Computer Science

CSC380: Principles of Data Science

Nonlinear Models 1

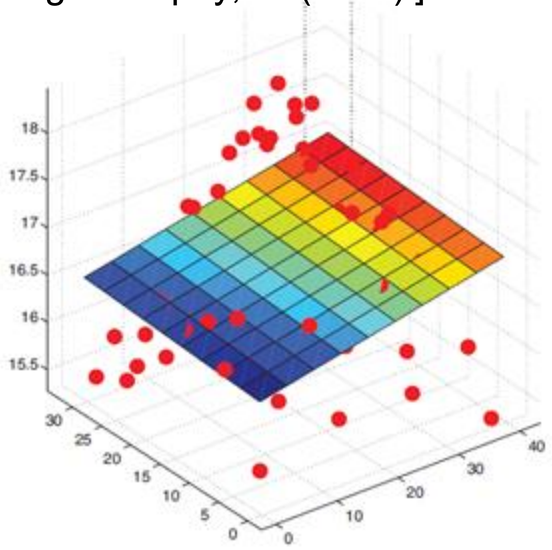
Xinchen Yu

Outline

- Basis Functions
- Support Vector Machine
- Neural Networks

Linear Models

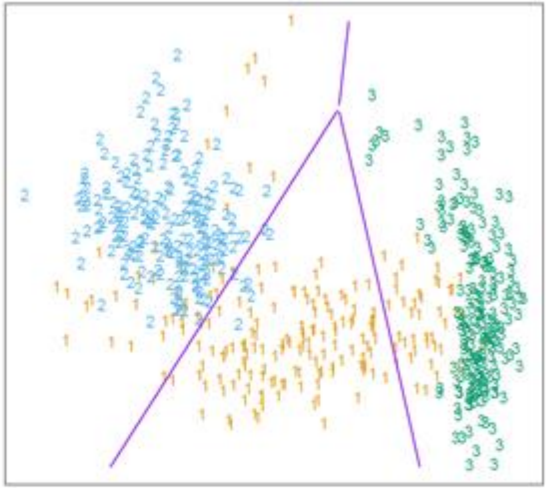
[Image: Murphy, K. (2012)]



Linear Regression Fit a *linear function* to the data,

$$y = w^T x$$

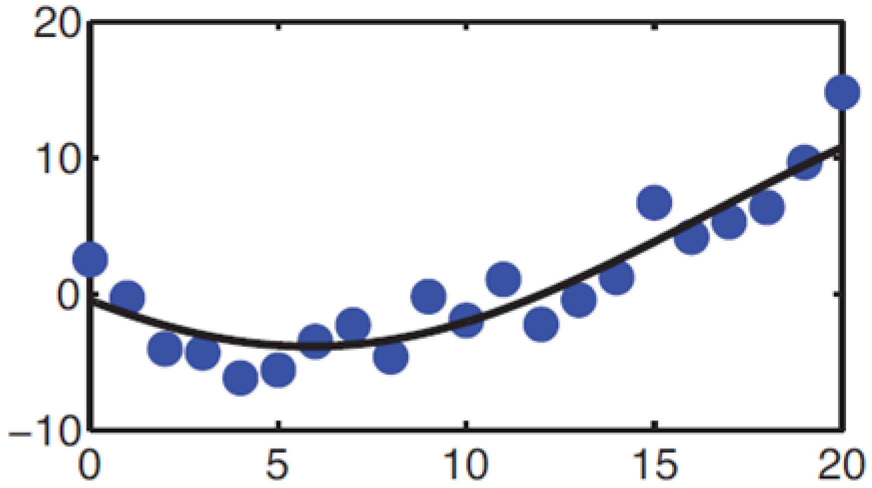
[Image: Hastie et al. (2001)]



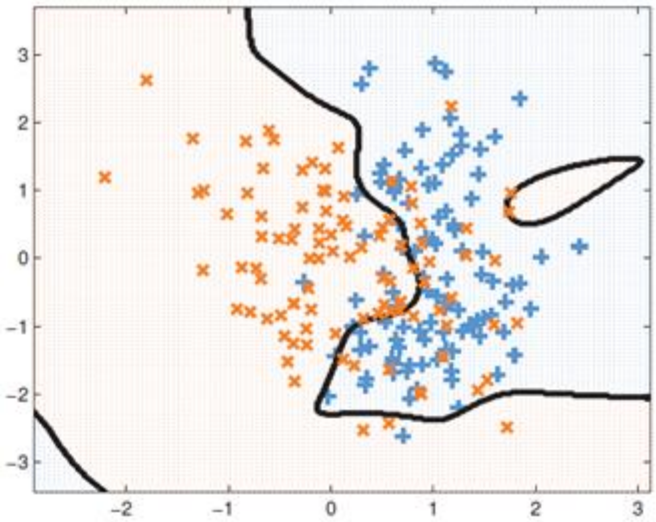
Logistic Regression Learn a decision boundary that is *linear in the data*,

$$y = \mathbf{I}\{w^\top x \geq 0\}$$

Nonlinear Data



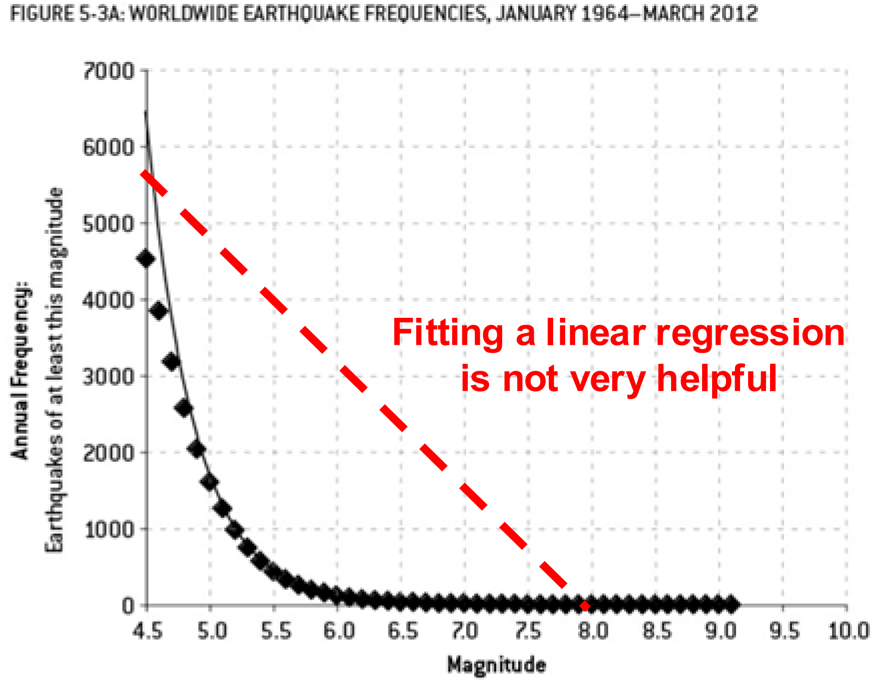
What if our data are *not* well-described by a linear function?



What if classes cannot be well-distinguished by a linear function?

Example: Earthquake Prediction

Suppose that we want to predict the number of earthquakes that occur of a certain magnitude. Our data are given by,



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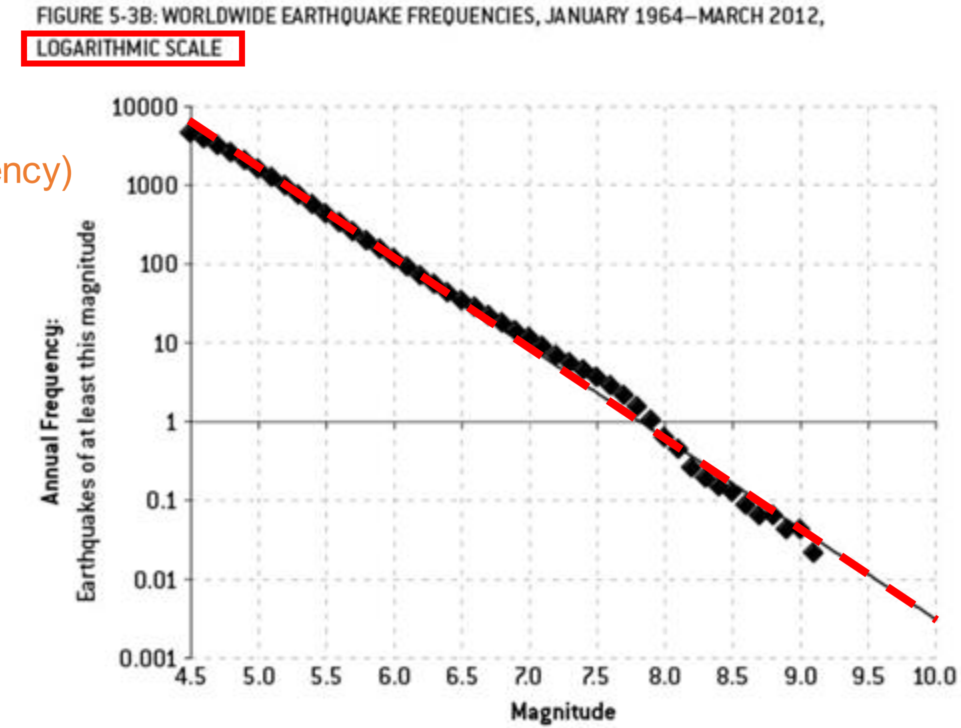

