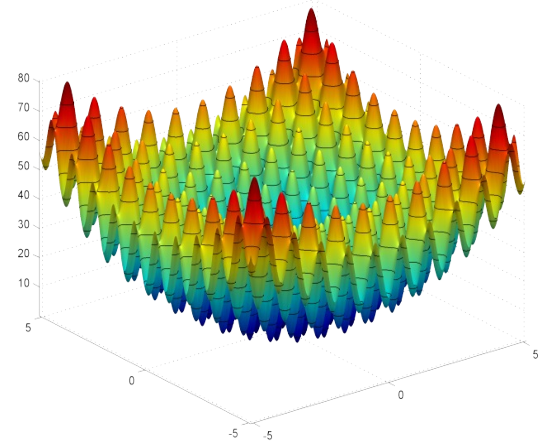
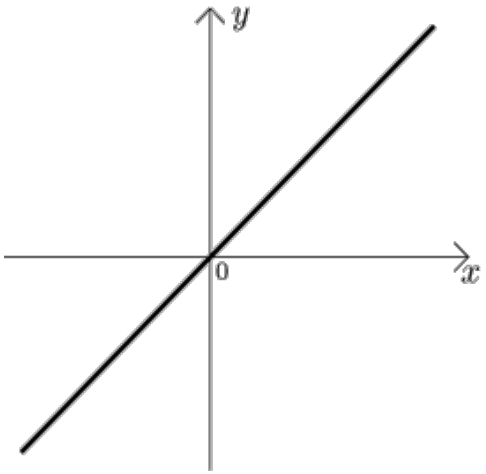
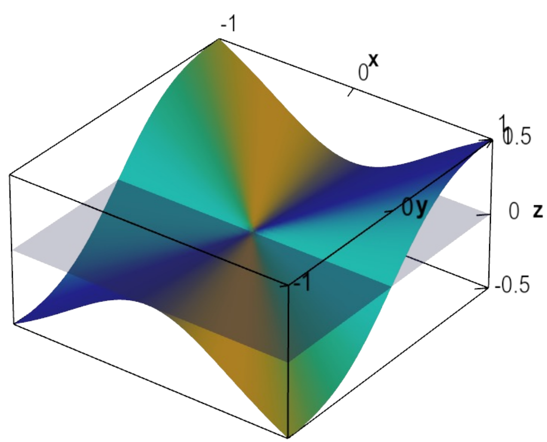
Kernel Methods

Linear Classification Methods

- Linear Regression
- Logistic Regression
- Perceptron $\hat{y} = \mathrm{sign}(w \cdot x)$
- Support Vector Machines



