CPSC 340:
Machine Learning and Data Mining

Kernel Trick

Fall 2017

Admin

- Assignment 3:
  - Due Friday.

- Midterm:
  - Can view your exam during instructor office hours or after class this week.

Digression: the "other" Normal Equations

- Recall the L2-regularized least squares objective:

$$f(w) = \frac{1}{2}\|Xw - y\|^2 + \frac{\lambda}{2}\|w\|^2$$

- We showed that the minimum is given by

$$w = \underbrace{(X^TX + \lambda I)^{-1}}_{d \times d} X^Ty$$

(in practice you still solve the linear system, since inverse can be numerically unstable – see CPSC 302)

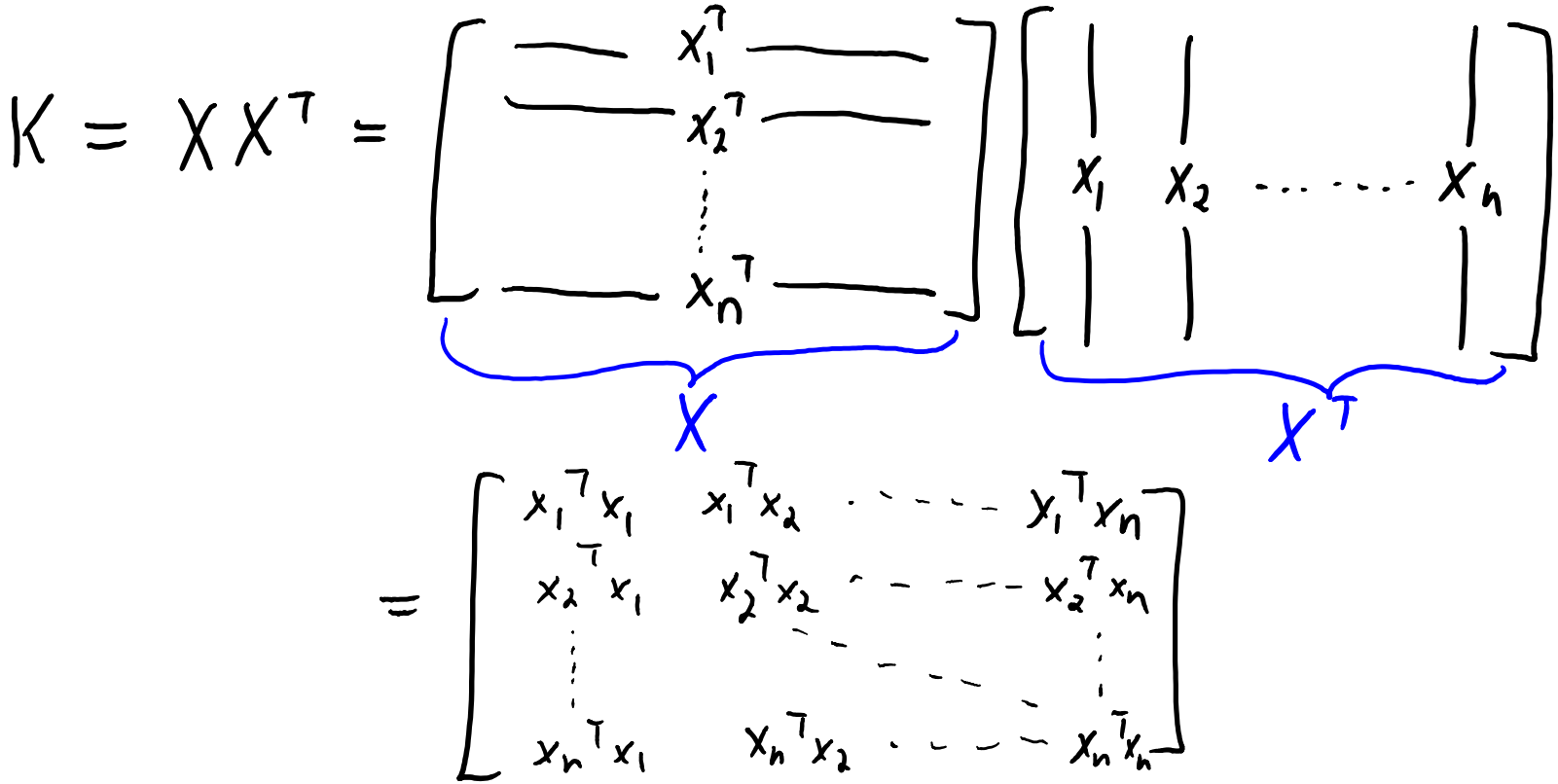
- With some work (bonus), this can equivalently be written as:

$$w = X^T\underbrace{(XX^T + \lambda I)^{-1}}_{n \times n} y$$

- This is faster if n << d:
  - Cost is $O(n^2d + n^3)$ instead of $O(nd^2 + d^3)$.

