Unit 8
Support Vector Machines

EL-GY 6143/CS-GY 6923: INTRODUCTION TO MACHINE LEARNING

PROF. PEI LIU

Midterm

- Midterm
  - March 29 (Monday), 11:00AM-1:30PM ET via Zoom
  - Zoom link will be emailed later this week
  - Exam questions via Google form
    - https://docs.google.com/forms/d/e/1FAIpQLSe8Ugqv7UhBv2B6zd7nYwhzX78cno7EnPjvfrdHaRKtBnBujQ/viewform?usp=sf_link
- Policy
  - Close-book exam
  - 2 piece of paper cheatsheet, can write on both sides.
  - Attendance at exams is mandatory
- What will be included in the midterm?
  - All materials taught in Lecture 1 to Lecture 7
  - Not include Lecture 8: SVM
  - 6-7 questions, very similar to homework

Requirements for Midterm

- ❑Please join the meeting on 15 minutes before 11AM, and use your full name when you join.
- ❑Each student is required to open Zoom and turn on their video, making sure the camera captures your hands and your computer screen/keyboard. The whole exam will be recorded. To clearly capture the video of exam taking, it is recommended that:
  - A student can use an external webcam connected to the computer;
  - Or use another device (smartphone/ipad/laptop with power plugged in);
  - In both cases, adjust the position/orientation of the camera so that it clearly captures the keyboard, screen and both hands.
- ❑During the exam, you should keep your video on all the time. If there is anything wrong with your Zoom connection, please recoonect ASAP. If you cannot reconnect, please email ASAP.

Midterm Submission

- Students can read exam questions from computer screen, and write answers on BLANK papers using pen/pencil. If you have a printer, you can also print the questions and answer directly on the question papers.
  - Use a separate page for each question, and clear mark the questions on the top of the page.
- At 1:30PM, submit a single PDF to newclasses.nyu.edu, under the assignment named "Midterm Exam".
  - Use Adobe Scan APP/iPhone Notes APP/etc to scan your answers;
  - Don't upload several photos;
  - The DEADLINE for submission is in 10 minutes .If you never used your phone to scan a documents, give it a try before the exam;
  - Before you leave the exam, it's your responsibility to make sure all your answers are uploaded.

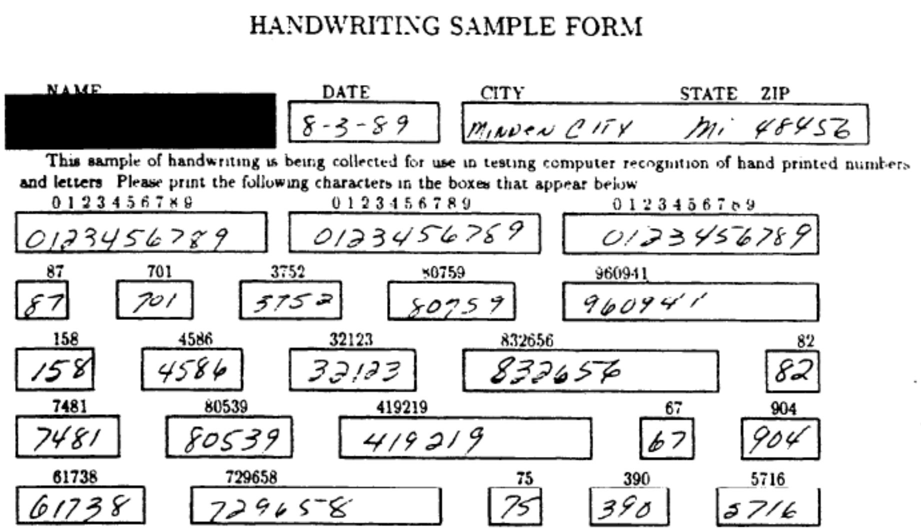
Learning Objectives

- ❑Interpret weights in linear classification of images
- ❑Describe why linear classification for images does not work
- ❑Define the margin in linear classification
- ❑Describe the SVM classification problem.
- ❑Write equations for solutions of constrained optimization using the Lagrangian.
- ❑Describe a kernel SVM problem for non-linear classification
- ❑Implement SVM classifiers in python
- ❑Select SVM parameters from cross-validation

Outline

- Motivating example: Recognizing handwritten digits
  - Why logistic regression doesn't work well.
- Maximum margin classifiers
- Support vector machines
- Kernel trick
- Constrained optimization

MNIST Digit Classification


HANDWRITING SAMPLE FORM

NAME [redacted] DATE 8-3-89 CITY MINDEN CITY STATE MI ZIP 48456

This sample of handwriting is being collected for use in testing computer recognition of hand printed numbers and letters. Please print the following characters in the boxes that appear below.

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

87   701   3752   80759   960941

158   4586   32123   832656   82

7481   80539   419219   67   904

61738   729658   75   390   5716

- Problem: Recognize hand-written digits
- Original problem:
  - Census forms
  - Automated processing
- Classic machine learning problem
- Benchmark

From Patrick J. Grother, NIST Special Database, 1995

A Widely-Used Benchmark

- We will look at SVM today
- Not the best algorithm
- But quite good
- ...and illustrates the main points

Classifiers [edit]

This is a table of some of the machine learning methods used on the database and their error rates, by type of classifier:

Type	Classifier	Distortion	Preprocessing	Error rate (%)
Linear classifier	Pairwise linear classifier	None	Deskewing	7.6[9]
K-Nearest Neighbors	K-NN with non-linear deformation (P2DHMDM)	None	Shiftable edges	0.52[14]
Boosted Stumps	Product of stumps on Haar features	None	Haar features	0.87[15]
Non-Linear Classifier	40 PCA + quadratic classifier	None	None	3.3[9]
Support vector machine	Virtual SVM, deg-9 poly, 2-pixel jittered	None	Deskewing	0.56[16]
Neural network	2-layer 784-800-10	None	None	1.6[17]
Neural network	2-layer 784-800-10	elastic distortions	None	0.7[17]
Deep neural network	6-layer 784-2500-2000-1500-1000-500-10	elastic distortions	None	0.35[18]
Convolutional neural network	Committee of 35 conv. net, 1-20-P-40-P-150-10	elastic distortions	Width normalizations	0.23[8]

Downloading MNIST

```
import tensorflow as tf

(Xtr,ytr),(Xts,yts) = tf.keras.datasets.mnist.load_data()

print('Xtr shape: %s' % str(Xtr.shape))
print('Xts shape: %s' % str(Xts.shape))

ntr = Xtr.shape[0]
nts = Xts.shape[0]
nrow = Xtr.shape[1]
ncol = Xtr.shape[2]
```

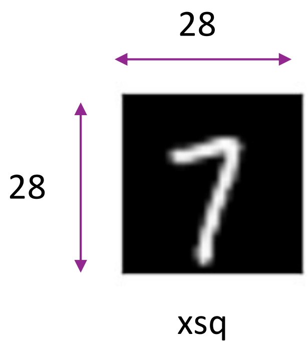
```
Xtr shape: (60000, 28, 28)
Xts shape: (10000, 28, 28)
```

- MNIST data is available in many sources
  - Note: It has been removed from sklearn
- Tensorflow version:
  - 60000 training samples
  - 10000 test samples
- Each sample is a 28 x 28 images
- Grayscale: Pixel values $\in \{0,1,\ldots,255\}$
  - 0 = Black and
  - 255 = White

Matrix and Vector Representation

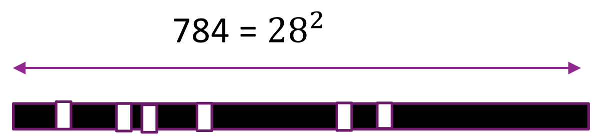
- For this demo, we reshape data from $N\times 28\times 28$ to $N\times 784$
- But, you can easily go back and forth
- Also, scale the pixel values from -1 to 1

```python
npix = nrow*ncol
Xtr = 2*(Xtr/255 - 0.5)
Xtr = Xtr.reshape((ntr,npix))

Xts = 2*(Xts/255 - 0.5)
Xts = Xts.reshape((nts,npix))
```




```python
x = xsq.ravel()
```

```python
xsq = x.reshape((28,28))
```



$$S = \mathrm{Mat}(x) = \begin{bmatrix} s_{11} & \cdots & s_{1,28} \\ \vdots & \vdots & \vdots \\ s_{28,1} & \cdots & s_{28,28} \end{bmatrix}$$

$$x = \mathrm{vec}(S) = [x_1 \quad \cdots \quad x_{784}]$$

Displaying Images in Python

4 random images in the dataset

A human can classify these easily

```
def plt_digit(x):
    nrow = 28
    ncol = 28
    xsq = x.reshape((nrow,ncol))
    plt.imshow(xsq,  cmap='Greys_r')
    plt.xticks([])
    plt.yticks([])

# Convert data to a matrix
X = mnist.data
y = mnist.target

# Select random digits
nplt = 4
nsamp = X.shape[0]
Iperm = np.random.permutation(nsamp)

# Plot the images using the subplot command
for i in range(nplt):
    ind = Iperm[i]
    plt.subplot(1,nplt,i+1)
    plt_digit(X[ind,:])
```

Key command

Sample permutation is necessary for this dataset, as the original data is ordered by digits

Try a Logistic Classifier

```
ntr1 = 5000
Xtr1 = Xtr[Iperm[:ntr1],:]
ytr1 = ytr[Iperm[:ntr1]]
```

