Machine Learning 1 Exercise 4

Group: BSSBCH

November 13, 2017

Matthias Bigalke, 339547, maku@win.tu-berlin.de Tolga Buz, 346836, buz_tolga@yahoo.de Alejandro Hernandez, 395678, alejandrohernandezmunuera@gmail.com Aitor Palacios Cuesta, 396276, aitor.palacioscuesta@campus.tu-berlin.de Christof Schubert, 344450, christof.schubert@campus.tu-berlin.de Daniel Steinhaus, 342563, dany.steinhaus@googlemail.com

1 Lagrange Multipliers

(a)

Find the parameter θ that minimizes $J(\theta)$ subject to the constraint $\theta^T b = 0$.

We have

$$\mathcal{L} = \sum_{k=1}^n ||oldsymbol{ heta} - oldsymbol{x}_k||^2 + \lambda oldsymbol{ heta}^T oldsymbol{b}$$

From this we get

$$0 = \frac{\partial}{\partial \boldsymbol{\theta}} \mathcal{L} \tag{1}$$

$$\Leftrightarrow 0 = \sum_{k=1}^{n} 2(\boldsymbol{\theta} - \boldsymbol{x}_k) + \lambda \boldsymbol{b}$$
 (2)

$$\Leftrightarrow 0 = \boldsymbol{\theta} - \overline{\boldsymbol{x}} + \frac{\lambda}{2n} \boldsymbol{b} \tag{3}$$

$$\Leftrightarrow \quad \boldsymbol{\theta} = \overline{x} - \frac{\lambda}{2n} \boldsymbol{b} \tag{4}$$

and

$$0 = \frac{\partial}{\partial \lambda} \mathcal{L} \tag{5}$$

$$\Leftrightarrow 0 = \boldsymbol{\theta}^T \boldsymbol{b} \tag{6}$$

$$\overset{(4)}{\Leftrightarrow} \quad 0 = (\overline{\boldsymbol{x}} - \frac{\lambda}{2n} \boldsymbol{b})^T \boldsymbol{b} \tag{7}$$

$$\Leftrightarrow 0 = \overline{\boldsymbol{x}}^T \boldsymbol{b} - \frac{\lambda}{2n} \boldsymbol{b}^T \boldsymbol{b}$$
 (8)

$$\overset{b \neq 0}{\Leftrightarrow} \quad \lambda = 2n \frac{\overline{x}^T b}{b^T b} \tag{9}$$

(10)

With (4) and (10) we finally get

$$oldsymbol{ heta} = \overline{oldsymbol{x}} - rac{\overline{oldsymbol{x}}^T oldsymbol{b}}{oldsymbol{b}^T oldsymbol{b}} oldsymbol{b} = \overline{oldsymbol{x}} - rac{\overline{oldsymbol{x}}^T oldsymbol{b}}{||oldsymbol{b}||} \cdot rac{oldsymbol{b}}{||oldsymbol{b}||}$$

Geometrical interpretation

 $\frac{\overline{x}^T b}{||b||}$ discribes a projection from \overline{x} on b. $\frac{\overline{x}^T b}{||b||} \cdot \frac{b}{||b||}$ gives us the projection point. So this constraint gives us a minimum at the shifted emperical mean in opposite direction of b by the value of the projection.

(b)

Find the parameter θ that minimizes $J(\theta)$ subject to the constraint $||\boldsymbol{\theta} - \boldsymbol{c}||^2 = 1$.

We have

$$\mathcal{L} = \sum_{k=1}^{n} ||oldsymbol{ heta} - oldsymbol{x}_k||^2 + \lambda ||oldsymbol{ heta} - oldsymbol{c}||^2 - \lambda$$

