Kernel Density Estimation

An Introduction

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Overview

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2. Basic Estimators for Univariate KDE
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Densities and their Estimation

Probability Density Functions

We can assign probabilities to subsets of a continuous sample space Ω by integrating probability density functions (PDFs) p over them:

$$
\begin{aligned}
P(\text{event}) &= \int_{\text{event}} p(u)\, \mathrm{d}u \\
p(u_1)\, \mathrm{d}u &= P(\{u \in [u_1, u_1 + \mathrm{d}u]\})
\end{aligned}
$$

A PDF p is nonnegative, but can exceed unity, and $P(\Omega) = \int_{\Omega} p(u)\, \mathrm{d}u = 1$.

Parametric Estimation of Densities

If we have a parametric, generative model of the PDF, we can estimate its parameters from samples.

Example 1. Univariate Normal (Gaussian) Distribution

$$
\begin{aligned}
p(x;\mu,\sigma) &= \frac{1}{\sqrt{2\pi}\,\sigma}\exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \\
\hat{\mu} &= \frac{1}{N}\sum_{i=1}^{N} x_i \\
\hat{\sigma}^2 &= \frac{1}{N}\sum_{i=1}^{N} (x_i - \mu)^2
\end{aligned}
$$

Parametric Estimation of Densities

Example 2. Mixture of Univariate Normal Distributions

$$p(x; \mu_1, \dots, \mu_K, \sigma_1, \dots, \sigma_K, w_1, \dots, w_{K-1}) = \sum_{k=1}^{K} w_k p(x; \mu_k, \sigma_k)$$

with mixture proportions w_k the prior probabilities that a given observation was produced by mixture component k, and $\sum_{k=1}^{K} w_k = 1$:

Expectation-Maximization, gradient descent over the parameters, ...

Nonparametric Estimation of Densities

Without a generative model, all we can use to estimate $\hat{p}(x)$ is our available sample $x_1, \ldots, x_N$.

Uses:

- Faithfully model arbitrary distributions from finite samples
- Intuitive presentation and exploration
- Identify multimodality
- Resample

Histogram

Bin the data into intervals $[x_0 + mh, x_0 + (m+1)h)$ of width h, for $m \in \mathbb{Z}$:

$$\hat{p}(x) = \frac{1}{Nh} |\{x_i \text{ in same bin as } x\}|$$

Issues:

- Sensitivity to x_0, h, and (for multivariate data) the coordinate directions
- Step function

Generalized histogram:

$$\hat{p}(x) = \frac{1}{N} \frac{|\{x_i \text{ in same bin as } x\}|}{\text{width of bin containing } x}$$

Naive Estimator

From the definition of a PDF:

$$p(x) = \lim_{h \to 0} \frac{1}{2h} P(x - h < X < x + h)$$

Thus, we can further generalize our histogram:

$$\begin{aligned} \hat{p}(x) &= \frac{1}{2Nh} |\{x_i \text{ falling within } (x-h, x+h)\}| \\ &= \frac{1}{Nh} \sum_{i=1}^{N} w\left(\frac{x - x_i}{h}\right) \\ w(u) &= \begin{cases} \frac{1}{2} & \text{if } |u| < 1 \\ 0 & \text{otherwise} \end{cases} \end{aligned}$$

How many observations fall into a fixed-with box centered at x?

Issue:

- Step function

Basic Estimators for Univariate KDE

Kernel Estimator

Replace the weight function w by a kernel function K with $\int_{-\infty}^{\infty} K(x)\mathrm{d}x = 1$. Then, by analogy with the naive estimator,

$$\hat{p}(x) = \frac{1}{Nh}\sum_{i=1}^{N} K\left(\frac{x - x_i}{h}\right)$$

with *bandwidth* or *smoothing parameter* h.

Properties:

- If K is nonnegative, then it is a PDF, and so is $\hat{p}$.
- $\hat{p}$ inherits all continuity and differentiability properties from K.
- The fixed bandwidth may oversmooth in some regions and undersmooth in others.

Nearest Neighbor Estimator

Complementary to the naive estimator, *what is the smallest box containing a given number of observations*?

