# Support Vector Machines 

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## Outline

- Classification
- Support vector machines
- Nonlinear features
- Overfitting and regularization
- Dual problem
- Kernel SVM
- Training problem properties


## Binary classification

- Labels $y=0$ or $y=1$ (alternatively $y=-1$ or $y=1$ )
- Training problem

$$
\underset{\theta}{\operatorname{minimize}} \sum_{i=1}^{N} L\left(m\left(x_{i} ; \theta\right), y_{i}\right)
$$

- Design loss $L$ to train model parameters $\theta$ such that:
- $m\left(x_{i} ; \theta\right)<0$ for pairs $\left(x_{i}, y_{i}\right)$ where $y_{i}=0$
- $m\left(x_{i} ; \theta\right)>0$ for pairs $\left(x_{i}, y_{i}\right)$ where $y_{i}=1$
- Predict class belonging for new data points $x$ with trained $\bar{\theta}$ :
- $m(x ; \bar{\theta})<0$ predict class $y=0$
- $m(x ; \bar{\theta})>0$ predict class $y=1$


## Binary classification - Cost functions

- Different cost functions $L$ can be used:
- $y=0$ : Small cost for $m(x ; \theta) \ll 0$ large for $m(x ; \theta) \gg 0$
- $y=1$ : Small cost for $m(x ; \theta) \gg 0$ large for $m(x ; \theta) \ll 0$



$$
L(u, y)=\log \left(1+e^{u}\right)-y u \text { (logistic loss) }
$$

## Binary classification - Cost functions

- Different cost functions $L$ can be used:
- $y=0$ : Small cost for $m(x ; \theta) \ll 0$ large for $m(x ; \theta) \gg 0$
- $y=1$ : Small cost for $m(x ; \theta) \gg 0$ large for $m(x ; \theta) \ll 0$

nonconvex (Neyman Pearson loss)


## Binary classification - Cost functions

- Different cost functions $L$ can be used:
- $y=0$ : Small cost for $m(x ; \theta) \ll 0$ large for $m(x ; \theta) \gg 0$
- $y=1$ : Small cost for $m(x ; \theta) \gg 0$ large for $m(x ; \theta) \ll 0$



$$
L(u, y)=\max (0, u)-y u
$$

## Binary classification - Cost functions

- Different cost functions $L$ can be used:
- $y=-1$ : Small cost for $m(x ; \theta) \ll 0$ large for $m(x ; \theta) \gg 0$
- $y=1$ : Small cost for $m(x ; \theta) \gg 0$ large for $m(x ; \theta) \ll 0$



$$
L(u, y)=\max (0,1-y u)(\text { hinge loss used in SVM })
$$

## Binary classification - Cost functions

- Different cost functions $L$ can be used:
- $y=-1$ : Small cost for $m(x ; \theta) \ll 0$ large for $m(x ; \theta) \gg 0$
- $y=1$ : Small cost for $m(x ; \theta) \gg 0$ large for $m(x ; \theta) \ll 0$



$$
L(u, y)=\max (0,1-y u)^{2} \text { (squared hinge loss) }
$$

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## Support vector machine

- SVM uses:
- affine parameterized model $m(x ; \theta)=w^{T} x+b$ (where $\theta=(w, b)$ )
- loss function $L(u, y)=\max (0,1-y u)$ (if labels $y=-1, y=1$ )
- Training problem, find model parameters by solving:

$$
\underset{\theta}{\operatorname{minimize}} \sum_{i=1}^{N} L\left(m\left(x_{i} ; \theta\right), y_{i}\right)=\sum_{i=1}^{N} \max \left(0,1-y_{i}\left(w^{T} x_{i}+b\right)\right)
$$

- Training problem convex in $\theta=(w, b)$ since:
- model $m(x ; \theta)$ is affine in $\theta$
- loss function $L(u, y)$ is convex in $u$




## Prediction

- Use trained model $m$ to predict label $y$ for unseen data point $x$
- Since affine model $m(x ; \theta)=w^{T} x+b$, prediction for $x$ becomes:
- If $w^{T} x+b<0$, predict corresponding label $y=-1$
- If $w^{T} x+b>0$, predict corresponding label $y=1$
- If $w^{T} x+b=0$, predict either $y=-1$ or $y=1$
- A hyperplane (decision boundary) separates class predictions:

$$
H:=\left\{x: w^{T} x+b=0\right\}
$$



## Training problem interpretation

- Every parameter choice $\theta=(w, b)$ gives hyperplane in data space:

$$
H:=\left\{x: w^{T} x+b=0\right\}=\{x: m(x ; \theta)=0\}
$$

- Training problem searches hyperplane to "best" separates classes
- Example - models with different parameters $\theta$ :



