12. Machine learning I

- Regression
- Overfitting
- Classification
- Example: Handwritten digit recognition
- Support vector machines (SVMs)

Regression

- Suppose we are given *N* pairs of a vector **x** and a scalar *d*

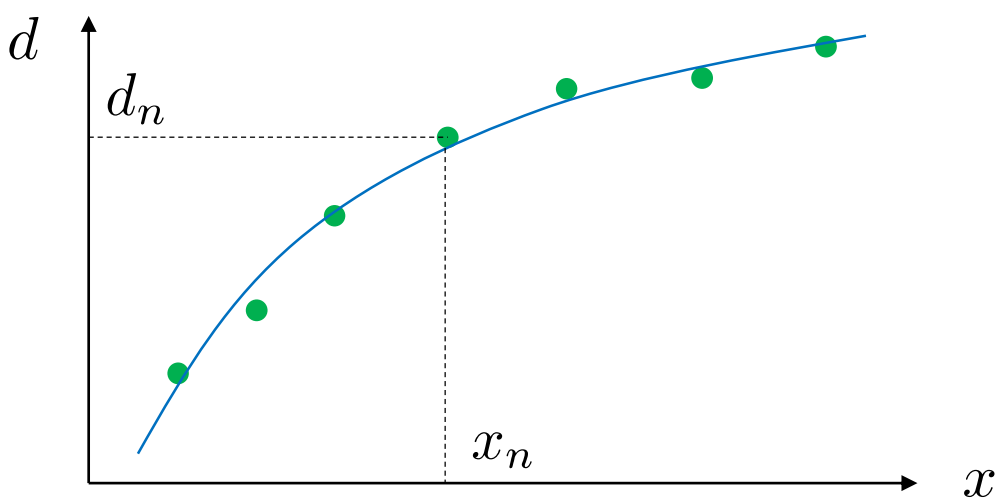
$$\{\mathbf{x}_n\}(n = 1, \ldots, N) \qquad \{d_n\}(n = 1, \ldots, N)$$

- We wish to predict *d* for a new input **x**
  - **x**, called an independent variable, is observation used for predicting
  - *d, called a dependent variable, is the target, or the desired value to predict*

- Toward this goal, we consider a function that approximately satisfies

$$y(\mathbf{x}_n) \sim d_n$$

  - You can use any arbitrary (analytical) function for y(x)



Fitting polynomial functions

- Consider fitting a n-order polynomial func., instead of a linear func. considered earlier

$$y = a_0 + a_1 x + a_2 x^2 + \cdots a_n x^n$$

$$\sum_{i=1}^{N} \| y_i - (a_0 + a_1 x_i + a_2 x_i^2 + \cdots a_n x_i^n) \|^2 \to \min$$

- `polyfit` performs this
  - E.g., You can fit a linear func. as follows, instead of using `pinv`

```
>> p=polyfit(x,y,1);
```

```
>> p=pinv(X)*y;
```

  - E.g., 3rd-order polynomial function

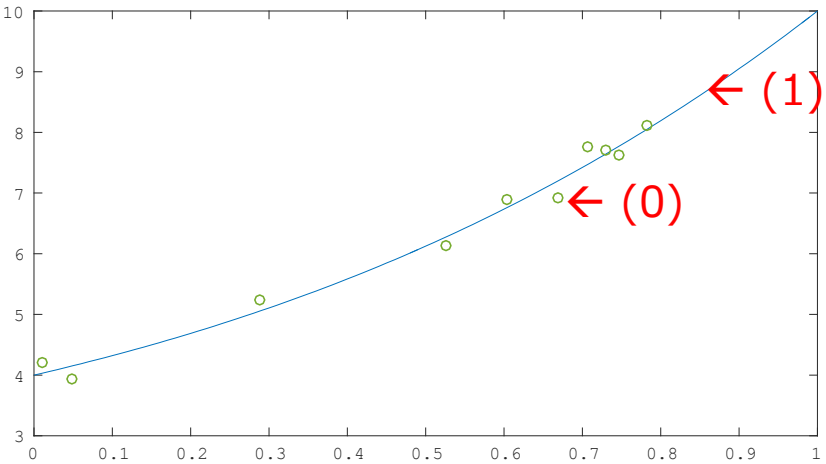
```
>> p=polyfit(x,y,3)
ans =
   -2.2455    3.8778   -1.3517    0.4603
```

