Statistical Learning V 29-11-2019

1. Support Vector Machines (Can create infinitely many features!)
   a) Optimal separating hyperplane
   b) SVMs
   c) Interpretation as penalized ERM with hinge loss
   d) Dual Formulation
   e) Kernel trick
   f) Derivation of dual formulation

Vapnik & Chervonenkis: foundational work on statistical learning starting in sixties and seventies, leading to SVMs ~1990.

Vapnik. 1998: "solve the problem directly and never solve a more general problem as an intermediate step"

1. SVMs

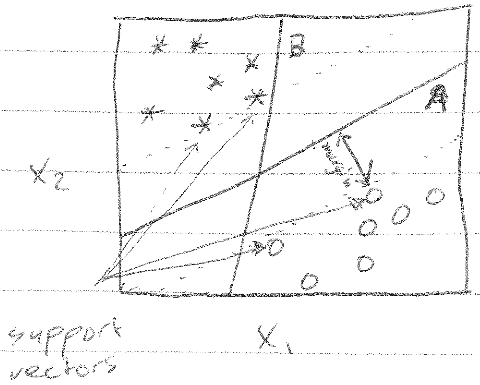
a) Optimal separating hyperplane

	estimate
generative:	$P(X,Y)$
discriminative:	$P(Y\|X)$
now:	decision boundary directly

Assume: 2 classes, linearly separable

$$\begin{pmatrix} Y_1 \\ X_1 \end{pmatrix}, \dots, \begin{pmatrix} Y_N \\ X_N \end{pmatrix} \qquad Y \in \{-1, +1\}$$

Linear Model: classifiers that compute $x^T\beta + \beta_0$ ← writing intercept separately and return its sign



Which decision boundary do you like best? A or B?

A has larger "margin" = distance to nearest point

Fig. 12.1, left

"Optimal" separating hyperplane maximizes the margin.

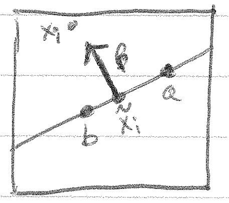
<u>support vectors:</u> points <u>on</u> the margin

decision boundary: $\{x : x^T\beta + \beta_0 = 0\}$

Let $f(x) = x^T\beta + \beta_0$. Then distance of x_i to decision boundary is $\frac{|f(x_i)|}{\|\beta\|}$

<u>margin:</u> $\frac{y_i \cdot f(x_i)}{\|\beta\|}$ $\leftarrow$ ~~$\frac{f(x_i)}{\|\beta\|}$~~ is distance if x_i classified correctly, is negative distance if classified incorrectly

<u>Optional:</u> for any a, b on decision boundary:



$(b-a)^T\beta = 0$, so $\frac{\beta}{\|\beta\|}$ is normal vector to the decision boundary of length 1.

suppose $\tilde{x}_i$ is projection of x_i onto decision boundary. Then

$$x_i = \tilde{x}_i + \alpha \cdot \frac{\beta}{\|\beta\|}$$

$|\alpha|$ is distance of x_i from decision boundary

$$\alpha \frac{\beta}{\|\beta\|} = x_i - \tilde{x}_i$$

$$\alpha \cdot \|\beta\| = (x_i - \tilde{x}_i)^T\beta \quad (\text{because } \beta^T\beta = \|\beta\|^2)$$

$$= x_i^T\beta - \tilde{x}_i^T\beta$$

$$= x_i^T\beta + \beta_0 \quad (\text{because } \tilde{x}_i \text{ on decision boundary})$$

$$= f(x_i)$$

$$\alpha = \frac{f(x_i)}{\|\beta\|}$$

How to express optimal separating hyperplane mathematically:

to maximize the margin M:

$$\max_{\beta, \beta_0, M} \quad M$$

subject to: $\underset{\substack{\uparrow \\ \text{margin of } \binom{y_i}{x_i}}}{\dfrac{y_i(x_i^T\beta + \beta_0)}{\|\beta\|}} \geq M$ for $i = 1, \ldots, N$

Same decision boundary and margin if we multiply β, β_0 by a constant, so can always choose this constant such that $\|\beta\| = \frac{1}{M}$:

$$\max_{\substack{\beta, \beta_0, M \\ \|\beta\| = \frac{1}{M}}} \quad M$$

s.t. $\quad \cancel{\dfrac{y_i(x_i^T\beta + \beta_0)}{\|\beta\|}} \geq M \cdot \|\beta\| \quad \forall i$

$$\max_{\beta, \beta_0} \quad \frac{1}{\|\beta\|}$$

s.t. $\quad y_i(x_i^T\beta + \beta_0) \geq 1 \quad \forall i$

solution achieved by same parameters β, β_0

convex function $\rightarrow$ $\displaystyle\min_{\beta, \beta_0} \frac{1}{2}\|\beta\|^2$

linear inequality constraints $\rightarrow$ s.t. $y_i(x_i^T\beta + \beta_0) \geq 1 \quad \forall i$

Can solve this optimization problem efficiently!