- ❑ Train on 5000 samples
  - To reduce training time.
  - In practice want to train with ~40k
- ❑ Select correct solver (lbfgs)
  - Others can be very slow. Even this will take minutes

```
from sklearn import linear_model
logreg = linear_model.LogisticRegression(verbose=10, solver='lbfgs',\
                                          multi_class='multinomial',max_iter=500)
logreg.fit(Xtr1,ytr1)
```

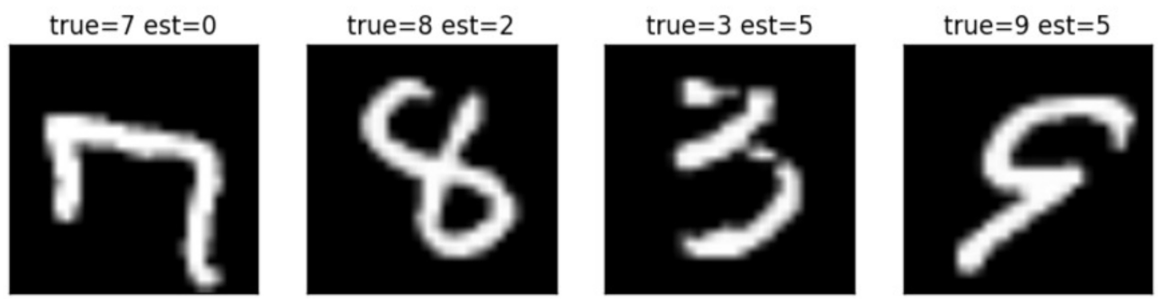
```
[Parallel(n_jobs=1)]: Using backend SequentialBackend with 1 concurrent workers.
C:\ProgramData\Anaconda3\lib\site-packages\sklearn\linear_model\logistic.py:758:
e. Increase the number of iterations.
  "of iterations.", ConvergenceWarning)
[Parallel(n_jobs=1)]: Done   1 out of   1 | elapsed:  1.3min remaining:    0.0s
[Parallel(n_jobs=1)]: Done   1 out of   1 | elapsed:  1.3min finished
```

Performance

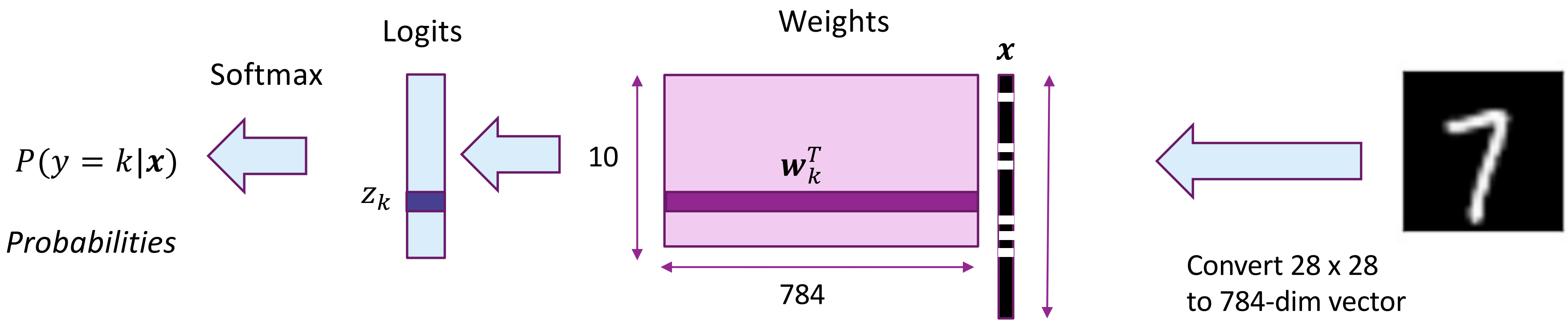
- Accuracy = 89%. Very bad
- Some of the errors seem like they should have been easy to spot
- What went wrong?

```
nts1 = 5000
Iperm_ts = np.random.permutation(nts)
Xts1 = Xts[Iperm_ts[:nts1],:]
yts1 = yts[Iperm_ts[:nts1]]
yhat = logreg.predict(Xts1)
acc = np.mean(yhat == yts1)
print('Accuaracy = {0:f}'.format(acc))
```

```
Accuaracy = 0.891000
```



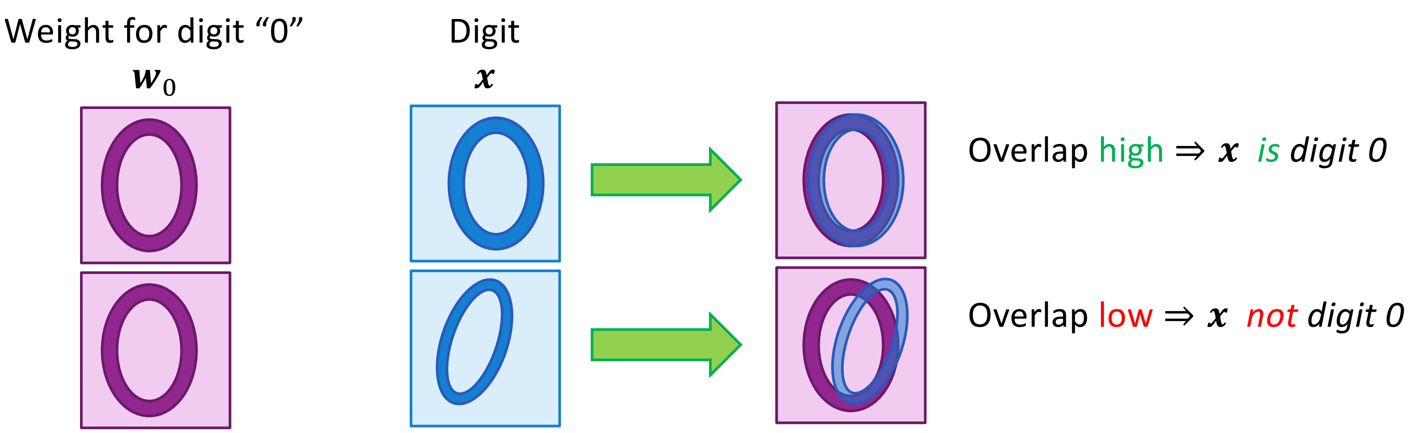
Recap: Logistic Classifier



- Each logit $z_k = \boldsymbol{w}_k^T \boldsymbol{x}$ = inner product with weight $\boldsymbol{w}_k$ with digit $\boldsymbol{x}$, $k = 0, \ldots, 9$
- Will select $\hat{y} = \arg\max_k P(y = k|x) = \arg\max_k z_k$
  - Output z_k which is largest
- When is z_k large?

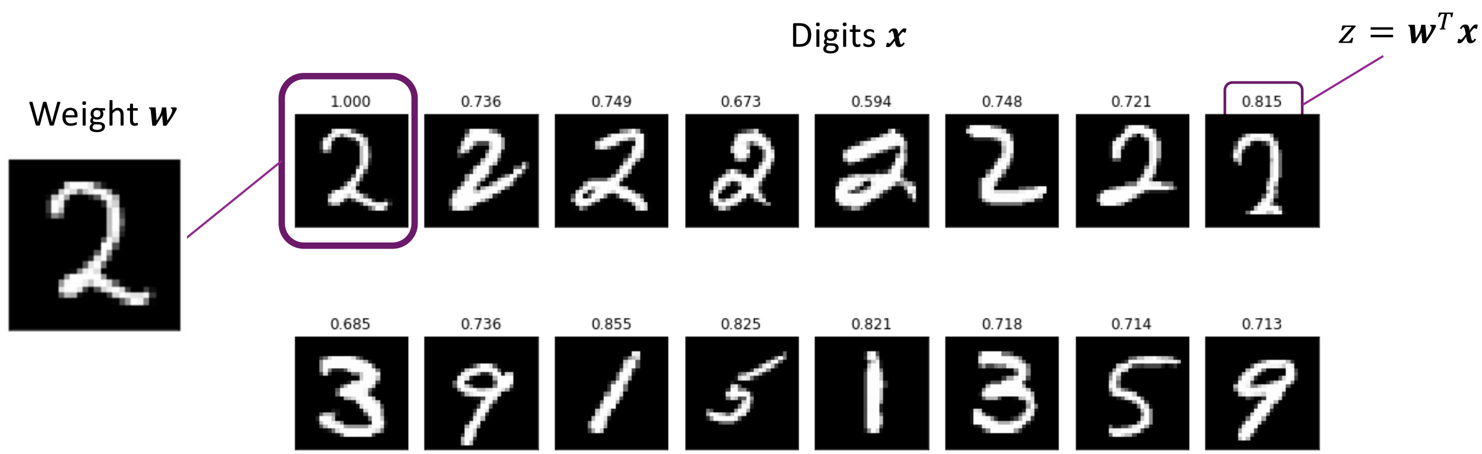
Interpreting the Logistic Classifier Weights

- A logit $z_k = \boldsymbol{w}_k^T \boldsymbol{x}$ is high when there is high overlap between $\boldsymbol{w}_k$ with digit $\boldsymbol{x}$
  - Visualize each weight as an image
  - Suppose pixels are 0 or 1
  - $z_k = \boldsymbol{w}_k^T \boldsymbol{x} = \sum_i w_{ki} x_i$ = number of pixels that overlap with $\boldsymbol{w}_k$ and $\boldsymbol{x}$
- Conclusion: Small variations in digits can cause low overlap



