Lecture 17 SVM (Part II) and Online Learning

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(some slides from my convex optimization class, originally taught by Ryan Tibshirani in CMU)

Recap: Support Vector Machines

Given $y \in \{-1, 1\}^n$, $X \in \mathbb{R}^{n \times p}$ having rows $x_1, \ldots x_n$, recall the support vector machine or SVM problem:

$$\begin{aligned} \min_{\beta, \beta_0, \xi} \quad & \frac{1}{2}\|\beta\|_2^2 + C\sum_{i=1}^n \xi_i \\ \text{subject to} \quad & \xi_i \geq 0, \; i = 1, \ldots n \\ & y_i(x_i^T\beta + \beta_0) \geq 1 - \xi_i, \; i = 1, \ldots n \end{aligned}$$

This is a quadratic program

Recap: Lagrange dual problem

Given a minimization problem

$$\begin{array}{ll} \min\limits_{x} & f(x) \\ \text{subject to} & h_i(x) \leq 0,\ i = 1, \ldots m \\ & \ell_j(x) = 0,\ j = 1, \ldots r \end{array}$$

we defined the Lagrangian:

$$L(x, u, v) = f(x) + \sum_{i=1}^{m} u_i h_i(x) + \sum_{j=1}^{r} v_j \ell_j(x)$$

and Lagrange dual function:

$$g(u, v) = \min_{x}\ L(x, u, v)$$

Recap: Lagrange dual problem

The subsequent dual problem is:

$$\begin{array}{ll} \max\limits_{u,v} & g(u,v) \\ \text{subject to} & u \geq 0 \end{array}$$

Important properties:

- Dual problem is always convex, i.e., g is always concave (even if primal problem is not convex)
- The primal and dual optimal values, $f^\star$ and $g^\star$, always satisfy weak duality: $f^\star \geq g^\star$
- Slater's condition: for convex primal, if there is an x such that

$$h_1(x) < 0, \ldots h_m(x) < 0 \quad \text{and} \quad \ell_1(x) = 0, \ldots \ell_r(x) = 0$$

then strong duality holds: $f^\star = g^\star$. Can be further refined to strict inequalities over the nonaffine h_i, $i = 1, \ldots m$

Recap: Deriving the dual of SVM

Introducing dual variables $v, w \geq 0$, we form the Lagrangian:

$$L(\beta, \beta_0, \xi, v, w) = \frac{1}{2}\|\beta\|_2^2 + C\sum_{i=1}^{n}\xi_i - \sum_{i=1}^{n} v_i\xi_i + \sum_{i=1}^{n} w_i\left(1 - \xi_i - y_i(x_i^T\beta + \beta_0)\right)$$

$$0 = \nabla_\beta L = \beta + \sum_{i=1}^{n} w_i(-y_i)\, x_i \quad (w_i(-y_i) \text{ scalar})$$

$$\nabla_{\beta_0} L = \sum_{i=1}^{n} -w_i y_i \qquad \beta_0\left(\sum_{i=1}^{n} -w_i y_i\right)$$

$$\nabla_{\xi_i} L = C - v_i - w_i \qquad \xi_i(C - v_i - w_i)$$

$v, w \geq 0$

$$g(w, v) = \begin{cases} -\infty & \text{if} \\ \text{---} & \text{next slide} \end{cases}$$

not satisfied

$$\begin{cases} -\sum_{i=1}^{n} w_i y_i = 0 \\ C - v_i - w_i = 0 \end{cases}$$

Constraints on w, v

Recap: Dual SVM

Minimizing over β, β_0, ξ gives Lagrange dual function:

$$g(v,w) = \begin{cases} -\frac{1}{2} w^T \tilde{X} \tilde{X}^T w + 1^T w & \text{if } w = C1 - v,\ w^T y = 0 \\ -\infty & \text{otherwise} \end{cases}$$

where $\tilde{X} = \mathrm{diag}(y) X$. Thus SVM dual problem, eliminating slack variable v, becomes

$$\begin{aligned} \max_w \quad & -\frac{1}{2} w^T \tilde{X} \tilde{X}^T w + 1^T w \\ \text{subject to} \quad & 0 \le w \le C1,\ w^T y = 0 \end{aligned}$$

