Machine Learning
(機器學習)

Lecture 11: Support Vector Machine (2)

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Roadmap

1. When Can Machines Learn?
2. Why Can Machines Learn?
3. How Can Machines Learn?
4. How Can Machines Learn Better?
5. Embedding Numerous Features: Kernel Models

Lecture 11: Support Vector Machine (2)

- Kernel Trick
- Polynomial Kernel
- Gaussian Kernel
- Comparison of Kernels
- Motivation and Primal Problem
- Dual Problem
- Messages behind Soft-Margin SVM
- Soft-Margin SVM as Regularized Model

Dual SVM Revisited

goal: SVM **without dependence on $\tilde{d}$**

half-way done:

$$\begin{aligned} \min_{\boldsymbol{\alpha}} \quad & \frac{1}{2}\boldsymbol{\alpha}^T \mathrm{Q_D} \boldsymbol{\alpha} - \mathbf{1}^T \boldsymbol{\alpha} \\ \text{subject to} \quad & \mathbf{y}^T \boldsymbol{\alpha} = 0; \\ & \alpha_n \geq 0, \text{for } n = 1, 2, \ldots, N \end{aligned}$$

- $q_{n,m} = y_n y_m \mathbf{z}_n^T \mathbf{z}_m$: inner product in $\mathbb{R}^{\tilde{d}}$
- need: $\mathbf{z}_n^T \mathbf{z}_m = \mathbf{\Phi}(\mathbf{x}_n)^T \mathbf{\Phi}(\mathbf{x}_m)$ calculated faster than $O(\tilde{d})$

can we do so?

Fast Inner Product for Φ_2

2nd order polynomial transform

$$\Phi_2(\mathbf{x}) = (1, x_1, x_2, \ldots, x_d, x_1^2, x_1x_2, \ldots, x_1x_d, x_2x_1, x_2^2, \ldots, x_2x_d, \ldots, x_d^2)$$

—include both x_1x_2 & x_2x_1 for '**simplicity**' **:-)**

$$\begin{aligned}
\Phi_2(\mathbf{x})^T\Phi_2(\mathbf{x}') &= 1 + \sum_{i=1}^{d} x_i x_i' + \sum_{i=1}^{d}\sum_{j=1}^{d} x_i x_j x_i' x_j' \\
&= 1 + \sum_{i=1}^{d} x_i x_i' + \sum_{i=1}^{d} x_i x_i' \sum_{j=1}^{d} x_j x_j' \\
&= 1 + \mathbf{x}^T\mathbf{x}' + (\mathbf{x}^T\mathbf{x}')(\mathbf{x}^T\mathbf{x}')
\end{aligned}$$

for Φ_2, transform + inner product can be carefully done in $O(d)$ instead of $O(d^2)$

Kernel: Transform + Inner Product

transform $\boldsymbol{\Phi} \Longleftrightarrow$ **kernel function**: $K_{\boldsymbol{\Phi}}(\mathbf{x}, \mathbf{x}') \equiv \boldsymbol{\Phi}(\mathbf{x})^T \boldsymbol{\Phi}(\mathbf{x}')$

$\boldsymbol{\Phi}_2 \Longleftrightarrow K_{\boldsymbol{\Phi}_2}(\mathbf{x}, \mathbf{x}') = 1 + (\mathbf{x}^T\mathbf{x}') + (\mathbf{x}^T\mathbf{x}')^2$

- quadratic coefficient $q_{n,m} = y_n y_m \mathbf{z}_n^T \mathbf{z}_m = y_n y_m K(\mathbf{x}_n, \mathbf{x}_m)$
- optimal bias b? from SV $(\mathbf{x}_s, y_s)$,

$$b = y_s - \mathbf{w}^T \mathbf{z}_s = y_s - \left(\sum_{n=1}^{N} \alpha_n y_n \mathbf{z}_n \right)^T \mathbf{z}_s = y_s - \sum_{n=1}^{N} \alpha_n y_n \Big(K(\mathbf{x}_n, \mathbf{x}_s) \Big)$$

- optimal hypothesis g_{SVM}: for test input $\mathbf{x}$,

$$g_{\text{SVM}}(\mathbf{x}) = \operatorname{sign}\left(\mathbf{w}^T \boldsymbol{\Phi}(\mathbf{x}) + b\right) = \operatorname{sign}\left(\sum_{n=1}^{N} \alpha_n y_n K(\mathbf{x}_n, \mathbf{x}) + b \right)$$

kernel trick: plug in **efficient kernel function** to avoid dependence on $\tilde{d}$

