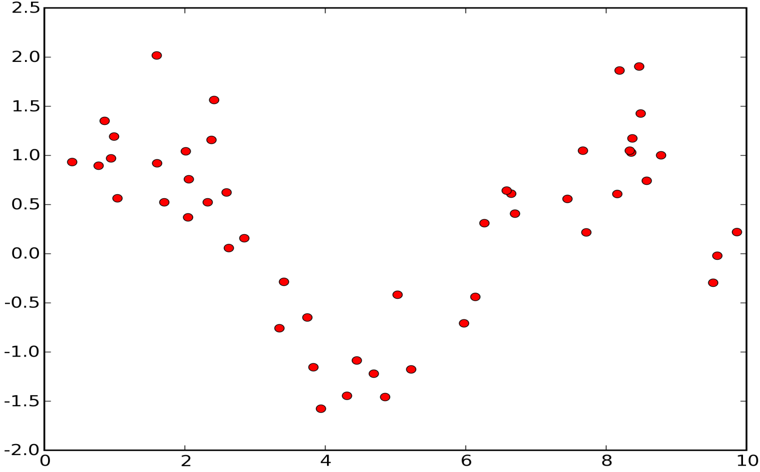
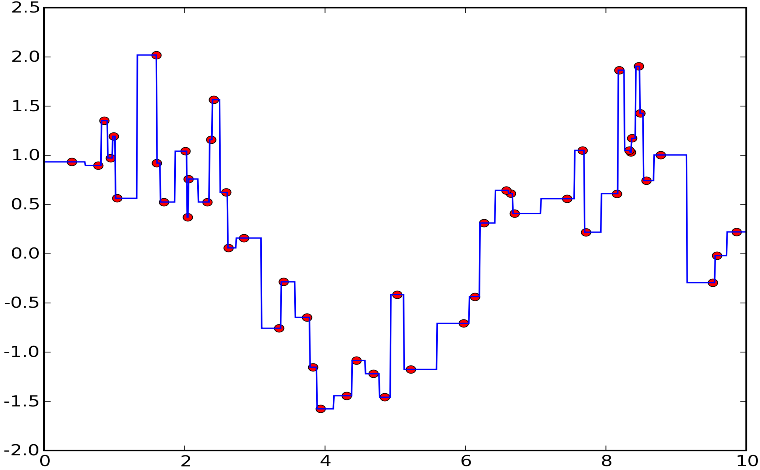


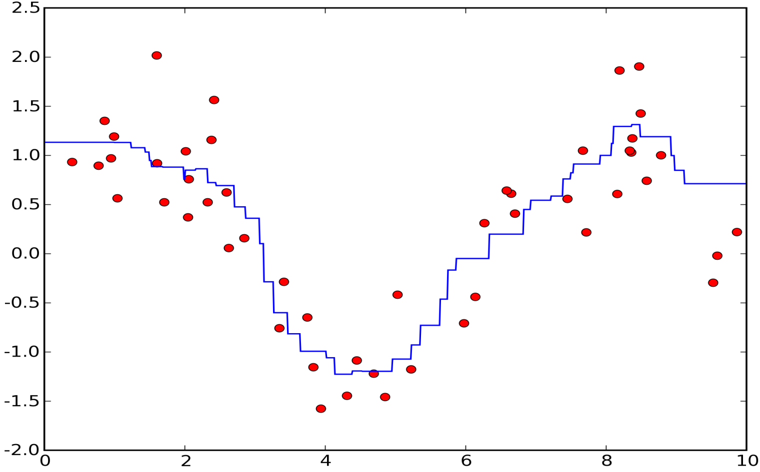
Regression Problem



Nearest Neighbor Regression



7 Nearest Neighbors Regression



Mini Summary

Nearest Neighbor Rule

Predict same label as nearest neighbor

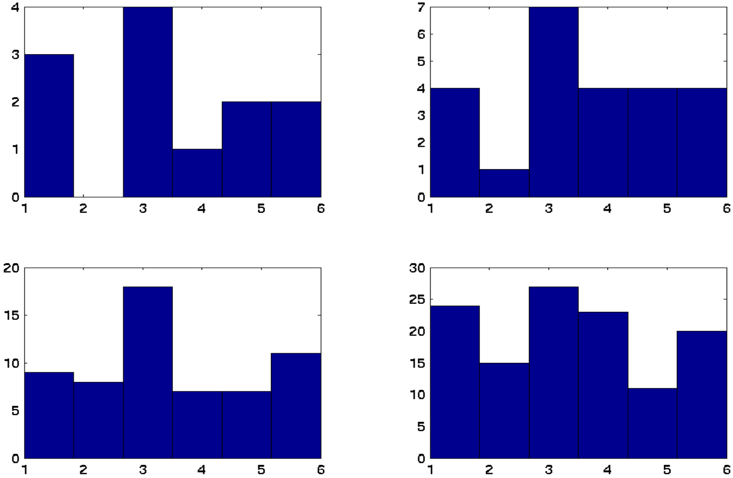
***k*-Nearest Neighbor Rule**

Average estimates over k neighbors

Details

- Easy to implement
- No training required
- Slow if lots of training data
- Not so great performance

Tossing a dice (again)



Priors to the Rescue

Big Problem

Only sampling *many times* gets the parameters right.

Rule of Thumb

We need at least 10-20 times as many observations.

Conjugate Priors

Often we know what we should expect. Using a conjugate prior helps. We **insert fake additional data** which we assume that it comes from the prior.

Conjugate Prior for Discrete Distributions

- Assume we see u_i additional observations of class i.

$$\pi_i = \frac{\#\text{occurrences of } i + u_i}{\#\text{trials} + \sum_j u_j}.$$

- Assuming that the dice is even, set $u_i = m_0$ for all $1 \leq i \leq 6$. For $u_i = 1$ this is the **Laplace Rule**.