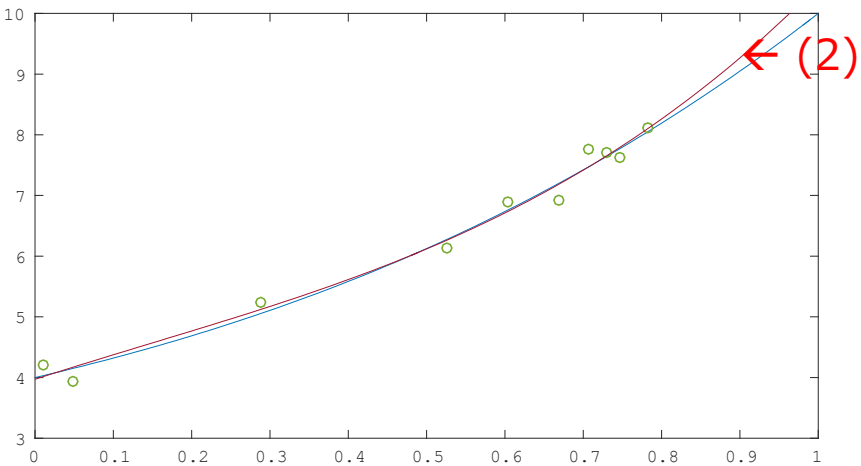
a_3 a_2 a_1 a_0

Fitting polynomial functions: an example

```
>> x=rand(10,1);
>> p0=[1.0,2.0,3.0,4.0];
>> y=p0(1)*x.^3+p0(2)*x.^2+p0(3)*x+p0(4)+0.2*randn(10,1);
>> plot(x,y,'o') ← (0)
>>
>> hold on
>> xx=0:0.01:1;
>> yy=p0(1)*xx.^3+p0(2)*xx.^2+p0(3)*xx+p0(4);
>> plot(xx,yy) ← (1)
>>
>> p=polyfit(x,y,3);
>> plot(xx,polyval(p,xx)) ← (2)
```

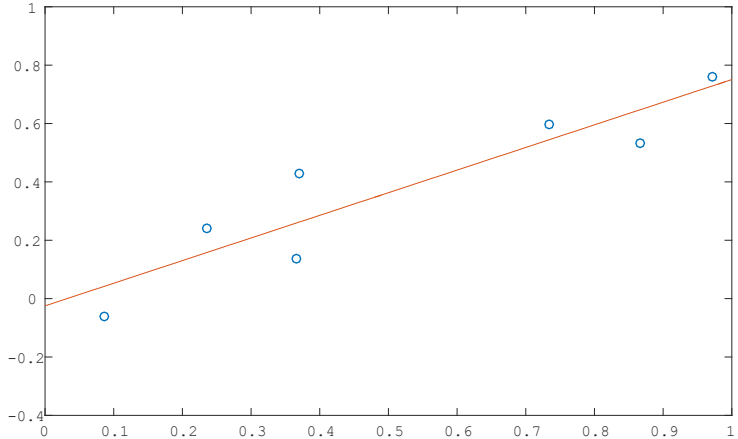
Data are synthesized here for the purpose of explanation



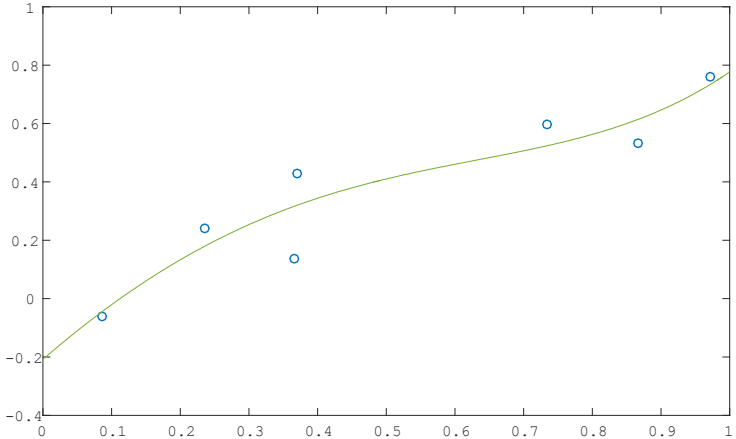


Overfitting (also called *overtraining*)

