

CPSC 340: Machine Learning and Data Mining

Kernel Trick

Admin

- **Assignment 4:**
 - Due Friday.
 - Hint for Q3.3 posted (and pinned) on Piazza.
- **Final exam:**
 - Saturday, April 14, 3:30pm-6pm
 - Location TBD

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

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

(in practice you don't actually invert the matrix because of numerical stability – see CPSC 302)

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

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

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

Gram Matrix

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

$$K = XX^T = \underbrace{\begin{bmatrix} \text{---} x_1^T \text{---} \\ \text{---} x_2^T \text{---} \\ \vdots \\ \text{---} x_n^T \text{---} \end{bmatrix}}_X \underbrace{\begin{bmatrix} | & | & \dots & | \\ x_1 & x_2 & \dots & x_n \\ | & | & \dots & | \end{bmatrix}}_{X^T}$$
$$= \begin{bmatrix} x_1^T x_1 & x_1^T x_2 & \dots & x_1^T x_n \\ x_2^T x_1 & x_2^T x_2 & \dots & x_2^T x_n \\ \vdots & \vdots & \ddots & \vdots \\ x_n^T x_1 & x_n^T x_2 & \dots & x_n^T x_n \end{bmatrix}$$

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

Jupyter demo (part 1)

Multi-Dimensional Polynomial Basis

- Recall fitting **polynomials** when we only have 1 feature:

$$\hat{y}_i = w_0 + w_1 x_i + w_2 x_i^2$$

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

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

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

Kernel Trick

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

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

- In general we have $O(d^p)$ terms (see bonus slides)
- For large 'd' and 'p', **we can't even store 'Z' or 'w'**.
- But, even though dimension of the basis, 'k', grows very rapidly with 'd' and 'p', for medium 'n' **we can use this basis efficiently** with the **kernel trick**.
- 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 using the "other" normal equations.

Kernel Trick

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

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

$$= \underbrace{\tilde{Z} Z^T}_{\tilde{K}} \underbrace{(ZZ^T + \lambda I)^{-1}}_K y$$

$${}^{t \times 1} = \underbrace{\tilde{K}}_{t \times n} \underbrace{(K + \lambda I)^{-1}}_{n \times n} \underbrace{y}_{n \times 1}$$

- Key observation behind **kernel trick**:

- Predictions \hat{y} only depend on features through K and \tilde{K} .
- If we have a function that computes K and \tilde{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.
- ‘ \tilde{K} ’ contains the inner products between training and test examples.
- Kernel trick summary:
 - I want to use a basis z_i that is too huge to store (very large ‘k’).
 - But I only need z_i to compute Gram matrix $K = ZZ^T$ and $\hat{K} = \hat{Z}Z^T$.
 - The sizes of these matrices are independent of k.
 - Everything we need to know about z_i is summarized by the n^2 values of $z_i^T z_j$.
 - 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 k-dimensional basis z_i explicitly.

Example: Degree-2 Kernel

- Consider two examples x_i and x_j with $d=2$:

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

- And consider a **particular basis with $k=3$** :

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

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

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

$$= (x_{i1} x_{j1} + x_{i2} x_{j2})^2 \quad \text{"completing the square"}$$

$$\underbrace{\hspace{10em}}_{x_i^T x_j}$$

$$= (x_i^T x_j)^2 \quad \leftarrow \text{No } \underline{\text{need}} \text{ for } z_i \text{ to compute } z_i^T z_j$$

Polynomial Kernel with Higher Degrees

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

$$z_i = [1 \quad \sqrt{2}x_{i1} \quad \sqrt{2}x_{i2} \quad x_{i1}^2 \quad \sqrt{2}x_{i1}x_{i2} \quad x_{i2}^2]^T$$

- I can compute **inner products** using:

$$\begin{aligned} (1 + x_i^T x_j)^2 &= 1 + 2x_i^T x_j + (x_i^T x_j)^2 \\ &= 1 + 2x_{i1}x_{j1} + 2x_{i2}x_{j2} + x_{i1}^2 x_{j1}^2 + 2x_{i1}x_{i2}x_{j1}x_{j2} + x_{i2}^2 x_{j2}^2 \end{aligned}$$

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

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 $x_{i1}^4, x_{i1}^3 x_{i2}, x_{i1}^2 x_{i2}^2, x_{i1} x_{i2}^3, x_{i2}^4, \dots$

- 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 \tilde{K} using:

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

\tilde{x}_i
test example
 x_j
train example

- Make predictions using:

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

\hat{y} (t x 1) \tilde{K} (t x n) $(K + \lambda I)^{-1}$ (n x n) y (n x 1)

- Training cost is only $O(n^2d + n^3)$, despite using $k=O(d^p)$ features.

