Support Vector Machines: Training with Stochastic Gradient Descent

Machine Learning
Spring 2020

The slides are mainly from Vivek Srikumar
Support vector machines

• Training by maximizing margin

• The SVM objective

• Solving the SVM optimization problem

• Support vectors, duals and kernels
SVM objective function

\[
\min_{w,b} \frac{1}{2} w^\top w + C \sum \max (0, 1 - y_i (w^\top x_i + b))
\]

Regularization term:
- Maximize the margin
- Imposes a preference over the hypothesis space and pushes for better generalization
- Can be replaced with other regularization terms which impose other preferences

Empirical Loss:
- Hinge loss
- Penalizes weight vectors that make mistakes
- Can be replaced with other loss functions which impose other preferences

A hyper-parameter that controls the tradeoff between a large margin and a small hinge-loss
Outline: Training SVM by optimization

1. Review of convex functions and gradient descent
2. Stochastic gradient descent
3. Gradient descent vs stochastic gradient descent
4. Sub-derivatives of the hinge loss
5. Stochastic sub-gradient descent for SVM
6. Comparison to perceptron
Outline: Training SVM by optimization

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Solving the SVM optimization problem

This function is convex in $w$, $b$

For convenience, use simplified notation:

$$w_0 \leftarrow w$$

$$w \leftarrow [w_0, b]$$

$$x_i \leftarrow [x_i, 1]$$

$$\min_w \frac{1}{2} w^\top w + C \sum \max(0, 1 - y_i(w^\top x_i + b))$$
Recall: Convex functions

A function $f$ is convex if for every $u, v$ in the domain, and for every $\lambda \in [0,1]$ we have

$$f(\lambda u + (1 - \lambda)v) \leq \lambda f(u) + (1 - \lambda)f(v)$$
Recall: Convex functions

A function $f$ is **convex** if for every $u, v$ in the domain, and for every $\lambda \in [0,1]$ we have

$$f(\lambda u + (1 - \lambda)v) \leq \lambda f(u) + (1 - \lambda)f(v)$$

From geometric perspective

Every tangent plane lies below the function

$$f(x) \geq f(u) + \nabla f(u)^T (x - u)$$
Convex functions

\[ f(x) = -x \]
Linear functions

\[ f(x) = x^2 \]

\[ f(x) = \max(0, x) \]
max is convex

Some ways to show that a function is convex:

1. Using the definition of convexity
2. Showing that the second derivative is nonnegative (for one dimensional functions)
3. Showing that the second derivative is positive semi-definite (for vector functions)
Not all functions are convex

\[ f(\lambda u + (1 - \lambda)v) \geq \lambda f(u) + (1 - \lambda)f(v) \]
Convex functions are convenient

A function $f$ is **convex** if for every $u, v$ in the domain, and for every $\lambda \in [0, 1]$ we have

$$f(\lambda u + (1 - \lambda)v) \leq \lambda f(u) + (1 - \lambda)f(v)$$

In general: Necessary condition for $x$ to be a minimum for the function $f$ is $\nabla f(x) = 0$
Convex functions are convenient

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In general: Necessary condition for $x$ to be a minimum for the function $f$ is $\nabla f(x) = 0$

For convex functions, this is both necessary *and* sufficient
Solving the SVM optimization problem

\[
\min_w \frac{1}{2} w_0^T w_0 + C \sum_i \max(0, 1 - y_i w^T x_i)
\]

This function is convex in \( w \)

- This is a quadratic optimization problem because the objective is quadratic

- Older methods: Used techniques from Quadratic Programming
  - Very slow

- No constraints, can use \textit{gradient descent}
  - Still very slow!
Gradient descent

General strategy for minimizing a function $J(w)$

• Start with an initial guess for $w$, say $w^0$

• Iterate till convergence:
  – Compute the gradient of $J$ at $w^t$
  – Update $w^t$ to get $w^{t+1}$ by taking a step in the opposite direction of the gradient

Intuition: The gradient is the direction of steepest increase in the function. To get to the minimum, go in the opposite direction

We are trying to minimize

$$J(w) = \frac{1}{2} w_0^T w_0 + C \sum_i \max(0, 1 - y_i w^T x_i)$$
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Intuition: The gradient is the direction of steepest increase in the function. To get to the minimum, go in the opposite direction.
Gradient descent for SVM

1. Initialize $\mathbf{w}^0$

2. For $t = 0, 1, 2, \ldots$
   1. Compute gradient of $J(\mathbf{w})$ at $\mathbf{w}^t$. Call it $\nabla J(\mathbf{w}^t)$
   2. Update $\mathbf{w}$ as follows:
      
      $$\mathbf{w}^{t+1} = \mathbf{w}^t - r \nabla J(\mathbf{w}^t)$$

      $r$: Called the learning rate.