Check: Slater's condition is satisfied, and we have strong duality. Further, from study of SVMs, might recall that at optimality

$$\beta = \tilde{X}^T w$$

$\text{Score}(x) = \beta^T x + \beta_0$

This is not a coincidence, as we'll later via the KKT conditions

"Kernel trick" in SVM

- The dual SVM depends only on inner products

$$\max_{w} \quad -\frac{1}{2} w^T \tilde{X}\tilde{X}^T w + 1^T w$$

$$\text{subject to} \quad 0 \le w \le C1,\ w^T y = 0$$

- How to make predictions?

This lecture

- KKT conditions
  - SVM as an example
- Online Learning

Optimality conditions: the conditions that characterizes the optimal solutions

- What you learned in high school

$$\min_{x \in \mathbb{R}} x^2 - 4x + 9 = f(x)$$

$x \in [0,1]$ $\quad \nabla f(x^*) = 0$ if $f''(x) \geq 0$

- Slight generalization: For convex and differentiable objective function

$$\min_{x \in \mathbb{R}^d} f(x) \qquad \nabla f(x) = 0 \qquad \nabla^2 f(x) \geq 0$$

Does not handle non-differentiable functions, does not handle constraints.

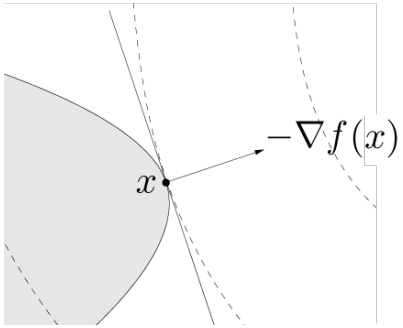
Handling constraints with first-order optimality conditions

For a convex problem

$$\min_x \ f(x) \ \text{ subject to } \ x \in C$$

and differentiable f, a feasible point x is optimal if and only if

$$\nabla f(x)^T (y - x) \geq 0 \ \text{ for all } y \in C$$



This is called the first-order condition for optimality

In words: all feasible directions from x are aligned with gradient $\nabla f(x)$

Important special case: if $C = \mathbb{R}^n$ (unconstrained optimization), then optimality condition reduces to familiar $\nabla f(x) = 0$

Handling non-differentiable functions with "subgradient"

Recall that for convex and differentiable f,

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

I.e., linear approximation always underestimates f

A subgradient of a convex function f at x is any $g \in \mathbb{R}^n$ such that

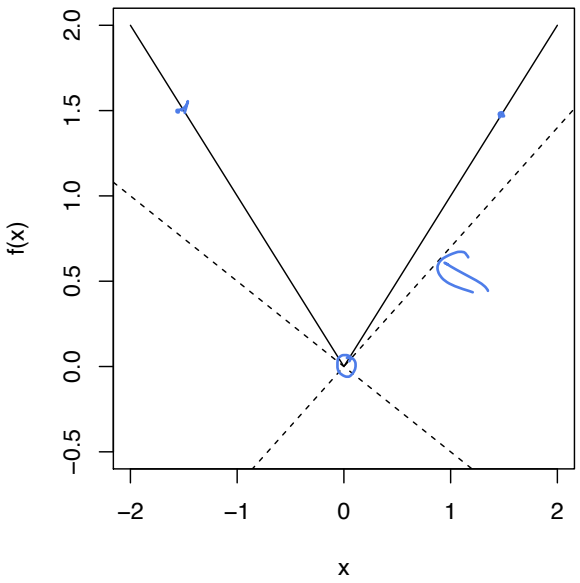
$$f(y) \geq f(x) + g^T (y - x) \quad \text{for all } y$$

- Always exists[1]
- If f differentiable at x, then $g = \nabla f(x)$ uniquely
- Same definition works for nonconvex f (however, subgradients need not exist)