- We can form 'K' in $O(n^2d)$, and we need to "invert" an 'n x n' matrix.

- Testing cost is $O(ndt)$, cost to form \tilde{K} .

Linear Regression vs. Kernel Regression

Linear Regression

Training

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

Testing

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

Kernel Regression

Training

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

Testing:

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

Non-parametric
↑

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 identical:
 - 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 $\sigma=1$, it corresponds to using this basis (bonus slide):

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

Kernel Trick for Non-Vector Data

- 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.

Kernel Trick for Other Methods

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

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

- 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 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 $O(mdt)$.
↑ Number of support vectors.⁹

Kernel trick continued

- Because of the support vectors, kernels are used with SVMs quite often, and much less so with logistic regression.

`sklearn.svm.SVC`

```
class sklearn.svm.SVC (C=1.0, kernel='rbf', degree=3, gamma='auto', coef0=0.0, shrinking=True, probability=False, tol=0.001, cache_size=200, class_weight=None, verbose=False, max_iter=-1, decision_function_shape=None, random_state=None)
```

[\[source\]](#)

`sklearn.linear_model.LogisticRegression`

```
class sklearn.linear_model.LogisticRegression (penalty='l2', dual=False, tol=0.0001, C=1.0, fit_intercept=True, intercept_scaling=1, class_weight=None, random_state=None, solver='liblinear', max_iter=100, multi_class='ovr', verbose=0, warm_start=False, n_jobs=1)
```

[\[source\]](#)

Jupyter demo (part 2)

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.

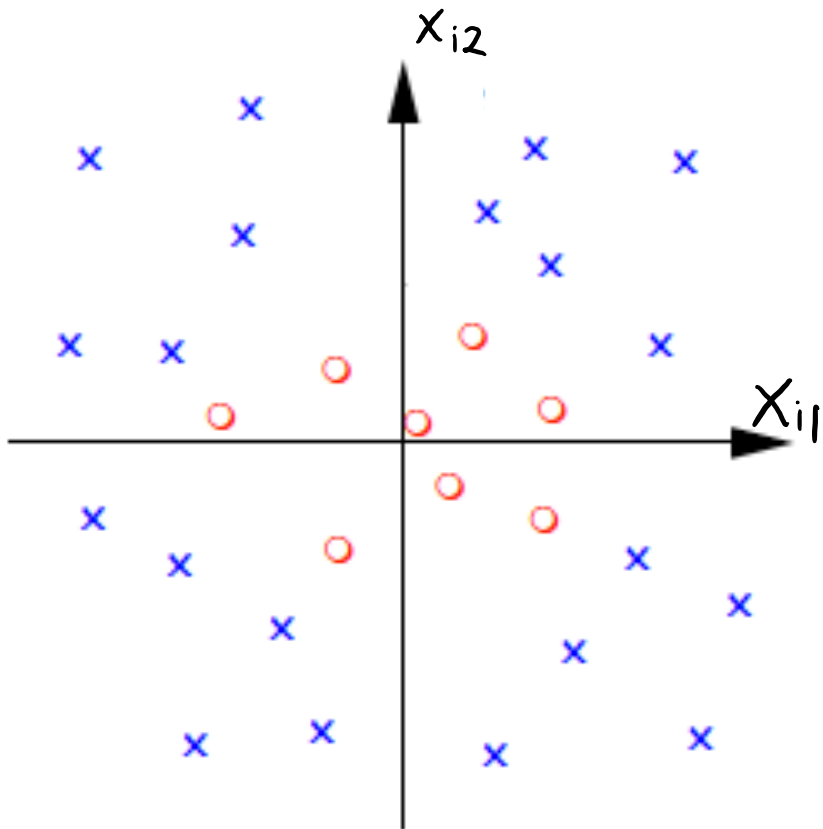
$$\hat{y} = \tilde{K} (K + \lambda I)^{-1} y$$

$t \times n$ matrix $\tilde{Z}Z^T$ 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.