Gram Matrix

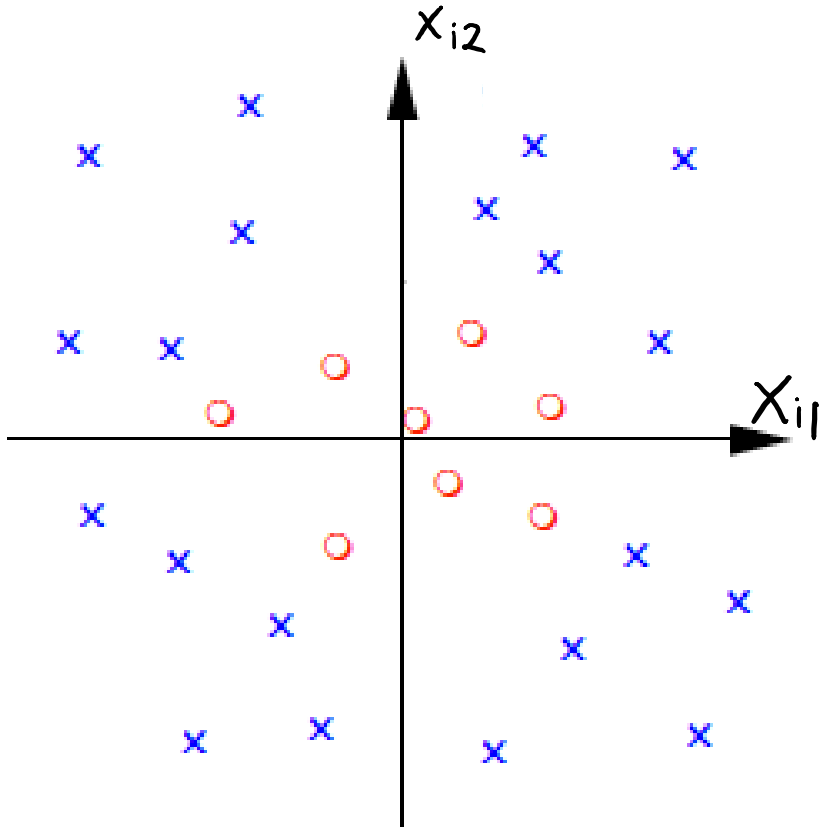
- The matrix XX^T is called the Gram matrix K.



- K contains the inner products between all training examples.
  - Similar to 'Z' in RBFs, but using dot product as "similarity" instead of distance.

Support Vector Machines for Non-Separable

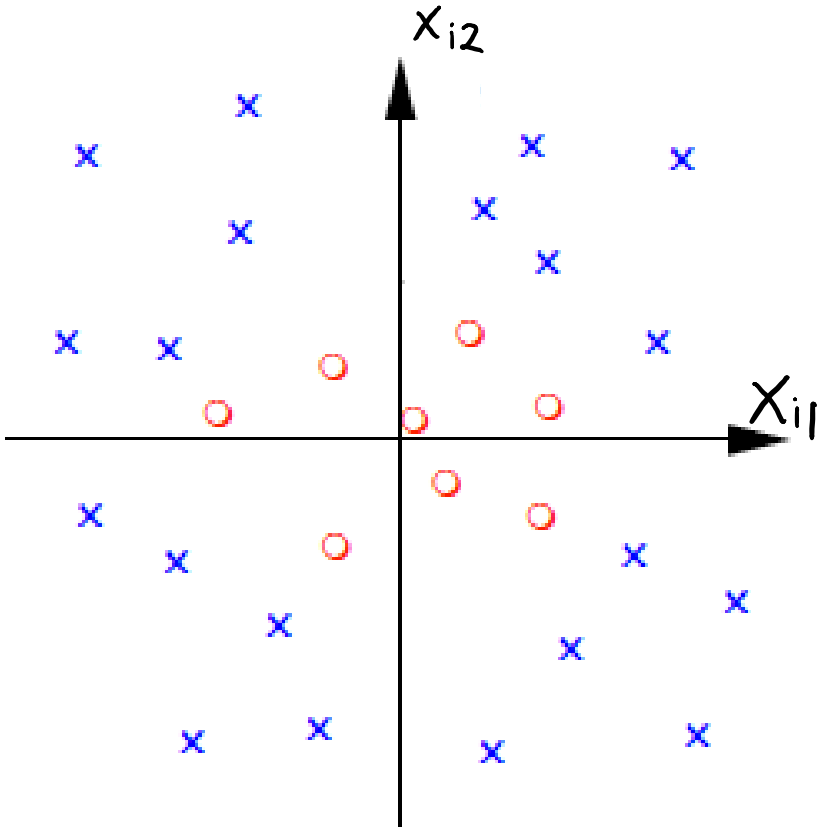
- What about data that is not even close to separable?

