Computer Science

CSC380: Principles of Data Science

Nonlinear Models 2

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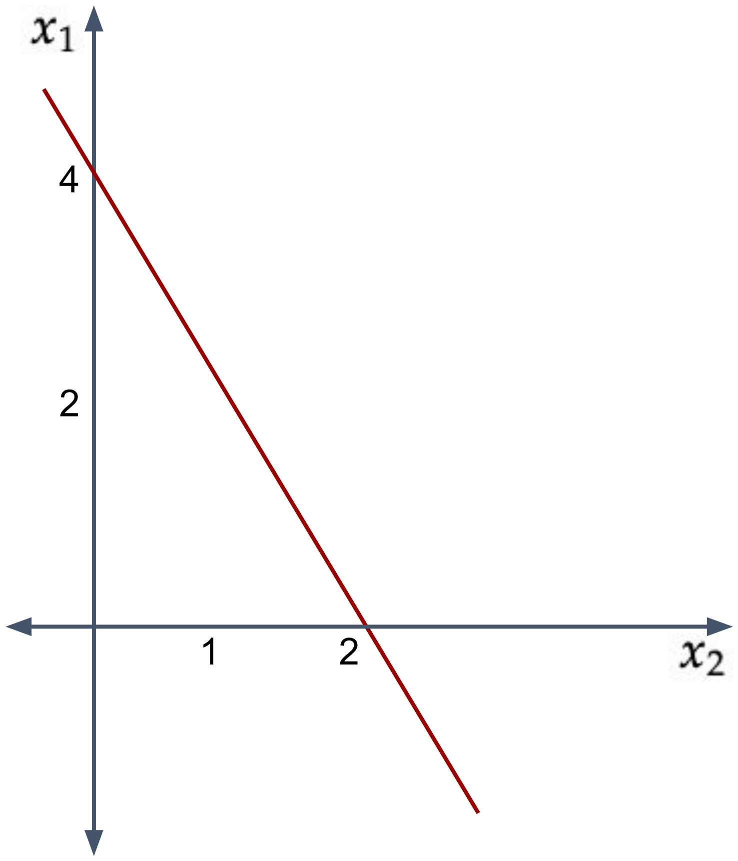
Hyperplane

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:

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



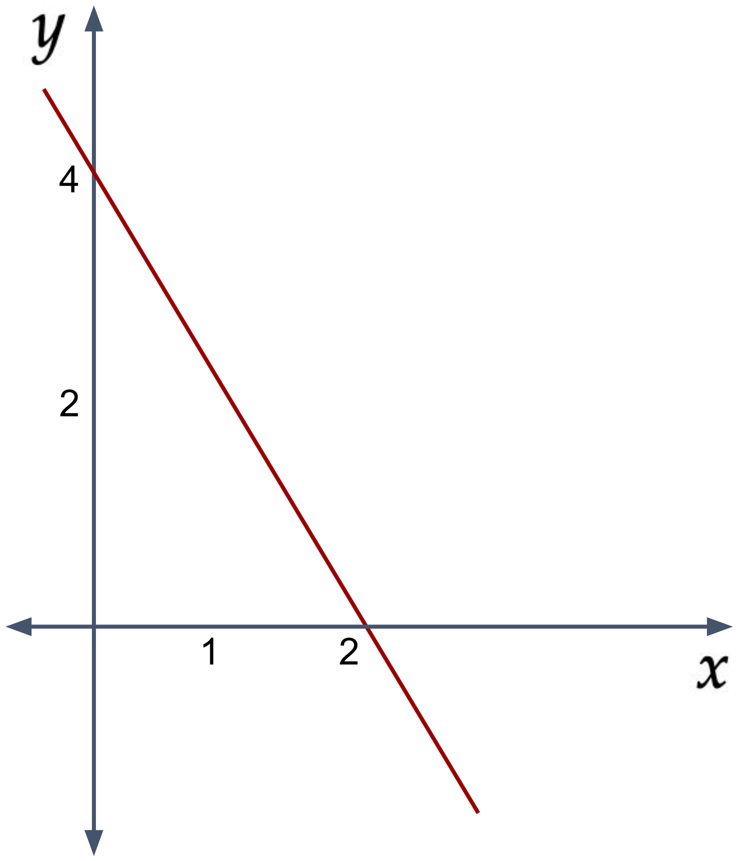
Hyperplane: an example

$$y = -2x + 4$$

$$y + 2x - 4 = 0$$

$$y \longrightarrow x_1$$
$$x \longrightarrow x_2$$

$$x_1 + 2x_2 - 4 = 0$$



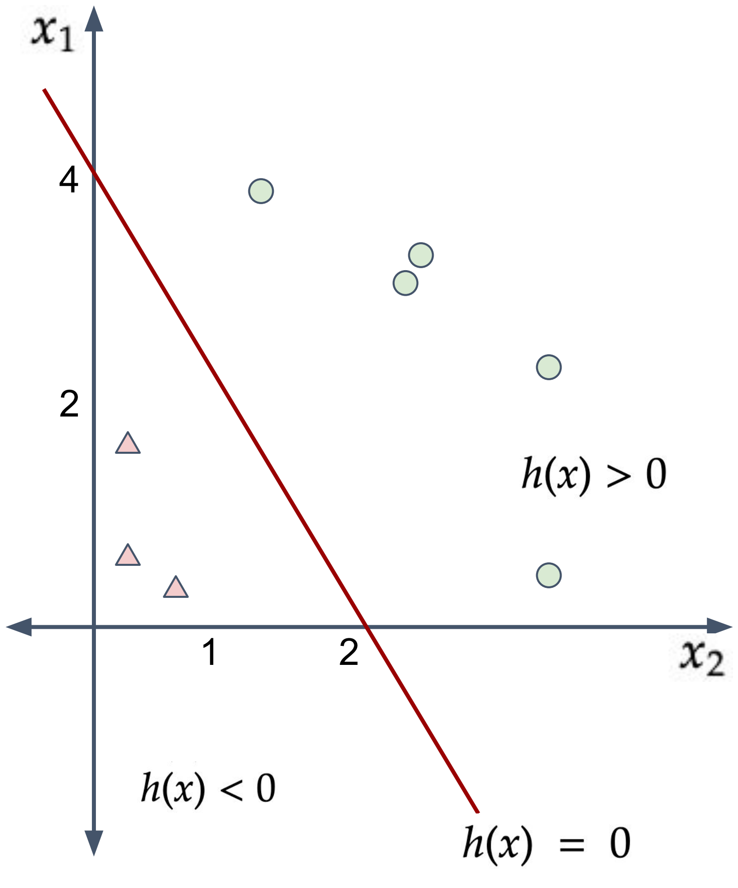
Separating Hyperplane

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

$$y = -2x + 4$$

○ $y > -2x + 4 \qquad y + 2x - 4 > 0$

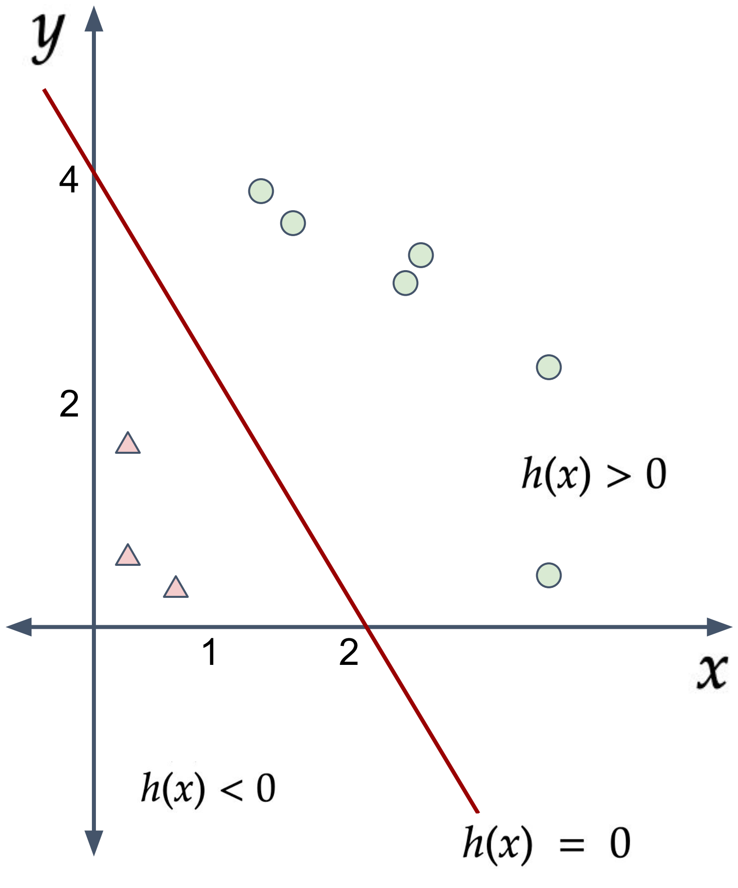
△ $y < -2x + 4 \qquad y + 2x - 4 < 0$

$$y \longrightarrow x_1$$
$$x \longrightarrow x_2$$

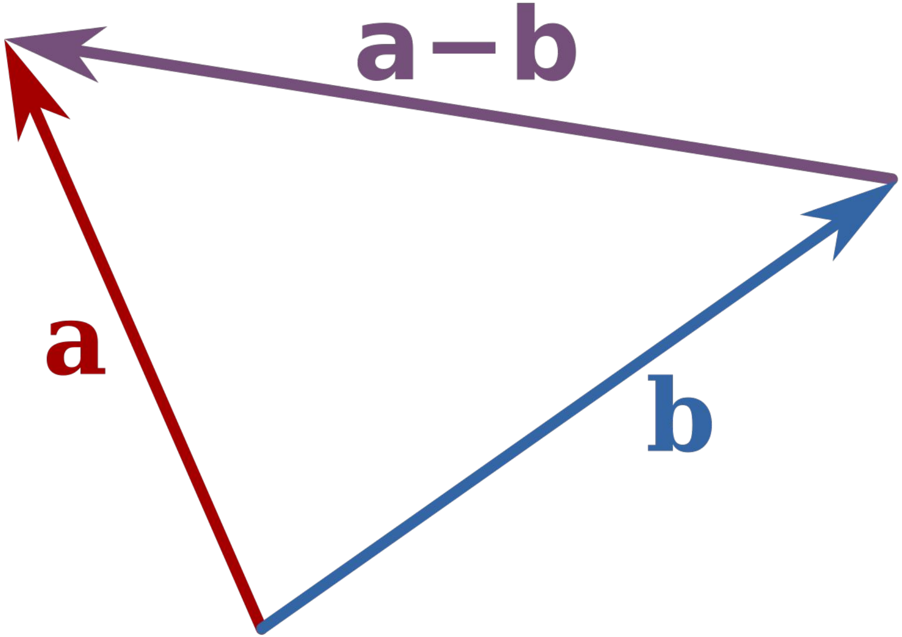
○ $x_1 + 2x_2 - 4 > 0$

△ $x_1 + 2x_2 - 4 < 0$

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



Vector subtraction



Separating Hyperplane: weight vector

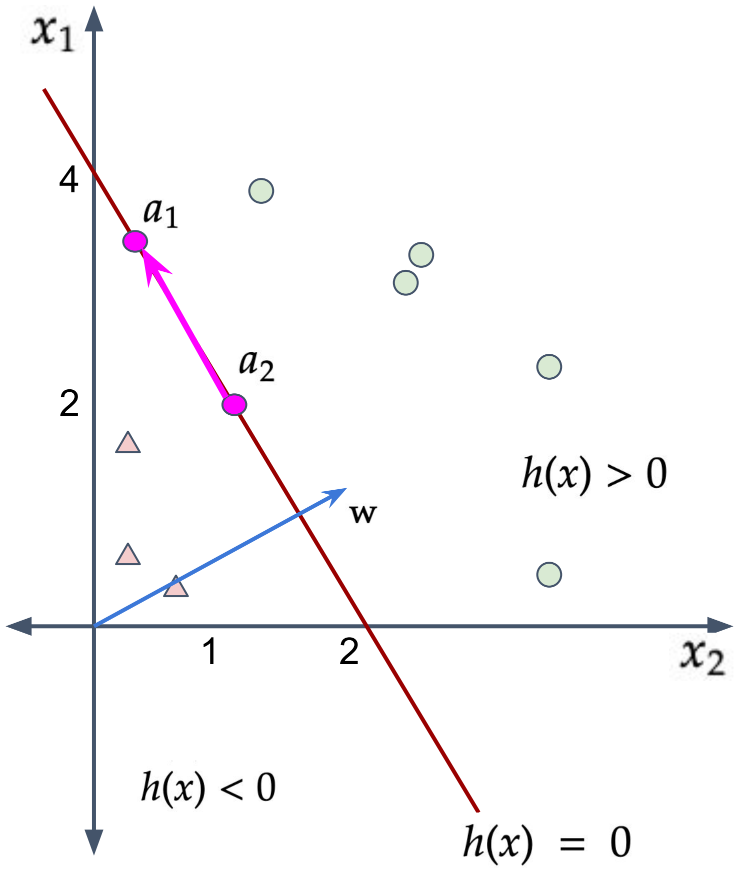
Let a_1 and a_2 be two arbitrary points that lie on the hyperplane, we have:

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

Subtracting one from the other:

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

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



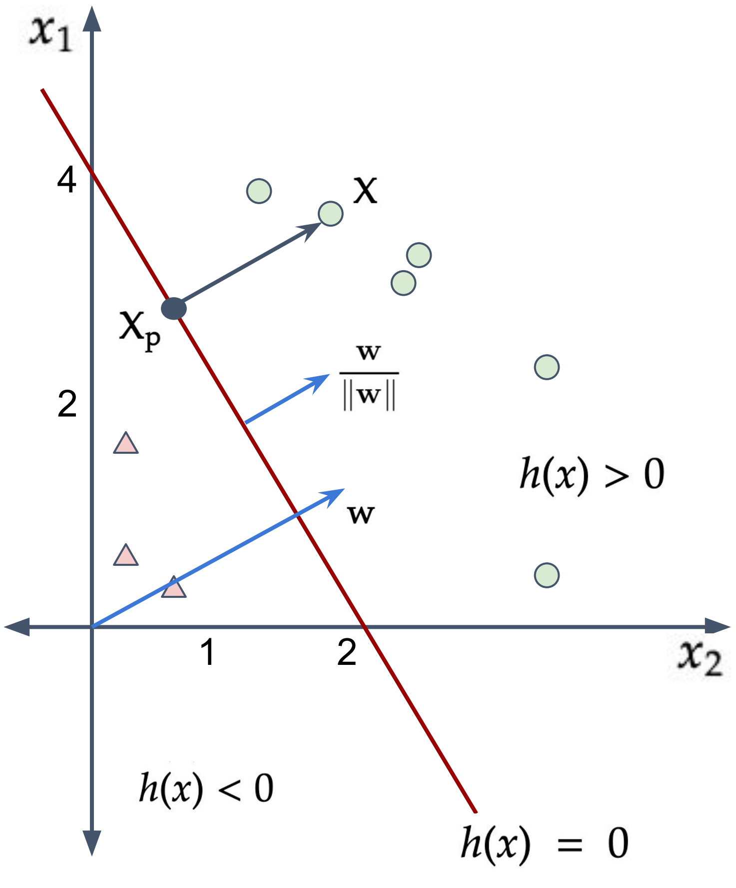
Distance of a Point to the Hyperplane

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.

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

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.

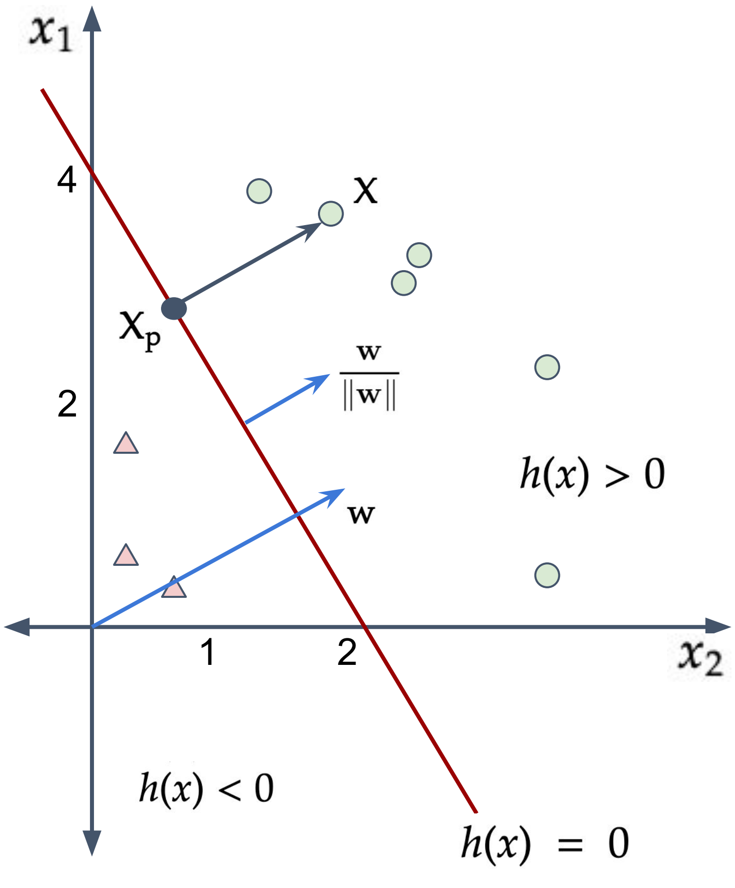
$$h(\mathbf{x}) = h(\mathbf{x}_p + r\frac{\mathbf{w}}{\|\mathbf{w}\|})$$

$$= \mathbf{w}^T\left(\mathbf{x}_p + r\frac{\mathbf{w}}{\|\mathbf{w}\|}\right) + b$$

$$= \underbrace{\mathbf{w}^T\mathbf{x}_p + b}_{h(\mathbf{x}_p)} + r\frac{\mathbf{w}^T\mathbf{w}}{\|\mathbf{w}\|}$$