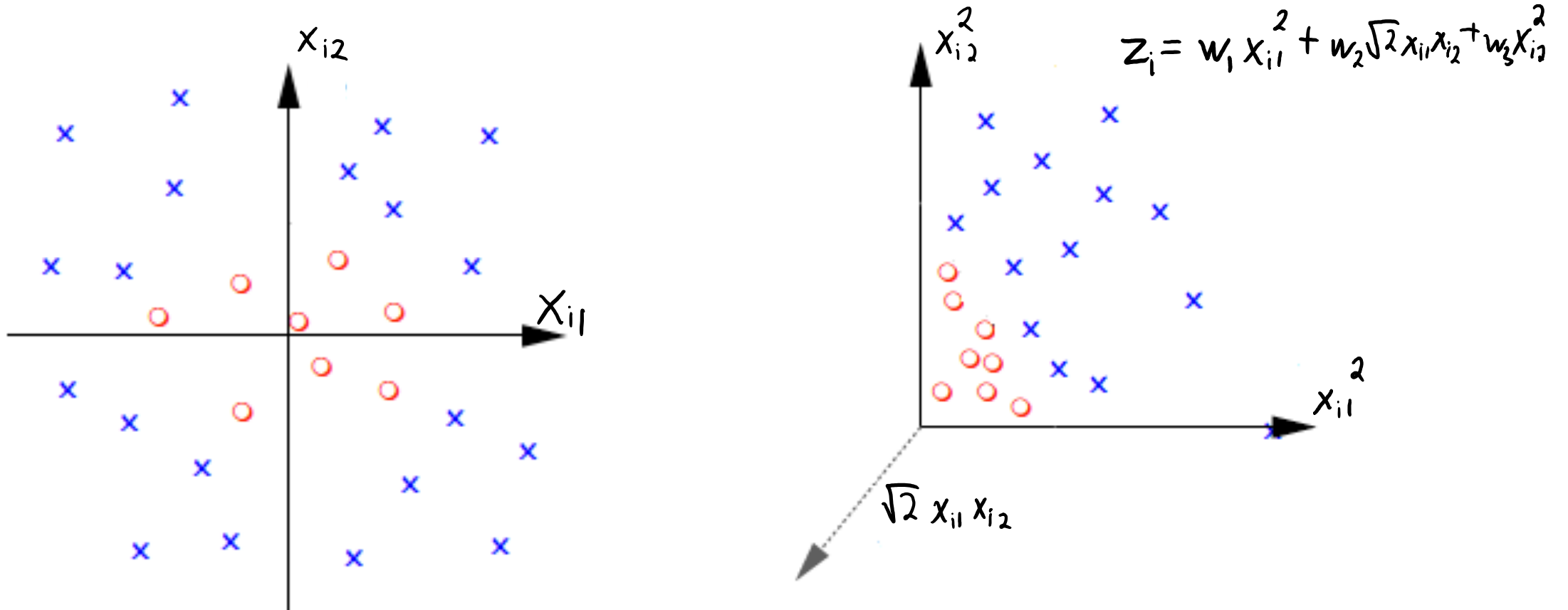
Support Vector Machines for Non-Separable