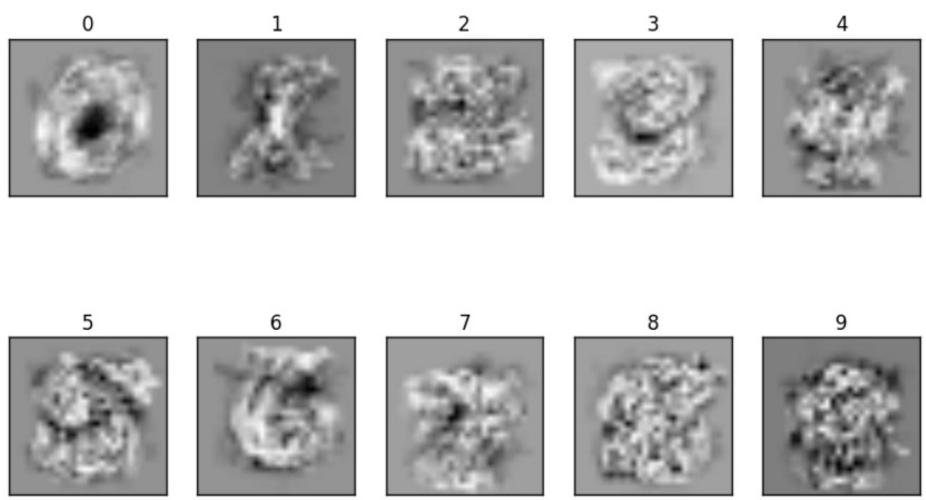
Example with Actual Digits

- Take weight $\boldsymbol{w}$ from a random digit "2"
- Inner products $z = \boldsymbol{w}^T\boldsymbol{x}$ are only slightly higher for other digits "2"
- Cannot tell which digit is correct from the inner product $z = \boldsymbol{w}^T\boldsymbol{x}$



Visualizing the Weights

- Optimized weights of the classifier
- Blurry versions of image to try to capture rotations, translations, …



Problems with Logistic Classifier

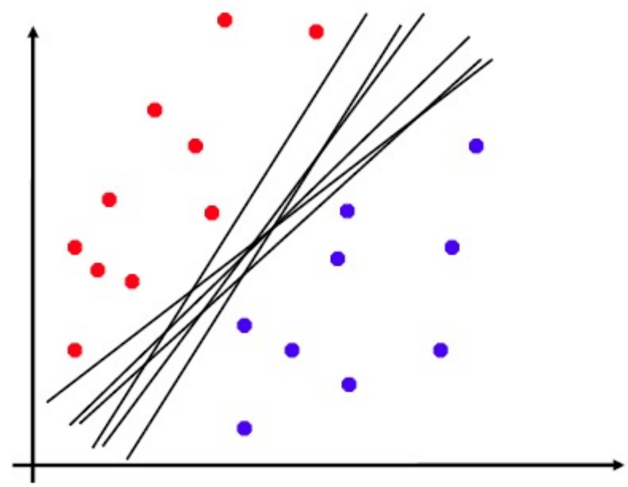
- Linear weighting cannot capture many deformities in image
  - Rotations
  - Translations
  - Variations in relative size of digit components
- Can be improved with preprocessing
  - E.g. deskewing, contrast normalization, many methods
- Is there a better classifier?

Outline

- Motivating example: Recognizing handwritten digits
  - Why logistic regression doesn’t work well.
- Maximum margin classifiers
- Support vector machines
- Kernel trick
- Constrained optimization

Non-Uniqueness of Separating Plane

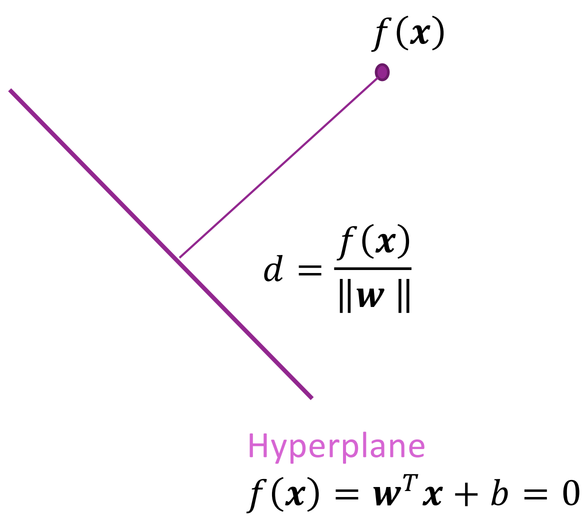
- Linearly separable data:
  - Can find a separating hyper-plane as a linear classifier.
- Separating hyper-plane is not unique
  - Fig. on right: Many separating planes



- Which one is optimal?

Hyperplane Basics

- Linear function: $f(\boldsymbol{x}) = \boldsymbol{w}^T\boldsymbol{x} + b, \boldsymbol{x} \in R^d$
- Hyperplane in d-dimensional: $f(\boldsymbol{x}) = 0$
- Parameters:
  - Weight $\boldsymbol{w}$ and bias b
  - Unique up to scaling:
  - $(b, \boldsymbol{w})$ and $(\alpha b, \alpha\boldsymbol{w})$ define the same plane.
  - For unique definition, we can require $\|\boldsymbol{w}\|=1$.
- Distance of any point **x** to the hyperplane:
  - $d = f(\boldsymbol{x})/\|\boldsymbol{w}\|$, where $f(\boldsymbol{x}) = b + \boldsymbol{w}^T\boldsymbol{x}$.
  - See ESL Sec. 4.5.
  - ESL: Hastie, Tibshirani, Friedman, "The Elements of Statistical Learning". 2nd Ed. Springer.

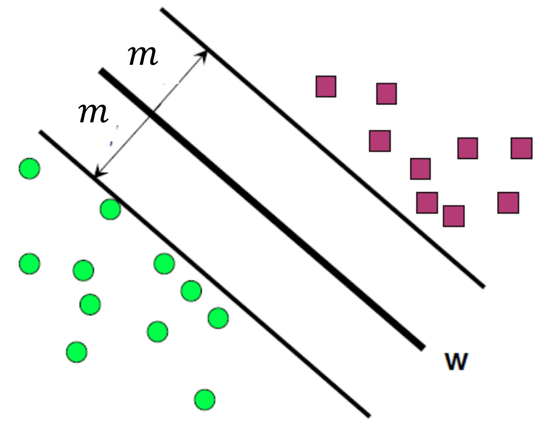


Linear Separability and Margin

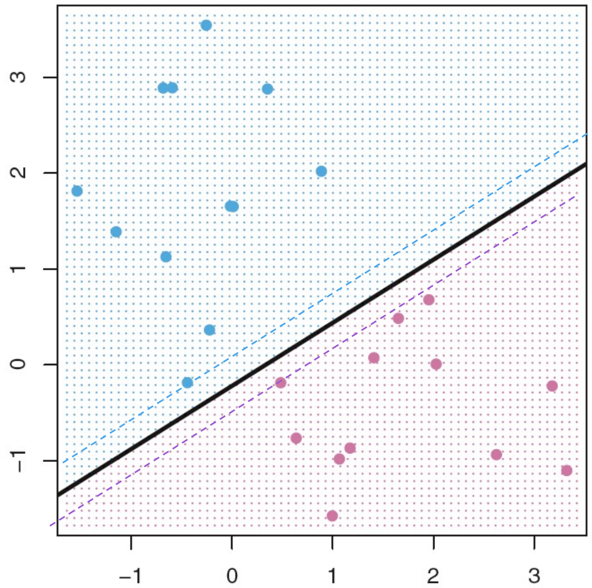
- Given training data $(\boldsymbol{x}_i, y_i), i = 1, \ldots, N$
  - Binary class label: $y_i = \pm 1$
- Suppose it is separable with parameters $(\boldsymbol{w}, b)$
- There must exist a $\gamma > 0$ s.t.:
  - $b + w_1 x_{i1} + \cdots w_d x_{id} > \gamma$ when $y_i = 1$
  - $b + w_1 x_{i1} + \cdots w_d x_{id} < -\gamma$ when $y_i = -1$
- Single equation form:

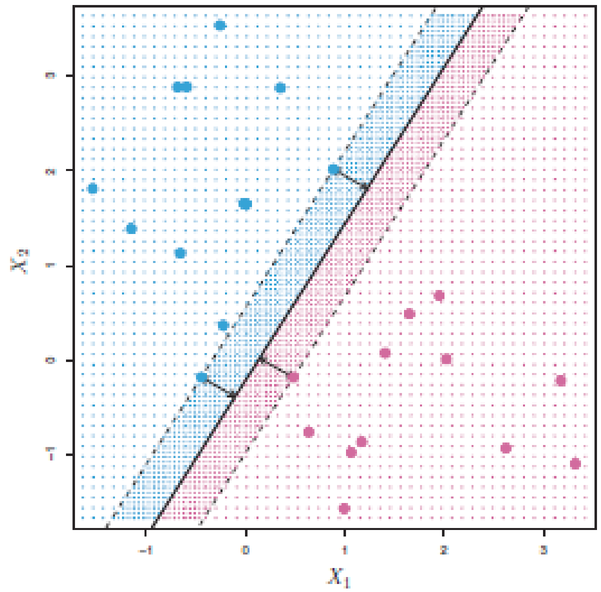
$$y_i(b + w_1 x_{i1} + \cdots w_d x_{id}) > \gamma \text{ for all } i = 1, \ldots, N$$

- Margin: $\mathrm{m} = \frac{\gamma}{\|\boldsymbol{w}\|}$: minimal distance of a sample to the plane
  - γ is the maximum value satisfying the above constraints



Which separating plane is better ?