$$= \underbrace{h(\mathbf{x}_p)}_{0} + r\|\mathbf{w}\|$$

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



Distance of a Point to the Hyperplane

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

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

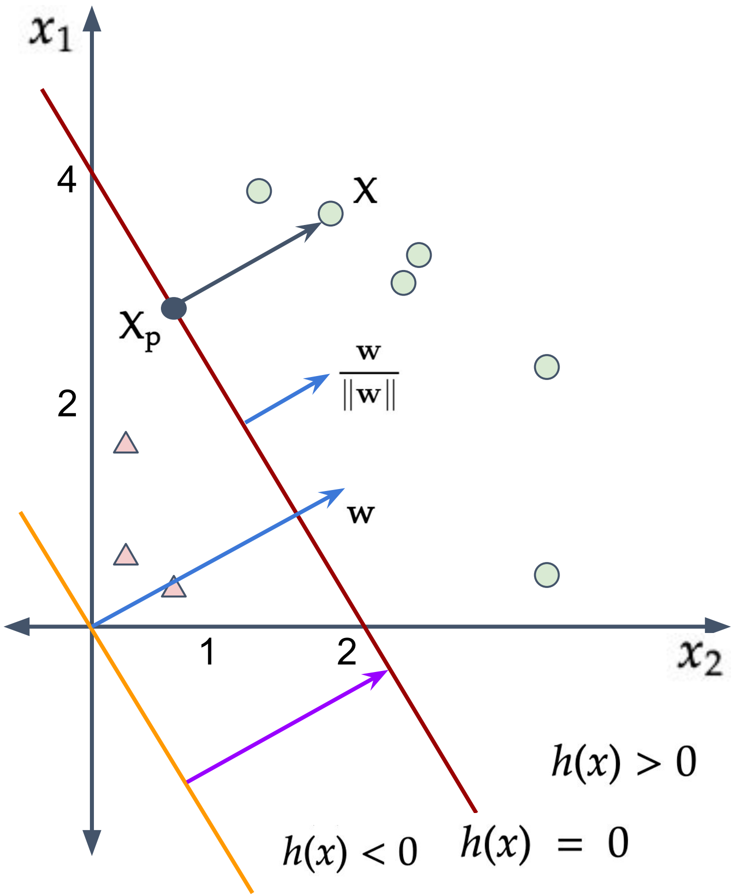
Example:

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

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

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

Q: how to deal with negative distance?



Distance of a Point to the Hyperplane

Q: How to deal with negative distance?

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

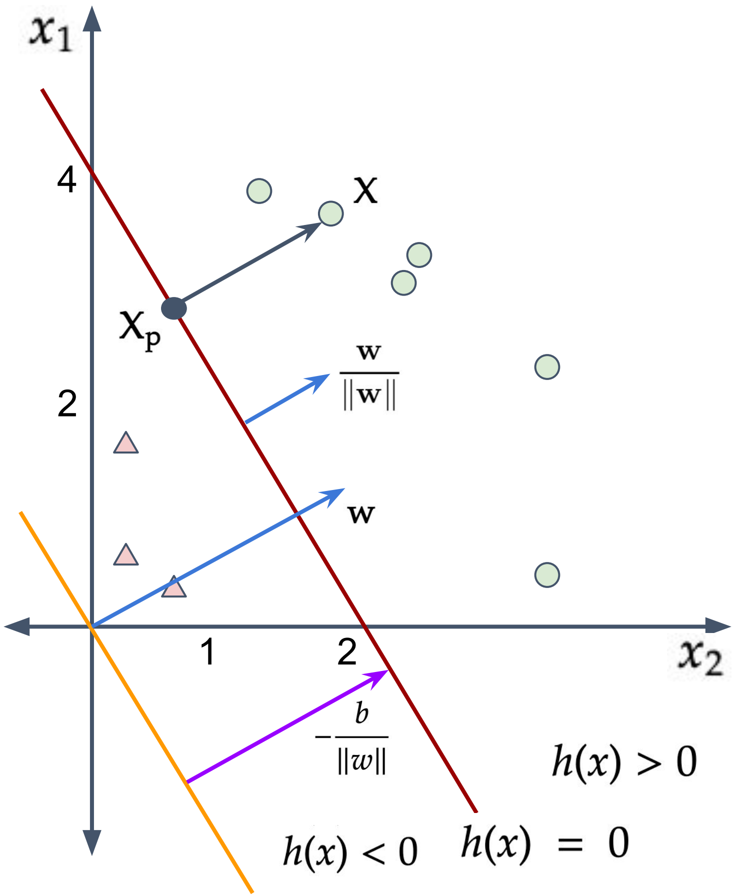
$$y = \begin{cases} +1 & \text{if } h(\mathbf{x}) > 0 \\ -1 & \text{if } h(\mathbf{x}) < 0 \end{cases}$$

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

Q: why not using absolute value?

Example (when point is the origin):

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



Distance of a Point to the Hyperplane

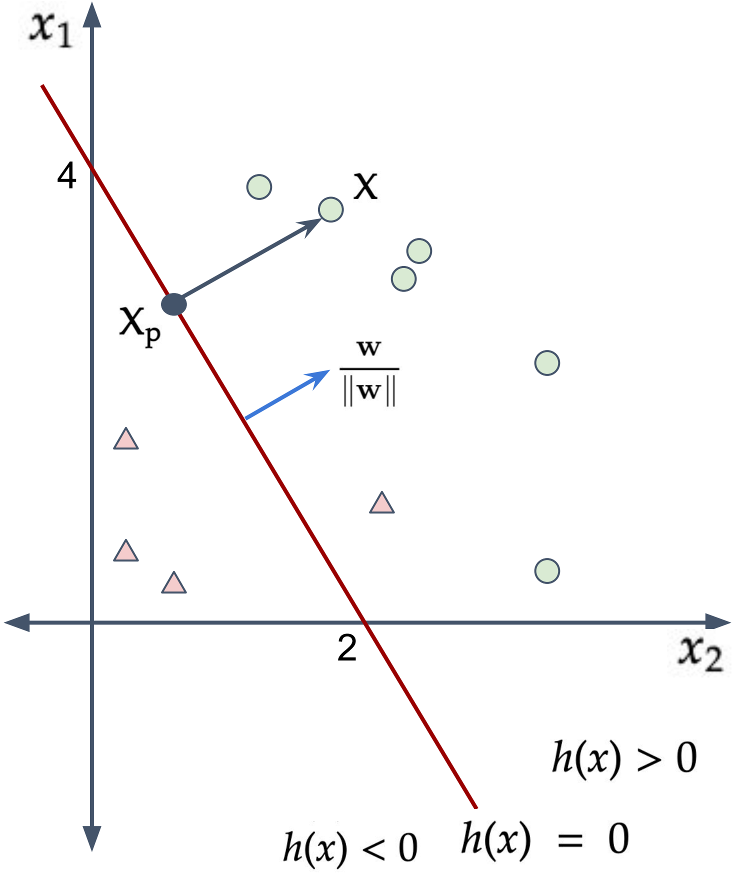
Q: How to deal with negative distance?