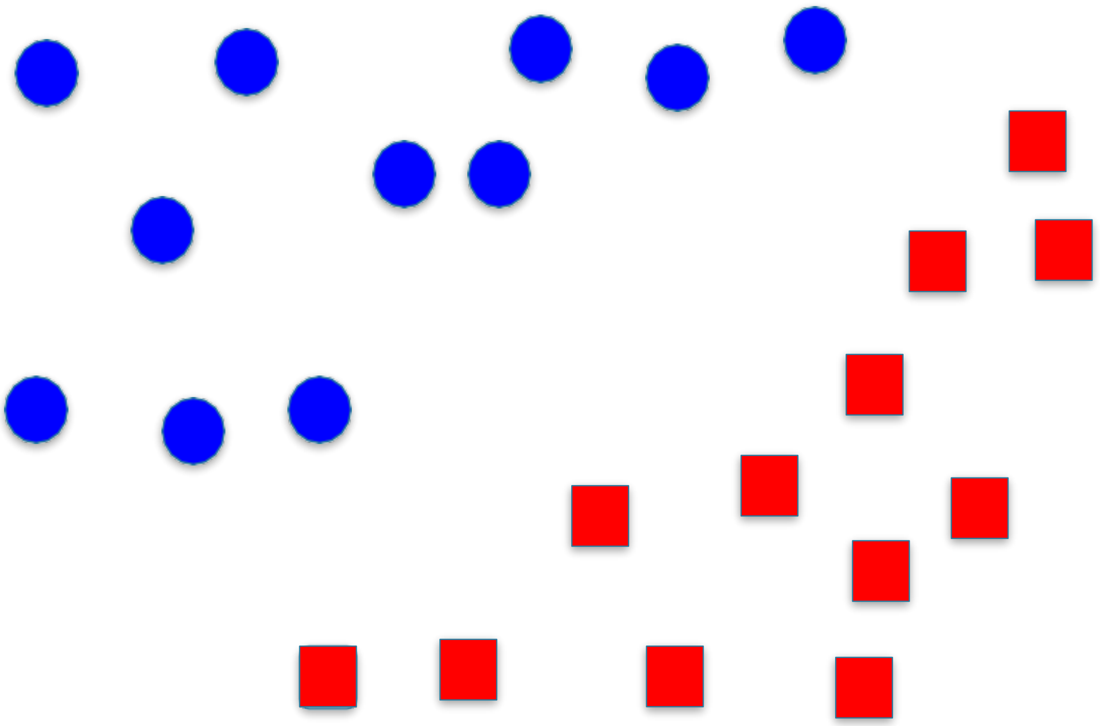




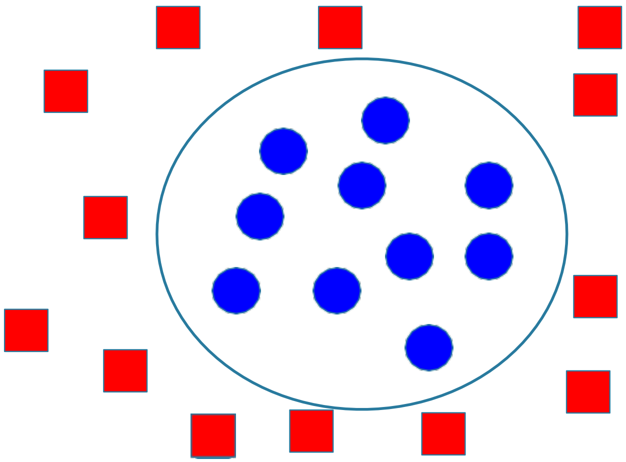
Review: Lingering Questions

- What would we do if we saw all of the data (batch)?
  - We'd pick the best separating hyperplane!
- Which separating hyperplane is the best?
  - The maximum margin separator
  - Use a quadratic regularizer on the weights
- What can we do for non-linear data?
  - It's not separable, use slack variables
  - Can we do better?

Linearly Separable



Not Linearly Separable



Handling Non-Linear Data

- Option 1: Add features by hand that make the data separable
  - Requires feature engineering
- Option 2: Learn a small number of additional features that will suffice
  - We'll see this eventually
- Option 3: Kernel trick
  - Today

Feature Mapping Functions

- Assuming a two dimensional vector x = [x(1),x(2)]
  - x(i) is the ith position of x
- Let's apply a feature mapping function

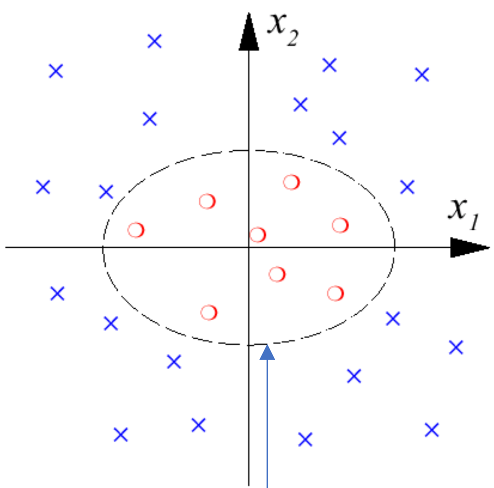
$$\phi([x_{(1)}, x_{(2)}]) = (x_{(1)}^2, \sqrt{2} \cdot x_{(1)}\, x_{(2)}, x_{(2)}^2)$$

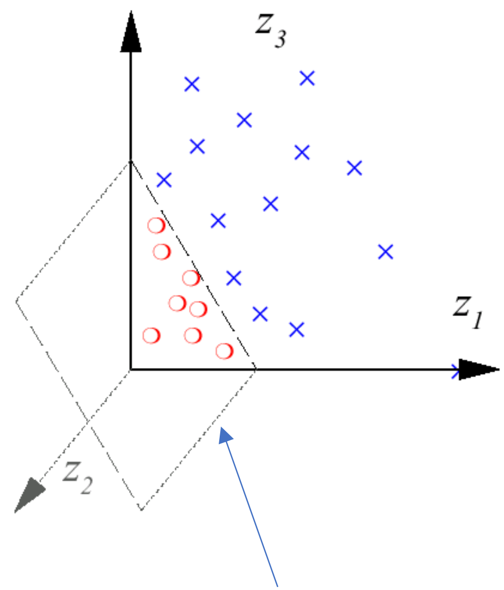
- Why is this useful?
  - Elliptical decision boundary:
  - Not linear in x, but linear in ϕ(x)
  - Boundaries defined by linear combinations of x2, y2, xy, x, and y are ellipses, parabolas, and hyperbolas in the original space.

