CSCI567 Machine Learning (Spring 2021)

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Outline

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Logistics

- HW 2 Is due today, and HW 3 will be assigned!

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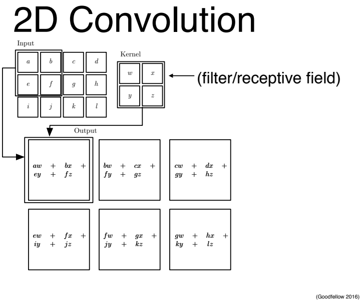
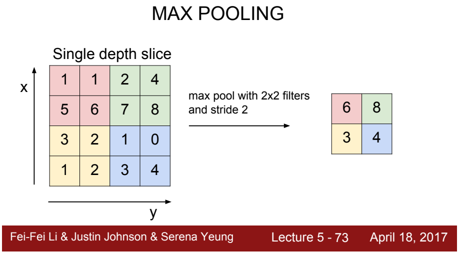
Convolutional Neural Nets

Typical architecture for CNNs:

Input → [[Conv → ReLU]*N → Pool?]*M → [FC → ReLU]*Q → FC





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Motivation

Recall the question: *how to choose nonlinear basis* $\phi : \mathbb{R}^{\mathsf{D}} \rightarrow \mathbb{R}^{\mathsf{M}}$?

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- neural network is one approach: learn ϕ from data
- **kernel method** is another one: sidestep the issue of choosing ϕ by using *kernel functions*

What are Kernels?

Consider the following example, where the data is not linearly separable in the **ambient** space but is separable **feature** space[1]

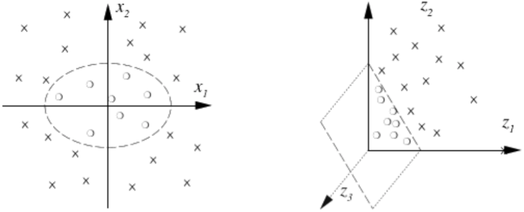

Figure 2.1 Toy example of a binary classification problem mapped into feature space. We assume that the true decision boundary is an ellipse in input space (left panel). The task of the learning process is to estimate this boundary based on empirical data consisting of training points in both classes (crosses and circles, respectively). When mapped into feature space via the nonlinear map $\Phi_2(x) = (z_1, z_2, z_3) = ([x]_1^2, [x]_2^2, \sqrt{2}\,[x]_1[x]_2)$ (right panel), the ellipse becomes a hyperplane (in the present simple case, it is parallel to the z_3 axis, hence all points are plotted in the (z_1, z_2) plane). This is due to the fact that ellipses can be written as linear equations in the entries of (z_1, z_2, z_3). Therefore, in feature space, the problem reduces to that of estimating a hyperplane from the mapped data points. Note that via the polynomial kernel (see (2.12) and (2.13)), the dot product in the three-dimensional space can be computed without computing Φ_2. Later in the book, we shall describe algorithms for constructing hyperplanes which are based on dot products (Chapter 7).

Schölkopf, Bernhard, and Alexander J. Smola. Learning with kernels: support vector machines, regularization, optimization, and beyond. MIT press, 2002.

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2. Statistical issue of **curse of dimensionality** kicks-in, which means that as dimension increases we may require exponentially more data samples!

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Don't need to know $\phi(\cdot)$: Since we use **Kernel function** we actually don't need to know the mapping $\phi(\cdot)$. This means that $\phi(\cdot)$ may be infinite dimensional but we can still evaluate the inner-products in an infinite dimensional feature space!!

Example

Let's take a closer look at the example. Here, we consider the following polynomial basis $\boldsymbol{\phi} : \mathbb{R}^2 \to \mathbb{R}^3$:

$$\boldsymbol{\phi}(\boldsymbol{x}) = \begin{pmatrix} x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \end{pmatrix}$$

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$$\boldsymbol{\phi}(\boldsymbol{x})^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}') = {x_1}^2{x_1'}^2 + 2x_1x_2x_1'x_2' + {x_2}^2{x_2'}^2$$

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Therefore, *the inner product in the new space is simply a function of the inner product in the original space*.

