CSCI567 Machine Learning (Fall 2018)

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Administration

HW 1 grading will be completed next week

HW 2 to be released very soon

- deadline is 10/07
- but solutions for written part will be released on 09/27

Midterm (10/03)

- location is finalized: THH 101 and THH 201
- coverage on Lecture 6 will be minimum
- you can start preparing after this lecture

Outline

1. Review of last lecture
2. Convolutional neural networks
3. Kernel methods

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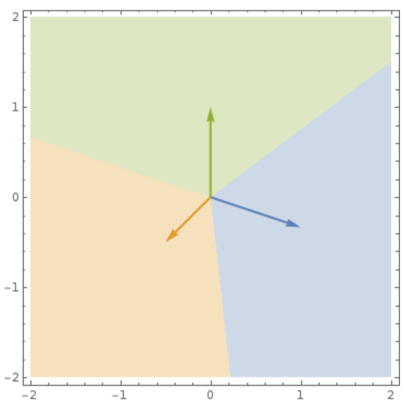
Linear models: from binary to multiclass



$\boldsymbol{w}_1 = (1, -\frac{1}{3})$
$\boldsymbol{w}_2 = (-\frac{1}{2}, -\frac{1}{2})$
$\boldsymbol{w}_3 = (0, 1)$

- Blue class: $\{\boldsymbol{x} : 1 = \text{argmax}_k \, \boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}\}$
- Orange class: $\{\boldsymbol{x} : 2 = \text{argmax}_k \, \boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}\}$
- Green class: $\{\boldsymbol{x} : 3 = \text{argmax}_k \, \boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}\}$

$$\mathcal{F} = \left\{ f(\boldsymbol{x}) = \underset{k\in[\mathsf{C}]}{\text{argmax}} \; \boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x} \mid \boldsymbol{w}_1, \ldots, \boldsymbol{w}_{\mathsf{C}} \in \mathbb{R}^{\mathsf{D}} \right\}$$

MLE = minimizing cross-entropy loss

Maximize probability of see labels $y_1, \ldots, y_{\mathsf{N}}$ given $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{\mathsf{N}}$

$$P(\boldsymbol{W}) = \prod_{n=1}^{\mathsf{N}} \mathbb{P}(y_n \mid \boldsymbol{x}_n; \boldsymbol{W}) = \prod_{n=1}^{\mathsf{N}} \frac{e^{\boldsymbol{w}_{y_n}^{\mathrm{T}}\boldsymbol{x}_n}}{\sum_{k\in[\mathsf{C}]} e^{\boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}_n}}$$

By taking **negative log**, this is equivalent to minimizing

$$F(\boldsymbol{W}) = \sum_{n=1}^{\mathsf{N}} \ln \left(\frac{\sum_{k\in[\mathsf{C}]} e^{\boldsymbol{w}_k^{\mathrm{T}}\boldsymbol{x}_n}}{e^{\boldsymbol{w}_{y_n}^{\mathrm{T}}\boldsymbol{x}_n}} \right) = \sum_{n=1}^{\mathsf{N}} \ln \left(1 + \sum_{k\neq y_n} e^{(\boldsymbol{w}_k - \boldsymbol{w}_{y_n})^{\mathrm{T}}\boldsymbol{x}_n} \right)$$

This is the *multiclass logistic loss*, a.k.a *cross-entropy loss*.

Comparisons of multiclass-to-binary reductions

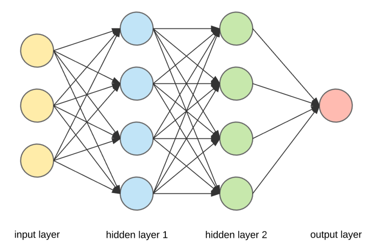
In big O notation,

Reduction	**#training points**	**test time**	**Idea**
OvA	CN	C	is class k or not?
OvO	CN	C^2	is class k or class k'?
ECOC	LN	L	is bit b on or off?
Tree	$(\log_2 \mathsf{C})\mathsf{N}$	$\log_2 \mathsf{C}$	belong to which half of the label set?

Math formulation of neural nets

An L-layer neural net can be written as

$$\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{h}_{\mathsf{L}} \left(\boldsymbol{W}_L \boldsymbol{h}_{\mathsf{L}-1} \left(\boldsymbol{W}_{L-1} \cdots \boldsymbol{h}_1 \left(\boldsymbol{W}_1 \boldsymbol{x} \right) \right) \right)$$



To ease notation, for a given input $\boldsymbol{x}$, define recursively

$$\boldsymbol{o}_0 = \boldsymbol{x}, \qquad \boldsymbol{a}_\ell = \boldsymbol{W}_\ell \boldsymbol{o}_{\ell-1}, \qquad \boldsymbol{o}_\ell = \boldsymbol{h}_\ell(\boldsymbol{a}_\ell) \qquad (\ell = 1, \ldots, \mathsf{L})$$

where

- $\boldsymbol{W}_\ell \in \mathbb{R}^{\mathsf{D}_\ell \times \mathsf{D}_{\ell-1}}$ is the weights for layer ℓ
- $\mathsf{D}_0 = \mathsf{D}, \mathsf{D}_1, \ldots, \mathsf{D}_{\mathsf{L}}$ are numbers of neurons at each layer
- $\boldsymbol{a}_\ell \in \mathbb{R}^{\mathsf{D}_\ell}$ is input to layer ℓ
- $\boldsymbol{o}_\ell \in \mathbb{R}^{\mathsf{D}_\ell}$ is output to layer ℓ
- $\boldsymbol{h} : \mathbb{R}^{\mathsf{D}_\ell} \rightarrow \mathbb{R}^{\mathsf{D}_\ell}$ is activation functions at layer ℓ

Backprop = SGD for neural nets

The **backpropagation** algorithm (**Backprop**)

Initialize $\boldsymbol{W}_1, \ldots, \boldsymbol{W}_\mathsf{L}$ (all $\mathbf{0}$ or randomly). Repeat:

1. randomly pick one data point $n \in [\mathsf{N}]$
2. **forward propagation**: for each layer $\ell = 1, \ldots, \mathsf{L}$
   - compute $\boldsymbol{a}_\ell = \boldsymbol{W}_\ell \boldsymbol{o}_{\ell-1}$ and $\boldsymbol{o}_\ell = \boldsymbol{h}_\ell(\boldsymbol{a}_\ell)$ $\qquad (\boldsymbol{o}_0 = \boldsymbol{x}_n)$
3. **backward propagation**: for each $\ell = L, \ldots, 1$
   - compute

$$\frac{\partial \mathcal{E}_n}{\partial \boldsymbol{a}_\ell} = \begin{cases} \left(\boldsymbol{W}_{\ell+1}^{\mathrm{T}} \frac{\partial \mathcal{E}_n}{\partial \boldsymbol{a}_{\ell+1}}\right) \circ \boldsymbol{h}'_\ell(\boldsymbol{a}_\ell) & \text{if } \ell < \mathsf{L} \\ 2(\boldsymbol{h}_\mathsf{L}(\boldsymbol{a}_\mathsf{L}) - \boldsymbol{y}_n) \circ \boldsymbol{h}'_\mathsf{L}(\boldsymbol{a}_\mathsf{L}) & \text{else} \end{cases}$$

   - update weights

$$\boldsymbol{W}_\ell \leftarrow \boldsymbol{W}_\ell - \eta \frac{\partial \mathcal{E}_n}{\partial \boldsymbol{W}_\ell} = \boldsymbol{W}_\ell - \eta \frac{\partial \mathcal{E}_n}{\partial \boldsymbol{a}_\ell} \boldsymbol{o}_{\ell-1}^{\mathrm{T}}$$

Think about how to do the last two steps properly!

Outline

Acknowledgements

Not much math, a lot of empirical intuitions

The materials borrow *heavily* from the following sources:

- Stanford Course Cs231n: `http://cs231n.stanford.edu/`
- Dr. Ian Goodfellow's lectures on deep learning: `http://deeplearningbook.org`

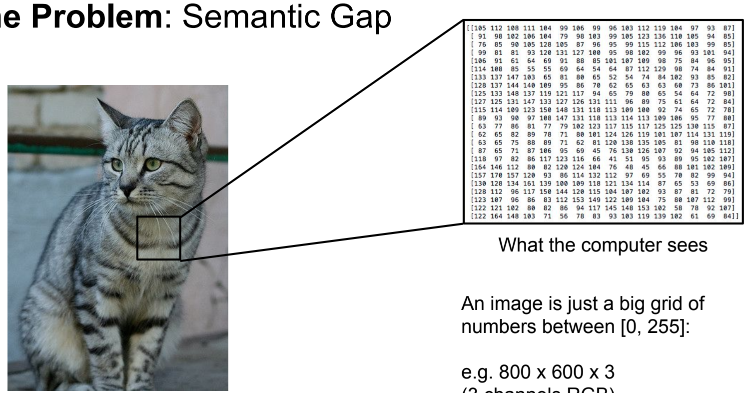
Both website provides tons of useful resources: notes, demos, videos, etc.

Image Classification: A core task in Computer Vision

(assume given set of discrete labels)
{dog, cat, truck, plane, ...}

→ cat

The Problem: Semantic Gap

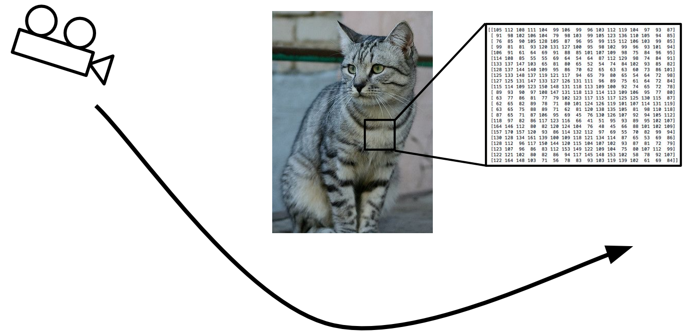


What the computer sees

An image is just a big grid of numbers between [0, 255]:

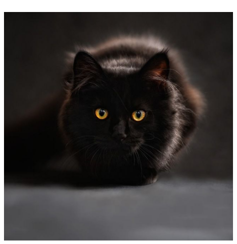
e.g. 800 x 600 x 3
(3 channels RGB)

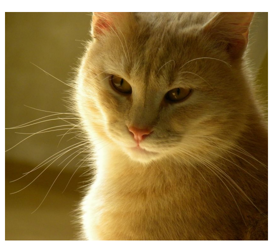
Challenges: Viewpoint variation

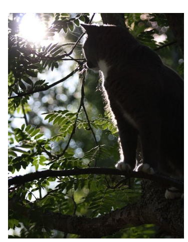


All pixels change when the camera moves!

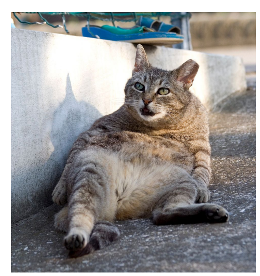
Challenges: Illumination

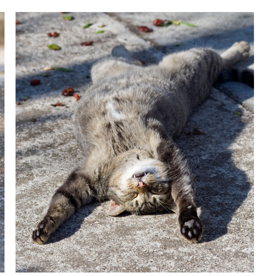


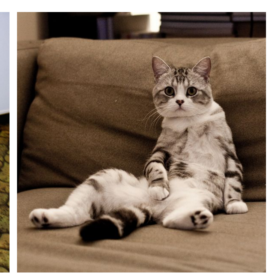




Challenges: Deformation







Challenges: Occlusion

Challenges: Background Clutter

Challenges: Intraclass variation

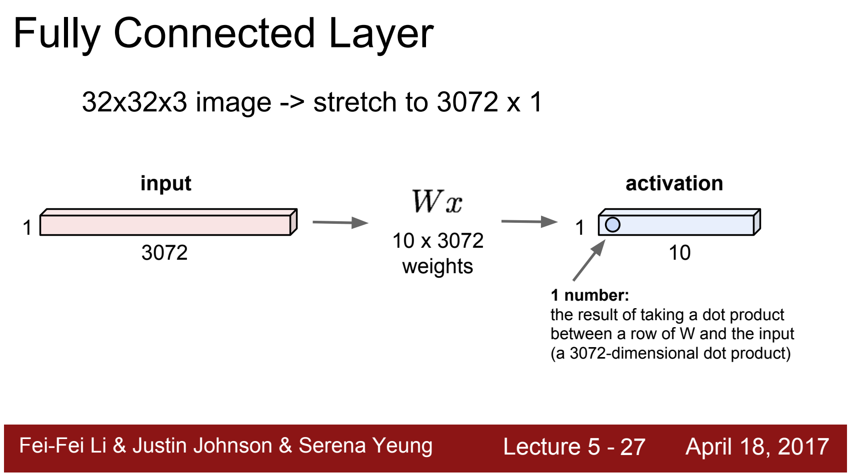
Fundamental problems in vision

The key challenge
How to train a model that can tolerate all those variations?

