Kernels and the Kernel Trick

Machine Learning

THE UNIVERSITY OF UTAH

Support vector machines

- Training by maximizing margin
- The SVM objective
- Solving the SVM optimization problem
- Support vectors, duals and kernels

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This lecture

1. Support vectors

2. Kernels

3. The kernel trick

4. Properties of kernels

5. Another example of the kernel trick

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1. **Support vectors**
2. Kernels
3. The kernel trick
4. Properties of kernels
5. Another example of the kernel trick

So far we have seen

- Support vector machines

- Hinge loss and optimizing the regularized loss

More broadly, different algorithms for learning linear classifiers

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- Hinge loss and optimizing the regularized loss

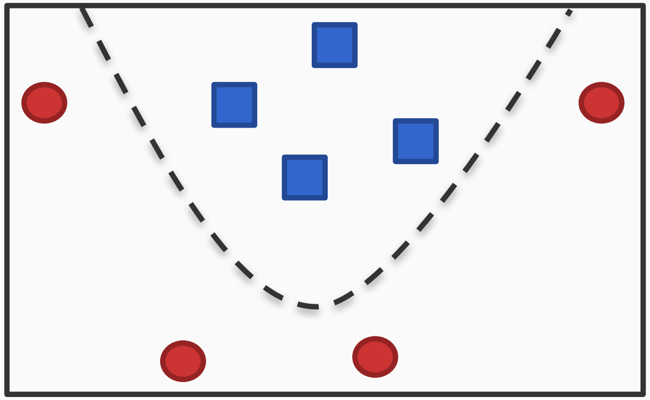
More broadly, different algorithms for learning linear classifiers

What about non-linear models?

One way to learn non-linear models

Explicitly introduce non-linearity into the feature space

If the true separator is quadratic



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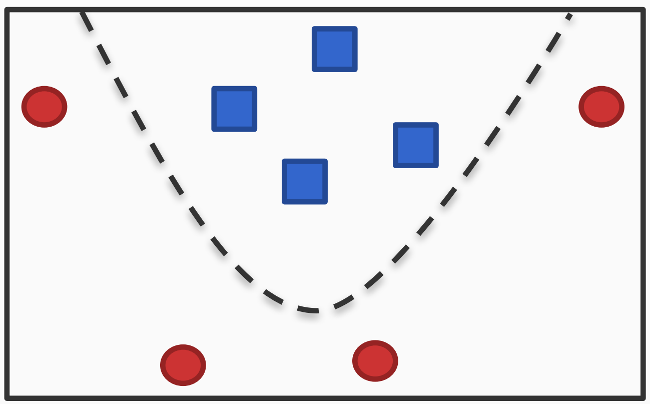

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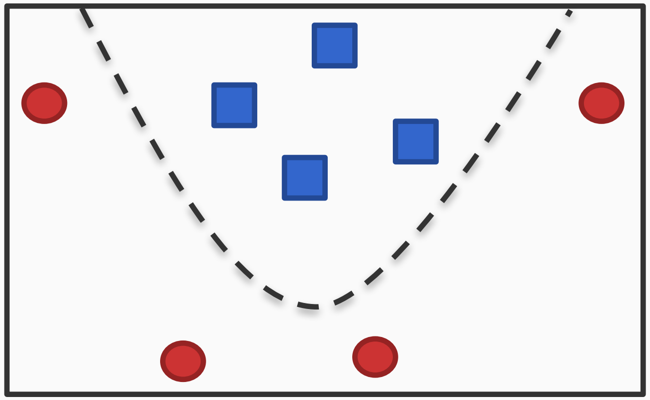

Transform all input points as

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Now, we can try to find a weight vector in this higher dimensional space

That is, predict using $\mathbf{w}^T \phi(x_1, x_2) \geq b$

SVM: Primals and duals

The SVM objective

$$\begin{aligned} \min_{\mathbf{w},\xi} \quad & & \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_i \xi_i \\ \text{s.t.} \quad & \forall i, & y_i \mathbf{w}^T \mathbf{x}_i \geq 1 - \xi_i \\ & \forall i, & \xi_i \geq 0. \end{aligned}$$