From Fig. 9.2 and Fig. 9.3 in ISL.

Maximum Margin Classifier

- For the classifier to be more robust to noise, we want to maximize the margin!

- Define maximum margin classifier

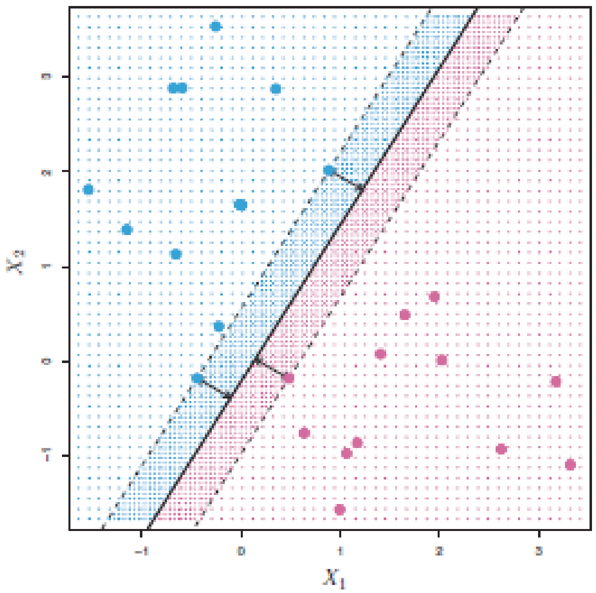
$\max_{w,b} \gamma$ — Maximizes the margin

  - Such that $y_i(b + \boldsymbol{w}^T \boldsymbol{x}) \geq \gamma \quad \text{for all } i$ — Ensures all points are correctly classified
  - $\sum_{j=1}^{d} w_j^2 \leq 1$ — Scaling on weights

- Called a constrained optimization
  - Objective function and constraints
  - More on this later.

- See closed form solution in Sec. 4.5.2 in ESL. Note notation difference.

Visualizing Maximum Margin Classifier



- Fig. 9.3 of ISL
- Margin determined by closest points to the line
  - The maximal margin hyperplane represents the mid-line of the widest "slab" that we can insert between two classes
- In this figure, there are 3 points at the margin

ISL: James, Witten, Hastie, Tibshirani, An Introduction to Statistical Learning, Springer. 2013.

Problems with MM classifier

- Data is often not perfectly separable
  - Only want to correctly separate most points

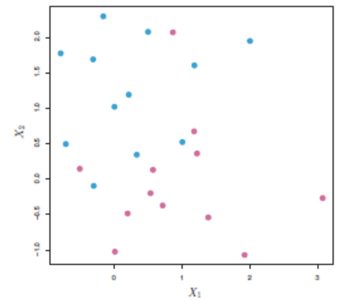


Fig. 9.4

- MM classifier is not robust
  - A single sample can radically change line

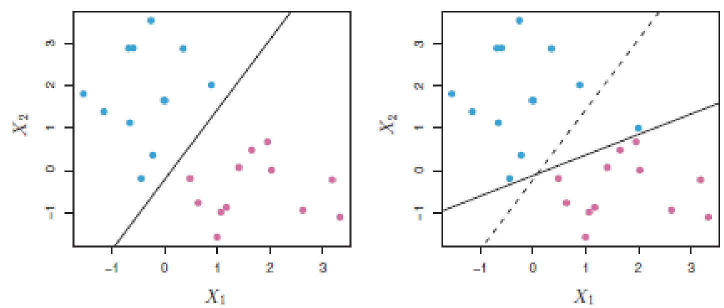


Fig. 9.5

In-Class Exercise

- Found in github site: svm_inclass.ipynb

Problem 1. Margin

For the points below with binary labels:

- Create a scatter plot of the points with different markers for the two classes
- Find the weight and bias of the classifier that separates the two classes
- Compute the distance to the classifier boundary for the points
- Find the margin

```
X = np.array([[0.5,0.5], [1,0.5],[0.5,1.75], [0.75,2.75], [1.1,2.2], [2,1], [3,1.5]])
y = np.array([1,1,1,0,0,0,0])
```

Outline

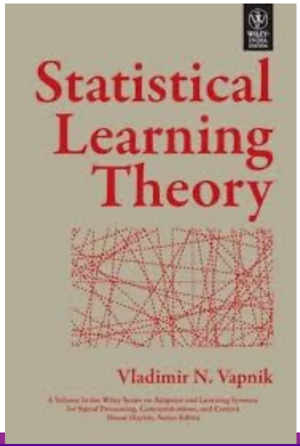
- ❑ Motivating example: Recognizing handwritten digits
  - Why logistic regression doesn't work well.
- ❑ Maximum margin classifiers
- ❑ Support vector machines
- ❑ Kernel trick
- ❑ Constrained optimization

Support Vector Machine

- Support Vector Machine (SVM)
  - Vladimir Vapnik, 1963
  - But became widely-used with kernel trick, 1993
  - More on this later

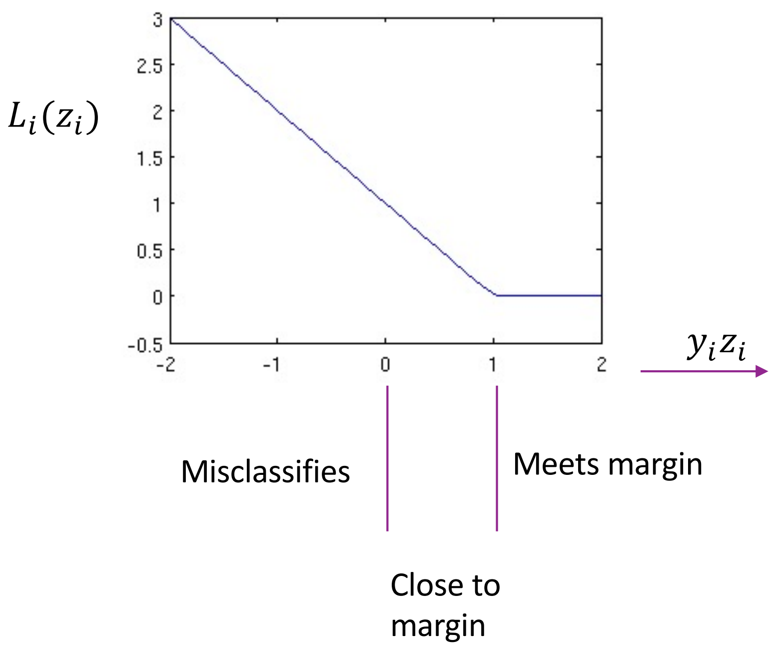
- Got best results on character recognition

- Key idea: Allow "slack" in the classification
  - Support vector classifier (SVC): Directly use raw features. Good when the original feature space is roughly linearly separable
  - Support vector machine (SVM): Map the raw features to some other domain through a kernel function



Hinge Loss

- Fix $\gamma = 1$
- Want ideally: $y_i(\boldsymbol{w}^T\boldsymbol{x} + b) \geq 1$ for all samples i
  - Equivalently, $y_i z_i \geq 1, \quad z_i = b + \boldsymbol{w}^T\boldsymbol{x}$
- But perfect separation may not be possible
- Define hinge loss or soft margin:
  - $L_i(\boldsymbol{w}, b) = \max(0, 1 - y_i z_i)$
- Starts to increase as sample is misclassified:
  - $y_i z_i \geq 1 \;\Rightarrow$ Sample meets margin target, $L_i(w) = 0$
  - $y_i z_i \in [0,1) \;\Rightarrow$ Sample margin too small, small loss
  - $y_i z_i \leq 0 \;\Rightarrow$ Sample misclassified, large loss



SVM Optimization

- Given data $(\boldsymbol{x}_i, y_i)$
- Optimization $\min_{w,b} J(\boldsymbol{w}, b)$

$$J(\boldsymbol{w}, b) = C \sum_{i=1}^{N} \max(0, 1 - y_i(\boldsymbol{w}^T \boldsymbol{x}_i + b)) + \frac{1}{2} \|\boldsymbol{w}\|^2$$

C controls final margin

Hinge loss term
Attempts to reduce
Misclassifications

margin=$1/\|\boldsymbol{w}\|$

- Constant $C > 0$ will be discussed below
- Note: ISL book uses different naming conventions.
  - We have followed convention in sklearn

Alternate Form of SVM Optimization

- Equivalent optimization:

$$\min J_1(\boldsymbol{w}, b, \boldsymbol{\epsilon}), \qquad J_1(\boldsymbol{w}, b, \boldsymbol{\epsilon}) = C \sum_{i=1}^{N} \epsilon_i + \frac{1}{2} \|\boldsymbol{w}\|^2$$

- Subject to constraints:

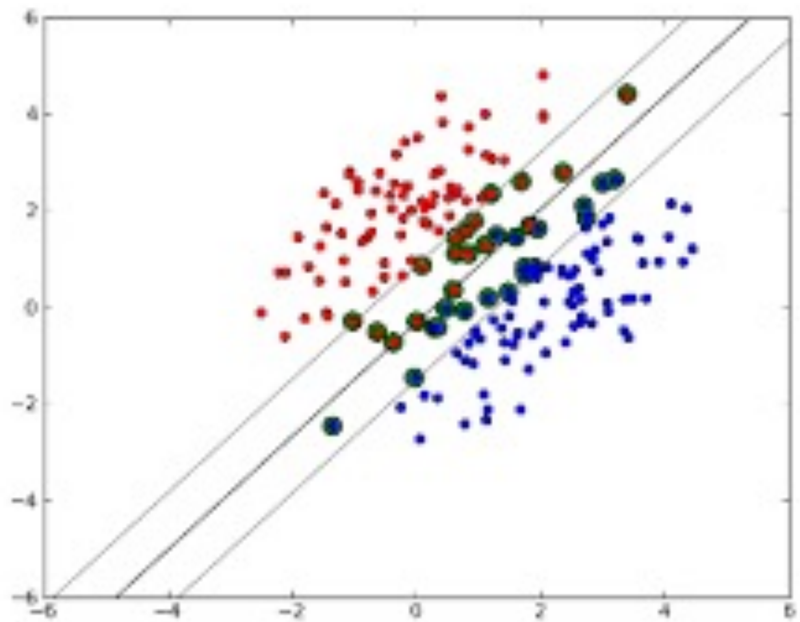
$$y_i(\boldsymbol{w}^T \boldsymbol{x}_i + b) \geq 1 - \epsilon_i \ \text{ for all } i = 1, \ldots, N$$
$$\epsilon_i \geq 0 \ \text{ for all } i = 1, \ldots, N$$

  - ϵ_i = amount sample i misses margin target

- Sometimes write as $J_1(\boldsymbol{w}, b, \boldsymbol{\epsilon}) = C\|\boldsymbol{\epsilon}\|_1 + \frac{1}{2}\|\boldsymbol{w}\|^2$
  - $\|\boldsymbol{\epsilon}\|_1 = \sum_{i=1}^{N} \epsilon_i$ called the "one-norm"
  - Generally one-norm would have absolute sign over ϵ_i.
  - But in this case, when the constraint is met, ϵ_i>=0.

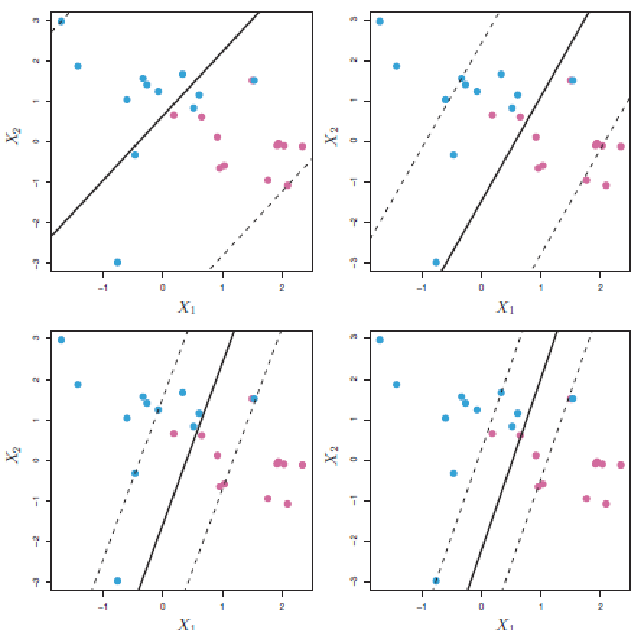
Support Vectors

- Support vectors: Samples that either:
  - Are exactly on margin: $y_{\mathrm{i}}(\boldsymbol{w}^T\boldsymbol{x}_i + b) = 1$
  - Or, on wrong side of margin: $y_{\mathrm{i}}(\boldsymbol{w}^T\boldsymbol{x}_i + b) \leq 1$
- Changing samples that are not SVs
  - Does not change solution
  - Provides robustness



Illustrating Effect of C

Low $C = C_1$ C_2



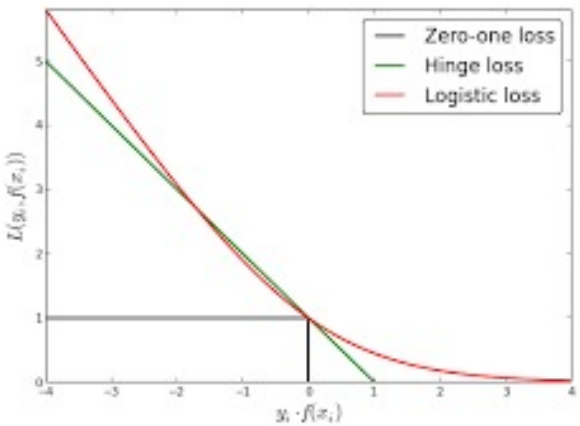
C_3 High C_4

- Fig. 9.7 of ISL
  - Note: C has opposite meaning in ISL than python
  - Here, we use python meaning
- Low C:
  - Leads to large margin
  - But allow many violations of margin.
  - Many more SVs
  - Reduces variance by using more samples
- Large C:
  - Leads to small margin
  - Reduce number of violations, and fewer SVs.
  - Highly fit to data. Low bias, higher variance
  - More chance to overfit

Relation to Logistic Regression

- Logistic regression also minimizes a loss function:

$$J(\boldsymbol{w}, b) = \sum_{i=1}^{N} L_i(w, b)\,, \qquad L_i(w, b) = \ln P(y_i|\boldsymbol{x}_i) = -\ln(1 + e^{-y_i z_i})$$



In-Class Exercise

Problem 2. Minimizing the Hinge Loss

For the data below, first create a scatter plot of the points with different markers for the two classes. You should see that the data is not linearly separable.

Then, consider a set of classifiers:

```
yhat = sign(z),    z = w.dot(x)+b
```

Use the the `w` below, plot the hinge loss as a function of the bias `b` where the hinge loss is:

```
J  = sum( maximum(0, 1-ypm*z) )
```

Here `ypm=2*y-1` so that it is a value +1 or -1. Find the `b` that minimizes the hinge loss and plot the boundary of the classifier.

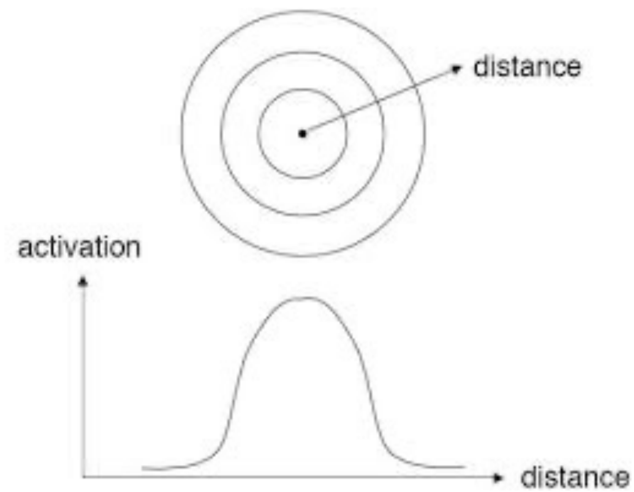
```
X = np.array([[0.5,0.5], [1,0.5],[0.5,1.75], [2,2], [0.75,0.75], [0.75,2.75], [1.1,2.2], [2,1], [3,1.5]])
y = np.array([1,1,1,1,0,0,0,0,0])

w = np.array([1.5, 1])
w = w / np.linalg.norm(w)
```

Outline

- Motivating example: Recognizing handwritten digits
  - Why logistic regression doesn't work well.
- Maximum margin classifiers
- Support vector machines
- Kernel trick
- Constrained optimization

The Kernel Function

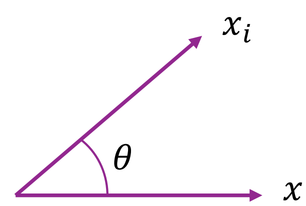
- Kernel function:
  - Function $K(\boldsymbol{x}_i, \boldsymbol{x})$
  - Key function for SVMs and kernel classifiers
  - Measures "similarity" between new sample $\boldsymbol{x}$ and training sample $\boldsymbol{x}_i$



- Typical property
  - $\boldsymbol{x}_i, \boldsymbol{x}$ close $\Rightarrow K(\boldsymbol{x}_i, \boldsymbol{x})$ maximum value
  - $\boldsymbol{x}_i, \boldsymbol{x}$ far $\Rightarrow K(\boldsymbol{x}_i, \boldsymbol{x}) \approx 0$

Common Kernels

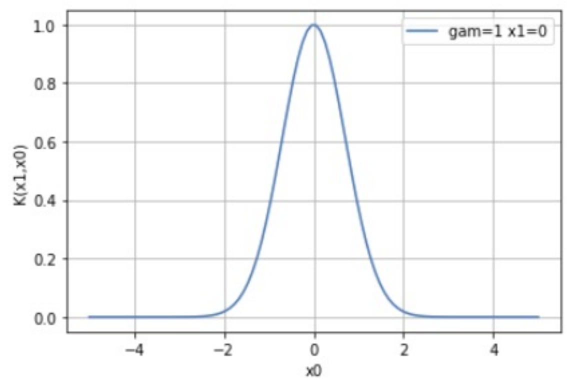
- Linear SVM:
  - $K(x_i, x) = x_i^T x = \|x_i\|\|x\| \cos\theta$
  - Maximum when angle between vectors is small



