# Lecture 8: Support Vector Machines Advanced Topics in Machine Learning: COMPGI13 

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## Overview

- The representer theorem
- Review of convex optimization
- Support vector classification, the $C-S V$ and $\nu$-SV machines


## Representer theorem

## Learning problem: setting

Given a set of paired observations $\left(x_{1}, y_{1}\right), \ldots\left(x_{n}, y_{n}\right)$ (regression or classification).
Find the function $f^{*}$ in the RKHS $\mathcal{H}$ which satisfies

$$
\begin{equation*}
J\left(f^{*}\right)=\min _{f \in \mathcal{H}} J(f) \tag{1}
\end{equation*}
$$

where

$$
J(f)=L_{y}\left(f\left(x_{1}\right), \ldots, f\left(x_{n}\right)\right)+\Omega\left(\|f\|_{\mathcal{H}}^{2}\right)
$$

$\Omega$ is non-decreasing, and $y$ is the vector of $y_{i}$.

- Classification: $L_{y}\left(f\left(x_{1}\right), \ldots, f\left(x_{n}\right)\right)=\sum_{i=1}^{n} \mathbb{I}_{y_{i} f\left(x_{i}\right) \leq 0}$
- Regression: $L_{y}\left(f\left(x_{1}\right), \ldots, f\left(x_{n}\right)\right)=\sum_{i=1}^{n}\left(y_{i}-f\left(x_{i}\right)\right)^{2}$


## Representer theorem

The representer theorem: solution to

$$
\min _{f \in \mathcal{H}}\left[L_{y}\left(f\left(x_{1}\right), \ldots, f\left(x_{n}\right)\right)+\Omega\left(\|f\|_{\mathcal{H}}^{2}\right)\right]
$$

takes the form

$$
f^{*}=\sum_{i=1}^{n} \alpha_{i} k\left(x_{i}, \cdot\right)
$$

If $\Omega$ is strictly increasing, all solutions have this form.

## Representer theorem: proof

Proof: Denote $f_{s}$ projection of $f$ onto the subspace

$$
\begin{equation*}
\operatorname{span}\left\{k\left(x_{i}, \cdot\right): 1 \leq i \leq n\right\}, \tag{2}
\end{equation*}
$$

such that

$$
f=f_{s}+f_{\perp},
$$

where $f_{s}=\sum_{i=1}^{n} \alpha_{i} k\left(x_{i}, \cdot\right)$.
Regularizer:

$$
\|f\|_{\mathcal{H}}^{2}=\left\|f_{s}\right\|_{\mathcal{H}}^{2}+\left\|f_{\perp}\right\|_{\mathcal{H}}^{2} \geq\left\|f_{s}\right\|_{\mathcal{H}}^{2}
$$

then

$$
\Omega\left(\|f\|_{\mathcal{H}}^{2}\right) \geq \Omega\left(\left\|f_{s}\right\|_{\mathcal{H}}^{2}\right),
$$

so this term is minimized for $f=f_{s}$.

## Representer theorem: proof

Proof (cont.): Individual terms $f\left(x_{i}\right)$ in the loss:

$$
f\left(x_{i}\right)=\left\langle f, k\left(x_{i}, \cdot\right)\right\rangle_{\mathcal{H}}=\left\langle f_{s}+f_{\perp}, k\left(x_{i}, \cdot\right)\right\rangle_{\mathcal{H}}=\left\langle f_{s}, k\left(x_{i}, \cdot\right)\right\rangle_{\mathcal{H}}
$$

SO

$$
L_{y}\left(f\left(x_{1}\right), \ldots, f\left(x_{n}\right)\right)=L_{y}\left(f_{s}\left(x_{1}\right), \ldots, f_{s}\left(x_{n}\right)\right)
$$

Hence

- Loss $L(\ldots)$ only depends on the component of $f$ in the data subspace,
- Regularizer $\Omega(\ldots)$ minimized when $f=f_{s}$.
- If $\Omega$ is strictly non-decreasing, then $\left\|f_{\perp}\right\|_{\mathcal{H}}=0$ is required at the minimum.


## Short overview of convex optimization

## Convex set


(Figure from Boyd and Vandenberghe)
Leftmost set is convex, remaining two are not.
Every point in the set can be seen from any other point in the set, along a straight line that never leaves the set.