Main ideas

- need a lot of data that exhibits those variations
- need more specialized models to capture the invariance

Issues of standard NN for image inputs

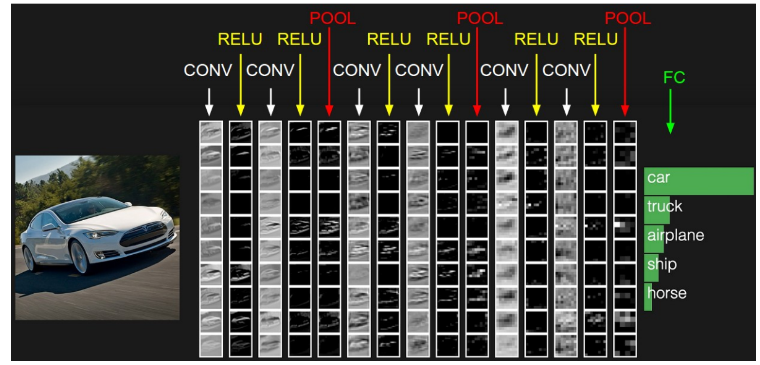


Spatial structure is lost!

Solution: Convolutional Neural Net (ConvNet/CNN)

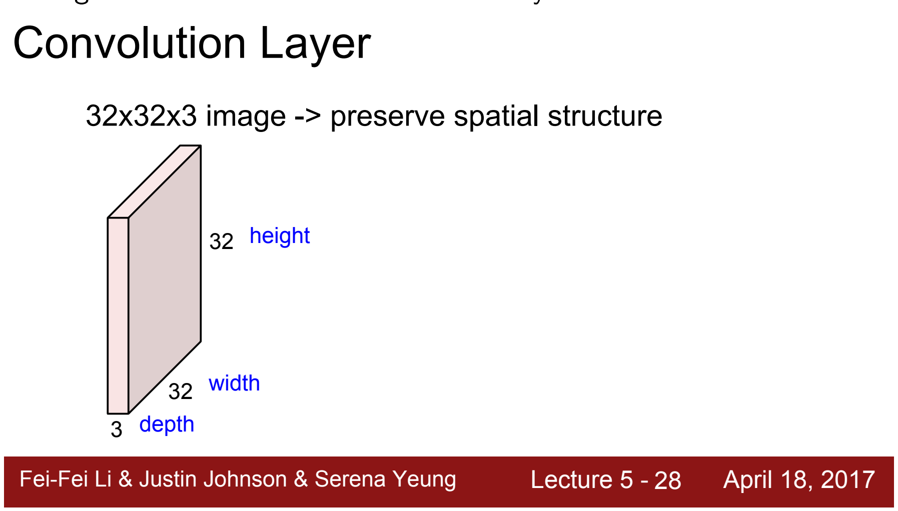
A special case of fully connected neural nets

- usually consist of **convolution layers**, ReLU layers, **pooling layers**, and regular fully connected layers
- key idea: *learning from low-level to high-level features*

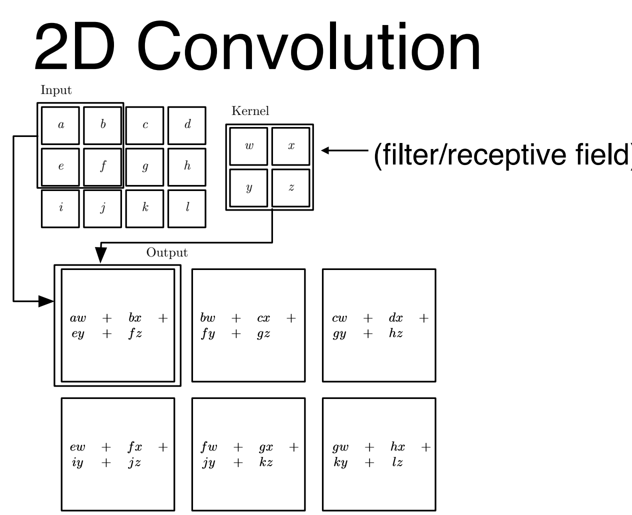


Convolution layer

Arrange neurons as a **3D volume** naturally



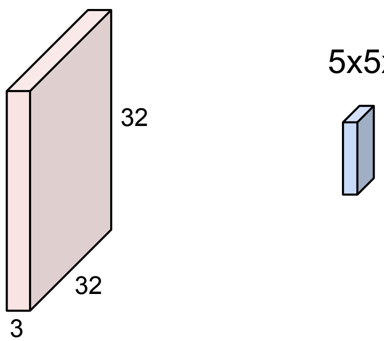
Convolution



Convolution Layer

32x32x3 image

5x5x3 filter



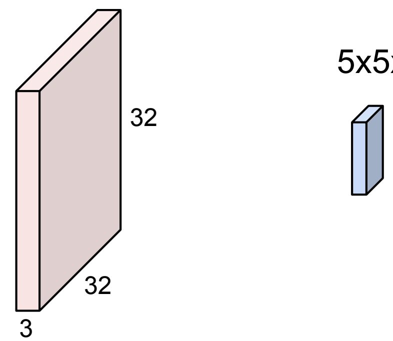
Convolve the filter with the image
i.e. “slide over the image spatially, computing dot products”

Convolution Layer

Filters always extend the full depth of the input volume

32x32x3 image

5x5x3 filter

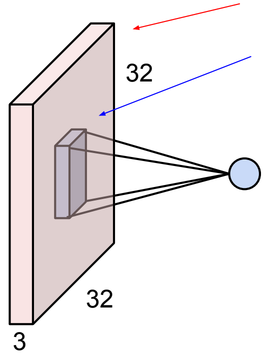


Convolve the filter with the image
i.e. “slide over the image spatially, computing dot products”