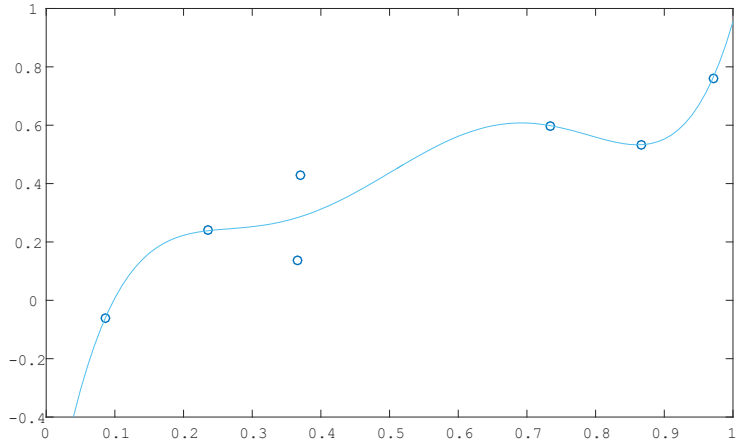
- If you fit 1st, 3rd, 5th, and 6th-order funcs to seven data points…
  - Models with excessively large degrees of freedom can explain data perfectly even including their noises, which is totally meaningless!



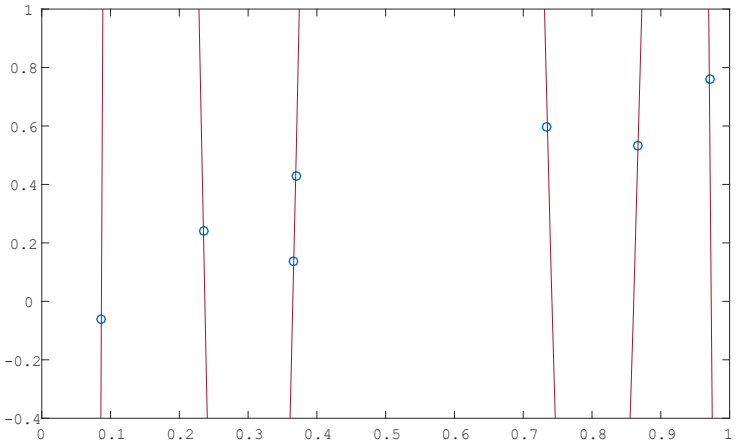
1st order (a line)



3rd-order



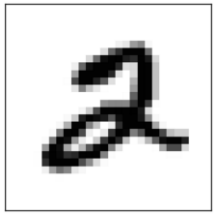
5th-order



6th-order

Classification

- Consider a variable **x** belonging to one of *K* classes
- Classification = assigning an input **x** with one of *K* class labels
  - E.g., **x** is an image of a digit; we wish to answer what digit it is



$\mathbf{x}$

0,1,2,3,4,5,6,7,8,9

- Supposing that *N* pairs of input **x** and its true class label *d* are given

$$\{\mathbf{x}_n\}(n = 1, \ldots, N) \qquad \{d_n\}(n = 1, \ldots, N)$$

we wish to predict which class a new input **x** belongs to

Example: Handwritten digit recognition

- We use *MNIST*, a famous dataset of handwritten digit recognition

  `http://yann.lecun.com/exdb/mnist/`

  - Download and unzip the following file from the course page

    `mnist-data.zip`

  - We use the following two files today:

    `t10k-images-idx3-ubyte` & `t10k-labels-idx1-ubyte`

- We use *support vector machines* (*SVMs*) for classification
- For this purpose, we use *liblinear*, a software library of SVM