But plotting outputs on a logarithmic scale reveals a strong linear relationship…

it's like $y = e^{-ax+b}$

Beyond linearity: Transformation in x

- Recall: for 1d problem, we embedded the feature: $x' = (x, 1) \in \mathbb{R}^2$ so we can encode the intercept term.

$$\phi_0(x) = 1 \qquad \phi_1(x) = x \qquad y = \boldsymbol{w}^\top \Phi_{\text{lin}}(x) = \phi_0(x)w_0 + \phi_1(x)w_1 = w_0 + w_1 x$$

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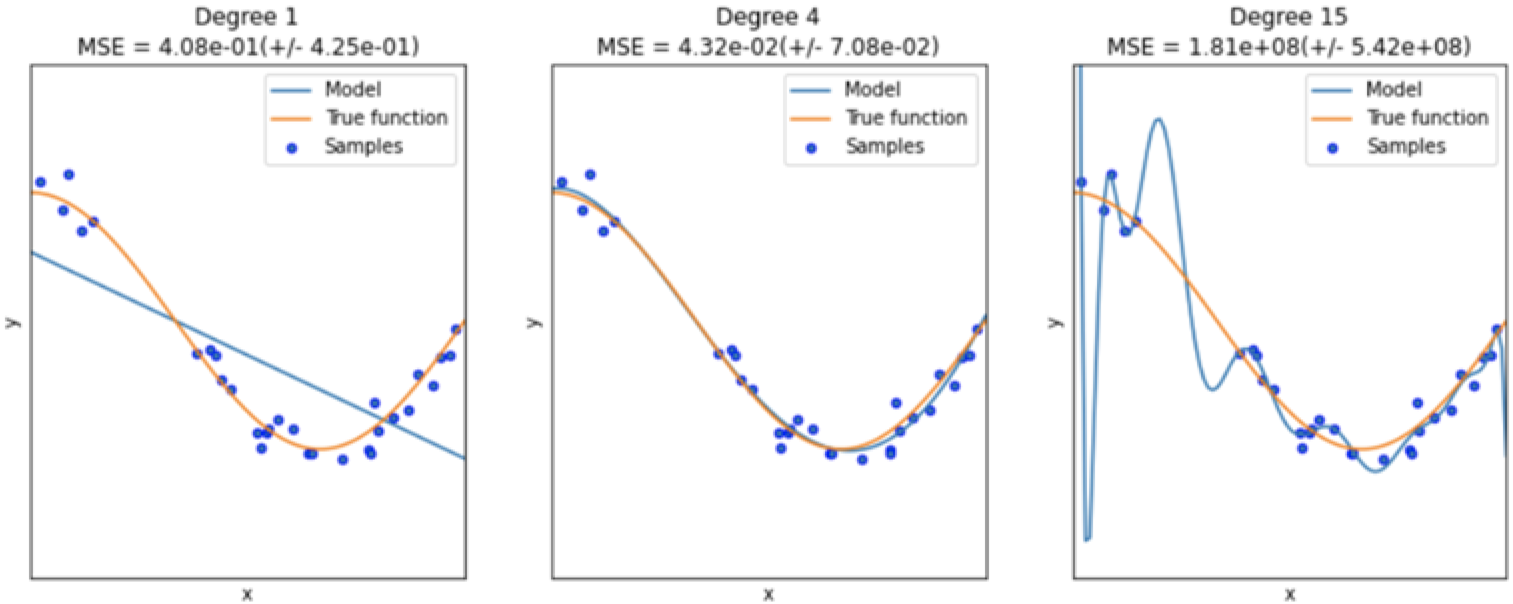
$$\phi_0(x) = 1 \qquad \phi_1(x) = x \qquad y = \boldsymbol{w}^\top \Phi_{\text{lin}}(x) = \phi_0(x)w_0 + \phi_1(x)w_1 = w_0 + w_1 x$$

- Actually, the embedding trick is stronger.
  - $(x^2, x, 1)$: 2nd order polynomial with respect to x
  - $(x^d, x^{d-1}, \ldots, 1)$: d-th order polynomial (= degree d)

$$\phi_0(x) = 1 \qquad \phi_1(x) = x \qquad \phi_2(x) = x^2$$

$$y = \boldsymbol{w}^\top \Phi_{\text{lin}}(x) = \phi_0(x)w_0 + \phi_1(x)w_1 + \phi_2(x)w_2 = w_0 + w_1 x + w_2 x^2$$

Feature embedding trick



$(x, 1)$ $(x^4, x^3, x^2, x, 1)$ $(x^{15}, \ldots, x^3, x^2, x, 1)$

higher-order polynomial = higher complexity = prone to overfitting!

from https://datascience.foundation/sciencewhitepaper/underfitting-and-overfitting-in-machine-learning

Basis Functions

- A **basis function** can be any function of the input features X
- Define a set of B basis functions $\phi_1(x), \ldots, \phi_B(x)$
- Fit a linear regression model in terms of basis functions,

$$y = \sum_{b=1}^{B} w_b \phi_b(x) = w^T \phi(x)$$

notation:
$\phi(x) := [\phi_1(x), \ldots, \phi_B(x)]$

- The model is *linear in the transformed basis/induced features* $\phi(x)$.
- The model is *nonlinear in the data* X

Recall the ordinary least squares solution is given by,

$$\mathbf{X} = \begin{pmatrix} 1 & x_{11} & \dots & x_{1D} \\ 1 & x_{21} & \dots & x_{2D} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_{m1} & \dots & x_{mD} \end{pmatrix} \qquad \mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_m \end{pmatrix} \qquad w^{\text{OLS}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Design Matrix
(each training input on a column)

Vector of
Training labels

Can similarly solve in terms of basis functions,

$$\mathbf{\Phi} = \begin{pmatrix} 1 & \phi_1(x_1) & \dots & \phi_B(x_1) \\ 1 & \phi_1(x_2) & \dots & \phi_B(x_2) \\ \vdots & \vdots & \vdots & \vdots \\ 1 & \phi_1(x_m) & \dots & \phi_B(x_m) \end{pmatrix} \qquad w^{\text{OLS}} = (\mathbf{\Phi}^T\mathbf{\Phi})^{-1}\mathbf{\Phi}^T\mathbf{y}$$

sklearn.preprocessing.PolynomialFeatures

degree : *int or tuple (min_degree, max_degree), default=2*

If a single int is given, it specifies the maximal degree of the polynomial features. If a tuple `(min_degree, max_degree)` is passed, then `min_degree` is the minimum and `max_degree` is the maximum polynomial degree of the generated features. Note that `min_degree=0` and `min_degree=1` are equivalent as outputting the degree zero term is determined by `include_bias`.

interaction_only : *bool, default=False*

If `True`, only interaction features are produced: features that are products of at most `degree` *distinct* input features, i.e. terms with power of 2 or higher of the same input feature are excluded:

- included: `x[0]`, `x[1]`, `x[0] * x[1]`, etc.
- excluded: `x[0] ** 2`, `x[0] ** 2 * x[1]`, etc.

include_bias : *bool, default=True*

If `True` (default), then include a bias column, the feature in which all polynomial powers are zero (i.e. a column of ones - acts as an intercept term in a linear model).

order : *{'C', 'F'}, default='C'*

Order of output array in the dense case. `'F'` order is faster to compute, but may slow down subsequent estimators.

