Kernel Logistic Regression

这篇笔记开始介绍SVM的一些实际应用，本篇是对于logistic regression的改进

一、SVM as Regularization Model

Recap:

Wrap-Up

Hard-Margin Primal

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

Soft-Margin Primal

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

Hard-Margin Dual

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

Soft-Margin Dual

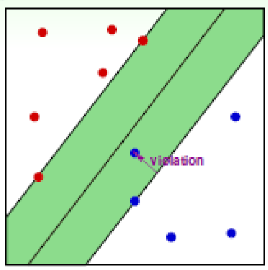
$$\min_{\alpha} \quad \frac{1}{2}\alpha^T Q\alpha - \mathbf{1}^T\alpha$$
$$\text{s.t.} \quad \mathbf{y}^T\alpha = 0$$
$$0 \le \alpha_n \le C$$

对于松弛变量ξ_n的解释

Slack Variables ξ_n

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

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



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

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

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

我们就得到了ξ_n的公式：

$$\xi_n = \max(1 - y_n(w^T)z_n + b, 0) \tag{1}$$

由此观之，SVM项可以看作是regularization项，这就得到了SVM Loss

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

我们总结一下各种regularization：

其中L2 regularization是对regularization constraint的一种改进：

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

C越大，正则化的程度就越小！

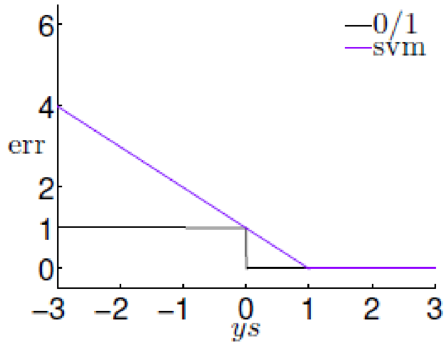
二、SVM and Logistic Regression

对比0/1 loss 和 SVM loss：

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

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 $\mathrm{err}_{0/1}$

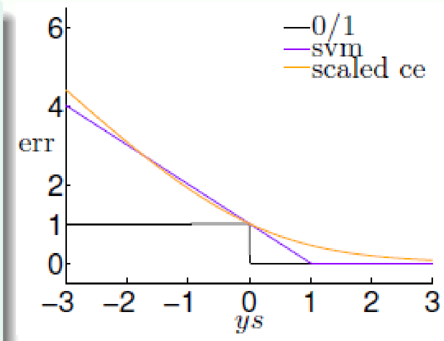
注意一个结论：如果loss function 是0/1-loss的 upper bound，那么就可以优化该loss-function来进行操作

