Kernel Regression

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Overview

1. Preliminaries
2. k nearest neighbor
3. Kernel Density Estimation
4. Kernel Density Classification

Preliminaries

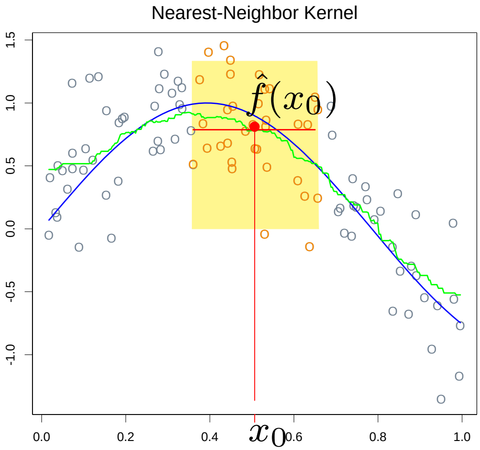
- Linear models, even those based on basis expansion, have high bias.
- In contrast, kernel methods fit many models to each point using the observations close to that point.
- Localization is based on a weighting function $K_\lambda(x_0; x_i)$ that assigns a weight to each observation x_i based on distance to a query point.
- Typically, the kernel function has only a single parameter (λ) to determine width of neighborhood.
- The "model" is the entire training data set.
- While undoubtedly effective in many instances, kernel methods lack interpretability that is often desired for scientific applications.

k Nearest Neighbor (kNN)

- Simplest possible model for prediction - even simpler than linear regression!
- Given a set of observations, we take the average of the k nearest neighbors as an estimate.

$$E[Y|X=x] = \hat{f}(x) = Ave(y_i|x_i \in N_k(x))$$

- Prediction is bumpy, i.e., changes in average are discrete at the boundary between the inclusion and exclusion of a point.



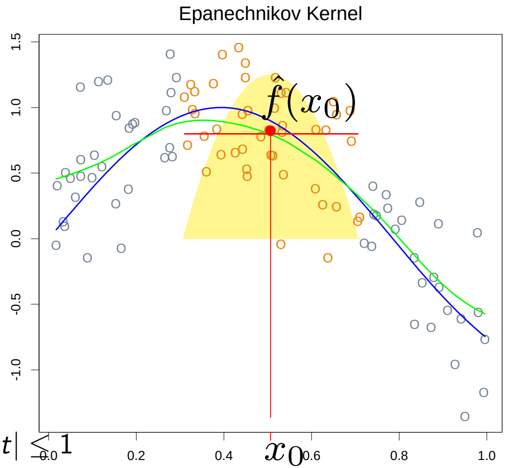
Improving on kNN

- kNN gives equal weight to all points that falls within the k nearest neighbor region.
- Solution: use a weighted kernel that goes to zero smoothly with distance from point.
- Nadaraya-Watson kernel-weighted average:

$$\hat{f}(x) = \frac{\sum_{i=1}^{N} K_\lambda(x_0, x_i) y_i}{\sum_{i=1}^{N} K_\lambda(x_0, x_i)}$$

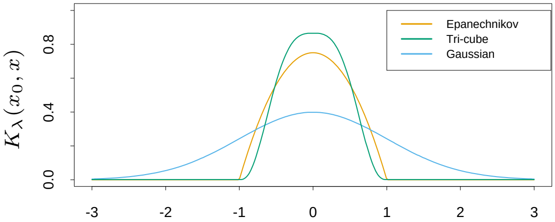
- Epanechnikov quadratic kernel:

$$K_\lambda(x_0, x) = D\left(\frac{|x - x_0|}{\lambda}\right), D(t) = \frac{3}{4}(1-t^2) \text{ if } |t| \leq 1$$



Considerations

- Smoothing parameter λ determines the width of the local neighborhood. Large λ means lower variance but higher bias.
- Metric window widths: As local density increases, vias decreases.
- Epanechnikov kernel is compact. Tri-cube kernel $D(t) = (1 - |t|^3)^3$ if $|t| \leq 1$ is another compact kernel that is flatter and differentiable at bounday.
- Gaussian kernel is a popular *non-compact* kernel. Standard deviation controls width of kernel.