Example: Polynomial Basis Functions

Create three two-dimensional data points [0,1], [2,3], [4,5]:

```
>>> X = np.arange(6).reshape(3, 2)
>>> X
array([[0, 1],
       [2, 3],
       [4, 5]])
```

Compute quadratic features $(1, x_1, x_2, x_1^2, x_1 x_2, x_2^2)$,

```
>>> poly = PolynomialFeatures(degree=2)
>>> poly.fit_transform(X)
array([[ 1.,   0.,   1.,   0.,   0.,   1.],
       [ 1.,   2.,   3.,   4.,   6.,   9.],
       [ 1.,   4.,   5.,  16.,  20.,  25.]])
```

These are now our new data and ready to fit a model…

Example: Polynomial Basis Functions

Create a 3-rd order polynomial (cubic) function,

```
f = lambda x: (x-1)*(x-2)*(x-3)
import numpy.random as ra
ra.seed(20)
train_x = np.arange(5)
train_y = f(train_x) + 1*ra.randn(len(train_x))
train_y
```

✓ 0.3s

```
array([-5.11610689,  0.19586502,  0.35753652, -2.34326191,  4.91516741])
```

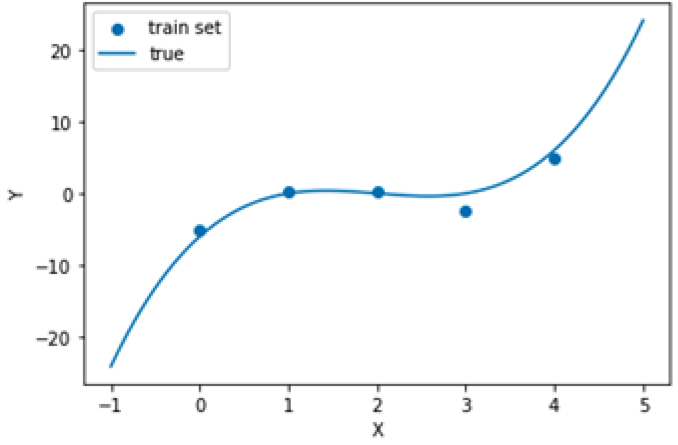
Plot train set and the actual function

```
test_x = np.linspace(-1,5,400)

from matplotlib import pyplot as plt
plt.scatter(train_x,train_y)

plt.plot(test_x, f(test_x))
plt.legend(['train set', 'true'])
plt.xlabel('X')
plt.ylabel('Y')
plt.show()
```

✓ 0.4s



Example: Polynomial Basis Functions

Create cubic features $(1, x, x^2, x^3)$

```
poly = PolynomialFeatures(degree=3)
train_xx = poly.fit_transform(train_x[:,np.newaxis])
train_xx
```

✓ 0.4s

turns train_x (length 5 array) into a matrix (5 by 1 matrix)

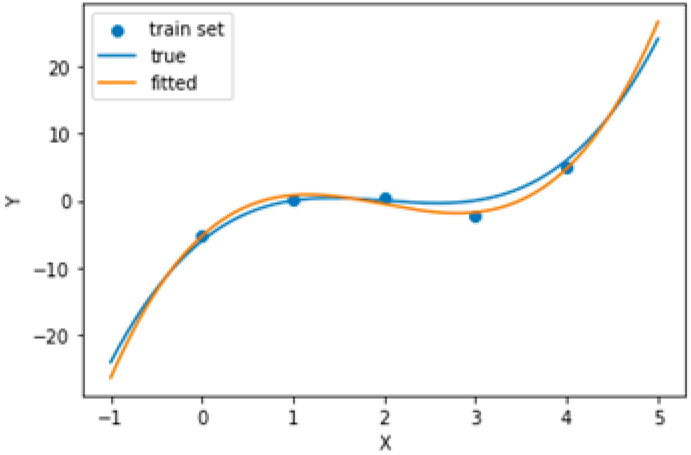
```
array([[ 1.,  0.,  0.,  0.],
       [ 1.,  1.,  1.,  1.],
       [ 1.,  2.,  4.,  8.],
       [ 1.,  3.,  9., 27.],
       [ 1.,  4., 16., 64.]])
```

Perform linear regression; plot it

```
from matplotlib import pyplot as plt
from sklearn.linear_model import LinearRegression
model = LinearRegression().fit(train_xx, train_y)
test_x = np.linspace(-1,5,400)
test_xx = poly.fit_transform(test_x[:,np.newaxis])
pred_y = model.predict(test_xx)

plt.scatter(train_x,train_y)
plt.plot(test_x, f(test_x))
plt.plot(test_x, pred_y)
plt.legend(['train set', 'true', 'fitted'])
plt.xlabel('X')
plt.ylabel('Y')
plt.show()
```

✓ 0.2s



Data Preprocessing

- Generally the first step in data science involves *preprocessing* or transforming data in some way
  - Filling in missing values (imputation)
  - Centering / normalizing / standardizing
  - Etc.

- We then fit our models to this preprocessed data

- One way to view preprocessing is simply as computing some basis function $\phi(x)$, nothing more

Basis Functions

PROs

- More flexible modeling that is nonlinear in the original data
- Increases model expressivity

CONs

- Typically requires **more parameters** to be learned
- More sensitive to **overfitting** training data (due to expressivity)
- Requires more **regularization** to avoid overfitting
- Need to find *good* basis functions (feature engineering)

Outline

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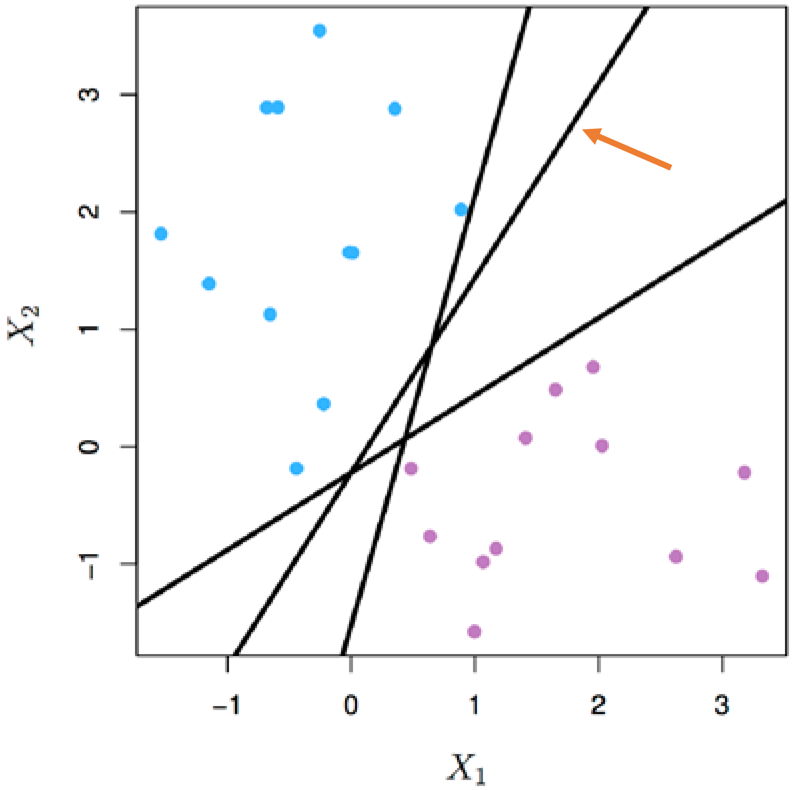
- Neural Networks

Linear Decision Boundary

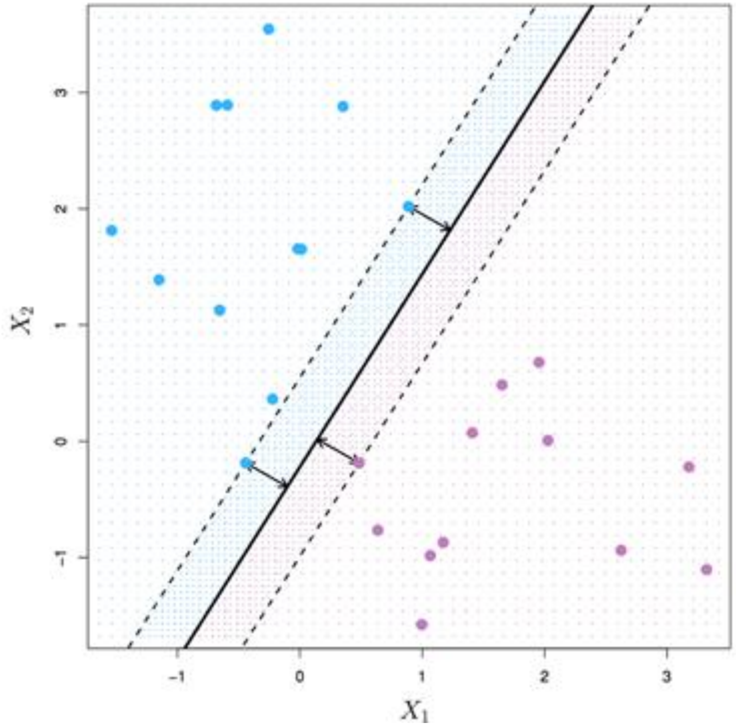
Forget about the 'regression' point of view for now..