This is called the *primal form* of the objective

This can be converted to its *dual form*, which will let us prove a very useful property

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Another optimization problem

Has the property that max Dual = min Primal

This is called the *primal form* of the objective

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Support vector machines

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Let **w** be the minimizer of the SVM problem for some dataset with m examples: $\{(\mathbf{x}_i, y_i)\}$

Then, for i = 1…m, there exist $\alpha_i \geq 0$ such that the optimum w can be written as

$$\mathbf{w} = \sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i$$

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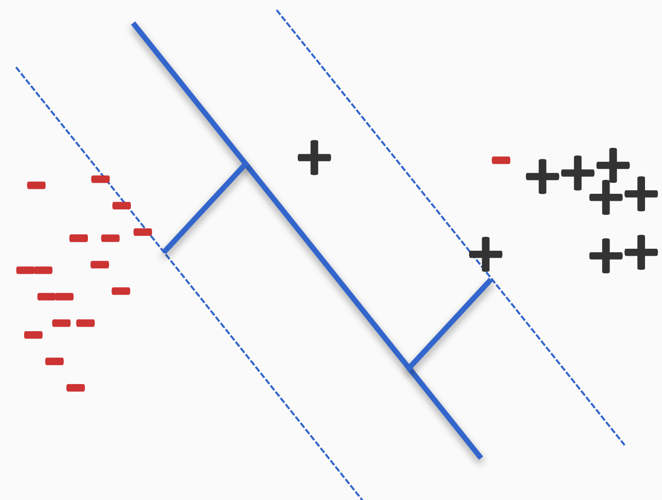

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$\alpha_i = 0 \quad\quad \Rightarrow y_i \mathbf{w}^T x_i \geq 1$

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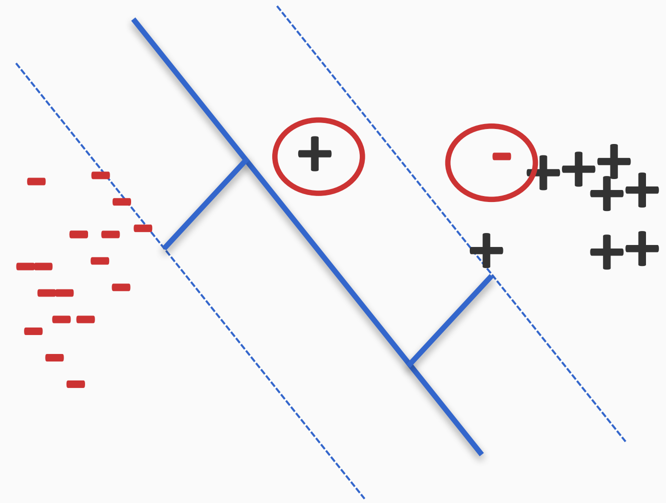

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All points on the wrong side of the margin

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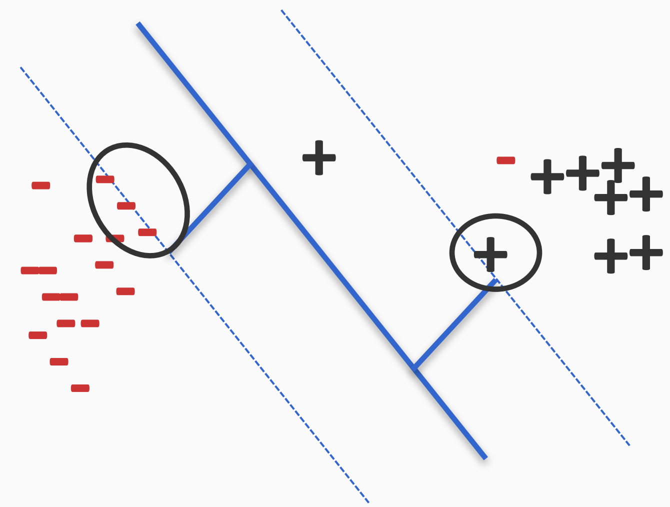