## Definition

$C$ is convex if for all $x_{1}, x_{2} \in C$ and any $0 \leq \theta \leq 1$ we have $\theta x_{1}+(1-\theta) x_{2} \in C$, i.e. every point on the line between $x_{1}$ and $x_{2}$ lies in $C$.

## Convex function: no local optima


(Figure from Boyd and Vandenberghe)

## Definition (Convex function)

A function $f$ is convex if its domain domf is a convex set and if $\forall x, y \in \operatorname{dom} f$, and any $0 \leq \theta \leq 1$,

$$
f(\theta x+(1-\theta) y) \leq \theta f(x)+(1-\theta) f(y)
$$

The function is strictly convex if the inequality is strict for $x \neq y$.

## Optimization and the Lagrangian

Optimization problem on $x \in \mathbb{R}^{n}$,

$$
\begin{array}{rlr}
\operatorname{minimize} & f_{0}(x) & \\
\text { subject to } & f_{i}(x) \leq 0 & i=1, \ldots, m  \tag{3}\\
& h_{i}(x)=0 & i=1, \ldots p
\end{array}
$$

- $p^{*}$ the optimal value of (3)
- $\mathcal{D}:=\bigcap_{i=0}^{m} \operatorname{dom} f_{i} \cap \bigcap_{i=1}^{p} \operatorname{dom} h_{i}$ (nonempty).

The Lagrangian $L: \mathbb{R}^{n} \times \mathbb{R}^{m} \times \mathbb{R}^{p} \rightarrow \mathbb{R}$ associated with problem (3) is written


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The Lagrangian $L: \mathbb{R}^{n} \times \mathbb{R}^{m} \times \mathbb{R}^{p} \rightarrow \mathbb{R}$ associated with problem (3) is written

$$
L(x, \lambda, \nu):=f_{0}(x)+\sum_{i=1}^{m} \lambda_{i} f_{i}(x)+\sum_{i=1}^{p} \nu_{i} h_{i}(x)
$$

and has domain dom $L:=\mathcal{D} \times \mathbb{R}^{m} \times \mathbb{R}^{p}$. The vectors $\lambda$ and $\nu$ are called Lagrange multipliers or dual variables.

## Lower bound interpretation of Lagrangian

Idealy we would want an unconstrained problem

$$
\operatorname{minimize} f_{0}(x)+\sum_{i=1}^{m} I_{-}\left(f_{i}(x)\right)+\sum_{i=1}^{p} I_{0}\left(h_{i}(x)\right)
$$

where $I_{-}(u)=\left\{\begin{array}{ll}0 & u \leq 0 \\ \infty & u>0\end{array} \quad\right.$ and $I_{0}(u)$ is the indicator of 0 .
To get a lower bound, we require $\lambda \succeq 0$.



## Lagrange dual: lower bound on optimum p*

Lagrange dual: minimize Lagrangian (lower bound) over all $x \in \mathcal{D}$ When $\lambda \succeq 0$ and $f_{i}(x) \leq 0$, Lagrange dual function is

$$
\begin{equation*}
g(\lambda, \nu):=\inf _{x \in \mathcal{D}} L(x, \lambda, \nu) \leq p^{*} \tag{4}
\end{equation*}
$$

A dual feasible pair $(\lambda, \nu)$ is a pair for which $\lambda \succeq 0$ and $(\lambda, \nu) \in \operatorname{dom}(g)$. (Figure from Boyd and Vandenberghe)


## Reminders:

- $f_{0}$ is function to be minimized.
- $f_{1} \leq 0$ is inequality constraint
- $\lambda \geq 0$ is Lagrange multiplier
- $p^{*}$ is minimum $f_{0}$ in constraint set


## Lagrange dual: lower bound on optimum $p^{*}$

When $\lambda \succeq 0$, then for all $\nu$ we have

$$
\begin{equation*}
g(\lambda, \nu) \leq p^{*} \tag{5}
\end{equation*}
$$

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Reminders:

- $g(\lambda, \nu):=$ $\inf _{x \in \mathcal{D}} L(x, \lambda)$
- $\lambda \geq 0$ is Lagrange multiplier
- $p^{*}$ is minimum $f_{0}$ in constraint set


## Lagrange dual is lower bound on $p^{*}$ (proof)

We now give a formal proof that Lagrange dual function $g(\lambda, \nu)$ lower bounds $p^{*}$.
Proof: Assume $\tilde{x}$ is feasible, i.e. $f_{i}(\tilde{x}) \leq 0, h_{i}(\tilde{x})=0, \tilde{x} \in \mathcal{D}$, $\lambda \succeq 0$. Then


