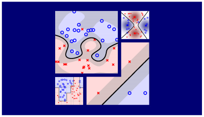
Machine Learning Techniques
(機器學習技法)



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

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

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

Wrap-Up

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Hard-Margin Dual

$$\min_{\boldsymbol{\alpha}} \quad \frac{1}{2}\boldsymbol{\alpha}^T \mathrm{Q}\boldsymbol{\alpha} - \mathbf{1}^T\boldsymbol{\alpha}$$

$$\text{s.t.} \quad \mathbf{y}^T\boldsymbol{\alpha} = 0$$

$$0 \leq \alpha_n$$

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

Slack Variables ξ_n

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

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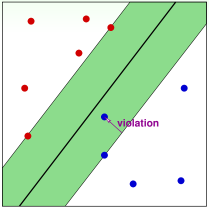

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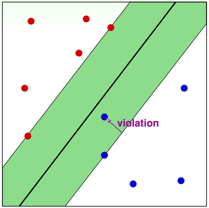

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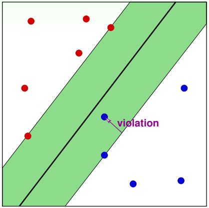

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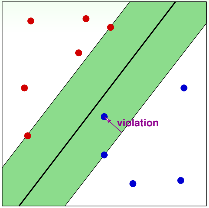

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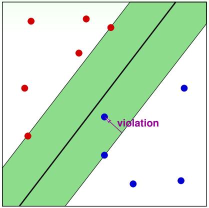

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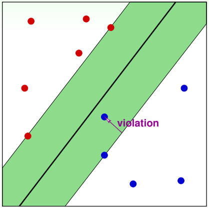

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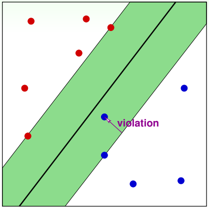

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'unconstrained' form of soft-margin SVM:

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

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just L2 regularization

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

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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]

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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

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2. a smaller λ, that is, stronger regularization
3. a larger λ, that is, weaker regularization
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Reference Answer: ④

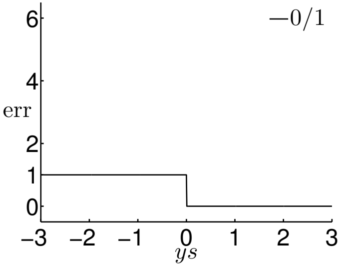
Comparing the formulations on page 4 of the slides, we see that *C* corresponds to $\frac{1}{2\lambda}$. So larger *C* corresponds to smaller λ, which surely means weaker regularization.

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

- $\text{err}_{0/1}(s, y) = [\![ys \le 0]\!]$



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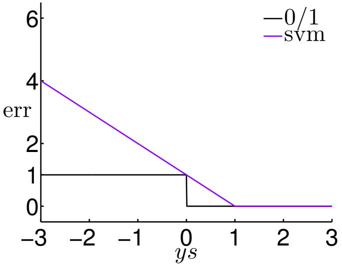

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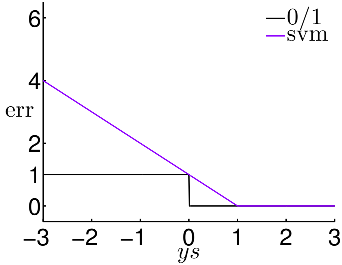

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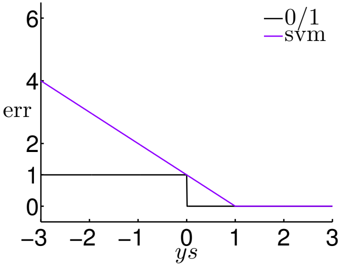

$\widehat{\text{err}}_{\text{SVM}}$: **algorithmic error measure**
by **convex upper bound** of $\text{err}_{0/1}$

Connection between SVM and Logistic Regression

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

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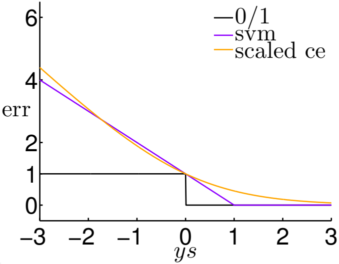
- $\text{err}_{\text{SCE}}(s, y) = \log_2(1 + \exp(-ys))$: another upper bound of $\text{err}_{0/1}$ used in **logistic regression**