Geometric Interpretation

$$\phi([x_{(1)}, x_{(2)}]) = (x_{(1)}^2, \sqrt{2} \cdot x_{(1)}\, x_{(2)}, x_{(2)}^2)$$

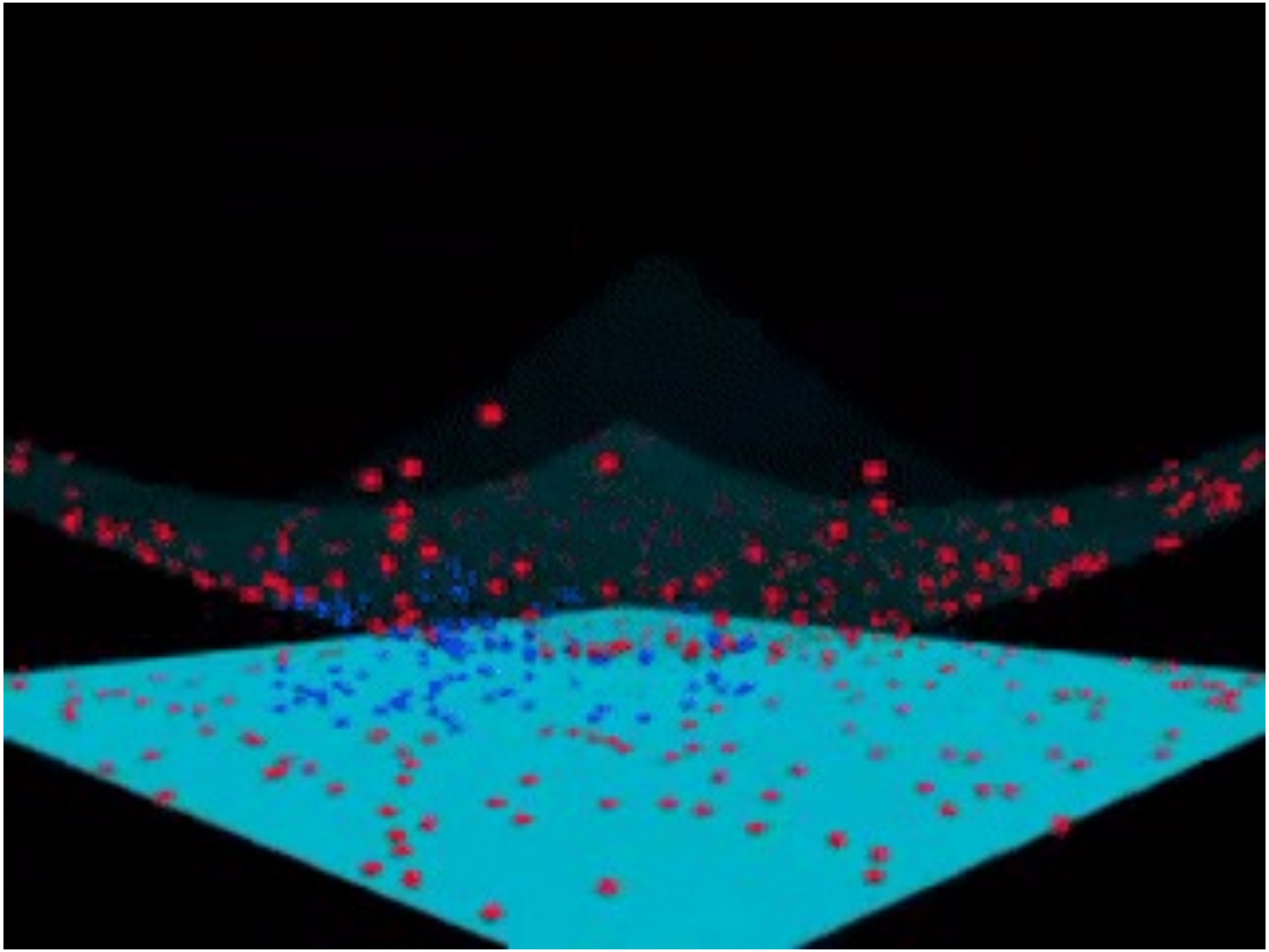
$$z_1 \qquad\qquad z_2 \qquad\qquad z_3$$





$$a x_{(1)}^2 + b x_{(2)}^2 < c \qquad a\phi(x)_{(1)} + b\phi(x)_{(3)} < c$$

Geometric Interpretation



Why Feature Mapping Functions?

