The Kernel Trick

CS771: Introduction to Machine Learning

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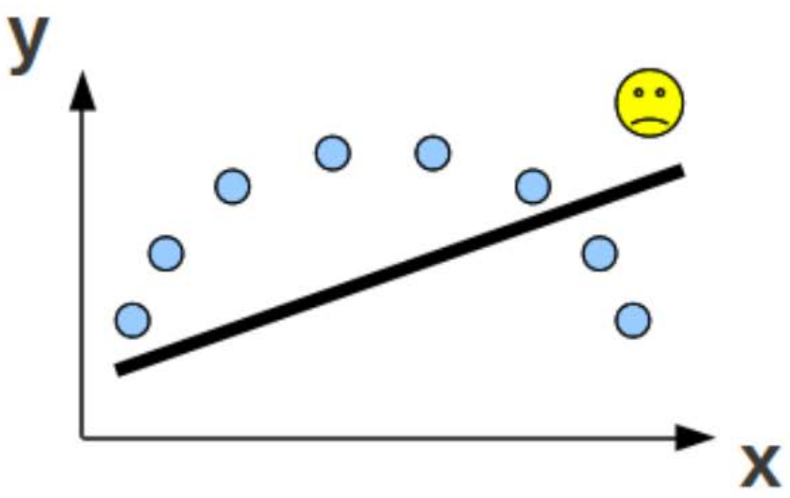
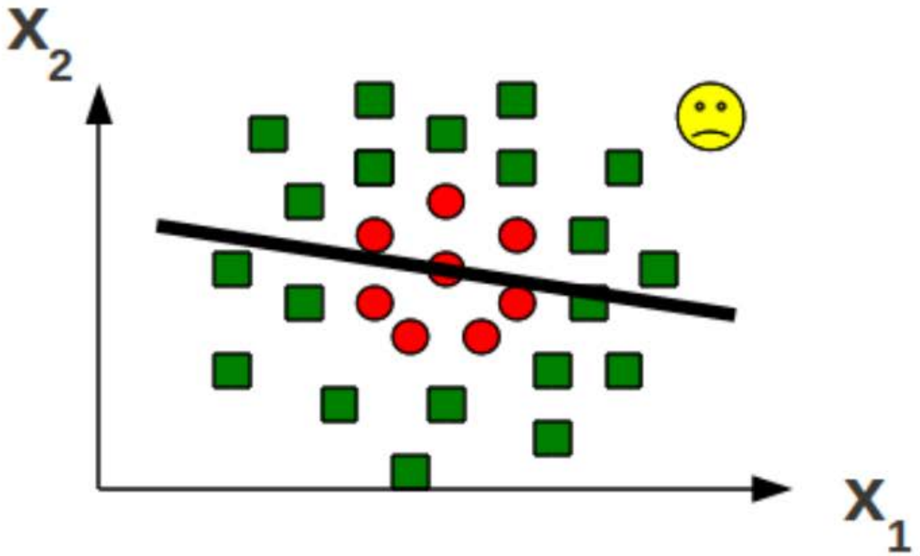
Logistics

- By now, all of you should have your mid sem results
  - Anyone who doesn't have them should email their TA, cc-ing me
- Assignment 3 will be released after Wednesday's class
  - Will be due next weekend (you will have 10 days)
- Quiz 3 will be this Friday
  - Syllabus is everything we covered until the last class
- Your TA will share complete course marks for all assessments in the course so far later this week
  - Please cross-check your marks and submit regrading requests if you find any discrepancies

Limits of linear Models

- Nice and interpretable but can’t learn nonlinear patterns

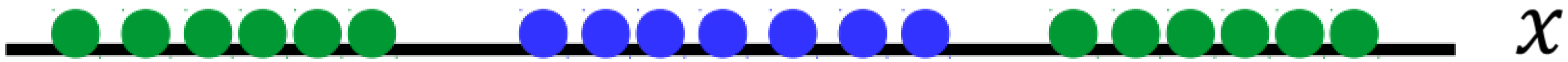




- So, are linear models useless for such problems?