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



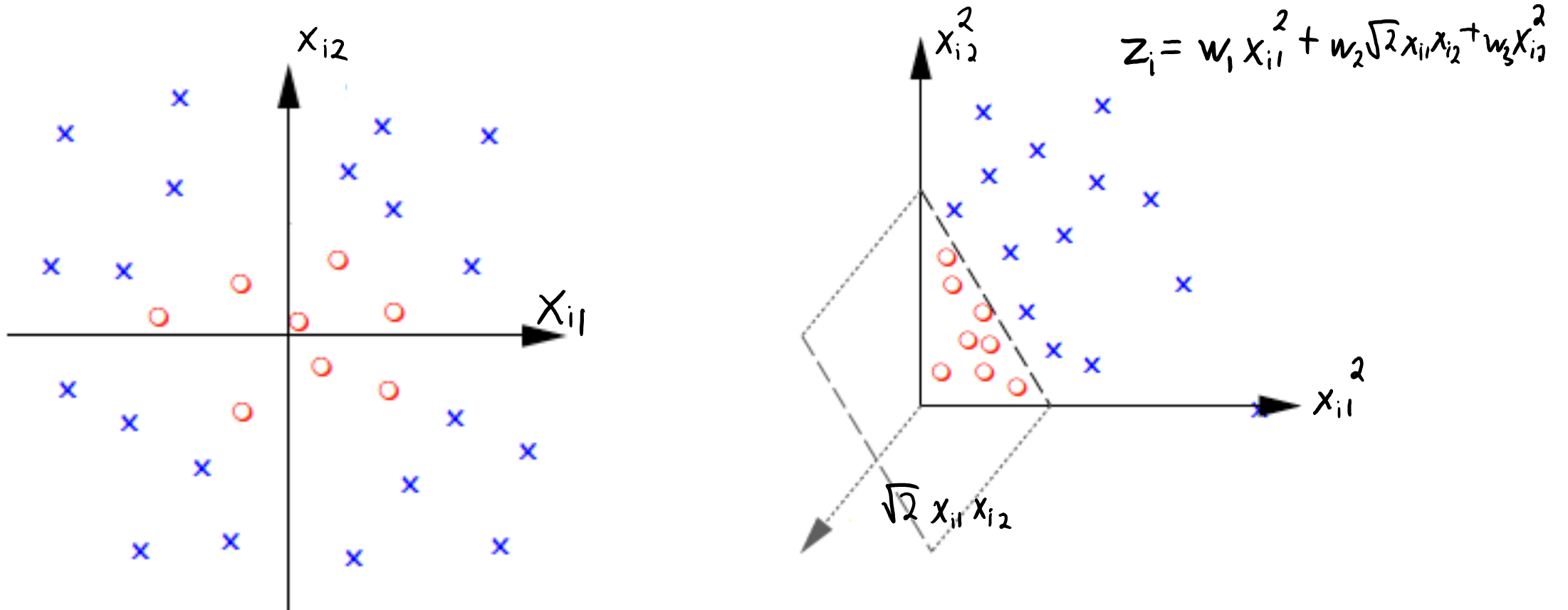
Support Vector Machines for Non-Separable

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



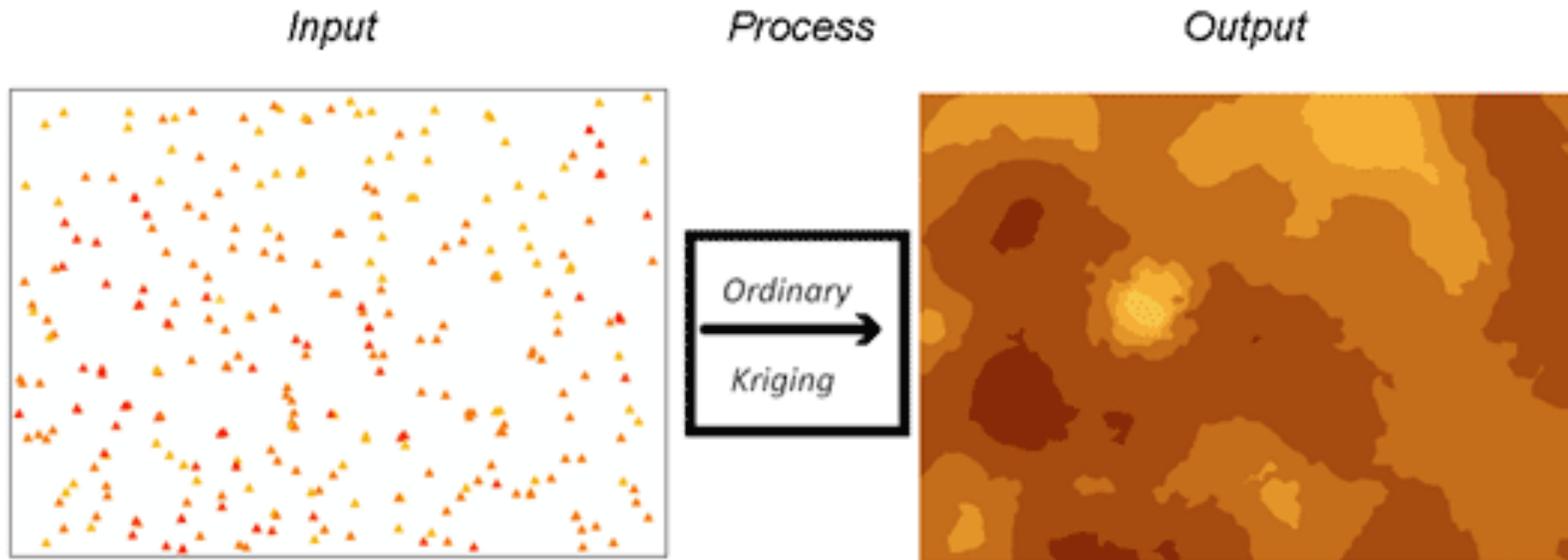
Support Vector Machines for Non-Separable