## What is "best" separation?

- The "best" separation is the one that minimizes the loss function
- Hyperplane for model $m(\cdot ; \theta)$ with parameter $\theta=\theta_{1}$ :

- Training loss:



## What is "best" separation?

- The "best" separation is the one that minimizes the loss function
- Hyperplane for model $m(\cdot ; \theta)$ with parameter $\theta=\theta_{2}$ :

- Training loss:



## What is "best" separation?

- The "best" separation is the one that minimizes the loss function
- Hyperplane for model $m(\cdot ; \theta)$ with parameter $\theta=\theta_{3}$ :

- Training loss:



## What is "best" separation?

- The "best" separation is the one that minimizes the loss function
- Hyperplane for model $m(\cdot ; \theta)$ with parameter $\theta=\theta_{4}$ :

- Training loss:



## What is "best" separation?

- The "best" separation is the one that minimizes the loss function
- Hyperplane for model $m(\cdot ; \theta)$ with parameter $\theta=\theta^{*}$ :

- Training loss:



$$
=0.0
$$

## Fully separable data - Solution

- Let $\bar{\theta}=(\bar{w}, \bar{b})$ give model that separates data:

- Let $H_{\bar{\theta}}:=\left\{x: m(x ; \bar{\theta})=\bar{w}^{T} x+\bar{b}=0\right\}$ be hyperplane separates
- Training loss:



## Fully separable data - Solution

- Also $2 \bar{\theta}=(2 \bar{w}, 2 \bar{b})$ separates data:

- Hyperplane $H_{2 \bar{\theta}}:=\left\{x: m(x ; 2 \bar{\theta})=2\left(\bar{w}^{T} x+\bar{b}\right)=0\right\}=H_{\bar{\theta}}$ same
- Training loss reduced since input $m(x ; 2 \bar{\theta})=2 m(x ; \bar{\theta})$ further out:




## Fully separable data - Solution

- And $3 \bar{\theta}=(3 \bar{w}, 3 \bar{b})$ also separates data:

- Hyperplane $H_{3 \bar{\theta}}:=\left\{x: m(x ; 3 \bar{\theta})=3\left(\bar{w}^{T} x+\bar{b}\right)=0\right\}=H_{\bar{\theta}}$ same
- Training loss further reduced since input $m(x ; 3 \bar{\theta})=3 m(x ; \bar{\theta})$ :




## Fully separable data - Solution

- And $3 \bar{\theta}=(3 \bar{w}, 3 \bar{b})$ also separates data:

- Hyperplane $H_{3 \bar{\theta}}:=\left\{x: m(x ; 3 \bar{\theta})=3\left(\bar{w}^{T} x+\bar{b}\right)=0\right\}=H_{\bar{\theta}}$ same
- Training loss


- As soon as $\left|m\left(x_{i} ; \theta\right)\right| \geq 1$ (with correct sign) for all $x_{i}$, cost is 0


## Margin classification and support vectors

- Support vector machine classifiers for separable data
- Classes separated with margin, o marks support vectors



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## Nonlinear example

- Can classify nonlinearly separable data using lifting



## Adding features

- Create feature map $\phi: \mathbb{R}^{n} \rightarrow \mathbb{R}^{p}$ of training data
- Data points $x_{i} \in \mathbb{R}^{n}$ replaced by featured data points $\phi\left(x_{i}\right) \in \mathbb{R}^{p}$
- Example: Polynomial feature map with $n=2$ and degree $d=3$

$$
\phi(x)=\left(x_{1}, x_{2}, x_{1}^{2}, x_{1} x_{2}, x_{2}^{2}, x_{1}^{3}, x_{1}^{2} x_{2}, x_{1} x_{2}^{2}, x_{2}^{3}\right)
$$

