3 Fundamental Algorithms (part 4 of 5)

Support Vector Machine (SVM)

Recall from §1: hard-margin SVM

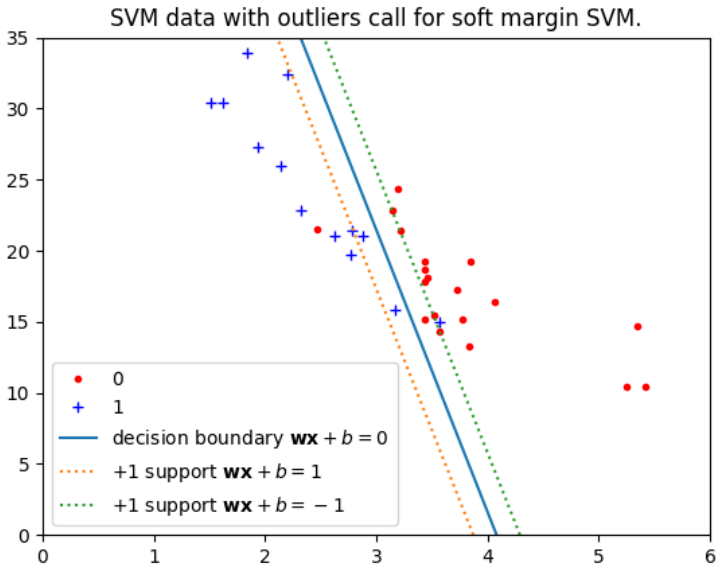
- A hard margin support vector machine (SVM) addresses the case where binary-labeled subsets of examples $\{(\mathbf{x}_i, y_i)\}_{i=1}^N$ are _____.
- It finds a linear decision hyperplane $\mathbf{wx}+b=0$ (center of a road)[1] that separates $+1$ examples from -1 examples by minimizing $||\mathbf{w}||$ subject to $y_i(\mathbf{wx}_i+b) \geq 1$ for $i=1,\ldots,N$.
- Minimizing $||\mathbf{w}||$ maximizes $\frac{2}{||w||}$, the distance from the $+1$ margin $\mathbf{wx}_i+b=1$ (one edge of road) to the -1 margin $\mathbf{wx}_i+b=-1$ (other edge).

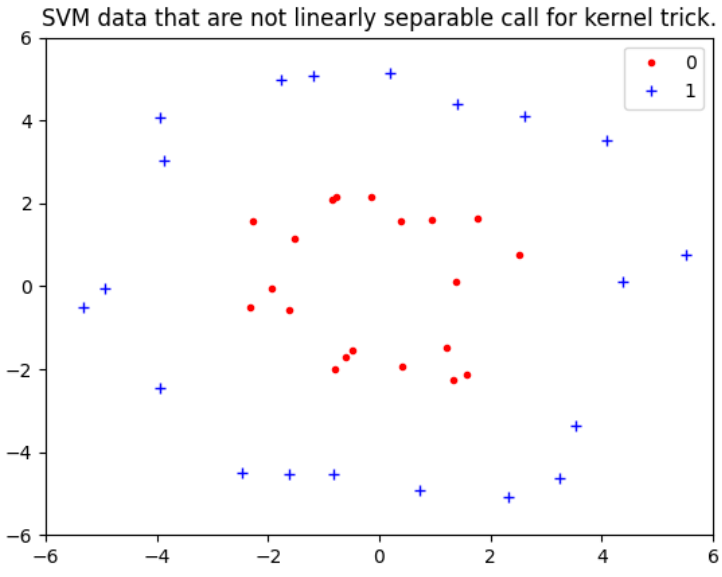
Two problems and §3 solutions (below):

- Outlying examples may violate the boundary (noise):

  A *soft margin* SVM can include a *hyperparameter* (parameter controling learning; not trained) that penalizes misclassification of _____ (positives on the negative side of the boundary or negatives on the positive side).
- For some data, the $+1$ and -1 examples cannot be separated by a hyperplane but could be separated by a polynomial or other _____ boundary: an SVM can include a *kernel* that allows a nonlinear decision boundary.

e.g.[2]

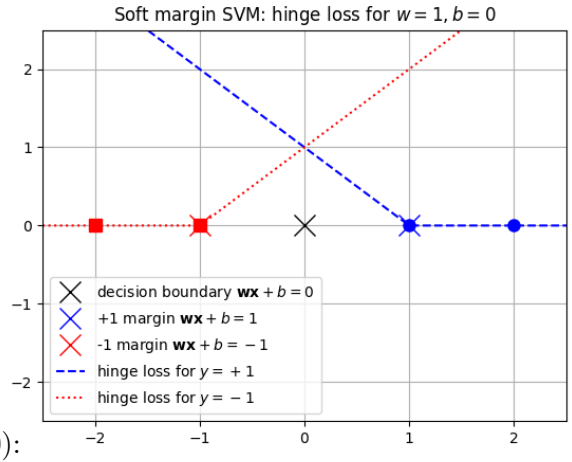




[1] Recall: Burkov uses $\mathbf{wx}-b=0$. I use $\mathbf{wx}+b=0$ to match scikit-learn.

