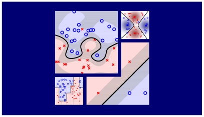
Machine Learning Techniques
(機器學習技法)



Lecture 5: Kernel Logistic Regression

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Roadmap

1. Embedding Numerous Features: Kernel Models

Lecture 4: Soft-Margin Support Vector Machine

allow some **margin violations** ξ_n while penalizing them by C; equivalent to **upper-bounding** α_n by C

Lecture 5: Kernel Logistic Regression

- Soft-Margin SVM as Regularized Model
- SVM versus Logistic Regression
- SVM for Soft Binary Classification
- Kernel Logistic Regression

2. Combining Predictive Features: Aggregation Models
3. Distilling Implicit Features: Extraction Models

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

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

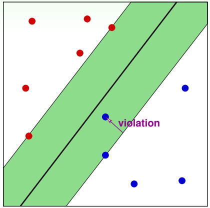
soft-margin preferred in practice;
linear: LIBLINEAR; non-linear: LIBSVM

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 $(b, \mathbf{w})$, ξ_n = **margin violation** $= \max\left(1 - y_n(\mathbf{w}^T\mathbf{z}_n + b), 0\right)$

- $(\mathbf{x}_n, y_n)$ 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:

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

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? :-)

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

just L2 regularization

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

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}	$\mathbf{w}^T\mathbf{w} \le C$
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

Fun Time

When viewing soft-margin SVM as regularized model, a larger C corresponds to

1. a larger λ, that is, stronger regularization
2. a smaller λ, that is, stronger regularization
3. a larger λ, that is, weaker regularization
4. a smaller λ, that is, weaker regularization

Fun Time

When viewing soft-margin SVM as regularized model, a larger C corresponds to

1. a larger λ, that is, stronger regularization
2. a smaller λ, that is, stronger regularization
3. a larger λ, that is, weaker regularization
4. a smaller λ, that is, weaker regularization

Reference Answer: 4

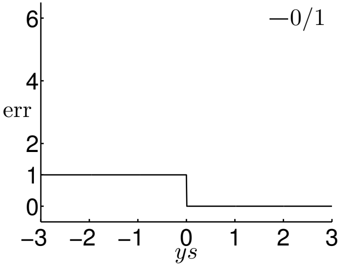
Comparing the formulations on page 4 of the slides, we see that C corresponds to $\frac{1}{2\lambda}$. So larger C corresponds to smaller λ, which surely means weaker regularization.

Algorithmic Error Measure of SVM

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

linear score $s = \mathbf{w}^T\mathbf{z}_n + b$

- $\mathrm{err}_{0/1}(s, y) = [\![ys \le 0]\!]$
- $\widehat{\mathrm{err}}_{\mathrm{SVM}}(s, y) = \max(1 - ys, 0)$: upper bound of $\mathrm{err}_{0/1}$ —often called **hinge error measure**



$\widehat{\mathrm{err}}_{\mathrm{SVM}}$: **algorithmic error measure**
by **convex upper bound** of $\mathrm{err}_{0/1}$

Algorithmic Error Measure of SVM

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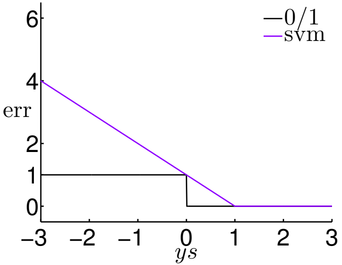
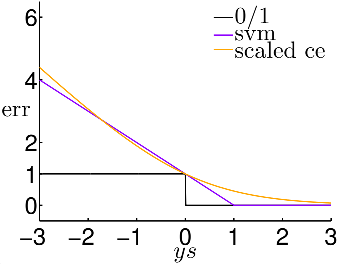


$\widehat{\mathrm{err}}_{\mathrm{SVM}}$: **algorithmic error measure**
by **convex upper bound** of $\mathrm{err}_{0/1}$

