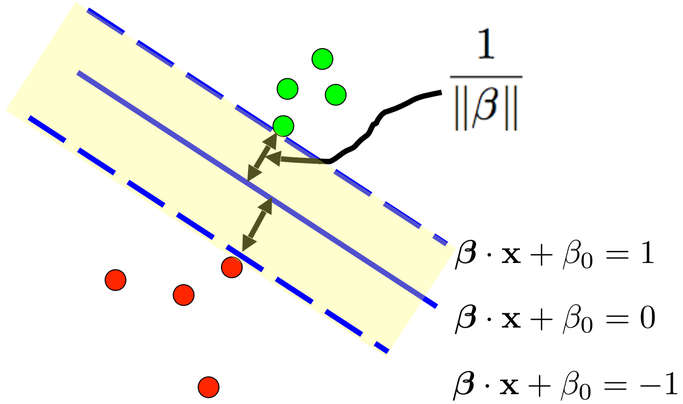
Hard Margin

Linear SVM for Separable Data

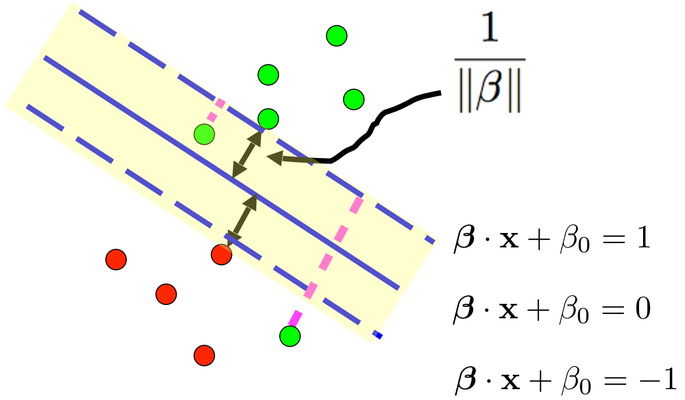


Kernel Machine

Nonlinear SVM for Separable/Non-separable Data

Soft Margin

Linear SVM for Non-separable/Separable Data



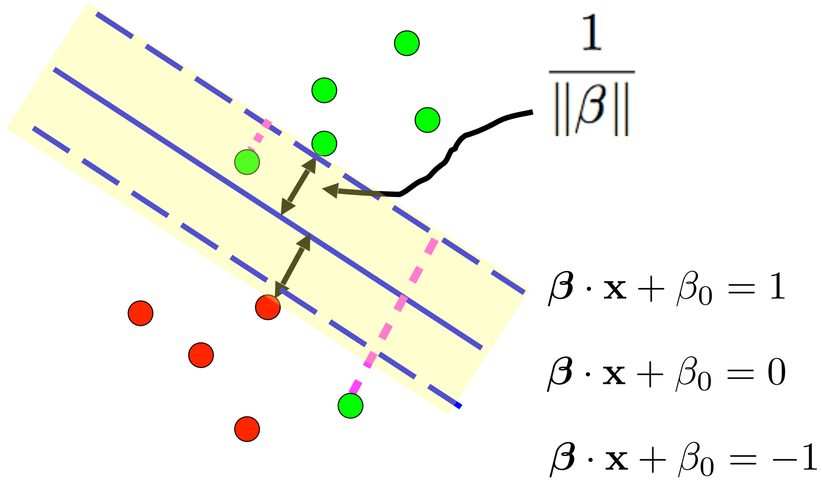
1. Formulate the **Primal** Problem (dim = p+1)
2. Solve the **Dual** Problem (dim = n)
3. **KKT Conditions** link the two sets of solutions
4. **SV**: data points on the dashed lines or on the wrong side of the datelines

Some Practical Issues

1. Binary decision to probability
2. Multiclass SVM

Some Practical Issues

1. From binary decision to probability



Run a logistic regression wrt f(x_i).

$$f(\mathbf{x}) = \boldsymbol{\beta} \cdot \mathbf{x} + \beta_0$$

Some Practical Issues

Consider MNIST Data

- **One-vs-all** Fit 10 SVMs
- **One-vs-one** Fit 45 SVMs

Can we formulate the concept of margin as some kind of area/volume of the ball (or some kind of convex region) that separate the K classes? Not a fan of this idea.