Example: Dice

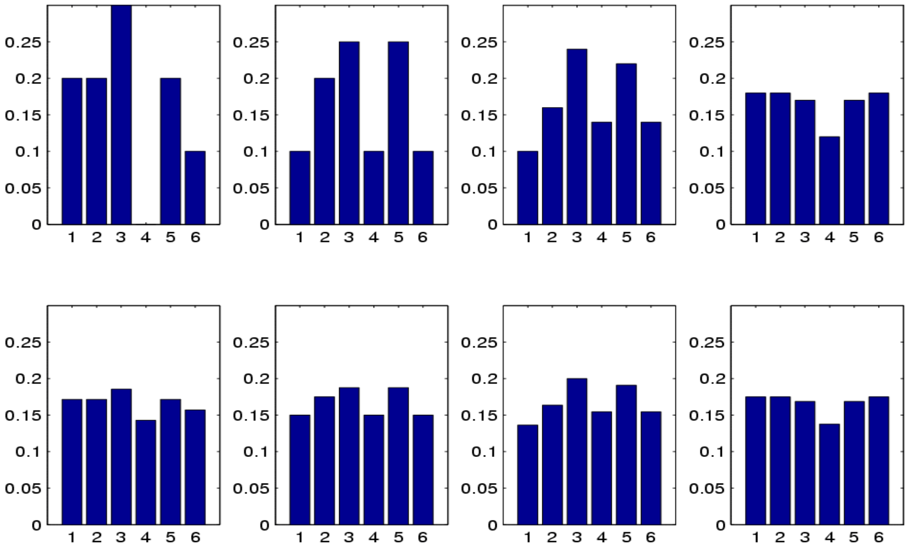
20 tosses of a dice

Outcome	1	2	3	4	5	6
Counts	3	6	2	1	4	4
MLE	0.15	0.30	0.10	0.05	0.20	0.20
MAP ($m_0 = 6$)	0.25	0.27	0.12	0.08	0.19	0.19
MAP ($m_0 = 100$)	0.16	0.19	0.16	0.15	0.17	0.17

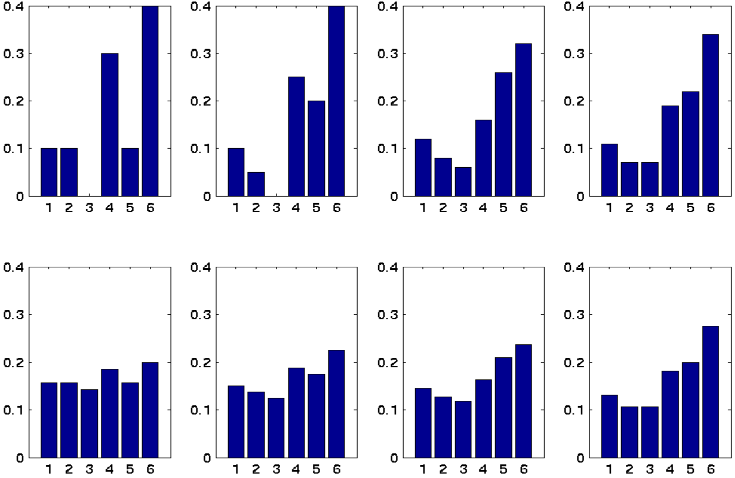
Consequences

- Stronger prior brings the estimate closer to uniform distribution.
- More robust against outliers
- But: Need more data to detect deviations from prior

Correct dice



Tainted dice



Mini Summary

Maximum Likelihood Solution

- Count number of observations per event
- Set probability to empirical frequency of occurrence.

Maximum a Posteriori Solution

- We have a good guess about solution
- Use conjugate prior
- Corresponds to inventing extra data
- Set probability to take additional observations into account

Extension

- Works also for other estimates, such as means and covariance matrices.

Density Estimation

Data

Continuous valued random variables.

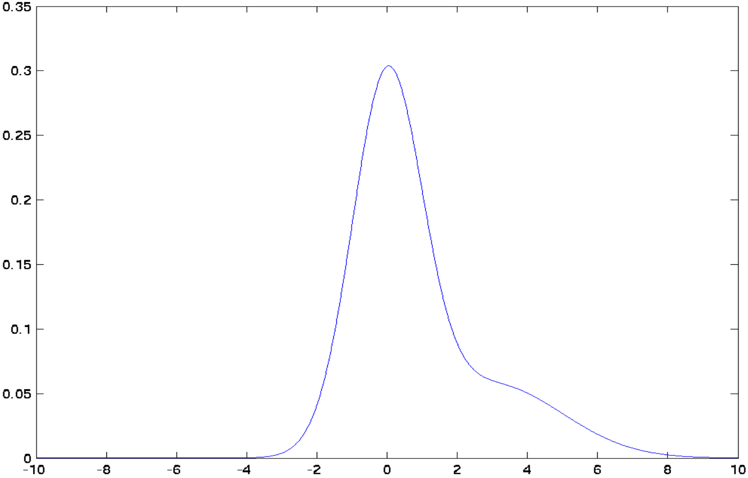
Naive Solution

Apply the bin-counting strategy to the continuum. That is, we discretize the domain into bins.

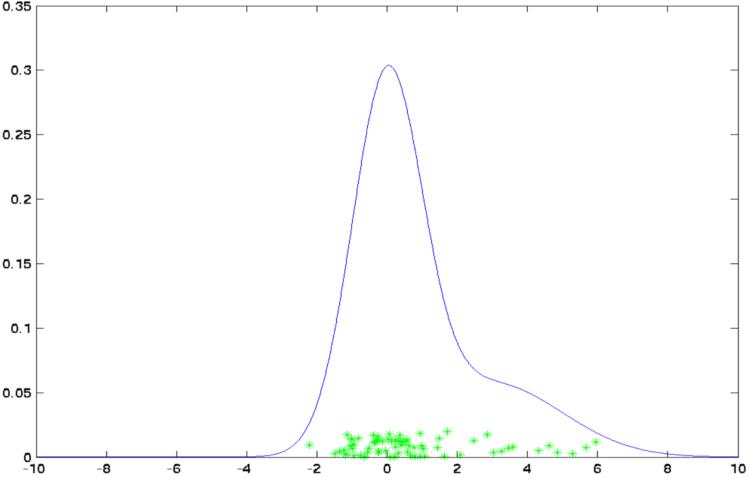
Problems

- We need lots of data to fill the bins
- In more than one dimension the number of bins grows exponentially:
- Assume 10 bins per dimension, so we have 10 in $\mathbb{R}^1$
- 100 bins in $\mathbb{R}^2$
- 10^{10} bins (10 billion bins) in $\mathbb{R}^{10}$ …