Linear Models for Nonlinear Problems

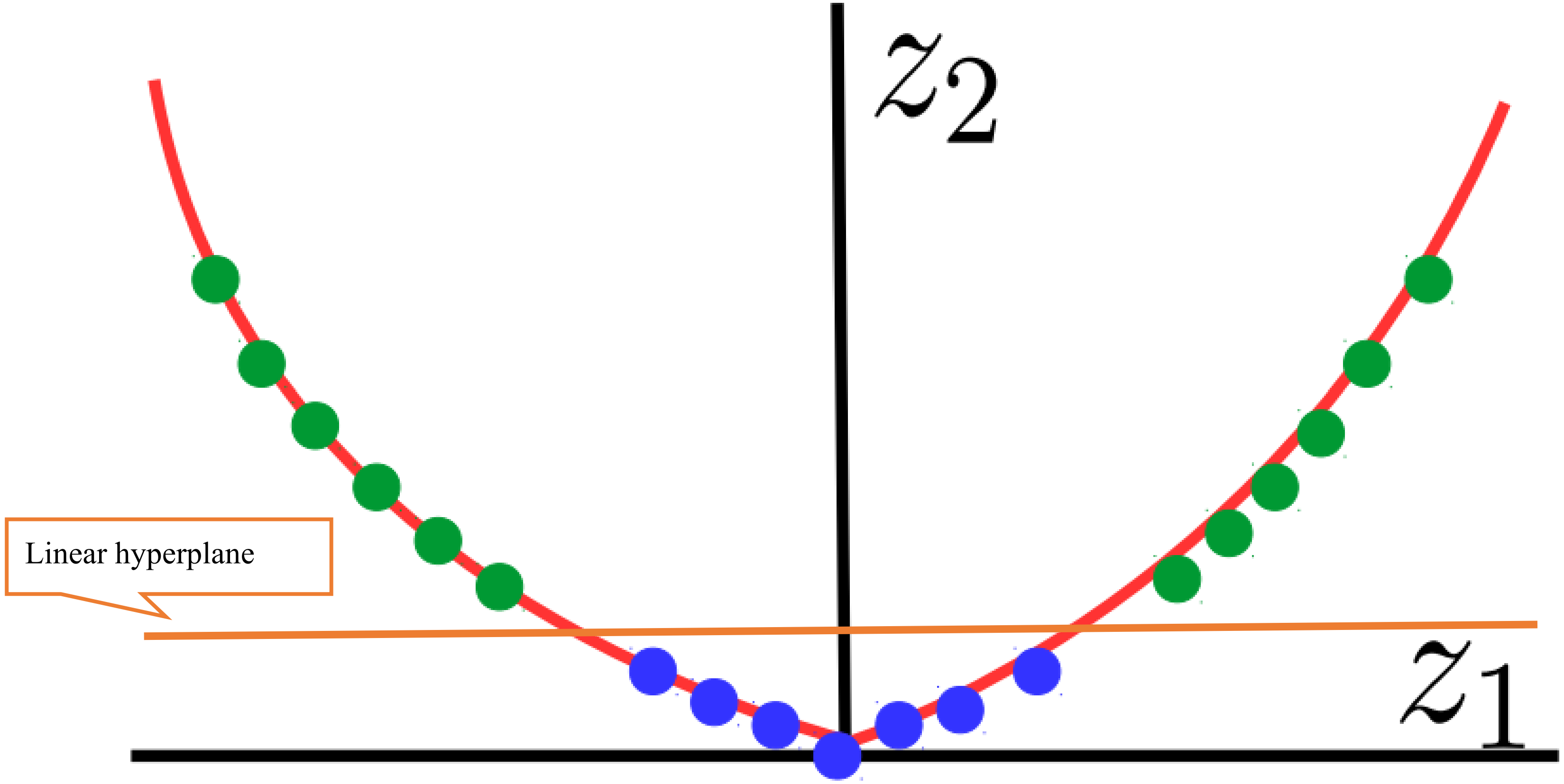
- Consider the following one-dimensional inputs from two classes



- Can't separate using a linear hyperplane

Linear Models for Nonlinear Problems

- Consider mapping each x to two-dimensions as $x \to \mathbf{z} = [z_1, z_2] = [x, x^2]$