[1] On the relative interior of $\mathrm{dom}(f)$

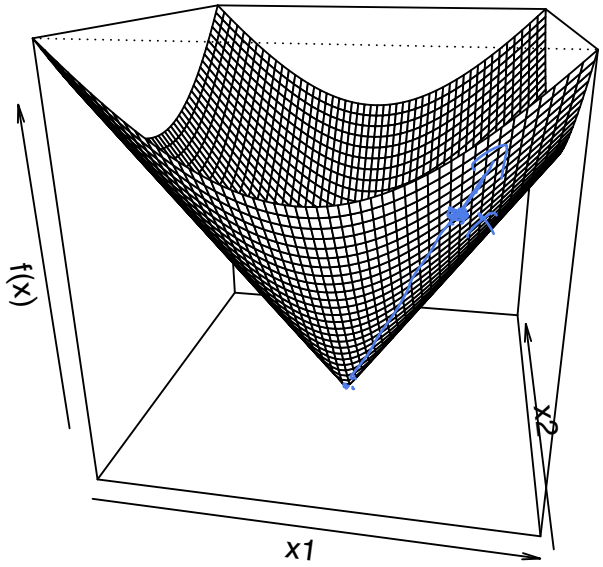
Examples of subgradients

Consider $f : \mathbb{R} \to \mathbb{R}$, $f(x) = |x|$



- For $x \neq 0$, unique subgradient $g = \text{sign}(x)$
- For $x = 0$, subgradient g is any element of $[-1, 1]$

Consider $f : \mathbb{R}^n \to \mathbb{R}$, $f(x) = \|x\|_2$



- For $x \neq 0$, unique subgradient $g = x/\|x\|_2$
- For $x = 0$, subgradient g is any element of $\{z : \|z\|_2 \leq 1\}$

Subdifferential

Set of all subgradients of convex f is called the subdifferential:

$$\partial f(x) = \{g \in \mathbb{R}^n : g \text{ is a subgradient of } f \text{ at } x\}$$

- Nonempty (only for convex f)
- $\partial f(x)$ is closed and convex (even for nonconvex f)
- If f is differentiable at x, then $\partial f(x) = \{\nabla f(x)\}$
- If $\partial f(x) = \{g\}$, then f is differentiable at x and $\nabla f(x) = g$

First order optimality condition with subgradient

For any f (convex or not),

$$f(x^\star) = \min_x f(x) \iff 0 \in \partial f(x^\star)$$

I.e., $x^\star$ is a minimizer if and only if 0 is a subgradient of f at $x^\star$. This is called the subgradient optimality condition

Why? Easy: $g = 0$ being a subgradient means that for all y

$$f(y) \geq f(x^\star) + 0^T(y - x^\star) = f(x^\star)$$

Note the implication for a convex and differentiable function f, with $\partial f(x) = \{\nabla f(x)\}$

Karush-Kuhn-Tucker conditions

Given general problem

$$\begin{aligned} \min_x \quad & f(x) \\ \text{subject to} \quad & h_i(x) \leq 0, \; i = 1, \ldots m \\ & \ell_j(x) = 0, \; j = 1, \ldots r \end{aligned}$$

The Karush-Kuhn-Tucker conditions or KKT conditions are:

- $0 \in \partial \left(f(x) + \sum_{i=1}^m u_i h_i(x) + \sum_{j=1}^r v_j \ell_j(x) \right)$ (stationarity)
- $u_i \cdot h_i(x) = 0$ for all i (complementary slackness)
- $h_i(x) \leq 0, \; \ell_j(x) = 0$ for all i, j (primal feasibility)
- $u_i \geq 0$ for all i (dual feasibility)

Necessity

Let $x^\star$ and $u^\star, v^\star$ be primal and dual solutions with zero duality gap (strong duality holds, e.g., under Slater's condition). Then

$$f(x^\star) = g(u^\star, v^\star)$$

$$= \min_x \; f(x) + \sum_{i=1}^m u_i^\star h_i(x) + \sum_{j=1}^r v_j^\star \ell_j(x)$$

$$\leq f(x^\star) + \sum_{i=1}^m u_i^\star h_i(x^\star) + \sum_{j=1}^r v_j^\star \ell_j(x^\star)$$

$$\leq f(x^\star)$$

In other words, all these inequalities are actually equalities

Two things to learn from this:

- The point $x^\star$ minimizes $L(x, u^\star, v^\star)$ over $x \in \mathbb{R}^n$. Hence the subdifferential of $L(x, u^\star, v^\star)$ must contain 0 at $x = x^\star$—this is exactly the stationarity condition
- We must have $\sum_{i=1}^m u_i^\star h_i(x^\star) = 0$, and since each term here is ≤ 0, this implies $u_i^\star h_i(x^\star) = 0$ for every i—this is exactly complementary slackness

Primal and dual feasibility hold by virtue of optimality. Therefore:

> If $x^\star$ and $u^\star, v^\star$ are primal and dual solutions, with zero duality gap, then $x^\star, u^\star, v^\star$ satisfy the KKT conditions

(Note that this statement assumes nothing a priori about convexity of our problem, i.e., of f, h_i, ℓ_j)

Sufficiency

If there exists $x^\star, u^\star, v^\star$ that satisfy the KKT conditions, then

$$\begin{aligned} g(u^\star, v^\star) &= f(x^\star) + \sum_{i=1}^m u_i^\star h_i(x^\star) + \sum_{j=1}^r v_j^\star \ell_j(x^\star) \\ &= f(x^\star) \end{aligned}$$

where the first equality holds from stationarity, and the second holds from complementary slackness

Therefore the duality gap is zero (and $x^\star$ and $u^\star, v^\star$ are primal and dual feasible) so $x^\star$ and $u^\star, v^\star$ are primal and dual optimal. Hence, we've shown:

> If $x^\star$ and $u^\star, v^\star$ satisfy the KKT conditions, then $x^\star$ and $u^\star, v^\star$ are primal and dual solutions

Putting it together

In summary, KKT conditions:

- always sufficient
- necessary under strong duality

Putting it together:

For a problem with strong duality (e.g., assume Slater's condition: convex problem and there exists x strictly satisfying non-affine inequality contraints),

$$x^\star \text{ and } u^\star, v^\star \text{ are primal and dual solutions}$$
$$\iff x^\star \text{ and } u^\star, v^\star \text{ satisfy the KKT conditions}$$

(Warning, concerning the stationarity condition: for a differentiable function f, we cannot use $\partial f(x) = \{\nabla f(x)\}$ unless f is convex! There are other versions of KKT conditions that deal with local optima.)

Example: support vector machines

Given $y \in \{-1, 1\}^n$, and $X \in \mathbb{R}^{n \times p}$, the support vector machine problem is:

$$\begin{aligned} \min_{\beta, \beta_0, \xi} \quad & \frac{1}{2}\|\beta\|_2^2 + C\sum_{i=1}^n \xi_i \\ \text{subject to} \quad & \xi_i \geq 0, \ i = 1, \ldots n \\ & y_i(x_i^T\beta + \beta_0) \geq 1 - \xi_i, \ i = 1, \ldots n \end{aligned}$$

Introduce dual variables $v, w \geq 0$. KKT stationarity condition:

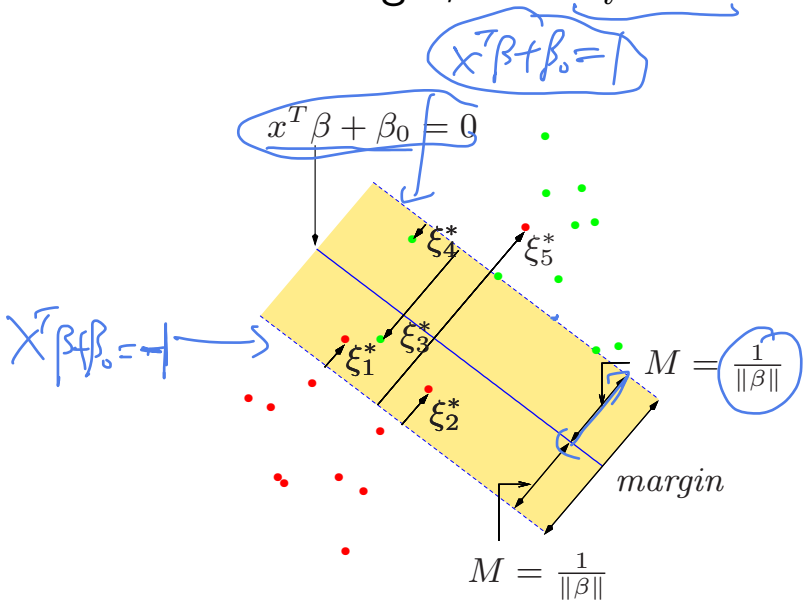
$$0 = \sum_{i=1}^n w_i y_i, \quad \beta = \sum_{i=1}^n w_i y_i x_i, \quad w = C1 - v$$