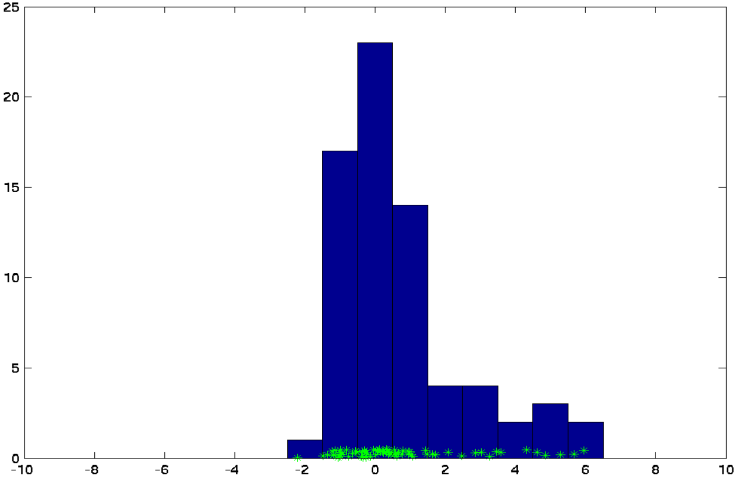
Mixture Density



Sampling from $p(x)$



Bin counting



Parzen Windows

Naive approach

Use the empirical density

$$p_{\text{emp}}(x) = \frac{1}{m} \sum_{i=1}^{m} \delta(x, x_i).$$

which has a delta peak for every observation.

Problem

What happens when we see slightly different data?

Idea

Smear out p_{emp} by convolving it with a kernel $k(x, x')$. Here $k(x, x')$ satisfies

$$\int_{\mathcal{X}} k(x, x') dx' = 1 \text{ for all } x \in \mathcal{X}.$$

Parzen Windows

Estimation Formula

Smooth out p_{emp} by convolving it with a kernel $k(x, x')$.

$$p(x) = \frac{1}{m} \sum_{i=1}^{m} k(x_i, x)$$

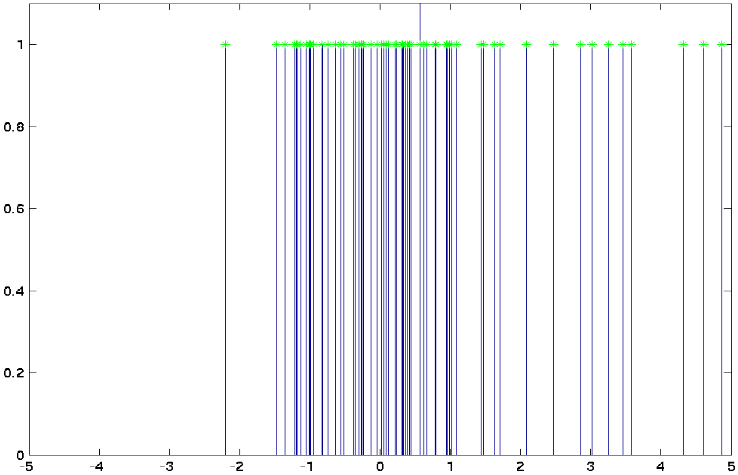
Adjusting the kernel width

- Range of data should be adjustable
- Use kernel function $k(x, x')$ which is a proper kernel.
- Scale kernel by radius r. This yields

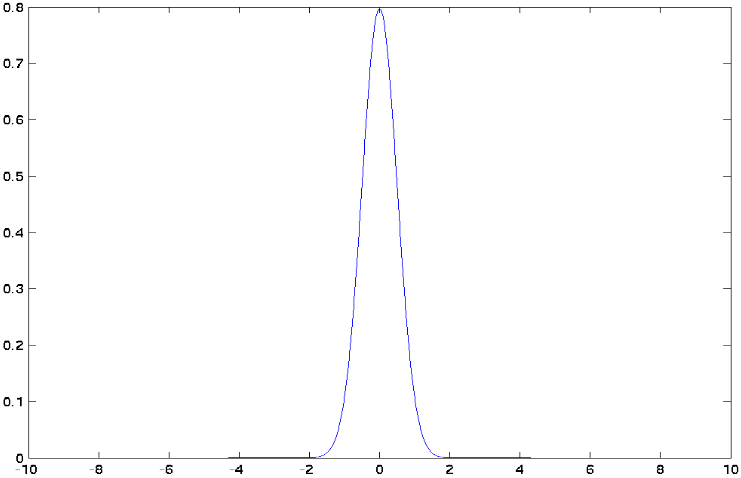
$$k_r(x, x') := r^n k(rx, rx')$$

Here n is the dimensionality of x.