From this we get

$$0 = \frac{\partial}{\partial \theta} \mathcal{L} \tag{11}$$

$$\Leftrightarrow 0 = \sum_{k=1}^{n} 2\theta - 2x_k + 2\lambda(\theta - c)$$
 (12)

$$\Leftrightarrow 0 = n\theta - \sum_{k=1}^{n} x_k + \lambda \theta - \lambda c$$
 (13)

$$\Leftrightarrow 0 = \theta - \overline{x} + \frac{\lambda}{n}\theta - \frac{\lambda}{n}c$$
 (14)

$$\Leftrightarrow \frac{n+\lambda}{n}\boldsymbol{\theta} = \overline{\boldsymbol{x}} + \frac{\lambda}{n}\boldsymbol{c} \tag{15}$$

$$\Leftrightarrow \quad \boldsymbol{\theta} = \frac{n}{n+\lambda} \overline{\boldsymbol{x}} + \frac{\lambda}{n+\lambda} \boldsymbol{c} \tag{16}$$

and

$$0 = \frac{\partial}{\partial \lambda} \mathcal{L} \tag{17}$$

$$\Leftrightarrow 0 = ||\boldsymbol{\theta} - \boldsymbol{c}||^2 - 1 \tag{18}$$

$$\Leftrightarrow 0 = ||\boldsymbol{\theta} - \boldsymbol{c}||^2 - 1 \qquad \text{eq (16)}$$

$$\Leftrightarrow 0 = \left| \left| \frac{n}{n+\lambda} \overline{x} + \frac{\lambda}{n+\lambda} c - c \right| \right|^2 - 1$$
 (20)

$$\Leftrightarrow 0 = \left| \left| \frac{n}{n+\lambda} \overline{x} - \frac{n}{n+\lambda} c \right| \right|^2 - 1 \tag{21}$$

$$\Leftrightarrow 1 = \frac{n^2}{(n+\lambda)^2} ||\overline{x} - c||^2 \tag{22}$$

$$\Leftrightarrow (n+\lambda)^2 = n^2 ||\overline{x} - c||^2$$
(23)

$$\Rightarrow \lambda = n \cdot (||\overline{x} - c|| - 1) \tag{24}$$

With Eq (16) and Eq (24) we get

$$\begin{aligned} \boldsymbol{\theta} &= \frac{n}{n+n||\overline{x}-\boldsymbol{c}||-n} \overline{x} + \frac{n||\overline{x}-\boldsymbol{c}||-n}{n+n||\overline{x}-\boldsymbol{c}||-n} \boldsymbol{c} \\ &= \frac{1}{||\overline{x}-\boldsymbol{c}||} \overline{x} + \frac{||\overline{x}-\boldsymbol{c}||-1}{||\overline{x}-\boldsymbol{c}||} \boldsymbol{c} \\ &= \frac{1}{||\overline{x}-\boldsymbol{c}||} \overline{x} - \frac{1}{||\overline{x}-\boldsymbol{c}||} \boldsymbol{c} + \boldsymbol{c} \\ &= \frac{1}{||\overline{x}-\boldsymbol{c}||} (\overline{x}-\boldsymbol{c}) + \boldsymbol{c} \end{aligned}$$

Geometrical interpretation

2 Bounds on Eigenvalues

(a)

Show that $\sum_{i=1}^{d} S_{ii} \ge \lambda_1$.

Assumptions

Since S is a scatter matrix we can infer:

- (I) S is symmetrical
- (II) S is positive semi definite

Proof

We have

$$\lambda_1 \leq \sum_{i=1}^d S_{ii} = Tr(S) \stackrel{(I)}{=} \sum_{i=1}^d \lambda_i$$

$$\Leftrightarrow \quad 0 \leq \sum_{i=2}^d \lambda_i$$

which is fullfilled because with (II) we get $\forall i \in \{1, ..., d\} : \lambda_i \geq 0$.

- (b)
- (c)
- (d)

3 Iterative PCA

- (a)
- (b)

Programming

```
See next page.
```

[11pt]article

[T1]fontenc mathpazo

graphicx caption no label label format=no label

adjustbox xcolor enumerate geometry amsmath amssymb textcomp upquote eurosym [mathletters]ucs [utf8x]inputenc fancyvrb grffile hyperref longtable booktabs [inline]enumitem [normalem]ulem