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\sum_{i=1}^{m} \lambda_{i} f_{i}(\tilde{x})+\sum_{i=1}^{p} \nu_{i} h_{i}(\tilde{x}) \leq 0
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\sum_{i=1}^{m} \lambda_{i} f_{i}(\tilde{x})+\sum_{i=1}^{p} \nu_{i} h_{i}(\tilde{x}) \leq 0
$$

Thus

$$
\begin{aligned}
g(\lambda, \nu) & :=\inf _{x \in \mathcal{D}}\left(f_{0}(x)+\sum_{i=1}^{m} \lambda_{i} f_{i}(x)+\sum_{i=1}^{p} \nu_{i} h_{i}(x)\right) \\
& \leq f_{0}(\tilde{x})+\sum_{i=1}^{m} \lambda_{i} f_{i}(\tilde{x})+\sum_{i=1}^{p} \nu_{i} h_{i}(\tilde{x}) \\
& \leq f_{0}(\tilde{x})
\end{aligned}
$$

This holds for every feasible $\tilde{x}$, hence lower bound holds.

## Best lower bound: maximize the dual

Best lower bound $g(\lambda, \nu)$ on the optimal solution $p^{*}$ of (3): Lagrange dual problem

$$
\begin{array}{cl}
\text { maximize } & g(\lambda, \nu) \\
\text { subject to } & \lambda \succeq 0 . \tag{6}
\end{array}
$$

Dual feasible: $(\lambda, \nu)$ with $\lambda \succeq 0$ and $g(\lambda, \nu)>-\infty$. Dual optimal: solutions $\left(\lambda^{*}, \nu^{*}\right)$ to the dual problem, $d^{*}$ is optimal value (dual always easy to maximize: next slide). Weak duality always holds:
...but what is the point of finding a best lower bound on a minimization problem?

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$$
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$$

Strong duality: (does not always hold, conditions given later):

$$
d^{*}=p^{*}
$$

If S.D. holds: solve the easy (concave) dual problem to find $p_{\underline{\underline{\underline{n}}}}^{*}$

## Maximizing the dual is always easy

The Lagrange dual function: minimize Lagrangian (lower bound)

$$
g(\lambda, \nu)=\inf _{x \in \mathcal{D}} L(x, \lambda, \nu)
$$

Dual function is a pointwise infimum of affine functions of $(\lambda, \nu)$, hence concave in $(\lambda, \nu)$ with convex constraint set $\lambda \succeq 0$.


## Example:

One inequality constraint,

$$
L(x, \lambda)=f_{0}(x)+\lambda f_{1}(x)
$$

and assume there are only four possible values for $x$. Each line represents a different $x$.

## How do we know if strong duality holds?

Conditions under which strong duality holds are called constraint qualifications (they are sufficient, but not necessary)
(Probably) best known sufficient condition: Strong duality

- Primal problem is convex, i.e. of the form

for convex $f_{0}, \ldots, f_{m}$, and
- Slater's condition holds: there exists some strictly feasible point ${ }^{1} \tilde{x} \in \operatorname{relint}(\mathcal{D})$ such that


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\begin{align*}
\operatorname{minimize} & f_{0}(x) \\
\text { subject to } & f_{i}(x) \leq 0  \tag{8}\\
& A x=b
\end{align*} \quad i=1, \ldots, n
$$

for convex $f_{0}, \ldots, f_{m}$, and

- Slater's condition holds: there exists some strictly feasible point $^{1} \tilde{x} \in \operatorname{relint}(\mathcal{D})$ such that

$$
f_{i}(\tilde{x})<0 \quad i=1, \ldots, m \quad A \tilde{x}=b .
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for convex $f_{0}, \ldots, f_{m}$, and

- Slater's condition for the case of affine $f_{i}$ is trivial:

$$
f_{i}(\tilde{x}) \leq 0 \quad i=1, \ldots, m \quad A \tilde{x}=b
$$

## A consequence of strong duality...

Assume primal is equal to the dual. What are the consequences?