- Number of features $p+1=\binom{n+d}{d}=\frac{(n+d)!}{d!n!}$ grows fast!
- SVM training problem

$$
\underset{\theta}{\operatorname{minimize}} \sum_{i=1}^{N} \max \left(0,1-y_{i}\left(w^{T} \phi\left(x_{i}\right)+b\right)\right)
$$

still convex since features fixed

## Nonlinear example - Polynomial features

- SVM and polynomial features of degree 2



## Nonlinear example - Polynomial features

- SVM and polynomial features of degree 3



## Nonlinear example - Polynomial features

- SVM and polynomial features of degree 4



## Nonlinear example - Polynomial features

- SVM and polynomial features of degree 5



## Nonlinear example - Polynomial features

- SVM and polynomial features of degree 6



## Nonlinear example - Polynomial features

- SVM and polynomial features of degree 7



## Nonlinear example - Polynomial features

- SVM and polynomial features of degree 8



## Nonlinear example - Polynomial features

- SVM and polynomial features of degree 9



## Nonlinear example - Polynomial features

- SVM and polynomial features of degree 10



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## Overfitting and regularization

- SVM is prone to overfitting if model too expressive
- Regularization using $\|\cdot\|_{1}$ (for sparsity) or $\|\cdot\|_{2}^{2}$
- Tikhonov regularization with $\|\cdot\|_{2}^{2}$ especially important for SVM
- Regularize only linear terms $w$, not bias $b$
- Training problem with Tikhonov regularization of $w$

$$
\underset{\theta}{\operatorname{minimize}} \sum_{i=1}^{N} \max \left(0,1-y_{i}\left(w^{T} \phi\left(x_{i}\right)+b\right)\right)+\frac{\lambda}{2}\|w\|_{2}^{2}
$$

(note that features are used $\phi\left(x_{i}\right)$ )

## Nonlinear example revisited

- Regularized SVM and polynomial features of degree 6
- Regularization parameter: $\lambda=0.00001$



## Nonlinear example revisited

- Regularized SVM and polynomial features of degree 6
- Regularization parameter: $\lambda=0.00006$



## Nonlinear example revisited

- Regularized SVM and polynomial features of degree 6
- Regularization parameter: $\lambda=0.00036$



## Nonlinear example revisited

- Regularized SVM and polynomial features of degree 6
- Regularization parameter: $\lambda=0.0021$



## Nonlinear example revisited

- Regularized SVM and polynomial features of degree 6
- Regularization parameter: $\lambda=0.013$



## Nonlinear example revisited

- Regularized SVM and polynomial features of degree 6
- Regularization parameter: $\lambda=0.077$



## Nonlinear example revisited

- Regularized SVM and polynomial features of degree 6
- Regularization parameter: $\lambda=0.46$



## Nonlinear example revisited

- Regularized SVM and polynomial features of degree 6
- Regularization parameter: $\lambda=2.78$



## Nonlinear example revisited

- Regularized SVM and polynomial features of degree 6
- Regularization parameter: $\lambda=16.7$

- $\lambda$ and polynomial degree chosen using cross validation/holdout


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## SVM problem reformulation

- Consider Tikhonov regularized SVM:

$$
\underset{w, b}{\operatorname{minimize}} \sum_{i=1}^{N} \max \left(0,1-y_{i}\left(w^{T} \phi\left(x_{i}\right)+b\right)\right)+\frac{\lambda}{2}\|w\|_{2}^{2}
$$

- Derive dual from reformulation of SVM:

$$
\underset{w, b}{\operatorname{minimize}} \mathbf{1}^{T} \max \left(\mathbf{0}, \mathbf{1}-\left(X_{\phi, Y} w+Y b\right)\right)+\frac{\lambda}{2}\|w\|_{2}^{2}
$$

where max is vector valued and

$$
X_{\phi, Y}=\left[\begin{array}{c}
y_{1} \phi\left(x_{1}\right)^{T} \\
\vdots \\
y_{N} \phi\left(x_{N}\right)^{T}
\end{array}\right], \quad Y=\left[\begin{array}{c}
y_{1} \\
\vdots \\
y_{N}
\end{array}\right]
$$

