Kernel Methods : Homework 2

Thibaud Ehret & Sammy Khalife

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1)

The formula for the projection on the i^{th} eigenvector is $\sum_{j=1}^{n} \alpha_j^{(i)}(\Phi(x_j) - m)$.

$$
\begin{aligned}
\sum_{j=1}^{n} \alpha_j^{(i)}(\Phi(x_j) - m) &= \sum_{j=1}^{n} \alpha_j^{(i)}\Phi(x_j) - \sum_{j=1}^{n} \alpha_j^{(i)} m \\
&= \sum_{j=1}^{n} \alpha_j^{(i)}\Phi(x_j) - m\left(\sum_{j=1}^{n} \alpha_j^{(i)}\right) \\
&= \sum_{j=1}^{n} \alpha_j^{(i)}\Phi(x_j) - \frac{1}{n}\left(\sum_{u=1}^{n} \Phi(x_u)\right)\left(\sum_{j=1}^{n} \alpha_j^{(i)}\right) \\
&= \sum_{j=1}^{n} \alpha_j^{(i)}\Phi(x_j) - \left(\sum_{u=1}^{n} \frac{1}{n}\left(\sum_{j=1}^{n} \alpha_j^{(i)}\right)\Phi(x_u)\right) \\
&= \sum_{j=1}^{n} \alpha_j^{(i)}\Phi(x_j) - \left(\sum_{j=1}^{n} \frac{1}{n}\left(\sum_{u=1}^{n} \alpha_u^{(i)}\right)\Phi(x_j)\right) \\
&= \sum_{j=1}^{n} \left(\alpha_j^{(i)} - \frac{1}{n}\left(\sum_{u=1}^{n} \alpha_u^{(i)}\right)\right)\Phi(x_j)
\end{aligned}
$$

We note $\beta_j = \alpha_j^{(i)} - \frac{1}{n}\left(\sum_{u=1}^n \alpha_u^{(i)}\right)$, so that the vector can be written $\sum_{j=1}^n \beta_j^{(i)}\Phi(x_j)$. Therefore after injecting into the expression of Ψ,

$$\begin{aligned}
\Psi(x) &= \sum_{i=1}^d \langle \sum_{j=1}^n \beta_j^{(i)}\Phi(x_j), \Phi(x) - m\rangle \left(\sum_{j=1}^n \beta_j^{(i)}\Phi(x_j)\right) + m \\
&= \sum_{i=1}^d \left(\sum_{j=1}^n \beta_j^{(i)}\langle\Phi(x_j), \Phi(x)\rangle\right)\left(\sum_{j=1}^n \beta_j^{(i)}\Phi(x_j)\right) - \sum_{i=1}^d \left(\sum_{j=1}^n \beta_j^{(i)}\langle\Phi(x_j), m\rangle\right)\left(\sum_{j=1}^n \beta_j^{(i)}\Phi(x_j)\right) + m \\
&= \sum_{i=1}^d \left(\sum_{j=1}^n \beta_j^{(i)} K(x_j, x)\right)\left(\sum_{j=1}^n \beta_j^{(i)}\Phi(x_j)\right) - \sum_{i=1}^d \left(\sum_{j=1}^n \beta_j^{(i)}\langle\Phi(x_j), \frac{1}{n}\sum_{u=1}^n \Phi(x_u)\rangle\right)\left(\sum_{j=1}^n \beta_j^{(i)}\Phi(x_j)\right) \\
&\quad + \frac{1}{n}\sum_{u=1}^n \Phi(x_u) \\
&= \sum_{i=1}^d \left(\sum_{j=1}^n \beta_j^{(i)} K(x_j, x)\right)\left(\sum_{j=1}^n \beta_j^{(i)}\Phi(x_j)\right) - \sum_{i=1}^d \left(\sum_{j=1}^n \beta_j^{(i)}\frac{1}{n}\sum_{u=1}^n K(x_j, x_u)\right)\left(\sum_{j=1}^n \beta_j^{(i)}\Phi(x_j)\right) \\
&\quad + \frac{1}{n}\sum_{u=1}^n \Phi(x_u) \\
&= \sum_{i=1}^d \left(\sum_{j=1}^n \beta_j^{(i)} K(x_j, x)\right)\left(\sum_{j=1}^n \beta_j^{(i)}\Phi(x_j)\right) - \sum_{i=1}^d \left(\sum_{j=1}^n \beta_j^{(i)}\frac{1}{n}\sum_{u=1}^n K(x_j, x_u)\right)\left(\sum_{j=1}^n \beta_j^{(i)}\Phi(x_j)\right) \\
&\quad + \frac{1}{n}\sum_{u=1}^n \Phi(x_u) \\
&= \sum_{j=1}^n \left(\sum_{u=1}^n \left(\sum_{i=1}^d \beta_u^{(i)}\beta_j^{(i)}\right) K(x_u, x) - \sum_{u=1}^n \left(\sum_{i=1}^d \beta_u^{(i)}\beta_j^{(i)}\right)\left(\frac{1}{n}\sum_{v=1}^n K(x_u, x_v)\right) + \frac{1}{n}\right)\Phi(x_j)
\end{aligned}$$