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

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

Q: why not using absolute value of h(x)?

We not only care about the distance of a point to the hyperplane, but also care if the point is correctly labeled: using absolute value only gets the distance (because always positive).



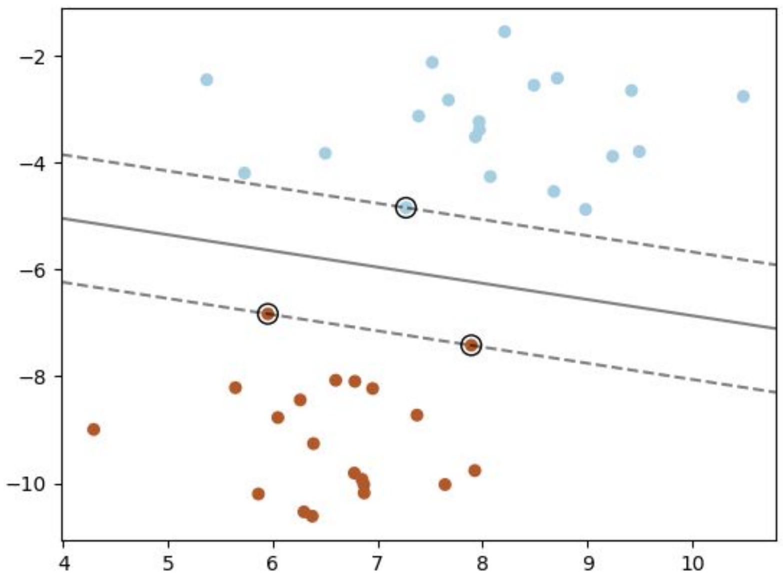
Margin and Support Vectors

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***.