Installing *liblinear*, a software library for SVM

- liblinear
  - One of the most popular libraries in machine learning created by *Machine Learning Group* at *National Taiwan University*
- Download files from the URL:
  - https://www.csie.ntu.edu.tw/~cjlin/liblinear
- Extract the downloaded file and change the current directory to `liblinear-x.xx/matlab`
  - `cd /Users/xxxx/Octave/liblinear-2.11/matlab`
- Run make.m
  - `>> make`
- Add the folder to search paths
  - `>> addpath('/Users/xxxx/Octave/liblinear-2.11/matlab')`

Support vector machines (SVMs) (1/2)*

- Consider two-class classification : $d_n = 1 \text{ or } -1$
- A set of samples are given : $(\boldsymbol{x}_1, d_1), (\boldsymbol{x}_2, d_2), \cdots, (\boldsymbol{x}_N, d_N)$
- We employ the following method for classification:

$$y(\mathbf{x}) = \begin{cases} 1 & \text{if } u(\mathbf{x}) > 0 \\ -1 & \text{otherwise} \end{cases}$$

where $u(\mathbf{x}, \mathbf{w}) = w_0 + w_1 x_1 + \cdots + w_I x_I = w_0 + \mathbf{w}^\top \mathbf{x}$

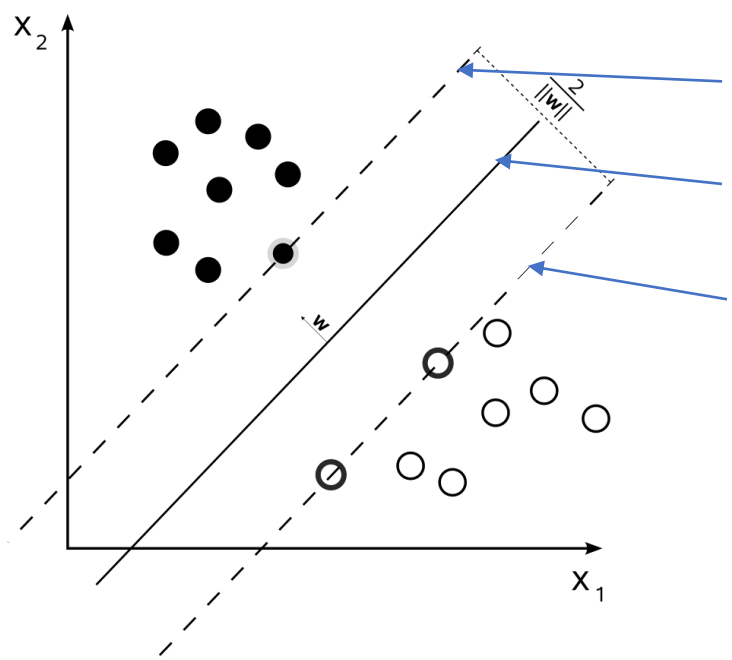
- **w**, called weights, is a parameter to be determined
- Consider determining w as follows:
  - Known as a *hard-margin SVM*

Minimize $\|\mathbf{w}\| \quad \text{subject to} \quad d_n(w_0 + \mathbf{w}^\top \mathbf{x}) \geq 1$

Support vector machines (SVMs) (2/2)*

- We consider two parallel planes separating data points correctly into two corresponding classes that have the maximum distance
  - For simplicity we assume here that the data points can be separated by a plane (called *linearly separable*)
- We then choose the parallel plane in the exact middle of the two parallel plane; we use its parameters w_0 and **w**
  - Why do we do this? → It will be safe to choose the plane having the maximum distances to the nearest data points for the purpose of classifying new inputs **x**'s correctly