urlcolorrgb0,.145,.698 linkcolorrgb.71,0.21,0.01 citecolorrgb.12,.54,.11

ansi-black
HTML3E424D ansi-black-intenseHTML282C36 ansi-red
HTMLE75C58 ansi-red-intenseHTMLB22B31 ansi-green
HTML00A250 ansi-green-intenseHTML007427 ansi-yellow
HTMLDDB62B ansi-yellow-intenseHTMLB27D12 ansi-blue
HTML208FFB ansi-blue-intenseHTML0065CA ansi-magenta
HTMLD160C4 ansi-magenta-intenseHTMLA03196 ansi-cyan
HTML60C6C8 ansi-cyan-intenseHTML258F8F ansi-white
HTMLC5C1B4

ansi-white-intenseHTMLA1A6B2 HighlightingVerbatimcommandchars=

{}

sheet04

incolorrgb0.0, 0.0, 0.5 outcolorrgb0.545, 0.0, 0.0

breaklinks=true, colorlinks=true, urlcolor=urlcolor, linkcolor=linkcolor, cite-color=citecolor,

verbose,tmargin=1in,bmargin=1in,lmargin=1in,rmargin=1in

4 Principal Component Analysis

4.1 Introduction

In this exercise, you will experiment with two different techniques to compute the principal components of a dataset:

- Basic PCA: The standard technique based on singular value decomposition.
- **Iterative PCA**: A technique that progressively optimizes the PCA objective function.

Principal component analysis is applied here to modeling handwritten characters data (characters "O" and "I") using the dataset introduced in the paper "L.J.P. van der Maaten. 2009. A New Benchmark Dataset for Handwritten Character Recognition". The dataset consists of black and white images of 28×28 pixels, each representing a handwritten character. For the purpose of the PCA analysis, these images are interpreted as 784-dimensional vectors with values between 0 and 1. Three methods are provided for your convenience and are available in the module utils that is included in the zip archive. The methods are the following:

- utils.load() load data from the file characters.csv and stores them in a data matrix of size 4631×784 . (The subset ofthe original dataset available here: http://lvdmaaten.github.io/publications/misc/characters.zip)
- utils.scatterplot(...) produces a scatter plot from a two-dimensional data set. Each point in the scatter plot represents one handwritten character. This method provides a convenient way to produce two-dimensional PCA plots.
- utils.render(...) takes a matrix of size $n \times 784$ as input, interprets it as n images of size 28×28 , and renders these images in the IPython notebook.

A demo code that makes use of these methods is given below. It performs basic data analysis, for example, plotting simple statistics for each data point in the dataset, or rendering a few examples randomly selected from the dataset. [commandchars=

```
\{\}\} In [1]: [rgb]0.00,0.50,0.00import [rgb]0.00,0.00,1.00utils[rgb]0.40,0.40,0.40,[rgb]0.00,0.00,1.00numpy [rgb]0.40,0.40,0.40%[rgb]0.00,0.50,0.00matplotlib inline [rgb]0.25,0.50,0.50# Load the characters "O" and "I" from the handwritten
```

characters dataset X [rgb]0.40,0.40,0.40= utils[rgb]0.40,0.40,0.40.load()

[rgb]0.00,0.50,0.00**print**([rgb]0.73,0.13,0.13'[rgb]0.73,0.13,0.13dataset size:

 $[rgb]0.73, 0.40, 0.53\% s [rgb]0.73, 0.13, 0.13 \\ [rgb]0.40, 0.40, 0.40 \\ [rgb]0.00, 0.50, 0.00 \\ \textbf{str}(X.shape))$

[rgb]0.25, 0.50, 0.50 # Plot some statistics of the data using the scatterplot func-

xlabel[rgb]0.40,0.40,0.40=[rgb]0.73,0.13,0.13'[rgb]0.73,0.13,0.13Averageylapixels 1...392[rgb]0.73,0.13,0.13', bel[rgb]0.40,0.40,0.40 = [rgb]0.73,0.13,0.13'[rgb]0.73,0.13,0.13Average value of $pixels\ 393...784[rgb]0.73,0.13,0.13')\ utils[rgb]0.40,0.40,0.40.scatterplot(X[:,::[rgb]0.40,0.40,0.402][rgb]0.40,0.40,0.40,0.40]$ xlabel[rgb]0.40,0.40,0.40=[rgb]0.73,0.13,0.13'[rgb]0.73,0.13,0.13Averagevalue pixels[rgb]0.73,0.13,0.13', of even ylabel[rgb]0.40,0.40,0.40 = [rgb]0.73,0.13,0.13'[rgb]0.73,0.13,0.13Averagevalue of odd pixels[rgb]0.73,0.13,0.13') [rgb]0.25, 0.50, 0.50 #randomly examplesRendersomeselectedR[rgb]0.40, 0.40, 0.40 = numpy[rgb]0.40, 0.40, 0.40, 0.40, random[rgb]0.40, 0.40, 0.40, randimt([rgb]0.40, 0.40,utils[rgb]0.40,0.40,0.40.render(X[R]) [commandchars=