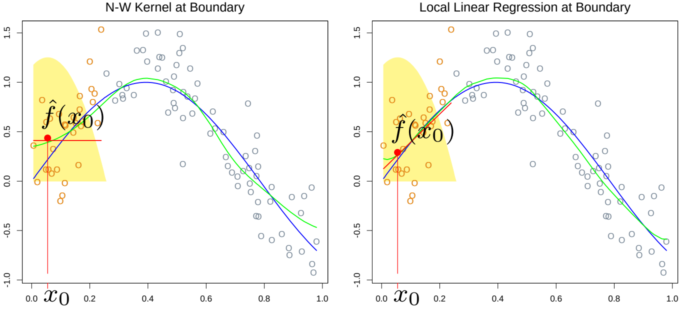
Code

```python
from sklearn.neighbors import KNeighborsRegressor
from sklearn.model_selection import cross_val_predict, KFold


kfold = KFold(n_splits=5, shuffle=True, random_state=42)
knn = KNeighborsRegressor(n_neighbors=14)
yhat_knn = cross_val_predict(knn, x, y, cv=kfold)
```

Local linear/polynomial regression

- Local linear/polynomial regression can be used, which corrects bias at boundary regions at the expense of higher variance.
- For higher dimensions especially, local linear regression is preferred to local constant fit.



- Often used to interpolate within a region of feature space.

Kernel Density Estimation

- Estimate the probability density function $\hat{f}_X(x)$ as:

$$\hat{f}_X(x_0) = \frac{\# x_i \in N(x_0)}{N\lambda}$$

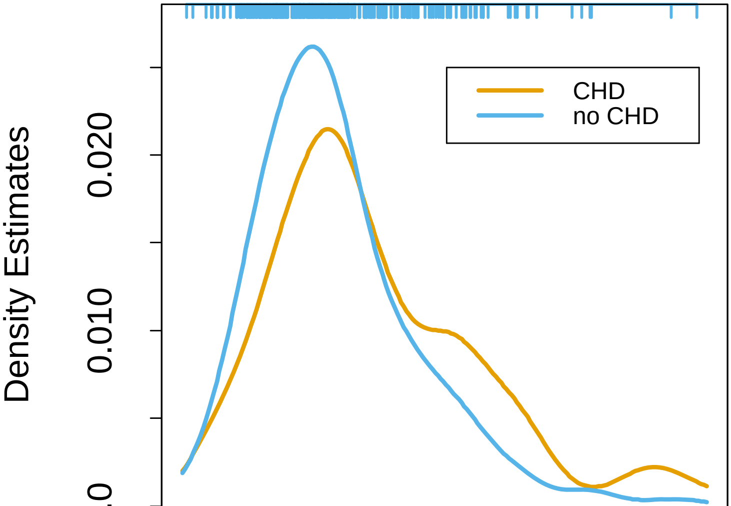
where λ is the width of the bin and $N(x_0)$ is the neighbor of x_0 and N is the total data count.

- Often, the smooth Parzen estimate is used.

$$\hat{f}_X(x_0) = \frac{1}{N\lambda} \sum_{i=1}^{N} K_\lambda(x_0, x_i)$$

- Popular choice of K_λ is the Gaussian kernel $\phi(\frac{x-x_0}{\lambda})$.
- Essentially $f_X(x)$ is the convolution of the sample distribution with the Gaussian distribution with standard deviation λ.

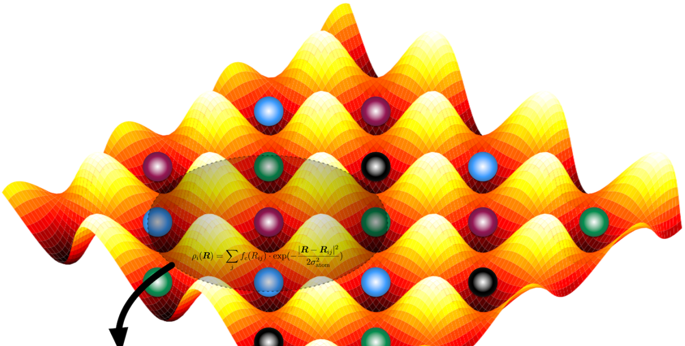
Gaussian KDE



Example of Gaussian Density Estimation in Interatomic Potential

- Gaussian Approximation Potential[1] uses a smooth-overlap of atomic positions (SOAP) kernel in a Gaussian process model:

$$\rho_i(\boldsymbol{R}) = \sum_j f_c(R_{ij}) \cdot \exp(-\frac{|\boldsymbol{R} - \boldsymbol{R}_{ij}|^2}{2\sigma^2_{\mathrm{atom}}}) = \sum_{nlm} c_{nlm}\; g_n(R) Y_{lm}(\hat{\boldsymbol{R}}),$$