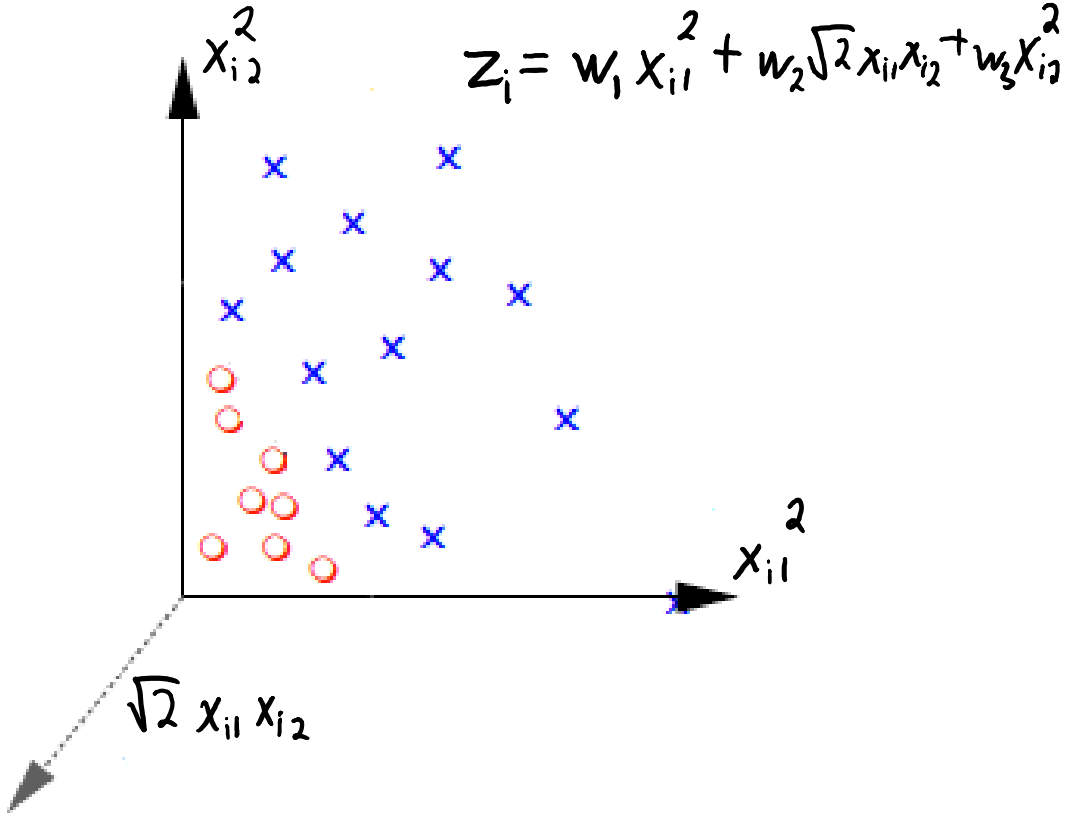


http://math.stackexchange.com/questions/353607/how-do-inner-product-space-determine-half-planes

Support Vector Machines for Non-Separable

- What about data that is not even close to separable?
  - It may be separable under change of basis (or closer to separable).

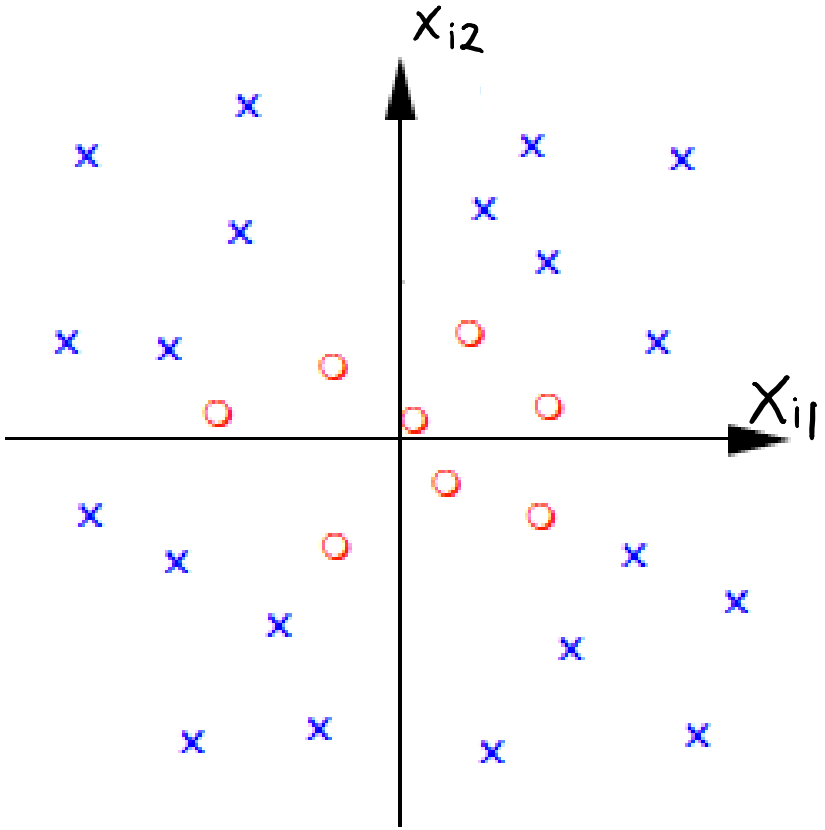


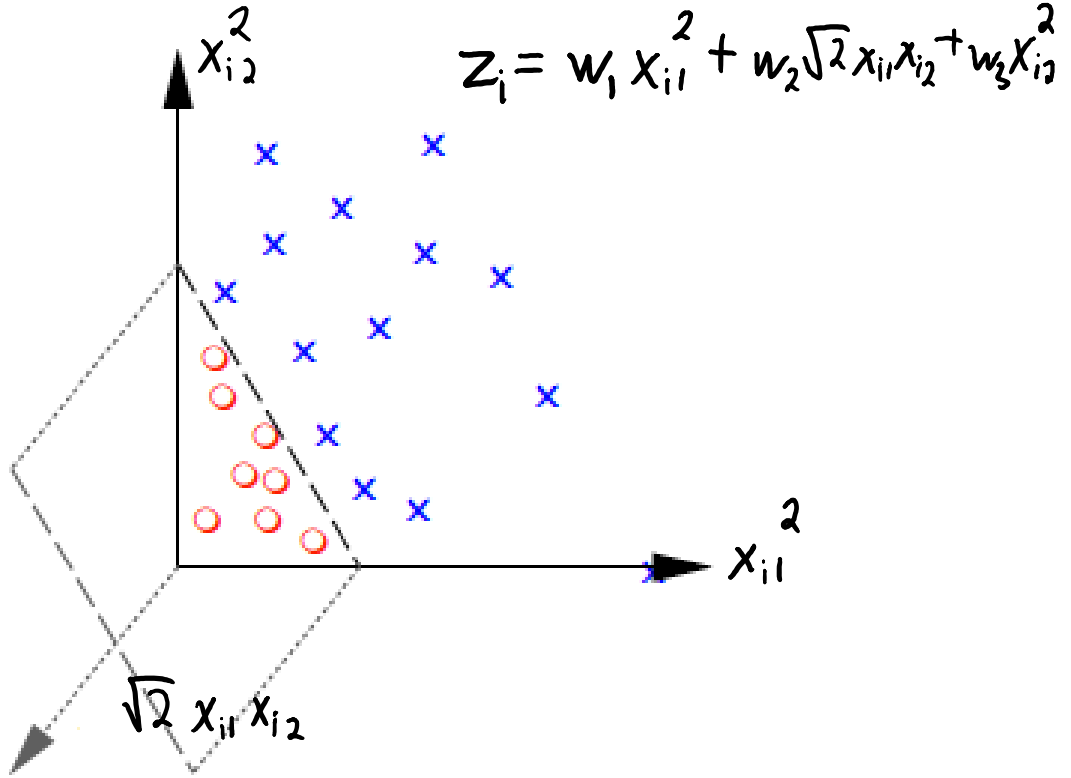


http://math.stackexchange.com/questions/353607/how-do-inner-product-space-determine-half-planes