- Recall that to make something linearly separable I can just add a unique feature to every example
- Any dataset is linearly separable if we use enough dimensions
  - In an n-dimensional space, almost any set of up to n+1 labeled points is linearly separable!
- We can obtain linear separability by projecting data into higher dimensional spaces
  - Use smarter techniques to obtain generalizeable separability

Feature Functions + SVM

- Replace x with a feature mapping function

$$\underset{w}{\operatorname{argmin}} \|w\|_2^2$$

$$s.t. \quad y_i(w^T \phi(x_i)) \geq 1, \forall i$$

- The dot product is now taken over a higher dimensional feature space
  - If ϕ is quadratic then the feature space is a quadratic space in terms of the inputs

Limitations

- We still have to learn w
  - w will grow in size of the feature space
  - e.g. quadratic kernel: $|x| = 100 \rightarrow |\phi(x)| = 10000$
- Feature functions just increase the feature space in a non-linear way
- Too limiting

SVMs and w

- Wait a minute, there is no w!

$$\sum_{i=1}^{N} \alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} y_i y_j \alpha_i \alpha_j \left(\phi(x_i)^T \phi(x_j)\right)$$

- There is no modeling constraint that prevents us from making $\phi(x)$ very large
- αs do not grow in the size of $\phi(x)$
- Thank you dual!

Kernels

- Let's replace $\left(\phi(x_i)^T\phi(x_j)\right)$ with a kernel function K

$$\sum_{i=1}^{N}\alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} y_i y_j \alpha_i \alpha_j K\left(x_i, x_j\right)$$

where

$$\phi(x)^T w = \phi(x)^T \sum_{i=1}^{N}[\alpha_i y_i \phi(x_i)] = \sum_{i=1}^{N} \alpha_i y_i K(x, x_i)$$

Why?

- We have removed all dependencies in the SVM on the size of the feature space
    - The feature space $\phi(x)$ appears only in the kernel
- As long as the Kernel function does the work, we can handle any feature space

Intuition About Over-Fitting

- Wait a minute!
- Assuming we project features then even using the simple projection shown so far, we'd have way to many features!
- Didn't we learn that too many features means over-fitting?

Saved by the Dual

- We aren't free to choose a parameter for each feature
- w is a linear combination of the inputs
  - We can only choose the parameters for αs
  - There are only n αs, no matter how large our feature space projection
- The inputs x put a constraint on our flexibility in high dimensional space

The Kernel Trick

- Take a linear SVM
- Substitute a non-linear kernel
- Optimize objective in the dual
- We get non-linear classification!
- Without
  - Over-fitting
  - Learning too many parameters
  - Computing a large feature space

What is a Kernel?

- A kernel is a scalar product between two high dimensional feature vectors
$$K(x, x') = \phi(x)^T \phi(x')$$
- A proposed kernel function can be written in this form
- We can define any mapping function and then compute the kernel

Quadratic Kernel

- Let's take the cross product of all features (quadratic)

$$K(x, x') = (x^T \cdot x')^2$$

- Why is the quadratic a valid kernel?
- It's actually just a scalar product of the two vectors

$$\begin{aligned} K(x, x') &= (x^T x')^2 \\ &= (x_1 x'_1 + x_2 x'_2)^2 \\ &= x_1^2 x'^2_1 + 2 x_1 x'_1 x_2 x'_2 + x_2^2 x'^2_2 \\ &= (x_1^2, \sqrt{2} x_1 x_2, x_2^2) \cdot (x'^2_1, \sqrt{2} x'_1 x'_2, x'^2_2) \\ &= \phi(x) \cdot \phi(x') \end{aligned}$$