Complementary slackness:

$$v_i \xi_i = 0, \ w_i\big(1 - \xi_i - y_i(x_i^T\beta + \beta_0)\big) = 0, \quad i = 1, \ldots n$$

Hence at optimality we have $\beta = \sum_{i=1}^{n} w_i y_i x_i$, and w_i is nonzero only if $y_i(x_i^T\beta + \beta_0) = 1 - \xi_i$. Such points i are called the support points

- For support point i, if $\xi_i = 0$, then x_i lies on edge of margin, and $w_i \in (0, C]$;
- For support point i, if $\xi_i \neq 0$, then x_i lies on wrong side of margin, and $w_i = C$



$\frac{1-0}{\|\beta\|_2}$ distance between two hyperplanes

KKT conditions do not really give us a way to find solution, but gives a better understanding

In fact, we can use this to screen away non-support points before performing optimization

Checkpoint: KKT conditions and SVM

- A generalized set of conditions that characterizes the optimal solutions
  - Stationarity, complementary slackness, primal / dual feasibility
  - Always sufficient for optimality
  - Necessary when we have strong duality

- Complementary slackness implies
  - SVM dual solutions are sparse!
  - The number of “support vector”s is small

This lecture

- KKT conditions
  - SVM as an example

- Online Learning

Batch

Recap: Statistical Learning Setting

$(x_1, y_1) \cdots (x_n, y_n) \overset{iid}{\sim} D$ $\quad x \in \mathcal{X} = \mathbb{R}^d$ or $\{0,1\}^d$

$y \in \mathcal{Y} = \{0,1\}$

$\mathcal{H}$ hypothesis class $\quad h \in \mathcal{H} \quad h : \mathcal{X} \to \mathcal{Y}$

Realizable case $\quad \exists h^* \in \mathcal{H}$ s.t. w.p. 1 $\quad h^*(x) = y$

$(x, y) \sim D$

Goal of learning: find $h \in \mathcal{H}$ s.t.

$$err_D(h) = \underset{(x,y)\sim D}{\mathbb{E}} \left[\mathbb{1}\left(\underbrace{h^*(x)}_{\text{function of data}} \neq h(x) \right) \right] \xrightarrow{n \to \infty} 0$$

(Adversarial) Online Learning Setting

- Data points show up sequentially (non-iid), learner makes online predictions

x_1 chosen by nature

$h_1 \Leftarrow x_1$, predict $\hat{y}_1 = h_1(x_1)$

y_1 is revealed by nature

⋮

$h_t \Leftarrow (x_1, y_1), \ldots, (x_{t-1}, y_{t-1}), x_t$, predict $h_t(x_t)$, receive y_t

$\text{loss}_t = \mathbb{1}(\hat{y}_t \neq y_t)$

- Performance metric: Mistake bounds M

If Alg A satisfies # of mistakes A makes $\leq M$

for all seq. of $(x_1, h^*(x_1)), (x_2, h^*(x_2)), \ldots$

then Alg A has a mistake bound of M.

Algorithm A "Consistency"

1. $V_1 = H$
2. for $t = 1, 2, 3, \ldots$
   - Receive x_t, pick any $h \in V_t$
   - prediction $\hat{y}_t = h(x_t)$
   - Receive $y_t = h^*(x_t)$
   - update $V_{t+1} = \{h \in V_t \mid h(x_t) = y_t\}$

Check: $\forall h \in V_{t+1}$, $h^*(x_i) = y_i$ for $\forall i = 1, 2, \ldots, t$