## Dual problem

- Let $L=\left[X_{\phi, Y}, Y\right]$ and write problem as

$$
\underset{w, b}{\operatorname{minimize}} \underbrace{\mathbf{1}^{T} \max \left(\mathbf{0}, \mathbf{1}-\left(X_{\phi, Y} w+Y b\right)\right)}_{f(L(w, b))}+\underbrace{\frac{\lambda}{2}\|w\|_{2}^{2}}_{g(w, b)}
$$

where

- $f(\psi)=\sum_{i=1}^{N} f_{i}\left(\psi_{i}\right)$ and $f_{i}\left(\psi_{i}\right)=\max \left(0,1-\psi_{i}\right)$ (hinge loss)
- $g(w, b)=\frac{\lambda}{2}\|w\|_{2}^{2}$, i.e., does not depend on $b$
- Dual problem

$$
\underset{\nu}{\operatorname{minimize}} f^{*}(\nu)+g^{*}\left(-L^{T} \nu\right)
$$

## Conjugate of $g$

- Conjugate of $g(w, b)=\frac{\lambda}{2}\|w\|_{2}^{2}=: g_{1}(w)+g_{2}(b)$ is

$$
g^{*}\left(\mu_{w}, \mu_{b}\right)=g_{1}^{*}\left(\mu_{w}\right)+g_{2}^{*}\left(\mu_{b}\right)=\frac{1}{2 \lambda}\left\|\mu_{w}\right\|_{2}^{2}+\iota_{\{0\}}\left(\mu_{b}\right)
$$

- Evaluated at $-L^{T} \nu=-\left[X_{\phi, Y}, Y\right]^{T} \nu$ :

$$
\begin{aligned}
g^{*}\left(-L^{T} \nu\right) & =g^{*}\left(-\left[\begin{array}{c}
X_{\phi, Y}^{T} \\
Y^{T}
\end{array}\right] \nu\right)=\frac{1}{2 \lambda}\left\|-X_{\phi, Y}^{T} \nu\right\|_{2}^{2}+\iota_{\{0\}}\left(-Y^{T} \nu\right) \\
& =\frac{1}{2 \lambda} \nu^{T} X_{\phi, Y} X_{\phi, Y}^{T} \nu+\iota_{\{0\}}\left(Y^{T} \nu\right)
\end{aligned}
$$

## Conjugate of $f$

- Conjugate of $f_{i}\left(\psi_{i}\right)=\max \left(0,1-\psi_{i}\right)$ (hinge-loss):

$$
f_{i}^{*}\left(\nu_{i}\right)= \begin{cases}\nu_{i} & \text { if }-1 \leq \nu_{i} \leq 0 \\ \infty & \text { else }\end{cases}
$$

- Conjugate of $f(\psi)=\sum_{i=1}^{N} f_{i}\left(\psi_{i}\right)$ is sum of individual conjugates:

$$
f^{*}(\nu)=\sum_{i=1}^{N} f_{i}^{*}\left(\nu_{i}\right)=\mathbf{1}^{T} \nu+\iota_{[-\mathbf{1}, \mathbf{0}]}(\nu)
$$

## SVM dual

- The SVM dual is

$$
\underset{\nu}{\operatorname{minimize}} f^{*}(\nu)+g^{*}\left(-L^{T} \nu\right)
$$

- Inserting the above computed conjugates gives dual problem

$$
\begin{array}{ll}
\underset{\nu}{\operatorname{minimize}} & \sum_{i=1}^{N} \nu_{i}+\frac{1}{2 \lambda} \nu^{T} X_{\phi, Y} X_{\phi, Y}^{T} \nu \\
\text { subject to } & -\mathbf{1} \leq \nu \leq \mathbf{0} \\
& Y^{T} \nu=0
\end{array}
$$

- Since $Y \in \mathbb{R}^{N}, Y^{T} \nu=0$ is a hyperplane constraint
- If no bias term $b$; dual same but without hyperplane constraint


## Primal solution recovery

- Meaningless to solve dual if we cannot recover primal
- Necessary and sufficient primal-dual optimality conditions

$$
0 \in\left\{\begin{array}{l}
\partial f^{*}(\nu)-L(w, b) \\
\partial g^{*}\left(-L^{T} \nu\right)-(w, b)
\end{array}\right.
$$

- From dual solution $\nu$, find $(w, b)$ that satisfies both of the above
- For SVM, second condition is

$$
\partial g^{*}\left(-L^{T} \nu\right)=\left[\begin{array}{c}
\frac{1}{\lambda}\left(-X_{\phi, Y}^{T} \nu\right) \\
\partial \iota_{\{0\}}\left(-Y^{T} \nu\right)
\end{array}\right] \ni\left[\begin{array}{c}
w \\
b
\end{array}\right]
$$

which gives optimal $w=-\frac{1}{\lambda} X_{\Phi, Y}^{T} \nu$ (since unique)