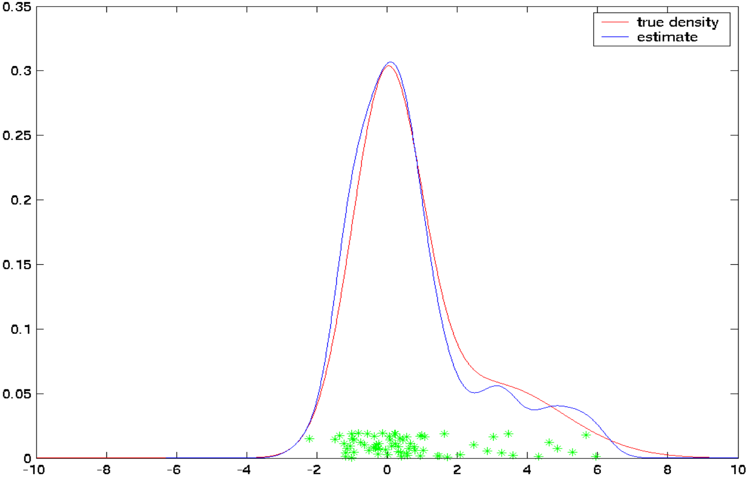
Discrete Density Estimate



Smoothing Function



Density Estimate



Examples of Kernels

Gaussian Kernel

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

Laplacian Kernel

$$k(x, x') = \lambda^n 2^{-n} \exp\left(-\lambda\|x - x'\|_1\right)$$

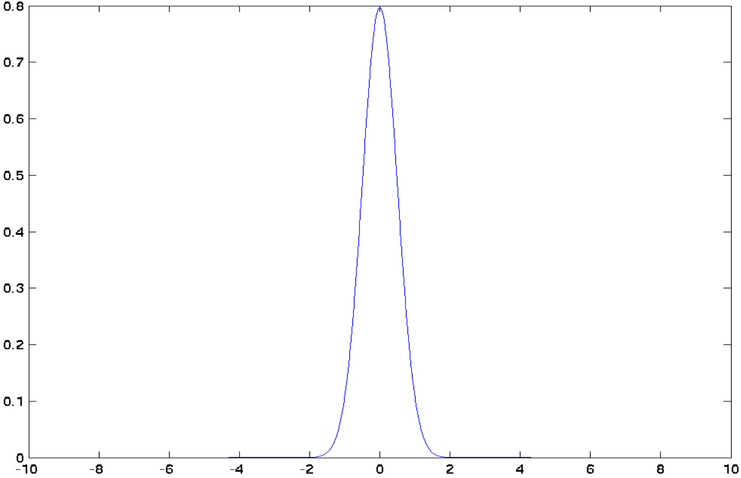
Indicator Kernel

$$k(x, x') = 1_{[-0.5,0.5]}(x - x')$$

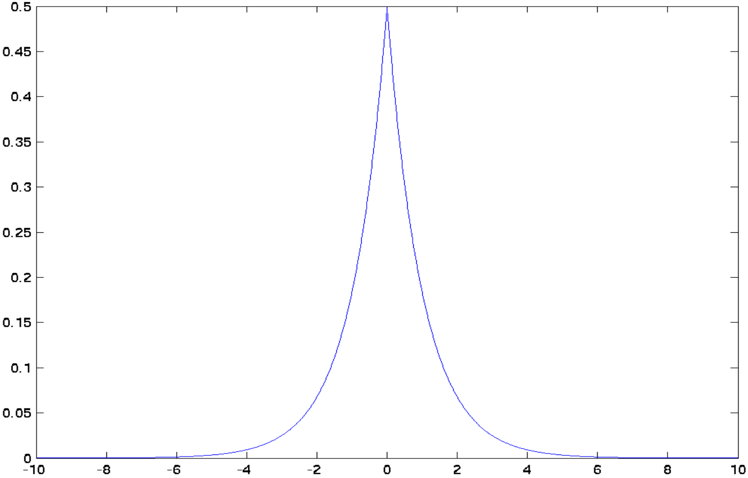
Important Issue

Width of the kernel is usually much more important than **type**.