$$\Updownarrow$$



$$w_0 + \mathbf{w}^\top \mathbf{x} = 1$$

$$w_0 + \mathbf{w}^\top \mathbf{x} = 0$$

$$w_0 + \mathbf{w}^\top \mathbf{x} = -1$$

&

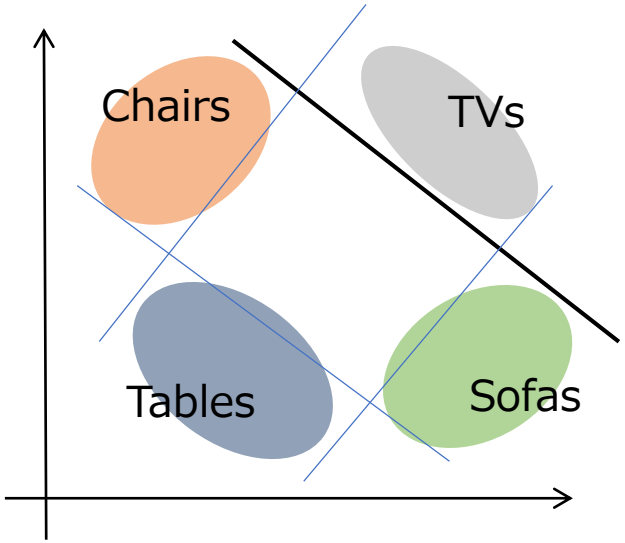
Minimize $\|\mathbf{w}\|$ subject to $d_n(w_0 + \mathbf{w}^\top \mathbf{x}) \geq 1$

Classification of multiple classes*

- Two-class classifier is trained for each class to distinguish it from the others
  - Called the *one-versus-the-rest* classifier

1. k^{th} model $y_k(x)$ is trained to classify class k and other classes
2. Regarding the output of each model as *score* of the model, we classify an input sample to the class with the largest score

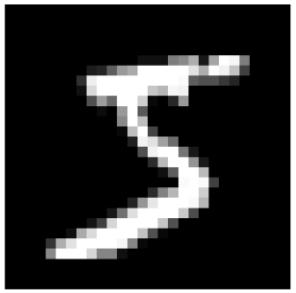
$$\underset{k}{\operatorname{argmax}}\, y_k(\mathbf{x})$$



Reading data from MNIST files

- Loading images to Octave:
  - File ‘test-images-idx3-ubyte’ contains 10,000 images of 28x28 pixels
  - Skip the first four integers (32bits) and load the remaining numerical data into a variable named `data`
  - To display images, first reshape the image data into a tensor of appropriate size and use `imshow(matrix, [brightness_min, brightness_max])`

```
>> fid=fopen('t10k-images-idx3-ubyte','r','b');
>> fread(fid,4,'int32')
>> data=fread(fid,[28*28,10000],'uint8');
>> fclose(fid);
>> img=reshape(data,28,28,10000);
>> imshow(img(:,:,1)',[0,255])
>> imshow(img(:,:,100)',[0,255])
```



- Loading labels to Octave:
  - File ‘test-labels-idx1-ubyte’ contains labels of the images in the same order
  - Skip the first two integers (32bits) and load the remaining integers into a variable named `label`

```
>> fid=fopen('t10k-labels-idx1-ubyte','r','b');
>> fread(fid,2,'int32')
>> label=fread(fid,10000,'uint8');
```

Check the contents of this variable

Training and testing a classifier

- Train a classifier using, say, 5,000 samples (images) from the data
  - Train a model (SVM) using samples with indices 1,⋯,5000:

```
>> tr_label = label(1:5000);
>> tr_data = data(:,1:5000);
>> model = train(tr_label,sparse(tr_data)');
...
Objective value = -0.081903
nSV = 910
```

Status of training, which you can ignore (as long as the training went well)

- Evaluate the performance of the classifier using the remaining samples
  - Test the model using samples with indices 5001,⋯,6000:

```
>> te_label = label(5001:6000);
>> te_data = data(:,5001:6000);
>> pred_label = predict(te_label,sparse(te_data)',model)
Accuracy = 84.6% (846/1000)
pred_label =
    2
    3
...
```

Classification accuracy for the input 1,000 samples is shown

Predicted labels for the 1,000 samples; note that the numbers do not correspond to the true digits; these numbers correspond to the indices of model.Label, which stores the true labels of digits