Another example

$\boldsymbol{\phi} : \mathbb{R}^{\mathsf{D}} \to \mathbb{R}^{2\mathsf{D}}$ is parameterized by θ:

$$\boldsymbol{\phi}_{\theta}(\boldsymbol{x}) = \begin{pmatrix} \cos(\theta x_1) \\ \sin(\theta x_1) \\ \vdots \\ \cos(\theta x_{\mathsf{D}}) \\ \sin(\theta x_{\mathsf{D}}) \end{pmatrix}$$

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Once again, *the inner product in the new space is a simple function of the features in the original space*.

More complicated example

Based on ϕ_θ, define $\phi_L : \mathbb{R}^{\mathsf{D}} \to \mathbb{R}^{2\mathsf{D}(L+1)}$ for some integer L:

$$\phi_L(\boldsymbol{x}) = \begin{pmatrix} \phi_0(\boldsymbol{x}) \\ \phi_{\frac{2\pi}{L}}(\boldsymbol{x}) \\ \phi_{2\frac{2\pi}{L}}(\boldsymbol{x}) \\ \vdots \\ \phi_{L\frac{2\pi}{L}}(\boldsymbol{x}) \end{pmatrix}$$

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What is the inner product between $\phi_L(\boldsymbol{x})$ and $\phi_L(\boldsymbol{x}')$?

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$$\boldsymbol{\phi}_\infty(\boldsymbol{x})^{\mathrm{T}} \boldsymbol{\phi}_\infty(\boldsymbol{x}') = \int_0^{2\pi} \sum_{d=1}^{\mathsf{D}} \cos(\theta(x_d - x'_d))\, d\theta$$

$$= \sum_{d=1}^{\mathsf{D}} \frac{\sin(2\pi(x_d - x'_d))}{x_d - x'_d}$$

Again, a simple function of the original features.

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Note that using this mapping in linear regression, we are *learning a weight $\boldsymbol{w}^*$ with infinite dimension!*

Kernel functions

Definition: a function $k : \mathbb{R}^{\mathsf{D}} \times \mathbb{R}^{\mathsf{D}} \to \mathbb{R}$ is called a *(positive semidefinite) kernel function* if there exists a function $\boldsymbol{\phi} : \mathbb{R}^{\mathsf{D}} \to \mathbb{R}^{\mathsf{M}}$ so that for any $\boldsymbol{x}, \boldsymbol{x}' \in \mathbb{R}^{\mathsf{D}}$,

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Examples we have seen

$$k(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x}^{\mathrm{T}} \boldsymbol{x}')^2$$

$$k(\boldsymbol{x}, \boldsymbol{x}') = \sum_{d=1}^{\mathsf{D}} \frac{\sin(2\pi(x_d - x'_d))}{x_d - x'_d}$$

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Gram/kernel matrix needs to be *positive semi-definite* and *symmetric*

$$\boldsymbol{K} = \boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathrm{T}} = \begin{pmatrix} k(\boldsymbol{x}_1, \boldsymbol{x}_1) & k(\boldsymbol{x}_1, \boldsymbol{x}_2) & \cdots & k(\boldsymbol{x}_1, \boldsymbol{x}_N) \\ k(\boldsymbol{x}_2, \boldsymbol{x}_1) & k(\boldsymbol{x}_2, \boldsymbol{x}_2) & \cdots & k(\boldsymbol{x}_2, \boldsymbol{x}_N) \\ \vdots & \vdots & \vdots & \vdots \\ k(\boldsymbol{x}_N, \boldsymbol{x}_1) & k(\boldsymbol{x}_N, \boldsymbol{x}_2) & \cdots & k(\boldsymbol{x}_N, \boldsymbol{x}_N) \end{pmatrix}$$

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In fact, k is a kernel if and only if $\boldsymbol{K}$ is positive semidefinite for *any N and any $\boldsymbol{x}_1$, $\boldsymbol{x}_2$, …, $\boldsymbol{x}_N$* (formalized by the **Mercer theorem**).

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- useful for proving that a function is not a kernel

Examples that are not kernels

Function

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More examples of kernel functions

Two most commonly used kernel functions in practice:

Polynomial kernel

$$k(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x}^{\mathrm{T}}\boldsymbol{x}' + c)^d$$

for $c \geq 0$ and d is a positive integer.