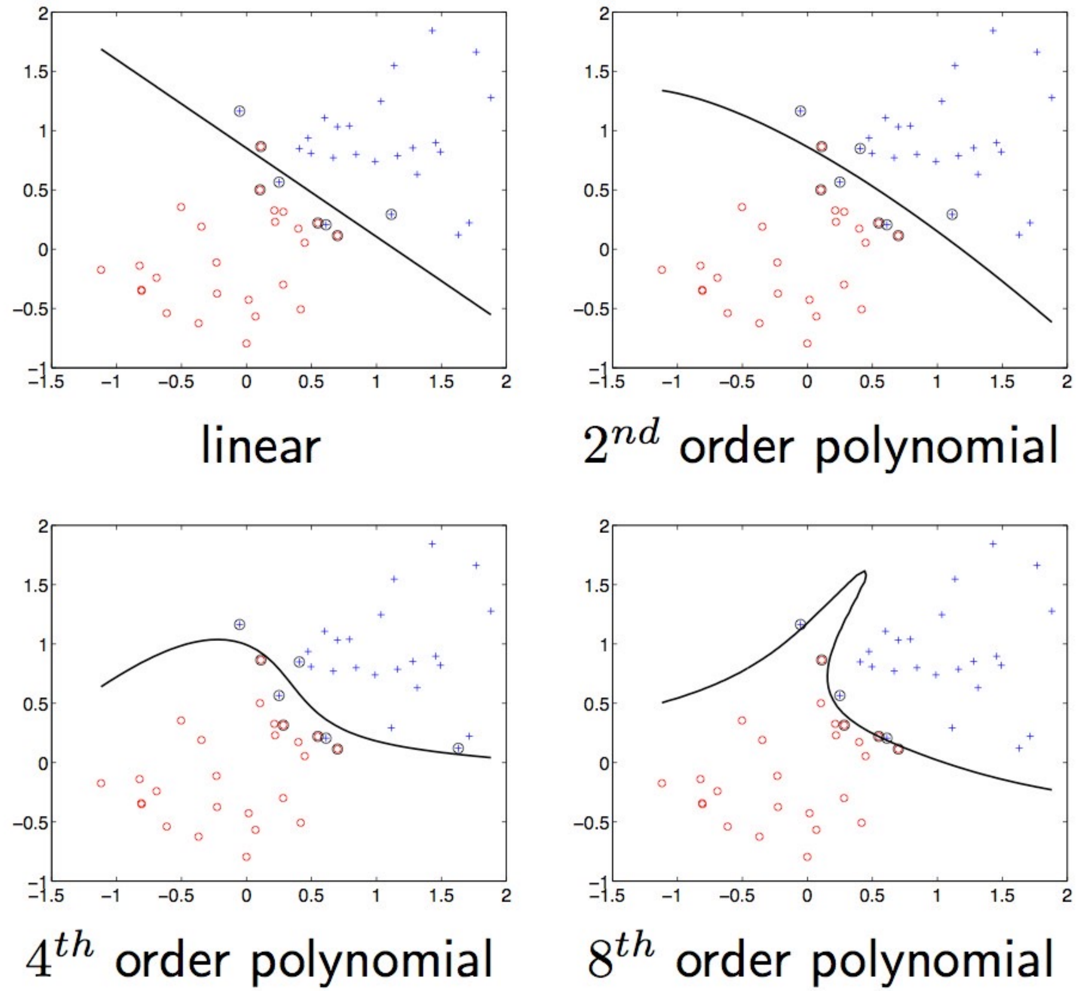
- $\phi(x)$ is the feature mapping function used for the ellipse example
  - This is true for arbitrary dimensions of x

Polynomial Kernel

- In fact, this is true of any exponent p
$$K(x, x') = (1 + x^T x')^p$$
- This is the polynomial kernel
  - To get the feature vectors we would concatenate all elements up to the pth order polynomial terms of the components of x (weighted appropriately)

Polynomial Kernel

- In the given feature space the separators are non-linear
- In the high dimensional space they are linear
- Support vectors are circled



Decision Boundary

- How does the kernel influence the decision boundary?
- Recall prediction given by

$$\phi(x)^T w = \sum_{i=1}^{N} \alpha_i y_i K(x, x_i)$$

- The larger $K(x, x_i)$ the more x_i contributes to the decision for x
- x receives a label based on those support vectors (examples with large α) with highest $K(x, x_i)$

Similarity Function?

- Does that mean $K(x, x_i)$ is a similarity function?
  - Give same label as most similar examples
- Sort of
  - Recall:

$$\cos\psi = \frac{x \cdot x'}{\|x\|\|x'\|}$$

  - Therefore

$$x \cdot x' = \|x\|\|x'\| \cos\psi$$

  - So

$$\alpha K(x, x') = \alpha\phi(x) \cdot \phi(x') = \alpha\|\phi(x)\|\|\phi(x')\| \cos\theta$$

Similarity Function?

$$\alpha K(x, x') = \alpha\phi(x) \cdot \phi(x')$$
$$= \alpha\|\phi(x)\|\|\phi(x')\| \cos\theta$$

- Note
  - $\phi(x)$: constant across all x' in the prediction
  - $\alpha\phi(x')$: α is scaled per x' so this just weighs importance
  - $\cos\theta$: the angle between the vectors
    - When θ is 0, this is 1 so larger values for more similar vectors

Kernel Definitions

- A scalar product of two vectors in high dimensional space
- OR
- Mercer’s theorem

Mercer’s Theorem

- Suppose K is a valid kernel
- Define Kernel matrix (Gram matrix) as
$$K_{i,j} = K(x_i, x_j)$$
- K must be symmetric
$$K_{i,j} = K\left(x_i, x_j\right) = \phi(x_i) \cdot \phi\left(x_j\right) = \phi\left(x_j\right) \cdot \phi(x_i)$$
$$= K\left(x_j, x_i\right) = K_{j,i}$$

Mercer's Theorem

- $\phi_k(x)$ kth position of vector

$$
\begin{aligned}
z^T K z &= \sum_i \sum_j z_i K_{ij} z_j \\
&= \sum_i \sum_j z_i \phi(x_i)^T \phi(x_j) z_j \\
&= \sum_i \sum_j z_i \left(\sum_k \phi_k(x_i) \phi_k(x_j)\right) z_j \\
&= \sum_k \sum_i \sum_j z_i \phi_k(x_i) \phi_k(x_j)\, z_j \\
&= \sum_k \left(\sum_i z_i \phi_k(x_i)\right)^2 \\
&\geq 0
\end{aligned}
$$

Mercer's Theorem

- Let K : R^M x R^M -> R be given. Then for K to be a valid (Mercer) kernel, it is necessary and sufficient that for any finite data set, the corresponding kernel matrix is symmetric positive semi-definite.