Support Vector Machines for Non-Separable

- What about data that is not even close to separable?
  - It may be separable under change of basis (or closer to separable).





http://math.stackexchange.com/questions/353607/how-do-inner-product-space-determine-half-planes

Multi-Dimensional Polynomial Basis

- Recall fitting polynomials when we only have 1 feature:

$$y_i = w_0 + w_1 x_i + w_2 x_i^2$$

- We can fit these models using a change of basis:

$$X = \begin{bmatrix} 0.2 \\ -0.5 \\ 1 \\ 4 \end{bmatrix} \qquad Z = \begin{bmatrix} 1 & 0.2 & (0.2)^2 \\ 1 & -0.5 & (-0.5)^2 \\ 1 & 1 & (1)^2 \\ 1 & 4 & (4)^2 \end{bmatrix}$$

- How can we do this when we have a lot of features?

Multi-Dimensional Polynomial Basis

- Polynomial basis for d=2 and p=2:

$$X = \begin{bmatrix} 0.2 & 0.3 \\ 1 & 0.5 \\ -0.5 & -0.1 \end{bmatrix} \longrightarrow Z = \begin{bmatrix} 1 & 0.2 & 0.3 & (0.2)^2 & (0.3)^2 & (0.1)(0.3) \\ 1 & 1 & 0.5 & (1)^2 & (0.5)^2 & (1)(0.5) \\ 1 & 0.5 & -0.1 & (0.5)^2 & (-0.1)^2 & (-0.5)(-0.1) \end{bmatrix}$$

bias x_{i1} x_{i2} $(x_{i1})^2$ $(x_{i2})^2$ $(x_{i1})(x_{i2})$

- With d=4 and p=3, the polynomial basis would include:
  - Bias variable and the x_{ij}: 1, x_{i1}, x_{i2}, x_{i3}, x_{i4}.
  - The x_{ij} squared and cubed: $(x_{i1})^2$, $(x_{i2})^2$, $(x_{i3})^2$, $(x_{i4})^2$, $(x_{i1})^3$, $(x_{i2})^3$, $(x_{i3})^3$, $(x_{i4})^3$.
  - Two-term interactions: $x_{i1}x_{i2}$, $x_{i1}x_{i3}$, $x_{i1}x_{i4}$, $x_{i2}x_{i3}$, $x_{i2}x_{i4}$, $x_{i3}x_{i4}$.
  - Cubic interactions: $x_{i1}x_{i2}x_{i3}$, $x_{i2}x_{i3}x_{i4}$, $x_{i1}x_{i3},x_{i4}$,
    $x_{i1}^2x_{i2}$, $x_{i1}^2x_{i3}$, $x_{i1}^2x_{i4}$, $x_{i1}x_{i2}^2$, $x_{i2}^2x_{i3}$, $x_{i2}^2x_{i4}$, $x_{i1}x_{i3}^2$, $x_{i2}x_{i3}^2$,$x_{i3}^2x_{i4}$, $x_{i1}x_{i4}^2$, $x_{i2}x_{i4}^2$, $x_{i3}x_{i4}^2$.

Kernel Trick

- If we go to degree p=5, we'll have $O(d^5)$ quintic terms:

$$x_{i1}^5, x_{i1}^4 x_{i2}, x_{i1}^4 x_{i3}, \ldots, x_{i1}^4 x_{id}, x_{i1}^3 x_{i2}^2, x_{i1}^3 x_{i3}^2, \ldots, x_{i1}^3 x_{id}^2, \ldots, x_{i2}^5, x_{i2}^4 x_{i3}, \ldots, x_{id}^5$$

  - For large 'd' and 'p', we can't even store 'Z' or 'w'.

- But, we can use this basis efficiently with the kernel trick (medium 'n').

- Basic idea:
  - We can sometimes efficiently compute dot product $z_i^T z_j$ directly from x_i and x_j.
  - Use this to make the Gram matrix ZZ^T and make predictions.

Kernel Trick

- Given test data $\hat{X}$, predict $\hat{y}$ by forming and $\hat{Z}$ using:

$$\hat{y} = \hat{Z}w \quad \leftarrow \quad w = Z^T(ZZ^T + \lambda I)^{-1}y$$

$$= \hat{Z}Z^T(ZZ^T + \lambda I)^{-1}y$$

$$= \hat{K}(K + \lambda I)^{-1}y$$

($\hat{K}$: $t \times n$, K: $n \times n$, y: $n \times 1$, result: $t \times 1$)

- Key observation behind kernel trick:
  - Predictions $\hat{y}$ only depend on features through K and $\hat{K}$.
  - If we have a function that computes K and $\hat{K}$, we don't need the features.

Kernel Trick

- 'K' contains the inner products between all training examples.
  - Intuition: inner product can be viewed as a measure of similarity, so this matrix gives a similarity between each pair of examples.
- '$\widehat{K}$' contains the inner products between training and test examples.

- Kernel trick:
  - I want to use a basis z_i that is too huge to store (very large 'd').
  - But I only need z_i to compute Gram matrix $K = ZZ^T$ and $\widehat{K} = \hat{Z}Z^T$.
    - The sizes of these matrices are independent of d.
    - Everything we need to know about z_i is summarized by the $z_i^T z_j$.
  - I can use this basis if I have a kernel function that computes $k(x_i,x_j) = z_i^T z_j$.
    - I don't need to compute the basis z_i explicitly.