Kernel SVM with QP

Kernel Hard-Margin SVM Algorithm

1. $q_{n,m} = y_n y_m K(\mathbf{x}_n, \mathbf{x}_m)$; $\mathbf{p} = -\mathbf{1}_N$; $(\mathrm{A}, \mathbf{c})$ for equ./bound constraints
2. $\boldsymbol{\alpha} \leftarrow \mathrm{QP}(\mathrm{Q}_\mathrm{D}, \mathbf{p}, \mathrm{A}, \mathbf{c})$
3. $b \leftarrow \left(y_s - \sum_{\text{SV indices } n} \alpha_n y_n K(\mathbf{x}_n, \mathbf{x}_s) \right)$ with SV $(\mathbf{x}_s, y_s)$
4. return SVs and their α_n as well as b such that for new $\mathbf{x}$,

$$g_{\text{SVM}}(\mathbf{x}) = \text{sign}\left(\sum_{\text{SV indices } n} \alpha_n y_n K(\mathbf{x}_n, \mathbf{x}) + b \right)$$

- 1: time complexity $O(N^2) \cdot$ (kernel evaluation)
- 2: QP with N variables and $N+1$ constraints
- 3 & 4: time complexity $O(\#\text{SV}) \cdot$ (kernel evaluation)

kernel SVM:

use computational shortcut to avoid $\tilde{d}$ & predict with SV only

Questions?

General Poly-2 Kernel

$$\Phi_2(\mathbf{x}) = (1, x_1, \ldots, x_d, x_1^2, \ldots, x_d^2) \quad \Leftrightarrow \quad K_{\Phi_2}(\mathbf{x}, \mathbf{x}') = 1 + \mathbf{x}^T\mathbf{x}' + (\mathbf{x}^T\mathbf{x}')^2$$

$$\Phi_2(\mathbf{x}) = (1, \sqrt{2}x_1, \ldots, \sqrt{2}x_d, x_1^2, \ldots, x_d^2) \quad \Leftrightarrow \quad K_2(\mathbf{x}, \mathbf{x}') = 1 + 2\mathbf{x}^T\mathbf{x}' + (\mathbf{x}^T\mathbf{x}')^2$$

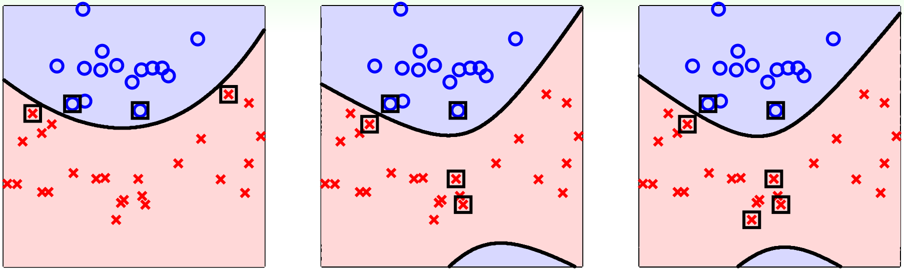
$$\Phi_2(\mathbf{x}) = (1, \sqrt{2\gamma}x_1, \ldots, \sqrt{2\gamma}x_d, \gamma x_1^2, \ldots, \gamma x_d^2)$$
$$\Leftrightarrow K_2(\mathbf{x}, \mathbf{x}') = 1 + 2\gamma\mathbf{x}^T\mathbf{x}' + \gamma^2(\mathbf{x}^T\mathbf{x}')^2$$

$$K_2(\mathbf{x}, \mathbf{x}') = (1 + \gamma\mathbf{x}^T\mathbf{x}')^2 \text{ with } \gamma > 0$$

- K_2: somewhat '**easier**' to calculate than K_{Φ_2}
- Φ_2 and Φ_2: equivalent **power**,
  different inner product $\Longrightarrow$ different **geometry**

K_2 commonly used

Poly-2 Kernels in Action



$(1 + 0.001\mathbf{x}^T\mathbf{x}')^2$ $\quad$ $1 + \mathbf{x}^T\mathbf{x}' + (\mathbf{x}^T\mathbf{x}')^2$ $\quad$ $(1 + 1000\mathbf{x}^T\mathbf{x}')^2$

- g_{SVM} **different**, $\boxed{\text{SVs}}$ **different**
  —'hard' to say which is better before learning
- change of kernel $\Leftrightarrow$ change of **margin definition**

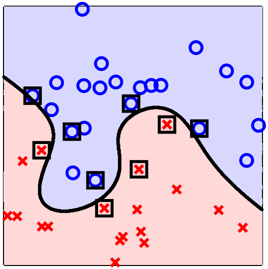
need selecting K, just like selecting $\boldsymbol{\Phi}$