Kernel Definitions

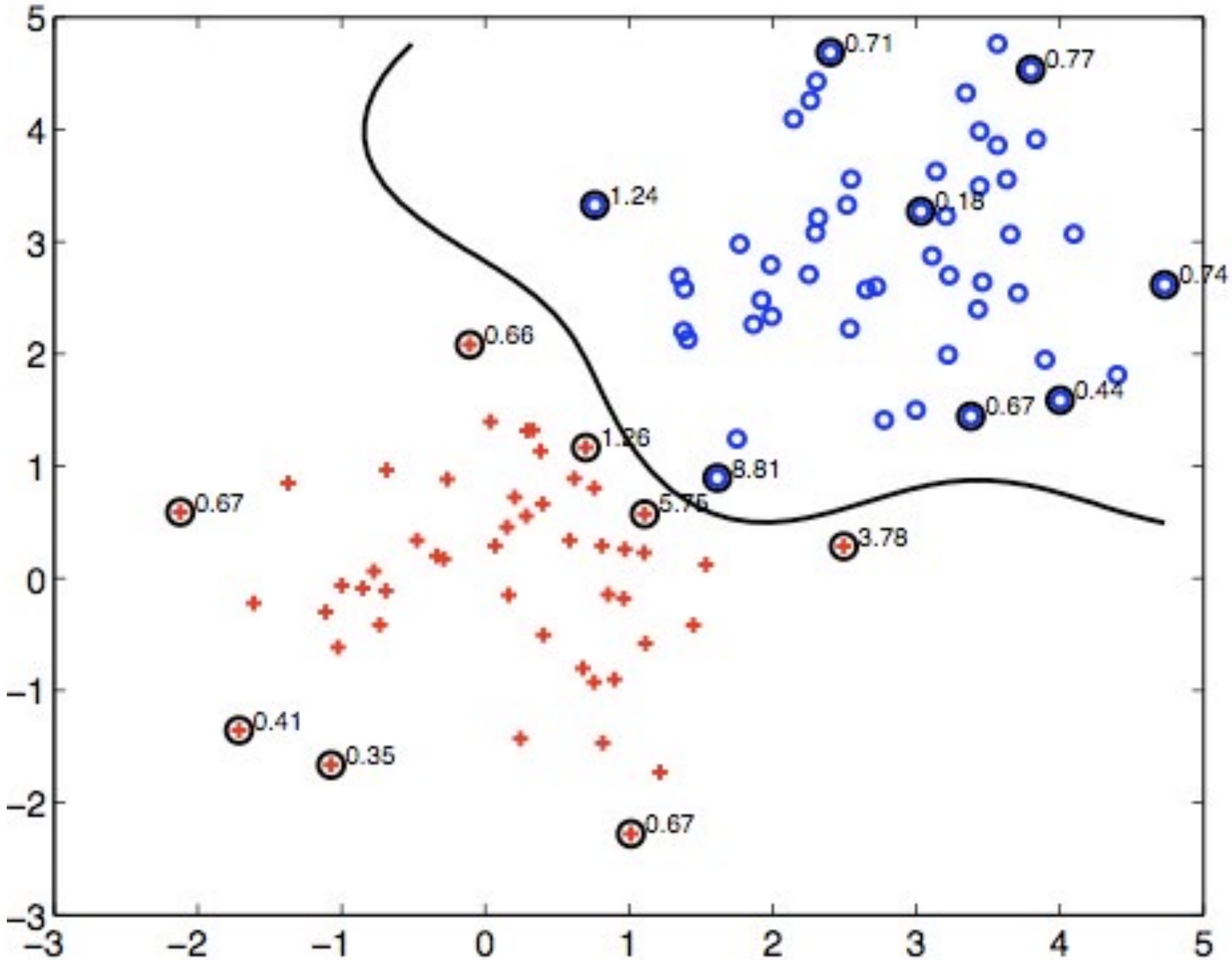
- A kernel is
  - A scalar product of two vectors in high dimensional space
  - Mercer's theorem
- How do we test a kernel without writing $\phi(x)$ explicitly?
- Equivalent definition
  - The Gram matrix $\boldsymbol{K}$ should be positive semidefinite for all x
  - Gram matrix $\boldsymbol{K}$: $K_{ij} = K(x_i, xj)$
- Positive semidefinite: $x^T\boldsymbol{M}x \geq 0$