- $x^{*}$ solution of original problem (minimum of $f_{0}$ under constraints),
- $\left(\lambda^{*}, \nu^{*}\right)$ solutions to dual

$$
\begin{aligned}
& f_{0}\left(x^{*}\right) \quad \underset{\text { (assumed) }}{=} g\left(\lambda^{*}, \nu^{*}\right) \\
& \underset{\text { (g definition) }}{=} \inf _{x \in \mathcal{D}}\left(f_{0}(x)+\sum_{i=1}^{m} \lambda_{i}^{*} f_{i}(x)+\sum_{i=1}^{p} \nu_{i}^{*} h_{i}(x)\right) \\
& \underset{\text { (inf definition) }}{\leq} f_{0}\left(x^{*}\right)+\sum_{i=1}^{m} \lambda_{i}^{*} f_{i}\left(x^{*}\right)+\sum_{i=1}^{p} \nu_{i}^{*} h_{i}\left(x^{*}\right) \\
& \underset{(4)}{\leq} \quad f_{0}\left(x^{*}\right),
\end{aligned}
$$

(4): $\left(x^{*}, \lambda^{*}, \nu^{*}\right)$ satisfies $\lambda^{*} \succeq 0, f_{i}\left(x^{*}\right) \leq 0$, and $h_{i}\left(x^{*}\right)=0$.

## ...is complementary slackness

From previous slide,

$$
\begin{equation*}
\sum_{i=1}^{m} \lambda_{i}^{*} f_{i}\left(x^{*}\right)=0 \tag{9}
\end{equation*}
$$

which is the condition of complementary slackness. This means

$$
\begin{aligned}
\lambda_{i}^{*}>0 & \Longrightarrow \quad f_{i}\left(x^{*}\right)=0 \\
f_{i}\left(x^{*}\right)<0 & \Longrightarrow \quad \lambda_{i}^{*}=0 .
\end{aligned}
$$

From $\lambda_{i}$, read off which inequality constraints are strict.

## KKT conditions for global optimum

Assume functions $f_{i}, h_{i}$ are differentiable and strong duality. Since $x^{*}$ minimizes $L\left(x, \lambda^{*}, \nu^{*}\right)$, derivative at $x^{*}$ is zero,

$$
\nabla f_{0}\left(x^{*}\right)+\sum_{i=1}^{m} \lambda_{i}^{*} \nabla f_{i}\left(x^{*}\right)+\sum_{i=1}^{p} \nu_{i}^{*} \nabla h_{i}\left(x^{*}\right)=0 .
$$

KKT conditions we are at global optimum, $(x, \lambda, \nu)=\left(x^{*}, \lambda^{*}, \nu^{*}\right)$ when strong duality holds, and


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$$

KKT conditions we are at global optimum, $(x, \lambda, \nu)=\left(x^{*}, \lambda^{*}, \nu^{*}\right)$ when strong duality holds, and

$$
\begin{aligned}
f_{i}(x) & \leq 0, i=1, \ldots, m \\
h_{i}(x) & =0, i=1, \ldots, p \\
\lambda_{i} & \geq 0, i=1, \ldots, m \\
\lambda_{i} f_{i}(x) & =0, i=1, \ldots, m \\
\nabla f_{0}(x)+\sum_{i=1}^{m} \lambda_{i} \nabla f_{i}(x)+\sum_{i=1}^{p} \nu_{i} \nabla h_{i}(x) & =0
\end{aligned}
$$

## KKT conditions for global optimum

In summary: if

- primal problem convex and
- constraint functions satisfy Slater's conditions and
- functions $f_{i}, h_{i}$ differentiable
then KKT conditions necessary and sufficient for optimality.


## Support vector classification

## Linearly separable points

Classify two clouds of points, where there exists a hyperplane which linearly separates one cloud from the other without error.


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## Linearly separable points

Classify two clouds of points, where there exists a hyperplane which linearly separates one cloud from the other without error.


Smallest distance from each class to the separating hyperplane $(w, b)$ is called the margin.