- Cannot recover $b$ from this condition


## Primal solution recovery - Bias term

- Necessary and sufficient primal-dual optimality conditions

$$
0 \in\left\{\begin{array}{l}
\partial f^{*}(\nu)-L(w, b) \\
\partial g^{*}\left(-L^{T} \nu\right)-(w, b)
\end{array}\right.
$$

- For SVM, row $i$ of first condition is $0 \in \partial f_{i}^{*}\left(\nu_{i}\right)-L_{i}(w, b)$ where

$$
\partial f_{i}^{*}\left(\nu_{i}\right)=\left\{\begin{array}{ll}
{[-\infty, 1]} & \text { if } \nu_{i}=-1 \\
\{1\} & \text { if }-1<\nu_{i}<0 \\
{[1, \infty]} & \text { if } \nu_{i}=0 \\
\emptyset & \text { else }
\end{array}, \quad L_{i}=y_{i}\left[\phi\left(x_{i}\right)^{T} 1\right]\right.
$$

- Pick $i$ with $\nu_{i} \in(-1,0)$, then unique subgradient $\partial f_{i}\left(\nu_{i}\right)$ is 1 and

$$
0=1-y_{i}\left(w^{T} \phi\left(x_{i}\right)+b\right)
$$

and optimal $b$ must satisfy $b=y_{i}-w^{T} \phi\left(x_{i}\right)$ for such $i$

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## SVM dual - A reformulation

- Dual problem

$$
\begin{array}{ll}
\underset{\nu}{\operatorname{minimize}} & \sum_{i=1}^{N} \nu_{i}+\frac{1}{2 \lambda} \nu^{T} X_{\phi, Y} X_{\phi, Y}^{T} \nu \\
\text { subject to } & -\mathbf{1} \leq \nu \leq \mathbf{0} \\
& Y^{T} \nu=0
\end{array}
$$

- Let $\kappa_{i j}:=\phi\left(x_{i}\right)^{T} \phi\left(x_{j}\right)$ and rewrite quadratic term:

$$
\begin{aligned}
\nu^{T} X_{\phi, Y} X_{\phi, Y}^{T} \nu & =\nu \operatorname{diag}(Y) \\
& =\nu \operatorname{diag}(Y) \underbrace{\left[\begin{array}{c}
\phi\left(x_{1}\right)^{T} \\
\vdots \\
\phi\left(x_{N}\right)^{T}
\end{array}\right]\left[\begin{array}{lll}
\phi\left(x_{1}\right) & \cdots & \left.\phi\left(x_{N}\right)\right] \operatorname{diag}(Y) \nu \\
\kappa_{11} & \cdots & \kappa_{1 N} \\
\vdots & \ddots & \vdots \\
\kappa_{N 1} & \cdots & \kappa_{N N}
\end{array}\right]}_{K} \operatorname{diag}(Y) \nu
\end{aligned}
$$

where $K$ is called Kernel matrix

## SVM dual - Kernel formulation

- Dual problem with Kernel matrix

$$
\begin{array}{ll}
\underset{\nu}{\operatorname{minimize}} & \sum_{i=1}^{N} \nu_{i}+\frac{1}{2 \lambda} \nu^{T} \operatorname{diag}(Y) K \operatorname{diag}(Y) \nu \\
\text { subject to } & -\mathbf{1} \leq \nu \leq \mathbf{0} \\
& Y^{T} \nu=0
\end{array}
$$

- Solved without evaluating features, only scalar products:

$$
\kappa_{i j}:=\phi\left(x_{i}\right)^{T} \phi\left(x_{j}\right)
$$

## Kernel methods

- We explicitly defined features and created Kernel matrix
- We can instead create Kernel that implicitly defines features


## Kernel operators

- Define:
- Kernel operator $\kappa(x, y): \mathbb{R}^{n} \times \mathbb{R}^{n} \rightarrow \mathbb{R}$
- Kernel shortcut $\kappa_{i j}=\kappa\left(x_{i}, x_{j}\right)$
- A Kernel matrix

$$
K=\left[\begin{array}{ccc}
\kappa_{11} & \cdots & \kappa_{1 N} \\
\vdots & \ddots & \vdots \\
\kappa_{N 1} & \cdots & \kappa_{N N}
\end{array}\right]
$$