We are trying to minimize

$$J(\mathbf{w}) = \frac{1}{2} \mathbf{w}_0^\top \mathbf{w}_0 + C \sum_i \max(0, 1 - y_i \mathbf{w}^\top \mathbf{x}_i)$$
Outline: Training SVM by optimization

✅ Review of convex functions and gradient descent

2. **Stochastic gradient descent**

3. Gradient descent vs stochastic gradient descent

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Gradient descent for SVM

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   1. Compute gradient of $J(w)$ at $w^t$. Call it $\nabla J(w^t)$

We are trying to minimize

$$J(w) = \frac{1}{2} w_0^T w_0 + C \sum_i \max(0, 1 - y_i w^T x_i)$$

Gradient of the SVM objective requires summing over the entire training set

Slow, does not really scale

$r$: Called the learning rate
Stochastic gradient descent for SVM

\[ J(w) = \frac{1}{2} w_0^T w_0 + C \sum_i \max(0, 1 - y_i w^T x_i) \]

Given a training set \( S = \{(x_i, y_i)\}, x \in \mathbb{R}^n, y \in \{-1, 1\} \)

1. Initialize \( w^0 = 0 \in \mathbb{R}^n \)
2. For epoch = 1 ... T:

3. Return final \( w \)
Stochastic gradient descent for SVM

Given a training set $S = \{(x_i, y_i)\}$, $x \in \mathbb{R}^n$, $y \in \{-1, 1\}$

1. Initialize $w^0 = 0 \in \mathbb{R}^n$
2. For epoch = 1 ... $T$:
   1. Pick a random example $(x_i, y_i)$ from the training set $S$

3. Return final $w$
Stochastic gradient descent for SVM

Given a training set \( S = \{(x_i, y_i)\}, \ x \in \mathbb{R}^n, \ y \in \{-1,1\} \)

1. Initialize \( \mathbf{w}^0 = 0 \in \mathbb{R}^n \)

2. For epoch = 1 \ldots T:
   1. Pick a random example \((x_i, y_i)\) from the training set \( S \)
   2. Repeat \((x_i, y_i)\) to make a full dataset and take the derivative of the SVM objective at the current \( \mathbf{w} \) to be \( \nabla J_t(\mathbf{w}) \)

3. Return final \( \mathbf{w} \)
Stochastic gradient descent for SVM

Given a training set \( S = \{ (x_i, y_i) \}, x \in \mathbb{R}^n, y \in \{-1, 1\} \)

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\[
J^t(w) = \frac{1}{2} w_0^T w_0 + C \sum \max(0, 1 - y_i w^T x_i)
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\[
J^t(w) = \frac{1}{2} w_0^\top w_0 + C \sum_i \max(0, 1 - y_i w^\top x_i)
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J^t(w) = \frac{1}{2} w_0^T w_0 + C \sum_i \max(0, 1 - y_i w^T x_i)
\]

3. Update: \( w \leftarrow w - \gamma_t \nabla J^t(w) \)

3. Return final \( w \)
Stochastic gradient descent for SVM

Given a training set \( S = \{ (x_i, y_i) \}, x \in \mathbb{R}^n, y \in \{-1,1\} \)

1. Initialize \( w^0 = 0 \in \mathbb{R}^n \)
2. For epoch = 1 ... T:
   1. Pick a random example \((x_i, y_i)\) from the training set \( S \)
   2. Repeat \((x_i, y_i)\) to make a full dataset and take the derivative of the SVM objective at the current \( w \) to be \( \nabla J_t(w) \)
   3. Update: \( w \leftarrow w - \gamma_t \nabla J_t(w) \)
3. Return final \( w \)

This algorithm is guaranteed to converge to the minimum of \( J \) if \( \gamma_t \) is small enough.

\[
J(w) = \frac{1}{2} w_0^T w_0 + C \sum_i \max(0, 1 - y_i w^T x_i)
\]
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✓ Review of convex functions and gradient descent
✓ Stochastic gradient descent

3. Gradient descent vs stochastic gradient descent
4. Sub-derivatives of the hinge loss
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Gradient Descent vs SGD

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Many more updates than gradient descent, but each individual update is less computationally expensive.