Connection between SVM and Logistic Regression

linear score $s = \mathbf{w}^T \mathbf{z}_n + b$

- $\text{err}_{0/1}(s, y) = [\![ys \le 0]\!]$
- $\widehat{\text{err}}_{\text{SVM}}(s, y) = \max(1 - ys, 0)$: upper bound of $\text{err}_{0/1}$
- $\text{err}_{\text{SCE}}(s, y) = \log_2(1 + \exp(-ys))$: another upper bound of $\text{err}_{0/1}$ used in **logistic regression**



$-\infty$	$\longleftarrow$	ys	$\longrightarrow$	$+\infty$
$\approx -ys$		$\widehat{\text{err}}_{\text{SVM}}(s, y)$		$= 0$
$\approx -ys$		$(\ln 2) \cdot \text{err}_{\text{SCE}}(s, y)$		≈ 0

SVM $\approx$ L2-regularized **logistic regression**

Linear Models for Binary Classification

PLA	soft-margin SVM	regularized logistic regression for classification
minimize $\mathrm{err}_{0/1}$ specially	minimize regularized $\widehat{\mathrm{err}}_{\mathrm{SVM}}$ by QP	minimize regularized $\mathrm{err}_{\mathrm{SCE}}$ by GD/SGD/...
• pros: **efficient if lin. separable**	• pros: **'easy' optimization** & theoretical guarantee	• pros: **'easy' optimization** & regularization guard
• cons: works only if lin. separable, otherwise needing **pocket**	• cons: loose bound of $\mathrm{err}_{0/1}$ for very negative *ys*	• cons: loose bound of $\mathrm{err}_{0/1}$ for very negative *ys*

regularized LogReg $\Longrightarrow$ approximate SVM

SVM $\Longrightarrow$ approximate LogReg (?)

Fun Time

We know that $\widehat{\mathrm{err}}_{\mathsf{SVM}}(s, y)$ is an upper bound of $\mathrm{err}_{0/1}(s, y)$. When is the upper bound tight? That is, when is $\widehat{\mathrm{err}}_{\mathsf{SVM}}(s, y) = \mathrm{err}_{0/1}(s, y)$?

1. $ys \geq 0$
2. $ys \leq 0$
3. $ys \geq 1$
4. $ys \leq 1$

Fun Time

We know that $\widehat{\text{err}}_{\text{SVM}}(s, y)$ is an upper bound of $\text{err}_{0/1}(s, y)$. When is the upper bound tight? That is, when is $\widehat{\text{err}}_{\text{SVM}}(s, y) = \text{err}_{0/1}(s, y)$?

1. $ys \geq 0$
2. $ys \leq 0$
3. $ys \geq 1$
4. $ys \leq 1$

Reference Answer: 3

By plotting the figure, we can easily see that $\widehat{\text{err}}_{\text{SVM}}(s, y) = \text{err}_{0/1}(s, y)$ if and only if $ys \geq 1$. In that case, both error functions evaluate to 0.

SVM for Soft Binary Classification

Naïve Idea 1

1. run SVM and get $(b_{\text{SVM}}, \mathbf{w}_{\text{SVM}})$
2. return $g(\mathbf{x}) = \theta(\mathbf{w}_{\text{SVM}}^T \mathbf{x} + b_{\text{SVM}})$

- 'direct' use of similarity —works reasonably well
- **no LogReg flavor**

Naïve Idea 2

1. run SVM and get $(b_{\text{SVM}}, \mathbf{w}_{\text{SVM}})$
2. run LogReg with $(b_{\text{SVM}}, \mathbf{w}_{\text{SVM}})$ as $\mathbf{w}_0$
3. return LogReg solution as $g(\mathbf{x})$

- not really 'easier' than original LogReg
- **SVM flavor (kernel?) lost**

want: flavors from both sides

A Possible Model: Two-Level Learning

$$g(\mathbf{x}) = \theta(A \cdot (\mathbf{w}_{\text{SVM}}^T \mathbf{\Phi}(\mathbf{x}) + b_{\text{SVM}}) + B)$$