Define $d_1(x) = \| x - x_{n_1} \| \leq \ldots \leq d_N(x) = \| x - x_{n_N} \|$. Then, the k***th nearest neighbor density estimate*** is defined by

$$\hat{p}(x) = \frac{k}{2Nd_k(x)}.$$

Properties:

- *Bandwidth depends on the density of observations around the query value x.*
- Derivative full of discontinuities
- $\int_{-\infty}^{\infty} \hat{p}(x) \mathrm{d}x = \infty$

Nearest Neighbor Estimator (Continued)

This can be generalized by introducing a kernel function:

$$\hat{p}(x) = \frac{1}{N d_k(x)} \sum_{i=1}^{N} K\left(\frac{x - x_i}{d_k(x)}\right)$$

Variable Kernel Estimator

$$\hat{p}(x) = \frac{1}{Nh}\sum_{i=1}^{N}\frac{1}{d_k(x_i)}K\left(\frac{x-x_i}{hd_k(x_i)}\right)$$

The bandwidth depends on the densities around the observations x_i.

Properties: Same as for the basic kernel density estimator.

Remarks

Estimators for Multivariate Densities

All discussed methods extend straightforwardly.

Sampling from a Kernel Density Estimate

Basically:

1. Choose an observation at random.
2. Sample from the kernel centered at that observation.

In general, methods exist for sampling from arbitrary PDFs (inverse transform sampling, rejection sampling, …).

For many specific kernel functions, more efficient, specialized methods exist (normal distributions: Box-Muller transform, …).

Methods for Particular Domains

Bounded Domains

- Outside of the boundaries, set $\hat{p}$ to zero:
  - $\int \hat{p}(x)\mathrm{d}x < 1$
  - Observations near the boundaries contribute less to $\hat{p}$, and $\hat{p}$ is underestimated near the boundaries.
- Take logs: e.g., for positive data, if $\hat{q}$ is the density estimated from the logarithm of the data, then

$$\hat{p}(x) = \frac{1}{x}\hat{q}(\log x).$$

  - There will be a spike at the singularity.

Bounded Domains (Continued)

- Reflect the data: e.g., for positive data, if $\hat{q}$ is the density estimated from this augmented data set, then

$$\hat{p}(x) = \begin{cases} 2\hat{q}(x) & \text{for } x \geq 0 \\ 0 & \text{for } x < 0. \end{cases}$$

Circular Domains

For example, replicate angular data twice, shifted by $\pm 2\pi$ (or even more copies, if necessary).

Then, apply a conventional estimator.

A similar trick applies to toroidal domains.

Spherical Domains

For example, represent data as unit vectors $\mathbf{x}_i \in \mathbb{R}^d$, and use a von Mises–Fisher kernel:

$$\hat{p}(\mathbf{x};\kappa) = \frac{1}{Nc_d(\kappa)}\sum_{i=1}^{N}\exp(\kappa\mathbf{x}^T\mathbf{x}_i)$$

where κ is a concentration parameter. [Mardia and Jupp 1999]

The normalizing constant $c_d(\kappa)$ is messy to compute explicitly and can in practice be determined by numerical integration.