Visualization of weights*

- `predict` performs the following computation

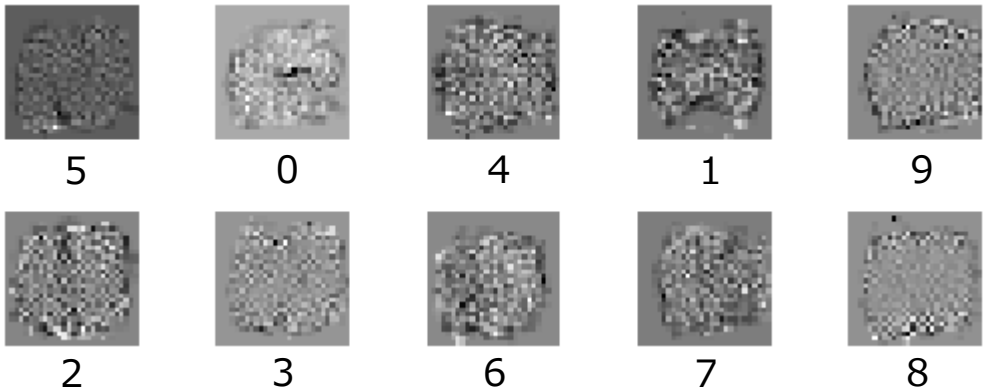
```
>> for i=1:10,model.w(i,:)*reshape(te_data(:,4),28*28,1)+model.bias,end
ans = -5.3081
...
...
ans = -17.245
ans =  2.5717
...
```

```
>> te_label(4)
ans =  6
>> model.Label
ans =

   5
   0
   4
   1
   9
   2
   3
   6
   7
   8
```

- Visualize the trained weights as images
  - Can you tell where in the image the model looks at to classify each digit?

```
>> figure
>> for i=1:10,subplot(2,5,i),imshow(reshape(model.w(i,:),28,28),[min(model.w(i,:)),max(model.w(i,:))]),end
```



The order of weights is specified by `model.Label`

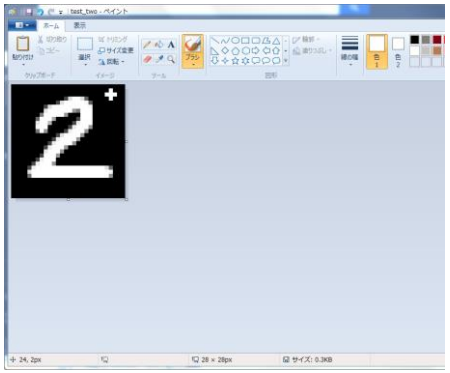
Exercise 12.1 (Make the model recognize your handwritten digit)

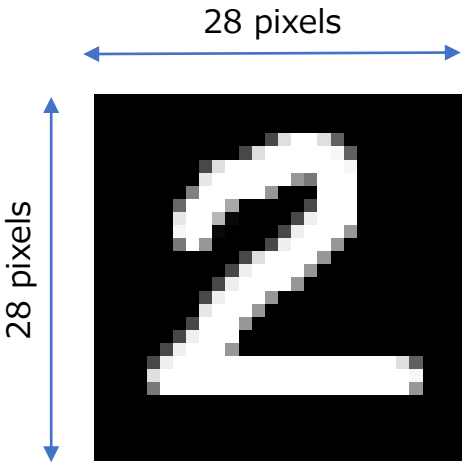
- Make two hand-written images; one can be recognized correctly by your trained model, and another is which cannot be recognized correctly.

  - You can make hand-written digit images in paint tool.
  - Load your image and try your SVM model.

Black background and white foreground in “png” format

For assignment, please attach your images in addition to script and PDF.





Hint：How to test your png file on your trained model

```
>> sample = imread('a_number_I_wrote.png');
>> sample = mean(sample,3);
```

Convert your image into grayscale if it is a color image

True label

```
>> predict([2], sparse(reshape(sample',1,28*28)), model)
Accuracy = 100% (1/1)
ans =  2
```

Predicted label; this is correct!