Non-parametric Methods

Oliver Schulte - CMPT 726

Bishop PRML Ch. 2.5

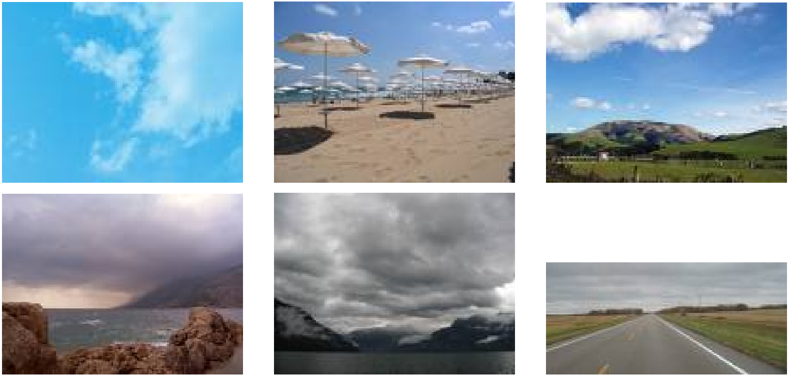
Outline

Kernel Density Estimation

Nearest-neighbour

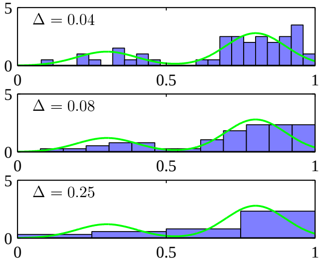
- These are non-parametric methods
  - Rather than having a fixed set of parameters (e.g. weight vector for regression, μ, Σ for Gaussian) we have a possibly infinite set of parameters based on each data point
- Fundamental Distinction in Machine Learning:
  - Model-Based, Parametric. What's the rule, law, pattern?
  - Instance-Based, non-parametric. What have I seen before that's similar?

Histograms



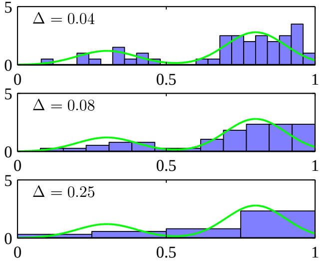
- Consider the problem of modelling the distribution of brightness values in pictures taken on sunny days versus cloudy days
- We could build histograms of pixel values for each class

Histograms



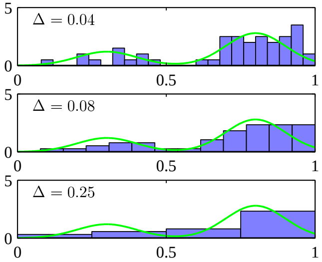
- E.g. for sunny days
- Count n_i number of datapoints (pixels) with brightness value falling into each bin: $p_i = \frac{n_i}{N\Delta_i}$
- Sensitive to bin width Δ_i
- Discontinuous due to bin edges
- In D-dim space with M bins per dimension, M^D bins

Histograms



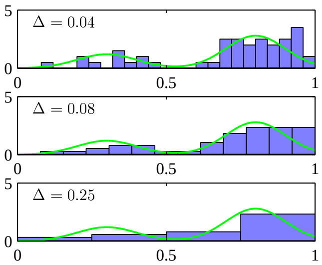
- E.g. for sunny days
- Count n_i number of datapoints (pixels) with brightness value falling into each bin: $p_i = \frac{n_i}{N\Delta_i}$
- Sensitive to bin width Δ_i
- Discontinuous due to bin edges
- In D-dim space with M bins per dimension, M^D bins

Histograms



- E.g. for sunny days
- Count n_i number of datapoints (pixels) with brightness value falling into each bin: $p_i = \frac{n_i}{N\Delta_i}$
- Sensitive to bin width Δ_i
- Discontinuous due to bin edges
- In D-dim space with M bins per dimension, M^D bins

Histograms



- E.g. for sunny days
- Count n_i number of datapoints (pixels) with brightness value falling into each bin: $p_i = \frac{n_i}{N\Delta_i}$
- Sensitive to bin width Δ_i
- Discontinuous due to bin edges
- In D-dim space with M bins per dimension, M^D bins