[2] Burkov and the user guide (linked below) use $y \in \{-1,1\}$. scikit-learn seems also to allow $y \in \{0,1\}$.

Soft Margin SVM



To handle noise, use the *hinge loss*, $\max(0, 1 - y_i(\mathbf{w}\mathbf{x}_i + b)) =$

$$\begin{cases} 0, \text{ if constraint } y_i(\mathbf{w}\mathbf{x}_i + b) \geq 1 \text{ is } \_\_\_\_\_ \\ \text{proportional to distance from constraint edge, otherwise} \end{cases}$$

e.g. Here are a few typical hinge losses (pictured for $w = 1, b = 0$):

For $(\mathbf{x}, y = 1)$:	$\max(0, 1 - y(\mathbf{wx} + b))$
above the $\mathbf{wx} + b = 1$ margin (so $\mathbf{wx} + b > 1$)	_____ (constraint satisfied)
on the $\mathbf{wx} + b = 1$ margin	_____ (constraint just satisfied)
on the $\mathbf{wx} + b = 0$ decision boundary	_____ (constraint failed; neutral decision)
on the $\mathbf{wx} + b = -1$ margin	_____ (wrong decision)
below the $\mathbf{wx} + b = -1$ margin (so $\mathbf{wx} + b < -1$)	_____ (wrong decision)

Hard margin SVM's minimizing $||\mathbf{w}||$ is equivallent to minimizing $\frac{1}{2}||\mathbf{w}||^2$.

To get a *soft margin* SVM, we minimize the cost function

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

where hyperparameter C decides the tradeoff between _____ the separation between $+1$ and -1 examples and ensuring that each $\mathbf{x}_i$ is on the correct side.[3]

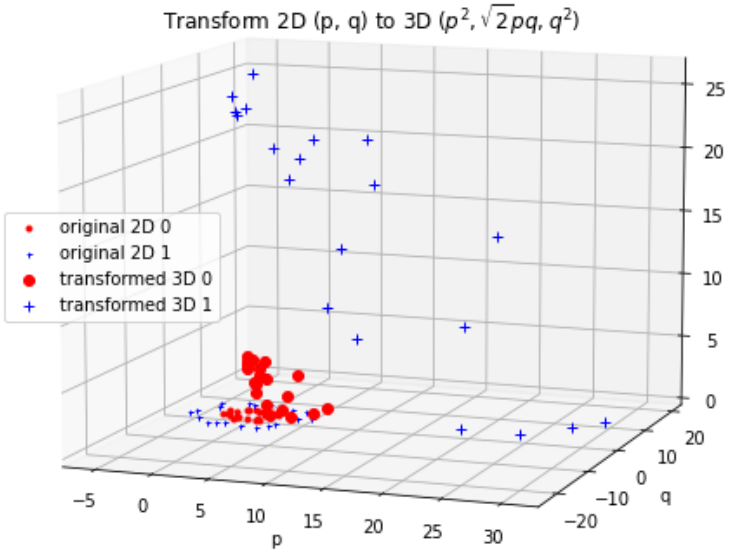
- Increasing C yields a smaller margin and classifies _____ examples better.
- Decreasing C yields a larger margin suited to noisy data, making more errors on training examples but generalizing better to new (_____) examples.

Nonlinear Boundary

- For a nonlinear boundary, we may be able to use some $\phi : \mathbf{x} \mapsto \phi(\mathbf{x})$ to transform the feature space into a higher-dimension space in which we can make a linear separation.

  e.g. In the right-hand figure above, the concentric red and blue rings are not linearly separable. However, we can use $\phi(\mathbf{x}) = \phi(p, q) = (p^2, \sqrt{2}pq, q^2)$ to map each 2D point to a _____ point:

[3] Burkov puts the C on the $\frac{1}{2}||\mathbf{w}||^2$ term. I put it on the hinge loss term to match scikit-learn.



In 3D, the red and blue points are linearly separable by a plane.

Transforming data and trying several $\phi(\mathbf{x})$ functions while seeking linear separation in a higher dimension can be computationally _____.

- Using a function to make a transformation *implicitly* is called the *kernel trick* and can be much less expensive. It facilitates a nonlinear boundary in the original feature space.