General Polynomial Kernel

$$
\begin{aligned}
K_2(\mathbf{x}, \mathbf{x}') &= (\zeta + \gamma \mathbf{x}^T \mathbf{x}')^2 \text{ with } \gamma > 0, \zeta \geq 0 \\
K_3(\mathbf{x}, \mathbf{x}') &= (\zeta + \gamma \mathbf{x}^T \mathbf{x}')^3 \text{ with } \gamma > 0, \zeta \geq 0 \\
&\vdots \\
K_Q(\mathbf{x}, \mathbf{x}') &= (\zeta + \gamma \mathbf{x}^T \mathbf{x}')^Q \text{ with } \gamma > 0, \zeta \geq 0
\end{aligned}
$$

- embeds $\mathbf{\Phi}_Q$ specially with parameters (γ, ζ)
- allows computing large-margin polynomial classification without dependence on $\tilde{d}$

SVM + Polynomial Kernel: Polynomial SVM



10-th order polynomial with margin 0.1

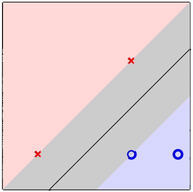
Special Case: Linear Kernel

$$K_1(\mathbf{x}, \mathbf{x}') = (0 + 1 \cdot \mathbf{x}^T\mathbf{x}')^1$$

$$\vdots$$

$$K_Q(\mathbf{x}, \mathbf{x}') = (\zeta + \gamma\mathbf{x}^T\mathbf{x}')^Q \text{ with } \gamma > 0, \zeta \geq 0$$

- K_1: just **usual inner product**, called **linear kernel**
- 'even easier': can be solved (often in primal form) **efficiently**



linear first, remember? :-)

Questions?

Kernel of Infinite Dimensional Transform

infinite dimensional $\boldsymbol{\Phi}(\mathbf{x})$? Yes, if $K(\mathbf{x}, \mathbf{x}')$ **efficiently computable**!

when $\mathbf{x} = (x)$, $K(x, x')$

$$
\begin{aligned}
K(x, x') &= \exp(-(x - x')^2) \\
&= \exp(-(x)^2)\exp(-(x')^2)\exp(2xx') \\
&\overset{\text{Taylor}}{=} \exp(-(x)^2)\exp(-(x')^2)\left(\sum_{i=0}^{\infty}\frac{(2xx')^i}{i!}\right) \\
&= \sum_{i=0}^{\infty}\left(\exp(-(x)^2)\exp(-(x')^2)\sqrt{\frac{2^i}{i!}}\sqrt{\frac{2^i}{i!}}(x)^i(x')^i\right) \\
&= \boldsymbol{\Phi}(x)^T\boldsymbol{\Phi}(x')
\end{aligned}
$$

with infinite dimensional $\boldsymbol{\Phi}(x) = \exp(-x^2) \cdot \left(1, \sqrt{\frac{2}{1!}}x, \sqrt{\frac{2^2}{2!}}x^2, \ldots\right)$

more generally, **Gaussian kernel** $K(\mathbf{x}, \mathbf{x}') = \exp\left(-\gamma\|\mathbf{x} - \mathbf{x}'\|^2\right)$ with $\gamma > 0$

Hypothesis of Gaussian SVM

Gaussian kernel $K(\mathbf{x}, \mathbf{x}') = \exp\left(-\gamma\|\mathbf{x} - \mathbf{x}'\|^2\right)$

$$
\begin{aligned}
g_{\mathrm{SVM}}(\mathbf{x}) &= \mathrm{sign}\left(\sum_{\mathrm{SV}} \alpha_n y_n K(\mathbf{x}_n, \mathbf{x}) + b\right) \\
&= \mathrm{sign}\left(\sum_{\mathrm{SV}} \alpha_n y_n \exp\left(-\gamma\|\mathbf{x} - \mathbf{x}_n\|^2\right) + b\right)
\end{aligned}
$$

- linear combination of Gaussians centered at SVs $\mathbf{x}_n$
- also called Radial Basis Function (RBF) kernel

Gaussian SVM:
find α_n to combine Gaussians centered at $\mathbf{x}_n$
& achieve large margin in infinite-dim. space

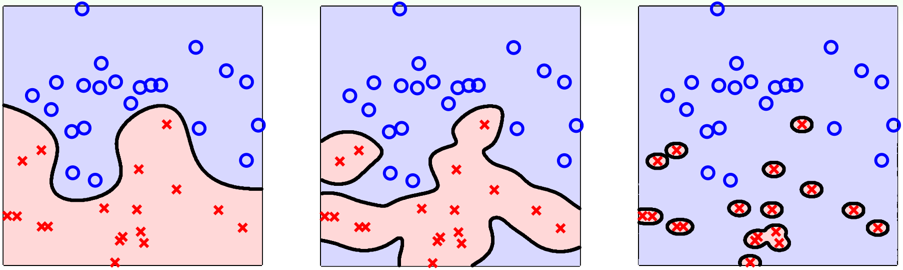
Support Vector Mechanism

	large-margin **hyperplanes** **+ higher-order transforms** with **kernel trick**
#	**not many**
boundary	**sophisticated**