Stochastic Gradient descent
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4. **Sub-derivatives of the hinge loss**
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Stochastic gradient descent for SVM

Given a training set $S = \{(x_i, y_i)\}$, $x \in \mathbb{R}^n$, $y \in \{-1,1\}$

1. Initialize $w^0 = 0 \in \mathbb{R}^n$
2. For epoch = 1 ... T:
   1. Pick a random example $(x_i, y_i)$ from the training set $S$
   2. Treat $(x_i, y_i)$ as a full dataset and take the derivative of the SVM objective at the current $w$ to be $\nabla J^t(w)$
   3. Update: $w \leftarrow w - \gamma_t \nabla J^t(w)$
3. Return final $w$

What is the derivative of the hinge loss with respect to $w$? (The hinge loss is not a differentiable function!)
Hinge loss is not differentiable!

What is the derivative of the hinge loss with respect to $w$?

$$J^t(w) = \frac{1}{2}w_0^T w_0 + C \cdot N \max(0, 1 - y_i w^T x_i)$$
Detour: Sub-Gradients

Generalization of gradients to non-differentiable functions

(Remember that every tangent lies below the function for convex functions)

Informally, a sub-tangent line at a point is any line that crosses the point and lies below the entire function.

A sub-gradient is the slope of the sub-tangent line
Sub-gradients

Formally, $g$ is a subgradient to $f$ at $x$ if

$$f(y) \geq f(x) + g^T(y - x) \quad \text{for all } y$$

[Example from Boyd]
Sub-gradients

Formally, $g$ is a subgradient to $f$ at $x$ if

$$f(y) \geq f(x) + g^T(y - x) \quad \text{for all } y$$

$f$ is differentiable at $x_1$
Tangent at this point

$$f(x_1) + g_1^T(x - x_1)$$

$g_1$ is a gradient at $x_1$
Sub-gradients

Formally, $g$ is a subgradient to $f$ at $x$ if

$$f(y) \geq f(x) + g^T(y - x) \quad \text{for all } y$$

$f$ is differentiable at $x_1$

Tangent at this point

$f(x_1) + g_1^T(x - x_1)$

$g_1$ is a gradient at $x_1$

$g_2$ and $g_3$ are both subgradients at $x_2$
Sub-gradient of the SVM objective

\[ J^t(w) = \frac{1}{2} w_0^\top w_0 + C \cdot N \max(0, 1 - y_i w^\top x_i) \]

**General strategy:** First solve the max and compute the gradient for each case.
Sub-gradient of the SVM objective

\[ J^t(w) = \frac{1}{2} w_0^T w_0 + C \cdot N \max(0, 1 - y_i w^T x_i) \]

**General strategy:** First solve the max and compute the gradient for each case

\[ \nabla J^t = \begin{cases} 
[w_0; 0] & \text{if } \max(0, 1 - y_i w^T x_i) = 0 \\
[w_0; 0] - C \cdot N y_i x_i & \text{otherwise}
\end{cases} \]
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Stochastic sub-gradient descent for SVM

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Given a training set \( S = \{(x_i, y_i)\}, x \in \mathbb{R}^n, y \in \{-1,1\} \)

1. Initialize \( w^0 = 0 \in \mathbb{R}^n \)

3. Return \( w \)
Stochastic sub-gradient descent for SVM

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1. Initialize \( w^0 = 0 \in \mathbb{R}^n \)
2. For epoch = 1 ... T:

3. Return \( w \)
Stochastic **sub-gradient** descent for SVM

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[w_0; 0] & \text{if } \max(0, 1 - y_i w^T x_i) = 0 \\
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Given a training set \( S = \{(x_i, y_i)\}, x \in \mathbb{R}^n, y \in \{-1, 1\} \)

1. Initialize \( w^0 = 0 \in \mathbb{R}^n \)

2. For epoch = 1 ... T:
   1. For each training example \( (x_i, y_i) \in S \):
      
         Update \( w \leftarrow w - \gamma_t \nabla J^t \)

3. Return \( w \)
Stochastic sub-gradient descent for SVM

\[ \nabla J^t = \begin{cases} 
[w_0; 0] & \text{if } \max(0, 1 - y_i w^T x_i) = 0 \\
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\end{cases} \]

Given a training set \( S = \{(x_i, y_i)\}, \ x \in \mathbb{R}^n, y \in \{-1,1\} \)