This problem can be expressed as follows:

$$
\begin{equation*}
\max _{w, b}(\operatorname{margin})=\max _{w, b}\left(\frac{2}{\|w\|}\right) \tag{10}
\end{equation*}
$$

subject to

$$
\begin{cases}\min \left(w^{\top} x_{i}+b\right)=1 & i: y_{i}=+1  \tag{11}\\ \max \left(w^{\top} x_{i}+b\right)=-1 & i: y_{i}=-1\end{cases}
$$

The resulting classifier is

$$
y=\operatorname{sign}\left(w^{\top} x+b\right)
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We can rewrite to obtain

$$
\max _{w, b} \frac{1}{\|w\|} \quad \text { or } \quad \min _{w, b}\|w\|^{2}
$$

subject to

$$
\begin{equation*}
y_{i}\left(w^{\top} x_{i}+b\right) \geq 1 \tag{12}
\end{equation*}
$$

Allow "errors": points within the margin, or even on the wrong side of the decision boudary. Ideally:

$$
\min _{w, b}\left(\frac{1}{2}\|w\|^{2}+C \sum_{i=1}^{n} \mathbb{I}\left[y_{i}\left(w^{\top} x_{i}+b\right)<0\right]\right)
$$

where $C$ controls the tradeoff between maximum margin and loss.
Replace with convex upper bound:

with hinge loss,


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where $C$ controls the tradeoff between maximum margin and loss. Replace with convex upper bound:

$$
\min _{w, b}\left(\frac{1}{2}\|w\|^{2}+C \sum_{i=1}^{n} \theta\left(y_{i}\left(w^{\top} x_{i}+b\right)\right)\right) .
$$

with hinge loss,

$$
\theta(\alpha)=(1-\alpha)_{+}= \begin{cases}1-\alpha & 1-\alpha>0 \\ 0 & \text { otherwise }\end{cases}
$$

## Hinge loss

Hinge loss:

$$
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## Support vector classification

Substituting in the hinge loss, we get

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\min _{w, b}\left(\frac{1}{2}\|w\|^{2}+C \sum_{i=1}^{n} \theta\left(y_{i}\left(w^{\top} x_{i}+b\right)\right)\right) .
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How do you implement hinge loss with simple inequality constraints (for optimization)?

subject to ${ }^{2}$


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How do you implement hinge loss with simple inequality constraints (for optimization)?

$$
\begin{equation*}
\min _{w, b, \xi}\left(\frac{1}{2}\|w\|^{2}+C \sum_{i=1}^{n} \xi_{i}\right) \tag{13}
\end{equation*}
$$

subject to ${ }^{2}$

$$
\xi_{i} \geq 0 \quad y_{i}\left(w^{\top} x_{i}+b\right) \geq 1-\xi_{i}
$$

${ }^{2}$ Either $y_{i}\left(w^{\top} x_{i}+b\right) \geq 1$ and $\xi_{i}=0$ as before, or $y_{i}\left(w^{\top} x_{i}+b\right)<1$, and then $\xi_{i}>0$ takes the value satisfying $y_{i}\left(w^{\top} x_{i}+b\right)=1-\xi_{i}$.

## Support vector classification



## Does strong duality hold?

(C) Is the optimization problem convex wrt the variables $w, b, \xi$ ?
minimize

$$
f_{0}(w, b, \xi):=\frac{1}{2}\|w\|^{2}+C \sum_{i=1}^{n} \xi_{i}
$$

subject to $\quad f_{i}(w, b, \xi):=1-\xi_{i}-y_{i}\left(w^{\top} x_{i}+b\right) \leq 0 \quad i=1$

$$
A x=b \quad(\text { absent })
$$

Each of $f_{0}, f_{1}, \ldots, f_{n}$ are convex.
(2) Does Slater's condition hold? Trivial since inequality constraints affine, and there always exists some

$$
\begin{aligned}
\xi_{i} & \geq 0 \\
y_{i}\left(w^{\top} x_{i}+b\right) & \geq 1-\xi_{i}
\end{aligned}
$$

Thus strong duality holds, the problem is differentiable, hence the


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subject to $\quad f_{i}(w, b, \xi):=1-\xi_{i}-y_{i}\left(w^{\top} x_{i}+b\right) \leq 0 \quad i=1, \ldots, n$

$$
A x=b \quad \text { (absent) }
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Thus strong duality holds, the problem is differentiable, hence the KKT conditions hold at the global optimum.

## Support vector classification: Lagrangian

The Lagrangian: $L(w, b, \xi, \alpha, \lambda)$
$=\frac{1}{2}\|w\|^{2}+C \sum_{i=1}^{n} \xi_{i}+\sum_{i=1}^{n} \alpha_{i}\left(1-y_{i}\left(w^{\top} x_{i}+b\right)-\xi_{i}\right)+\sum_{i=1}^{n} \lambda_{i}\left(-\xi_{i}\right)$
with dual variable constraints

$$
\alpha_{i} \geq 0, \quad \lambda_{i} \geq 0 .
$$

Minimize wrt the primal variables $w, b$, and $\xi$.