利用SVM-Loss的regression叫做：hinge regression

引入logistic regression里面的loss function

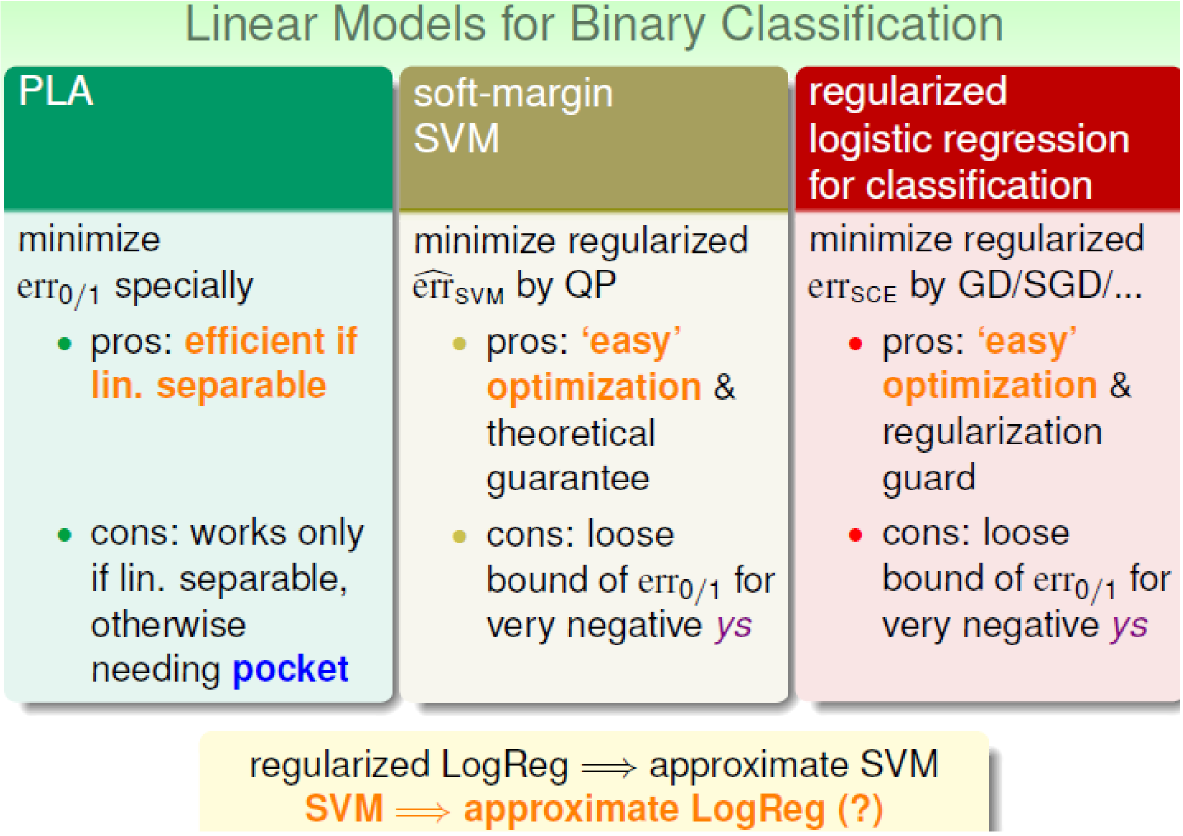
linear score $s = \mathbf{w}^T\mathbf{z}_n + b$

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



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

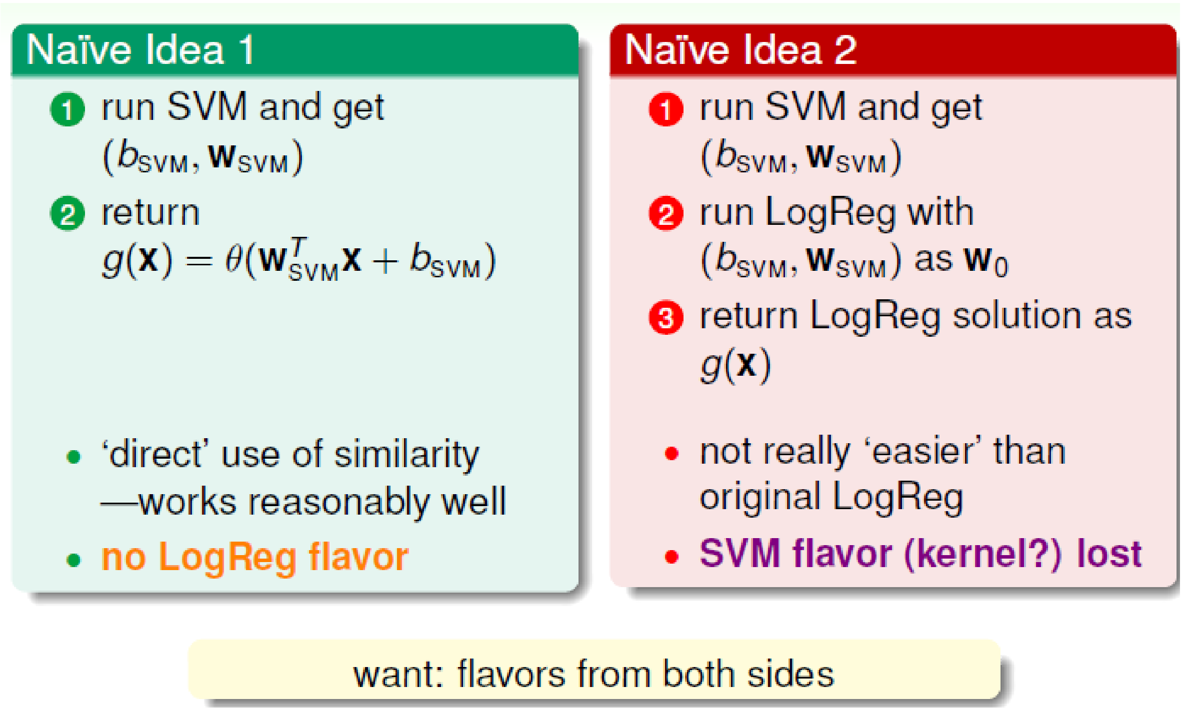
对比三者，发现SVM-Loss 和 L2-regularized logistic regression类似！