At the end of the day, we just want a line that separates the two classes well.



Q: but if you have to choose one, which one will you choose?

Classifier Margin



*The **margin** measures minimum distance between each class and the decision boundary*

Observation Decision boundaries with larger margins are more likely to generalize to unseen data

Idea Learn the classifier with the largest margin that still separates the data…

…we call this a ***max-margin classifier***

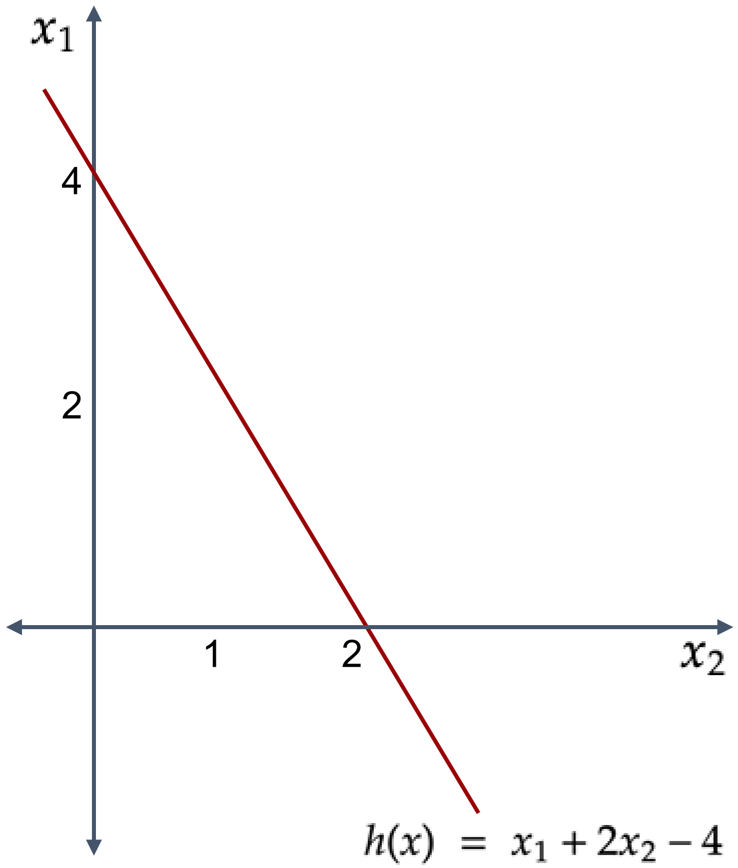
Hyperplane

A linear discriminant function in D dimensions is given by a hyperplane, defined as follows:

$$h(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$$
$$= w_1x_1 + w_2x_2 + \cdots + w_dx_d + b$$

For points that lie on the hyperlane, we have:

$$h(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b = 0$$



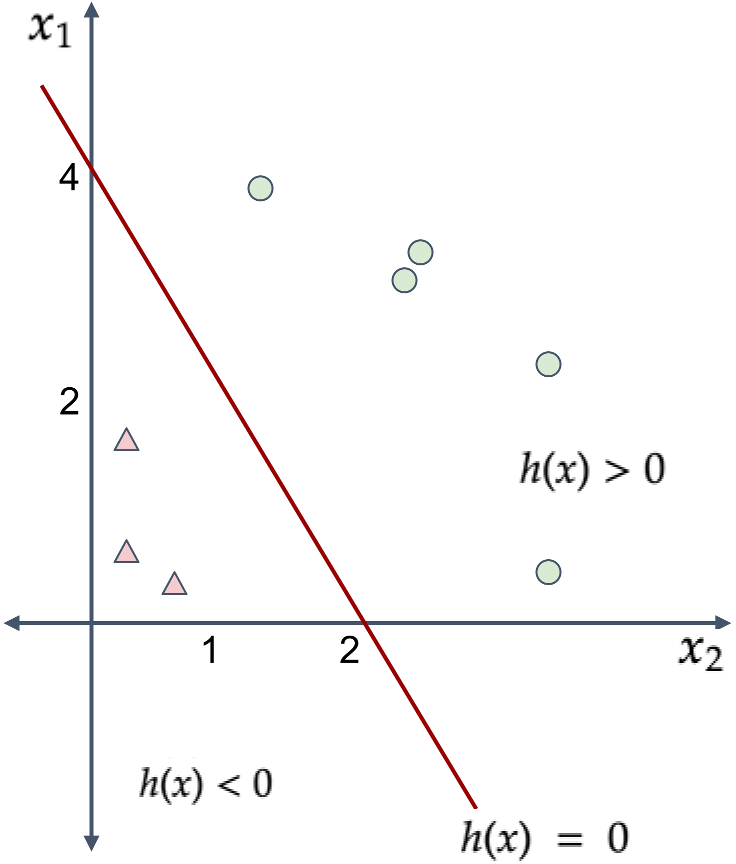
Separating Hyperplane

A hyperplane h(x) splits the original d-dimensional space into two half-spaces. If the input dataset is linearly separable:

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

Example:

$$h(x) = x_1 + 2x_2 - 4$$



Separating Hyperplane: weight vector

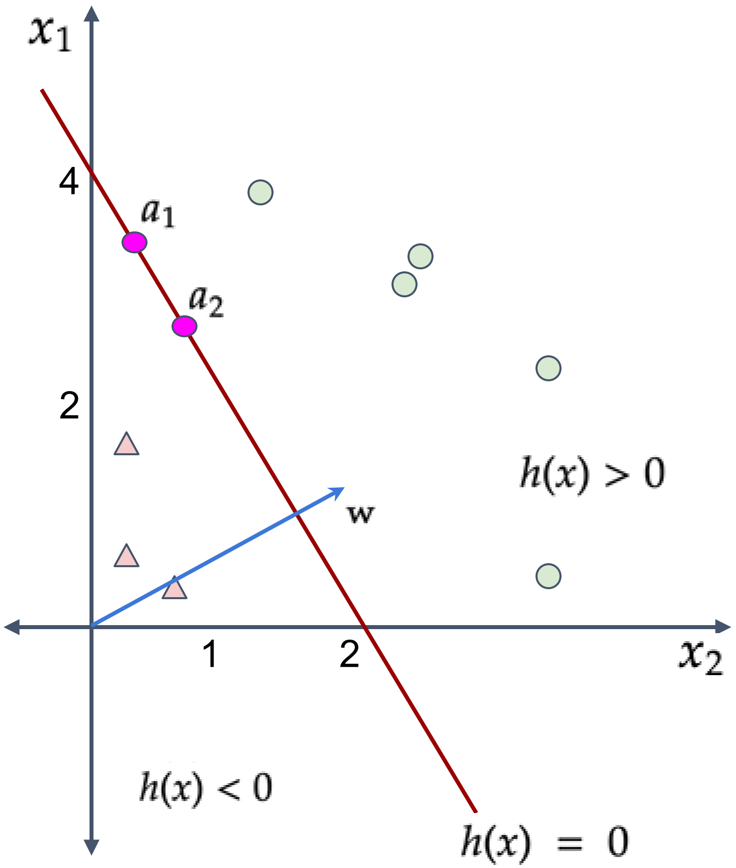
Let a_1 and a_2 be two arbitrary points that lie on the hyperplane, we have:

$$h(\mathbf{a}_1) = \mathbf{w}^T\mathbf{a}_1 + b = 0$$
$$h(\mathbf{a}_2) = \mathbf{w}^T\mathbf{a}_2 + b = 0$$

Subtracting one from the other:

$$\mathbf{w}^T(\mathbf{a}_1 - \mathbf{a}_2) = 0$$

The weight vector **w** is orthogonal to the hyperplane.