- A Kernel operator $\kappa: \mathbb{R}^{n} \times \mathbb{R}^{n} \rightarrow \mathbb{R}$ is:
- symmetric if $\kappa(x, y)=\kappa(y, x)$
- positive semidefinite (PSD) if symmetric and

$$
\sum_{i, j}^{m} a_{i} a_{j} \kappa\left(x_{i}, x_{j}\right) \geq 0
$$

for all $m \in \mathbb{N}, \alpha_{i}, \alpha_{j} \in \mathbb{R}$, and $x_{i}, x_{j} \in \mathbb{R}^{n}$

- All Kernel matrices PSD if Kernel operator PSD


## Mercer's theorem

- Assume $\kappa$ is a positive semidefinite Kernel operator
- Mercer's theorem:

There exists continuous functions $\left\{e_{j}\right\}_{j=1}^{\infty}$ and nonnegative

$$
\begin{gathered}
\left\{\lambda_{j}\right\}_{j=1}^{\infty} \text { such that } \\
\kappa(x, y)=\sum_{j=1}^{\infty} \lambda_{j} e_{j}(x) e_{j}(y)
\end{gathered}
$$

- Let $\phi(x)=\left(\sqrt{\lambda_{1}} e_{1}(x), \sqrt{\lambda_{2}} e_{2}(x), \ldots\right)$ be a feature map, then

$$
\kappa(x, y)=\langle\phi(x), \phi(y)\rangle
$$

where scalar product in $\ell_{2}$ (space of square summable sequences)

- A PSD kernel operator implicitly defines features


## Kernel SVM dual and corresponding primal

- SVM dual from Kernel $\kappa$ with Kernel matrix $K_{i j}=\kappa\left(x_{i}, x_{j}\right)$

$$
\begin{array}{ll}
\underset{\nu}{\operatorname{minimize}} & \sum_{i=1}^{N} \nu_{i}+\frac{1}{2 \lambda} \nu \operatorname{diag}(Y) K \operatorname{diag}(Y) \nu \\
\text { subject to } & -\mathbf{1} \leq \nu \leq \mathbf{0} \\
& Y^{T} \nu=0
\end{array}
$$

- Due to Mercer's theorem, this is dual to primal problem

$$
\underset{\theta}{\operatorname{minimize}} \sum_{i=1}^{N} \max \left(0,1-y_{i}\left(\left\langle w, \phi\left(x_{i}\right)\right\rangle+b\right)\right)+\frac{\lambda}{2}\|w\|^{2}
$$

with potentially an infinite number of features $\phi$ and variables $w$

## Primal recovery and class prediction

- Assume we know Kernel operator, dual solution, but not features
- Can recover: Label prediction and primal solution $b$
- Cannot recover: Primal solution $w$ (might be infinite dimensional)
- Primal solution $b=y_{i}-w^{T} \phi\left(x_{i}\right)$ :

$$
w^{T} \phi\left(x_{i}\right)=-\frac{1}{\lambda} \nu^{T} X_{\phi, Y} \phi\left(x_{i}\right)=-\frac{1}{\lambda} \nu^{T}\left[\begin{array}{c}
y_{1} \phi\left(x_{1}\right)^{T} \\
\vdots \\
y_{N} \phi\left(x_{N}\right)^{T}
\end{array}\right] \phi\left(x_{i}\right)=-\frac{1}{\lambda} \nu^{T}\left[\begin{array}{c}
y_{1} \kappa_{1 i} \\
\vdots \\
y_{N} \kappa_{N i}
\end{array}\right]
$$

- Label prediction for new data $x$ (sign of $\left.w^{T} \phi(x)+b\right)$ :

$$
w^{T} \phi(x)+b=-\frac{1}{\lambda} \nu^{T}\left[\begin{array}{c}
y_{1} \phi\left(x_{1}\right)^{T} \phi(x) \\
\vdots \\
y_{N} \phi\left(x_{N}\right)^{T} \phi(x)
\end{array}\right]+b=-\frac{1}{\lambda} \nu^{T}\left[\begin{array}{c}
y_{1} \kappa\left(x_{1}, x\right) \\
\vdots \\
y_{N} \kappa\left(x_{N}, x\right)
\end{array}\right]+b
$$