Convolution Layer

32x32x3 image

5x5x3 filter w



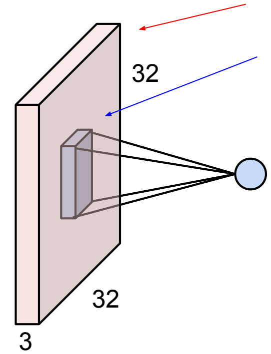
1 number:
the result of taking a dot product between the filter and a small 5x5x3 chunk of the image
(i.e. 5*5*3 = 75-dimensional dot product + bias)

$$w^T x + b$$

Convolution Layer

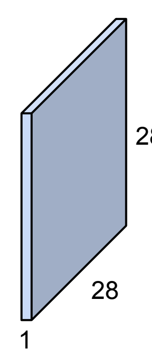
32x32x3 image

5x5x3 filter



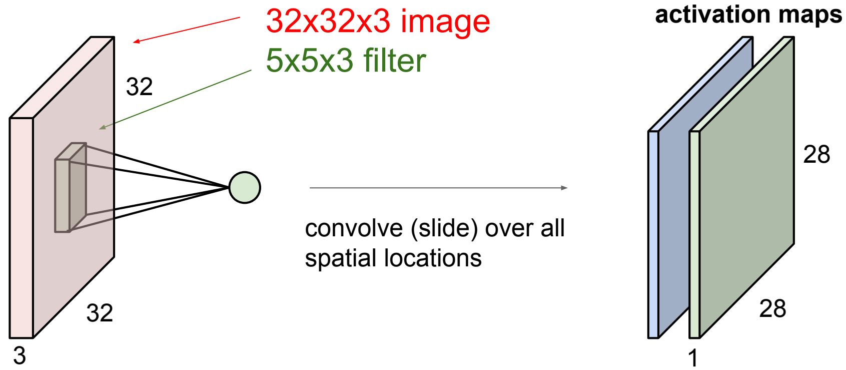
convolve (slide) over all spatial locations

activation map

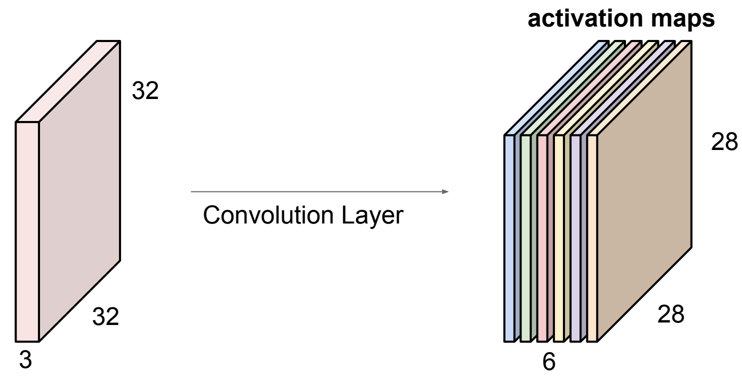


Convolution Layer

consider a second, green filter

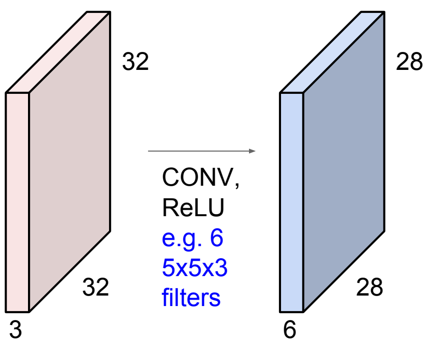


For example, if we had 6 5x5 filters, we'll get 6 separate activation maps:

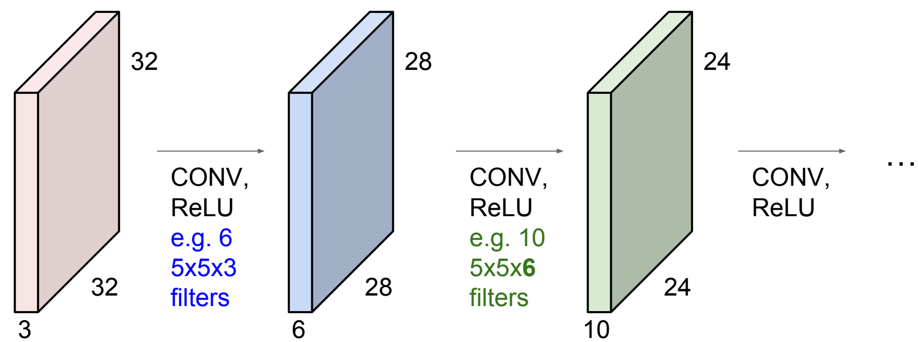


We stack these up to get a "new image" of size 28x28x6!

Preview: ConvNet is a sequence of Convolution Layers, interspersed with activation functions



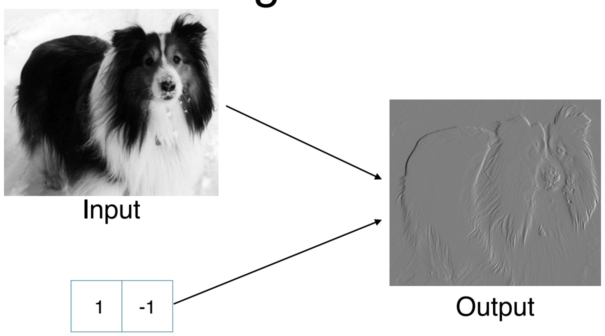
Preview: ConvNet is a sequence of Convolutional Layers, interspersed with activation functions



Why convolution makes sense?

Main idea: **if a filter is useful at one location, it should be useful at other locations.**

A simple example why filtering is useful



Connection to fully connected NNs

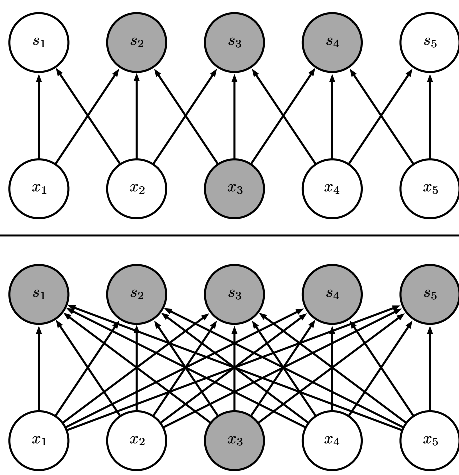
A convolution layer is a special case of a fully connected layer:

- filter = weights with **sparse connection**

Local Receptive Field Leads to Sparse Connectivity (affects less)

Sparse connections due to small convolution kernel

Dense connections



(Goodfellow 2016)

Sparse connectivity: being affected by less

Sparse connections due to small convolution kernel

Dense connections

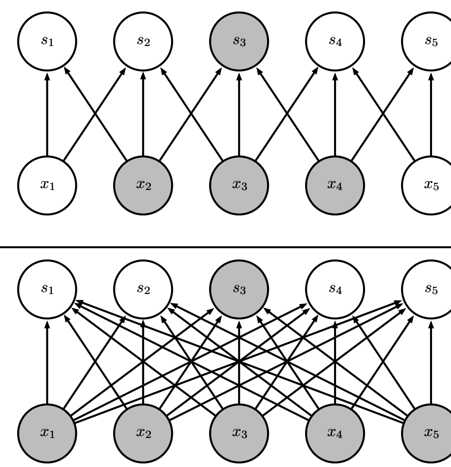


Figure 9.3

(Goodfellow 2016)