Distance of a Point to the Hyperplane

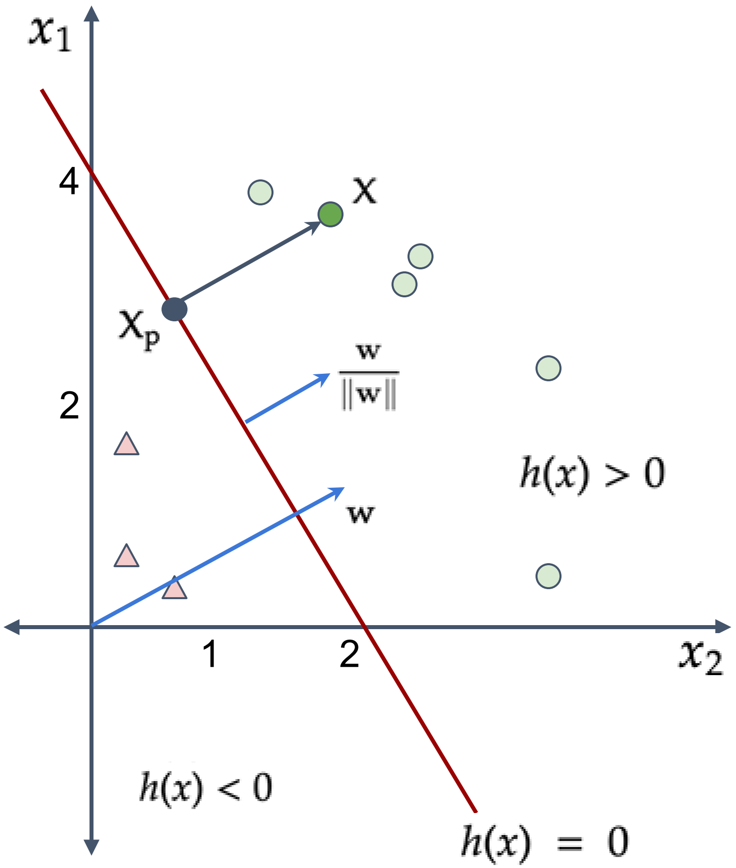
Consider a point X not on the hyperplane. Let X_p be the projection of X on the hyperplane.

Let r be the steps need to walk from X_p to X.

$$\mathbf{x} = \mathbf{x}_p + r\frac{\mathbf{w}}{\|\mathbf{w}\|}$$

$$\|w\| = \sqrt{w^T w} = \sqrt{\sum_i w_i^2}$$

Q: how many steps/direct distance do we need to walk?

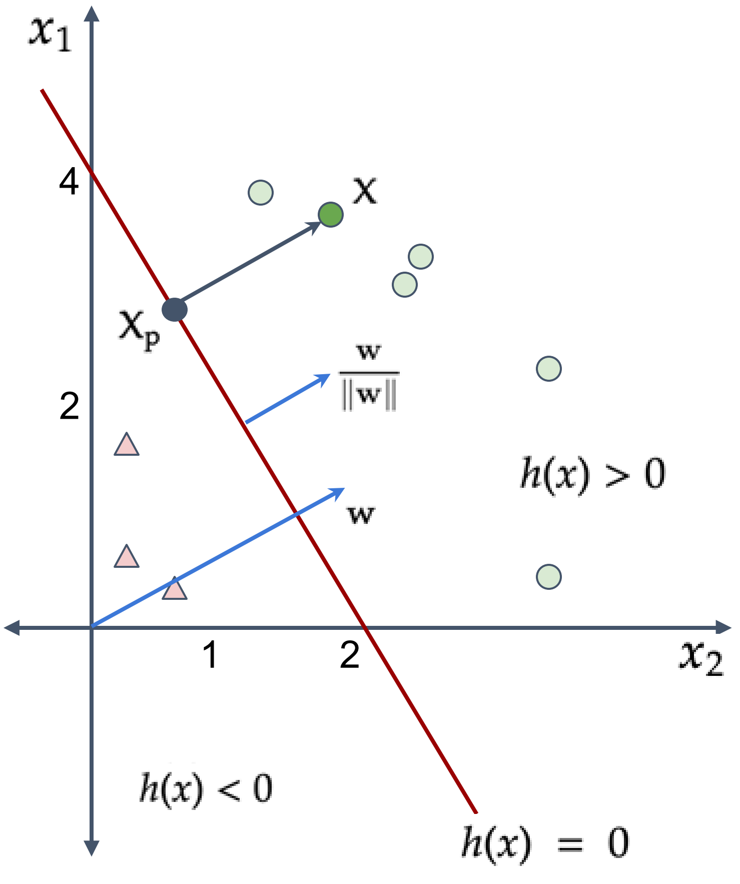


Distance of a Point to the Hyperplane

Consider a point X not on the hyperplane. Let X_p be the projection of X on the hyperplane.

Let r be the steps need to walk from X_p to X.

$$
\begin{aligned}
h(\mathbf{x}) &= h(\mathbf{x}_p + r\frac{\mathbf{w}}{\|\mathbf{w}\|}) \\
&= \mathbf{w}^T\left(\mathbf{x}_p + r\frac{\mathbf{w}}{\|\mathbf{w}\|}\right) + b \\
&= \underbrace{\mathbf{w}^T\mathbf{x}_p + b}_{h(\mathbf{x}_p)} + r\frac{\mathbf{w}^T\mathbf{w}}{\|\mathbf{w}\|} \\
&= \underbrace{h(\mathbf{x}_p)}_{0} + r\|\mathbf{w}\| \\
&= r\|\mathbf{w}\|
\end{aligned}
\qquad r = \frac{h(\mathbf{x})}{\|\mathbf{w}\|}
$$



Distance of a Point to the Hyperplane

Q: What is the direct distance from origin (x=0) to the hyperplane?

$$r = \frac{h(\mathbf{x})}{\|\mathbf{w}\|} \qquad r = \frac{h(\mathbf{0})}{\|\mathbf{w}\|} = \frac{\mathbf{w}^T\mathbf{0} + b}{\|\mathbf{w}\|} = \frac{b}{\|\mathbf{w}\|}$$

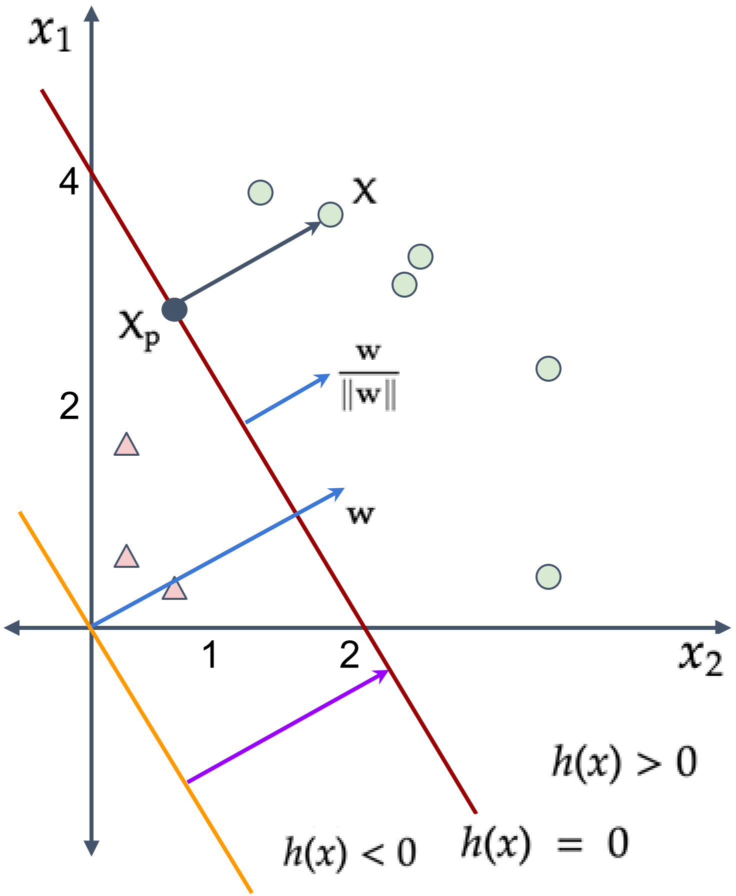
Example:

$$h(x) = x_1 + 2x_2 - 4$$

$$w^T x + b = (1 \;\; 2)\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} - 4$$

$$\frac{b}{\|w\|} = -\frac{4}{\sqrt{5}}$$

Q: how to deal with negative distance?



Distance of a Point to the Hyperplane

Q: How to deal with negative distance?

