

SDS 383D, Exercises 3: Linear smoothing and Gaussian processes

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Curve fitting by linear smoothing

- (A) Linear smoothing Suppose we want to estimate the value of the regression function y^* at some new point x^* , denoted $\hat{f}(x^*)$. Assume for the moment that $f(x)$ is linear, and that y and x have already had their means subtracted, in which case $y_i = \beta x_i + \epsilon_i$.

Show that for the one-predictor case, your prediction $\hat{y}^* = \hat{f}(x^*) = \hat{\beta}x^*$ may be expressed as:

$$\hat{f}(x^*) = \sum_{i=1}^n w(x_i, x^*) y_i$$

We can express $\hat{\beta}$ in matrix notation as,

$$\hat{\beta} = (X^T X)^{-1} X^T Y.$$

Plugging this in to find our predictor, \hat{y}^* we get,

$$\begin{aligned} \hat{y}^* &= x^* (X^T X)^{-1} X^T Y \\ &= \frac{X^T Y}{X^T X} \\ &= \frac{\sum_{i=1}^n x_i x^* y_i}{\sum_{i=1}^n x_i^2} \end{aligned}$$

The result is of the form $\hat{f}(x^*) = \sum_{i=1}^n w(x_i, x^*) y_i$ with the weights expressed as,

$$w(x_i, x^*) = \frac{\sum_{i=1}^n x_i x^*}{\sum_{i=1}^n x_i^2}.$$

This resultant *smoother* has constant weights and produces predictions that lie on the line with slope $\hat{\beta}$. If the data is binned, this estimate is similar to a running line average.

$$w_K(x_i, x^*) = \begin{cases} 1/K, & x_i \text{ one of the } K \text{ closest sample points to } x^*, \\ 0, & \text{otherwise.} \end{cases}$$

With *K-nearest-neighbor smoothing* \hat{y}^* is essentially the arithmetic mean of the K y_i 's nearest x^* .

- (B) A *kernel function* $K(x)$ is a smooth function satisfying

$$\int_{\mathbb{R}} K(x) dx = 1, \quad \int_{\mathbb{R}} x K(x) dx = 0, \quad \int_{\mathbb{R}} x^2 K(x) dx > 0.$$

A very simple example is the uniform kernel,

$$K(x) = \frac{1}{2}I(x) \quad \text{where} \quad I(x) = \begin{cases} 1, & |x| \leq 1 \\ 0, & \text{otherwise.} \end{cases}$$

Another common example is the Gaussian kernel:

$$K(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}.$$

Kernels are used as weighting functions for taking local averages. Specifically, define the weighting function

$$w(x_i, x^*) = \frac{1}{h} K\left(\frac{x_i - x^*}{h}\right),$$

where h is the bandwidth. Using this weighting function in a linear smoother is called *kernel regression*. (The weighting function gives the unnormalized weights; you should normalize the weights so that they sum to 1.)

```
from __future__ import division
import numpy as np
import matplotlib.pyplot as plt
import sys
sys.path.append('../scripts/')
from smoothers import kernel_smoother
```

```
# Create noisy data, y_i = sin(x_i) + e_i
x = np.linspace(0, 2*np.pi, num = 20)
y = np.sin(x) + np.random.normal(scale=0.2, size=x.shape)

# Create vector for fitting purposes
x_star = np.linspace(0, 2*np.pi)

# Instantiate array of bandwidths
h = np.array([0.25, 1.0])
```

```
# Instantiate a list to append kernel_smoother objects
H = []

# Iterates through array of bandwidths and passes the feature vector, response vector, and ↵
# bandwidth to kernel_smoother object
for i in range(len(h)):
    H.append(kernel_smoother(x, y, x_star, h=h[i]))
```

```
# Plots data
plt.figure()
plt.plot(x, y, '.k', label='Noisy response')
plt.plot(x, np.sin(x), '--k', label='True function')
# Iterates over the smoother objects and plots functions for the uniform and gaussian kernels
for i in range(len(h)):
    plt.plot(x_star, H[i].predictor(kernel='uniform'), label='Uniform Kernel, h='+str(h[i]))
    plt.plot(x_star, H[i].predictor(kernel='gaussian'), label='Gaussian Kernel, h='+str(h[i]))
plt.legend(loc=0)
# plt.show()
plt.savefig('figures/kernel_smoother.pdf')
plt.close()
```