{}] dataset size: (4631, 784)

 $\max \text{ size}=0.90.9 \text{sheet} 04_f iles/sheet 04_{11}.png$

max size=0.90.9sheet $04_files/sheet<math>04_{12}.png$

max size=0.90.9sheet $04_files/sheet<math>04_{13}.png$

The preliminary data analysis above does not reveal particularly interesting structure in the data. For example scatter plots fail to let appear the two types of characters present in the dataset ("O" and "I"). Therefore, we would like to gain more insight on the dataset by performing a more sophisticated analysis based on PCA.

4.2 PCA with Singular Value Decomposition (15 P)

As shown during the lecture, principal components can be found by solving the eigenvalue problem

$$Sw = \lambda w$$
.

While we could eigendecompose the scatter matrix to find the desired eigenvalues and eigenvectors (for example, by using the function numpy.linalg.eigh), we usually prefer to recover principal components directly from singular value decomposition

$$X = U \Sigma V^{\top}$$
.

where the principal components and projection of data onto these components can also be retrieved from the matrices U, Σ and V.

Tasks:

• Compute the principal components of the data using the function numpy.linalg.svd.

- Measure the computational time required to find the principal components. Use the function time.time() for that purpose. Do not include in your estimate the computation overhead caused by loading the data, plotting and rendering.
- Plot the projection of the dataset on the first two principal components using the function utils.scatterplot.
- Visualize the 25 leading principal components using the function utils.render.

Note that if the algorithm runs for more than 1 minute, you might be doing

something wrong. [commandchars= {}] In [2]: [rgb]0.00,0.50,0.00**import** [rgb]0.00,0.00,1.00**time** [rgb]0.40,0.40,0.40 =time[rgb]0.40,0.40,0.40.time()t.1 X.c[rgb]0.40,0.40,0.40 =X [rgb]0.40,0.40,0.40-X[rgb]0.40,0.40,0.40,.40.mean(axis[rgb]0.40,0.40,0.40=[rgb]0.40,0.40,0.400,dtype[rgb]0.40, 0.40, 0.40 = numpy[rgb]0.40, 0.40, 0.40, float64)u.s.v [rgb]0.40,0.40,0.40 = numpv[rgb]0.40,0.40,0.40.linalg[rgb]0.40,0.40,0.40.svd(X'c)W[rgb]0.40,0.40,0.40 = v[numpv[rgb]0.40,0.40,0.40.argsort(s)[[rgb]0.40,0.40,0.40][rgb]0.40,0.40,0.402:],:] [rgb]0.40,0.40,0.40 =W W[::[rgb]0.40,0.40,0.40-[rgb]0.40,0.40,0.40 =[rgb]0.40,0.40,0.401,:] **PCA** W[rgb]0.40,0.40,0.40,dot(X'c[rgb]0.40,0.40,0.40,T)[rgb]0.00, 0.50, 0.00**print** [rgb]0.73,0.13,0.13" [rgb]0.73,0.13,0.13Time: [rgb]0.73,0.13,0.13" [rgb]0.40,0.40,0.40+[rgb]0.00,0.50,0.00str(time[rgb]0.40,0.40,0.40.time())[rgb]0.40,0.40,0.40-t1 [rgb]0.40,0.40,0.40+[rgb]0.73,0.13,0.13 [rgb]0.73,0.13,0.13seconds.[rgb]0.73,0.13,0.13" utils[rgb]0.40,0.40,0.40.scatterplot(PCA[[rgb]0.40,0.40,0.400,:],PCA[[rgb]0.40,0.40,0.401,:],xlabel[rgb]0.40,0.40,0.40=[rgb]0.73,0.13,0.13'[rgb]0.73,0.13,0.13PCA1[rgb]0.73, 0.13, 0.13', ylabel[rgb]0.40, 0.40, 0.40 = [rgb]0.73, 0.13, 0.13'[rgb]0.73, 0.13, 0.13PCA2[rgb]0.73,0.13,0.13') eig[rgb]0.40,0.40,0.40 = v[numpy[rgb]0.40,0.40,0.40.argsort(s)][rgb]0.40,0.40,0.40[rgb]0.40.0.40.0.4025:],:] eig [rgb]0.40,0.40,0.40 = eig[::[rgb]0.40,0.40,0.40[rgb]0.40,0.40,0.401,:] utils[rgb]0.40,0.40,0.40.render(eig) [commandchars= {}] Time: 9.75734400749 seconds.