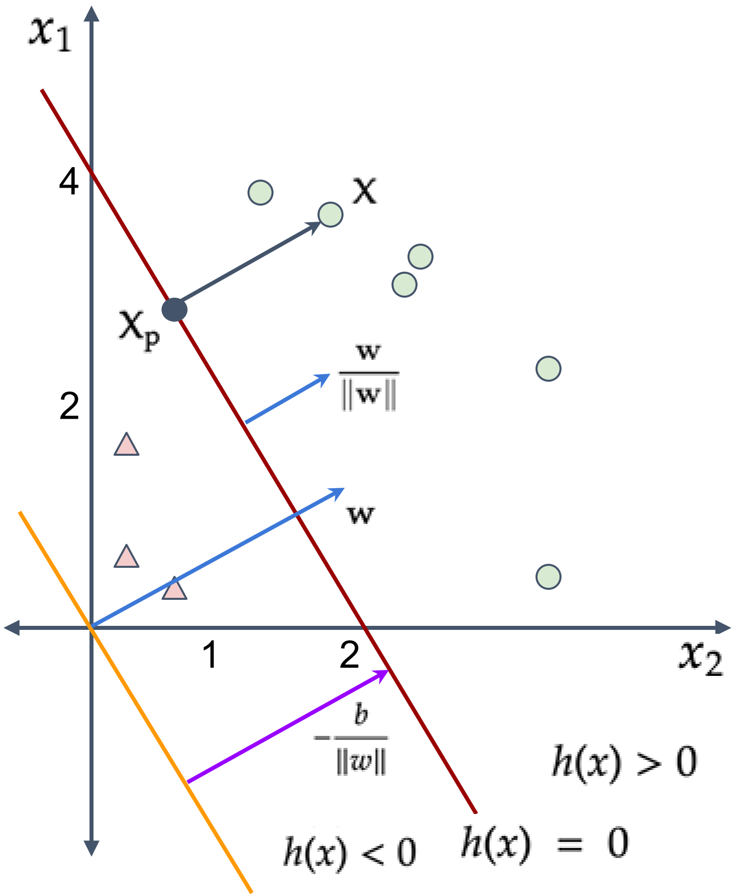
$$r = \frac{h(\mathbf{x})}{\|\mathbf{w}\|}$$

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

$$\delta = y\,r = \frac{y\,h(\mathbf{x})}{\|\mathbf{w}\|}$$

Example (when point is the origin):

$$(-1) \cdot \frac{b}{\|w\|} = \frac{4}{\sqrt{5}}$$

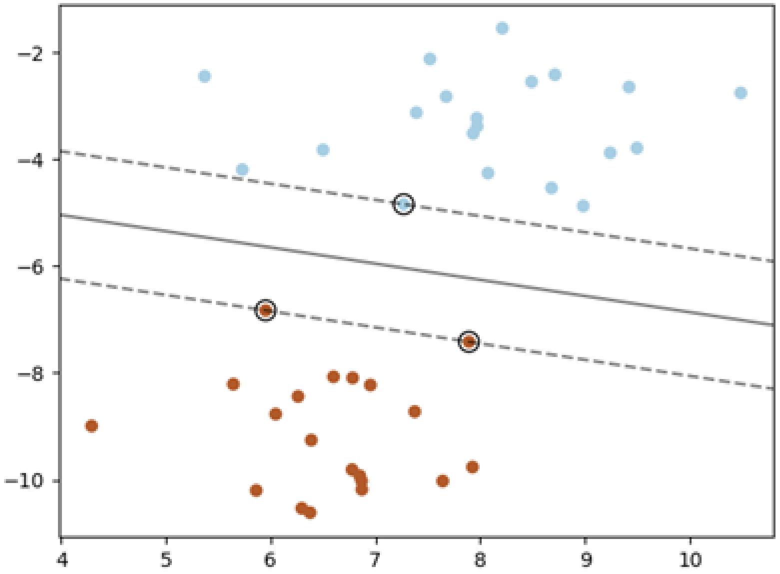


Margin and Support Vectors

$$\delta = y\, r = \frac{y\, h(\mathbf{x})}{\|\mathbf{w}\|}$$

Over all the n points, the ***margin*** of the linear classifier is the minimum distance of a point from the separating hyperplane:

$$\delta^* = \min_{\mathbf{x}_i} \left\{ \frac{y_i(\mathbf{w}^T\mathbf{x}_i + b)}{\|\mathbf{w}\|} \right\}$$



All the points that achieve this minimum distance are called ***support vectors***.

Max-Margin Classifier (Linear Separable Case)

For training data $\{(x^{(i)}, y^{(i)})\}_{i=1}^{m}$, a classifier $f(x) = w^\top x + b$ with 0 train error will satisfy

$$y^{(i)} f(x^{(i)}) = y^{(i)}(w^\top x^{(i)} + b) > 0$$

↓ negative margin when misclassifying it!

The distance for ($x^{(i)}$, $y^{(i)}$) to separating hyperplane

$$\frac{y^{(i)}(w^\top x^{(i)} + b)}{\|w\|}$$

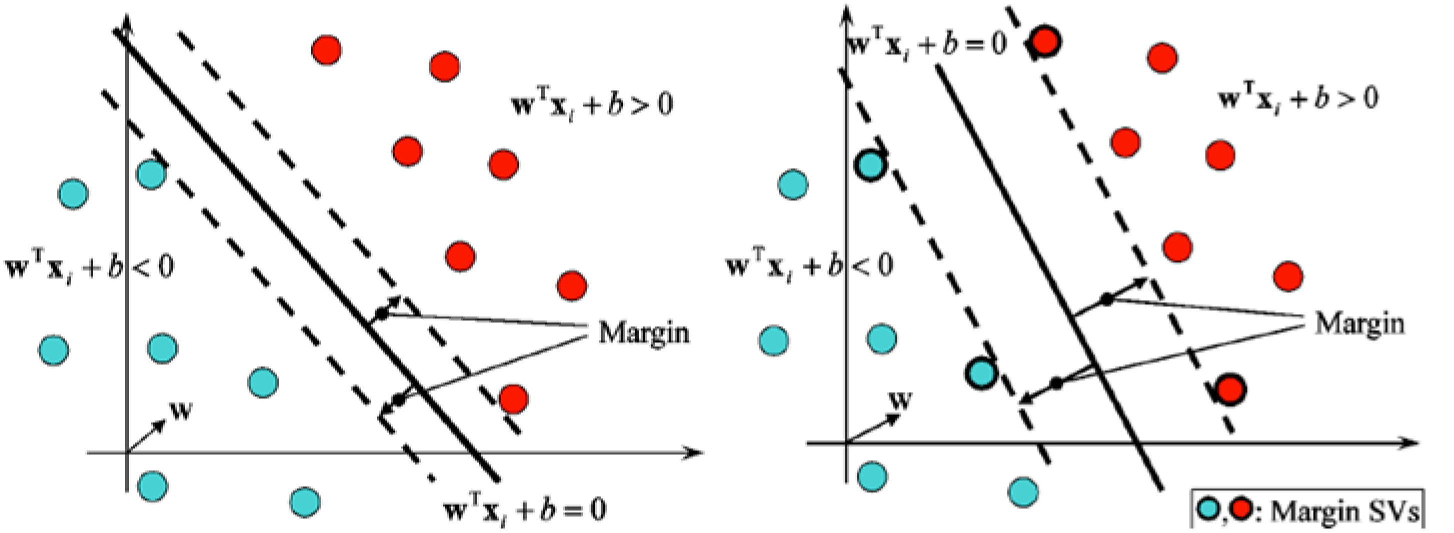
The margin of a classifier $f(x)$ is

$$\min_i \frac{y^{(i)}(w^\top x^{(i)} + b)}{\|w\|}$$

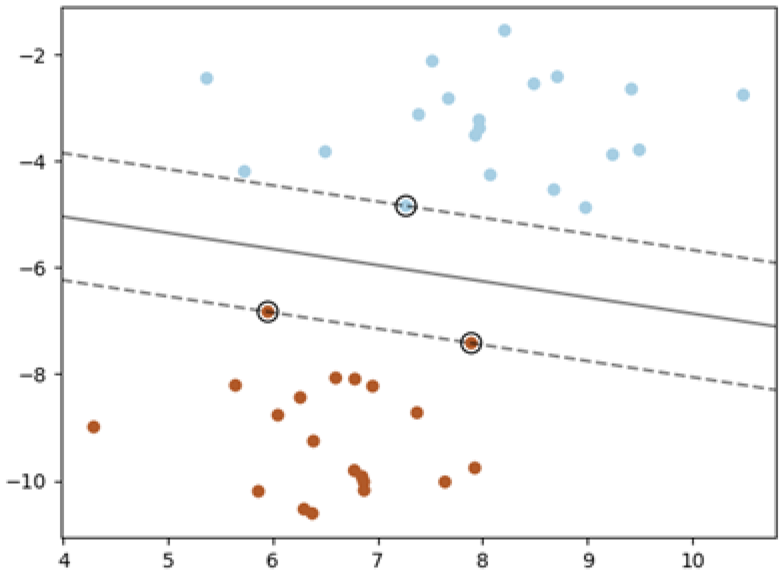
Find f that maximize margin

$$\arg\max_{w,b} \min_i \frac{y^{(i)}(w^\top x^{(i)} + b)}{\|w\|}$$

Max-Margin Classifier (Linear Separable Case)