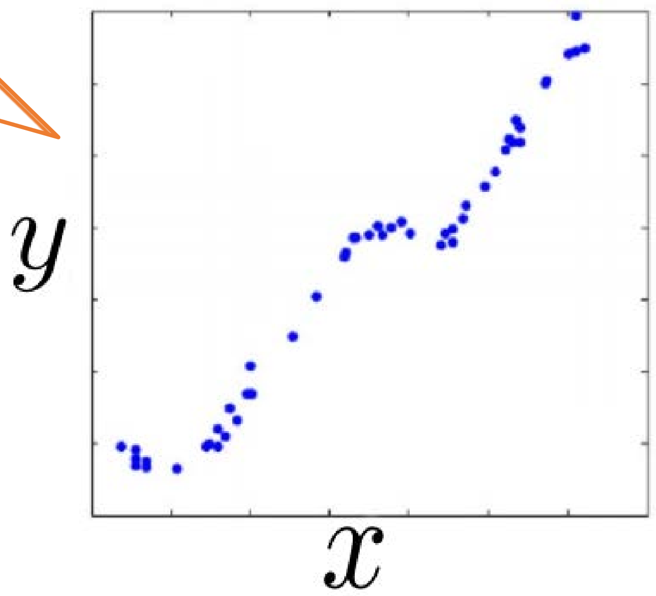
- Classes are now linearly separable in the two-dimensional space

Linear Models for Nonlinear Problems

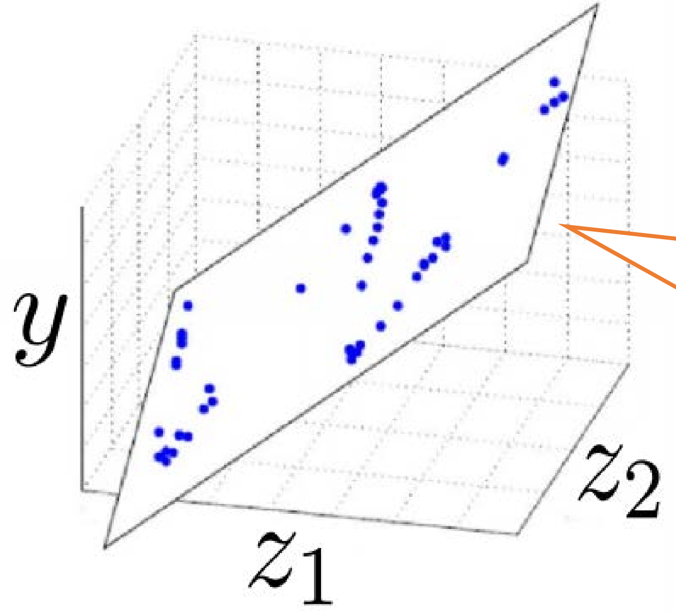
- The same idea can be applied for nonlinear regression as well

Not a linear relationship between inputs (x) and outputs (y)

A linear regression model will not work well



$$x \rightarrow \boldsymbol{z} = [z_1, z_2] = [x, \cos(x)]$$



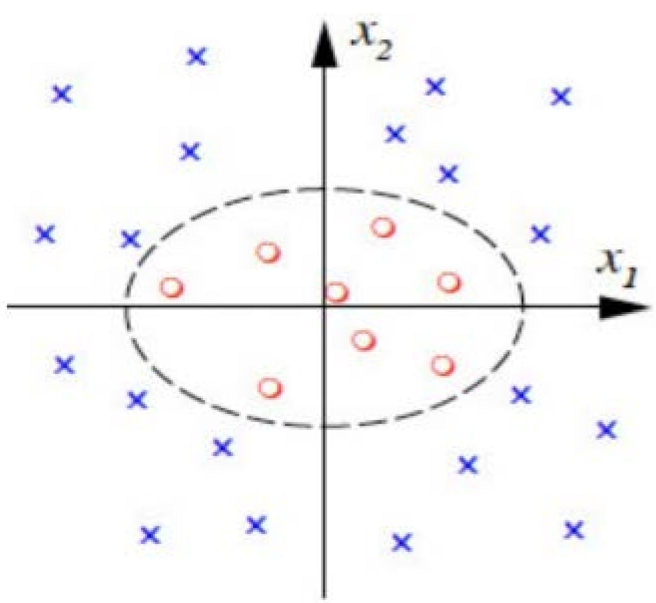
A linear regression model will work well with this new two-dim representation of the original one-dim inputs