- transformed vector $\mathbf{z} = \mathbf{\Phi}(\mathbf{x}) \Longrightarrow$ efficient kernel $K(\mathbf{x}, \mathbf{x}')$
- store optimal $\mathbf{w} \Longrightarrow$ store a few SVs and α_n

new possibility by Gaussian SVM:
infinite-dimensional linear classification, with generalization 'guarded by' large-margin **:-)**

Gaussian SVM in Action



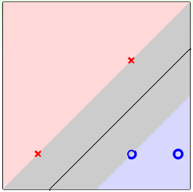
$\exp(-1\|\mathbf{x}-\mathbf{x}'\|^2)$ $\exp(-10\|\mathbf{x}-\mathbf{x}'\|^2)$ $\exp(-100\|\mathbf{x}-\mathbf{x}'\|^2)$

- large $\gamma \Longrightarrow$ sharp Gaussians $\Longrightarrow$ 'overfit'?
- **warning: SVM can still overfit :-(**

Gaussian SVM: need careful selection of γ

Questions?

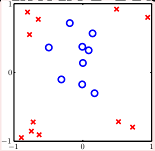
Linear Kernel: Cons and Pros



$$K(\mathbf{x}, \mathbf{x}') = \mathbf{x}^T \mathbf{x}'$$

Cons

- restricted
  —**not always separable?!**

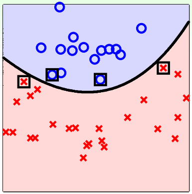


Pros

- safe—**linear first, remember? :-)**
- fast—with **special QP solver** in primal
- very explainable—**w and SVs** say something

linear kernel: an important **basic** tool

Polynomial Kernel: Cons and Pros



$$K(\mathbf{x}, \mathbf{x}') = (\zeta + \gamma \mathbf{x}^T \mathbf{x}')^Q$$

Cons

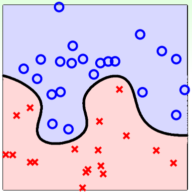
- **numerical difficulty** for large Q
  - $|\zeta + \gamma \mathbf{x}^T \mathbf{x}'| < 1$: $K \to 0$
  - $|\zeta + \gamma \mathbf{x}^T \mathbf{x}'| > 1$: $K \to$ big
- three parameters (γ, ζ, Q) —**more difficult to select**

Pros

- **less restricted** than linear
- strong physical control —'knows' **degree Q**

polynomial kernel: perhaps **small-Q only**
—sometimes efficiently done by **linear on $\boldsymbol{\Phi}_Q(\mathbf{x})$**

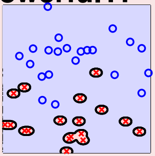
Gaussian Kernel: Cons and Pros



$$K(\mathbf{x}, \mathbf{x}') = \exp(-\gamma\|\mathbf{x}-\mathbf{x}'\|^2)$$

Cons

- **mysterious**—no **w**
- **slower** than linear
- **too powerful?!**



Pros

- **more powerful than linear/poly.**
- bounded—**less numerical difficulty than poly.**
- one parameter only—**easier to select than poly.**

Gaussian kernel: **one of most popular** but shall **be used with care**

Other Valid Kernels

- kernel represents **special** similarity: $\boldsymbol{\Phi}(\mathbf{x})^T\boldsymbol{\Phi}(\mathbf{x}')$
- any similarity $\Longrightarrow$ valid kernel? **not really**
- necessary **& sufficient** conditions for valid kernel: **Mercer's condition**
  - symmetric
  - let $k_{ij} = K(\mathbf{x}_i, \mathbf{x}_j)$, the matrix K

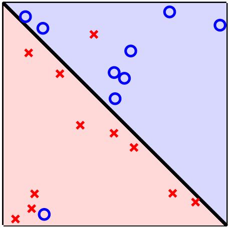
$$
\begin{aligned}
&= \begin{bmatrix} \boldsymbol{\Phi}(\mathbf{x}_1)^T\boldsymbol{\Phi}(\mathbf{x}_1) & \boldsymbol{\Phi}(\mathbf{x}_1)^T\boldsymbol{\Phi}(\mathbf{x}_2) & \ldots & \boldsymbol{\Phi}(\mathbf{x}_1)^T\boldsymbol{\Phi}(\mathbf{x}_N) \\ \boldsymbol{\Phi}(\mathbf{x}_2)^T\boldsymbol{\Phi}(\mathbf{x}_1) & \boldsymbol{\Phi}(\mathbf{x}_2)^T\boldsymbol{\Phi}(\mathbf{x}_2) & \ldots & \boldsymbol{\Phi}(\mathbf{x}_2)^T\boldsymbol{\Phi}(\mathbf{x}_N) \\ \ldots & \ldots & \ldots & \ldots \\ \boldsymbol{\Phi}(\mathbf{x}_N)^T\boldsymbol{\Phi}(\mathbf{x}_1) & \boldsymbol{\Phi}(\mathbf{x}_N)^T\boldsymbol{\Phi}(\mathbf{x}_2) & \ldots & \boldsymbol{\Phi}(\mathbf{x}_N)^T\boldsymbol{\Phi}(\mathbf{x}_N) \end{bmatrix} \\
&= \begin{bmatrix} \mathbf{z}_1 & \mathbf{z}_2 & \ldots & \mathbf{z}_N \end{bmatrix}^T \begin{bmatrix} \mathbf{z}_1 & \mathbf{z}_2 & \ldots & \mathbf{z}_N \end{bmatrix} \\
&= \mathrm{Z}\mathrm{Z}^T \text{ must **always** be **positive semi-definite**}
\end{aligned}
$$

