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Kernel Methods: Motivation

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![Diagram](image)

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- Kernels give such mappings **for (almost) free**
  - In most cases, the mappings need not be even computed
  - .. using the **Kernel Trick**!
Classifying non-linearly separable data

- Consider this binary classification problem
- Each example represented by a **single feature** $x$
- No linear separator exists for this data
Classifying non-linearly separable data

- Consider this binary classification problem

![Graph showing a single feature x]

- Each example represented by a single feature $x$
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- Now map each example as $x \rightarrow \{x, x^2\}$
- Each example now has two features ("derived" from the old representation)
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- Data now becomes linearly separable in the new representation
Classifying non-linearly separable data

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  ![Graph showing non-linearly separable data]

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  ![Graph showing linear separability in the new representation]

  Linear in the new representation $\equiv$ nonlinear in the old representation
Classifying non-linearly separable data

Let’s look at another example:

Each example defined by a two features $\mathbf{x} = \{x_1, x_2\}$
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Classifying non-linearly separable data

- Let’s look at another example:

Each example defined by a **two features** \( x = \{x_1, x_2\} \)

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- Now map each example as \( x = \{x_1, x_2\} \rightarrow z = \{x_1^2, \sqrt{2}x_1x_2, x_2^2\} \)

- Each example now has **three features** ("derived" from the old representation)
Let’s look at another example:

Each example defined by two features \( x = \{x_1, x_2\} \)

No linear separator exists for this data

Now map each example as \( x = \{x_1, x_2\} \rightarrow z = \{x_1^2, \sqrt{2}x_1x_2, x_2^2\} \)

Each example now has three features ("derived" from the old representation)

Data now becomes linearly separable in the new representation
Feature Mapping

Consider the following mapping $\phi$ for an example $\mathbf{x} = \{x_1, \ldots, x_D\}$

$$\phi: \mathbf{x} \rightarrow \{x_1^2, x_2^2, \ldots, x_D^2, x_1x_2, x_1x_2, \ldots, x_1x_D, \ldots \ldots, x_{D-1}x_D\}$$
Consider the following mapping $\phi$ for an example $\mathbf{x} = \{x_1, \ldots, x_D\}$

$$
\phi : \mathbf{x} \rightarrow \{x_1^2, x_2^2, \ldots, x_D^2, x_1x_2, x_1x_2, \ldots, x_1x_D, \ldots, x_{D-1}x_D\}
$$

It’s an example of a quadratic mapping

- Each new feature uses a pair of the original features
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**Problem:** Mapping usually leads to the number of features blow up!
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$$\phi: \mathbf{x} \rightarrow \{x_1^2, x_2^2, \ldots, x_D^2, x_1x_2, x_1x_3, \ldots, x_1x_D, \ldots, x_{D-1}x_D\}$$

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Thankfully, Kernels help us avoid both these issues!
Feature Mapping

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Thankfully, Kernels help us avoid both these issues!

- The mapping doesn’t have to be explicitly computed
- Computations with the mapped features remain efficient
Consider two examples $\mathbf{x} = \{x_1, x_2\}$ and $\mathbf{z} = \{z_1, z_2\}$
Consider two examples $x = \{x_1, x_2\}$ and $z = \{z_1, z_2\}$

Let's assume we are given a function $k$ (kernel) that takes as inputs $x$ and $z$

$$k(x, z) = (x^T z)^2$$
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k(x, z) = (x^T z)^2 = (x_1 z_1 + x_2 z_2)^2
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Consider two examples \( x = \{x_1, x_2\} \) and \( z = \{z_1, z_2\} \). Let's assume we are given a function \( k \) (kernel) that takes as inputs \( x \) and \( z \):

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Let's assume we are given a function $k$ (kernel) that takes as inputs $\mathbf{x}$ and $\mathbf{z}$

$$k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^\top \mathbf{z})^2$$
$$= (x_1 z_1 + x_2 z_2)^2$$
$$= x_1^2 z_1^2 + x_2^2 z_2^2 + 2x_1 x_2 z_1 z_2$$
$$= (x_1^2, \sqrt{2}x_1 x_2, x_2^2)^\top (z_1^2, \sqrt{2}z_1 z_2, z_2^2)$$
Kernels as High Dimensional Feature Mapping

Consider two examples $\mathbf{x} = \{x_1, x_2\}$ and $\mathbf{z} = \{z_1, z_2\}$

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\]
\[
= \phi(\mathbf{x})^\top \phi(\mathbf{z})
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Consider two examples \( x = \{x_1, x_2\} \) and \( z = \{z_1, z_2\} \).