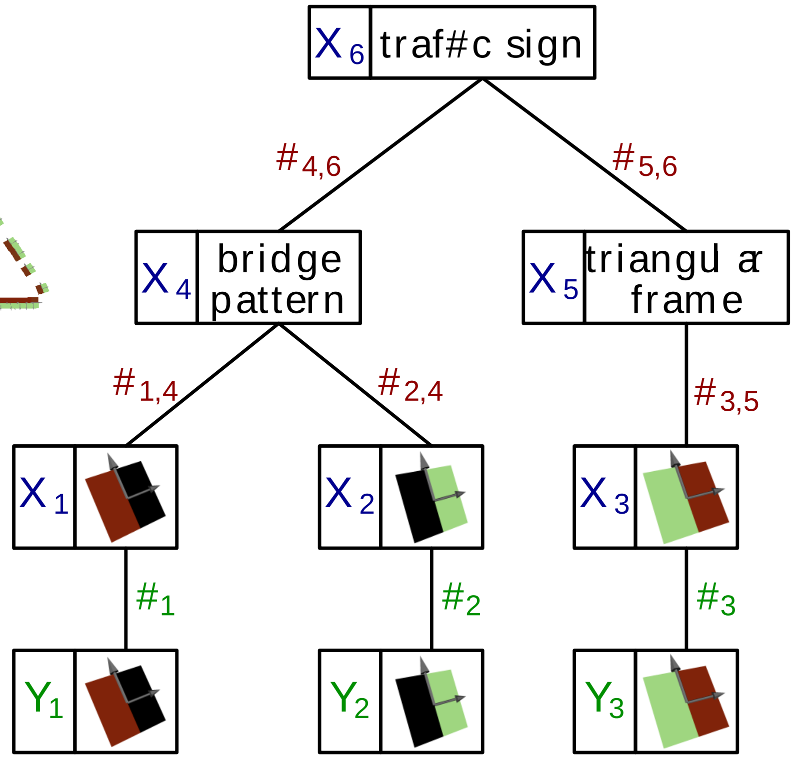
For axial domains, use a Dimroth-Watson kernel (inner product squared):

- $\kappa > 0$: antipodal
- $\kappa = 0$: uniform
- $\kappa < 0$: girdle

Case Study: Pose Estimation
Renaud Detry

[Detry et al. 2009]

Local Appearance + Spatial Relations



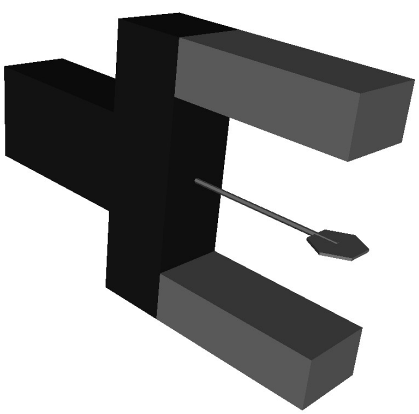
Vertex (random variable): distribution of *positions*

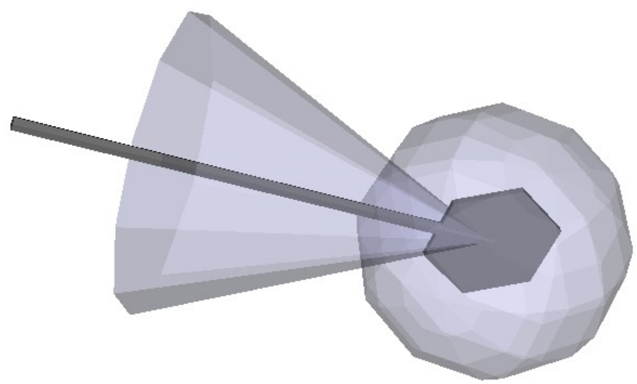
Edge (potential): distribution of *spatial relations* Ψ

Object Model (Markov network): structure; potentials Ψ, Φ

A Kernel for Pose Densities

- Pose $\mathbf{x} \in SE(3) = \mathbb{R}^3 \times SO(3)$
- Assuming that positions and orientations are independent, use an $SE(3)$ kernel $K(\mathbf{x}; \boldsymbol{\mu}, \sigma)$ that factors into
  - a location kernel $N(\mathbf{x}_{pos}; \boldsymbol{\mu}_{pos}, \sigma_{pos})$ (normal)
  - an orientation kernel $c(\sigma_{or}) \exp(\sigma_{or} (\boldsymbol{\mu}_{or}^{qT} \mathbf{x}_{or}^{q})^2)$ (Dimroth-Watson), with q denoting quaternion representations.





Uses of KDE

Sampling:

- from weighted-particle representations
- for forming message products
- for stochastic integration of products of densities (convolutions)

Finding maximum:

- for determining the maximum-likelihood pose
- to find the best gripper pose for grasping

Uses of KDE (Continued)

To sample in $\mathrm{SE}(3)$**:**

1. Choose an observation at random.
2. Sample from the position part of the kernel centered at that observation.
3. Sample from the orientation part of the kernel centered at that observation [Wood 1994].

Conclusion

References

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