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$$0 \leq \alpha_i \leq C \quad \Rightarrow y_i \mathbf{w}^T x_i = 1$$

All points on the margin

Support vectors

The weight vector is completely defined by training examples whose α_is are not zero

$$\mathbf{w} = \sum_{i=1}^{m} \alpha_i y_i \mathbf{x}_i$$

These examples are called the *support vectors*

This lecture

✓ Support vectors

2. **Kernels**

3. The kernel trick

4. Properties of kernels

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Predicting with linear classifiers

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  - We only need to compute dot products between training examples and the new example **x**
- This is true even if we map examples to a high dimensional space

$$\mathbf{w}^T\phi(\mathbf{x}) = \sum_i \alpha_i y_i \phi(\mathbf{x}_i)^T\phi(\mathbf{x})$$

Predicting with linear classifiers

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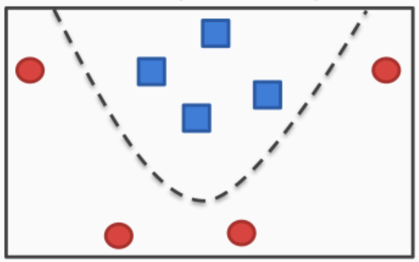

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because $\mathbf{w}^T \phi(\mathbf{x}) = \sum_i \alpha_i y_i \phi(\mathbf{x}_i)^T \phi(\mathbf{x})$

Kernel based methods

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What does this new formulation give us?

If we have to compute ϕ every time anyway, we gain nothing

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If we can compute the value of K without explicitly writing the blown up representation, then we will have a computational advantage.

This lecture

✓ Support vectors

✓ Kernels

3. **The kernel trick**

4. Properties of kernels

5. Another example of the kernel trick

Example: Polynomial Kernel

- Given two examples **x** and **z** we want to map them to a high dimensional space [for example, quadratic]

$$\phi(x_1, x_2, \cdots, x_n) = [1, x_1, x_2, \cdots, x_n, x_1^2, x_2^2, \cdots x_n^2, x_1 x_2, \cdots, x_{n-1} x_n]^T$$

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All degree zero terms

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and compute the dot product A = ϕ(**x**)^Tϕ (**z**) [takes time]

- Instead, in the original space, compute

$$B = K(\mathbf{x}, \mathbf{z}) = \left(1 + \mathbf{x}^T \mathbf{z}\right)^2$$

Claim: A = B (Coefficients do not really matter)

Example: Two dimensions, quadratic kernel

A = $\phi(\mathbf{x})^T\phi(\mathbf{z})$ $\quad$ $B = K(\mathbf{x},\mathbf{z}) = \left(1+\mathbf{x}^T\mathbf{z}\right)^2$

$$\phi(x_1, x_2) = \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ x_1^2 \\ x_2^2 \\ x_1 x_2 \end{bmatrix}$$

The Kernel Trick

Suppose we wish to compute $K(\mathbf{x}, \mathbf{z}) = \phi(\mathbf{x})^T \phi(\mathbf{z})$

Here ϕ maps **x** and **z** to a high dimensional space

The Kernel Trick: Save time/space by computing the value of $K(\mathbf{x}, \mathbf{z})$ by performing operations in the original space (without a feature transformation!)

Computing dot products efficiently

Kernel Trick: You want to work with degree 2 polynomial features, ϕ(x). Then, your dot product will be operate using vectors in a space of dimensionality n(n+1)/2.

The kernel trick allows you to save time/space and compute dot products in an n dimensional space.