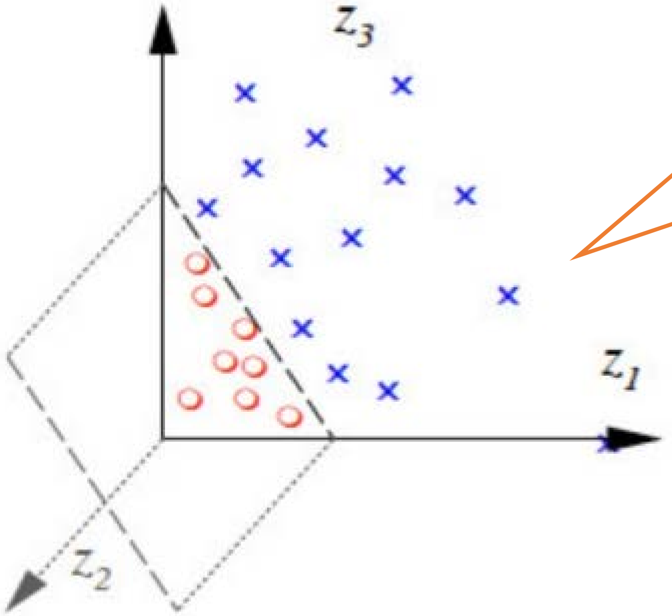
Linear Models for Nonlinear Problems

- Can assume a feature mapping $\boldsymbol{\phi}$ that maps/transforms the inputs to a “nice” space

$$\phi : \mathbb{R}^2 \rightarrow \mathbb{R}^3$$

$$(x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt(2)x_1x_2, x_2^2)$$



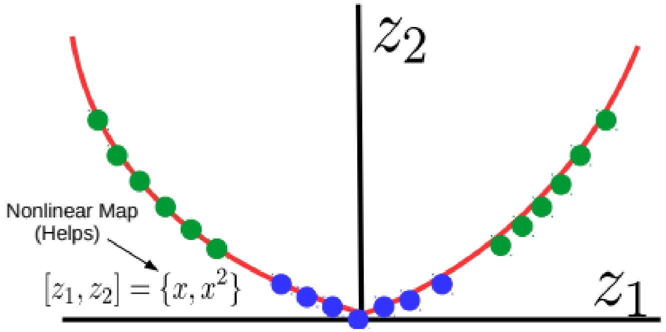


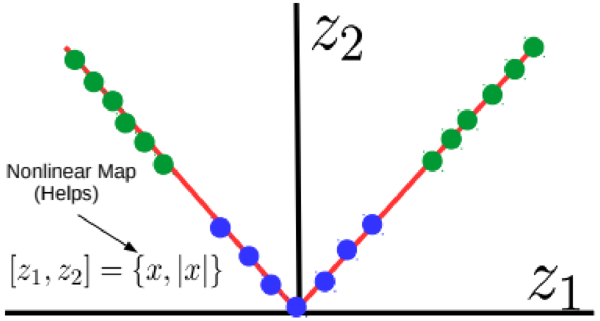
The linear model in the new feature space corresponds to a nonlinear model in the original feature space

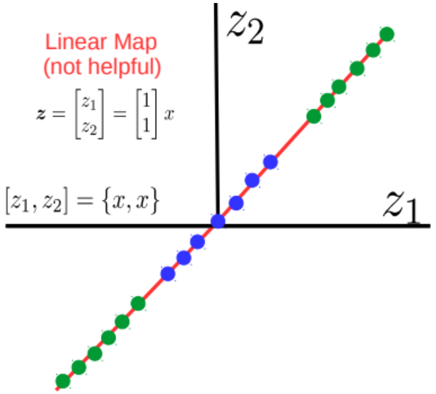
- .. and then happily apply a linear model in the new space!

Not Every Mapping is Helpful

- Not every higher-dim mapping helps in learning nonlinear patterns
- Must be a nonlinear mapping
- For the nonlinear classification problem we saw earlier, consider some possible mappings







How to get these “good” (nonlinear) mappings?

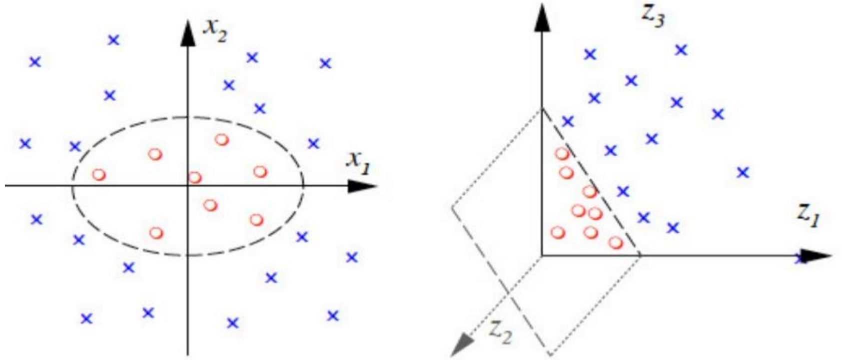
- Can try to learn the mapping from the data itself (e.g., using deep learning - later)
- Can use pre-defined “good” mappings (e.g., defined by kernel functions - today’s topic)