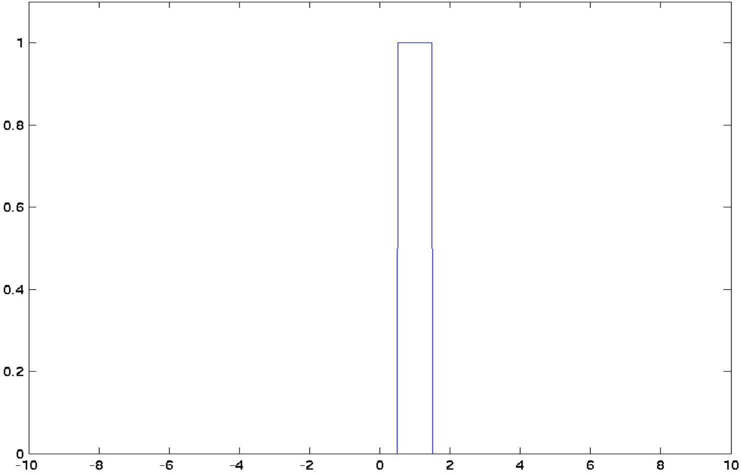
Gaussian Kernel



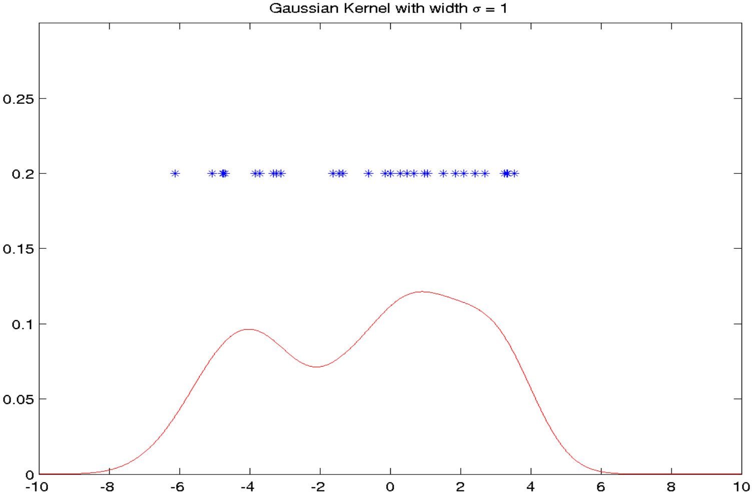
Laplacian Kernel



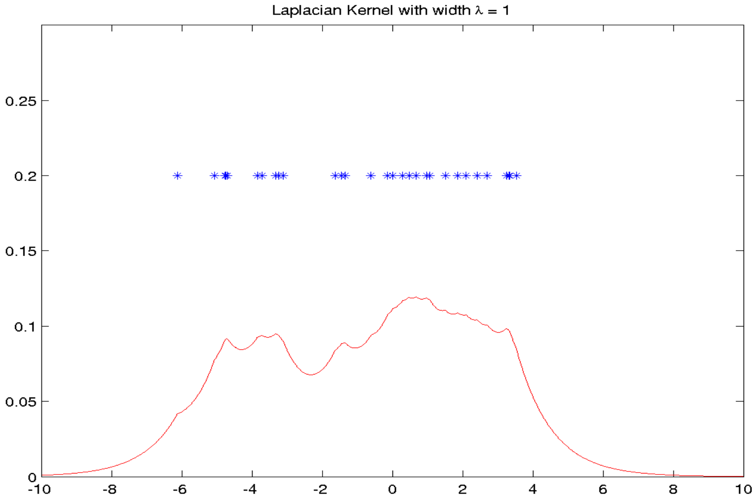
Indicator Kernel



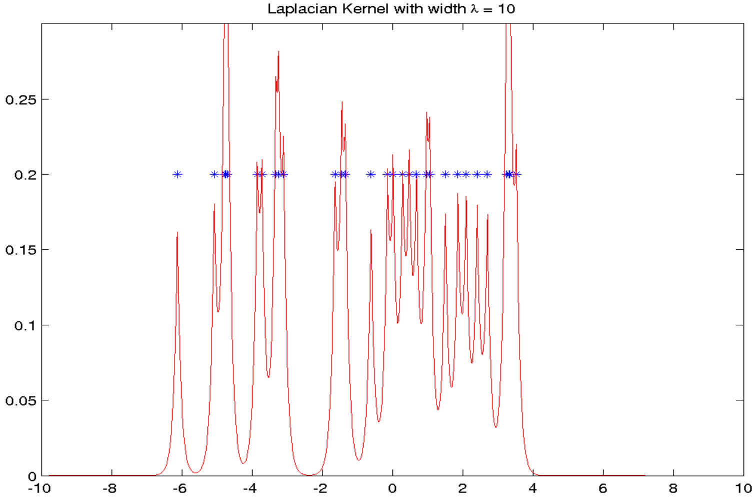
Gaussian Kernel



Laplacian Kernel



Laplacian Kernel



Selecting the Kernel Width

Goal

We need a method for adjusting the kernel width.

Problem

The likelihood keeps on increasing as we narrow the kernels.

Reason

The likelihood estimate we see is distorted (we are being overly optimistic through optimizing the parameters).

Possible Solution

Check the performance of the density estimate on an unseen part of the data. This can be done e.g. by

- Leave-one-out crossvalidation
- Ten-fold crossvalidation

Expected log-likelihood

What we really want

- A parameter such that in expectation the likelihood of the data is maximized

$$p_r(X) = \prod_{i=1}^{m} p_r(x_i)$$

or equivalently $$\frac{1}{m} \log p_r(X) = \frac{1}{m} \sum_{i=1}^{m} \log p_r(x_i).$$

- However, if we optimize r for the seen data, we will always overestimate the likelihood.

Solution: Crossvalidation

- Test on unseen data
- Remove a fraction of data from X, say X', estimate using $X \backslash X'$ and test on X'.

Crossvalidation Details

Basic Idea

Compute $p(X'|\theta(X \backslash X'))$ for various subsets of X and average over the corresponding log-likelihoods.

Practical Implementation

Generate subsets $X_i \subset X$ and compute the log-likelihood estimate

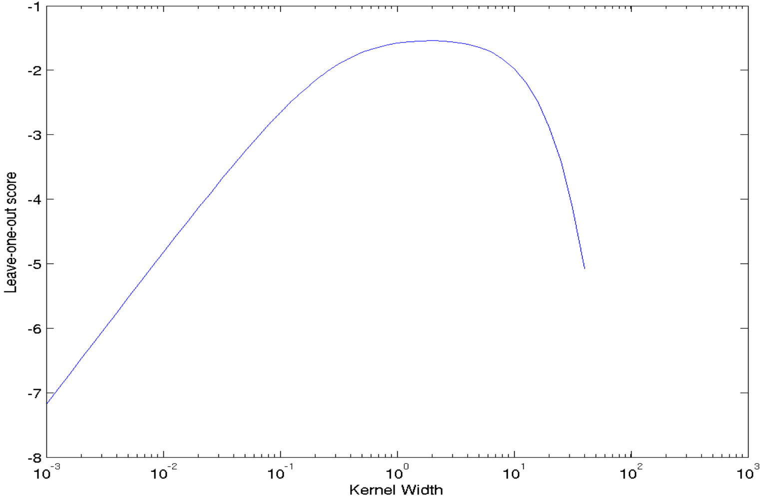
$$\frac{1}{n}\sum_{i}^{n}\frac{1}{|X_i|}\log p(X_i|\theta(X|\backslash X_i))$$

Pick the parameter which maximizes the above estimate.

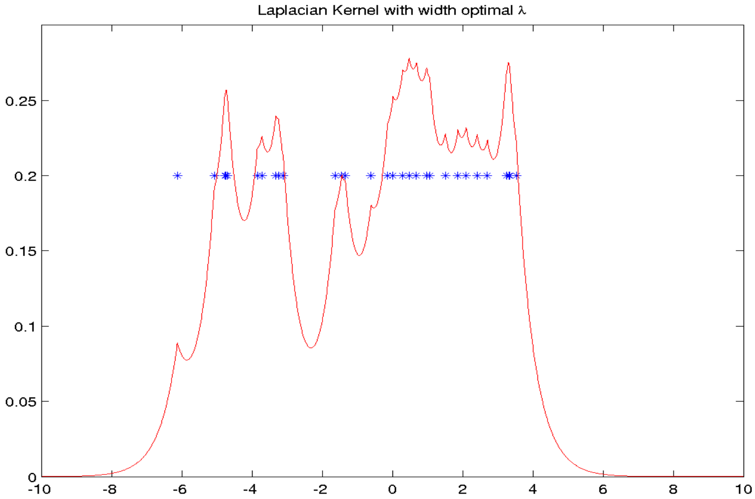
Special Case: Leave-one-out Crossvalidation

$$p_{X\backslash x_i}(x_i) = \frac{m}{m-1}p_X(x_i) - \frac{1}{m-1}k(x_i, x_i)$$

Cross Validation



Best Fit ($\lambda = 1.9$)



Mini Summary

Discrete Density

- Bin counting
- Problems for continuous variables
- Really big problems for variables in high dimensions (curse of dimensionality)

Parzen Windows

- Smooth out discrete density estimate.
- Smoothing kernel integrates to 1 (allows for similar observations to have some weight).
- Density estimate is average over kernel functions
- Scale kernel to accommodate spacing of data

Tuning it

- Cross validation
- Expected log-likelihood

Application: Novelty Detection

Goal

Find the least likely observations x_i from a dataset X. Alternatively, identify low-density regions, given X.