define your own kernel: possible, **but hard**

Questions?

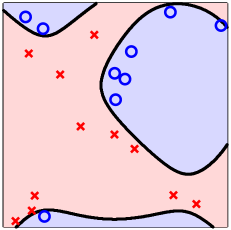
Cons of Hard-Margin SVM

recall: SVM can still overfit :-(



$\mathbf{\Phi}_1$

- part of reasons: $\mathbf{\Phi}$
- other part: **separable**



$\mathbf{\Phi}_4$

if always insisting on **separable** ($\Longrightarrow$ **shatter**), have power to **overfit to noise**

Give Up on Some Examples

want: **give up** on some noisy examples

min.-error perceptron

$$\min_{b,\mathbf{w}} \sum_{n=1}^{N} [\![y_n \neq \text{sign}(\mathbf{w}^T\mathbf{z}_n + b)]\!]$$

hard-margin SVM

$$\min_{b,\mathbf{w}} \frac{1}{2}\mathbf{w}^T\mathbf{w}$$

$$\text{s.t.} \quad y_n(\mathbf{w}^T\mathbf{z}_n + b) \geq 1 \text{ for all } n$$

combination:

$$\min_{b,\mathbf{w}} \frac{1}{2}\mathbf{w}^T\mathbf{w} + C \cdot \sum_{n=1}^{N} [\![y_n \neq \text{sign}(\mathbf{w}^T\mathbf{z}_n + b)]\!]$$

$$\text{s.t.} \quad y_n(\mathbf{w}^T\mathbf{z}_n + b) \geq 1 \text{ for } \textbf{correct } n$$

$$y_n(\mathbf{w}^T\mathbf{z}_n + b) \geq -\infty \text{ for } \textbf{incorrect } n$$

C: trade-off of large margin & noise tolerance

Soft-Margin SVM (1/2)

$$\min_{b,\mathbf{w}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w} + C \cdot \sum_{n=1}^{N} [\![y_n \neq \text{sign}(\mathbf{w}^T\mathbf{z}_n + b)]\!]$$

$$\text{s.t.} \quad y_n(\mathbf{w}^T\mathbf{z}_n + b) \geq 1 - \infty \cdot [\![y_n \neq \text{sign}(\mathbf{w}^T\mathbf{z}_n + b)]\!]$$

- $[\![\cdot]\!]$: non-linear, **not QP anymore :-(**
  —what about dual? kernel?
- cannot distinguish **small error** (slightly away from fat boundary) or **large error** (a...w...a...y... from fat boundary)

- record '**margin violation**' by ξ_n—**linear constraints**
- penalize with **margin violation** instead of **error count**
  —**quadratic objective**

soft-margin SVM: $$\min_{b,\mathbf{w},\boldsymbol{\xi}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w} + C \cdot \sum_{n=1}^{N} \xi_n$$

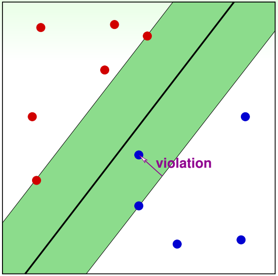
$$\text{s.t.} \quad y_n(\mathbf{w}^T\mathbf{z}_n + b) \geq 1 - \xi_n \text{ and } \xi_n \geq 0 \text{ for all } n$$

Soft-Margin SVM (2/2)

- record '**margin violation**' by ξ_n
- penalize with **margin violation**

$$\min_{b,\mathbf{w},\boldsymbol{\xi}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w} + C \cdot \sum_{n=1}^{N} \xi_n$$

$$\text{s.t.} \quad y_n(\mathbf{w}^T\mathbf{z}_n + b) \geq 1 - \xi_n \text{ and } \xi_n \geq 0 \text{ for all } n$$



- parameter C: trade-off of large margin & margin violation
  - large C: want less margin violation
  - small C: want large margin
- QP of $\tilde{d} + 1 + N$ variables, $2N$ constraints

next: remove dependence on $\tilde{d}$ by soft-margin SVM primal $\Rightarrow$ **dual**?