## Support vector classification: Lagrangian

Derivative wrt $w$ :

$$
\begin{equation*}
\frac{\partial L}{\partial w}=w-\sum_{i=1}^{n} \alpha_{i} y_{i} x_{i}=0 \quad w=\sum_{i=1}^{n} \alpha_{i} y_{i} x_{i} \tag{14}
\end{equation*}
$$

Derivative wrt $b$ :

$$
\begin{equation*}
\frac{\partial L}{\partial b}=\sum_{i} y_{i} \alpha_{i}=0 \tag{15}
\end{equation*}
$$

Derivative wrt $\xi_{i}$ :

$$
\begin{equation*}
\frac{\partial L}{\partial \xi_{i}}=C-\alpha_{i}-\lambda_{i}=0 \quad \alpha_{i}=C-\lambda_{i} \tag{16}
\end{equation*}
$$

Noting that $\lambda_{i} \geq 0$,

$$
\alpha_{i} \leq C
$$

## Support vector classification: Lagrangian

Now use complementary slackness:

```
Non-margin SVs: }\mp@subsup{\alpha}{i}{}=C\not=0
    (1) We immediately have 1- \xii= yi}(\mp@subsup{w}{}{\top}\mp@subsup{x}{i}{}+b
    (2) Also, from condition 的=C - \lambdai, we have }\mp@subsup{\lambda}{i}{}=0\mathrm{ , hence
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Non-SVs: }\mp@subsup{\alpha}{i}{}=
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```


## Support vector classification: Lagrangian

Now use complementary slackness:
Non-margin SVs: $\alpha_{i}=C \neq 0$ :
(1) We immediately have $1-\xi_{i}=y_{i}\left(w^{\top} x_{i}+b\right)$.
(2) Also, from condition $\alpha_{i}=C-\lambda_{i}$, we have $\lambda_{i}=0$, hence $\xi_{i}>0$.
Margin SVs: $0<\alpha_{i}<C$ :
(1) We again have $1-\xi_{i}=y_{i}\left(w^{\top} x_{i}+b\right)$
(2) This time, from $\alpha_{i}=C-\lambda_{i}$, we have $\lambda_{i} \neq 0$, hence $\xi_{i}=0$.

Non-SVs: $\alpha_{i}=0$
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(2) From $\alpha_{i}=C-\lambda_{i}$, we have $\lambda_{i} \neq 0$, hence $\xi_{i}=0$.

We observe:
(1) The solution is sparse: points which are not on the margin, or "margin errors", have $\alpha_{i}=0$
(2) The support vectors: only those points on the decision boundary, or which are margin errors, contribute.
(3) Influence of the non-margin SVs is bounded, since their weight cannot exceed $C$.

## Support vector classification: dual function

Thus, our goal is to maximize the dual,

$$
\begin{aligned}
g(\alpha, \lambda)= & \frac{1}{2}\|w\|^{2}+C \sum_{i=1}^{n} \xi_{i}+\sum_{i=1}^{n} \alpha_{i}\left(1-y_{i}\left(w^{\top} x_{i}+b\right)-\xi_{i}\right) \\
& +\sum_{i=1}^{n} \lambda_{i}\left(-\xi_{i}\right) \\
= & \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i}^{\top} x_{j}+C \sum_{i=1}^{m} \xi_{i}-\sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i}^{\top} x_{j} \\
& -b \underbrace{b \sum_{i=1}^{m} \alpha_{i} y_{i}}+\sum_{i=1}^{m} \alpha_{i}-\sum_{i=1}^{m} \alpha_{i} \xi_{i}-\sum_{i=1}^{m}\left(C-\alpha_{i}\right) \xi_{i} \\
= & \sum_{i=1}^{m} \alpha_{i}-\underbrace{\frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i}^{\top} x_{j} .}_{i=1}
\end{aligned}
$$

## Support vector classification: dual function

Maximize the dual,

$$
g(\alpha)=\sum_{i=1}^{m} \alpha_{i}-\frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i}^{\top} x_{j}
$$

subject to the constraints

$$
0 \leq \alpha_{i} \leq C, \quad \sum_{i=1}^{n} y_{i} \alpha_{i}=0
$$

This is a quadratic program.