- We are really interested in label prediction, not primal solution


## Valid kernels

- Polynomial kernel of degree $d: \kappa(x, y)=\left(1+x^{T} y\right)^{d}$
- Radial basis function kernels:
- Gaussian kernel: $\kappa(x, y)=e^{-\frac{\|x-y\|_{2}^{2}}{2 \sigma^{2}}}$
- Laplacian kernel: $\kappa(x, y)=e^{-\frac{\|x-y\|_{2}}{\sigma}}$
- Bias term $b$ often not needed with Kernel methods


## Example - Laplacian Kernel

- Regularized SVM with Laplacian Kernel with $\sigma=1$
- Regularization parameter: $\lambda=0.01$



## Example - Laplacian Kernel

- Regularized SVM with Laplacian Kernel with $\sigma=1$
- Regularization parameter: $\lambda=0.035938$



## Example - Laplacian Kernel

- Regularized SVM with Laplacian Kernel with $\sigma=1$
- Regularization parameter: $\lambda=0.12915$



## Example - Laplacian Kernel

- Regularized SVM with Laplacian Kernel with $\sigma=1$
- Regularization parameter: $\lambda=0.46416$



## Example - Laplacian Kernel

- Regularized SVM with Laplacian Kernel with $\sigma=1$
- Regularization parameter: $\lambda=1.6681$



## Example - Laplacian Kernel

- Regularized SVM with Laplacian Kernel with $\sigma=1$
- Regularization parameter: $\lambda=5.9948$



## Example - Laplacian Kernel

- Regularized SVM with Laplacian Kernel with $\sigma=1$
- Regularization parameter: $\lambda=21.5443$



## Example - Laplacian Kernel

- What if there is no structure in data? (Labels are randomly set)


## Example - Laplacian Kernel

- What if there is no structure in data? (Labels are randomly set)
- Regularized SVM Laplacian Kernel, regularization parameter: $\lambda=0.01$

- Linearly separable in high dimensional feature space
- Can be prone to overfitting $\Rightarrow$ Regularize and use cross validation


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## Composite optimization - Dual SVM

Dual SVM problems

$$
\begin{array}{ll}
\underset{\nu}{\operatorname{minimize}} & \sum_{i=1}^{N} \nu_{i}+\frac{1}{2 \lambda} \nu^{T} X_{\phi, Y} X_{\phi, Y}^{T} \nu \\
\text { subject to } & -\mathbf{1} \leq \nu \leq \mathbf{0} \\
& Y^{T} \nu=0
\end{array}
$$

can be written on the form

$$
\underset{\nu}{\operatorname{minimize}} h_{1}(\nu)+h_{2}\left(-X_{\phi, Y}^{T} \nu\right)
$$

where

- $h_{1}(\nu)=\mathbf{1}^{T} \nu+\iota_{[-\mathbf{1}, \mathbf{0}]}(\nu)+\iota_{\{0\}}\left(Y^{T} \nu\right)$
- First part $\mathbf{1}^{T} \nu+\iota_{[-\mathbf{1}, \mathbf{0}]}(\nu)$ is conjugate of sum of hinge losses
- Second part $\iota_{\{0\}}\left(Y^{T} \nu\right)$ comes from that bias $b$ not regularized
- $h_{2}(\mu)=\frac{1}{2 \lambda}\|\mu\|_{2}^{2}$ is conjugate to Tikhonov regularization $\frac{\lambda}{2}\|w\|_{2}^{2}$


## Gradient and function properties

- Gradient of $\left(h_{2} \circ-X_{\phi, Y}^{T}\right)$ satisfies:

$$
\begin{aligned}
\nabla\left(h_{2} \circ-X_{\phi, Y}^{T}\right)(\nu) & =\nabla\left(\frac{1}{2 \lambda} \nu^{T} X_{\phi, Y} X_{\phi, Y}^{T} \nu\right)=\frac{1}{\lambda} X_{\phi, Y} X_{\phi, Y}^{T} \nu \\
& =\frac{1}{\lambda} \operatorname{diag}(Y) K \operatorname{diag}(Y) \nu
\end{aligned}
$$

where $K$ is Kernel matrix

- Function properties
- $h_{2}$ is convex and $\lambda^{-1}$-smooth, $h_{2} \circ-X_{\phi, Y}^{T}$ is $\frac{\left\|X_{\phi, Y}\right\|_{2}^{2}}{\lambda}$-smooth
- $h_{1}$ is convex and nondifferentiable, use prox in algorithms