Questions?

Lagrange Dual

primal: $$\min_{b,\mathbf{w},\boldsymbol{\xi}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w} + C \cdot \sum_{n=1}^{N} \xi_n$$

s.t. $y_n(\mathbf{w}^T\mathbf{z}_n + b) \geq 1 - \xi_n$ and $\xi_n \geq 0$ for all n

Lagrange function with Lagrange multipliers α_n and β_n

$$\mathcal{L}(b, \mathbf{w}, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = \frac{1}{2}\mathbf{w}^T\mathbf{w} + C \cdot \sum_{n=1}^{N} \xi_n + \sum_{n=1}^{N} \alpha_n \cdot \left(1 - \xi_n - y_n(\mathbf{w}^T\mathbf{z}_n + b)\right) + \sum_{n=1}^{N} \beta_n \cdot (-\xi_n)$$

want: Lagrange dual

$$\max_{\alpha_n \geq 0,\ \beta_n \geq 0} \left(\min_{b,\mathbf{w},\boldsymbol{\xi}} \quad \mathcal{L}(b, \mathbf{w}, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta}) \right)$$

Simplify ξ_n and β_n

$$\max_{\alpha_n \geq 0,\ \beta_n \geq 0} \left(\min_{b, \mathbf{w}, \boldsymbol{\xi}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w} + C \cdot \sum_{n=1}^{N} \xi_n + \sum_{n=1}^{N} \alpha_n \cdot (1 - \xi_n - y_n(\mathbf{w}^T\mathbf{z}_n + b)) + \sum_{n=1}^{N} \beta_n \cdot (-\xi_n) \right)$$

- $\frac{\partial \mathcal{L}}{\partial \xi_n} = 0 = C - \alpha_n - \beta_n$
- no loss of optimality if solving with implicit constraint $\beta_n = C - \alpha_n$ and explicit constraint $0 \leq \alpha_n \leq C$: β_n removed

ξ can also be removed :-), like how we removed b

$$\max_{0 \leq \alpha_n \leq C,\ \beta_n = C - \alpha_n} \left(\min_{b, \mathbf{w}, \xi} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w} + \sum_{n=1}^{N} \alpha_n (1 - y_n(\mathbf{w}^T\mathbf{z}_n + b)) \cancel{+ \sum_{n=1}^{N} (C - \alpha_n - \beta_n) \cdot \xi_n} \right)$$

Other Simplifications

$$\max_{0 \le \alpha_n \le C,\ \beta_n = C - \alpha_n} \left(\min_{b,\mathbf{w}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w} + \sum_{n=1}^{N} \alpha_n (1 - y_n(\mathbf{w}^T\mathbf{z}_n + b)) \right)$$

familiar? :-)

- inner problem **same as hard-margin SVM**
- $\frac{\partial \mathcal{L}}{\partial b} = 0$: no loss of optimality if solving with constraint $\sum_{n=1}^{N} \alpha_n y_n = 0$
- $\frac{\partial \mathcal{L}}{\partial w_i} = 0$: no loss of optimality if solving with constraint $\mathbf{w} = \sum_{n=1}^{N} \alpha_n y_n \mathbf{z}_n$

standard dual can be derived
using the same steps as Lecture 10

Standard Soft-Margin SVM Dual

$$\min_{\boldsymbol{\alpha}} \quad \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m \mathbf{z}_n^T \mathbf{z}_m - \sum_{n=1}^{N} \alpha_n$$

$$\text{subject to} \quad \sum_{n=1}^{N} y_n \alpha_n = 0;$$

$$0 \le \alpha_n \le C, \text{ for } n = 1, 2, \ldots, N;$$

$$\text{implicitly} \quad \mathbf{w} = \sum_{n=1}^{N} \alpha_n y_n \mathbf{z}_n;$$

$$\beta_n = C - \alpha_n, \text{ for } n = 1, 2, \ldots, N$$

—only difference to hard-margin: upper bound on α_n

another (convex) **QP**,
with N variables & $2N + 1$ constraints

Questions?