2. Multi-Class SVM

Recall how logistic regression and QDA/LDA/ NB handle multi-class?

Vanilla extension to multiclass

- **One-vs-all**
- **One-vs-one**

Formulate a multi-class SVM

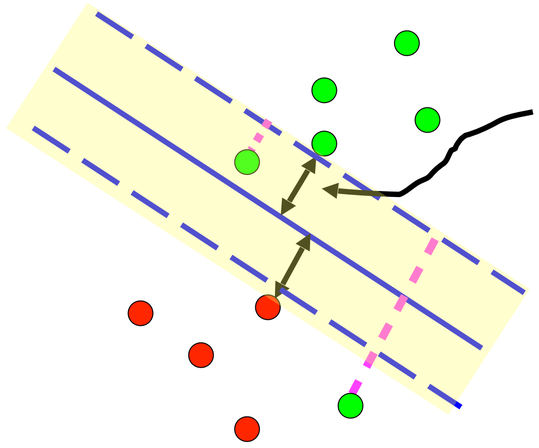
$$\min_{\boldsymbol{\beta},\beta_0,\xi_{1:n}} \frac{1}{2}\|\boldsymbol{\beta}\|^2 + \gamma \sum \xi_i$$
$$\text{subj to } y_i(\mathbf{x}_i \cdot \boldsymbol{\beta} + \beta_0) \geq 1 - \xi_i,$$
$$\xi_i \geq 0$$

$$f_k(\mathbf{x}) = \boldsymbol{\beta}_k \cdot \mathbf{x} + \beta_{k0}$$

$$\min_{\boldsymbol{\beta},\beta_0,\xi_{1:n}} \frac{1}{2}\sum_{k=1}^{K}\|\boldsymbol{\beta}_k\|^2 + \gamma \sum \xi_i$$
$$\text{subj to } f_{y_i}(\mathbf{x}_i) - f_y(\mathbf{x}_i) \geq 1 - \xi_i,$$
$$\xi_i \geq 0$$

Some Practical Issues

1. From binary decision to probability



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Linear SVM

Primal

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$$\text{subj to } y_i(\mathbf{x}_i \cdot \boldsymbol{\beta} + \beta_0) \geq 1 - \xi_i,$$

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Dual

$$\max_{\lambda_{1:n}} \quad \sum \lambda_i - \frac{1}{2} \sum_{i,j} \lambda_i \lambda_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j)$$

$$\text{subj to } \sum \lambda_i y_i = 0, \ \gamma \geq \lambda_i \geq 0$$

Prediction

$$\text{sign}\Big(\sum_{i \in N_s} \lambda_i y_i (\mathbf{x}_i \cdot \mathbf{x}_*) + \hat{\beta}_0\Big)$$

Note that we **do not need to compute beta's**. In practice, we just need to solve for lambda_i's from the Dual, and then use lambda_i's to make predictions.

Linear SVM

Primal

$$\min_{\boldsymbol{\beta},\beta_0,\xi_{1:n}} \quad \frac{1}{2}\|\boldsymbol{\beta}\|^2 + \gamma \sum \xi_i$$

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Prediction

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Nonlinear SVM

Nonlinear Feature Mapping

$$(x_1, x_2) \Longrightarrow (x_1, x_2, x_1 x_2, x_1^2, x_2^2)$$

$$\mathbf{x} \Longrightarrow \Phi(\mathbf{x}) = (\phi_1(\mathbf{x}), \phi_2(\mathbf{x}), \dots)$$

Kernel Trick: We do not even need to construct the mapping. All we need is $K_\Phi(\mathbf{x}, \mathbf{z}) = \langle \Phi(\mathbf{x}), \Phi(\mathbf{z}) \rangle$

Dual

$$\max_{\lambda_{1:n}} \sum \lambda_i - \frac{1}{2}\sum_{i,j} \lambda_i \lambda_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

$$\text{subj to } \sum \lambda_i y_i = 0, \ \gamma \geq \lambda_i \geq 0$$

Prediction

$$\text{sign}\Big(\sum_{i \in N_s} \lambda_i y_i K(\mathbf{x}_i, \mathbf{x}_*) + \hat{\beta}_0\Big)$$

The Kernel Function K

The bivariate function **K** is often referred to as the **reproducing kernel** (r.k.) function. We can view K(x, z) as a similarity measure between x and z, which generalizes the ordinary Euclidean inner product between x and z.