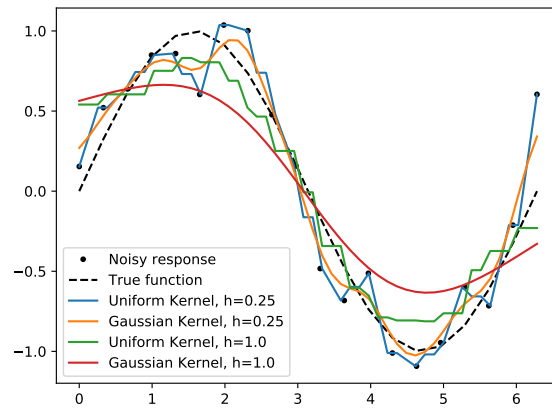


Figure 1: Uniform and Gaussian Kernel smoothing for different bandwidths

A Kernel Smoothing Code

```
from __future__ import division
import numpy as np

class kernels:
    """
    This class contains kernel functions for kernel smoothing
    """
    def __init__(self):
        pass

    def uniform(x):
        """
        Parameters
        -----
        x: float
            argument to be evaluated

        Returns
        -----
        k: float
            uniform kernel evaluation at x
            .. math:: k(x) = 1/2 I(x), \text{ with } I(x) = 1, \text{ if } |x| \leq 1, 0 \text{ otherwise}
        """
        if np.abs(x) <= 1:
            k = 0.5
        else:
            k = 0
        return k

    def gaussian(x):
        """
        Parameters
        -----
        x: float
            argument to be evaluated

        Returns
        -----
        k: float
            gaussian kernel evaluation at x
            .. math:: k(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}
        """
        return 1/np.sqrt(2*np.pi)*np.exp(-x**2/2)

class kernel_smoother:
    """
    This class returns a vector of smoothed values given feature and response vectors
    """
    def __init__(self, x, y, x_star, h=0.5):
        """
        Parameters
        -----
        x: float
            Feature vector

        y: float
            Response vector

        x_star: float
            Scalar or vector to be evaluated

        h: float (optional)
            Bandwidth
        """
        self.x = x
```

```

self.y = y
self.x_star = x_star
self.h = h

def predictor(self, kernel='gaussian'):
    """
    Parameters
    -----
        kernel: str (optional)
            Kernel type to be used: Available kernels are uniform, gaussian,

    Returns
    -----
        y_star: float, len(x_star)
            Predictor for x_star
        .. math:: y_i^* = \sum_{i=1}^n w(x_i, x^*) y_i
        .. math:: w(x_i, x^*) = \frac{1}{2} K\left(\frac{x_i - x^*}{h}\right), \sum_{i=1}^n w(x_i, x^*) = 1
    """
    # Instantiate y_star
    y_star = np.zeros(self.x_star.shape)

    # Iterate through each value in y_star
    for i in range(y_star.shape[0]):

        # Instantiate a weights vector
        weights = np.zeros(self.x.shape)

        # Iterates through feature/response vectors
        for j in range(self.x.shape[0]):

            #  $X = \frac{(x_i - x^*)}{h}$ 
            X = (self.x[j] - self.x_star[i])/self.h

            #  $w(x_i, x^*) = \frac{1}{h} K(X)$ 
            weights[j] = 1/self.h*getattr(kernels, kernel)(X)

        # Normalizes weights such that  $\sum_{i=1}^n w(x_i, x^*) = 1$ 
        weights = weights/weights.sum()

        #  $y_i^* = \sum_{i=1}^n w(x_i, x^*) y_i$ 
        y_star[i] = (weights*self.y).sum()

    return y_star

```