Idea

Perform density estimate $p_X(x)$ and declare all x_i with $p_X(x_i) < p_0$ as novel.

Algorithm

Simply compute $f(x_i) = \sum_j k(x_i, x_j)$ for all i and sort according to their magnitude.

Applications

Network Intrusion Detection

Detect whether someone is trying to hack the network, downloading tons of MP3s, or doing anything else *unusual* on the network.

Jet Engine Failure Detection

You can't destroy jet engines just to see *how* they fail.

Database Cleaning

We want to find out whether someone stored bogus information in a database (typos, etc.), mislabelled digits, ugly digits, bad photographs in an electronic album.

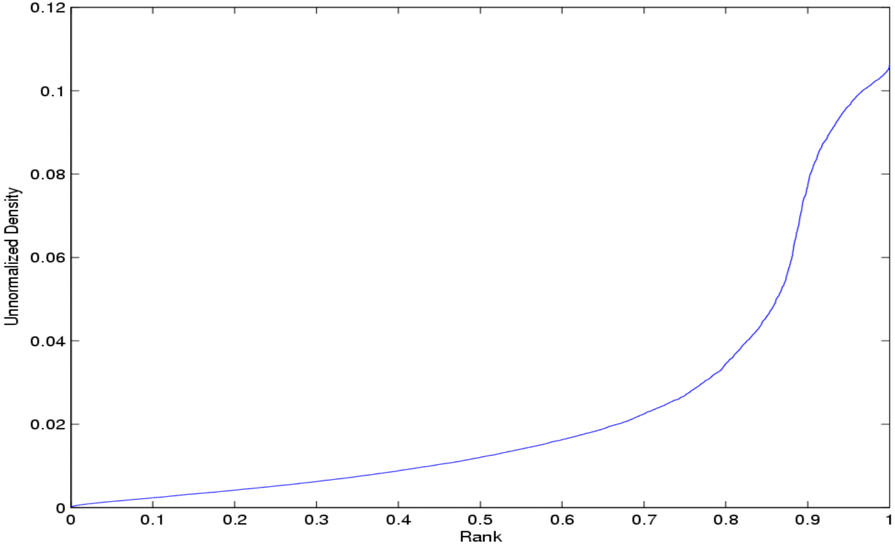
Fraud Detection

Credit Cards, Telephone Bills, Medical Records

Self calibrating alarm devices

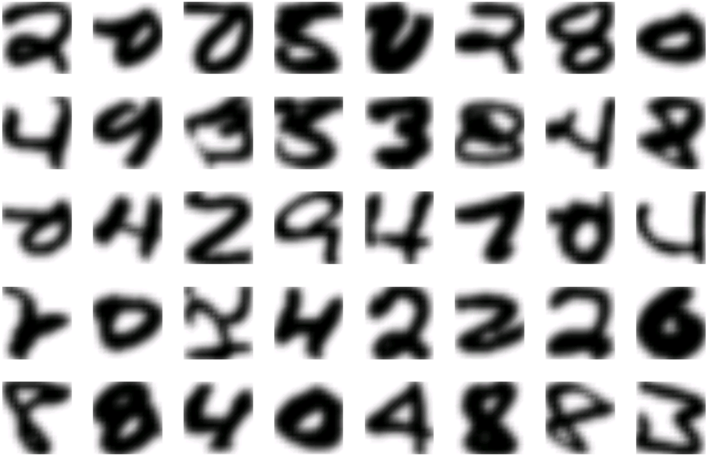
Car alarms (adjusts itself to where the car is parked), home alarm (furniture, temperature, windows, etc.)

Order Statistic of Densities



Typical Data

Outliers



Silverman's Automatic Adjustment

Problem

One 'width fits all' does not work well whenever we have regions of high and of low density.

Idea

Adjust width such that neighbors of a point are included in the kernel at a point. More specifically, adjust range h_i to yield

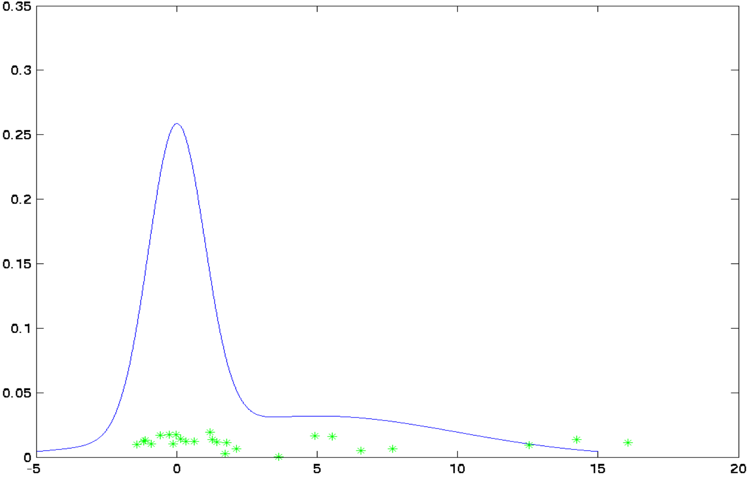
$$h_i = \frac{r}{k} \sum_{x_j \in \mathrm{NN}(x_i, k)} \|x_j - x_i\|$$

where $\mathrm{NN}(x_i, k)$ is the set of k nearest neighbors of x_i and r is typically chosen to be 0.5.

