CS639: Data Management for Data Science

Lecture 17: Linear Classifiers and Support Vector Machines

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(lecture by Ankur Goswami many slides from David Sontag)
Today’s Lecture

1. Linear classifiers
2. The Perceptron Algorithm
3. Support Vector Machines
Linear classifier

• Let’s simplify life by assuming:
  • Every instance is a vector of real numbers, $\mathbf{x} = (x_1, \ldots, x_n)$. (Notation: boldface $\mathbf{x}$ is a vector.)
  • There are only two classes, $y = (+1)$ and $y = (-1)$

• A linear classifier is vector $\mathbf{w}$ of the same dimension as $\mathbf{x}$ that is used to make this prediction:

$$ \hat{y} = \text{sign}(w_1 x_1 + w_2 x_2 + \ldots + w_n x_n) = \text{sign}(\mathbf{w} \cdot \mathbf{x}) $$

$$ \text{sign}(x) = \begin{cases} +1 & \text{if } x \geq 0 \\ -1 & \text{if } x < 0 \end{cases} $$
Example: Linear classifier

- Imagine 3 features (spam is “positive” class):
  1. free (number of occurrences of “free”)
  2. money (occurrences of “money”)
  3. BIAS (intercept, always has value 1)

\[
\sum_i w_i \cdot f_i(x) = w \cdot f(x)
\]

\[
\begin{array}{|c|c|c|}
\hline
x & f(x) & w \\
\hline
BIAS & 1 & -3 \\
free & 1 & 4 \\
money & 1 & 2 \\
\ldots & \ldots & \ldots \\
\hline
\end{array}
\]

\[
(1)(-3) + (1)(4) + (1)(2) + \ldots = 3
\]

\[w \cdot f(x) > 0 \rightarrow \text{SPAM}!!\]
The Perceptron Algorithm to learn a Linear Classifier

- Start with weight vector = \( \vec{0} \)
- For each training instance \((x_i, y_i^*)\):
  - Classify with current weights
    \[
    y_i = \begin{cases} 
    +1 & \text{if } w \cdot f(x_i) \geq 0 \\
    -1 & \text{if } w \cdot f(x_i) < 0 
    \end{cases}
    \]
  - If correct (i.e., \( y = y_i^* \)), no change!
  - If wrong: update
    \[
    w = w + y_i^* f(x_i)
    \]
Definition: Linearly separable data

\[ \exists w \text{ such that } \forall t \quad y_t(w \cdot x_t) \geq \gamma > 0 \]

Called the margin

Equivalently, for \( y_t = +1 \),
\[ w \cdot x_t \geq \gamma \]
and for \( y_t = -1 \),
\[ w \cdot x_t \leq -\gamma \]
Does the perceptron algorithm work?

- Assume the data set $D$ is linearly separable with margin $\gamma$, i.e.,
  \[ \exists w^*, \|w^*\|_2 = 1, \forall t, y_t x_t^T w^* \geq \gamma \]

- Assume $\|x_t\|_2 \leq R, \forall t$

- **Theorem**: The maximum number of mistakes made by the perceptron algorithm is bounded by $R^2/\gamma^2$

[Rong Jin]
Properties of the perceptron algorithm

- **Separability**: some parameters get the training set perfectly correct.

- **Convergence**: if the training is **linearly separable**, perceptron will eventually converge.
Problems with the perceptron algorithm

- **Noise**: if the data isn’t linearly separable, no guarantees of convergence or accuracy

- Frequently the training data is linearly separable! Why?
  - When the number of features is much larger than the number of data points, there is lots of flexibility
  - As a result, Perceptron can significantly overfit the data *[We will see next week]*

- **Averaged** perceptron is an algorithmic modification that helps with both issues
  - Averages the weight vectors across all iterations
Linear separators

- Which of these linear separators is optimal?
Support Vector Machines

- SVMs (Vapnik, 1990’s) choose the linear separator with the largest margin

- Robust to outliers!

- Good according to intuition, theory, practice

- SVM became famous when, using images as input, it gave accuracy comparable to neural-network with hand-designed features in a handwriting recognition task
Normal to a plane

\[ \mathbf{w} \]  -- unit vector parallel to \( \mathbf{w} \)

\[ \mathbf{X}_j \]  -- projection of \( \mathbf{x}_j \) onto the plane

\[ \mathbf{x}_j - \mathbf{X}_j = \lambda \frac{\mathbf{w}}{||\mathbf{w}||} \]

\( \lambda \) is the length of the vector, i.e.

\[ ||\mathbf{x}_j - \mathbf{X}_j|| = \frac{\lambda}{||\mathbf{w}||} ||\mathbf{w}|| = \lambda \]
Scale invariance

Any other ways of writing the same dividing line?

- \( \mathbf{w} \cdot \mathbf{x} + b = 0 \)
- \( 2\mathbf{w} \cdot \mathbf{x} + 2b = 0 \)
- \( 1000\mathbf{w} \cdot \mathbf{x} + 1000b = 0 \)
- .....
Scale invariance

During learning, we set the scale by asking that, for all $t$,

- for $y_t = +1$, $w \cdot x_t + b \geq 1$
- and for $y_t = -1$, $w \cdot x_t + b \leq -1$

That is, we want to satisfy all of the **linear** constraints

$$y_t (w \cdot x_t + b) \geq 1 \quad \forall t$$
What is $\gamma$ as a function of $w$?