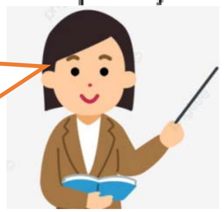
Even if I knew a good mapping, it seems I need to apply it for every input. Won’t this be computationally expensive?

Also, the number of features will increase? Will it not slow down the learning algorithm?

$$\phi : \mathbb{R}^2 \to \mathbb{R}^3$$

$$(x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt(2)x_1x_2, x_2^2)$$





Thankfully, using kernels, you don’t need to compute these mappings explicitly

The kernel will define an “implicit” feature mapping

Important: The idea can be applied to any ML algo in which training and test stage only require computing pairwise similarities b/w inputs

In a high-dim space implicitly defined by an underlying mapping $\boldsymbol{\phi}$ associated this this kernel function $\boldsymbol{k}(.,.)$

- Kernel: A function $\boldsymbol{k}(.,.)$ that gives dot product similarity b/w two inputs, say $\boldsymbol{x}_n$ and $\boldsymbol{x}_m$

Important: As we will see, computing $\boldsymbol{k}(.,.)$ does not require computing the mapping $\boldsymbol{\phi}$

$$k(\boldsymbol{x}_n, \boldsymbol{x}_m) = \phi(\boldsymbol{x}_n)^\top \phi(\boldsymbol{x}_m)$$

Kernels as (Implicit) Feature Maps

- Consider two inputs (in the same two-dim feature space): $\boldsymbol{x} = [x_1, x_2], \boldsymbol{z} = [z_1, z_2]$
- Suppose we have a function $k(.,.)$ which takes two inputs $\boldsymbol{x}$ and $\boldsymbol{z}$ and computes

Called the "kernel function"

$$k(\boldsymbol{x}, \boldsymbol{z}) = (\boldsymbol{x}^\top \boldsymbol{z})^2$$

Can think of this as a notion of similarity b/w $\boldsymbol{x}$ and $\boldsymbol{z}$

This is not a dot/inner product similarity but similarity using a more general function of $\boldsymbol{x}$ and $\boldsymbol{z}$ (square of dot product)

$$= (x_1 z_1 + x_2 z_2)^2$$

$$= x_1^2 z_1^2 + x_2^2 z_2^2 + 2 x_1 x_2 z_1 z_2$$

$$= (x_1^2, \sqrt{2} x_1 x_2, x_2^2)^\top (z_1^2, \sqrt{2} z_1 z_2, z_2^2)$$

$$= \phi(\boldsymbol{x})^\top \phi(\boldsymbol{z})$$

Didn't need to compute $\phi(x)$ explicitly. Just using the definition of the kernel $k(x, z) = (x^\top z)^2$ implicitly gave us this mapping for each input

Thus kernel function $k(\boldsymbol{x}, \boldsymbol{z}) = (\boldsymbol{x}^\top \boldsymbol{z})^2$ implicitly defined a feature mapping ϕ such that for $\boldsymbol{x} = [x_1, x_2]$, $\phi(\boldsymbol{x}) = (x_1^2, \sqrt{2} x_1 x_2, x_2^2)$

Dot product similarity in the new feature space defined by the mapping ϕ

Remember that a kernel does two things: Maps the data implicitly into a new feature space (feature transformation) and computes pairwise similarity between any two inputs under the new feature representation

- Also didn't have to compute $\phi(\boldsymbol{x})^\top \phi(\boldsymbol{z})$. Defn $k(\boldsymbol{x}, \boldsymbol{z}) = (\boldsymbol{x}^\top \boldsymbol{z})^2$ gives that

Kernel Functions

As we saw, kernel function $k(\boldsymbol{x},\boldsymbol{z}) = (\boldsymbol{x}^\top \boldsymbol{z})^2$ implicitly defines a feature mapping $\boldsymbol{\phi}$ such that for a two-dim $\boldsymbol{x} = [x_1, x_2]$, $\boldsymbol{\phi}(\boldsymbol{x}) = (x_1^2, \sqrt{2}x_1 x_2, x_2^2)$