$$\delta^* = \frac{y^*(\mathbf{w}^T \mathbf{x}^* + b)}{\|\mathbf{w}\|}$$



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

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

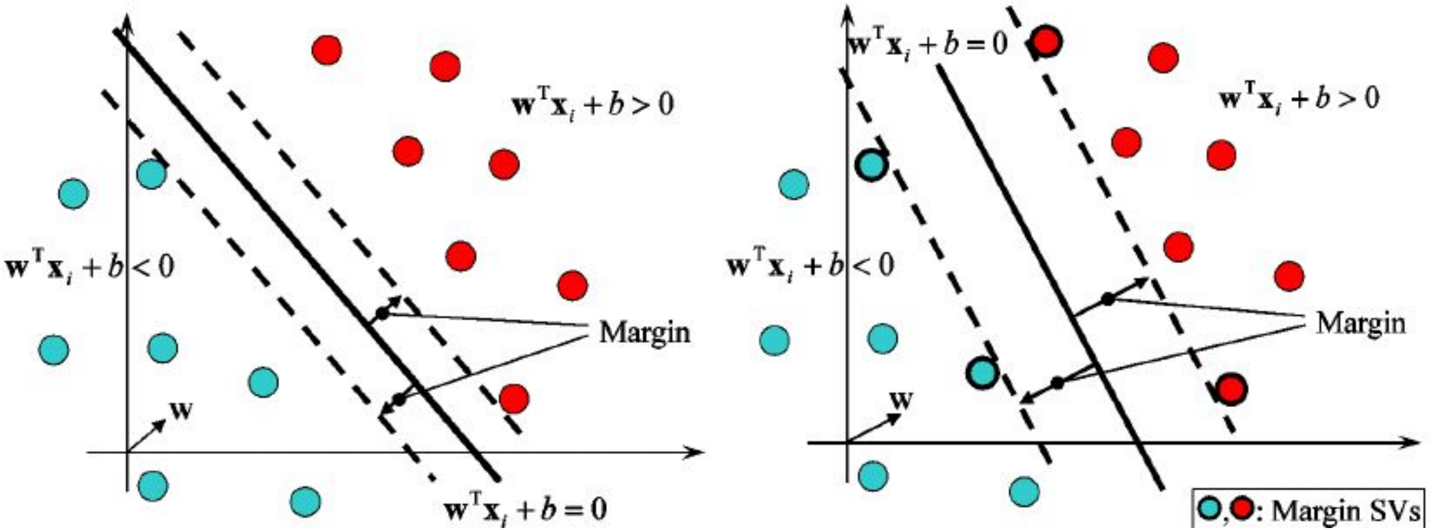
The margin of a classifier $f(x)$ is

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

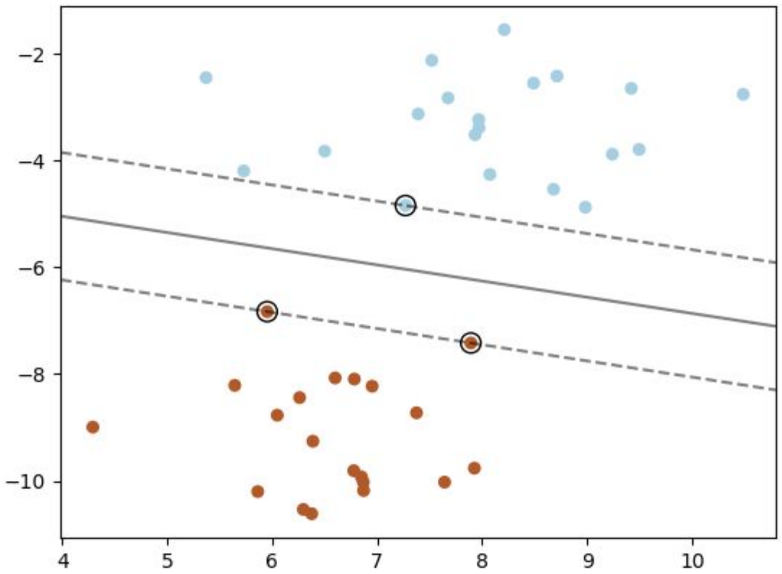
Find f that maximize margin

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

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

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

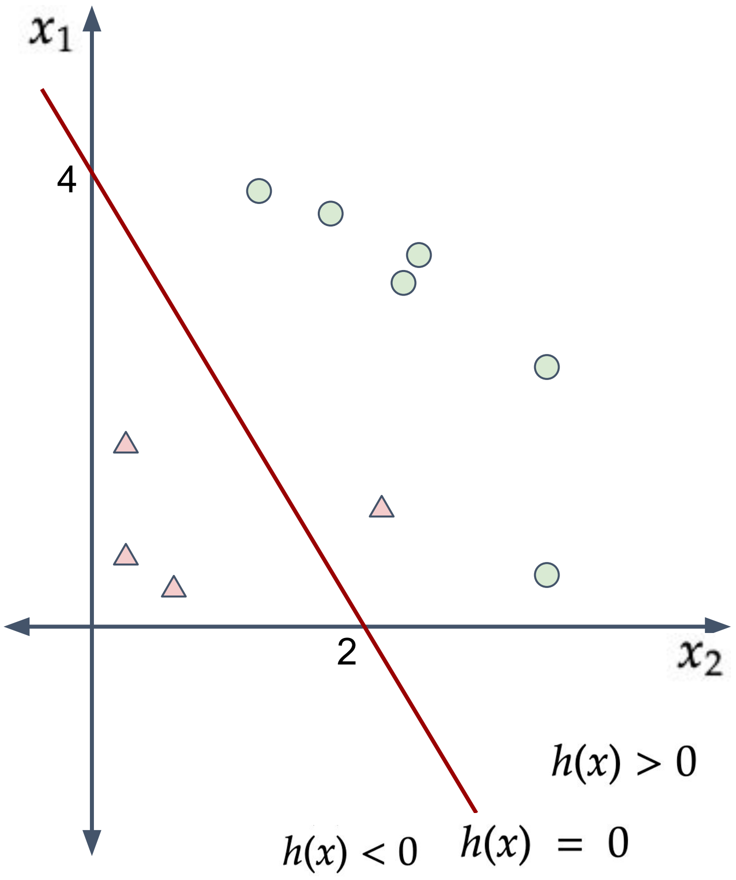
Issue: infinite equivalent hyperplanes result in infinite solutions:

- Multiplying on both sides by some scalars yields an equivalent hyperplane

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

Example of equivalent hyperplanes:

$$h(x) = x_1 + 2x_2 - 4$$
$$h(x) = 2x_1 + 4x_2 - 8$$



Canonical Hyperplane

Way to solve this issue:

- Choose the scalar s such that the absolute distance of a ***support vector*** from the hyperplane is 1.

$$sy^*(\mathbf{w}^T\mathbf{x}^* + b) = 1$$

$$s = \frac{1}{y^*(\mathbf{w}^T\mathbf{x}^* + b)} = \frac{1}{y^* h(\mathbf{x}^*)}$$

$$y_i\ (\mathbf{w}^T\mathbf{x}_i + b) \geq 1, \text{ for all points } \mathbf{x}_i \in \mathbf{D}$$

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

1

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

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

Canonical Hyperplane: an example

$$h'(\mathbf{x}) = \begin{pmatrix}5\\2\end{pmatrix}^T \mathbf{x} - 20 = 0$$

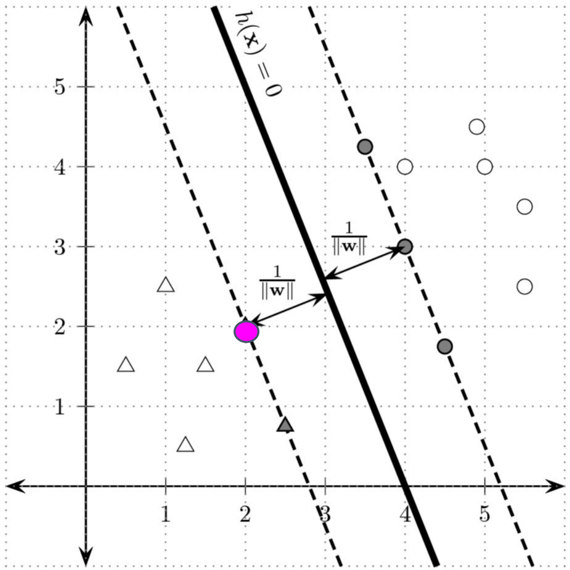
support vector $\mathbf{x}^* = (2,2)$, with class $y^* = -1$

$$s = \frac{1}{y^* h'(\mathbf{x}^*)} = \frac{1}{-1\left(\begin{pmatrix}5\\2\end{pmatrix}^T \begin{pmatrix}2\\2\end{pmatrix} - 20\right)} = \frac{1}{6}$$

$$\mathbf{w} = \frac{1}{6}\begin{pmatrix}5\\2\end{pmatrix} = \begin{pmatrix}5/6\\2/6\end{pmatrix} \qquad b = \frac{-20}{6}$$

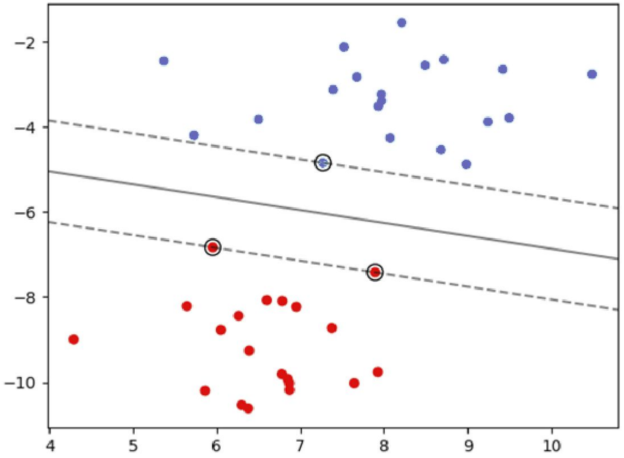
$$h(\mathbf{x}) = \begin{pmatrix}5/6\\2/6\end{pmatrix}^T \mathbf{x} - 20/6 = \begin{pmatrix}0.833\\0.333\end{pmatrix}^T \mathbf{x} - 3.33$$

$$\delta^* = \frac{y^*\ h(\mathbf{x}^*)}{\|\mathbf{w}\|} = \frac{-1\left(\begin{pmatrix}5/6\\2/6\end{pmatrix}^T \begin{pmatrix}2\\2\end{pmatrix} - 20/6\right)}{\sqrt{(\frac{5}{6})^2 + (\frac{2}{6})^2}} = \frac{1}{\frac{\sqrt{29}}{6}} = 1.114$$