Example: Degree-2 Kernel

- Consider two examples x_i and x_j for a 2-dimensional dataset:

$$x_i = (x_{i1}, x_{i2}) \qquad x_j = (x_{j1}, x_{j2})$$

- And consider a particular degree-2 basis:

$$z_i = (x_{i1}^2, \sqrt{2}\, x_{i1} x_{i2}, x_{i2}^2) \qquad z_j = (x_{j1}^2, \sqrt{2}\, x_{j1} x_{j2}, x_{j2}^2)$$

- We can compute inner product $z_i^T z_j$ without forming z_i and z_j:

$$\begin{aligned} z_i^T z_j &= x_{i1}^2 x_{j1}^2 + (\sqrt{2}\, x_{i1} x_{i2})(\sqrt{2}\, x_{j1} x_{j2}) + x_{i2}^2 x_{j2}^2 \\ &= x_{i1}^2 x_{j1}^2 + 2 x_{i1} x_{i2} x_{j1} x_{j2} + x_{i1}^2 x_{i2}^2 \\ &= (x_{i1} x_{j1} + x_{i2} x_{j2})^2 \qquad \text{"completing the square"} \\ &\qquad (x_{i1} x_{j1} + x_{i2} x_{j2} = x_i^T x_j) \\ &= (x_i^T x_j)^2 \end{aligned}$$

← No need for z_i to compute $z_i^T z_j$

Polynomial Kernel with Higher Degrees

- Let's add a bias and linear terms to our degree-2 basis:

$$z_i = \begin{bmatrix} 1 & \sqrt{2}x_{i1} & \sqrt{2}x_{i2} & x_{i1}^2 & \sqrt{2}x_{i1}x_{i2} & x_{i2}^2 \end{bmatrix}^T$$

- I can compute inner products using:

$$(1 + x_i^T x_j)^2 = 1 + 2x_i^T x_j + (x_i^T x_j)^2$$

$$= 1 + 2x_{i1}x_{j1} + 2x_{i2}x_{j2} + x_{i1}^2 x_{j1}^2 + 2x_{i1}x_{i2}x_{j1}x_{j2} + x_{i2}^2 x_{j2}^2$$

$$= \underbrace{\begin{bmatrix} 1 & \sqrt{2}x_{i1} & \sqrt{2}x_{i2} & x_{i1}^2 & \sqrt{2}x_{i1}x_{i2} & x_{i2}^2 \end{bmatrix}}_{z_i^T} \underbrace{\begin{bmatrix} 1 \\ \sqrt{2}x_{j1} \\ \sqrt{2}x_{j2} \\ x_{j2}^2 \\ \sqrt{2}x_{j1}x_{j2} \\ x_{j2}^2 \end{bmatrix}}_{z_j}$$

$$= z_i^T z_j$$

Polynomial Kernel with Higher Degrees

- To get all degree-4 "monomials" I can use:

$$z_i^T z_j = (x_i^T x_j)^4$$

Equivalent to using a z_i with weighted versions of $x_{i1}^4, x_{i1}^3 x_{i2}, x_{i1}^2 x_{i2}^2, x_{i1} x_{i2}^3, x_{i2}^4, \ldots$

- To also get lower-order terms use $z_i^T z_j = (1 + x_i^T x_j)^4$
- The general degree-p polynomial kernel function:

$$k(x_i, x_j) = (1 + x_i^T x_j)^p$$

  - Works for any number of features 'd'.
  - But cost of computing one $z_i^T z_j$ is $O(d)$ instead of $O(d^p)$.
  - Take-home message: I can compute dot-products without the features.

Kernel Trick with Polynomials

- Using polynomial basis of degree 'p' with the kernel trick:
  - Compute K and $\hat{K}$ using:

$$K_{ij} = (1 + x_i^T x_j)^p \qquad \hat{K}_{ij} = (1 + \hat{x}_i^T x_j)^p$$

test example; train example

  - Make predictions using:

$$\hat{y} = \hat{K}(K + \lambda I)^{-1} y$$

$\hat{y}$: $t \times 1$; $\hat{K}$: $t \times n$; $(K + \lambda I)^{-1}$: $n \times n$; y: $n \times 1$

- Training cost is only $O(n^2d + n^3)$, despite using $O(d^p)$ features.
  - We can form 'K' in $O(n^2d)$, and we need to "invert" an 'n x n' matrix.
  - Testing cost is only O(ndt), cost to formd $\hat{K}$.

Linear Regression vs. Kernel Regression

Linear Regression

Training

1. Form basis Z from X.
2. Compute $w = (Z^T Z + \lambda I)^{-1} \backslash (Z^T y)$

Testing

1. Form basis $\hat{Z}$ from $\hat{X}$
2. Compute $\hat{y} = \hat{Z} w$

Kernel Regression

Training:

1. Form inner products K from X.
2. Compute $v = (K + \lambda I)^{-1} \backslash y$

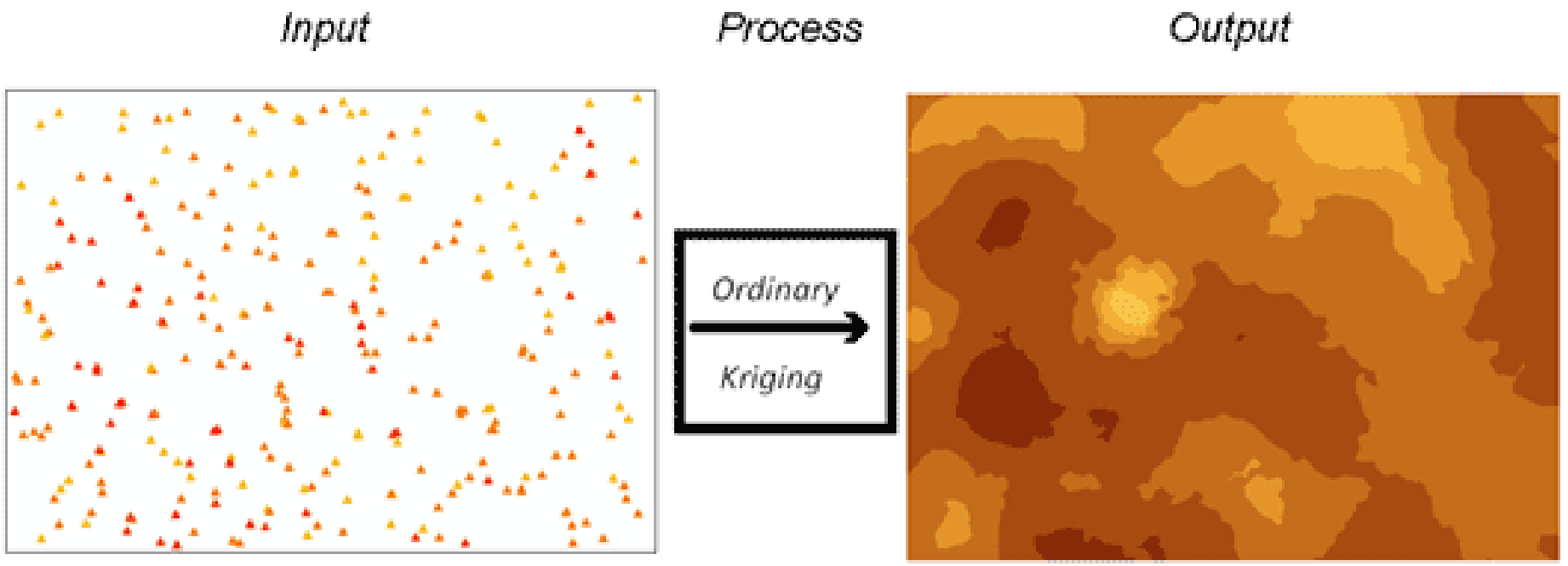
Non-parametric

Testing:

1. Form inner products $\hat{K}$ from X and $\hat{X}$
2. Compute $\hat{y} = \hat{K} v$

Motivation: Finding Gold

- Kernel methods first came from mining engineering ("Kriging"):
  - Mining company wants to find gold.
  - Drill holes, measure gold content.
  - Build a kernel regression model (typically use RBF kernels).



http://www.bisolutions.us/A-Brief-Introduction-to-Spatial-Interpolation.php

Gaussian-RBF Kernel

- Most common kernel is the Gaussian RBF kernel:

$$k(x_i, x_j) = \exp\left(-\frac{\|x_i - x_j\|^2}{2\sigma^2}\right)$$

- Same formula and behaviour as RBF basis, but not equivalent:
  - Before we used RBFs as a basis, now we're using them as inner-product.

- Basis z_i giving Gaussian RBF kernel is infinite-dimensional:
  - If d=1 and σ=1, it corresponds to using this basis (bonus slide):

$$z_i = \exp(-x_i^2)\left[1 \quad \sqrt{\frac{2}{1!}}x_i \quad \sqrt{\frac{2^2}{2!}}x_i^2 \quad \sqrt{\frac{2^3}{3!}}x_i^3 \quad \sqrt{\frac{2^4}{4!}}x_i^4 \quad \cdots\right]$$

Kernel Trick for Non-Vector Data

- Consider data that doesn't look like this:

$$X = \begin{bmatrix} 0.5377 & 0.3188 & 3.5784 \\ 1.8339 & -1.3077 & 2.7694 \\ -2.2588 & -0.4336 & -1.3499 \\ 0.8622 & 0.3426 & 3.0349 \end{bmatrix}, \quad y = \begin{bmatrix} +1 \\ -1 \\ -1 \\ +1 \end{bmatrix},$$

- But instead looks like this:

$$X = \begin{bmatrix} \text{Do you want to go for a drink sometime?} \\ \text{J'achète du pain tous les jours.} \\ \text{Fais ce que tu veux.} \\ \text{There are inner products between sentences?} \end{bmatrix}, y = \begin{bmatrix} +1 \\ -1 \\ -1 \\ +1 \end{bmatrix}.$$

- Kernel trick lets us fit regression models without explicit features:
  - We can interpret $k(x_i,x_j)$ as a "similarity" between objects x_i and x_j.
  - We don't need features if we can compute 'similarity' between objects.
  - There are "string kernels", "image kernels", "graph kernels", and so on.

Valid Kernels

- What kernel functions $k(x_i,x_j)$ can we use?

- Kernel 'k' must be an inner product in some space:
  - There must exist a mapping from x_i to some z_i such that $k(x_i,x_j) = z_i^T z_j$.

- It can be hard to show that a function satisfies this.
  - Infinite-dimensional eigenvalue equation.

- But like convex functions, there are some simple rules for constructing "valid" kernels from other valid kernels (bonus slide).

Kernel Trick for Other Methods

- Besides L2-regularized least squares, when can we use kernels?
  - We can compute Euclidean distance with kernels:

$$\|z_i - z_j\|^2 = z_i^T z_i - 2 z_i^T z_j + z_j^T z_j = k(x_i, x_i) - 2k(x_i, x_j) + k(x_j, x_j)$$

  - All of our distance-based methods have kernel versions:
    - Kernel k-nearest neighbours.
    - Kernel clustering k-means (allows non-convex clusters)
    - Kernel density-based clustering.
    - Kernel hierarchical clustering.
    - Kernel distance-based outlier detection.
    - Kernel “Amazon Product Recommendation”.