(Not just for degree 2 polynomials)

This lecture

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✓ The kernel trick

4. Properties of kernels

5. Another example of the kernel trick

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- General condition: construct the Gram matrix $\{K(\mathbf{x}_i, \mathbf{z}_j)\}$; check that it's positive semi definite

Reminder: Positive semi-definite matrices

A symmetric matrix M is positive semi-definite if it is

- For any vector non-zero **z**, we have $\mathbf{z}^T M \mathbf{z} \geq 0$

(A useful property characterizing many interesting mathematical objects)

The Kernel Matrix

- The Gram matrix of a set of n vectors S = $\{\mathbf{x}_1 \ldots \mathbf{x}_n\}$ is the $n \times n$ matrix $\mathbf{G}$ with $\mathbf{G}_{ij} = \mathbf{x}_i^T \mathbf{x}_j$
  - The kernel matrix is the Gram matrix of $\{\phi(\mathbf{x}_1), \ldots, \phi(\mathbf{x}_n)\}$
  - (size depends on the # of examples, not dimensionality)

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- Showing that a function K is a valid kernel
  - Direct approach: If you have the $\phi(\mathbf{x}_i)$, you have the Gram matrix (and it's easy to see that it will be positive semi-definite). *Why?*
  - Indirect: If you have the Kernel, write down the Kernel matrix K_{ij}, and show that it is a legitimate kernel, without an explicit construction of $\phi(\mathbf{x}_i)$

Mercer's condition

Let K($\mathbf{x}$, $\mathbf{z}$) be a function that maps two n dimensional vectors to a real number

K is a valid kernel if for every finite set $\{x_1, x_2, \cdots\}$, for any choice of real valued $c_1, c_2, \cdots$, we have

$$\sum_i \sum_j c_i c_j K(\mathbf{x}_i, \mathbf{x}_j) \geq 0$$

Polynomial kernels

- Linear kernel: $k(\mathbf{x}, \mathbf{z}) = \mathbf{x}^T\mathbf{z}$

- Polynomial kernel of degree *d*: $k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^T\mathbf{z})^d$
  - only *d*th-order interactions

- Polynomial kernel up to degree *d*: $k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^T\mathbf{z} + c)^d$ ($c>0$)
  - all interactions of order *d* or lower

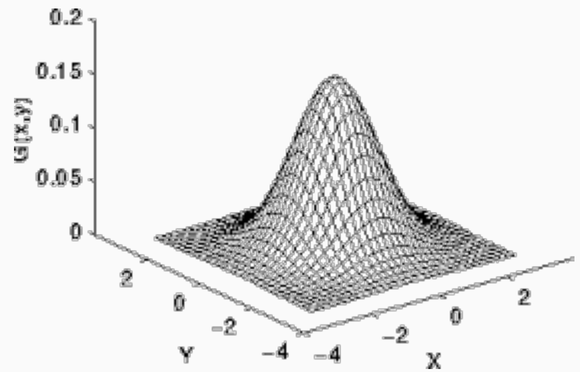
Gaussian Kernel

(or the radial basis function kernel)

$$K_{rbf}(\mathbf{x}, \mathbf{z}) = \exp\left(-\frac{||\mathbf{x} - \mathbf{z}||^2}{c}\right)$$

– $(x - z)^2$: squared Euclidean distance between **x** and **z**
– $c = \sigma^2$: a free parameter
– very small c: K ≈ identity matrix (every item is different)
– very large c: K ≈ unit matrix (all items are the same)

– k(**x**, **z**) ≈ 1 when **x**, **z** close
– k(**x**, **z**) ≈ 0 when **x**, **z** dissimilar



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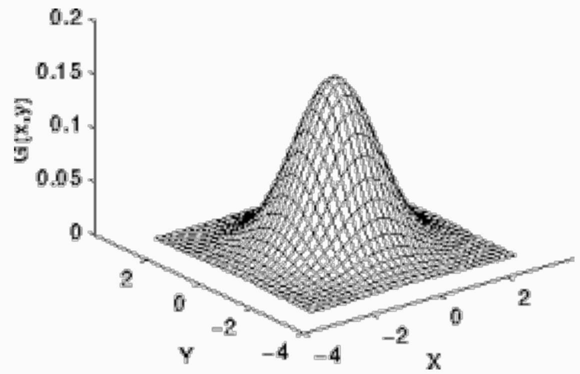

Exercises:
1. Prove that this is a kernel.
2. What is the "blown up" feature space for this kernel?