对比一下,$y_s \geq 1$的时候hinge和0/1一样

三、SVM 用作 binary classification

1. naive idea： 直接拿SVM-loss来代替logistic regression 或者 把SVM的结果作为gradient descent的初始解



2. 融合两个模型进行一步操作：

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:

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

two-level learning:
LogReg on SVM-transformed data

我们就有一个新的SVM模型了

3. 我们总结一下流程: Patt's Model

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?

做的比较好的时候，一般A>0,B≈0

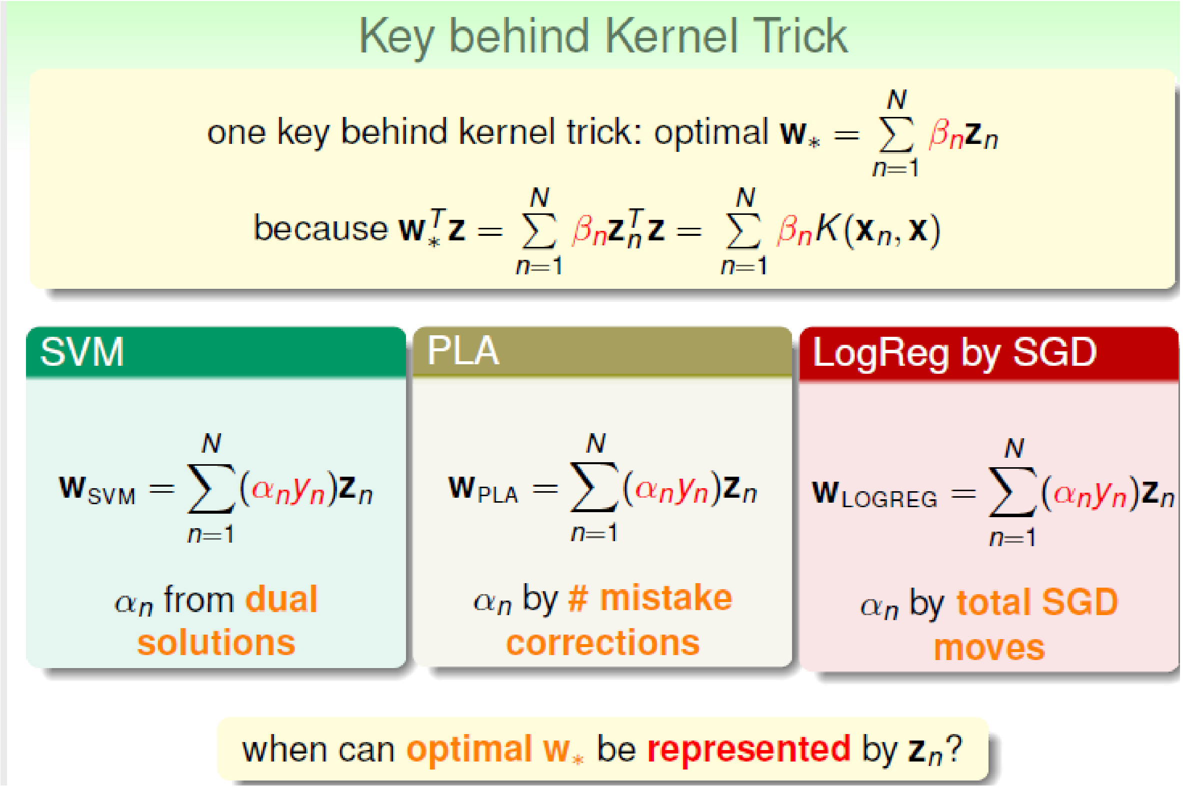
4. 存在的问题:

没有办法直接在 $z - space$里面找到自己想要的解!