NB. We cannot efficiently compute an ERM solution for 0/1-loss in general, but we see here that for separable data this gives a computationally efficient way to find one of the ERM solutions!

b) SVMs

What if classes are not linearly separable?

Greek letter "xi"

Fig. 12.1, right: introduce slack variable $\xi_i \geq 0$ for each data point $i = 1, \ldots, N$

$$\max_{\beta, \beta_0, M, \xi_i} \quad M$$

$$\text{subject to:} \quad \xi_i \geq 0, \quad \frac{y_i (x_i^T \beta + \beta_0)}{\|\beta\|} \geq M(1-\xi_i) \quad i = 1, \ldots, N$$

$$\sum_{i=1}^{N} \xi_i \leq t$$

parameter of alg. ← Assume we take large enough to have a solution

support vectors: all points inside the margin

$$\min_{\beta, \beta_0, \xi_i} \quad \frac{1}{2}\|\beta\|^2$$

$$\text{s.t.} \quad \xi_i \geq 0, \quad y_i (x_i^T \beta + \beta_0) \geq 1 - \xi_i \quad i = 1, \ldots, N$$

$$\sum_{i=1}^{N} \xi_i \leq t$$

equivalent

$$\min_{\beta, \beta_0, \xi_i} \quad \frac{1}{2}\|\beta\|^2 + \underset{\text{Parameter}}{C} \cdot \sum_{i=1}^{N} \xi_i \qquad (*)$$

$$\text{s.t.} \quad \xi_i \geq 0, \quad y_i (x_i^T \beta + \beta_0) \geq 1 - \xi_i \quad i = 1, \ldots, N$$

c.) Interpretation as penalized ERM

see slides 4

$L(y_i, f(x_i)) = \max\{0, 1 - y_i \cdot f(x_i)\}$ is "hinge loss"

$$\min_{\beta,\beta_0,\xi_i} \quad \tfrac{1}{2}\|\beta\|^2 + C\sum_{i=1}^{N}\xi_i$$

s.t. $\underbrace{\xi_i \geq 0 \quad , \quad \xi_i \geq 1 - y_i(x_i^T\beta+\beta_0)}_{\xi_i \geq L(y_i,\, x_i^T\beta+\beta_0)}$ $\quad i = 1, \dots, N$

$$\min_{\beta,\beta_0} \quad \sum_{i=1}^{N} L(y_i, x_i^T\beta+\beta_0) + \frac{1}{2C}\|\beta\|^2$$

ERM for hinge loss with L_2-penalty, $\lambda = \frac{1}{2C}$.

d) Dual Formulation

$$\max_{\alpha_1,\dots,\alpha_N} \quad \sum_{i=1}^{N}\alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{k=1}^{N}\alpha_i\alpha_k y_i y_k \overset{= x_i^T x_k}{\langle x_i, x_k\rangle}$$

subject to $0 \leq \alpha_i \leq C$ and $\sum_{i=1}^{N}\alpha_i y_i = 0$

Then solution to (*) is:

$$\hat{\beta} = \sum_{i=1}^{N}\hat{\alpha}_i y_i x_i$$ ← very different, but reminiscent of nearest neighbor, because also defined in terms of training data

$\hat{\alpha}_i = 0$ for x_i outside margin and on right side of decision boundary

$0 < \hat{\alpha}_i < C$ for x_i on margin and on right side of decision boundary

$\hat{\alpha}_i = C$ for x_i inside margin or on wrong side of decision boundary

solve $\hat{\beta}_0$ from $\hat{\alpha}_i[y_i(x_i^T\hat{\beta}+\hat{\beta}_0) - 1] = 0$
for any i s.t. $0 < \hat{\alpha}_i < C$

e) Kernel trick

Fig. 2.5: how to learn something like this with linear classifier?

map features x to a larger set of features h(x)!
e.g.

$$h\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \\ x_1 \cdot x_2 \\ x_1^2 \\ x_2^2 \end{pmatrix}$$

Then $\langle x_i, x_k \rangle$ in dual formulation becomes $\langle h(x_i), h(x_k) \rangle$

kernel trick: don't need to specify h, only need to know the kernel function

really nice if this were a simple function..., so turn things around and start by defining $K(x_i, x_k)$ → $K(x_i, x_k) = \langle h(x_i), h(x_k) \rangle$ ← measure of similarity, larger if x_i, x_k more similar.

h(x) may even be infinite-dimensional!