Therefore

$$\gamma_j = \sum_{u=1}^n \left(\sum_{i=1}^d \beta_u^{(i)}\beta_j^{(i)}\right) K(x_u, x) - \sum_{u=1}^n \left(\sum_{i=1}^d \beta_u^{(i)}\beta_j^{(i)}\right)\left(\frac{1}{n}\sum_{v=1}^n K(x_u, x_v)\right) + \frac{1}{n}$$

2)

$$\begin{aligned}
f(y) &= \|\Phi(y) - \Psi(x)\|^2 \\
&= \langle \Phi(y) - \Psi(x), \Phi(y) - \Psi(x)\rangle \\
&= \langle \Phi(y), \Phi(y)\rangle - 2\langle \Phi(y), \Psi(x)\rangle + \langle \Psi(x), \Psi(x)\rangle \\
&= K(y, y) - 2\langle \Phi(y), \Psi(x)\rangle + \langle \Psi(x), \Psi(x)\rangle
\end{aligned}$$

Using the the fact that $\Psi(x) = \sum_{i=1}^{n} \gamma_i \Phi(x_i)$,

$$\begin{aligned} f(y) &= K(y,y) - 2\langle \Phi(y), \sum_{i=1}^{n} \gamma_i \Phi(x_i\rangle + \langle \sum_{i=1}^{n} \gamma_i \Phi(x_i), \sum_{i=1}^{n} \gamma_i \Phi(x_i)\rangle \\ &= K(y,y) - 2\sum_{i=1}^{n} \gamma_i \langle \Phi(y), \Phi(x_i)\rangle + \sum_{i=1}^{n}\sum_{j=1}^{n} \gamma_i \gamma_j \langle \Phi(x_i), \Phi(x_j)\rangle \\ &= K(y,y) - 2\sum_{i=1}^{n} \gamma_i K(y, x_i) + \sum_{i=1}^{n}\sum_{j=1}^{n} \gamma_i \gamma_j K(x_i, x_j) \end{aligned}$$

The idea behind $\Psi(x)$ is to denoise x in the feature space, by keeping only the participation over the d first principal components we can hope to have consider the signal without its noise. Therefore ooptimizing $f(y)$ corresponds to finding the best y in the original space such that it is as close as possible to the "denoised" version in the feature space, therefore the y that optimizes f for a given x correspond to the best denoised version in the original space.

3)

In the case of $K(x,x') = exp(-\frac{||x-x'||^2}{2\sigma^2})$,

$$f(y) = \sum_{i=1}^{n}\sum_{j=1}^{n} \gamma_i \gamma_j exp(-\frac{||x_i - x_j'||^2}{2\sigma^2}) - 2\sum_{i=1}^{n} \gamma_i exp(-\frac{||y - x_i||^2}{2\sigma^2})$$

$$\nabla f(y) = \frac{2}{\sigma^2} \sum_{i=1}^{n} (y - x_i) \gamma_i exp(-\frac{||y - x_i||^2}{2\sigma^2})$$

We can here use a gradient descent method to find local minimum of f. We see that a stationary point satisfies :

$$y = \frac{\sum_{i=1}^{n} x_i \gamma_i exp(-\frac{||y-x_i||^2)}{2\sigma^2})}{\sum_{i=1}^{n} \gamma_i exp(\frac{-||y-x_i||^2)}{2\sigma^2})}$$

We can apply a fixed point method :

$$y_{k+1} = \frac{\sum_{i=1}^{n} x_i \gamma_i exp(-\frac{||y_k-x_i||^2)}{2\sigma^2})}{\sum_{i=1}^{n} \gamma_i exp(\frac{-||y_k-x_i||^2)}{2\sigma^2})}$$

With initialization at different points.