四、Kernel Logistic Regression

1. Recap:

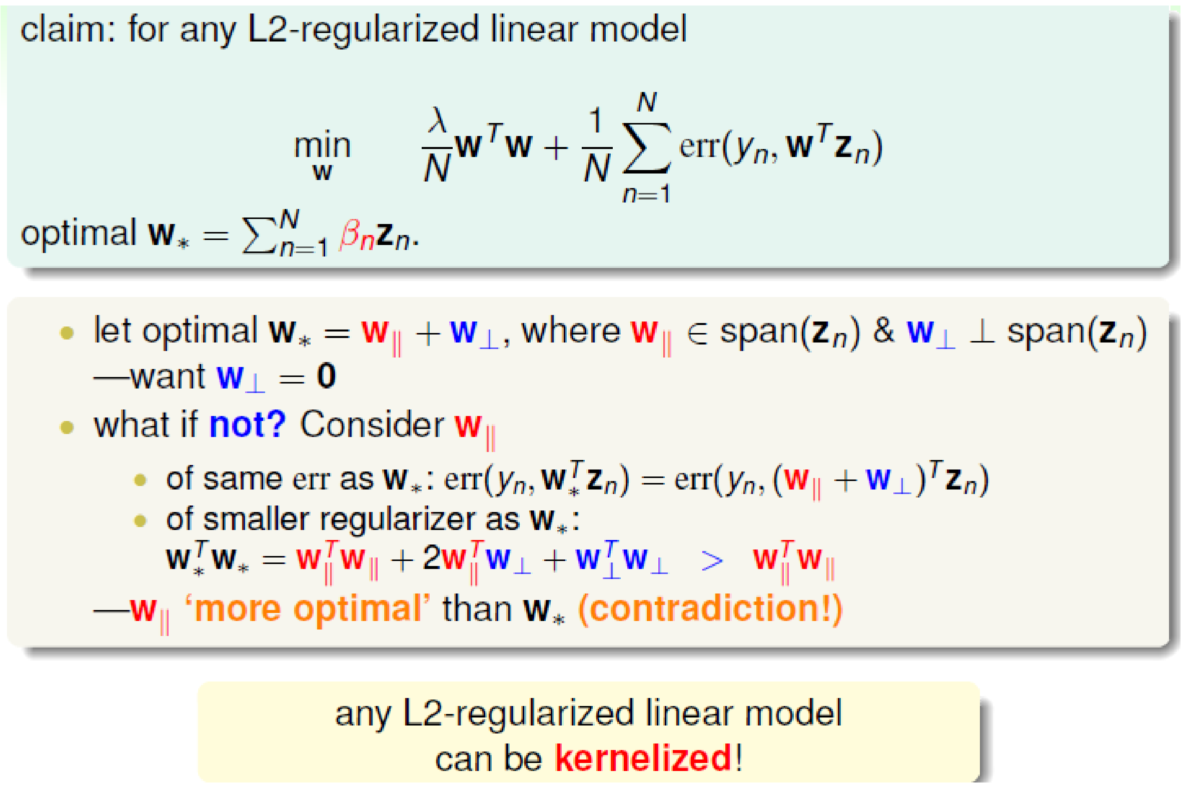
   我们可以使用kernel trick的一个原因是因为W可以表示成关于Z的一个线性组合，进而我们算出来的score就是关于Z的一个内积。



Key: W是Z的线性组合!

模型的系数是模型的本质差异

2. Representer Theorem: 表示定理



L2正则化的模型，我们最优的结果W一定都是关于Z的一个线性组合

2. KLR：

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 β instead of $\mathbf{w}$

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

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

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

我们利用结论，把关于w的最佳化问题转化成了关于β的最佳化问题。我们有如下的结论：

Kernel Logistic Regression　*Kernel Logistic Regression*

Kernel Logistic Regression (KLR) : Another View

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

- $\sum_{m=1}^{N}\beta_m K(\mathbf{x}_m,\mathbf{x}_n)$: inner product between variables β 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 $\beta^T\mathrm{K}\beta$
- KLR = linear model of β
  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!