- Radial basis function:

$$K(x_i, x\ ) = \exp[-\gamma\|x - x_i\|^2]$$

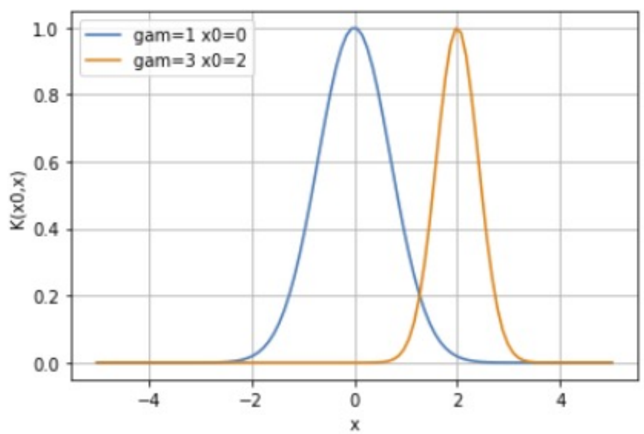
  - $1/\gamma$ indicates width of kernel



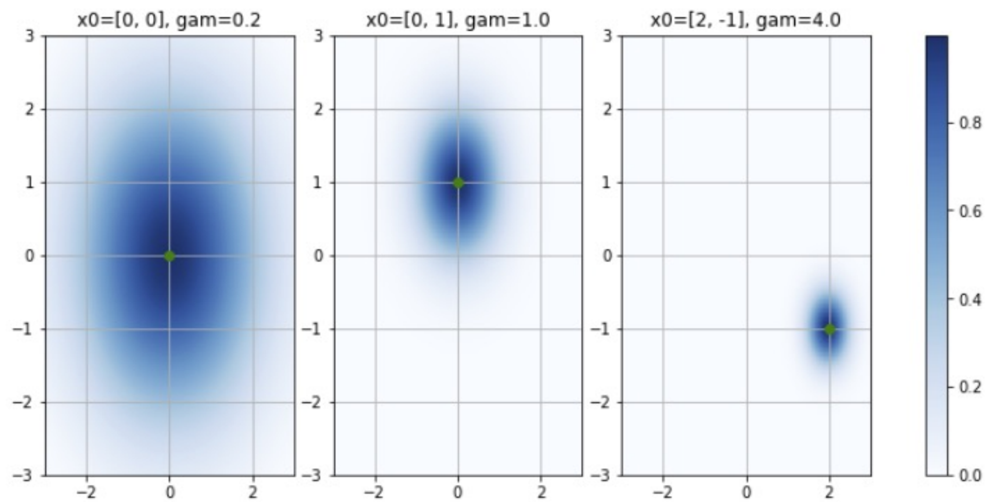
- Polynomial kernel: $K(x_i, x) = \left|x_i^T x\right|^d$
  - Typically d=2

RBF Kernel Examples

- RBF kernel: $K(x_0, x) = \exp[-\gamma \|x - x_0\|^2]$
  - Peak value of 1 at $x = x_0$
  - Width $\propto \frac{1}{\gamma}$



RBFs in 1D



RBFs in 2D

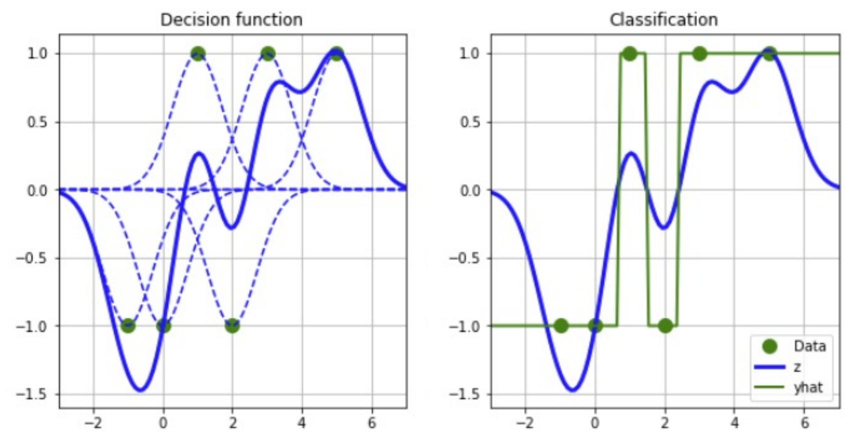
Kernel Classifier

- Given:
  - Training data (x_i, y_i) with binary labels $y_i = \pm 1$
  - Kernel $K(x_i, x)$
- To classify a new point x:
  - Decision function: $z = \sum_{i=1}^{n} y_i K(x_i, x)$
  - Classify: $\hat{y} = sign(z)$
- Idea:
  - z is large positive when x is close to samples x_i with $y_i = 1$
  - z is large negative when x is close to samples x_i with $y_i = -1$
- Kernel classifiers are a subject on their own
  - We just mention them here to explain connection to SVMs

Example in 1D

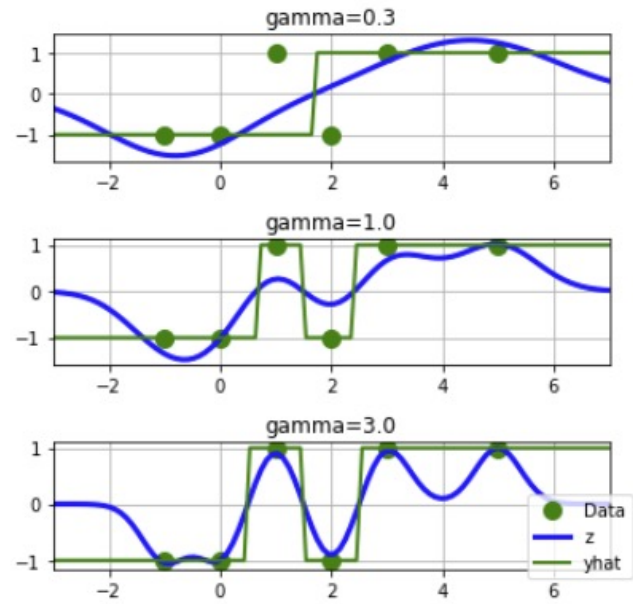
- Example data with 6 points (x_i, y_i)
  - RBF kernel: $K(x_i, x) = e^{-\gamma(x_i - x)^2}$, $\gamma = 1$
- Decision function:
  - $z = \sum_{i=1}^{n} y_i K(x_i, x)$
  - Sum of bell curves
  - Positive when near positive samples
  - Negative when near negative samples
- Classification:
  - $\hat{y} = sign(z)$

i	1	2	3	4	5	6
x_i	-1	0	1	2	3	5
y_i	-1	-1	1	-1	1	1



Effect of Gamma

- Same data as before
- RBF kernel: $K(x_i, x) = e^{-\gamma(x_i - x)^2}$
- As γ increases:
  - Decision function $z \approx y_i$ when $x = x_i$
  - Classifier fits training data better
  - Classification region more complex
- As a classifier, higher γ results in:
  - Lower bias error
  - But, higher variance error

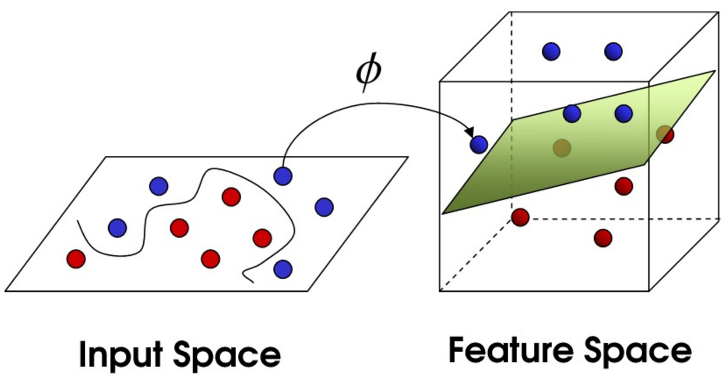


SVMs with Non-Linear Transformations

- Non-linear transformation:
  - Replace $\boldsymbol{x}$ with $\phi(\boldsymbol{x})$
  - Enables more rich, non-linear classifiers
  - Examples: polynomial classification

$$\phi(x) = [1, x, x^2, \dots, x^{d-1}]$$

- Tries to find separation in a feature space



- Kernel trick in SVMs:
  - Makes applying non-linear transformations easy

SVM with the Transformation

- Consider SVM model with $\boldsymbol{x}$ replaced by $\phi(\boldsymbol{x})$
- Minimize SVM cost function as before (i.e. Hinge loss + inverse margin)
- Theorem: The optimal weight is of the form:

$$\boxed{\boldsymbol{w} = \sum_{i=1}^{N} \alpha_i y_i \phi(\boldsymbol{x}_i)}$$

  - $\alpha_i \geq 0$ for all i
  - $\alpha_i > 0$ if and only if sample i is a support vector
  - Will show this fact later using results in constrained optimization
- Consequence: The linear discriminant on any other sample x is:

$$z = b + \boldsymbol{w}^T \phi(\boldsymbol{x}) = b + \sum_{i=1}^{N} \alpha_i y_i \boxed{\phi(\boldsymbol{x}_i)^T \phi(\boldsymbol{x})}$$

$K(\boldsymbol{x}_i, \boldsymbol{x})$ = "kernel"