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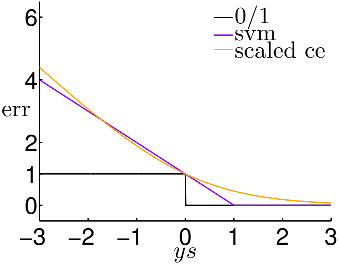

$-\infty \quad \longleftarrow \quad ys \quad \longrightarrow \quad +\infty$

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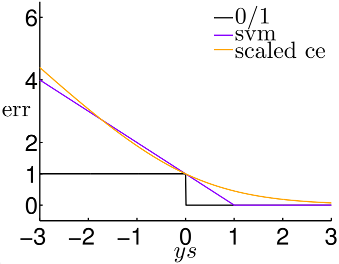

$-\infty \quad \longleftarrow \quad ys \quad \longrightarrow \quad +\infty$

$\widehat{\text{err}}_{\text{SVM}}(s, y)$

Connection between SVM and Logistic Regression

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

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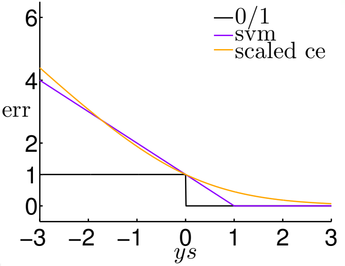

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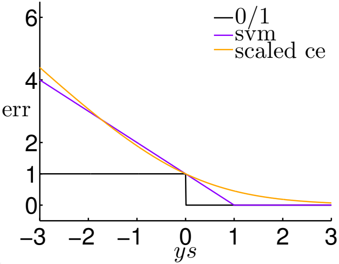

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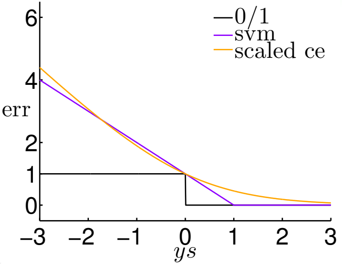

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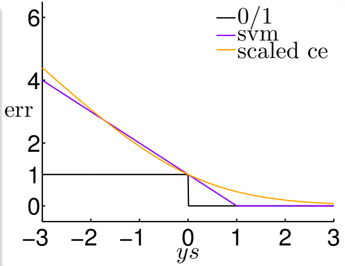

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SVM $\approx$ L2-regularized **logistic regression**

Linear Models for Binary Classification

PLA

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SVM $\Longrightarrow$ approximate LogReg (?)

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 $\widehat{\text{err}}_{\text{SVM}}(s, y) = \text{err}_{0/1}(s, y)$?

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2. $ys \leq 0$
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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.

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Naïve Idea 1

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want: flavors from both sides

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two-level learning:
LogReg on SVM-transformed data

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Platt's Model of Probabilistic SVM for Soft Binary Classification

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

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

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SVM

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

α_n from **dual solutions**

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

Representer Theorem

claim: for any L2-regularized linear model

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

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

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

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—how?

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

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

Kernel Logistic Regression (KLR) : Another View

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

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- $\sum_{m=1}^{N} \beta_m K(\mathbf{x}_m, \mathbf{x}_n)$: inner product between variables $\boldsymbol{\beta}$ and transformed data $(K(\mathbf{x}_1, \mathbf{x}_n), K(\mathbf{x}_2, \mathbf{x}_n), \ldots, K(\mathbf{x}_N, \mathbf{x}_n))$

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- $\sum_{n=1}^{N} \sum_{m=1}^{N} \beta_n \beta_m K(\mathbf{x}_n, \mathbf{x}_m)$: a special regularizer $\boldsymbol{\beta}^T \mathrm{K} \boldsymbol{\beta}$

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- KLR = linear model of $\boldsymbol{\beta}$
  with kernel as transform & kernel regularizer;

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  = linear model of $\mathbf{w}$
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- similar for SVM

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

Fun Time

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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