Support Vector Machine (Hard Margin)

… it leads to



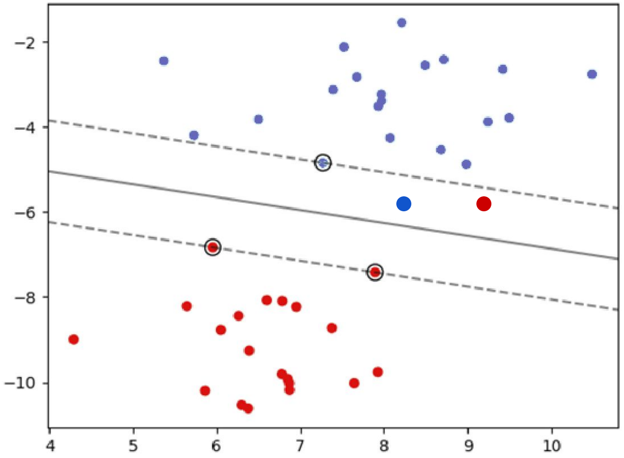
$$\min_{w,b} \frac{1}{2}\|w\|^2$$
$$\text{subject to}$$
$$y^{(i)}(w^\top x^{(i)} + b) \geq 1 \qquad \text{for } i = 1, \ldots, m$$

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,



error

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

subject to

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

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

Tradeoff between margin and the error!

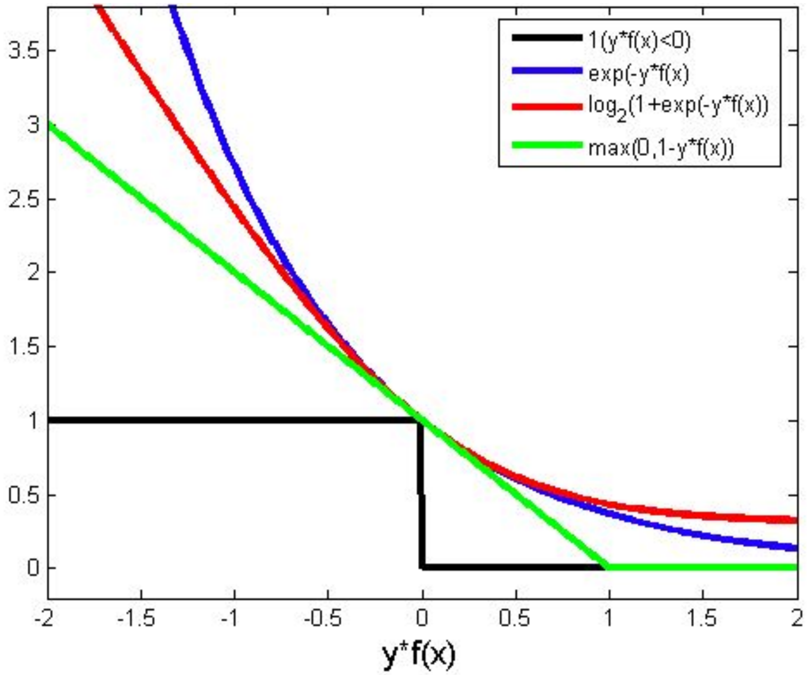
Support Vector Machine

$$\text{minimize } \frac{1}{2}\|w\|^2 + C \cdot \sum_{i=1}^{m} \xi_i$$

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

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

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

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

SVM - Soft Margin: an example

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

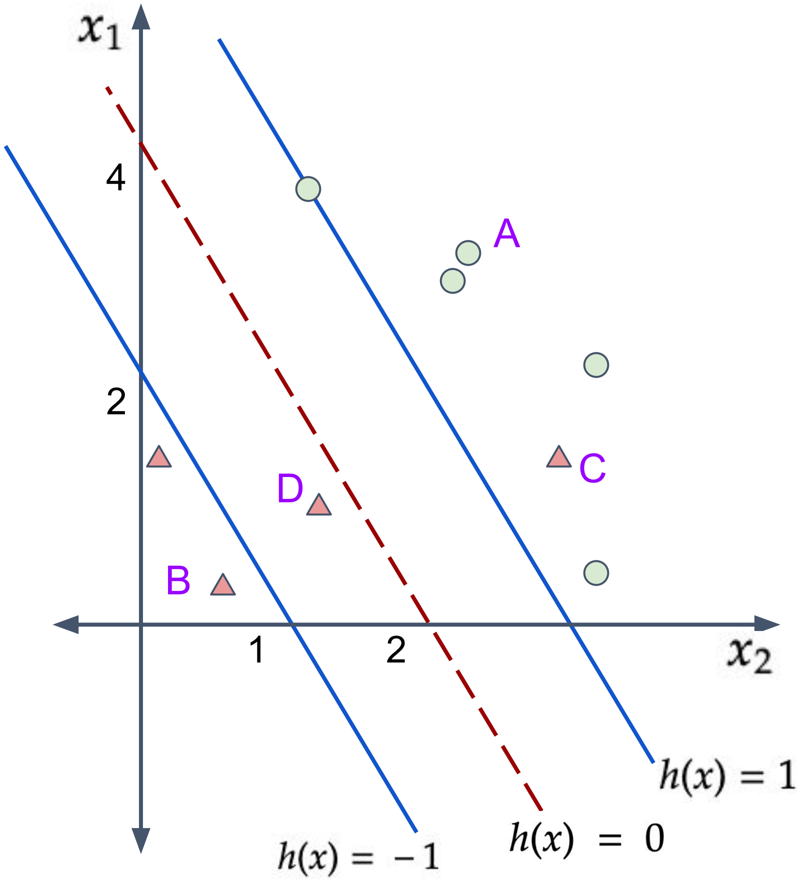
$$A:\ max(0,\ 1 - 1 \cdot (>1)) \rightarrow 0$$