Offset $b$ : for the margin SVs, we have $1=y_{i}\left(w^{\top} x_{i}+b\right)$. Obtain $b$ from any of these, or take an average.

## Support vector classification: kernel version



Taken from Schoelkopf and Smola (2002)

Maximum margin classifier in RKHS: write the hinge loss formulation

$$
\min _{w}\left(\frac{1}{2}\|w\|_{\mathcal{H}}^{2}+C \sum_{i=1}^{n} \theta\left(y_{i}\left\langle w, k\left(x_{i}, \cdot\right)\right\rangle_{\mathcal{H}}\right)\right)
$$

for the RKHS $\mathcal{H}$ with kernel $k(x, \cdot)$. Use the result of the representer theorem,

$$
w(\cdot)=\sum_{i=1}^{n} \beta_{i} k\left(x_{i}, \cdot\right) .
$$

Maximizing the margin equivalent to minimizing $\|w\|_{\mathcal{H}}^{2}$ : for many RKHSs a smoothness constraint (e.g. Gaussian kernel).

## Support vector classification: kernel version

Substituting and introducing the $\xi_{i}$ variables, get

$$
\begin{equation*}
\min _{w, b}\left(\frac{1}{2} \beta^{\top} K \beta+C \sum_{i=1}^{n} \xi_{i}\right) \tag{17}
\end{equation*}
$$

where the matrix $K$ has $i$, jth entry $K_{i j}=k\left(x_{i}, x_{j}\right)$, subject to

$$
\xi_{i} \geq 0 \quad y_{i} \sum_{j=1}^{n} \beta_{j} k\left(x_{i}, x_{j}\right) \geq 1-\xi_{i}
$$

Convex in $\beta$ since $K$ is positive definite: hence strong duality holds.

subject to the constraints $0 \leq \alpha_{i} \leq C$, and


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$$

Convex in $\beta$ since $K$ is positive definite: hence strong duality holds. Dual:

$$
g(\alpha)=\sum_{i=1}^{m} \alpha_{i}-\frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_{i} \alpha_{j} y_{i} y_{j} k\left(x_{i}, x_{j}\right)
$$

subject to the constraints $0 \leq \alpha_{i} \leq C$, and

$$
w(\cdot)=\sum_{i=1}^{n} y_{i} \alpha_{i} k(x, \cdot)
$$

## Support vector classification: the $\nu$-SVM

Hard to interpret $C$. Modify the formulation to get a more intuitive parameter $\nu$.
Again, we drop $b$ for simplicity. Solve

$$
\min _{w, \rho, \xi}\left(\frac{1}{2}\|w\|^{2}-\nu \rho+\frac{1}{n} \sum_{i=1}^{n} \xi_{i}\right)
$$

subject to

$$
\begin{aligned}
\rho & \geq 0 \\
\xi_{i} & \geq 0 \\
y_{i} w^{\top} x_{i} & \geq \rho-\xi_{i},
\end{aligned}
$$

(now directly adjust margin width $\rho$ ).

$$
\frac{1}{2}\|w\|_{\mathcal{H}}^{2}+\frac{1}{n} \sum_{i=1}^{n} \xi_{i}-\nu \rho+\sum_{i=1}^{n} \alpha_{i}\left(\rho-y_{i} w^{\top} x_{i}-\xi_{i}\right)+\sum_{i=1}^{n} \beta_{i}\left(-\xi_{i}\right)+\gamma(-\rho)
$$

for dual variables $\alpha_{i} \geq 0, \beta_{i} \geq 0$, and $\gamma \geq 0$.
Differentiating and setting to zero for each of the primal variables
$w, \xi, \rho$,

## From $\beta_{i} \geq 0$, equation (18) implies

$\frac{1}{2}\|w\|_{\mathcal{H}}^{2}+\frac{1}{n} \sum_{i=1}^{n} \xi_{i}-\nu \rho+\sum_{i=1}^{n} \alpha_{i}\left(\rho-y_{i} w^{\top} x_{i}-\xi_{i}\right)+\sum_{i=1}^{n} \beta_{i}\left(-\xi_{i}\right)+\gamma(-\rho)$
for dual variables $\alpha_{i} \geq 0, \beta_{i} \geq 0$, and $\gamma \geq 0$.
Differentiating and setting to zero for each of the primal variables $w, \xi, \rho$,

$$
\begin{align*}
w & =\sum_{i=1}^{n} \alpha_{i} y_{i} x_{i} \\
