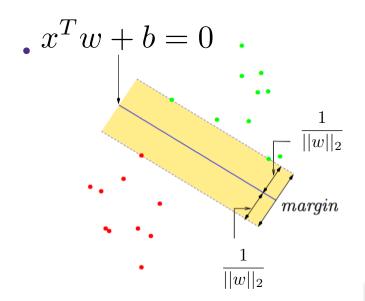
Kernels



What if the data is not linearly separable?



some points don't satisfy margin constraint:

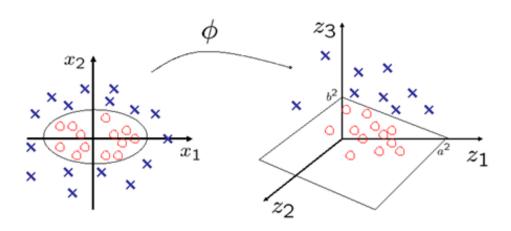
$$\min_{w,b} ||w||_2^2$$
$$y_i(x_i^T w + b) \ge 1 \quad \forall i$$

Two options:

- 1. Introduce slack to this optimization problem
- 2. Lift to higher dimensional space

What if the data is not linearly separable?

Use features of features of features...



Creating Features

Transformed data:

 $h: \mathbb{R}^d \to \mathbb{R}^p$ maps original features to a rich, possibly high-dimensional space

in d=1:
$$h(x) = \begin{bmatrix} h_1(x) \\ h_2(x) \\ \vdots \\ h_p(x) \end{bmatrix} = \begin{bmatrix} x \\ x^2 \\ \vdots \\ x^p \end{bmatrix}$$

for d>1, generate

$$\{u_j\}_{j=1}^p \subset \mathbb{R}^d$$

$$h_j(x) = (u_j^T x)^2$$

$$h_j(x) = \frac{1}{1 + \exp(u_j^T x)}$$

$$h_j(x) = \cos(u_j^T x)$$

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Feature space can get really large really quickly!

Degree-d Polynomials

How do we deal with high-dimensional lifts/data?

A fundamental trick in ML: use kernels

A function $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a kernel for a map ϕ if $K(x, x') = \phi(x) \cdot \phi(x')$ for all x, x'.

So, if we can represent our algorithms/decision rules as dot products and we can find a kernel for our feature map then we can avoid explicitly dealing with $\phi(x)$.

Linear Regression as Kernels

Dot-product of polynomials

 $\Phi(\mathbf{u}) \cdot \Phi(\mathbf{v}) = \text{polynomials of degree exactly d}$

$$d = 1 : \phi(u) = \begin{vmatrix} u_1 \\ u_2 \end{vmatrix} \quad \langle \phi(u), \phi(v) \rangle = u_1 v_1 + u_2 v_2$$

$$d = 2 : \phi(u) = \begin{bmatrix} u_1^2 \\ u_2^2 \\ u_1 u_2 \\ u_2 u_1 \end{bmatrix} \quad \langle \phi(u), \phi(v) \rangle = u_1^2 v_1^2 + u_2^2 v_2^2 + 2u_1 u_2 v_1 v_2$$

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Feature space can get really large really quickly!

General d: Dimension of $\phi(u)$ is roughly p^d if $u \in \mathbb{R}^p$

Feature expansion can be written **implicitly** $K(\mathbf{u}, \mathbf{v}) = (\mathbf{u} \cdot \mathbf{v})^p$

Examples of Kernels

Polynomials of degree exactly d

$$K(\mathbf{u}, \mathbf{v}) = (\mathbf{u} \cdot \mathbf{v})^p$$

Polynomials of degree up to d

$$K(\mathbf{u}, \mathbf{v}) = (\mathbf{u} \cdot \mathbf{v} + 1)^p$$

Gaussian (squared exponential) kernel

$$K(\mathbf{u}, \mathbf{v}) = \exp\left(-\frac{||\mathbf{u} - \mathbf{v}||^2}{2\sigma^2}\right)$$

Sigmoid

$$K(u, v) = \tanh(\gamma \cdot u^T v + r)$$

The Kernel Trick

Pick a kernel K

For a linear predictor, show $w = \sum_i \alpha_i x_i$

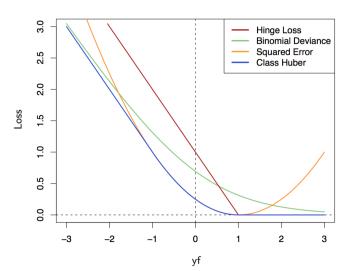
Change loss function/decision rule to only access data through dot products

Substitute $K(x_i, x_j)$ for $x_i^T x_j$

Loss Functions

$$\{(x_i, y_i)\}_{i=1}^n \quad x_i \in \mathbb{R}^d$$

$$y_i \in \mathbb{R}$$



Loss functions:

$$\sum_{i=1}^{n} \ell_i(w)$$

Squared error Loss: $\ell_i(w) = (y_i - x_i^T w)^2$

Logistic Loss: $\ell_i(w) = \log(1 + \exp(-y_i x_i^T w))$

 $0/1 \text{ loss: } \ell_i(w) = \mathbb{I}[\operatorname{sign}(y_i) \neq \operatorname{sign}(x_i^T w)]$

Hinge Loss: $\ell_i(w) = \max\{0, 1 - y_i x_i^T w\}$

The Kernel Trick for regularized least squares

$$\widehat{w} = \arg\min_{w} \sum_{i=1}^{n} (y_i - x_i^T w)^2 + \lambda ||w||_w^2$$

There exists an
$$\alpha \in \mathbb{R}^n$$
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$$\widehat{\alpha} = \arg\min_{\alpha} \sum_{i=1}^{n} (y_i - \sum_{j=1}^{n} \alpha_j \langle x_j, x_i \rangle)^2 + \lambda \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j \langle x_i, x_j \rangle$$

$$= \arg\min_{\alpha} \sum_{i=1}^{n} (y_i - \sum_{j=1}^{n} \alpha_j K(x_i, x_j))^2 + \lambda \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j K(x_i, x_j)$$

$$= \arg\min_{\alpha} ||\mathbf{y} - \mathbf{K}\alpha||_2^2 + \lambda \alpha^T \mathbf{K}\alpha$$

$$K(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle$$