Connection to fully connected NNs

A convolution layer is a special case of a fully connected layer:

- filter $=$ weights with **sparse connection**
- **parameters sharing**

Parameter Sharing

Convolution shares the same parameters across all spatial locations

Traditional matrix multiplication does not share any parameters

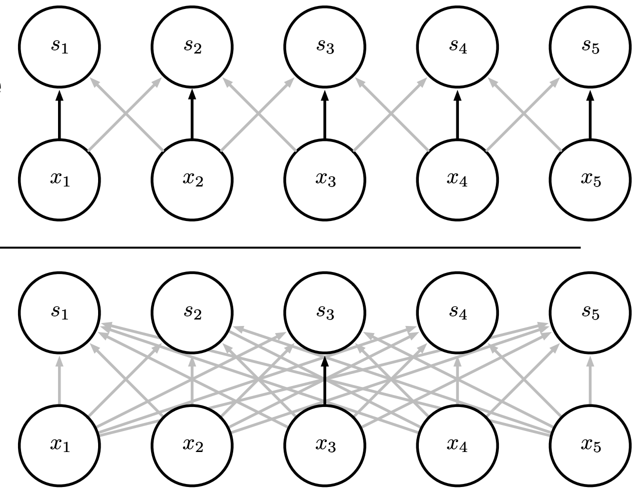


Figure 9.5

(Goodfellow 2016)

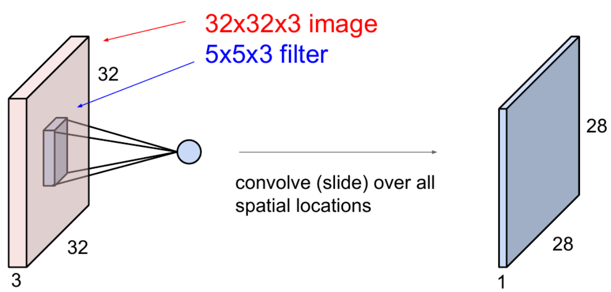
Connection to fully connected NNs

A convolution layer is a special case of a fully connected layer:

- filter $=$ weights with **sparse connection**
- **parameters sharing**

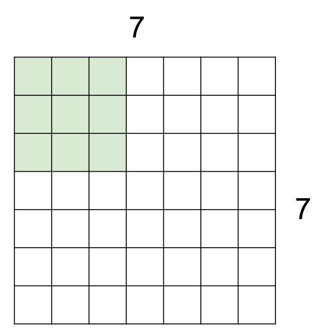
Much less parameters! Example (ignore bias terms):

- FC: $(32 \times 32 \times 3) \times (28 \times 28) \approx 2.4M$
- CNN: $5 \times 5 \times 3 = 75$



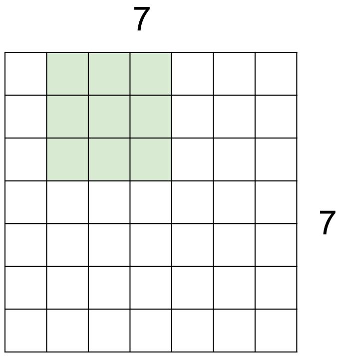
Spatial arrangement: stride and padding

A closer look at spatial dimensions:



7x7 input (spatially)
assume 3x3 filter

A closer look at spatial dimensions:



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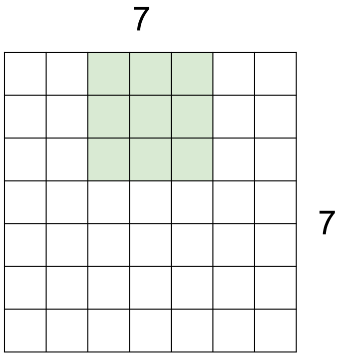

7x7 input (spatially)
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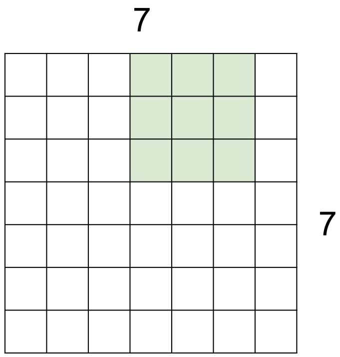
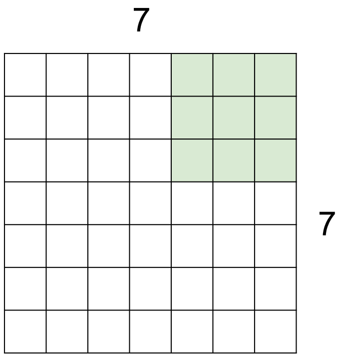
A closer look at spatial dimensions:



7x7 input (spatially)
assume 3x3 filter

A closer look at spatial dimensions:

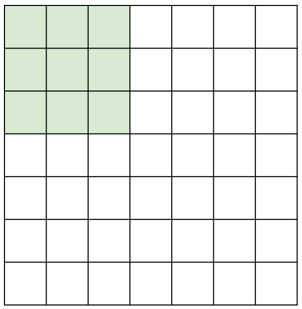


7x7 input (spatially)
assume 3x3 filter

=> 5x5 output

A closer look at spatial dimensions:

7

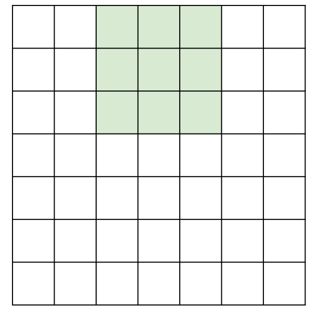


7

7x7 input (spatially)
assume 3x3 filter
applied **with stride 2**

A closer look at spatial dimensions:

7

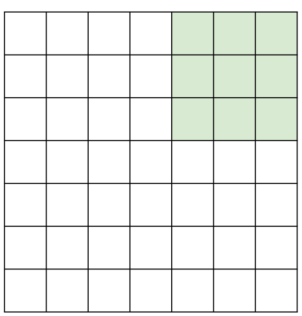


7

7x7 input (spatially)
assume 3x3 filter
applied **with stride 2**

A closer look at spatial dimensions:

7

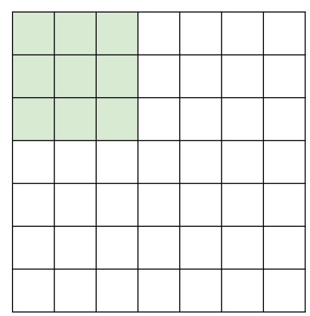


7

7x7 input (spatially)
assume 3x3 filter
applied **with stride 2**
=> 3x3 output!