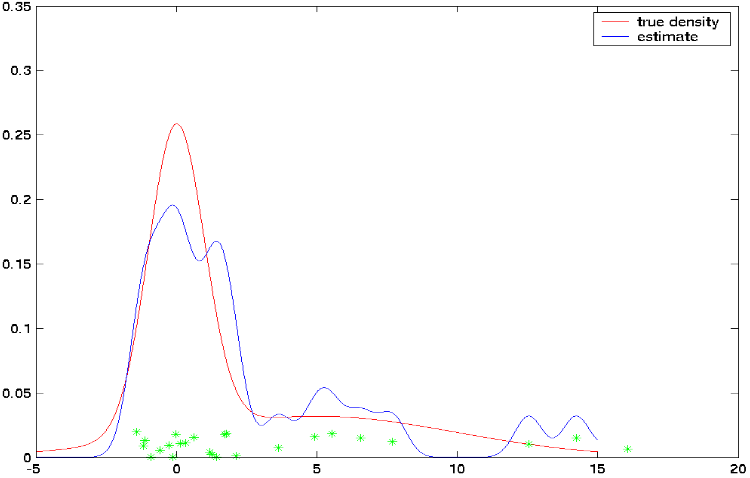
Result

State of the art density estimator, regression estimator and classifier.

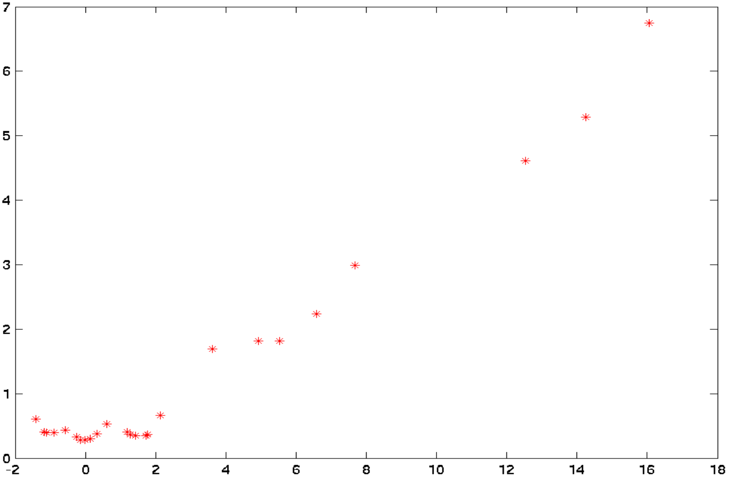
Sampling from $p(x)$



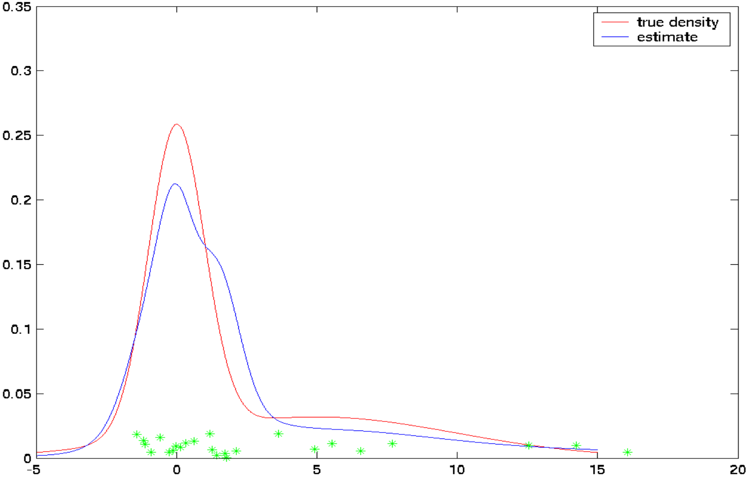
Uneven Scales



Neighborhood Scales



Adjusted Width



Watson-Nadaraya Estimator

Goal

Given pairs of observations (x_i, y_i) with $y_i \in \{\pm 1\}$ find estimator for conditional probability $\Pr(y|x)$.

Idea

Use definition $p(x, y) = p(y|x)p(x)$ and estimate both $p(x)$ and $p(x, y)$ using Parzen windows. Using Bayes rule this yields

$$\Pr(y = 1|x) = \frac{P(y = 1, x)}{P(x)} = \frac{m^{-1} \sum_{y_i = 1} k(x_i, x)}{m^{-1} \sum_i k(x_i, x)}$$

Bayes optimal decision

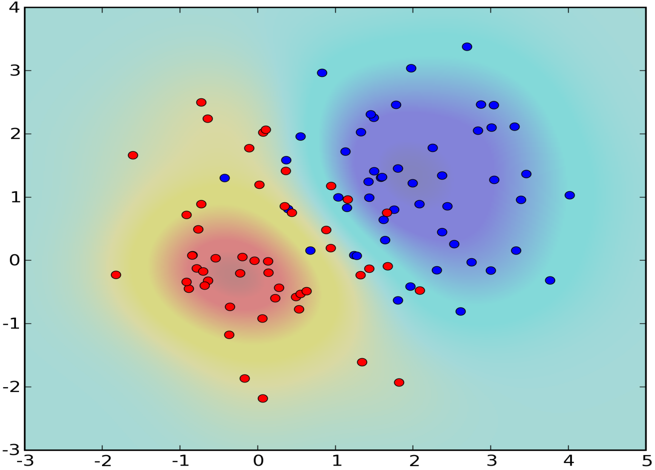
We want to classify $y = 1$ for $\Pr(y = 1|x) > 0.5$. This is equivalent to checking the sign of