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

The above \( k \) implicitly defines a mapping \( \phi \) to a higher dimensional space:

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Simply defining the kernel a certain way gives a higher dim. mapping \( \phi \).
Consider two examples $x = \{x_1, x_2\}$ and $z = \{z_1, z_2\}$

Let’s assume we are given a function $k$ (kernel) that takes as inputs $x$ and $z$

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Simply defining the kernel a certain way gives a higher dim. mapping $\phi$

Moreover the kernel $k(x, z)$ also computes the dot product $\phi(x)^\top \phi(z)$

$\phi(x)^\top \phi(z)$ would otherwise be much more expensive to compute explicitly
Consider two examples $\mathbf{x} = \{x_1, x_2\}$ and $\mathbf{z} = \{z_1, z_2\}$.

Let's assume we are given a function $k$ (kernel) that takes as inputs $\mathbf{x}$ and $\mathbf{z}$:

$$k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^T \mathbf{z})^2$$

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

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

$$= \phi(\mathbf{x})^T \phi(\mathbf{z})$$

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Simply defining the kernel a certain way gives a higher dim. mapping $\phi$.

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$\phi(\mathbf{x})^T \phi(\mathbf{z})$ would otherwise be much more expensive to compute explicitly.

All kernel functions have these properties.
Recall: Each kernel $k$ has an associated feature mapping $\phi$
Kernels: Formally Defined

- Recall: Each kernel $k$ has an associated feature mapping $\phi$
- $\phi$ takes input $x \in \mathcal{X}$ (input space) and maps it to $\mathcal{F}$ ("feature space")
Kernels: Formally Defined

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- $\phi$ takes input $x \in \mathcal{X}$ (input space) and maps it to $\mathcal{F}$ ("feature space")
- Kernel $k(x, z)$ takes two inputs and gives their similarity in $\mathcal{F}$ space

\[
\phi : \mathcal{X} \rightarrow \mathcal{F} \\
k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}, \quad k(x, z) = \phi(x)^T \phi(z)
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Recall: Each kernel $k$ has an associated feature mapping $\phi$

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Kernel $k(x, z)$ takes two inputs and gives their similarity in $\mathcal{F}$ space

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

$\mathcal{F}$ needs to be a vector space with a dot product defined on it

- Also called a Hilbert Space
Kernels: Formally Defined

- Recall: Each kernel \( k \) has an associated feature mapping \( \phi \).
- \( \phi \) takes input \( x \in \mathcal{X} \) (input space) and maps it to \( \mathcal{F} \) (“feature space”).
- Kernel \( k(x, z) \) takes two inputs and gives their similarity in \( \mathcal{F} \) space:
  \[
  k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}, \quad k(x, z) = \phi(x)\top \phi(z)
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- \( \mathcal{F} \) needs to be a vector space with a dot product defined on it.
  - Also called a Hilbert Space.
- Can just any function be used as a kernel function?
Kernels: Formally Defined

- Recall: Each kernel $k$ has an associated feature mapping $\phi$

- $\phi$ takes input $x \in X$ (input space) and maps it to $F$ ("feature space")

- Kernel $k(x, z)$ takes two inputs and gives their similarity in $F$ space

- $\phi : X \rightarrow F$

- $k : X \times X \rightarrow \mathbb{R}, \quad k(x, z) = \phi(x)^\top \phi(z)$

- $F$ needs to be a vector space with a dot product defined on it

- Also called a Hilbert Space

- Can just any function be used as a kernel function?

- No. It must satisfy Mercer’s Condition
Mercer’s Condition

- For $k$ to be a kernel function
Mercer’s Condition

- For $k$ to be a kernel function
  - There must exist a Hilbert Space $\mathcal{F}$ for which $k$ defines a dot product
Mercer’s Condition

For $k$ to be a kernel function:

- There must exist a Hilbert Space $\mathcal{F}$ for which $k$ defines a dot product.
- The above is true if $K$ is a positive definite function.

\[
\int dx \int dz f(x)k(x,z)f(z) > 0 \quad (\forall f \in L_2)
\]
Mercer’s Condition

- For $k$ to be a kernel function
  - There must exist a Hilbert Space $\mathcal{F}$ for which $k$ defines a dot product
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Mercer’s Condition

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- Let $k_1$, $k_2$ be two kernel functions then the following are as well:
Mercer’s Condition