- **SVM flavor**: fix hyperplane direction by $\mathbf{w}_{\text{SVM}}$—**kernel** applies
- **LogReg flavor**: fine-tune hyperplane to match maximum likelihood by scaling (A) and shifting (B)
  - often $A > 0$ if $\mathbf{w}_{\text{SVM}}$ reasonably good
  - often $B \approx 0$ if b_{SVM} reasonably good

new LogReg Problem:

$$\min_{A,B} \quad \frac{1}{N}\sum_{n=1}^{N} \log\left(1 + \exp\left(-y_n\left(A \cdot \underbrace{(\mathbf{w}_{\text{SVM}}^T \mathbf{\Phi}(\mathbf{x}_n) + b_{\text{SVM}}}_{\mathbf{\Phi}_{\text{SVM}}(\mathbf{x}_n)}) + B\right)\right)\right)$$

two-level learning:
LogReg on SVM-transformed data

Probabilistic SVM

Platt's Model of Probabilistic SVM for Soft Binary Classification

1. run **SVM** on $\mathcal{D}$ to get $(b_{\text{SVM}}, \mathbf{w}_{\text{SVM}})$ [or the equivalent α], and transform $\mathcal{D}$ to $\mathbf{z}'_n = \mathbf{w}_{\text{SVM}}^T \mathbf{\Phi}(\mathbf{x}_n) + b_{\text{SVM}}$
   —actual model performs this step in a more complicated manner
2. run **LogReg** on $\{(\mathbf{z}'_n, y_n)\}_{n=1}^N$ to get (A, B)
   —actual model adds some special regularization here
3. return $g(\mathbf{x}) = \theta(A \cdot (\mathbf{w}_{\text{SVM}}^T \mathbf{\Phi}(\mathbf{x}) + b_{\text{SVM}}) + B)$

- **soft binary classifier** not having the same boundary as **SVM classifier**
  —because of B
- how to solve **LogReg**: GD/SGD/**or better**
  —because only **two variables**

kernel SVM $\Longrightarrow$ approx. LogReg in $\mathcal{Z}$-space
exact LogReg in $\mathcal{Z}$-space?

Fun Time

Recall that the score $\mathbf{w}_{\text{SVM}}^T \mathbf{\Phi}(\mathbf{x}) + b_{\text{SVM}} = \sum_{\text{SV}} \alpha_n y_n K(\mathbf{x}_n, \mathbf{x}) + b_{\text{SVM}}$ for the kernel SVM. When coupling the kernel SVM with (A, B) to form a probabilistic SVM, which of the following is the resulting $g(\mathbf{x})$?

1. $\theta\left(\sum_{\text{SV}} B\alpha_n y_n K(\mathbf{x}_n, \mathbf{x}) + b_{\text{SVM}}\right)$
2. $\theta\left(\sum_{\text{SV}} B\alpha_n y_n K(\mathbf{x}_n, \mathbf{x}) + Bb_{\text{SVM}} + A\right)$
3. $\theta\left(\sum_{\text{SV}} A\alpha_n y_n K(\mathbf{x}_n, \mathbf{x}) + b_{\text{SVM}}\right)$
4. $\theta\left(\sum_{\text{SV}} A\alpha_n y_n K(\mathbf{x}_n, \mathbf{x}) + Ab_{\text{SVM}} + B\right)$

Fun Time

Recall that the score $\mathbf{w}_{\text{SVM}}^T \mathbf{\Phi}(\mathbf{x}) + b_{\text{SVM}} = \sum_{\text{SV}} \alpha_n y_n K(\mathbf{x}_n, \mathbf{x}) + b_{\text{SVM}}$ for the kernel SVM. When coupling the kernel SVM with (A, B) to form a probabilistic SVM, which of the following is the resulting $g(\mathbf{x})$?