1. Initialize \( w^0 = 0 \in \mathbb{R}^n \)
2. For epoch = 1 ... T:
   1. For each training example \( (x_i, y_i) \in S \):
      If \( y_i \, w^T \, x_i \leq 1 \),
         \[ w \leftarrow w - \gamma_t \left[ w_0; 0 \right] + \gamma_t C N y_i \, x_i \]
      else
         \[ w_0 \leftarrow (1 - \gamma_t) \, w_0 \]
3. Return \( w \)
Stochastic sub-gradient descent for SVM

Given a training set $S = \{(x_i, y_i)\}$, $x \in \mathbb{R}^n$, $y \in \{-1, 1\}$

1. Initialize $w^0 = 0 \in \mathbb{R}^n$

2. For epoch = 1 ... $T$:
   1. For each training example $(x_i, y_i) \in S$:
      
      If $y_i \mathbf{w}^T \mathbf{x}_i \leq 1$,
      $$
      w \leftarrow w - \gamma_t [w_0; 0] + \gamma_t C N y_i \mathbf{x}_i
      $$
      
      else
      $$
      w_0 \leftarrow (1 - \gamma_t) w_0
      $$

3. Return $w$

$\gamma_t$: learning rate, many tweaks possible

Important to shuffle examples at the start of each epoch
Stochastic sub-gradient descent for SVM

Given a training set $S = \{(x_i, y_i)\}, \ x \in \mathbb{R}^n, \ y \in \{-1, 1\}$

1. Initialize $w^0 = 0 \in \mathbb{R}^n$

2. For epoch = 1 ... T:
   1. Shuffle the training set
   2. For each training example $(x_i, y_i) \in S$:
      If $y_i \mathbf{w}^T x_i \leq 1$,
      \[ w \leftarrow w - \gamma_t [w_0; 0] + \gamma_t C N y_i x_i \]
      else
      \[ w_0 \leftarrow (1- \gamma_t) w_0 \]

3. Return $w$
Convergence and learning rates

With enough iterations, it will converge in expectation

Provided the step sizes are “square summable, but not summable”

• Step sizes $\gamma_t$ are positive
• Sum of squares of step sizes over $t = 1$ to $\infty$ is not infinite
• Sum of step sizes over $t = 1$ to $\infty$ is infinity

• Some examples: $\gamma_t = \frac{\gamma_0}{1 + \frac{\gamma_0 t}{C}}$ or $\gamma_t = \frac{\gamma_0}{1 + t}$
Convergence and learning rates

• Number of iterations to get to accuracy within $\varepsilon$

• For strongly convex functions, $N$ examples, $d$ dimensional:
  – Gradient descent: $O(Nd \ln(1/\varepsilon))$
  – Stochastic gradient descent: $O(d/\varepsilon)$

• More subtleties involved, but SGD is generally preferable when the data size is huge
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Stochastic sub-gradient descent for SVM

Given a training set \( S = \{(x_i, y_i)\}, \ x \in \mathbb{R}^n, \ y \in \{-1, 1\} \)

1. Initialize \( w^0 = 0 \in \mathbb{R}^n \)

2. For epoch = 1 ... T:
   1. Shuffle the training set
   2. For each training example \((x_i, y_i) \in S:\)
      - If \( y_i w^T x_i \leq 1, \)
        \[ w \leftarrow w - \gamma_t [w_0; 0] + \gamma_t C N y_i x_i \]
      - else
        \[ w_0 \leftarrow (1 - \gamma_t) w_0 \]

3. Return \( w \)

Compare with the Perceptron update:
If \( y_i w^T x_i \leq 0, \) update \( w \leftarrow w + r y_i x_i \)
Perceptron vs. SVM

• Perceptron: Stochastic sub-gradient descent for a different loss
  – No regularization though

\[ L_{Perceptron}(y, x, w) = \max(0, -yw^T x) \]

• SVM optimizes the hinge loss
  – With regularization

\[ L_{Hinge}(y, x, w) = \max(0, 1 - yw^T x) \]
SVM summary from optimization perspective

• Minimize regularized hinge loss

• Solve using stochastic sub-gradient descent
  – Very fast, run time does not depend on number of examples
  – Compare with Perceptron algorithm: similar framework with different objectives!
    – Compare with Perceptron algorithm: Perceptron does not maximize margin width
      • Perceptron variants can force a margin

• Other successful optimization algorithms exist
  – Eg: Dual coordinate descent, implemented in liblinear

Questions?