Example of a Kernel

- Polynomial kernel $K(x, x') = (1 + (x^T x'))^P$
- Radial Basis Function (RBF) kernel
  - Gaussian version
  - Infinite dimensional function

$$K(x, x') = \exp(-\frac{1}{2}\|x - x'\|^2)$$

Radial Basis Function



Building Kernels

- How do we build a kernel?
  - Decide on a projection that is meaningful for data
- How do we know something is valid?
  - Show it’s a scalar product
  - Show positive semidefinite kernel matrix
  - Best: compose new kernels from old kernels

Kernel Operations

- Many operations over kernels yield new kernels
  - $K(x, x') = cK_1(x, x')$
  - $K(x, x') = f(x)K_1(x, x')f(x')$
  - $K(x, x') = \exp(K_1(x, x'))$
  - $K(x, x') = K_1(x, x') + K_2(x, x')$
  - $K(x, x') = K_1(x, x')K_2(x, x')$

Gaussian Kernel

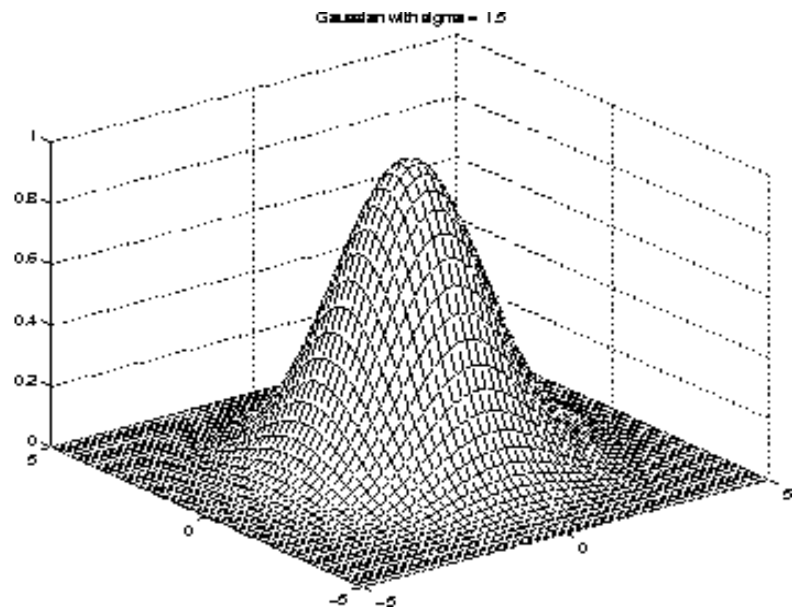
- Use a Gaussian to define a kernel
  - Since this is not a probability drop the normalization
    $$K(x, x') = \exp(-\|x - x'\|^2 / 2\sigma^2)$$
  - Why is this a valid kernel?
  - Expand the square
    $$\|x - x'\|^2 = x^T x + x'^T x' - 2x^T x'$$
  - Substitute

$K(x, x')$
$= \exp(-x^T x / 2\sigma^2) \exp(-x'^T x' / 2\sigma^2) \exp(2x^T x' / 2\sigma^2)$