$$\Pr(y = 1|x) - \Pr(y = -1|x) \propto \sum_i y_i k(x_i, x)$$

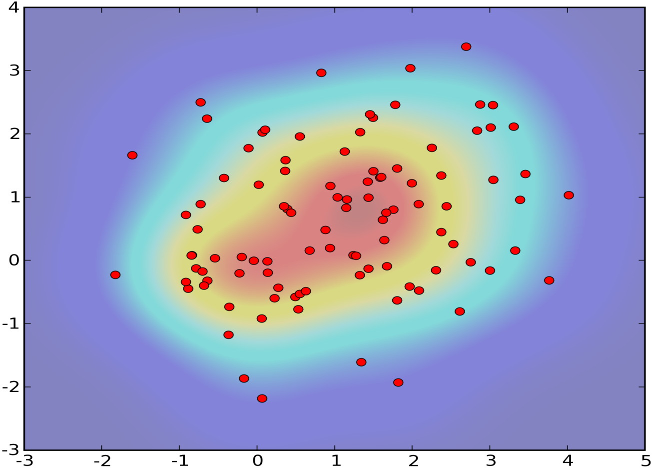
Python Pseudocode

```
# Kernel function
import elefant.kernels.vector
k = elefant.kernels.vector.CGaussKernel(1)

# Compute difference between densities
ytest = k.Expand(xtest, x, y)

# Compute density estimate (up to scalar)
density = k.Expand(xtest, x, ones(x.shape[0]))
```

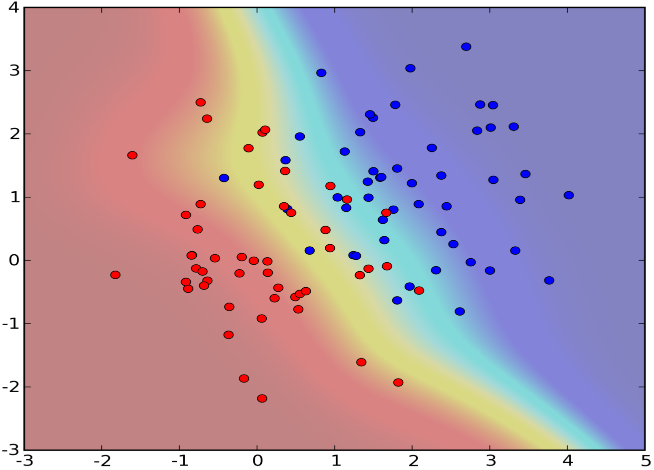
Parzen Windows Classifier



Parzen Windows Density Estimate



Parzen Windows Conditional



Watson Nadaraya Regression

Decision Boundary

Picking $y = 1$ or $y = -1$ depends on the sign of

$$\Pr(y = 1|x) - \Pr(y = -1|x) = \frac{\sum_i y_i k(x_i, x)}{\sum_i k(x_i, x)}$$

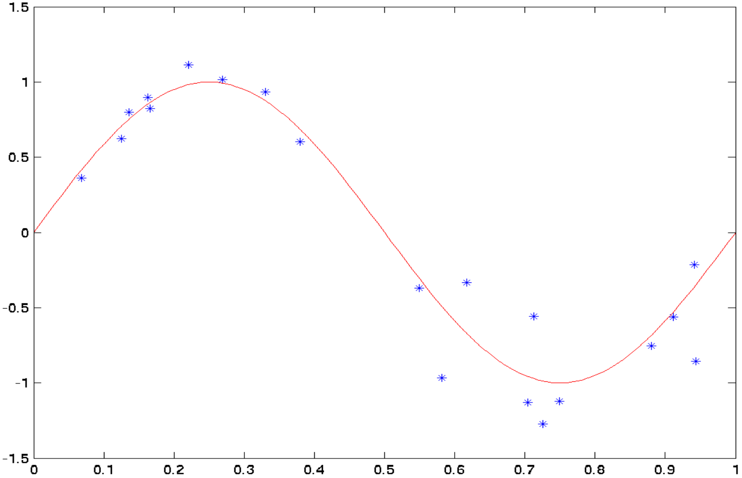
Extension to Regression

- Use the same equation for regression. This means that

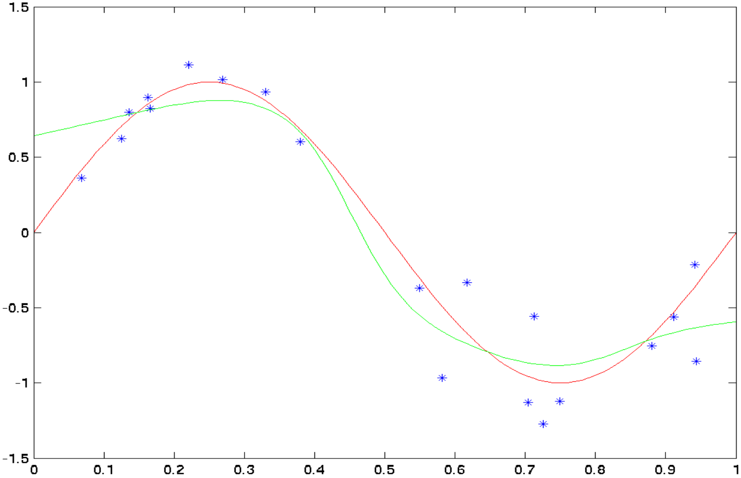
$$f(x) = \frac{\sum_i y_i k(x_i, x)}{\sum_i k(x_i, x)}$$

  where now $y_i \in \mathbb{R}$.
- We get a locally weighted version of the data

Regression Problem



Watson Nadaraya Regression



Mini Summary

Novelty Detection

- Observations in low-density regions are special (outliers).
- Applications to database cleaning, network security, etc.

Adaptive Kernel Width (Silverman's Trick)

- Kernels wide wherever we have low density

Watson Nadaraya Estimator

- Conditional density estimate
- Difference between class means (in feature space)
- Same expression works for regression, too

Summary

Density estimation

- empirical frequency, bin counting
- priors and Laplace rule

Parzen windows

- Smoothing out the estimates
- Examples

Adjusting parameters

- Cross validation
- Silverman's rule

Classification and regression with Parzen windows

- Watson-Nadaraya estimator
- Nearest neighbor classifier