Local Density Estimation

- In a histogram we use *nearby* points to estimate density.
- For a small region around x, estimate density as:

$$p(x) = \frac{K}{NV}$$

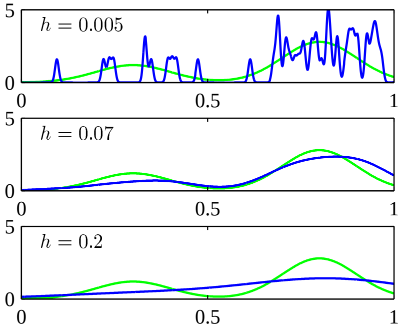
- K is number of points in region, V is volume of region, N is total number of datapoints
- Basic Principle: *high probability of* $x \iff x$ *is close to many points.*

Kernel Density Estimation

- Try to keep idea of using *nearby* points to estimate density, but obtain smoother estimate
- Estimate density by placing a small bump at each datapoint
  - Kernel function $k(\cdot)$ determines shape of these bumps
- Density estimate is

$$p(x) \propto \frac{1}{N} \sum_{n=1}^{N} k\left(\frac{x - x_n}{h}\right)$$

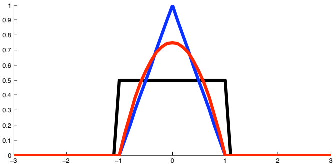
Kernel Density Estimation



- Example using Gaussian kernel:

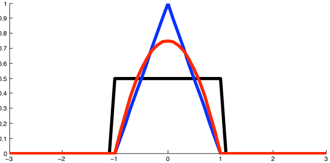
$$p(x) = \frac{1}{N} \sum_{n=1}^{N} \frac{1}{(2\pi h^2)^{1/2}} \exp\left\{ -\frac{||\boldsymbol{x} - \boldsymbol{x}_n||^2}{2h^2} \right\}$$