Kernel Soft-Margin SVM

Kernel Soft-Margin SVM Algorithm

1. $q_{n,m} = y_n y_m K(\mathbf{x}_n, \mathbf{x}_m)$; $\mathbf{p} = -\mathbf{1}_N$; $(\mathrm{A}, \mathbf{c})$ for equ./lower-bound/**upper-bound** constraints
2. $\alpha \leftarrow \mathrm{QP}(\mathrm{Q_D}, \mathbf{p}, \mathrm{A}, \mathbf{c})$
3. $b \leftarrow ?$
4. return SVs and their α_n as well as b such that for new $\mathbf{x}$,

$$g_{\mathrm{SVM}}(\mathbf{x}) = \mathrm{sign}\left(\sum_{\text{SV indices } n} \alpha_n y_n K(\mathbf{x}_n, \mathbf{x}) + b \right)$$

- almost the same as hard-margin
- more flexible than hard-margin —**primal/dual always solvable**

remaining question: step 3?

Solving for b

hard-margin SVM

complementary slackness:

$$\alpha_n(1 - y_n(\mathbf{w}^T\mathbf{z}_n + b)) = 0$$

- SV ($\alpha_s > 0$)
  $\Rightarrow b = y_s - \mathbf{w}^T\mathbf{z}_s$

soft-margin SVM

complementary slackness:

$$\alpha_n(1 - \xi_n - y_n(\mathbf{w}^T\mathbf{z}_n + b)) = 0$$

$$(C - \alpha_n)\xi_n = 0$$

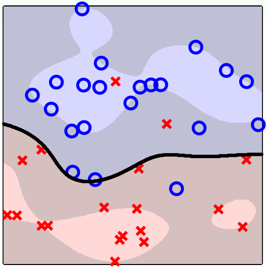
- SV ($\alpha_s > 0$)
  $\Rightarrow b = y_s - y_s\xi_s - \mathbf{w}^T\mathbf{z}_s$
- free ($\alpha_s < C$)
  $\Rightarrow \xi_s = 0$

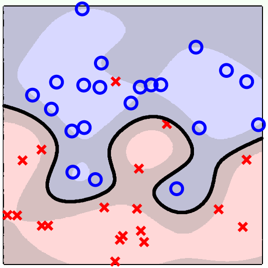
solve unique b with free SV $(\mathbf{x}_s, y_s)$:

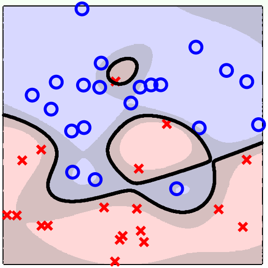
$$b = y_s - \sum_{\text{SV indices } n} \alpha_n y_n K(\mathbf{x}_n, \mathbf{x}_s)$$

—range of b otherwise

Soft-Margin Gaussian SVM in Action







$C = 1$ $C = 10$ $C = 100$

- large $C \Longrightarrow$ less noise tolerance $\Longrightarrow$ 'overfit'?
- **warning: SVM can still overfit :-(**

soft-margin Gaussian SVM:
need careful selection of (γ, C)

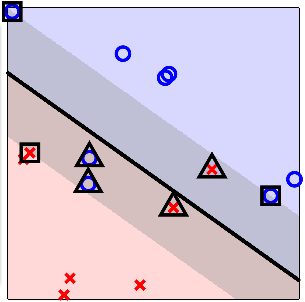
Physical Meaning of α_n

complementary slackness:

$$\alpha_n(1-\xi_n - y_n(\mathbf{w}^T\mathbf{z}_n + b)) = 0$$

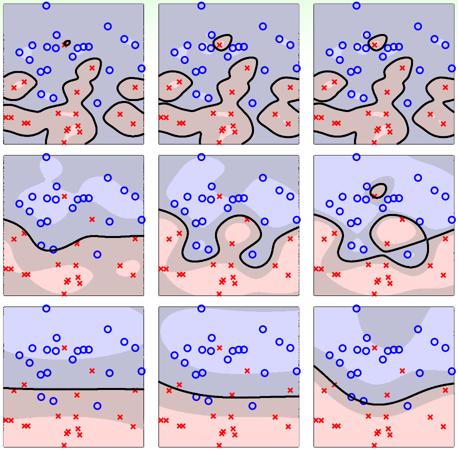
$$(C - \alpha_n)\xi_n = 0$$

- non SV ($0 = \alpha_n$): $\xi_n = 0$, 'away from'/on fat boundary
- $\square$ free SV ($0 < \alpha_n < C$): $\xi_n = 0$, on fat boundary, locates b
- $\triangle$ bounded SV ($\alpha_n = C$): $\xi_n =$ violation amount, 'violate'/on fat boundary



α_n can be used for **data analysis**

Practical Need: Model Selection



- complicated even for (C, γ) **of Gaussian SVM**
- more combinations if including other kernels or parameters

how to select? **validation :-)**

Questions?