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



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).



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:

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

- 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.

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:

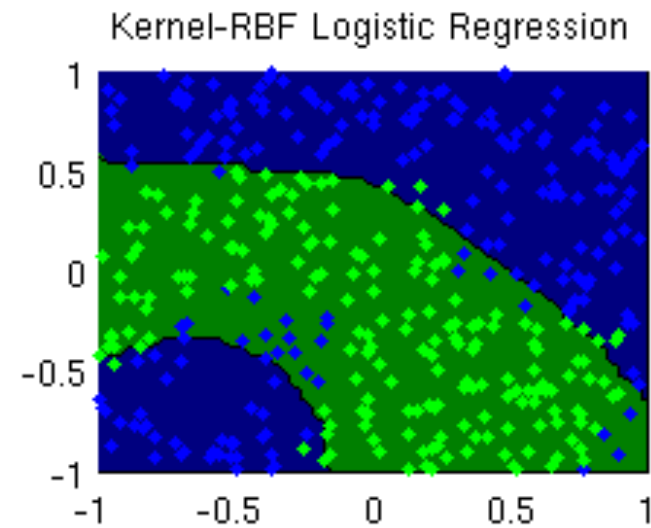
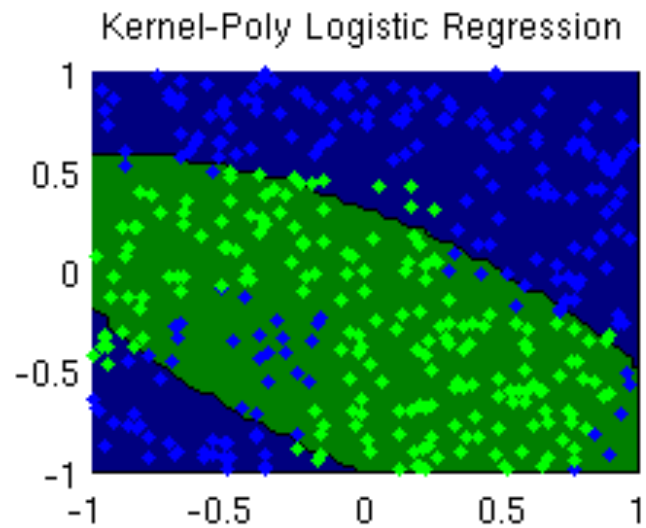
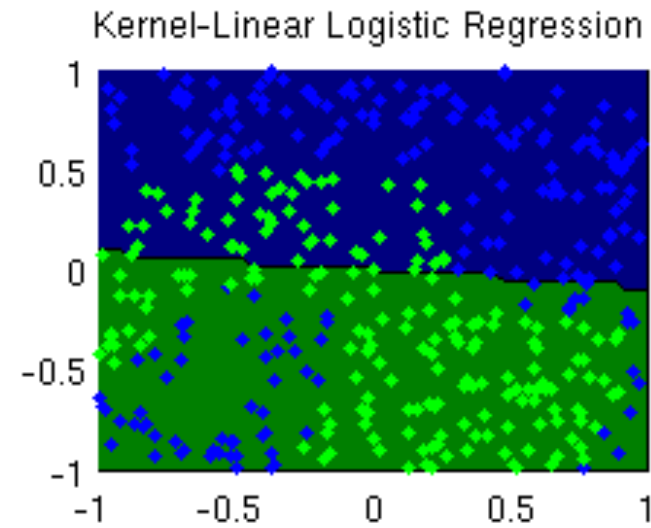
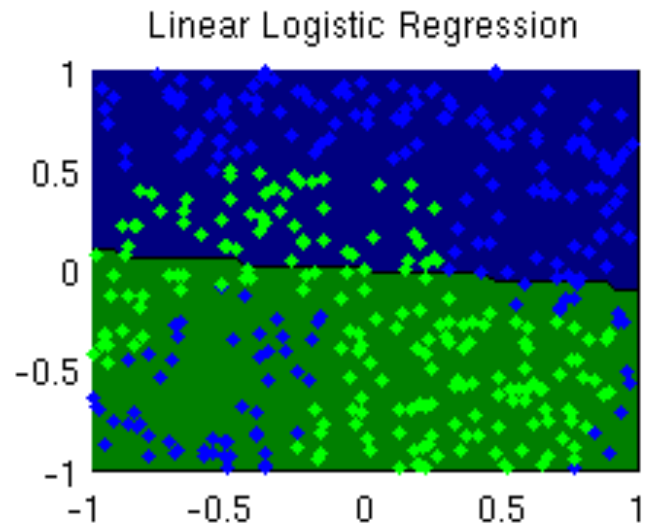
$$X = \begin{bmatrix} \text{Do you want to go for a drink sometime?} \\ \text{J'achète du pain tous les jours.} \\ \text{Fais ce que tu veux.} \\ \text{There are inner products between sentences?} \end{bmatrix}, \quad y = \begin{bmatrix} +1 \\ -1 \\ -1 \\ +1 \end{bmatrix}.$$