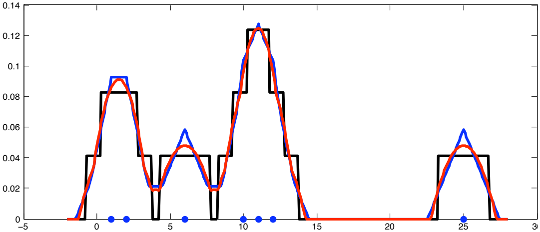
Kernel Density Estimation



- Other kernels: **Rectangle**, Triangle, Epanechnikov

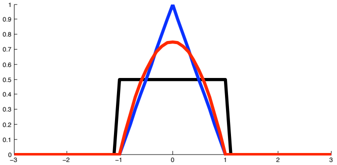
Kernel Density Estimation

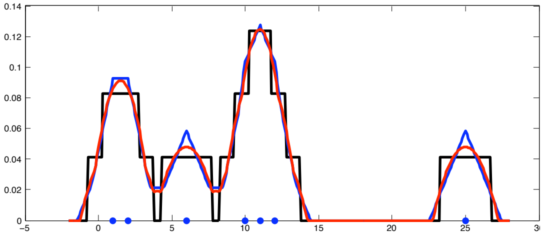




- Other kernels: **Rectangle**, Triangle, Epanechnikov

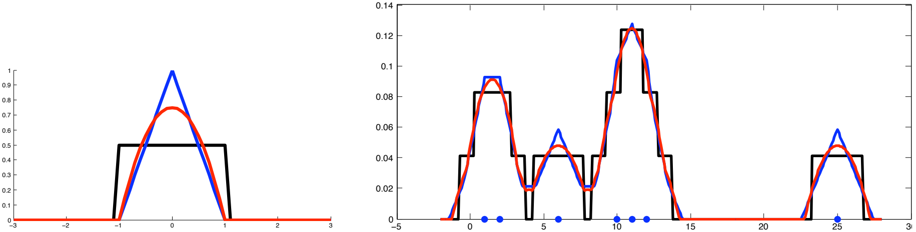
Kernel Density Estimation





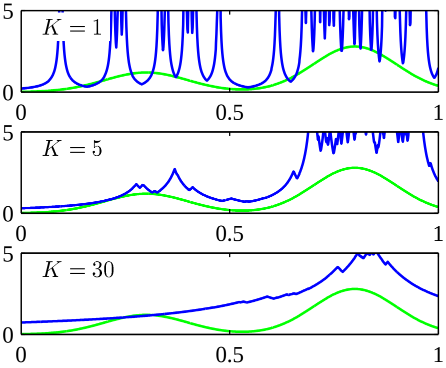
- Other kernels: **Rectangle**, Triangle, Epanechnikov
- Fast at training time, slow at test time – keep all datapoints

Kernel Density Estimation



- Other kernels: **Rectangle**, Triangle, Epanechnikov
- Fast at training time, slow at test time – keep all datapoints
- Sensitive to kernel bandwidth h

Nearest-neighbour



- Instead of relying on kernel bandwidth to get proper density estimate, fix number of nearby points K:

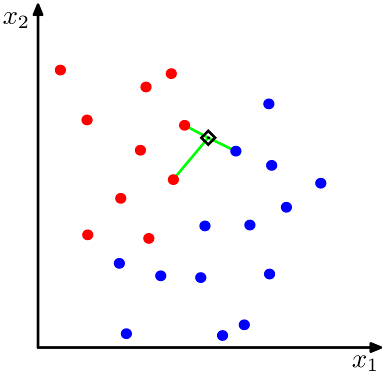
$$p(x) = \frac{K}{NV}$$

- Note: diverges, not proper density estimate

Nearest-neighbour for Classification

- K Nearest neighbour is often used for classification
  - Classification: predict labels t_i from x_i

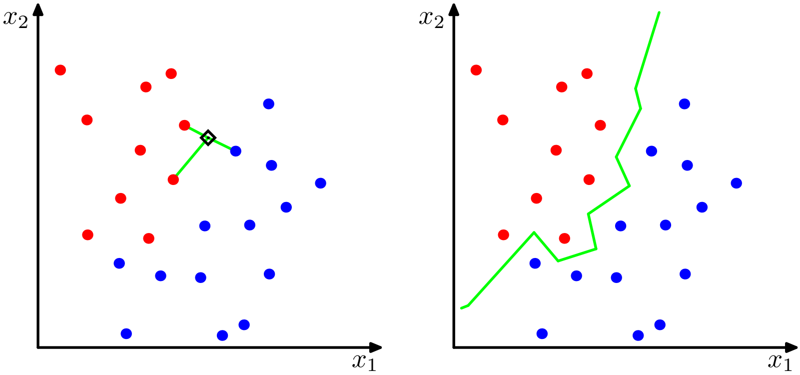
Nearest-neighbour for Classification



(a)

- K Nearest neighbour is often used for classification
  - Classification: predict labels t_i from x_i
  - e.g. $\boldsymbol{x}_i \in \mathbb{R}^2$ and $t_i \in \{0, 1\}$, 3-nearest neighbour

Nearest-neighbour for Classification



(a) (b)

- K Nearest neighbour is often used for classification
  - Classification: predict labels t_i from x_i
  - e.g. $\boldsymbol{x}_i \in \mathbb{R}^2$ and $t_i \in \{0, 1\}$, 3-nearest neighbour
- $K = 1$ referred to as nearest-neighbour

Nearest-neighbour for Classification

- Good baseline method
  - Slow, but can use fancy datastructures for efficiency (KD-trees, Locality Sensitive Hashing)
- Nice theoretical properties
  - As we obtain more training data points, space becomes more filled with labelled data
  - As $N \to \infty$ error no more than twice Bayes error

Conclusion

- Readings: Ch. 2.5
- Kernel density estimation
  - Model density $p(x)$ using kernels around training datapoints
- Nearest neighbour
  - Model density or perform classification using nearest training datapoints
- Multivariate Gaussian
  - Needed for next week's lectures, if you need a refresher read pp. 78-81