Examples: $K(x, x') = (1 + \langle x, x' \rangle)^d$: d-th degree polynomial

↳ e.g. $d = 2$, $x \in \mathbb{R}^2$:

$$K(x, x') = (1 + x_1 x_1' + x_2 x_2')^2$$
$$= \langle h(x), h(x') \rangle$$

for

$$h(x) = \begin{pmatrix} 1 \\ \sqrt{2}\, x_1 \\ \sqrt{2}\, x_2 \\ x_1^2 \\ x_2^2 \\ \sqrt{2}\, x_1 x_2 \end{pmatrix}$$

radial basis: $K(x, x') = e^{-\gamma \|x - x'\|^2}$

neural network: $K(x, x') = \tanh(a \langle x, x' \rangle + b)$

$$\tanh(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$

If K satisfies certain technical conditions (symmetric, positive definite) then there always exists some mapping h s.t. $K(x, x') = \langle h(x), h(x') \rangle$.

Classifying a new x:

$$\hat{f}(x) = h(x)^T\hat{\beta} + \hat{\beta}_0 = h(x)^T \sum_{i=1}^{N} \alpha_i y_i h(x_i) + \hat{\beta}_0$$

$$= \sum_{i=1}^{N} \alpha_i y_i \langle h(x), h(x_i)\rangle + \hat{\beta}_0$$

$$= \sum_{i=1}^{N} \alpha_i y_i K(x, x_i) + \hat{\beta}_0$$

Again no need to specify h; only need to know kernel.

Fig. 12.3

f.) Derivation of Dual Formulation ← optional!

$$\min_{\beta, \beta_0, \xi_i} \quad \tfrac{1}{2}\|\beta\|^2 + C \cdot \sum_{i=1}^{N} \xi_i$$

$$\text{s.t.} \quad \xi_i \geq 0, \quad y_i(x_i^T\beta + \beta_0) - (1-\xi_i) \geq 0 \qquad i = 1, \ldots, N$$

$$\min_{\beta, \beta_0, \xi_i} \ \sup_{\alpha_i, \mu_i \geq 0} \ \underbrace{\tfrac{1}{2}\|\beta\|^2 + C\sum_{i=1}^{N} \xi_i - \sum_{i=1}^{N} \alpha_i\left(y_i(x_i^T\beta + \beta_0) - (1-\xi_i)\right) - \sum_{i=1}^{N} \mu_i \xi_i}_{A}$$

(If β, β_0, ξ_i violate constraints, then α_i or μ_i becomes ∞ and $A = \infty$, so β, β_0, ξ_i only achieve minimum while satisfying constraints. And then α_i, μ_i become 0, so the constraints ~~don't~~ drop away and we are minimizing the previous objective.)

~~$\nabla_\beta A = 0 \Rightarrow \beta = \sum_{i=1}^{N} \alpha_i y_i x_i \qquad \nabla_{\beta_0} A = 0 \Rightarrow \sum_{i=1}^{N} \alpha_i y_i = 0$~~

~~$\nabla_{\xi_i} A = 0 \Rightarrow \mu_i = C - \alpha_i$~~

~~plugging~~

$$\min_{\beta,\beta_0,\xi_i} \sup_{\alpha_i,\mu_i \geq 0} A = \sup_{\alpha_i,\mu_i \geq 0} \underbrace{\min_{\beta,\beta_0,\xi_i} A}_{\text{can solve this}}.$$ by convex optimization theory (Slater's condition)

$$\nabla_\beta A = 0 \Rightarrow \beta = \sum_{i=1}^{N} \alpha_i y_i x_i \qquad \nabla_{\beta_0} A = 0 \Rightarrow \sum_{i=1}^{N} \alpha_i y_i = 0$$

$$\nabla_{\xi_i} A = 0 \Rightarrow \mu_i = C - \alpha_i$$

Plugging these in gives dual formulation.