A closer look at spatial dimensions:

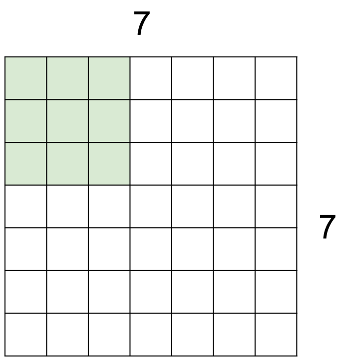
7



7

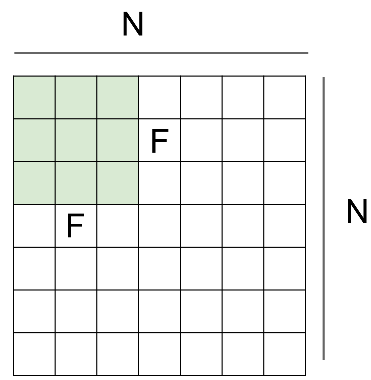
7x7 input (spatially)
assume 3x3 filter
applied **with stride 3?**

A closer look at spatial dimensions:



7x7 input (spatially)
assume 3x3 filter
applied **with stride 3?**

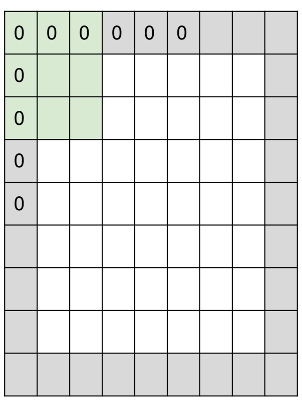
doesn't fit!
cannot apply 3x3 filter on
7x7 input with stride 3.



Output size:
(N - F) / stride + 1

e.g. N = 7, F = 3:
stride 1 => (7 - 3)/1 + 1 = 5
stride 2 => (7 - 3)/2 + 1 = 3
stride 3 => (7 - 3)/3 + 1 = 2.33 :\

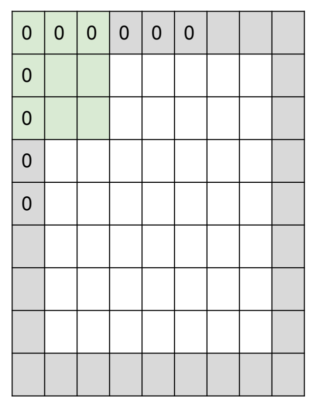
In practice: Common to zero pad the border



e.g. input 7x7
3x3 filter, applied with **stride 1**
pad with 1 pixel border => what is the output?

(recall:)
(N - F) / stride + 1

In practice: Common to zero pad the border



e.g. input 7x7
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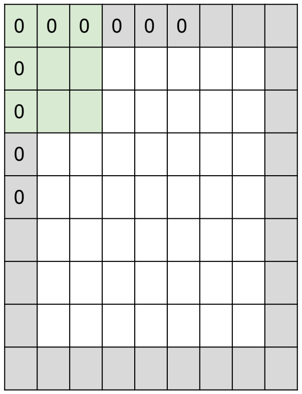
pad with 1 pixel border => what is the output?

7x7 output!

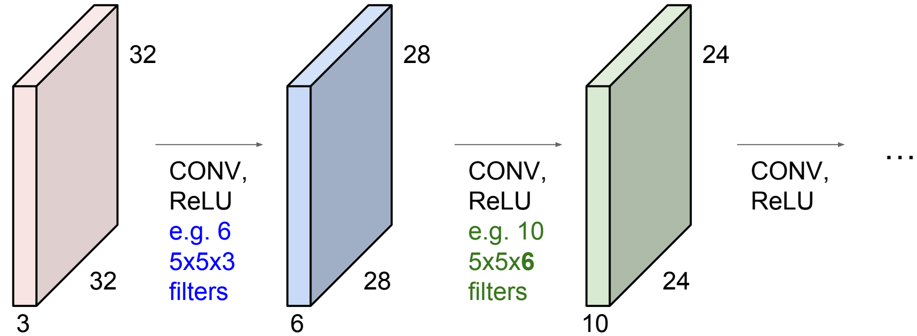
In practice: Common to zero pad the border



e.g. input 7x7
3x3 filter, applied with **stride 1**
pad with 1 pixel border => what is the output?

7x7 output!
in general, common to see CONV layers with stride 1, filters of size FxF, and zero-padding with (F-1)/2. (will preserve size spatially)
e.g. F = 3 => zero pad with 1
F = 5 => zero pad with 2
F = 7 => zero pad with 3

Remember back to…
E.g. 32x32 input convolved repeatedly with 5x5 filters shrinks volumes spatially! (32 -> 28 -> 24 ...). Shrinking too fast is not good, doesn't work well.



Summary for convolution layer

Input: a volume of size $W_1 \times H_1 \times D_1$

Hyperparameters:

- K filters of size $F \times F$
- stride S
- amount of zero padding P (for one side)

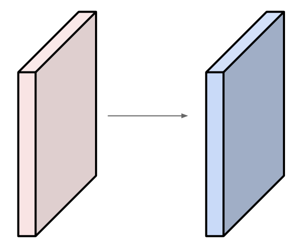
Output: a volume of size $W_2 \times H_2 \times D_2$ where

- $W_2 = (W_1 + 2P - F)/S + 1$
- $H_2 = (H_1 + 2P - F)/S + 1$
- $D_2 = K$

#parameters: $(F \times F \times D_1 + 1) \times K$ weights

Common setting: $F = 3, S = P = 1$

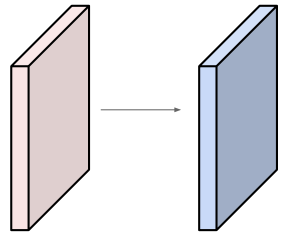
Examples time:



Input volume: **32x32x3**
10 5x5 filters with stride 1, pad 2

Output volume size: ?

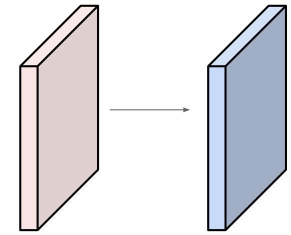
Examples time:



Input volume: **32x32x3**
10 5x5 filters with stride 1, pad 2

Output volume size:
(32+2*2-5)/1+1 = 32 spatially, so
32x32x10

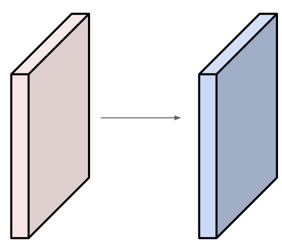
Examples time:



Input volume: **32x32x3**
10 5x5 filters with stride 1, pad 2

Number of parameters in this layer?