We also know that:

$$x_1 - x_2 = \gamma \frac{w}{||w||}$$

$$1 = w \cdot \left( \gamma \frac{w}{||w||} \right) = \frac{\gamma}{||w||} w \cdot w = \gamma ||w||$$

So, $\gamma = \frac{1}{||w||}$

**Final result:** can maximize margin by minimizing $||w||_2$!!!
Support Vector Machines (SVMs)

\[
\text{minimize}_{\mathbf{w}, b} \quad \mathbf{w} \cdot \mathbf{w} \\
(\mathbf{w} \cdot \mathbf{x}_j + b) y_j \geq 1, \quad \forall j
\]

- Example of a **convex optimization** problem
  - A quadratic program
  - Polynomial-time algorithms to solve!
- Hyperplane defined by **support vectors**
  - Could use them as a lower-dimension basis to write down line, although we haven’t seen how yet
- More on these later

**Non-support Vectors:**
- everything else
- moving them will not change \( \mathbf{w} \)

**Support Vectors:**
- data points on the canonical lines
What if the data is not separable?

\[
\begin{align*}
\text{minimize}_{w,b} & \quad w \cdot w + C \#(\text{mistakes}) \\
(w \cdot x_j + b) y_j & \geq 1, \forall j
\end{align*}
\]

- First Idea: Jointly minimize $w \cdot w$ and number of training mistakes
  - How to tradeoff two criteria?
  - Pick $C$ using held-out data

- Tradeoff #(mistakes) and $w \cdot w$
  - 0/1 loss
  - Not QP anymore
  - Also doesn’t distinguish near misses and really bad mistakes
  - NP hard to find optimal solution!!!
Allowing for slack: “Soft margin” SVM

\[ \text{minimize}_{w, b} \quad w \cdot w + C \sum_j \xi_j \]
\[ (w \cdot x_j + b) y_j \geq 1 - \xi_j, \quad \forall j \quad \xi_j \geq 0 \]

“slack variables”

Slack penalty \( C > 0 \):
- \( C = \infty \rightarrow \text{have to separate the data!} \)
- \( C = 0 \rightarrow \text{ignores the data entirely!} \)

For each data point:
- If margin \( \geq 1 \), don’t care
- If margin \( < 1 \), pay linear penalty
Allowing for slack: “Soft margin” SVM

minimize \( w, b \) \( w \cdot w + C \sum_j \xi_j \)

\[
(w \cdot x_j + b) \ y_j \geq 1 - \xi_j, \ \forall j, \ \xi_j \geq 0
\]

“slack variables”

What is the (optimal) value of \( \xi_j \) as a function of \( w \) and \( b \)?

If \( (w \cdot x_j + b) \ y_j \geq 1 \), then \( \xi_j = 0 \)

If \( (w \cdot x_j + b) \ y_j < 1 \), then \( \xi_j = 1 - (w \cdot x_j + b) \ y_j \)

Sometimes written as

\[
(1 - (w \cdot x_j + b) \ y_j)_+
\]

\[\xi_j = \max(0, 1 - (w \cdot x_j + b) \ y_j)\]
Equivalent Hinge Loss Formulation

\[
\text{minimize}_{w,b} \quad w \cdot w + C \sum_j \xi_j \\
\left(w \cdot x_j + b\right) y_j \geq 1 - \xi_j \quad , \forall j \quad \xi_j \geq 0
\]

Substituting \( \xi_j = \max (0, 1 - (w \cdot x_j + b) y_j) \) into the objective, we get:

\[
\min \|w\|^2 + C \sum_j \max (0, 1 - (w \cdot x_j + b) y_j)
\]

The hinge loss is defined as \( L(y, \hat{y}) = \max (0, 1 - \hat{y}y) \)

\[
\min_{w,b} \|w\|_2^2 + C \sum_j L(y_j, w \cdot x_j + b)
\]

This is called \textbf{regularization}; used to prevent overfitting!

This part is empirical risk minimization, using the hinge loss.
Hinge Loss vs 0-1 Loss

0-1 Loss:
\[ L(y, \hat{y}) = 1[\hat{y} \neq y] \]

Hinge loss:
\[ L(y, \hat{y}) = \max(0, 1 - \hat{y}y) \]

Hinge loss upper bounds 0/1 loss!
Multiclass SVM
One versus all classification

Learn 3 classifiers:

- vs \{0, +\}, weights \(w_-\)
- + vs \{0, -\}, weights \(w_+\)
- 0 vs \{+, -\}, weights \(w_0\)

Predict label using:

\[
\hat{y} \leftarrow \arg \max_k \ w_k \cdot x + b_k
\]

Any problems?

Could we learn this dataset? →
Multiclass SVM

Simultaneously learn 3 sets of weights:

• How do we guarantee the correct labels?

• Need new constraints!

The “score” of the correct class must be better than the “score” of wrong classes:

\[ w(y_j) \cdot x_j + b(y_j) > w(y) \cdot x_j + b(y) \quad \forall j, y \neq y_j \]
Multiclass SVM

As for the SVM, we introduce slack variables and maximize margin:

\[
\begin{align*}
\text{minimize}_{w, b} & \quad \sum_y w(y).w(y) + C \sum_j \xi_j \\
\quad & \quad w(y_j).x_j + b(y_j) \geq w(y').x_j + b(y') + 1 - \xi_j, \quad \forall y' \neq y_j, \quad \forall j \\
\quad & \quad \xi_j \geq 0, \quad \forall j
\end{align*}
\]

To predict, we use:

\[
\hat{y} \leftarrow \arg \max_k w_k \cdot x + b_k
\]

Now can we learn it? →
What you need to know

• Perceptron mistake bound
• Maximizing margin
• Derivation of SVM formulation
• Relationship between SVMs and empirical risk minimization
  – 0/1 loss versus hinge loss
• Tackling multiple class
  – One against All
  – Multiclass SVMs