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Gaussian kernel or Radial basis function (RBF) kernel

$$k(\boldsymbol{x}, \boldsymbol{x}') = e^{-\frac{\|\boldsymbol{x}-\boldsymbol{x}'\|_2^2}{2\sigma^2}}$$

for some $\sigma > 0$.

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Verify using the definition of kernel!

Case study: regularized linear regression

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$$\begin{aligned} \boldsymbol{w}^* &= \operatorname*{argmin}_{\boldsymbol{w}} F(\boldsymbol{w}) \\ &= \operatorname*{argmin}_{\boldsymbol{w}} \left(\|\boldsymbol{\Phi}\boldsymbol{w} - \boldsymbol{y}\|_2^2 + \lambda\|\boldsymbol{w}\|_2^2\right) \\ &= \left(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi} + \lambda\boldsymbol{I}\right)^{-1}\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{y} \end{aligned}$$

$$\boldsymbol{\Phi} = \begin{pmatrix} \boldsymbol{\phi}(\boldsymbol{x}_1)^{\mathrm{T}} \\ \boldsymbol{\phi}(\boldsymbol{x}_2)^{\mathrm{T}} \\ \vdots \\ \boldsymbol{\phi}(\boldsymbol{x}_{\mathsf{N}})^{\mathrm{T}} \end{pmatrix}, \quad \boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{\mathsf{N}} \end{pmatrix}$$

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Issue: *operate in space $\mathbb{R}^{\mathsf{M}}$ and M could be huge or even infinity!*
Our aim: pose these computation as inner-products between $\boldsymbol{\phi}(\cdot)$.

A closer look at the least square solution, where

By setting the gradient of $F(\boldsymbol{w}) = \|\boldsymbol{\Phi}\boldsymbol{w} - \boldsymbol{y}\|_2^2 + \lambda\|\boldsymbol{w}\|_2^2$ to be $\mathbf{0}$:

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we know

$$\boldsymbol{w}^* = \frac{1}{\lambda}\boldsymbol{\Phi}^{\mathrm{T}}(\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{w}^*) = \boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\alpha} = \sum_{n=1}^{N}\alpha_n\boldsymbol{\phi}(\boldsymbol{x}_n)$$

A closer look at the least square solution, where

By setting the gradient of $F(\boldsymbol{w}) = \|\boldsymbol{\Phi}\boldsymbol{w} - \boldsymbol{y}\|_2^2 + \lambda\|\boldsymbol{w}\|_2^2$ to be $\mathbf{0}$:

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Note this is true for perceptron and many other problems.

Of course, the above calculation does not show what $\boldsymbol{\alpha}$ is.

Why is this helpful?

Assuming we know $\boldsymbol{\alpha}$, the prediction of $\boldsymbol{w}^*$ on a new example $\boldsymbol{x}$ is

$$\boldsymbol{w}^{*\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}) = \sum_{n=1}^{N} \alpha_n \boldsymbol{\phi}(\boldsymbol{x}_n)^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}) = \sum_{n=1}^{N} \alpha_n k(\boldsymbol{x}_n, \boldsymbol{x})$$

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But we need to figure out what $\boldsymbol{\alpha}$ is first!

How to find $\boldsymbol{\alpha}$?

Plugging in $\boldsymbol{w} = \boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\alpha}$ into $F(\boldsymbol{w})$ gives

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This is sometime called the *dual formulation* of linear regression.

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$\boldsymbol{K} = \boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathrm{T}} \in \mathbb{R}^{\mathsf{N}\times\mathsf{N}}$ is called **Gram matrix** or **kernel matrix** where the (i, j) entry is

$$\boldsymbol{\phi}(\boldsymbol{x}_i)^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_j)$$

Examples of kernel matrix $\boldsymbol{K}$

3 data points in $\mathbb{R}$

$$x_1 = -1, x_2 = 0, x_3 = 1$$

$\boldsymbol{\phi}$ is polynomial basis with degree 4:

$$\boldsymbol{\phi}(x) = \begin{pmatrix} 1 \\ x \\ x^2 \\ x^3 \end{pmatrix}$$

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Calculation of the Gram matrix $\boldsymbol{K}$

$$\boldsymbol{\phi}(x_1) = \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix} \quad \boldsymbol{\phi}(x_2) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \boldsymbol{\phi}(x_3) = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