Popular kernel functions

- *d*-th degree polynomial

$$K(\mathbf{x}, \mathbf{z}) = (1 + \mathbf{x} \cdot \mathbf{z})^d$$

- Gaussian kernel

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

Kernel Trick: We only need the feature space to exist, as well as the K function.

How to Choose the K function?

1. Construct the feature mapping then we have the K function

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How to Choose the K function?

1. Construct the feature mapping then we have the K function

2. Can we use any symmetric bivariate function as K? K must satisfy the **Mercer's condition**: **symmetric, semi-positive definite function**

$$K(x, z) = \exp(-\sigma x^2) \exp(-\sigma z^2) \exp(2\sigma xz)$$

$$= \exp(-\sigma x^2)\exp(-\sigma z^2) \sum_{k=0}^{\infty} \frac{2^k x^k z^k}{k!}$$

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$$= \exp(-\sigma x^2)\exp(-\sigma z^2) \sum_{k=0}^{\infty} \frac{2^k x^k z^k}{k!}$$

3. Who cares. Use any symmetric function that can capture the similarity between x and z for your application/task (check our discussion on distance for KNN)

Convex Optimization

Primal

$$\min_{\boldsymbol{\beta},\beta_0,\xi_{1:n}} \quad \frac{1}{2}\|\boldsymbol{\beta}\|^2 + \gamma \sum \xi_i$$

$$\text{subj to } y_i(\mathbf{x}_i \cdot \boldsymbol{\beta} + \beta_0) \geq 1 - \xi_i,$$

$$\xi_i \geq 0$$

Dual

$$\max_{\lambda_{1:n}} \quad \sum \lambda_i - \frac{1}{2}\sum_{i,j} \lambda_i \lambda_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j)$$

$$\text{subj to } \sum \lambda_i y_i = 0, \ \gamma \geq \lambda_i \geq 0$$

Prediction

$$\text{sign}(\sum_{i \in N_s} \lambda_i y_i (\mathbf{x}_i \cdot \mathbf{x}_*) + \hat{\beta}_0)$$

Loss + Penalty

Primal

$$\min_{\boldsymbol{\beta},\beta_0} \sum_{i=1}^{n} \left[1 - y_i f(\mathbf{x}_i)\right]_+ + \nu\|\boldsymbol{\beta}\|^2$$

$$f(\mathbf{x}) = \boldsymbol{\beta} \cdot \mathbf{x} + \beta_0$$

Dual

$$f(\mathbf{x}) = \sum_i \lambda_i y_i (\mathbf{x}_i \cdot \mathbf{x}) + \beta_0 \qquad \boldsymbol{\beta} = \sum_i \lambda_i y_i \mathbf{x}_i$$

$$f(\mathbf{x}) = \sum_i \lambda_i y_i K(\mathbf{x}_i, \mathbf{x}) + \beta_0$$

$$= \sum_i \alpha_i K(\mathbf{x}_i, \mathbf{x}) + \alpha_0 \qquad \|\boldsymbol{\beta}\|^2 = \boldsymbol{\alpha}^t \mathbf{K}_{n \times n} \boldsymbol{\alpha}$$

$$= \alpha_1 K(\mathbf{x}_1, \mathbf{x}) + \cdots + \alpha_n K(\mathbf{x}_n, \mathbf{x}) + \alpha_0$$

The Kernel Machine

Kernel Model

$$f(\mathbf{x}) = \alpha_1 K(\mathbf{x}_1, \mathbf{x}) + \cdots + \alpha_n K(\mathbf{x}_n, \mathbf{x}) + \alpha_0$$