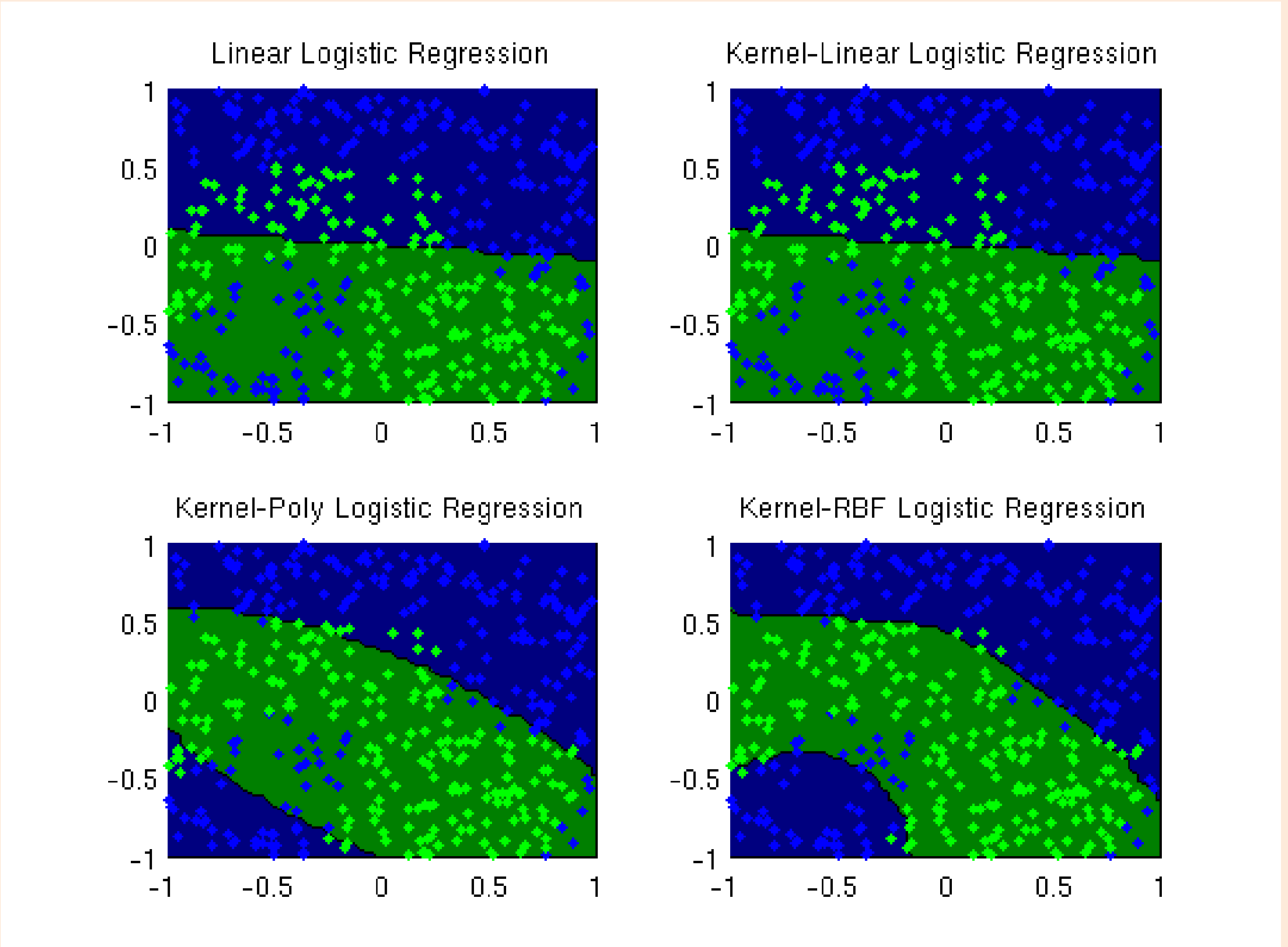
Kernel Trick for Other Methods

- Besides L2-regularized least squares, when can we use kernels?
  - "Representer theorems" (bonus slide) have shown that any L2-regularized linear model can be kernelized:
    - L2-regularized robust regression.
    - L2-regularized brittle regression.
    - L2-regularized logistic regression.
    - L2-regularized hinge loss (SVMs).

With a particular implementation, can reduce prediction cost from $O(ndt)$ to $O(mdt)$.

m: Number of support vectors.

Logistic Regression with Kernels



Summary

- High-dimensional bases allows us to separate non-separable data.
- Kernel trick allows us to use high-dimensional bases efficiently.
  - Write model to only depend on inner products between features vectors.

$$\hat{y} = \hat{K}(K + \lambda I)^{-1} y$$

$t \times n$ matrix $\hat{Z}Z^T$ containing inner products between test examples and training examples.

$n \times n$ matrix ZZ^T containing inner products between all training examples

- Kernels let us use similarity between objects, rather than features.
  - Allows some exponential- or infinite-sized feature sets.
  - Applies to L2-regularized linear models and distance-based models.

- Next time: how do we train on all of Gmail?

Why is inner product a similarity?

- It seems weird to think of the inner-product as a similarity.
- But consider this decomposition of squared Euclidean distance:

$$\frac{1}{2}\|x_i - x_j\|^2 = \frac{1}{2}\|x_i\|^2 - x_i^T x_j + \frac{1}{2}\|x_j\|^2$$

- If all training examples have the same norm, then minimizing Euclidean distance is equivalent to maximizing inner product.
  - So "high similarity" according to inner product is like "small Euclidean distance".
  - The only difference is that the inner product is biased by the norms of the training examples.
  - Some people explicitly normalize the x_i by setting $x_i = (1/||x_i||)x_i$, so that inner products act like the negation of Euclidean distances.