Each mistake, we can eliminate at least 1 hypothesis

trivial upper bound

$$M(\text{consistency}) \le |\mathcal{H}| - 1$$

Example: $\mathcal{X} = \{1, 2, \ldots, |\mathcal{H}|\}$

$\mathcal{H} = \{h_1, \ldots, h_{|\mathcal{H}|}\}$

$h_i(x) = \begin{cases} 0 & \text{if } x < i \\ 1 & \text{otherwise} \end{cases}$

$x_1 = 1, x_2 = 2, \ldots, x_{|\mathcal{H}|} = |\mathcal{H}|, \ldots$

$y_1 = 0, y_2 = 0, \ldots, y_{|\mathcal{H}|} = 1$

$h^* = h_{|\mathcal{H}|}$

predict $h_1, h_2, \ldots, h_{|\mathcal{H}|-1}, h_{|\mathcal{H}|}$

h_t classifies (x_i, y_i) $i = 1, \ldots, t-1$ but $h_t(x_t) \neq y_t$

Algorithm B "Halfing"

1. $V_1 = H$
2. for $t = 1, 2, 3, \ldots$

   Receive x_t

   predict $\hat{y}_t = \underset{h \in V_t}{\text{Vote}}(h(x_t)) = \underset{r \in \{0,1\}}{\text{argmax}} \left| \{ h \mid h \in V_t, h(x_t) = r \} \right|$

   receive $y_t = h^*(x_t)$

   update $V_{t+1} = \{ h \in V_t \mid h(x_t) = y_t \}$

Claim: $M(\text{halfing}) \leq \log_2(|H|)$

Proof: for each mistake, at least $\frac{|V_t|}{2}$ hypotheses are wrong.

$$|V_{t+1}| \leq |V_t| \cdot \frac{1}{2}$$

$$1 \leq |V_{t+M}| \leq |H| \cdot 2^{-M}$$

$$2^M \leq |H| \Rightarrow M \leq \log_2 |H| \quad \square$$

Now let's get rid of "Realizability". The setting is called "Agnostic learning"

Compete v.s. the best $h \in \mathcal{H}$ in hindsight

$$\text{Regret} = \sum_{t=1}^{T} \mathbb{1}(h_t(x_t) \neq y_t) - \min_{h \in \mathcal{H}} \sum_{t=1}^{T} \mathbb{1}(h(x_t) \neq y_t)$$

(x_t, y_t) chosen by adversary

as $T \to \infty$

If $\text{Regret}(T) = o(T)$

$\frac{1}{T}\text{Regret}(T) = o(1)$

Example: Stock forecasting

Alg C Weighted Majority

predict $\hat{y}_t = \mathbb{1}\left(\underbrace{\sum_{h \in H} w_h^t \cdot h(x_t)}_{\text{weighted "Up"}} \geq \underbrace{\frac{1}{2} \sum_{h \in H} w_h^t}_{\text{total weight}} \right)$

receive y_t: discount $w_h^{t+1} = w_h^t \cdot \frac{1}{2}$ for $\forall h$ that made a mistake

How do we fix "weighted majority"? Instead of discounting by 1/2, let's try discounting by 1-ϵ

- Following the same analysis

Fact: For all $0 \leq x \leq 0.5$

$$-x - x^2 \leq \log(1-x) \leq -x$$

Algorithm D: Randomized Weighted Majority

Analysis of RWM

From mistake bounds to loss minimization

- Loss function
- Regret
- The “Hedge” Algorithm:

Checkpoint: Online Learning

- Learning with expert advice
  - A summary of regret bound: # mistakes - Oracle # of mistakes

	Consistency	Halfing	Weighted Majority	Randomized WM
Realizable setting	$\min(T, \lvert\mathcal{H}\rvert)$	$\min(T, \log\lvert\mathcal{H}\rvert)$	$\min(T, \log\lvert\mathcal{H}\rvert)$	$\min(T, \log\lvert\mathcal{H}\rvert)$
Agnostic setting	n.a.	n.a.	$(1+\epsilon)m + \log\lvert\mathcal{H}\rvert/\epsilon$	$\sqrt{m\log\lvert\mathcal{H}\rvert} = O(\sqrt{T\log\lvert\mathcal{H}\rvert})$

Next lecture

- Online Learning (Part II)
  - Online Gradient Descent
- Reinforcement Learning
  - Markov Decision Processes