- Every kernel function k implicitly defines a feature mapping $\boldsymbol{\phi}$
- $\boldsymbol{\phi}$ takes input $\boldsymbol{x} \in \mathcal{X}$ (e.g., $\mathbb{R}^D$) and maps it to a new "feature space" $\mathcal{F}$
- The kernel function k can be seen as taking two points as inputs and computing their inner-product based similarity in the $\mathcal{F}$ space

For some kernels, as we will see shortly, $\boldsymbol{\phi}(x)$ (and thus the new feature space $\mathcal{F}$) can be very high-dimensional or even be infinite dimensional (but we don't need to compute it anyway, so it is not an issue)

$$\phi \; : \; \mathcal{X} \to \mathcal{F}$$

$$k \; : \; \mathcal{X} \times \mathcal{X} \to \mathbb{R}, \quad k(\boldsymbol{x},\boldsymbol{z}) = \phi(\boldsymbol{x})^\top \phi(\boldsymbol{z})$$

- $\mathcal{F}$ needs to be a vector space with a dot product defined on it (a.k.a. a Hilbert space)
- Is any function $k(\boldsymbol{x},\boldsymbol{z}) = \boldsymbol{\phi}(\boldsymbol{x})^\top \boldsymbol{\phi}(\boldsymbol{z})$ for some $\boldsymbol{\phi}$ a kernel function?
  - No. The function k must satisfy Mercer's Condition

Kernel Functions

- For k (.,.) to be a kernel function
  - k must define a dot product for some Hilbert Space
  - Above is true if k is symmetric and positive semi-definite (p.s.d.) function (though there are exceptions; there are also "indefinite" kernels)

Loosely speaking a PSD function here means that if we evaluation this function for N inputs (N^2 pairs) then the $N \times N$ matrix will be PSD (also called a kernel matrix)

$$k(\boldsymbol{x}, \boldsymbol{z}) = k(\boldsymbol{z}, \boldsymbol{x})$$

For all "square integrable" functions f (such functions satisfy $\int f(\boldsymbol{x})^2 d\boldsymbol{x} < \infty$

$$\iint f(\boldsymbol{x}) k(\boldsymbol{x}, \boldsymbol{z}) f(\boldsymbol{z}) d\boldsymbol{x} d\boldsymbol{z} \geq 0$$

  - The above condition is essentially known as Mercer's Condition

Can easily verify that the Mercer's Condition holds

- Let k_1, k_2 be two kernel functions then the following are as well
  - $k(\boldsymbol{x}, \boldsymbol{z}) = k_1(\boldsymbol{x}, \boldsymbol{z}) + k_2(\boldsymbol{x}, \boldsymbol{z})$: simple sum
  - $k(\boldsymbol{x}, \boldsymbol{z}) = \alpha k_1(\boldsymbol{x}, \boldsymbol{z})$: scalar product
  - $k(\boldsymbol{x}, \boldsymbol{z}) = k_1(\boldsymbol{x}, \boldsymbol{z}) k_2(\boldsymbol{x}, \boldsymbol{z})$: direct product of two kernels

Can also combine these rules and the resulting function will also be a kernel function

Some Pre-defined Kernel Functions

Several other kernels proposed for non-vector data, such as trees, strings, etc

Remember that kernels are a notion of similarity between pairs of inputs

Kernels can have a pre-defined form or can be learned from data (a bit advanced for this course)