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

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

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

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



General Principle

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

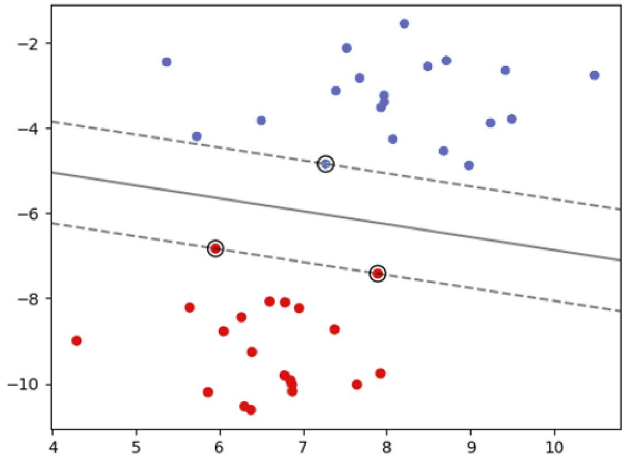
=> by setting $C = 1/\lambda$, it's equivalent to solve

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

SVM belongs to the general loss-oriented formulation!

$$\mathrm{Model} = \arg\min_{\mathrm{model}} \mathrm{Loss}(\mathrm{Model}, \mathrm{Data}) + \lambda \cdot \mathrm{Regularizer}(\mathrm{Model})$$

Support Vectors



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

subject to

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

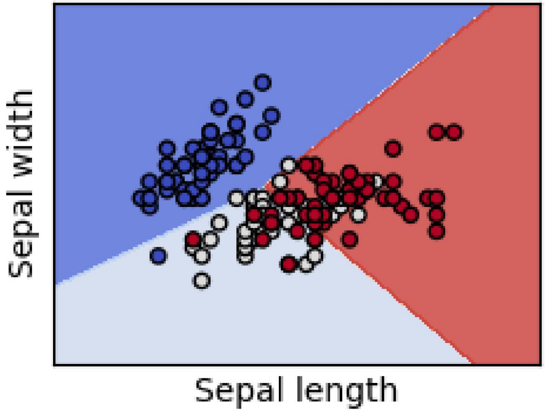
$$\xi_i \geq 0 \quad \text{for } i = 1, \ldots, m$$

Those data points achieving equality $y^{(i)}(w^\top x^{(i)} + b) = 1 - \xi_i$ are called **support vectors**.

Turns out, if you knew support vectors already, solving the optimization problem above with **just the support vectors as train set** leads to the same solution.

⇒ Leave-one-out cross validation can be done fast!

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))`.

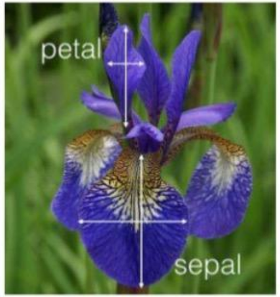
Example: Fisher’s Iris Dataset

Classify among 3 species of Iris flowers…

Iris setosa

Iris versicolor

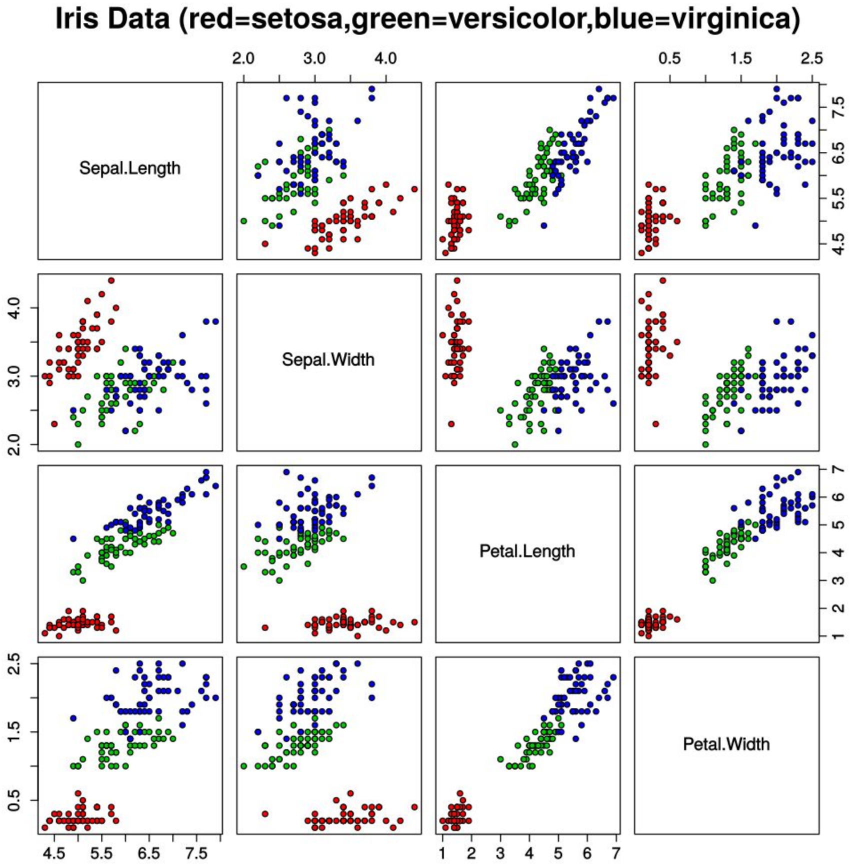
Iris virginica



Four features (in centimeters)

- Petal length / width
- Sepal length / width

Example: Fisher's Iris Dataset



Fairly easy to separate ***setosa*** *from others using a* *linear classifier*

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/]

Trick for Multi-Class

- Recall: logistic regression had a very natural extension to multi-class.
- What about SVM?

binary: $p(y = 1 \mid x) = \frac{1}{1+e^{-w^\top x}}$

multi-class: $p(y = j \mid x) = \frac{\exp\left({w^{(j)}}^\top x\right)}{\sum_{c=1}^{C} \exp\left({w^{(c)}}^\top x\right)}$

… Researchers have found a few, but it was not any better than a simple trick below.

[One-vs-the-rest trick]

- Given: dataset $D = \left\{\left(x^{(i)}, y^{(i)}\right)\right\}_{i=1}^{m}$
- For each class $c \in \{1, \dots, C\}$
  - Define label $z^{(i)} \in \{-1,1\}$ where 1 for class c and -1 for other classes, for all i=1,…,m.
  - Train a classifier f_c with $\left\{\left(x^{(i)}, z^{(i)}\right)\right\}_{i=1}^{m}$
- To classify x^*, compute $\hat{y} = \arg\max_{c\in\{1,\dots,C\}} \text{decision\_value}(f_c(x^*))$