- 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).

Logistic Regression with Kernels



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

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

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 $E^{-1} = (\frac{1}{\lambda}) I$), $F = X^T$, $H = -I$ (so $H^{-1} = -I$ too), and $G = X$:

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

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

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

Gaussian-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

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

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:

$$\begin{aligned} k(x_i, x_j) &= \exp\left(-\frac{\|x_i - x_j\|^2}{\sigma^2}\right) \\ &= \underbrace{\exp\left(-\frac{\|x_i\|^2}{\sigma^2}\right)}_{\phi(x_i)} \underbrace{\exp\left(\frac{2}{\sigma^2} \underbrace{x_i^T x_j}_{\text{valid}}\right)}_{\exp(\text{valid})} \underbrace{\exp\left(-\frac{\|x_j\|^2}{\sigma^2}\right)}_{\phi(x_j)}. \end{aligned}$$

Representer Theorem

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

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

- 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 be 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).³⁴

Representer Theorem

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

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

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

$$\begin{aligned} &= \operatorname{argmin}_{z \in \mathbb{R}^n} f(X X^T z) + \frac{\lambda}{2} z^T X X^T z \\ &= \operatorname{argmin}_{z \in \mathbb{R}^n} f(K z) + \frac{\lambda}{2} z^T K z. \end{aligned}$$

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

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

Number of polynomials of degree p

- We have 'd' features, plus a “dummy” feature that's 1.
- Now for each term we get to pick 'p' of these $d+1$ possibilities, with repetition allowed.
 - For example, if I pick feature 1 twice, that means I have $(x_{i_1})^2$ in my term
 - The dummy feature allows for lower order terms (total degree less than p)
- How many times can we pick 'p' objects from a set of $d+1$ distinct choices with replacement, where order doesn't matter?
 - See https://en.wikipedia.org/wiki/Combination#Number_of_combinations_with_repetition
 - In their notation, $n=d+1$ and $k=p$
 - Answer: $d+p$ choose p , which is $(d+p)!/d!p!$ or approximately $d^p/p!$. We call this $O(d^p)$ which is true, and also a reasonable bound when $d \gg p$, although perhaps $O((d/p)^p)$ would be better.

RBF kernel vs RBF features

- Like the RBF features, the RBF kernel...
 - can learn any decision boundary given enough data
 - as a result it is prone to overfitting, so we need to use regularization
 - σ parameter controls smoothness: larger σ means smoother boundaries
 - This is called "gamma" in sklearn and it's $1/\sigma$
 - λ parameter controls regularization: larger λ means more regularization
 - This is called "C" in sklearn and it's $1/\lambda$
- The RBF features are finite-dimensional (n features)
- The RBF kernel corresponds to infinitely many features
- Both are non-parametric methods