 $\max \text{ size} = 0.90.9 \text{sheet} 04_f iles/sheet 04_{32}.png$

 $\max \text{ size}=0.90.9 \text{sheet } 04_f iles/sheet 04_{31}.png$

4.3 Iterative PCA (15 P)

The objective that PCA optimizes is given by

$$J(\boldsymbol{w}) = \boldsymbol{w}^{\top} \boldsymbol{S} \boldsymbol{w}$$

subject to

$$\boldsymbol{w}^{\top} \boldsymbol{w} = 1.$$

The power iteration algorithm maximizes this objective using an iterative procedure. It starts with an initial weight vector \boldsymbol{w} , and iteratively applies the update rule

$$\boldsymbol{w} \leftarrow \frac{\boldsymbol{S}\boldsymbol{w}}{\|\boldsymbol{S}\boldsymbol{w}\|}$$

Tasks:

[rgb]0.00,0.50,0.00**if**

- Implement the iterative procedure. Use as a stopping criterion the value of J(w) between two iterations increasing by less than 0.01.
- Print the value of the objective function J(w) at each iteration.
- Measure the time taken to find the principal component.
- Visualize the the eigenvector w obtained after convergence using the function utils.render.

Note that if the algorithm runs for more than 1 minute, you might be doing

something wrong. [commandchars= {}] In [3]: [rgb]0.40,0.40,0.40 = time[rgb]0.40,0.40,0.40.time() Nt1[rgb]0.40,0.40,0.40 =X[rgb]0.40,0.40,0.40.shape[[rgb]0.40,0.40,0.400][rgb]0.40,0.40,0.40 =[rgb]0.40,0.40,0.40-Χ X[rgb]0.40,0.40,0.40.mean(axis[rgb]0.40,0.40,0.40=[rgb]0.40,0.40,0.400,dtype[rgb]0.40, 0.40, 0.40 = numpy[rgb]0.40, 0.40, 0.40, float64)[rgb]0.40,0.40,0.40 =[rgb]0.40,0.40,0.401.0[rgb]0.40,0.40,0.40/N $[rgb]0.40,0.40,0.40^* \text{ X'c}[rgb]0.40,0.40,0.40.\text{T}[rgb]0.40,0.40,0.40.\text{dot}(\text{X'c})$ w [rgb] 0.40, 0.40, 0.40 = numpy [rgb] 0.40, 0.40, 0.40, 0.40, random [rgb] 0.40, 0.40, 0.40, normal ([rgb] 0.40, 0.40, 0.40, 0.40, [rgb] 0.40, 0.40w [rgb] 0.40, 0.40, 0.40 = [rgb] 0.40, 0.40, 0.401 [rgb] 0.40, 0.40, 0.40 / numpy [rgb] 0.40, 0.40, 0.40. linalg [rgb] 0.40, 0.40, 0.40 / numpy [rgb] 0.40 / numpy[rgb]0.40,0.40,0.40* w j'last [rgb]0.40,0.40,0.40 =[rgb]0.40,0.40,0.40-[rgb]0.40,0.40,0.401 [rgb]0.40,0.40,0.40 =j current [rgb]0.40,0.40,0.40-[rgb]0.40,0.40,0.401 [rgb]0.40,0.40,0.40 =[rgb]0.40,0.40,0.400 [rgb]0.00,0.50,0.00**while** [rgb]0.00,0.50,0.00True: [rgb]0.40,0.40,0.40 =[rgb]0.40,0.40,0.40 =S[rgb]0.40,0.40,0.40,dot(w)[rgb]0.40,0.40,0.401[rgb]0.40,0.40,0.40/numpy[rgb]0.40,0.40,0.40.linalg[rgb]0.40,0.40,0.40.norm(w)[rgb]0.40,0.40,0.40* w i'last [rgb]0.40,0.40,0.40 = j current j current [rgb]0.40, 0.40, 0.40 = w[rgb]0.40, 0.40, 0.40, 0.40, T[rgb]0.40, 0.40, 0.40, 0.40, dot(S[rgb]0.40, 0.40, 0.40, dot(w))[rgb]0.00,0.50,0.00**print** [rgb]0.73,0.13,0.13" [rgb]0.73,0.13,0.13 iteration [rgb]0.73,0.13,0.13" [rgb]0.40,0.40,0.40+[rgb]0.00,0.50,0.00str(i)[rgb]0.40,0.40,0.40+[rgb]0.73,0.13,0.13"[rgb]0.73,0.13,0.13 [rgb]0.73,0.13,0.13" [rgb]0.40,0.40,0.40+J(w)[rgb]0.00,0.50,0.00str(j current[[rgb]0.40,0.40,0.400,[rgb]0.40,0.40,0.400])