1. $\theta\left(\sum_{\text{SV}} B\alpha_n y_n K(\mathbf{x}_n, \mathbf{x}) + b_{\text{SVM}}\right)$
2. $\theta\left(\sum_{\text{SV}} B\alpha_n y_n K(\mathbf{x}_n, \mathbf{x}) + Bb_{\text{SVM}} + A\right)$
3. $\theta\left(\sum_{\text{SV}} A\alpha_n y_n K(\mathbf{x}_n, \mathbf{x}) + b_{\text{SVM}}\right)$
4. $\theta\left(\sum_{\text{SV}} A\alpha_n y_n K(\mathbf{x}_n, \mathbf{x}) + Ab_{\text{SVM}} + B\right)$

Reference Answer: 4

We can simply plug the kernel formula of the score into $g(\mathbf{x})$.

Key behind Kernel Trick

one key behind kernel trick: optimal $\mathbf{w}_* = \sum_{n=1}^{N} \beta_n \mathbf{z}_n$

because $\mathbf{w}_*^T \mathbf{z} = \sum_{n=1}^{N} \beta_n \mathbf{z}_n^T \mathbf{z} = \sum_{n=1}^{N} \beta_n K(\mathbf{x}_n, \mathbf{x})$

SVM

$$\mathbf{w}_{\text{SVM}} = \sum_{n=1}^{N} (\alpha_n y_n) \mathbf{z}_n$$

α_n from **dual solutions**

PLA

$$\mathbf{w}_{\text{PLA}} = \sum_{n=1}^{N} (\alpha_n y_n) \mathbf{z}_n$$

α_n by **# mistake corrections**

LogReg by SGD

$$\mathbf{w}_{\text{LOGREG}} = \sum_{n=1}^{N} (\alpha_n y_n) \mathbf{z}_n$$

α_n by **total SGD moves**

when can **optimal $\mathbf{w}_*$** be **represented** by $\mathbf{z}_n$?

Representer Theorem

claim: for any L2-regularized linear model

$$\min_{\mathbf{w}} \quad \frac{\lambda}{N}\mathbf{w}^T\mathbf{w} + \frac{1}{N}\sum_{n=1}^{N} \mathrm{err}(y_n, \mathbf{w}^T\mathbf{z}_n)$$

optimal $\mathbf{w}_* = \sum_{n=1}^{N} \beta_n \mathbf{z}_n$.

- let optimal $\mathbf{w}_* = \mathbf{w}_\parallel + \mathbf{w}_\perp$, where $\mathbf{w}_\parallel \in \mathrm{span}(\mathbf{z}_n)$ & $\mathbf{w}_\perp \perp \mathrm{span}(\mathbf{z}_n)$ —want $\mathbf{w}_\perp = \mathbf{0}$
- what if **not?** Consider $\mathbf{w}_\parallel$
  - of same err as $\mathbf{w}_*$: $\mathrm{err}(y_n, \mathbf{w}_*^T\mathbf{z}_n) = \mathrm{err}(y_n, (\mathbf{w}_\parallel + \mathbf{w}_\perp)^T\mathbf{z}_n)$
  - of smaller regularizer as $\mathbf{w}_*$: $\mathbf{w}_*^T\mathbf{w}_* = \mathbf{w}_\parallel^T\mathbf{w}_\parallel + 2\mathbf{w}_\parallel^T\mathbf{w}_\perp + \mathbf{w}_\perp^T\mathbf{w}_\perp \quad > \quad \mathbf{w}_\parallel^T\mathbf{w}_\parallel$

—$\mathbf{w}_\parallel$ **'more optimal'** than $\mathbf{w}_*$ **(contradiction!)**

any L2-regularized linear model
can be **kernelized**!