Examples time:

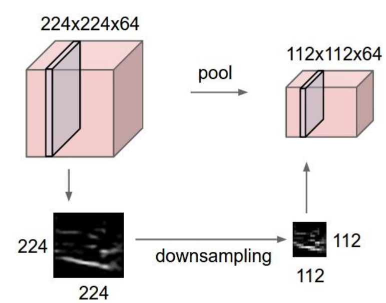


Input volume: **32x32x3**
10 5x5 filters with stride 1, pad 2

Number of parameters in this layer?
each filter has 5*5*3 + 1 = 76 params (+1 for bias)
=> 76*10 = **760**

Another element: pooling

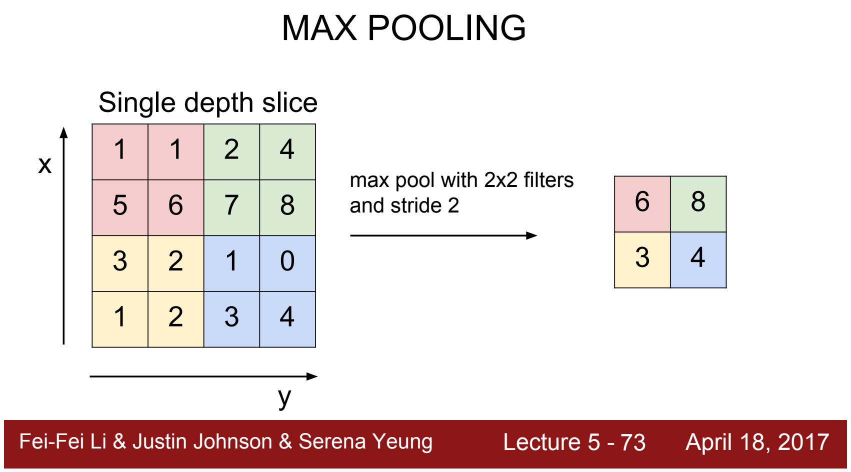
Pooling layer
- makes the representations smaller and more manageable
- operates over each activation map independently:



Types of pooling: average, L2-norm, max

Max pooling

Max pooling with 2×2 filter and stride 2 is very common



Putting everything together

Typical architecture for CNNs:

Input $\rightarrow$ [[Conv $\rightarrow$ ReLU]*N $\rightarrow$ Pool?]*M $\rightarrow$ [FC $\rightarrow$ ReLU]*Q $\rightarrow$ FC

Common choices: $N \leq 5, Q \leq 2$, M is large

Well-known CNNs: LeNet, AlexNet, ZF Net, GoogLeNet, VGGNet, etc.

All achieve excellent performance on image classification tasks.

How to train a CNN?

How do we learn the filters/weights?

Essentially the same as FC NNs: apply **SGD/backpropagation**

Outline

1. Review of last lecture
2. Convolutional neural networks
3. Kernel methods
   - Motivation
   - Dual formulation of linear regression
   - Kernel Trick

Motivation

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

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

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

Case study: regularized linear regression

Kernel methods work for *many problems* and we take **regularized linear regression** as an example.

Recall the regularized least square solution:

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

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

Issue: *operate in space $\mathbb{R}^M$ and M could be huge or even infinity!*

A closer look at the least square solution

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

$$\boldsymbol{\Phi}^{\mathrm{T}}(\boldsymbol{\Phi}\boldsymbol{w}^* - \boldsymbol{y}) + \lambda\boldsymbol{w}^* = \mathbf{0}$$

we know

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

Thus the least square solution is **a linear combination of features**!

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

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

Therefore we do not really need to know $\boldsymbol{w}^*$. *Only inner products in the new feature space matter!*

Kernel methods are exactly about computing inner products *without knowing ϕ*.

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

$$\begin{aligned}
G(\boldsymbol{\alpha}) &= F(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\alpha}) \\
&= \|\boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\alpha} - \boldsymbol{y}\|_2^2 + \lambda\|\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\alpha}\|_2^2 \\
&= \|\boldsymbol{K}\boldsymbol{\alpha} - \boldsymbol{y}\|_2^2 + \lambda\boldsymbol{\alpha}^{\mathrm{T}}\boldsymbol{K}\boldsymbol{\alpha} && (\boldsymbol{K} = \boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathrm{T}}) \\
&= \boldsymbol{\alpha}^{\mathrm{T}}\boldsymbol{K}^{\mathrm{T}}\boldsymbol{K}\boldsymbol{\alpha} - 2\boldsymbol{y}^{\mathrm{T}}\boldsymbol{K}\boldsymbol{\alpha} + \lambda\boldsymbol{\alpha}^{\mathrm{T}}\boldsymbol{K}\boldsymbol{\alpha} + \text{cnt.} \\
&= \boldsymbol{\alpha}^{\mathrm{T}}(\boldsymbol{K}^2 + \lambda\boldsymbol{K})\boldsymbol{\alpha} - 2\boldsymbol{y}^{\mathrm{T}}\boldsymbol{K}\boldsymbol{\alpha} + \text{cnt.} && (\boldsymbol{K}^{\mathrm{T}} = \boldsymbol{K})
\end{aligned}$$

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

$\boldsymbol{K} = \boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathrm{T}} \in \mathbb{R}^{\mathsf{N}\times\mathsf{N}}$ 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

3 data points in $\mathbb{R}$

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

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

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

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

Calculation of the Gram matrix

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

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**
$\boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathrm{T}}$	$\mathsf{N}\times\mathsf{N}$	$\boldsymbol{\phi}(\boldsymbol{x}_i)^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_j)$	both are **symmetric** and **positive semidefinite**
$\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}$	$\mathsf{M}\times\mathsf{M}$	$\sum_{n=1}^{N}\phi(\boldsymbol{x}_n)_i\phi(\boldsymbol{x}_n)_j$	

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

Minimize the dual formulation

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

Setting the derivative to $\boldsymbol{0}$ we have

$$\boldsymbol{0} = (\boldsymbol{K}^2 + \lambda \boldsymbol{K})\boldsymbol{\alpha} - \boldsymbol{K}\boldsymbol{y} = \boldsymbol{K}\left((\boldsymbol{K} + \lambda \boldsymbol{I})\boldsymbol{\alpha} - \boldsymbol{y}\right)$$