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- Let $k_1$, $k_2$ be two kernel functions then the following are as well:
  - $k(x, z) = k_1(x, z) + k_2(x, z)$: direct sum
Mercer’s Condition

- For \( k \) to be a kernel function
  - There must exist a Hilbert Space \( \mathcal{F} \) for which \( k \) defines a dot product
  - The above is true if \( K \) is a **positive definite function**

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\int dx \int dz f(x) k(x,z) f(z) > 0 \quad (\forall f \in L_2)
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Mercer’s Condition

- For $k$ to be a kernel function
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Mercer’s Condition

- For $k$ to be a kernel function
  - There must exist a Hilbert Space $\mathcal{F}$ for which $k$ defines a dot product
  - The above is true if $K$ is a positive definite function
    \[
    \int dxf(x)k(x, z)f(z) > 0 \quad (\forall f \in L_2)
    \]
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- Let $k_1, k_2$ be two kernel functions then the following are as well:
  - $k(x, z) = k_1(x, z) + k_2(x, z)$: direct sum
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  - $k(x, z) = k_1(x, z)k_2(x, z)$: direct product
- Kernels can also be constructed by composing these rules
The kernel function $k$ also defines the Kernel Matrix $K$ over the data.
The Kernel Matrix

- The kernel function $k$ also defines the Kernel Matrix $K$ over the data.

- Given $N$ examples $\{x_1, \ldots, x_N\}$, the $(i,j)$-th entry of $K$ is defined as:

$$K_{ij} = k(x_i, x_j) = \phi(x_i)^{\top} \phi(x_j)$$
The kernel function $k$ also defines the Kernel Matrix $\mathbf{K}$ over the data.

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$K_{ij}$: Similarity between the $i$-th and $j$-th example in the feature space $\mathcal{F}$.
The Kernel Matrix

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- Given $N$ examples $\{x_1, \ldots, x_N\}$, the $(i,j)$-th entry of $K$ is defined as:
  \[ K_{ij} = k(x_i, x_j) = \phi(x_i)^\top \phi(x_j) \]
- $K_{ij}$: Similarity between the $i$-th and $j$-th example in the feature space $F$
- $K$: $N \times N$ matrix of pairwise similarities between examples in $F$ space
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The kernel function \( k \) also defines the Kernel Matrix \( K \) over the data.

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- \( K_{ij} \): Similarity between the \( i \)-th and \( j \)-th example in the feature space \( \mathcal{F} \).
- \( K \): \( N \times N \) matrix of pairwise similarities between examples in \( \mathcal{F} \) space.
- \( K \) is a symmetric matrix.
- \( K \) is a positive definite matrix (except for a few exceptions).
The Kernel Matrix

- The kernel function $k$ also defines the Kernel Matrix $K$ over the data.

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- The Kernel Matrix $K$ is also known as the Gram Matrix.
Some Examples of Kernels

The following are the most popular kernels for real-valued vector inputs

- Linear (trivial) Kernel:

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**Note:** Kernel hyperparameters (e.g., \( d, \gamma \)) chosen via cross-validation
Using Kernels

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Recall: Kernel $k(x, z)$ represents a dot product in some high dimensional feature space $\mathcal{F}$.
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- Most learning algorithms are like that.
  
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  - Many of the unsupervised learning algorithms too can be kernelized (e.g., $K$-means clustering, Principal Component Analysis, etc.)
Recall the SVM dual Lagrangian:

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\text{Maximize } L_D(w, b, \xi, \alpha, \beta) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{m,n=1}^{N} \alpha_m \alpha_n y_m y_n (x_m \cdot x_n)
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subject to \( \sum_{n=1}^{N} \alpha_n y_n = 0, \quad 0 \leq \alpha_n \leq C; \quad n = 1, \ldots, N \)
Kernelized SVM Training

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  - This corresponds to a non-linear separator in the original space \( \mathcal{X} \)
Prediction for a test example $\mathbf{x}$ (assume $b = 0$)

$$y = \text{sign}(\mathbf{w}^\top \mathbf{x})$$
Kernelized SVM Prediction

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The learned decision boundary in the original space is nonlinear.
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- Kernels give a modular way to learn nonlinear patterns using linear models
  - All you need to do is replace the inner products with the kernel
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  The answer lies in the concepts of large margins and generalization
Intro to probabilistic methods for supervised learning
- Linear Regression (probabilistic version)
- Logistic Regression