Bonus Slide: Equivalent Form of Ridge Regression

Note that $\hat{X}$ and Y are the same on the left and right side, so we only need to show that

$$(X^T X + \lambda I)^{-1} X^T = X^T (X X^T + \lambda I)^{-1}. \tag{1}$$

A version of the matrix inversion lemma (Equation 4.107 in MLAPP) is

$$(E - FH^{-1}G)^{-1} FH^{-1} = E^{-1}F(H - GE^{-1}F)^{-1}.$$

Since matrix addition is commutative and multiplying by the identity matrix does nothing, we can re-write the left side of (1) as

$$(X^T X+\lambda I)^{-1} X^T = (\lambda I+X^T X)^{-1} X^T = (\lambda I+X^T I X)^{-1} X^T = (\lambda I-X^T(-I)X)^{-1} X^T = -(\lambda I-X^T(-I)X)^{-1} X^T(-I)$$

Now apply the matrix inversion with $E = \lambda I$ (so $E^{-1} = \left(\frac{1}{\lambda}\right) I$), $F = X^T$, $H = -I$ (so $H^{-1} = -I$ too), and $G = X$:

$$-(\lambda I - X^T(-I)X)^{-1} X^T(-I) = -(\frac{1}{\lambda}) I X^T(-I - X\left(\frac{1}{\lambda}\right) X^T)^{-1}.$$

Now use that $(1/\alpha)A^{-1} = (\alpha A)^{-1}$, to push the $(-1/\lambda)$ inside the sum as $-\lambda$,

$$-(\frac{1}{\lambda}) I X^T(-I - X\left(\frac{1}{\lambda}\right) X^T)^{-1} = X^T(\lambda I + X X^T)^{-1} = X^T(X X^T + \lambda I)^{-1}.$$

Guasian-RBF Kernels

- The most common kernel is the Gaussian-RBF (or 'squared exponential') kernel,

$$k(x_i, x_j) = \exp\left(-\frac{\|x_i - x_j\|^2}{\sigma^2}\right).$$

- What function $\phi(x)$ would lead to this as the inner-product?
  - To simplify, assume $d = 1$ and $\sigma = 1$,

$$\begin{aligned} k(x_i, x_j) &= \exp(-x_i^2 + 2x_i x_j - x_j^2) \\ &= \exp(-x_i^2)\exp(2x_i x_j)\exp(-x_j^2), \end{aligned}$$

  so we need $\phi(x_i) = \exp(-x_i^2)z_i$ where $z_i z_j = \exp(2x_i x_j)$.
    - For this to work for *all* x_i and x_j, z_i must be infinite-dimensional.
  - If we use that

$$\exp(2x_i x_j) = \sum_{k=0}^{\infty} \frac{2^k x_i^k x_j^k}{k!},$$

  then we obtain

$$\phi(x_i) = \exp(-x_i^2)\left[1 \quad \sqrt{\tfrac{2}{1!}}x_i \quad \sqrt{\tfrac{2^2}{2!}}x_i^2 \quad \sqrt{\tfrac{2^3}{3!}}x_i^3 \quad \cdots\right].$$

Constructing Valid Kernels

- If $k_1(x_i, x_j)$ and $k_2(x_i, x_j)$ are valid kernels, then the following are valid kernels:
  - $k_1(\phi(x_i), \phi(x_j))$.
  - $\alpha k_1(x_i, x_j) + \beta k_2(x_i, x_j)$ for $\alpha \geq 0$ and $\beta \geq 0$.
  - $k_1(x_i, x_j) k_2(x_i, x_j)$.
  - $\phi(x_i) k_1(x_i, x_j) \phi(x_j)$.
  - $\exp(k_1(x_i, x_j))$.
- Example: Gaussian-RBF kernel:

$$k(x_i, x_j) = \exp\left(-\frac{\|x_i - x_j\|^2}{\sigma^2}\right)$$

$$= \underbrace{\exp\left(-\frac{\|x_i\|^2}{\sigma^2}\right)}_{\phi(x_i)} \underbrace{\exp\left(\underbrace{\frac{2}{\sigma^2}}_{\alpha \geq 0} \underbrace{x_i^T x_j}_{\text{valid}}\right)}_{\exp(\text{valid})} \underbrace{\exp\left(-\frac{\|x_j\|^2}{\sigma^2}\right)}_{\phi(x_j)}.$$

Representer Theorem

- Consider linear model differentiable with losses f_i and L2-regularization,

$$\underset{w \in \mathbb{R}^d}{\text{argmin}} \sum_{i=1}^{n} f_i(w^T x_i) + \frac{\lambda}{2}\|w\|^2.$$

- Setting the gradient equal to zero we get

$$0 = \sum_{i=1}^{n} f_i'(w^T x_i) x_i + \lambda w.$$

- So any solution w^* can written as a linear combination of features x_i,

$$\begin{aligned} w^* &= -\frac{1}{\lambda} \sum_{i=1}^{n} f_i'((w^*)^T x_i) x_i = \sum_{i=1}^{n} z_i x_i \\ &= X^T z. \end{aligned}$$

- This is called a representer theorem (true under much more general conditions).

Representer Theorem

- Using representer theorem we can use $w = X^T z$ in original problem,

$$\begin{aligned}
&\underset{w \in \mathbb{R}^d}{\text{argmin}} \sum_{i=1}^{n} f_i(w^T x_i) + \frac{\lambda}{2}\|w\|^2 \\
&= \underset{z \in \mathbb{R}^n}{\text{argmin}} \sum_{i=1}^{n} f_i(\underbrace{z^T X x_i}_{x_i^T X^T z}) + \frac{\lambda}{2}\|X^T z\|^2
\end{aligned}$$

- Now defining $f(z) = \sum_{i=1}^{n} f_i(z_i)$ for a vector z we have

$$\begin{aligned}
&= \underset{z \in \mathbb{R}^n}{\text{argmin}}\, f(XX^T z) + \frac{\lambda}{2} z^T XX^T z \\
&= \underset{z \in \mathbb{R}^n}{\text{argmin}}\, f(Kz) + \frac{\lambda}{2} z^T K z.
\end{aligned}$$

- Similarly, at test time we can use the n variables z,

$$\hat{X} w = \hat{X} X^T z = \hat{K} z.$$