Constructing New Kernels

You can construct new kernels $k'(\mathbf{x}, \mathbf{x'})$ from existing ones:

- Multiplying $k(\mathbf{x}, \mathbf{x'})$ by a constant c

  $ck(\mathbf{x}, \mathbf{x'})$

- Multiplying $k(\mathbf{x}, \mathbf{x'})$ by a function f applied to $\mathbf{x}$ and $\mathbf{x'}$

  $f(\mathbf{x})k(\mathbf{x}, \mathbf{x'})f(\mathbf{x'})$

- Applying a polynomial (with non-negative coefficients) to $k(\mathbf{x}, \mathbf{x'})$

  $P(\ k(\mathbf{x}, \mathbf{x'})\ )$ with $P(z) = \sum_i a_i z^i$ and $a_i \geq 0$

- Exponentiating $k(\mathbf{x}, \mathbf{x'})$

  $\exp(k(\mathbf{x}, \mathbf{x'}))$

Constructing New Kernels (2)

- You can construct $k'(\mathbf{x}, \mathbf{x'})$ from $k_1(\mathbf{x}, \mathbf{x'})$, $k_2(\mathbf{x}, \mathbf{x'})$ by:
  - Adding $k_1(\mathbf{x}, \mathbf{x'})$ and $k_2(\mathbf{x}, \mathbf{x'})$:
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  - Multiplying $k_1(\mathbf{x}, \mathbf{x'})$ and $k_2(\mathbf{x}, \mathbf{x'})$:
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- Also:
  - If $\phi(\mathbf{x}) \in R^m$ and $k_m(\mathbf{z}, \mathbf{z'})$ a valid kernel in R^m,
    $k(\mathbf{x}, \mathbf{x}') = k_m(\phi(\mathbf{x}), \phi(\mathbf{x}'))$ is also a valid kernel
  - If $\mathbf{A}$ is a symmetric positive semi-definite matrix,
    $k(\mathbf{x}, \mathbf{x}') = \mathbf{xAx}'$ is also a valid kernel

Kernel Trick: An example

Let the blown up feature space represent the space of all 3^n conjunctions. Then,

$$K(\mathbf{x}, \mathbf{z}) = \sum_i \phi_i(\mathbf{x})\phi_i(\mathbf{z}) = 2^{same(\mathbf{x},\mathbf{z})}$$

where same(x,z) is the number of features that have the same value for both x and z

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Example: Take n=3; **x**=(001), **z**=(011), we have conjunctions of size 0,1,2,3

Kernel Trick: An example

Let the blown up feature space represent the space of all 3^n conjunctions. Then,

$$K(\mathbf{x}, \mathbf{z}) = \sum_i \phi_i(\mathbf{x})\phi_i(\mathbf{z}) = 2^{same(\mathbf{x},\mathbf{z})}$$

where same(x,z) is the number of features that have the same value for both x and z

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Conjunctions with literals outside this set disappear.

Exercises

1. Show that this argument works for a specific example
   - Take $X=\{x_1, x_2, x_3, x_4\}$
   - $\phi(\mathbf{x})$ = The space of all 3^n conjunctions ; $|\phi(\mathbf{x})| = 81$
   - Consider $\mathbf{x}=(1100)$, $\mathbf{z}=(1101)$
   - Write $\phi(\mathbf{x})$, $\phi(\mathbf{z})$, the representation of **x**, **z** in the ϕ space
   - Compute $\phi(\mathbf{x})^T\phi(\mathbf{z})$
   - Show that

     $$K(x,z) = \phi(\mathbf{x})^T\phi(\mathbf{z}) = \sum_i \phi_i(z)\, \phi_i(x) = 2^{same(\mathbf{x},\mathbf{z})} = 8$$

2. Try to develop another kernel, e.g., where the space of all conjunctions of size 3 (exactly)

Summary: Kernel trick

- To make the final prediction, we are computing dot products

- The kernel trick is a computational trick to compute dot products in higher dimensional spaces

- This is applicable not just to SVMs. The same idea can be extended to Perceptron too: the Kernel Perceptron

- Important: All the bounds we have seen (eg: Perceptron bound, etc) depend on the underlying dimensionality
  - By moving to a higher dimensional space, we are incurring a penalty on sample complexity