[rgb]0.40,0.40,0.40;

[rgb]0.40,0.40,0.400)

(j'last

```
[rgb]0.67,0.13,1.00and
                                               numpy[rgb]0.40,0.40,0.40.abs(j'last)
[rgb]0.40,0.40,0.40-
                      j current)
                                   [rgb]0.40,0.40,0.40; [rgb]0.40,0.40,0.400.01:
[rgb]0.00,0.50,0.00print
                                   [rgb]0.73,0.13,0.13"[rgb]0.73,0.13,0.13Stopping
               satisfied. [rgb]0.73, 0.13, 0.13"
                                                   [rgb]0.00, 0.50, 0.00break
creterion
[rgb]0.40,0.40,0.40+[rgb]0.40,0.40,0.40=[rgb]0.40,0.40,0.401
[rgb]0.00,0.50,0.00print
                                      [rgb]0.73,0.13,0.13"[rgb]0.73,0.13,0.13Time:
[rgb]0.73, 0.13, 0.13" [rgb]0.40, 0.40, 0.40 + [rgb]0.00, 0.50, 0.00 str(time[rgb]0.40, 0.40, 0.40, 0.40, time())
[rgb]0.40,0.40,0.40-t1) [rgb]0.40,0.40,0.40+ [rgb]0.73,0.13,0.13" [rgb]0.73,0.13,0.13
seconds.[rgb]0.73,0.13,0.13" utils[rgb]0.40,0.40,0.40.render(w[rgb]0.40,0.40,0.40.T)
```

[commandchars=

 $\{\}]$ iteration 0 J(w) = 2.9689384223 iteration 1 J(w) = 3.82131949849 iteration 2 J(w) = 4.84240465711 iteration 3 J(w) = 8.66375108562 iteration 4 J(w) = 12.2808867695 iteration 5 J(w) = 12.9987068232 iteration 6 J(w) = 13.0808942813 iteration 7 J(w) = 13.0896578376 Stopping creterion satisfied. Time: 0.211755037308 seconds.

max size=0.90.9sheet $04_files/sheet<math>04_{51}.png$

sheet04

November 13, 2017

1 Principal Component Analysis

1.1 Introduction

In this exercise, you will experiment with two different techniques to compute the principal components of a dataset:

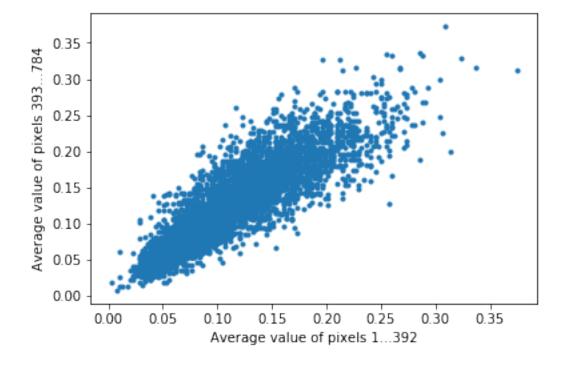
- Basic PCA: The standard technique based on singular value decomposition.
- Iterative PCA: A technique that progressively optimizes the PCA objective function.