Kernel Form of the SVM Classifier

- SVM classifier can be written with the kernel $K(\boldsymbol{x}_i, \boldsymbol{x})$ and values $\alpha_i \geq 0$:

$$z = b + \sum_{i=1}^{N} \alpha_i y_i K(\boldsymbol{x}_i, \boldsymbol{x}),$$

Decision function

$$\hat{y} = \text{sign}(z) = \begin{cases} 1 & \text{if } z > 0 \\ -1 & \text{if } z < 0 \end{cases}$$

Classification decision

- Key point: SVM classifier is approximately Kernel classifier
- But there are two differences:
  - Weights $\alpha_i \geq 0$ on the samples (the weights are only non-zero on the SVs)
  - A bias term b (can be positive or negative)

"Kernel Trick" and Dual Parameterization

- Kernel form of SVM classifier (previous slide):

$$z = b + \sum_{i=1}^{N} \alpha_i y_i K(\boldsymbol{x}_i, \boldsymbol{x}),$$
$$\hat{y} = \text{sign}(z)$$

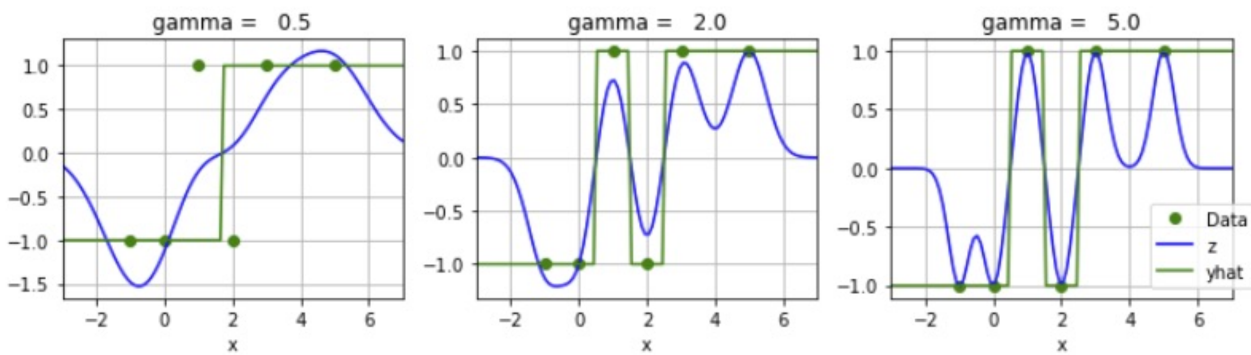
- Dual parameters: $\alpha_i \geq 0, i = 1, \dots, N$
  - Called the dual parameters due to constrained optimization – see next section

- Kernel trick:
  - Directly solve the parameters $\boldsymbol{\alpha}$ instead of the weights $\boldsymbol{w}$
  - Can show that the optimization only needs the kernel $K(\boldsymbol{x}_i, \boldsymbol{x})$
  - Does not need to explicitly use $\phi(\boldsymbol{x})$

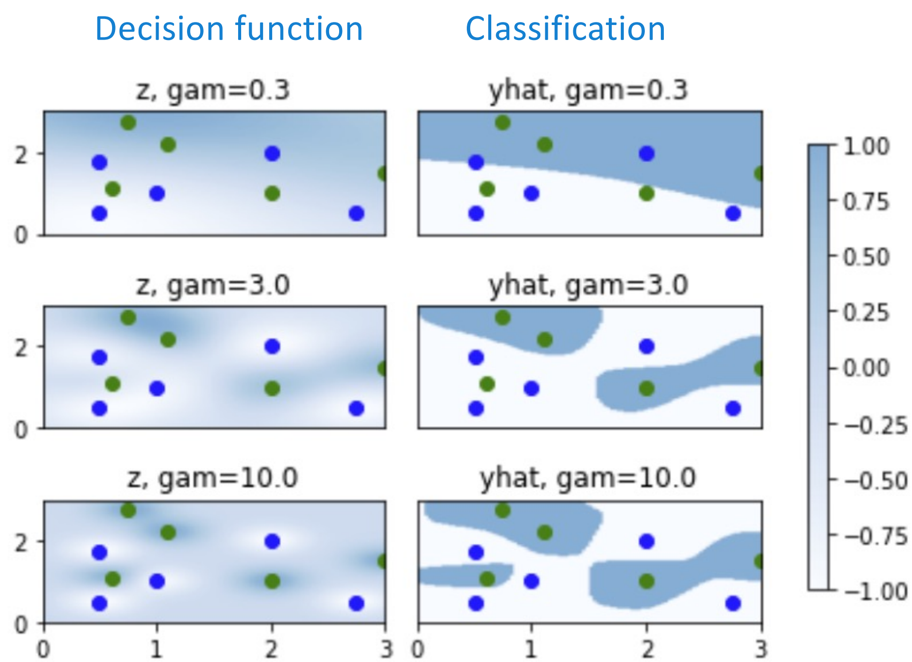
SVM Example in 1D

- Same data as in the Kernel classifier example
- Fit SVM with RBF with different γ
- Similar trends as kernel classifier: As γ increases
  - z “fits” data (x_i, y_i) closer
  - Leads to more complex decision regions.
  - Enables nonlinear decision regions

i	1	2	3	4	5	6
x_i	-1	0	1	2	3	5
y_i	-1	-1	1	-1	1	1



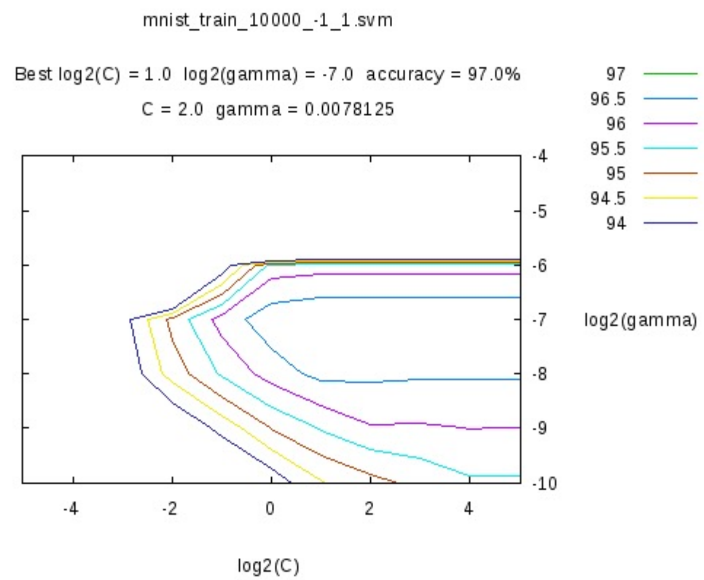
Example in 2D



- Example:
  - 10 data points with binary labels
  - Fit SVM with $C = 1$ and RBF
  - $\gamma = 0.3$, 3 and 10
- Plot:
  - z= linear discriminant
  - $\hat{y} = sign(z)$ = classification decision
- Observe: As γ increases
  - Fits training data better
  - More complex decision region

Parameter Selection

- For SVMs with RBFs we need to select:
  - Parameter $C > 0$ in the loss function
  - Kernel width $\gamma > 0$
- Higher C or γ
  - Fewer SVs
  - Classifiers averages over smaller set
  - Lower bias, but higher variance
- Typically select via cross-validation
  - Try out different (C, γ) pairs
  - Find which one provides highest accuracy on test set
- Python can automatically do grid search



http://peekaboo-vision.blogspot.com/2010/09/mnist-for-ever.html

Multi-Class SVMs

- Suppose there are K classes
- One-vs-one:
  - Train $\binom{K}{2}$ SVMs for each pair of classes
  - Test sample assigned to class that wins "majority of votes"
  - Best results but very slow
- One-vs-rest:
  - Train K SVMs: train each class k against all other classes
  - Pick class with highest z_k
- Sklearn has both options

MNIST Results

- Run classifier
- Very slow
  - Several minutes for 40,000 samples
  - Slow in training and test
  - Major drawback of SVM
- Accuracy ≈ 0.984
  - Much better than logistic regression
- Can get better with:
  - pre-processing
  - More training data
  - Optimal parameter selection

```
from sklearn import svm

# Create a classifier: a support vector classifier
svc = svm.SVC(probability=False,  kernel="rbf", C=2.8, gamma=.0073,verbose=10)
```

```
svc.fit(Xtr,ytr)
```

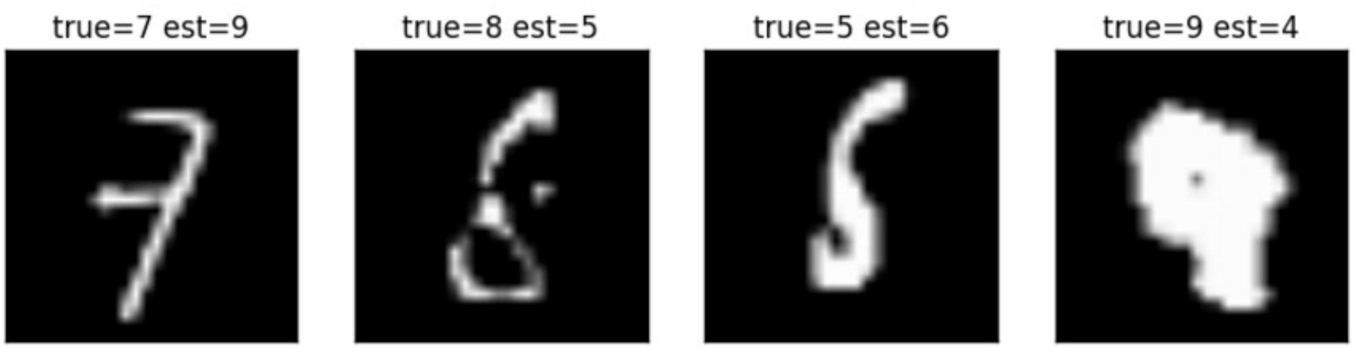
```
[LibSVM]

SVC(C=2.8, cache_size=200, class_weight=None, coef0=0.0,
  decision_function_shape=None, degree=3, gamma=0.0073, kernel='rbf',
  max_iter=-1, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=10)
```

```
yhat1 = svc.predict(Xts)
acc = np.mean(yhat1 == yts)
print('Accuaracy = {0:f}'.format(acc))
```

```
Accuaracy = 0.984000
```