Max-Margin Classifier (Linear Separable Case)



$$\overbrace{\arg\max_{w,b} \underbrace{\min_{i} \frac{y^{(i)}(w^{\top}x^{(i)} + b)}{\|w\|}}_{\text{Minimum margin over all training data}}}^{\text{Maximize the minimum margin}}$$

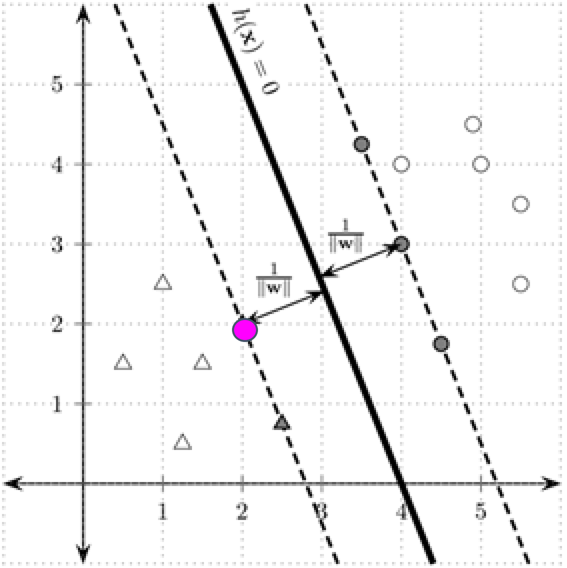
Find the parameters (w,b) that **maximize** the **smallest margin** over all the training data

Canonical Hyperplane

$$\arg\max_{w,b} \min_i \frac{\boxed{y^{(i)}(w^\top x^{(i)} + b)}}{\|w\|}$$ → 1 for support vectors

Issue: infinite equivalent hyperplanes result in infinite solutions

Solution: choose the scalar s such that the absolute distance of a ***support vector*** from the hyperplane is $\frac{1}{\|w\|}$

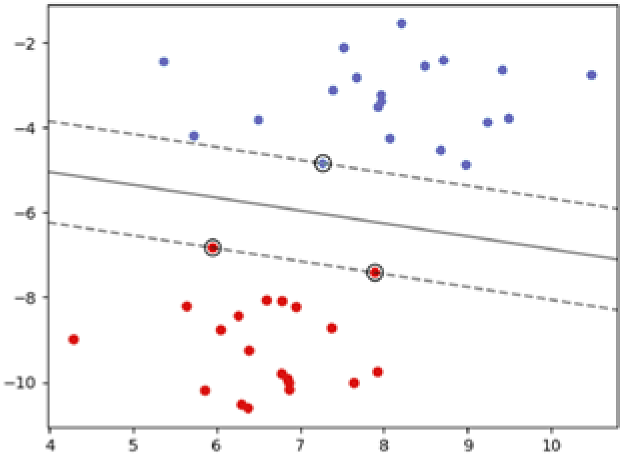


Margin: $\delta^* = \frac{1}{\|\mathbf{w}\|}$

Max margin: $h^* = \arg\max_h \{\delta_h^*\} = \arg\max_{\mathbf{w},b} \left\{\frac{1}{\|\mathbf{w}\|}\right\}$

Support Vector Machine (Hard Margin)

… it leads to



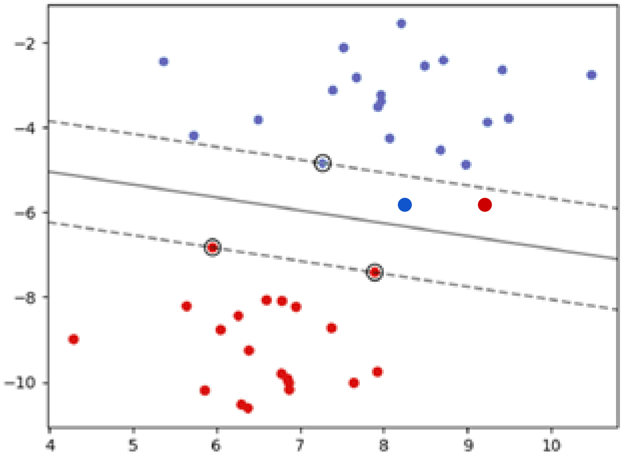
$$\min_{w,b} \frac{1}{2}\|w\|^2$$
subject to
$$y^{(i)}(w^\top x^{(i)} + b) \geq 1 \qquad \text{for } i = 1, \ldots, m$$

This is a convex (quadratic) optimization problem that can be solved efficiently

- Data are D-dimensional *vectors*
- Margins determined by nearest data points called ***support vectors***
- We call this a *support vector machine* (SVM)

Support Vector Machine (Soft Margin)

If the data is linearly not separable,



regularization   error

$$\min_{w,b} \frac{1}{2}\|w\|^2 + C \cdot \sum_{i=1}^{m} \xi_i$$

subject to

$$y^{(i)}(w^\top x^{(i)} + b) \geq 1 - \xi_i$$

$$\xi_i \geq 0 \quad \text{for } i = 1, \ldots, m$$

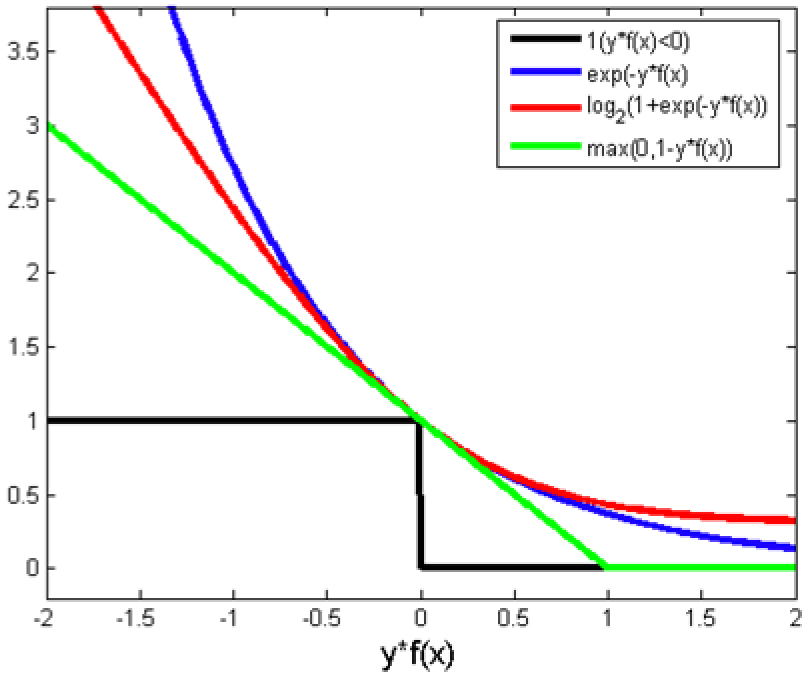
Equivalent formulation

$$\min_{\mathrm{w,b}} \frac{1}{2}\|w\|^2 + C \sum_{i=1}^{m} \left(1 - y^{(i)}(w^\top x^{(i)} + b)\right)_+$$

SVM - Soft Margin: hinge loss

Equivalent formulation

$$\min_{w,b} \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{m}\left(1 - y^{(i)}(w^\top x^{(i)} + b)\right)_+$$