Wrap-Up

Hard-Margin Primal

$$\min_{b,\mathbf{w}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w}$$
$$\text{s.t.} \quad y_n(\mathbf{w}^T\mathbf{z}_n + b) \geq 1$$

Soft-Margin Primal

$$\min_{b,\mathbf{w},\boldsymbol{\xi}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{n=1}^{N}\xi_n$$
$$\text{s.t.} \quad y_n(\mathbf{w}^T\mathbf{z}_n + b) \geq 1 - \xi_n, \xi_n \geq 0$$

Hard-Margin Dual

$$\min_{\boldsymbol{\alpha}} \quad \frac{1}{2}\boldsymbol{\alpha}^T\mathrm{Q}\boldsymbol{\alpha} - \mathbf{1}^T\boldsymbol{\alpha}$$
$$\text{s.t.} \quad \mathbf{y}^T\boldsymbol{\alpha} = 0$$
$$0 \leq \alpha_n$$

Soft-Margin Dual

$$\min_{\boldsymbol{\alpha}} \quad \frac{1}{2}\boldsymbol{\alpha}^T\mathrm{Q}\boldsymbol{\alpha} - \mathbf{1}^T\boldsymbol{\alpha}$$
$$\text{s.t.} \quad \mathbf{y}^T\boldsymbol{\alpha} = 0$$
$$0 \leq \alpha_n \leq C$$

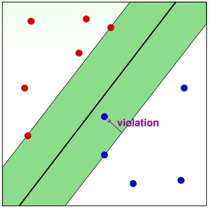
soft-margin preferred in practice;
linear: LIBLINEAR; non-linear: LIBSVM

Slack Variables ξ_n

- record '**margin violation**' by ξ_n
- penalize with **margin violation**

$$\min_{b,\mathbf{w},\boldsymbol{\xi}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w} + C \cdot \sum_{n=1}^{N} \xi_n$$

$$\text{s.t.} \quad y_n(\mathbf{w}^T\mathbf{z}_n + b) \geq 1 - \xi_n \text{ and } \xi_n \geq 0 \text{ for all } n$$



on any $(b, \mathbf{w})$, $\xi_n =$ **margin violation** $= \max\big(1 - y_n(\mathbf{w}^T\mathbf{z}_n + b), 0\big)$

- $(\mathbf{x}_n, y_n)$ violating margin: $\xi_n = 1 - y_n(\mathbf{w}^T\mathbf{z}_n + b)$
- $(\mathbf{x}_n, y_n)$ not violating margin: $\xi_n = 0$

'unconstrained' form of soft-margin SVM:

$$\min_{b,\mathbf{w}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w} + C \sum_{n=1}^{N} \max\big(1 - y_n(\mathbf{w}^T\mathbf{z}_n + b), 0\big)$$

Unconstrained Form

$$\min_{b,\mathbf{w}} \quad \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{n=1}^{N} \max\left(1 - y_n(\mathbf{w}^T\mathbf{z}_n + b), 0\right)$$

familiar? :-)

$$\min \quad \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum \widehat{\mathrm{err}}$$

just L2 regularization

$$\min \quad \frac{\lambda}{N}\mathbf{w}^T\mathbf{w} + \frac{1}{N}\sum \mathrm{err}$$

with shorter $\mathbf{w}$, another parameter, and special err

why not solve this? :-)

- not QP, **no (?) kernel trick**
- $\max(\cdot, 0)$ **not differentiable**, harder to solve

SVM as Regularized Model

	minimize	constraint
regularization by constraint	E_{in}	$\mathbf{w}^T\mathbf{w} \leq C$
hard-margin SVM	$\mathbf{w}^T\mathbf{w}$	$E_{\text{in}} = 0$ [and more]
L2 regularization	$\frac{\lambda}{N}\mathbf{w}^T\mathbf{w} + E_{\text{in}}$	
soft-margin SVM	$\frac{1}{2}\mathbf{w}^T\mathbf{w} + CN\widehat{E_{\text{in}}}$	

large margin $\Longleftrightarrow$ fewer hyperplanes $\Longleftrightarrow$ L2 regularization of short $\mathbf{w}$

soft margin $\Longleftrightarrow$ special $\widehat{\text{err}}$

larger C or C $\Longleftrightarrow$ smaller λ $\Longleftrightarrow$ less regularization

viewing SVM as regularized model:

allows **extending/connecting** to other learning models

Questions?

Summary

1 Embedding Numerous Features: Kernel Models

Lecture 11: Support Vector Machine (2)

- Kernel Trick
  kernel as shortcut of transform + inner product
- Polynomial Kernel
  embeds specially-scaled polynomial transform
- Gaussian Kernel
  embeds infinite dimensional transform
- Comparison of Kernels
  linear for efficiency or Gaussian for power
- Motivation and Primal Problem
  add margin violations ξ_n
- Dual Problem
  upper-bound α_n by C
- Messages behind Soft-Margin SVM
  bounded/free SVs for data analysis
- Soft-Margin SVM as Regularized Model
  L2-regularization with hinge error measure