  Optional: SVM's (hard-margin) minimization is implemented with the help of *Lagrange multipliers*, finding $\max_{\alpha_1,\ldots,\alpha_N} \left(\sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{k=1}^{N} y_i \alpha_i (\mathbf{x}_i \mathbf{x}_k) y_k \alpha_k \right)$ subject to $\sum_{i=1}^{N} \alpha_i y_i = 0$ and $\alpha_i \geq 0$ for $i = 1, \ldots, N$, which can be done with a quadratic programming algorithm.

  Here the feature vectors appear only as the _____$\mathbf{x}_i \mathbf{x}_k$.

- Instead of finding $\phi(\mathbf{x}_i)$ and $\phi(\mathbf{x}_k)$ and then $\phi(\mathbf{x}_i)\phi(\mathbf{x}_k)$ (expensive), we can use some *kernel function* $k(\mathbf{x}_i, \mathbf{x}_k)$ that is a function only of $\mathbf{x}_i$ and $\mathbf{x}_k$ (untransformed) and gives the same result, with no explicit application of $\phi()$ necessary.

  e.g. Instead of mapping $\mathbf{x}_i$ to $\phi(\mathbf{x}_i) = \phi(p_i, q_i) = (p_i^2, \sqrt{2} p_i q_i, q_i^2)$ and $\mathbf{x}_k$ to $\phi(\mathbf{x}_k) = \phi(p_k, q_k) = (p_k^2, \sqrt{2} p_k q_k, q_k^2)$ and then finding their 3D dot product $\mathbf{x}_i \mathbf{x}_k = p_i^2 p_k^2 + 2 p_i p_k q_i q_k + q_i^2 q_k^2$, we can find the 2D dot product $p_i p_k + q_i q_k$ and square it to get the same result. This is an example of the kernel trick using a quadratic kernel $k(\mathbf{x}_i, \mathbf{x}_k) = (\mathbf{x}_i \mathbf{x}_k)^2$.

  The most widely used of the many kernel functions is the *radial basis function (RBF) kernel*,

$$
\begin{aligned}
k(\mathbf{x}, \mathbf{x}') &= \exp\left(-\frac{||\mathbf{x} - \mathbf{x}'||^2}{2\sigma^2} \right) \text{ (Burkov's notation)} \\
&= \exp\left(-\gamma ||\mathbf{x} - \mathbf{x}'||^2 \right) \text{ (scikit-learn's notation, with } \gamma > 0) \,,
\end{aligned}
$$

  where the fraction's numerator is the squared *Euclidean distance* between the two vectors. Burkov asserts the space for the RBF kernel has ____ dimensions. Varying the hyperparameter $\gamma = \frac{1}{2\sigma^2}$ chooses between a smooth or curvy boundary in the original feature space.

Python

- `from sklearn import svm` (as in §01)
- `clf = svm.SVC(kernel='linear', C=1)` (as in §01)

  High `C` gives a hard-margin SVM (as in §01). Low `C` allows a larger margin on noisy data. Start with the default $C = 1$. Decrease to _____ better from noisy data. Increase for a narrower margin and better _____ performance.
- `clf = svm.SVC(kernel="rbf", C=1, gamma='scale')` uses the (RBF) kernel trick to allow a nonlinear decision boundary in the feature space.
  - `gamma='scale'` uses $\gamma = \frac{1}{D \cdot \texttt{X.var()}}$
  - `gamma='auto'` uses $\gamma = \frac{1}{D}$
  - or set `gamma` to a float

  The user guide says "`gamma` defines how much influence a single training example has. The larger `gamma` is, the closer other examples must be to be affected." A larger `gamma` allows more boundary curvature and more _____ of training data.
- `clf.fit(X, y)` fits the model to array $\texttt{X}_{N \times D}$ and $\texttt{y}_{N \times 1}$ (as in §1)
- `clf.coef_` gives $\mathbf{w}^*$ and `clf.intercept_` gives b^* (as in §1)
- `clf.predict(X)` does classification on examples in `X` (as in §1)
- `clf.predict_proba(X)[:, 1]` gives probabilities $\{P(y_i = 1)\}$ (`[:, 0]` gives $\{P(y_i = 0)\}$)
- `clf.score(X, y)` gives the average accuracy on `X` with respect to `y` (as in §1)

To learn more:

- User guide: `https://scikit-learn.org/stable/modules/svm.html` (as in §1)[4]
- Reference manual:

  `https://scikit-learn.org/stable/modules/generated/sklearn.svm.SVC.html` (as in §1)
- Advice on setting `C` and `gamma` for a nonlinear boundary is at

  `https://scikit-learn.org/stable/auto_examples/svm/plot_rbf_parameters.html`.
- The kernel trick is described at `https://en.wikipedia.org/wiki/Kernel_method`.

[4]The guide says SVM is not scale invariant, so we should scale each feature to $[0, 1]$ or $[-1, 1]$ or standardize each feature to have mean 0 and variance 1. We will discuss scaling in §05.