\alpha_{i}+\beta_{i} & =\frac{1}{n}  \tag{18}\\
\nu & =\sum_{i=1}^{n} \alpha_{i}-\gamma \tag{19}
\end{align*}
$$

From $\beta_{i} \geq 0$, equation (18) implies

$$
0 \leq \alpha_{i} \leq n^{-1}
$$

## Complementary slackness (1)

Complementary slackness conditions:
Assume $\rho>0$ at the global solution, hence $\gamma=0$, and

$$
\begin{equation*}
\sum_{i=1}^{n} \alpha_{i}=\nu \tag{20}
\end{equation*}
$$

Case of $\xi_{i}>0$ : complementary slackness states $\beta_{i}=0$, hence from (18) we have $\alpha_{i}=n^{-1}$. Denote this set as $N(\alpha)$. Then


SO

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$$
\sum_{i \in N(\alpha)} \frac{1}{n}=\sum_{i \in N(\alpha)} \alpha_{i} \leq \sum_{i=1}^{n} \alpha_{i}=\nu
$$

SO

$$
\frac{|N(\alpha)|}{n} \leq \nu
$$

and $\nu$ is an upper bound on the number of non-margin SVs.

## Complementary slackness (2)

Case of $\xi_{i}=0$ : then $\beta_{i}>0$ and so $\alpha_{i}<n^{-1}$. Denote by $M(\alpha)$ the set of points $n^{-1}>\alpha_{i}>0$. Then from (20),

$$
\nu=\sum_{i=1}^{n} \alpha_{i}=\sum_{i \in N(\alpha)} \frac{1}{n}+\sum_{i \in M(\alpha)} \alpha_{i} \leq \sum_{i \in M(\alpha) \cup N(\alpha)} \frac{1}{n},
$$

thus

$$
\nu \leq \frac{|N(\alpha)|+|M(\alpha)|}{n}
$$

and $\nu$ is a lower bound on the number of support vectors with non-zero weight (both on the margin, and "margin errors").

Substituting into the Lagrangian, we get

$$
\begin{aligned}
& \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i}^{\top} x_{j}+\frac{1}{n} \sum_{i=1}^{n} \xi_{i}-\rho \nu-\sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i}^{\top} x_{j} \\
& \quad+\sum_{i=1}^{n} \alpha_{i} \rho-\sum_{i=1}^{n} \alpha_{i} \xi_{i}-\sum_{i=1}^{n}\left(\frac{1}{n}-\alpha_{i}\right) \xi_{i}-\rho\left(\sum_{i=1}^{n} \alpha_{i}-\nu\right) \\
& =- \\
& \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i}^{\top} x_{j}
\end{aligned}
$$

Maximize:


## subject to



Substituting into the Lagrangian, we get

$$
\begin{aligned}
& \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i}^{\top} x_{j}+\frac{1}{n} \sum_{i=1}^{n} \xi_{i}-\rho \nu-\sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i}^{\top} x_{j} \\
& \quad+\sum_{i=1}^{n} \alpha_{i} \rho-\sum_{i=1}^{n} \alpha_{i} \xi_{i}-\sum_{i=1}^{n}\left(\frac{1}{n}-\alpha_{i}\right) \xi_{i}-\rho\left(\sum_{i=1}^{n} \alpha_{i}-\nu\right) \\
& =- \\
& \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i}^{\top} x_{j}
\end{aligned}
$$

Maximize:

$$
g(\alpha)=-\frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_{i} \alpha_{j} y_{i} y_{j} x_{i}^{\top} x_{j}
$$

subject to

$$
\sum_{i=1}^{n} \alpha_{i} \geq \nu \quad 0 \leq \alpha_{i} \leq \frac{1}{n}
$$

## Questions?




[^0]:    ${ }^{1}$ We denote by relint $(\mathcal{D})$ the relative interior of the set $\mathcal{D}$. This looks like the interior of the set, but is non-empty even when the set is a subspace of a

[^1]:    ${ }^{1}$ We denote by $\operatorname{relint}(\mathcal{D})$ the relative interior of the set $\mathcal{D}$. This looks like the interior of the set, but is non-empty even when the set is a subspace of a larger space.