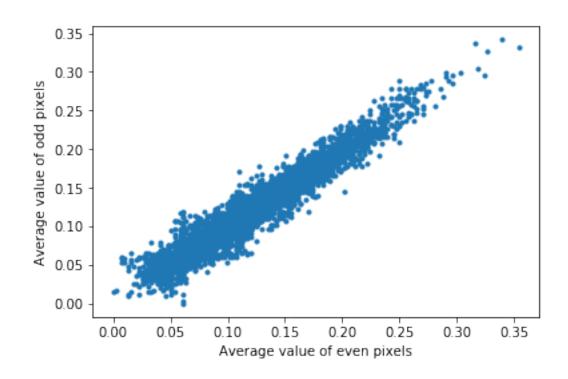
Principal component analysis is applied here to modeling handwritten characters data (characters "O" and "I") using the dataset introduced in the paper "L.J.P. van der Maaten. 2009. A New Benchmark Dataset for Handwritten Character Recognition". The dataset consists of black and white images of 28×28 pixels, each representing a handwritten character. For the purpose of the PCA analysis, these images are interpreted as 784-dimensional vectors with values between 0 and 1. Three methods are provided for your convenience and are available in the module utils that is included in the zip archive. The methods are the following:

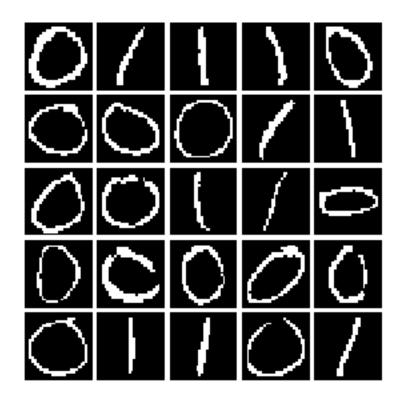
- utils.load() load data from the file characters.csv and stores them in a data matrix of size 4631 × 784. (The data is a subset of the original dataset available here: http://lvdmaaten.github.io/publications/misc/characters.zip)
- utils.scatterplot(...) produces a scatter plot from a two-dimensional data set. Each point in the scatter plot represents one handwritten character. This method provides a convenient way to produce two-dimensional PCA plots.
- utils.render(...) takes a matrix of size $n \times 784$ as input, interprets it as n images of size 28×28 , and renders these images in the IPython notebook.

A demo code that makes use of these methods is given below. It performs basic data analysis, for example, plotting simple statistics for each data point in the dataset, or rendering a few examples randomly selected from the dataset.

dataset size: (4631, 784)







The preliminary data analysis above does not reveal particularly interesting structure in the data. For example scatter plots fail to let appear the two types of characters present in the dataset ("O" and "I"). Therefore, we would like to gain more insight on the dataset by performing a more sophisticated analysis based on PCA.

1.2 PCA with Singular Value Decomposition (15 P)

As shown during the lecture, principal components can be found by solving the eigenvalue problem

$$Sw = \lambda w$$
.

While we could eigendecompose the scatter matrix to find the desired eigenvalues and eigenvectors (for example, by using the function numpy.linalg.eigh), we usually prefer to recover principal components directly from singular value decomposition

$$X = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^{\top}$$
,

where the principal components and projection of data onto these components can also be retrieved from the matrices U, Σ and V.

Tasks:

- Compute the principal components of the data using the function numpy.linalg.svd.
- Measure the computational time required to find the principal components. Use the function time.time() for that purpose. Do not include in your estimate the computation overhead caused by loading the data, plotting and rendering.
- Plot the projection of the dataset on the first two principal components using the function utils.scatterplot.
- Visualize the 25 leading principal components using the function utils.render.