MNIST Errors

- Some of the error are hard even for a human



Outline

- ❑Motivating example: Recognizing handwritten digits
  - Why logistic regression doesn't work well.
- ❑Maximum margin classifiers
- ❑Support vector machines
- ❑Kernel trick
- ❑Constrained optimization

Constrained Optimization

- In many problems, variables are constrained
- Constrained optimization formulation:
  - Objective: Minimize $f(\boldsymbol{w})$
  - Constraints: $g_1(\boldsymbol{w}) \leq 0, \ldots, g_M(\boldsymbol{w}) \leq 0$
- Examples:
  - Minimize the mpg of a car subject to a cost or meeting some performance
  - In ML: weight vector may have constraints from physical knowledge
- Often write constraints in vector form: Write $g(\boldsymbol{w}) \leq 0$

$$g(\boldsymbol{w}) = [g_1(\boldsymbol{w}), \ldots, g_m(\boldsymbol{w})]^T$$

Lagrangian

- Constrained optimization: Min $f(\boldsymbol{w})$ s.t. $g(\boldsymbol{w}) \leq 0$
- Consider first a single constraint: $g(\boldsymbol{w})$ is a scalar
- Define Lagrangian: $L(\boldsymbol{w}, \lambda) = f(\boldsymbol{w}) + \lambda g(\boldsymbol{w})$
  - $\boldsymbol{w}$ is called the primal variable
  - λ is called the dual variable
- Dual minimization: Given a dual parameter λ, minimize

$$\widehat{\boldsymbol{w}}(\lambda) = \arg\min_{\boldsymbol{w}} L(\boldsymbol{w}, \lambda), \qquad L^*(\lambda) = \min_{w} L(\boldsymbol{w}, \lambda)$$

  - Minimizes a weighted combination of objective and constraint.
  - Higher $\lambda \Rightarrow$ Weight constraint more (try to make $g(\boldsymbol{w})$ smaller)
  - Lower $\lambda \Rightarrow$ Weight objective more (try to make $f(\boldsymbol{w})$ smaller)

KKT Conditions

- Given objective $f(\boldsymbol{w})$ and constraint $g(\boldsymbol{w})$
- KKT Conditions: $\widehat{\boldsymbol{w}}, \hat{\lambda}$ satisfy:
  - $\widehat{\boldsymbol{w}}$ minimizes the Lagrangian: $\widehat{\boldsymbol{w}} = \arg\min_{\boldsymbol{w}} L(\boldsymbol{w}, \hat{\lambda})$
  - Either
    - $g(\widehat{\boldsymbol{w}}) = 0$ and $\hat{\lambda} \geq 0$ [active constraint]
    - $g(\widehat{\boldsymbol{w}}) < 0$ and $\hat{\lambda} = 0$ [inactive constraint]
- Theorem: Under some technical conditions,
  - if $\widehat{\boldsymbol{w}}, \hat{\lambda}$ are local mimima of the constrained optimization, they must satisfy KKT conditions

General Procedure for Single Constraint

- Suppose:
  - $\boldsymbol{w} = (w_1, \ldots, w_d)^T$: d unknown primal variables
  - $g(\boldsymbol{w}) \leq 0$: scalar constraint
- Case 1: Assume constraint is active:
  - Solve $\boldsymbol{w}$ and λ: $\partial L(\boldsymbol{w}, \lambda)/\partial w_j = 0$ and $g(\boldsymbol{w}) = 0$ (resulting from setting $\partial L(\boldsymbol{w}, \lambda)/\partial \lambda = 0$)
  - $d + 1$ unknowns and $d + 1$ equations
  - Verify that $\lambda \geq 0$
- Case 2: Assume constraint is inactive
  - Solve primal objective $\partial f(\boldsymbol{w})/\partial w_j = 0$ ignoring constraint
  - d unknowns and d equations
  - Verify that constraint is satisfied: $g(\boldsymbol{w}) \leq 0$

KKT Conditions Illustrated

- Example 1: Constraint is "active"

$$\min_{w} w^2 \quad s.t.\ w + 1 \le 0$$

- Example 2: Constraint is "inactive"

$$\min_{w} w^2 \quad s.t.\ w - 1 \le 0$$

- Examples worked on board with illustration

Multiple Constraints

- Now consider constraint: $g(\boldsymbol{w}) = [g_1(\boldsymbol{w}), \dots, g_M(\boldsymbol{w})]^T \leq 0$.
- Lagrangian is:

$$L(\boldsymbol{w}, \boldsymbol{\lambda}) = f(\boldsymbol{w}) + \boldsymbol{\lambda}^T g(\boldsymbol{w}) = f(\boldsymbol{w}) + \sum_{m=1}^{M} \lambda_m \, g_m(\boldsymbol{w})$$

  - Weighted sum of all M constraints
  - $\boldsymbol{\lambda}$ is called the dual vector

- KKT conditions extend to:
  - $\widehat{\boldsymbol{w}}$ minimizes the Lagrangian: $\widehat{\boldsymbol{w}} = \arg\min_{\boldsymbol{w}} L(\boldsymbol{w}, \hat{\lambda})$
  - For each $m = 1, \dots, M$
    - $g_m(\widehat{\boldsymbol{w}}) = 0$ and $\hat{\lambda}_m \geq 0$ [active constraint]
    - $g_m(\widehat{\boldsymbol{w}}) < 0$ and $\hat{\lambda}_m = 0$ [inactive constraint]

Multiple Constraints

- If there are M constraints, there could be 2^M cases to discuss

- In practice, the number of cases are much smaller

- For more information on KKT conditions, check the following lecture on youtube
  - UAMathCamp Lecture 40(A): Kuhn-Tucker Conditions: Conceptual and geometric insight
  - https://www.youtube.com/watch?v=HIm3Z0L90Co

SVM Constrained Optimization

- Recall: SVM constrained optimization

$$\min J_1(\boldsymbol{w}, b, \boldsymbol{\epsilon}), \qquad J_1(\boldsymbol{w}, b, \boldsymbol{\epsilon}) = C \sum_{i=1}^{N} \epsilon_i + \frac{1}{2} \|\boldsymbol{w}\|^2$$

  - Constraints: $y_i(\boldsymbol{w}^T \boldsymbol{x}_i + b) \geq 1 - \epsilon_i$ and $\epsilon_\mathrm{i} \geq 0$ for all $i = 1, \ldots, N$

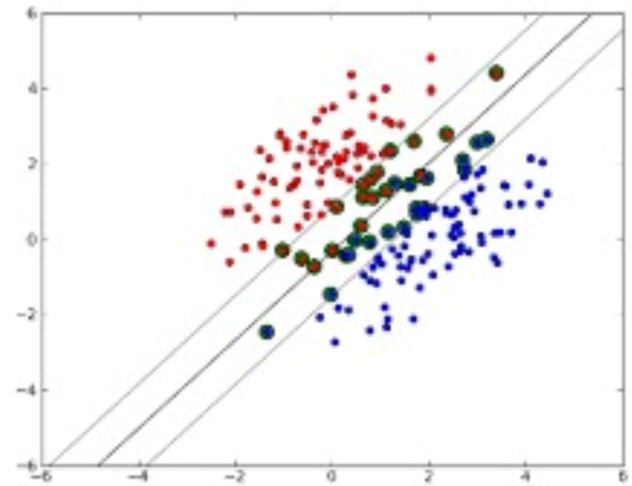
- After applying KKT conditions and some algebra [beyond this class], solution is
  - Optimal weight vector: $\boldsymbol{w} = \sum_{i=1}^{N} \alpha_i y_i \boldsymbol{x}_i$ linear combination of instances
  - Dual parameters α_i minimize

$$\sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y_i y_j \boldsymbol{x}_i^T \boldsymbol{x}_j \quad \text{s.t.} \;\; 0 \leq \alpha_i \leq C$$

  - Details can be found on textbook ESLII, section 12.2.1 Computing the Support Vector Classifier

Support Vectors

- Classifier weight is: $\boldsymbol{w} = \sum_{i=1}^{N} \alpha_i y_i \boldsymbol{x}_i$
- Can show that $\alpha_i > 0$ only when $\boldsymbol{x}_i$ is a support vector
  - On boundary or violating constraint
  - Otherwise $\alpha_i = 0$



What you should know

- Interpret weights in linear classification of images (logistic regression): Match filters
- Understand the margin in linear classification and maximum margin classifier
- SVM classifier: Allow violation of margin by introducing slack variables (More robust than linear classifier)
- Solve constrained optimization using the Lagrangian.
  - Understand KKT conditions for a single constraint
- Extend to nonlinear classifier by feature transformation: SVM with nonlinear kernels
- Select SVM parameters from cross-validation