$$K(x, x') = f(x) K_1(x, x') f(x')$$

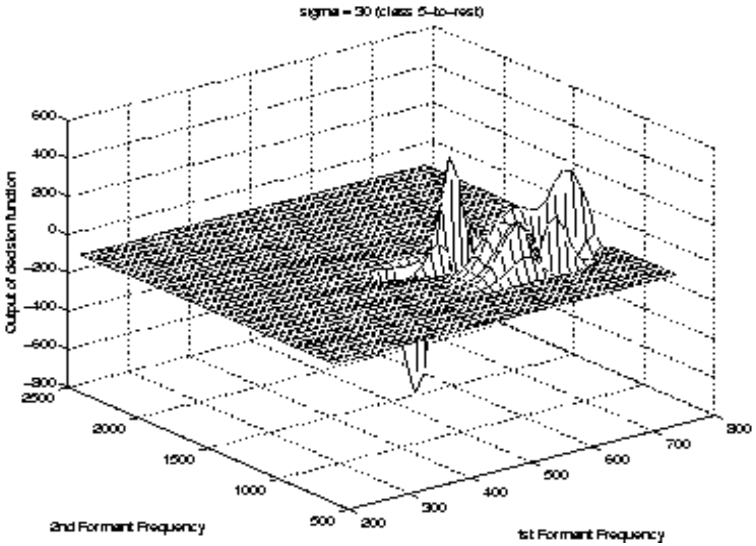
$$K(x, x') = \exp(K_1(x, x'))$$

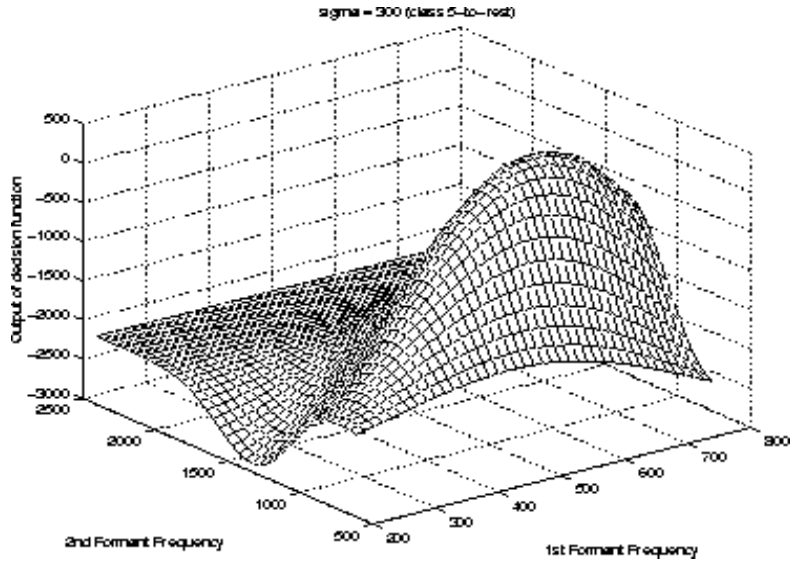
Gaussian Kernel



- Three dimensional Gaussian
  - σ determines the smoothness of the function
  - Large σ means the support vector has greater influence area
    - Less support vectors needed to cover boundaries

Decision Boundary





Smaller σ

Larger σ

Kernels for Objects

- We've talked about kernels as operating over $x \in \Re^M$
- However, we can define x as anything
  - As long as we can compute $K(x, x')$
- Kernels for
  - Strings
  - Trees/Graphs
  - Images

Kernels for Strings

- Represent a document as a feature vector
  - Each feature corresponds to a word in the document
  - Classify document based on the words
- Even better: each feature corresponds to a sub-string in the document
  - Include non-contiguous sub-strings
  - Value of feature is dependent on frequency of where it appears
- For sub-strings of size > 4 cannot compute this feature space
  - Way too many features!

Kernels for Strings

- String Subsequence Kernel

$$K(x, x') = \sum_{u \in \Sigma^d} \sum_{i: u = x[i]} \sum_{j: u = x\prime[j]} \lambda^{|i|+|j|}$$

  - For all string u of length d
  - For all substrings of x
  - For all substrings of x'
  - λ to the power of the size of the combined lengths
- Computing features would take $O(|\Sigma|^d)$ time
- Can compute the kernel for this feature representation using dynamic programming

Biology: Splice Site Recognition

- Find the boundary between exons and introns in eukaryotes (complex organism)
  - What part of DNA codes for genes
- Input is a sequence of DNA base pairs
- Normally each feature indicates a substring of base pairs appearing in the sequence

Biology: Splice Site Recognition

- Each possible substring of DNA is a new feature
- Use the kernel approach as for strings
- Problem for DNA: long substrings unlikely but still informative
- Solution: a kernel from many weighted spectrum kernels

Other Kernel Methods

Kernel Perceptron

- We showed a derivation for dual Perceptron

$$\hat{y} = sign(\sum_{i=1}^{N} \alpha_i y_i x_i x)$$

  - $\alpha_i = 1$ if we made a mistake on round i

- Replace the dot product with a kernel

$$\hat{y} = sign(\sum_{i=1}^{N} \alpha_i y_i K(x_i, x))$$

Kernel Linear Regression

- We can define linear regression with quadratic regularization using a linear combination of x

$$w = -\frac{1}{\lambda}\sum_{i=1}^{N}\{w^T\phi(x_i) - y_i\}\phi(x_i) = \sum_{i=1}^{N}\alpha_i\phi(x_i)$$

- So we can get a kernel version

$$w^T\phi(x) = k(x)^T(\boldsymbol{K} + \lambda\boldsymbol{I})^{-1}\boldsymbol{Y}$$
$$k_i(x)^T = K(x_i, x)$$

Kernel Logistic Regression

- We can do the same trick with logistic regression
- Represent w in terms of x and α

$$w = \sum_{i=1}^{N} \alpha_i \phi(x_i)$$

- Insert a kernel in place of a dot product in the model

$$P(y = 1|x, w) = \frac{1}{1 + \exp\{-\sum_{i=1}^{N} \alpha_i K(x, x_i) + b\}}$$

- Derive new gradient descent rule on α

Summary

- The good
  - Arbitrarily high dimensionality
  - Extensions to other data types
  - Non-linearity in a parametric linear framework
- The bad
  - What is a good kernel?
    - Whole field on designing kernels, learning kernels
  - Cannot handle large data
    - Kernel matrix grows quadratic in N