Note that if the algorithm runs for more than 1 minute, you might be doing something wrong.

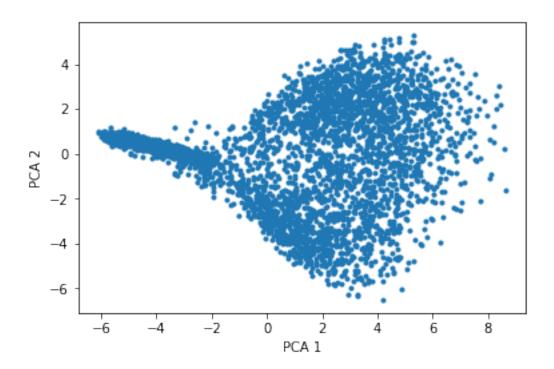
```
In [2]: import time

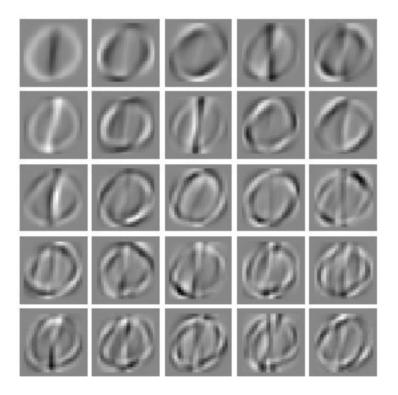
t1 = time.time()
X_c = X - X.mean(axis=0, dtype=numpy.float64)

u,s,v = numpy.linalg.svd(X_c)
W = v[numpy.argsort(s)[-2:],:]
W = W[::-1,:]
PCA = W.dot(X_c.T)
print "Time: " + str(time.time() - t1) + " seconds."

utils.scatterplot(PCA[0,:],PCA[1,:], xlabel='PCA 1', ylabel='PCA 2')
eig = v[numpy.argsort(s)[-25:],:]
eig = eig[::-1,:]
utils.render(eig)
```

Time: 9.75734400749 seconds.





1.3 Iterative PCA (15 P)

The objective that PCA optimizes is given by

$$I(w) = w^{\top} S w$$

subject to

$$\boldsymbol{w}^{\top}\boldsymbol{w}=1.$$

The power iteration algorithm maximizes this objective using an iterative procedure. It starts with an initial weight vector w, and iteratively applies the update rule

$$w \leftarrow rac{Sw}{\|Sw\|}$$

Tasks:

- Implement the iterative procedure. Use as a stopping criterion the value of J(w) between two iterations increasing by less than 0.01.
- Print the value of the objective function J(w) at each iteration.
- Measure the time taken to find the principal component.
- Visualize the the eigenvector w obtained after convergence using the function utils.render.

Note that if the algorithm runs for more than 1 minute, you might be doing something wrong.

```
In [3]: t1 = time.time()
        N = X.shape[0]
        X_c = X - X.mean(axis=0, dtype=numpy.float64)
        S = 1.0/N * X_c.T.dot(X_c)
        w = numpy.random.normal(0,1,size=(S.shape[0],1))
        w = 1/numpy.linalg.norm(w) * w
        j_last = -1
        j_current = -1
        i = 0
        while True:
            w = S.dot(w)
            w = 1/numpy.linalg.norm(w) * w
            j_last = j_current
            j_current = w.T.dot(S.dot(w))
            print "iteration " + str(i) + " J(w) = " + str(j_current[0,0])
            if (j_last > 0) and numpy.abs(j_last - j_current) < 0.01:
                print "Stopping creterion satisfied."
                break
```

```
i += 1

print "Time: " + str(time.time() - t1) + " seconds."
    utils.render(w.T)

iteration 0 J(w) = 2.9689384223
iteration 1 J(w) = 3.82131949849
iteration 2 J(w) = 4.84240465711
iteration 3 J(w) = 8.66375108562
iteration 4 J(w) = 12.2808867695
iteration 5 J(w) = 12.9987068232
iteration 6 J(w) = 13.0808942813
iteration 7 J(w) = 13.0896578376
Stopping creterion satisfied.
Time: 0.211755037308 seconds.
```