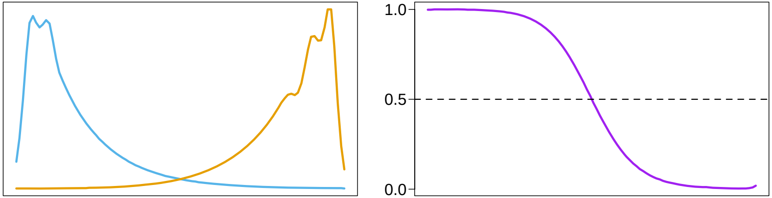


Kernel Density Classification

- Given the kernel density estimate for each class $\hat{f}_j(X)$ and class prior π_j, we can use Bayes theorem to perform classification:

$$P(G = j | X = x_0) = \frac{\pi_j \hat{f}_j(x_0)}{\sum_{k=1}^{J} \pi_k \hat{f}_k(x_0)}$$

- However, density estimation for each class is not necessary if we only need to perform classification.
- The key is to estimate the posterior decision boundary between classes accurately.



Naive Bayes

- Highly popular approach and often outperforms more sophisticated alternatives.
- Assumes features X_k are independent, i.e., $f_j(X) = \prod_{k=1}^{p} f_j k(X_k)$, i.e., class conditional probabilities can be estimated using 1D kernel densities!

$$
\begin{aligned}
\log \frac{P(G = l|X)}{P(G = k|X)} &= \log \frac{\pi_l}{\pi_j} + \sum_{k=1}^{p} \log \frac{f_{lk}(X_k)}{f_{jk}(X_k)} \\
&= \alpha_l + \sum_{k=1}^{p} g_{lk}(X_k)
\end{aligned}
$$

We are converting a high-dimensional problem into simpler generalized additive model (see later lecture on GAMs).

Radial Basis Functions

- Treat kernel functions as basis functions.

$$f(x) = \sum_{j=1}^{M} D\left(\frac{||x - \varepsilon_j||}{\lambda_j}\right)\beta_j$$

- Each basis function is index by location (ε_j) and scale parameter λ_j.
- Gaussian function is a common choice for D.
- Parameters are optimized, typically using a least squares approach.

Mixture Models

- Type of kernel model.

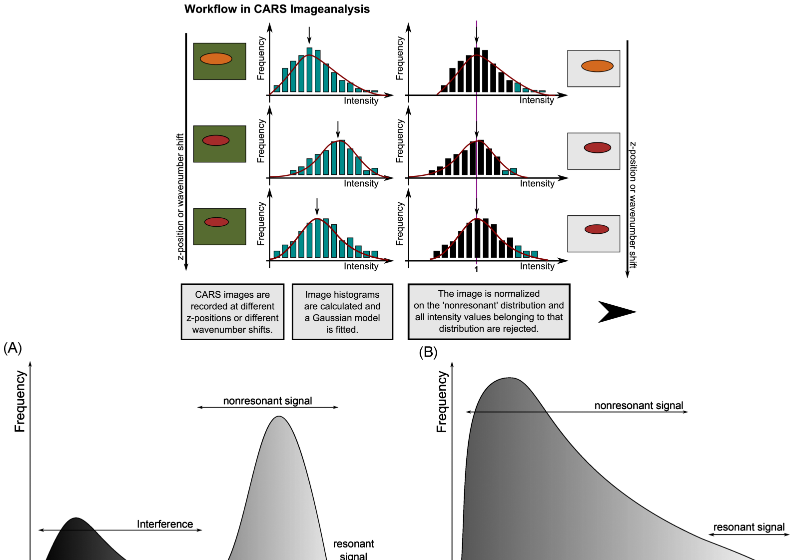
$$f(x) = \sum_{m=1}^{M} \alpha_m \phi(x; \mu_m, \Sigma_\mathrm{m})$$

- Again, Gaussian mixture model is by far the most common choice.
- If covariance matrices are constrained to be scalars. then it is similar to a radial basis expansion.
- Typically fitted using maximum likelihood approach / expectation maximization (next lecture).
- Probability that observation i belongs in component m is given by:

$$\hat{r}_{im} = \frac{\alpha_m \phi(x; \mu_m, \Sigma_\mathrm{m})}{\sum_{k=1}^{M} \alpha_k \phi(x; \mu_k, \Sigma_\mathrm{k})}$$

- Very often used in spectroscopy analysis.

CARS spectroscopy analysis using Gaussian Mixtures



Bibliography

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