- Linear kernel: $k(\boldsymbol{x},\boldsymbol{z}) = \boldsymbol{x}^\top \boldsymbol{z}$
- Quadratic Kernel: $k(\boldsymbol{x},\boldsymbol{z}) = (\boldsymbol{x}^\top \boldsymbol{z})^2$ or $k(\boldsymbol{x},\boldsymbol{z}) = (1 + \boldsymbol{x}^\top \boldsymbol{z})^2$
- Polynomial Kernel (of degree d): $k(\boldsymbol{x},\boldsymbol{z}) = (\boldsymbol{x}^\top \boldsymbol{z})^d$ or $k(\boldsymbol{x},\boldsymbol{z}) = (1 + \boldsymbol{x}^\top \boldsymbol{z})^d$
- Radial Basis Function (RBF) or "Gaussian" Kernel: $k(\boldsymbol{x},\boldsymbol{z}) = \exp[-\gamma \, ||\boldsymbol{x} - \boldsymbol{z}||^2]$
  - Gaussian kernel gives a similarity score between 0 and 1
  - $\gamma > 0$ is a hyperparameter (called the kernel bandwidth parameter)
  - The RBF kernel corresponds to an infinite dim. feature space $\mathcal{F}$ (i.e., you can't actually write down or store the map $\phi(\boldsymbol{x})$ explicitly – but we don't need to do that anyway ☺)
  - Also called "stationary kernel": only depends on the distance between $\boldsymbol{x}$ and $\boldsymbol{z}$ (translating both by the same amount won't change the value of $k(\boldsymbol{x},\boldsymbol{z})$)
- Kernel hyperparameters (e.g., d, γ) can be set via cross-validation

Controls how the distance between two inputs should be converted into a similarity

RBF Kernel = Infinite Dimensional Mapping

- We saw that the RBF/Gaussian kernel is defined as $k(\boldsymbol{x}, \boldsymbol{z}) = \exp[-\gamma \, ||\boldsymbol{x} - \boldsymbol{z}||^2]$
- Using this kernel corresponds to mapping data to infinite dimensional space

$$k(x, z) = \exp[-(x-z)^2] \quad \text{(assuming } \gamma = 1 \text{ and } x \text{ and } z \text{ to be scalars)}$$

$$= \exp(-x^2)\exp(-z^2)\exp(2xz)$$

$$= \exp(-x^2)\exp(-z^2)\sum_{k=1}^{\infty} \frac{2^k x^k z^k}{k!}$$

$$= \phi(x)^\top \phi(z)$$

Thus an infinite-dim vector (ignoring the constants coming from the 2^k and $k!$ terms

- Here $\phi(\boldsymbol{x}) = [\exp(-x^2)x^1, \exp\left(-x^2\right)x^2, \exp(-x^2)x^3, \ldots, \exp(-x^2)x^\infty]$
- But again, note that we never need to compute $\phi(\boldsymbol{x})$ to compute $k(x, z)$
  - $k(x, z)$ is easily computable from its definition itself ($\exp[-(x-z)^2]$ in this case)

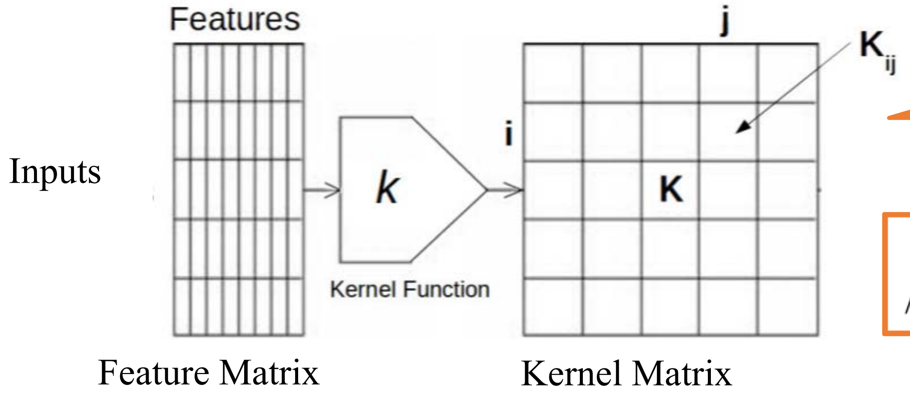
Kernel Matrix

- Kernel based ML algos work with kernel matrices rather than feature vectors
- Given $\boldsymbol{N}$ inputs, the kernel function $\boldsymbol{k}$ can be used to construct a Kernel Matrix $\boldsymbol{K}$
- The kernel matrix $\boldsymbol{K}$ is of size $\boldsymbol{N} \times \boldsymbol{N}$ with each entry defined as

$$K_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j) = \phi(\boldsymbol{x}_i)^\top \phi(\boldsymbol{x}_j)$$

Note again that we don't need to compute ϕ and this dot product explicitly

- K_{ij} : Similarity between the i^{th} and j^{th} inputs in the kernel induced feature space ϕ



K is a symmetric and positive semi-definite matrix

$$z^\top K z \geq 0 \; \forall z \in \mathbb{R}^N$$

Also, all eigenvalues of K are non-negative