Gram/Kernel matrix

$$\begin{aligned} \boldsymbol{K} &= \begin{pmatrix} \boldsymbol{\phi}(x_1)^{\mathrm{T}}\boldsymbol{\phi}(x_1) & \boldsymbol{\phi}(x_1)^{\mathrm{T}}\boldsymbol{\phi}(x_2) & \boldsymbol{\phi}(x_1)^{\mathrm{T}}\boldsymbol{\phi}(x_3) \\ \boldsymbol{\phi}(x_2)^{\mathrm{T}}\boldsymbol{\phi}(x_1) & \boldsymbol{\phi}(x_2)^{\mathrm{T}}\boldsymbol{\phi}(x_2) & \boldsymbol{\phi}(x_2)^{\mathrm{T}}\boldsymbol{\phi}(x_3) \\ \boldsymbol{\phi}(x_3)^{\mathrm{T}}\boldsymbol{\phi}(x_1) & \boldsymbol{\phi}(x_3)^{\mathrm{T}}\boldsymbol{\phi}(x_2) & \boldsymbol{\phi}(x_3)^{\mathrm{T}}\boldsymbol{\phi}(x_3) \end{pmatrix} \\ &= \begin{pmatrix} 4 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 4 \end{pmatrix} \end{aligned}$$

Gram matrix vs covariance matrix

	dimensions	**entry** (i,j)	**property**
$\mathbf{\Phi\Phi}^{\mathrm{T}}$			
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Minimize the dual formulation

$$G(\boldsymbol{\alpha}) = \boldsymbol{\alpha}^{\mathrm{T}}(\boldsymbol{K}^2 + \lambda \boldsymbol{K})\boldsymbol{\alpha} - 2\boldsymbol{y}^{\mathrm{T}}\boldsymbol{K}\boldsymbol{\alpha} + \text{cnt.}$$

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\end{aligned}
$$

Then what is the difference?

First, computing $(\mathbf{\Phi}\mathbf{\Phi}^{\mathrm{T}} + \lambda \boldsymbol{I})^{-1}$ can be more efficient than computing $(\mathbf{\Phi}^{\mathrm{T}}\mathbf{\Phi} + \lambda \boldsymbol{I})^{-1}$ when $\mathsf{N} \leq \mathsf{M}$.

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Now we can conclude that the exact form of $\boldsymbol{\phi}(\cdot)$ is not essential; *all we need is computing inner products* $\boldsymbol{\phi}(\boldsymbol{x})^T\boldsymbol{\phi}(\boldsymbol{x}')$.

For some $\boldsymbol{\phi}$ it is indeed possible to compute $\boldsymbol{\phi}(\boldsymbol{x})^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}')$ without computing/knowing $\boldsymbol{\phi}$. This is the *kernel trick*.

Kernelizing other ML algorithms

Kernel trick is applicable to **many ML algorithms**:

- nearest neighbor classifier
- perceptron
- logistic regression
- SVM
- $\cdots$

Example: Kernelized NNC

For NNC with **L2 distance**, the key is to compute for any two points $\boldsymbol{x}$, $\boldsymbol{x}'$

$$d(\boldsymbol{x}, \boldsymbol{x}') = \|\boldsymbol{x} - \boldsymbol{x}'\|_2^2 = \boldsymbol{x}^{\mathrm{T}}\boldsymbol{x} + \boldsymbol{x}'^{\mathrm{T}}\boldsymbol{x}' - 2\boldsymbol{x}^{\mathrm{T}}\boldsymbol{x}'$$

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With a kernel function k, we simply compute

$$d^{\mathrm{KERNEL}}(\boldsymbol{x}, \boldsymbol{x}') = k(\boldsymbol{x}, \boldsymbol{x}) + k(\boldsymbol{x}', \boldsymbol{x}') - 2k(\boldsymbol{x}, \boldsymbol{x}')$$

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which by definition is the **L2 distance in a new feature space**

$$d^{\mathrm{KERNEL}}(\boldsymbol{x}, \boldsymbol{x}') = \|\boldsymbol{\phi}(\boldsymbol{x}) - \boldsymbol{\phi}(\boldsymbol{x}')\|_2^2$$