Kernel Logistic Regression

solving L2-regularized logistic regression

$$\min_{\mathbf{w}} \quad \frac{\lambda}{N}\mathbf{w}^T\mathbf{w} + \frac{1}{N}\sum_{n=1}^{N}\log\left(1+\exp\left(-y_n\mathbf{w}^T\mathbf{z}_n\right)\right)$$

yields optimal solution $\mathbf{w}_* = \sum_{n=1}^{N} \beta_n \mathbf{z}_n$

with out loss of generality, can solve for optimal $\boldsymbol{\beta}$ instead of $\mathbf{w}$

$$\min_{\boldsymbol{\beta}} \frac{\lambda}{N}\sum_{n=1}^{N}\sum_{m=1}^{N}\beta_n\beta_m K(\mathbf{x}_n,\mathbf{x}_m) + \frac{1}{N}\sum_{n=1}^{N}\log\left(1+\exp\left(-y_n\sum_{m=1}^{N}\beta_m K(\mathbf{x}_m,\mathbf{x}_n)\right)\right)$$

—how? GD/SGD/... for **unconstrained optimization**

kernel logistic regression:
use **representer theorem** for kernel trick
on **L2-regularized logistic regression**

Kernel Logistic Regression (KLR) : Another View

$$\min_{\boldsymbol{\beta}} \frac{\lambda}{N} \sum_{n=1}^{N} \sum_{m=1}^{N} \beta_n \beta_m K(\mathbf{x}_n, \mathbf{x}_m) + \frac{1}{N} \sum_{n=1}^{N} \log \left(1 + \exp \left(-y_n \sum_{m=1}^{N} \beta_m K(\mathbf{x}_m, \mathbf{x}_n)\right)\right)$$

- $\sum_{m=1}^{N} \beta_m K(\mathbf{x}_m, \mathbf{x}_n)$: inner product between variables $\boldsymbol{\beta}$ and transformed data $(K(\mathbf{x}_1, \mathbf{x}_n), K(\mathbf{x}_2, \mathbf{x}_n), \ldots, K(\mathbf{x}_N, \mathbf{x}_n))$
- $\sum_{n=1}^{N} \sum_{m=1}^{N} \beta_n \beta_m K(\mathbf{x}_n, \mathbf{x}_m)$: a special regularizer $\boldsymbol{\beta}^T \mathrm{K} \boldsymbol{\beta}$
- KLR = linear model of $\boldsymbol{\beta}$
  with kernel as transform & kernel regularizer;
  = linear model of $\mathbf{w}$
  with embedded-in-kernel transform & L2 regularizer
- similar for SVM

warning: unlike coefficients α_n in SVM,
coefficients β_n in KLR often non-zero!

Fun Time

When viewing KLR as linear model of β with embedded-in-kernel transform & kernel regularizer, what is the dimension of the $\mathcal{Z}$ space that the linear model operates on?

1. d, the dimension of the original $\mathcal{X}$ space
2. N, the number of training examples
3. $\tilde{d}$, the dimension of some feature transform $\mathbf{\Phi}(\mathbf{x})$ that is embedded within the kernel
4. λ, the regularization parameter

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3. $\tilde{d}$, the dimension of some feature transform $\mathbf{\Phi}(\mathbf{x})$ that is embedded within the kernel
4. λ, the regularization parameter

Reference Answer: 2

For any $\mathbf{x}$, the transformed data is $(K(\mathbf{x}_1, \mathbf{x}), K(\mathbf{x}_2, \mathbf{x}), \ldots, K(\mathbf{x}_N, \mathbf{x}))$, which is N-dimensional.

Summary

1. Embedding Numerous Features: Kernel Models

Lecture 5: Kernel Logistic Regression

- Soft-Margin SVM as Regularized Model
  L2-regularization with hinge error measure
- SVM versus Logistic Regression
  $\approx$ **L2-regularized logistic regression**
- SVM for Soft Binary Classification
  common approach: two-level learning
- Kernel Logistic Regression
  representer theorem on L2-regularized LogReg

- **next: kernel models for regression**

2. Combining Predictive Features: Aggregation Models
3. Distilling Implicit Features: Extraction Models