Matrix Representation

$$\begin{pmatrix} f(\mathbf{x}_1) \\ f(\mathbf{x}_2) \\ \vdots \\ f(\mathbf{x}_n) \end{pmatrix} = \begin{pmatrix} K(\mathbf{x}_1, \mathbf{x}_1) & K(\mathbf{x}_1, \mathbf{x}_2) & \cdots & K(\mathbf{x}_1, \mathbf{x}_n) \\ K(\mathbf{x}_2, \mathbf{x}_1) & K(\mathbf{x}_2, \mathbf{x}_2) & \cdots & K(\mathbf{x}_2, \mathbf{x}_n) \\ \cdots & \cdots & \cdots & \cdots \\ K(\mathbf{x}_n, \mathbf{x}_1) & K(\mathbf{x}_n, \mathbf{x}_2) & \cdots & K(\mathbf{x}_n, \mathbf{x}_n) \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_n \end{pmatrix} + \alpha_0$$

$$= \mathbf{K}\boldsymbol{\alpha} + \alpha_0$$

Parameter Estimation via Regularization

$$\min_{\boldsymbol{\alpha}, \alpha_0} \sum_{i=1}^{n} \frac{1}{n} L\big(y_i, f(\mathbf{x}_i)\big) + \nu \boldsymbol{\alpha}^t \mathbf{K} \boldsymbol{\alpha}$$

The Kernel Machine

Kernel Model

$$f(\mathbf{x}) = \alpha_1 K(\mathbf{x}_1, \mathbf{x}) + \cdots + \alpha_n K(\mathbf{x}_n, \mathbf{x}) + \alpha_0$$

For this formulation, given a similarity function K(x, z) that doesn't need to satisfy the **Mercer's condition**, we just assume our model like this, and then estimate coefficients alpha's with a (generalized) ridge penalty.

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For SVM, we have
Hinge-Loss + Ridge-Penalty.
For SVM, the sparsity is from Hinge-Loss

The Kernel Machine

Kernel Model

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$$= \mathbf{K}\boldsymbol{\alpha} + \alpha_0$$

If K satisfies the Mercer's condition, what more we can say about this framework?

Parameter Estimation via Regularization

$$\min_{\boldsymbol{\alpha}, \alpha_0} \sum_{i=1}^{n} \frac{1}{n} L\big(y_i, f(\mathbf{x}_i)\big) + \nu \boldsymbol{\alpha}^t \mathbf{K} \boldsymbol{\alpha}$$

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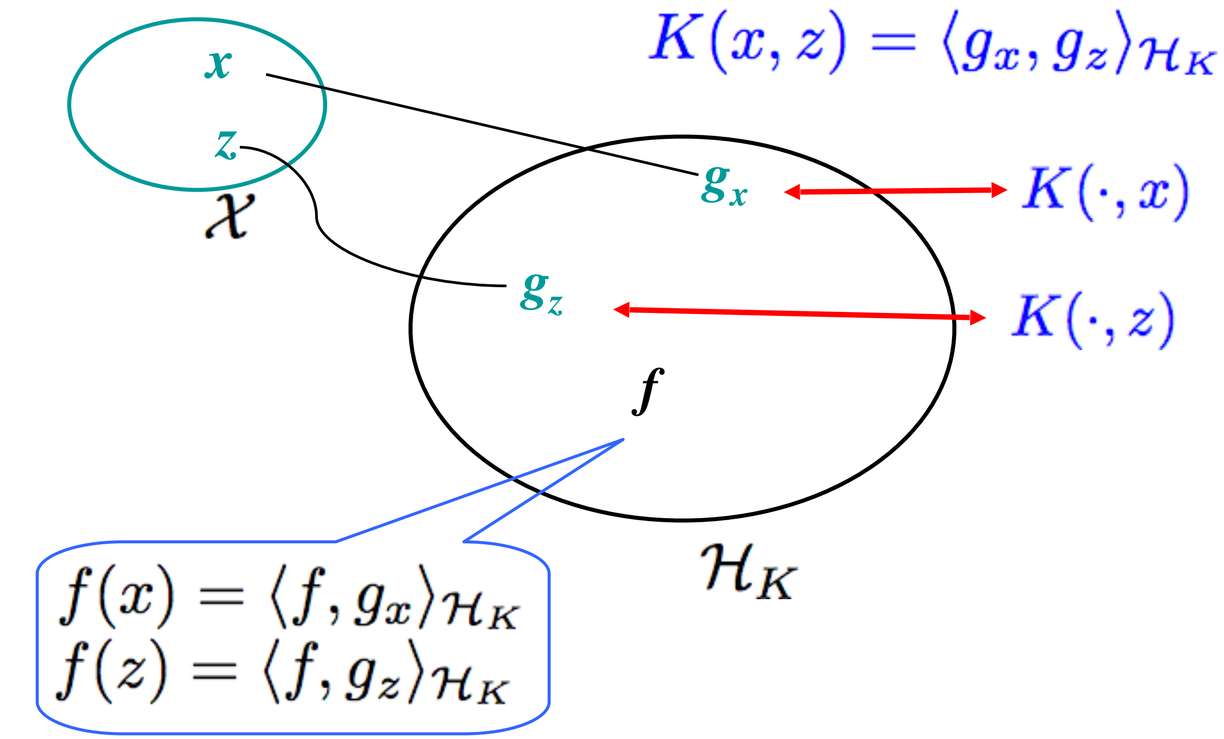
Reproducing Kernel Hilbert Space (RKHS)