Thus $\boldsymbol{\alpha} = (\boldsymbol{K} + \lambda \boldsymbol{I})^{-1}\boldsymbol{y}$ **is a minimizer** and we obtain

$$\boldsymbol{w}^* = \boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\alpha} = \boldsymbol{\Phi}^{\mathrm{T}}(\boldsymbol{K} + \lambda \boldsymbol{I})^{-1}\boldsymbol{y}$$

Exercise: *are there other minimizers?*

Comparing two solutions

Minimizing $F(\boldsymbol{w})$ gives $\boldsymbol{w}^* = (\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi} + \lambda \boldsymbol{I})^{-1}\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{y}$

Minimizing $G(\boldsymbol{\alpha})$ gives $\boldsymbol{w}^* = \boldsymbol{\Phi}^{\mathrm{T}}(\boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathrm{T}} + \lambda \boldsymbol{I})^{-1}\boldsymbol{y}$

Note $\boldsymbol{I}$ has different dimensions in two formulas.

Natural question: *are they the same or different?*

They are the same

$$\begin{aligned}
&(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi} + \lambda \boldsymbol{I})^{-1}\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{y} \\
&= (\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi} + \lambda \boldsymbol{I})^{-1}\boldsymbol{\Phi}^{\mathrm{T}}(\boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathrm{T}} + \lambda \boldsymbol{I})(\boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathrm{T}} + \lambda \boldsymbol{I})^{-1}\boldsymbol{y} \\
&= (\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi} + \lambda \boldsymbol{I})^{-1}(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathrm{T}} + \lambda \boldsymbol{\Phi}^{\mathrm{T}})(\boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathrm{T}} + \lambda \boldsymbol{I})^{-1}\boldsymbol{y} \\
&= (\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi} + \lambda \boldsymbol{I})^{-1}(\boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi} + \lambda \boldsymbol{I})\boldsymbol{\Phi}^{\mathrm{T}}(\boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathrm{T}} + \lambda \boldsymbol{I})^{-1}\boldsymbol{y} \\
&= \boldsymbol{\Phi}^{\mathrm{T}}(\boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathrm{T}} + \lambda \boldsymbol{I})^{-1}\boldsymbol{y}
\end{aligned}$$

Then what is the difference?

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

More importantly, computing $\boldsymbol{\alpha} = (\boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathrm{T}} + \lambda \boldsymbol{I})^{-1}$ also *only requires computing inner products in the new feature space!*

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

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*.

Example

Consider the following polynomial basis $\boldsymbol{\phi} : \mathbb{R}^2 \to \mathbb{R}^3$:

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

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

$$\begin{aligned}
\boldsymbol{\phi}(\boldsymbol{x})^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}') &= {x_1}^2{x_1'}^2 + 2x_1x_2x_1'x_2' + {x_2}^2{x_2'}^2 \\
&= (x_1x_1' + x_2x_2')^2 = (\boldsymbol{x}^{\mathrm{T}}\boldsymbol{x}')^2
\end{aligned}$$

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

Another example

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

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

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

$$\begin{aligned}\phi_\theta(\boldsymbol{x})^{\mathrm{T}}\phi_\theta(\boldsymbol{x}') &= \sum_{d=1}^{\mathsf{D}} \cos(\theta x_d)\cos(\theta x'_d) + \sin(\theta x_d)\sin(\theta x'_d) \\ &= \sum_{d=1}^{\mathsf{D}} \cos(\theta(x_d - x'_d))\end{aligned}$$

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:

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

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

$$\begin{aligned}\phi_L(\boldsymbol{x})^{\mathrm{T}}\phi_L(\boldsymbol{x}') &= \sum_{\ell=0}^{L} \phi_{\frac{2\pi\ell}{L}}(\boldsymbol{x})^{\mathrm{T}}\phi_{\frac{2\pi\ell}{L}}(\boldsymbol{x}') \\ &= \sum_{\ell=0}^{L}\sum_{d=1}^{\mathsf{D}} \cos\left(\frac{2\pi\ell}{L}(x_d - x'_d)\right)\end{aligned}$$

Infinite dimensional mapping

When $L \to \infty$, even if we cannot compute $\phi(x)$, a vector of *infinite dimension*, we can still compute inner product:

$$\begin{aligned}\phi_\infty(\boldsymbol{x})^{\mathrm{T}}\phi_\infty(\boldsymbol{x}') &= \int_0^{2\pi}\sum_{d=1}^{\mathsf{D}} \cos(\theta(x_d - x'_d))\, d\theta \\ &= \sum_{d=1}^{\mathsf{D}} \frac{\sin(2\pi(x_d - x'_d))}{x_d - x'_d}\end{aligned}$$

Again, a simple function of the original features.

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 $\phi : \mathbb{R}^{\mathsf{D}} \to \mathbb{R}^{\mathsf{M}}$ so that for any $\boldsymbol{x}, \boldsymbol{x}' \in \mathbb{R}^{\mathsf{D}}$,

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

Examples we have seen

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

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

Using kernel functions

Choosing a nonlinear basis ϕ becomes choosing a kernel function.

As long as computing the kernel function is more efficient, we should apply the kernel trick.

Gram/kernel matrix becomes:

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

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

Using kernel functions

The prediction on a new example $\boldsymbol{x}$ is

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

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.

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 $\sigma > 0$.

Think about *what the corresponding ϕ is* for each kernel.

Composing kernels

Creating more kernel functions using the following rules:

If $k_1(\cdot,\cdot)$ and $k_2(\cdot,\cdot)$ are kernels, the followings are kernels too

- **linear combination**: $\alpha k_1(\cdot,\cdot) + \beta k_2(\cdot,\cdot)$ if $\alpha, \beta \geq 0$
- **product**: $k_1(\cdot,\cdot)k_2(\cdot,\cdot)$
- **exponential**: $e^{k(\cdot,\cdot)}$
- $\cdots$

Verify using the definition of kernel!

Examples that are not kernels

Function

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

is *not a kernel*, why?

Example: if it is a kernel, the kernel matrix for two data points $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$:

$$\boldsymbol{K} = \begin{pmatrix} 0 & \|\boldsymbol{x}_1 - \boldsymbol{x}_2\|_2^2 \\ \|\boldsymbol{x}_1 - \boldsymbol{x}_2\|_2^2 & 0 \end{pmatrix}$$

must be positive semidefinite, *but is it?*

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 $\boldsymbol{x}$, $\boldsymbol{x}'$

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

With a kernel function k, we simply compute

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

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

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