$$\ell(f; x^{(i)}, y^{(i)}) = \left(1 - y^{(i)} f(x^{(i)})\right)_+$$

$$(X)_+ \coloneqq \max(X, 0)$$

SVM - Soft Margin: an example

$$Hinge\ loss = max\left(0,\ 1 - y_i\left(w^T x_i + b\right)\right)$$

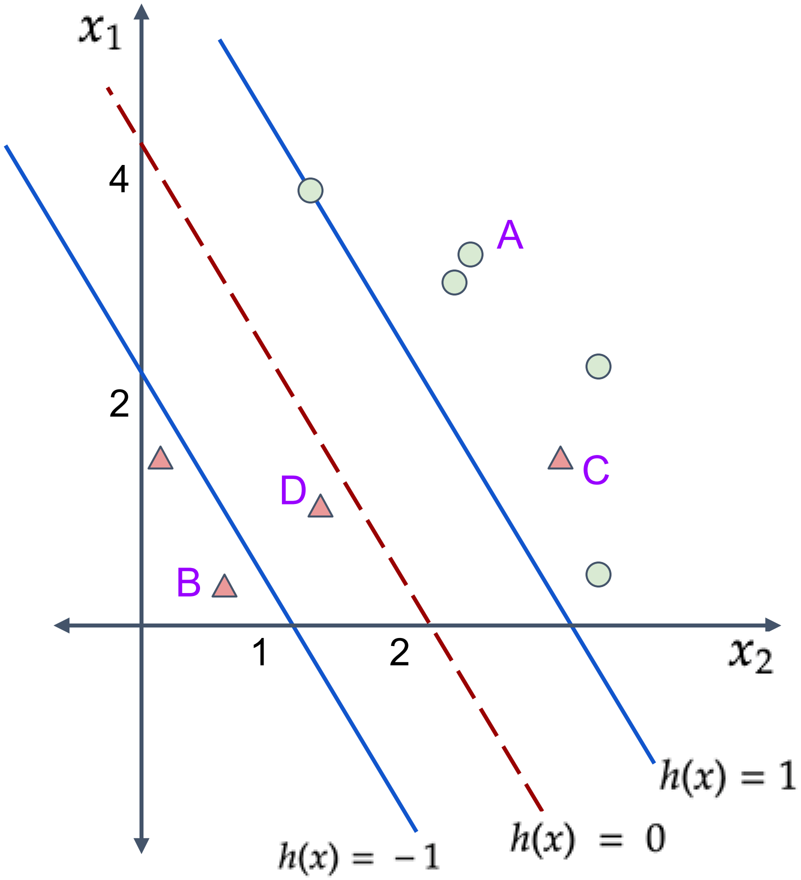
$$A:\ max(0,\ 1 - 1 \cdot (>1)) \rightarrow 0$$

$$B:\ max(0, 1 - (-1) \cdot (<-1)) \rightarrow 0$$

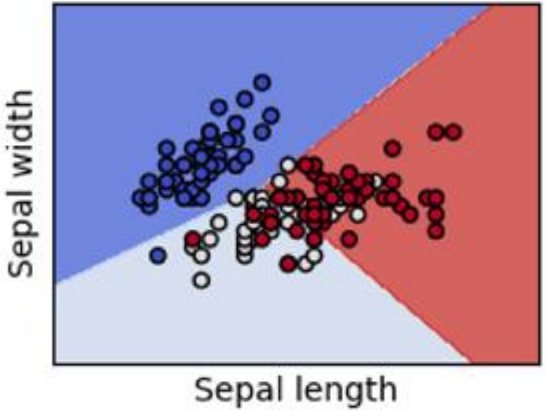
$$C:\ max(0,\ 1 - (-1) \cdot (>1)) \rightarrow\ >1$$

$$D:\ max(0, 1 - (-1) \cdot (between\ [-1, 0]))$$

$$\rightarrow between\ [0, 1]$$



SVM in Scikit-Learn



SVM with linear decision boundaries,

sklearn.svm.LinearSVC

Call options include…

penalty : *{'l1', 'l2'}, default='l2'*

Specifies the norm used in the penalization. The 'l2' penalty is the standard used in SVC. The 'l1' leads to `coef_` vectors that are sparse.

dual : *bool, default=True*

Select the algorithm to either solve the dual or primal optimization problem. Prefer dual=False when n_samples > n_features.

C : *float, default=1.0*

Regularization parameter. The strength of the regularization is inversely proportional to C. Must be strictly positive.

sklearn.svm.SVC

kernel : *{'linear', 'poly', 'rbf', 'sigmoid', 'precomputed'}, default='rbf'*

Specifies the kernel type to be used in the algorithm. It must be one of 'linear', 'poly', 'rbf', 'sigmoid', 'precomputed' or a callable. If none is given, 'rbf' will be used. If a callable is given it is used to pre-compute the kernel matrix from data matrices; that matrix should be an array of shape `(n_samples, n_samples)`.

gamma : *{'scale', 'auto'} or float, default='scale'*

Kernel coefficient for 'rbf', 'poly' and 'sigmoid'.

- if `gamma='scale'` (default) is passed then it uses 1 / (n_features * X.var()) as value of gamma,
- if 'auto', uses 1 / n_features.

for RBF,
small γ: complex decision boundary
large γ: more like linear decision boundary

max_iter : *int, default=-1*

Hard limit on iterations within solver, or -1 for no limit.

verbose : *bool, default=False*

Enable verbose output. Note that this setting takes advantage of a per-process runtime setting in libsvm that, if enabled, may not work properly in a multithreaded context.

class_weight : *dict or 'balanced', default=None*

Set the parameter C of class i to class_weight[i]*C for SVC. If not given, all classes are supposed to have weight one. The "balanced" mode uses the values of y to automatically adjust weights inversely proportional to class frequencies in the input data as `n_samples / (n_classes * np.bincount(y))`.

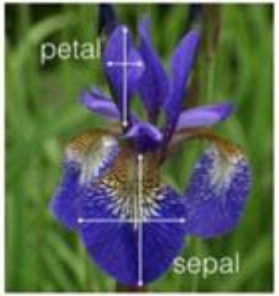
Example: Fisher's Iris Dataset

Classify among 3 species of Iris flowers…

Iris setosa

Iris versicolor

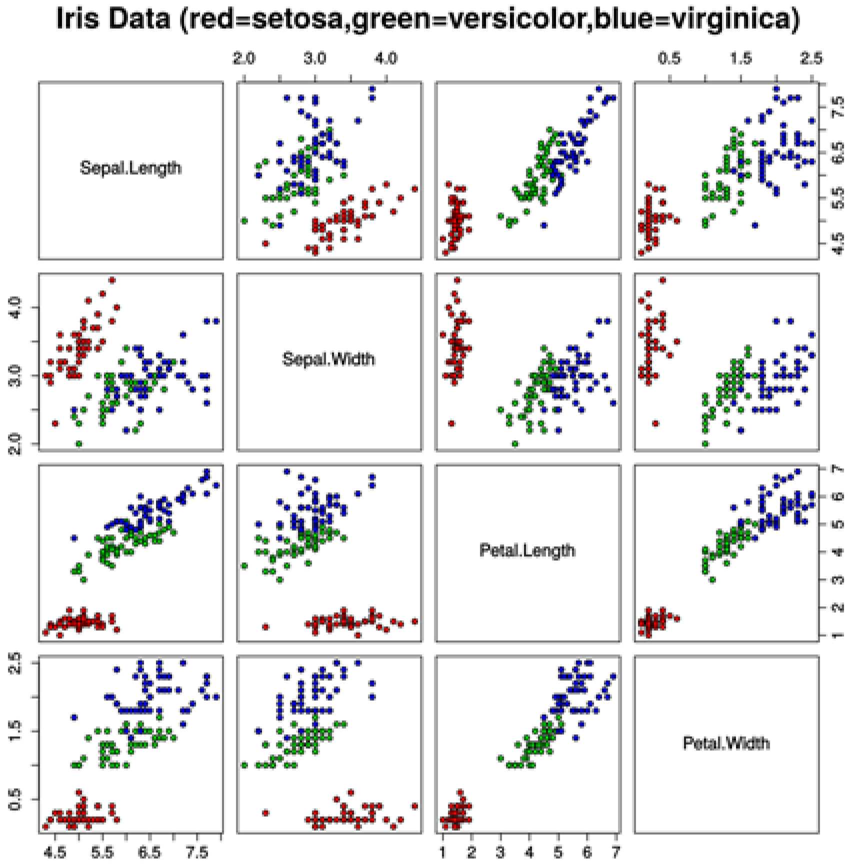
Iris virginica



Four features (in centimeters)

- Petal length / width
- Sepal length / width

Example: Fisher's Iris Dataset



Fairly easy to separate ***setosa*** *from others using a* *<u>linear classifier</u>*

Need to use nonlinear basis / kernel representation to better separate other classes

Example: Fisher's Iris Dataset

Train 8-degree polynomial kernel SVM classifier,

```
from sklearn.svm import SVC
svclassifier = SVC(kernel='poly', degree=8)
svclassifier.fit(X_train, y_train)
```

Generate predictions on held-out test data,

```
y_pred = svclassifier.predict(X_test)
```

Show confusion matrix and classification accuracy,

```
print(confusion_matrix(y_test, y_pred))
print(classification_report(y_test, y_pred))
```

```
[[11  0  0]
 [ 0 12  1]
 [ 0  0  6]]
```

```
                 precision    recall  f1-score   support

    Iris-setosa       1.00      1.00      1.00        11
Iris-versicolor       1.00      0.92      0.96        13
 Iris-virginica       0.86      1.00      0.92         6

    avg / total       0.97      0.97      0.97        30
```

[Source: https://stackabuse.com/implementing-svm-and-kernel-svm-with-pythons-scikit-learn/]