Or we can use the Newton step with the Hessian :

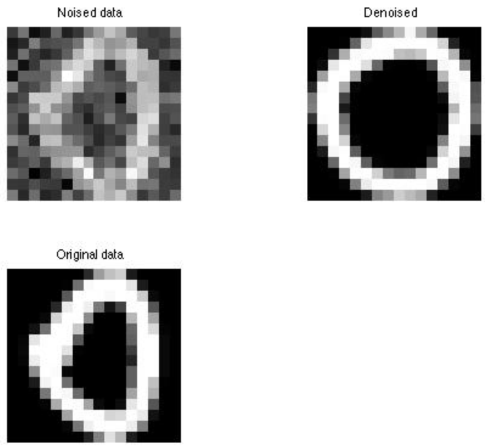
$$H_f(y) = \frac{2}{\sigma^2} \sum_{i=1}^{n} \gamma_i exp(-\frac{||y - x_i||^2}{2\sigma^2})[\frac{Id}{n} - (y - x_i)(y - x_i)^t]$$

$$y_{k+1} = y_k - H_f^{-1}(y_k) \nabla y_k$$

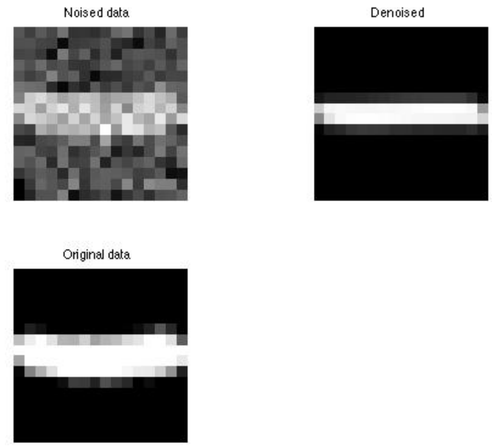
4)

Data used : (http://statweb.stanford.edu/ tibs/ElemStatLearn/datasets/zip.info.txt)

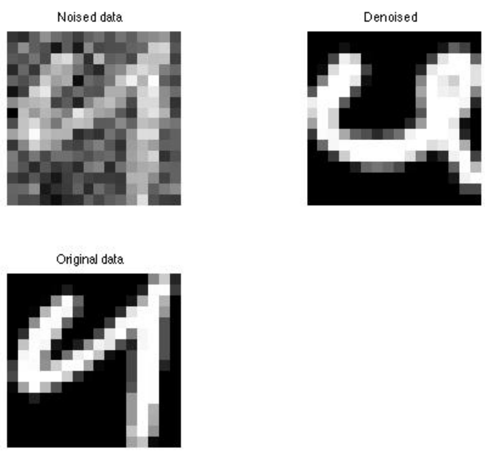
This dataset is composed of normalized handwritten digits, automatically scanned from envelopes by the U.S. Postal Service. The original scanned digits are binary and of different sizes and orientations; the images here have been deslanted and size normalized, resulting in 16 x 16 grayscale images.



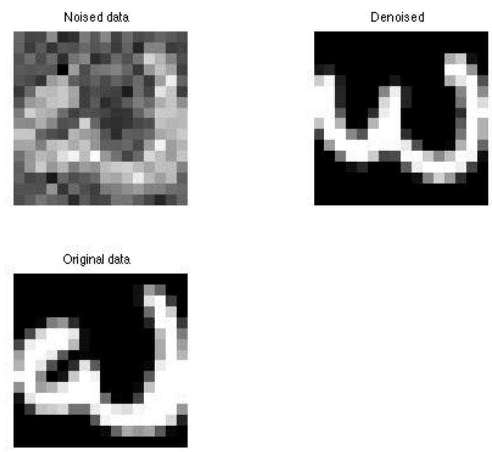
(a)



(b)



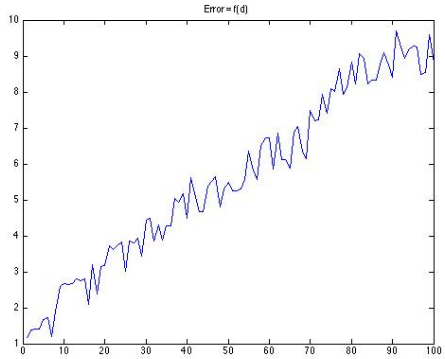
(c)



(d)

Figure 1: Results on different digits

These results have been obtained with **100 training samples**, and with **d=50**. We see that the minimization process that projects the noised data over the vector spanned by the eigenvectors simplify the geometry. Increasing d does not help to achieve better denoising, since we are closer and closer to the noised data x :



(a) Error plot as a function of d