Reproducing Property

Representer Theorem

$$\arg\min_{f \in \mathcal{H}_K} \sum_{i=1}^{n} \frac{1}{n} L\big(y_i, f(\mathbf{x}_i)\big) + \nu \|f\|_K^2$$
$$= \alpha_1 K(\mathbf{x}_1, \mathbf{x}) + \cdots + \alpha_n K(\mathbf{x}_n, \mathbf{x}) + \alpha_0$$

Proof : Let $\mathcal{H}_1 = \text{span}\{K(\cdot, x_1), \ldots, K(\cdot, x_n)\}$ and $\mathcal{H}_2 = \mathcal{H}_1^{\perp}$. Then for any function $f \in \mathcal{H}_K$, we can write

$$f = f_1 + f_2, \quad \text{where } f_1 \in \mathcal{H}_1 \text{ and } f_2 \in \mathcal{H}_2.$$

Then we have the following

1. $\|f\|^2 \geq \|f_1\|^2$;
2. $f(x_i) = f_1(x_i)$ for $i = 1, \ldots, n$, because

$$\big\langle f, K(\cdot, x_i) \big\rangle_{\mathcal{H}_K} = \big\langle f_1 + f_2, K(\cdot, x_i) \big\rangle_{\mathcal{H}_K} = \big\langle f_1, K(\cdot, x_i) \big\rangle_{\mathcal{H}_K}.$$

That is $\Omega(f) \geq \Omega(f_1)$. So to minimize $\Omega(f)$, it suffices to focus on subspace $\mathcal{H}_1$. (Does the proof sound familiar? Yes, it follows the same argument as the one in the proof for smoothing splines.)

Summary: SVMs

Primal

$$\min_{\boldsymbol{\beta},\beta_0,\xi_{1:n}} \quad \frac{1}{2}\|\boldsymbol{\beta}\|^2 + \gamma \sum \xi_i$$

$$\text{subj to } y_i(\mathbf{x}_i \cdot \boldsymbol{\beta} + \beta_0) \geq 1 - \xi_i,$$

$$\xi_i \geq 0$$

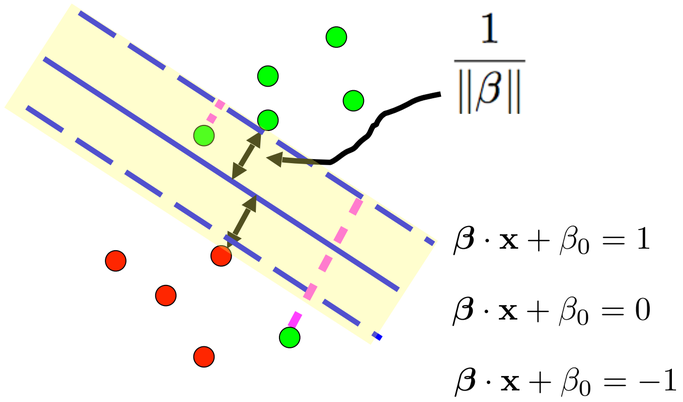
Dual

$$\max_{\lambda_{1:n}} \quad \sum \lambda_i - \frac{1}{2} \sum_{i,j} \lambda_i \lambda_j y_i y_j (\mathbf{x}_i \cdot \mathbf{x}_j)$$

$$\text{subj to } \sum \lambda_i y_i = 0, \ \gamma \geq \lambda_i \geq 0$$

Prediction

$$\text{sign}\Big(\sum_{i \in N_s} \lambda_i y_i (\mathbf{x}_i \cdot \mathbf{x}_*) + \hat{\beta}_0\Big)$$



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Here we can employ any loss function for regression/ classification, and any penalty function on alpha.