

# Introductions to Machine Learning and Deep Learning on Comet with examples for R, scaling R, and Convolution Networks with Python

Paul Rodriguez SDSC

# Outline

- I. Analytics, Machine Learning in a Nutshell
- II. R, Scaling in R, Parallel R
- III. Deep Learning in a Nutshell
- IV. Deep Learning Tutorial

# Lots of Terms:



Lior Rokach  
Department of Information Systems Engineering  
Ben-Gurion University of the Negev





# Machine Learning Models

- **Classification**
- **Regression/Predictive**

*Supervised (dependent variable or outcome labels given)*

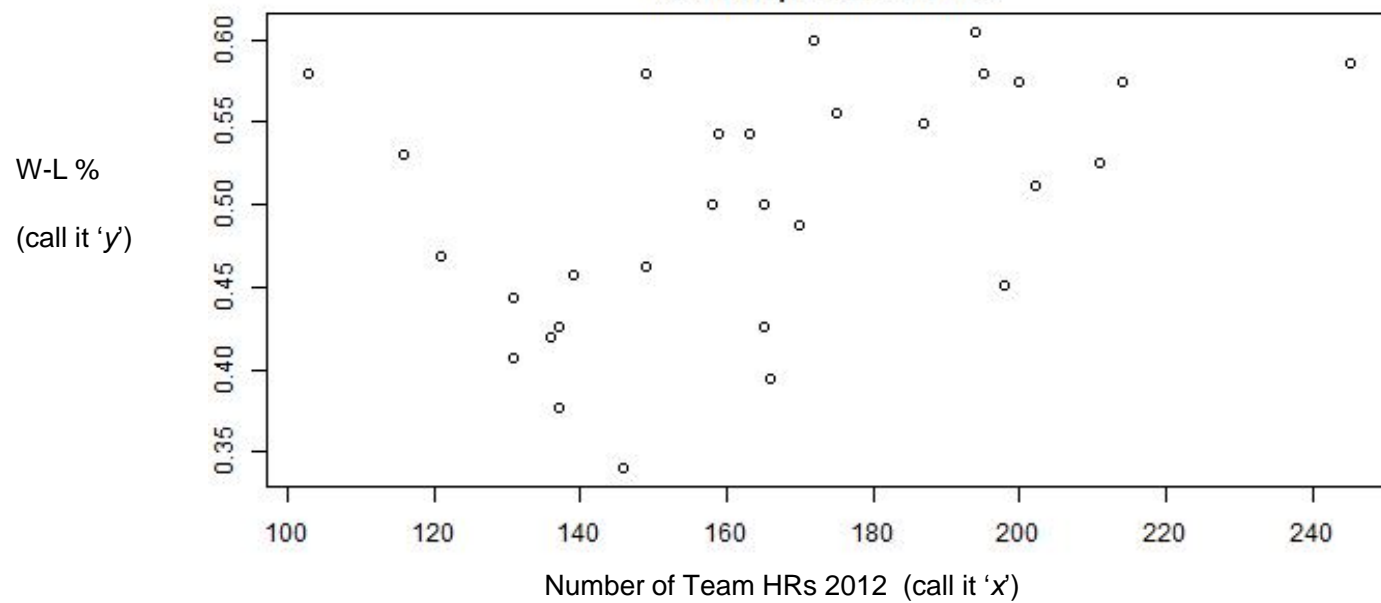
- **Cluster**
- **Matrix Factorization**

*Unsupervised (no labels)*

- **Bayesian (i.e. learning probability distributions)**

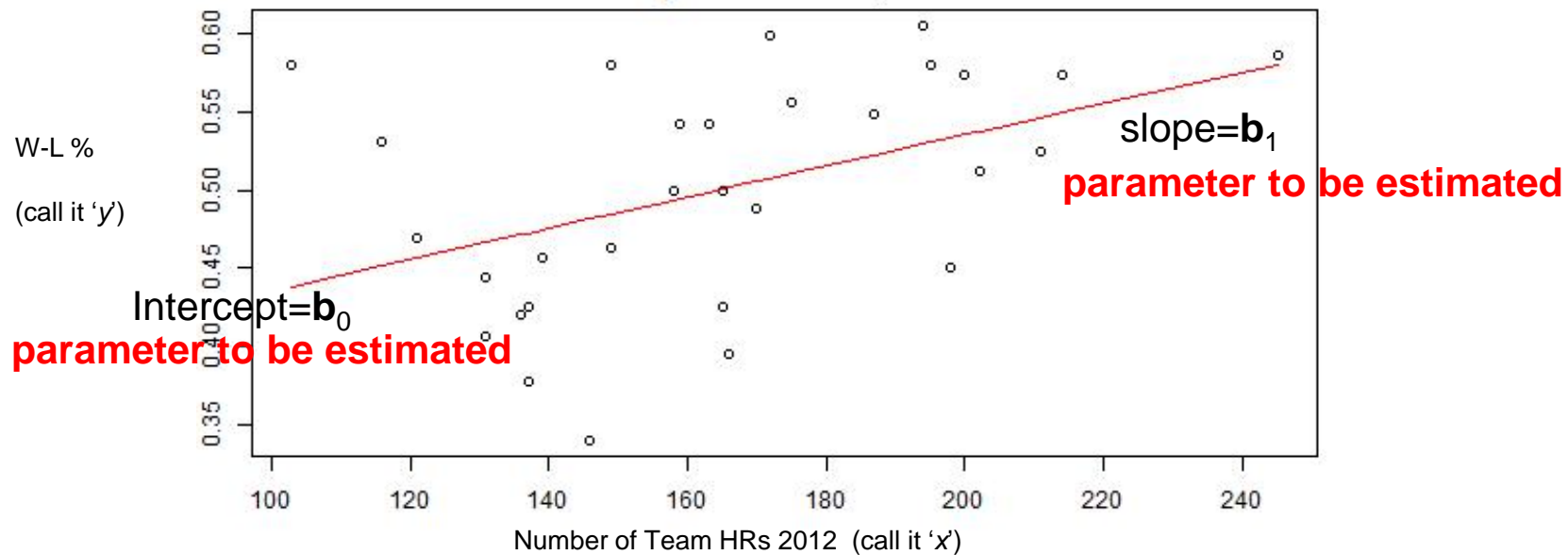
*Statistical but comes up in HPC settings*

# A data example: Home Runs and W-L percent



# Recall Linear Regression is Fitting a Line – to minimize error

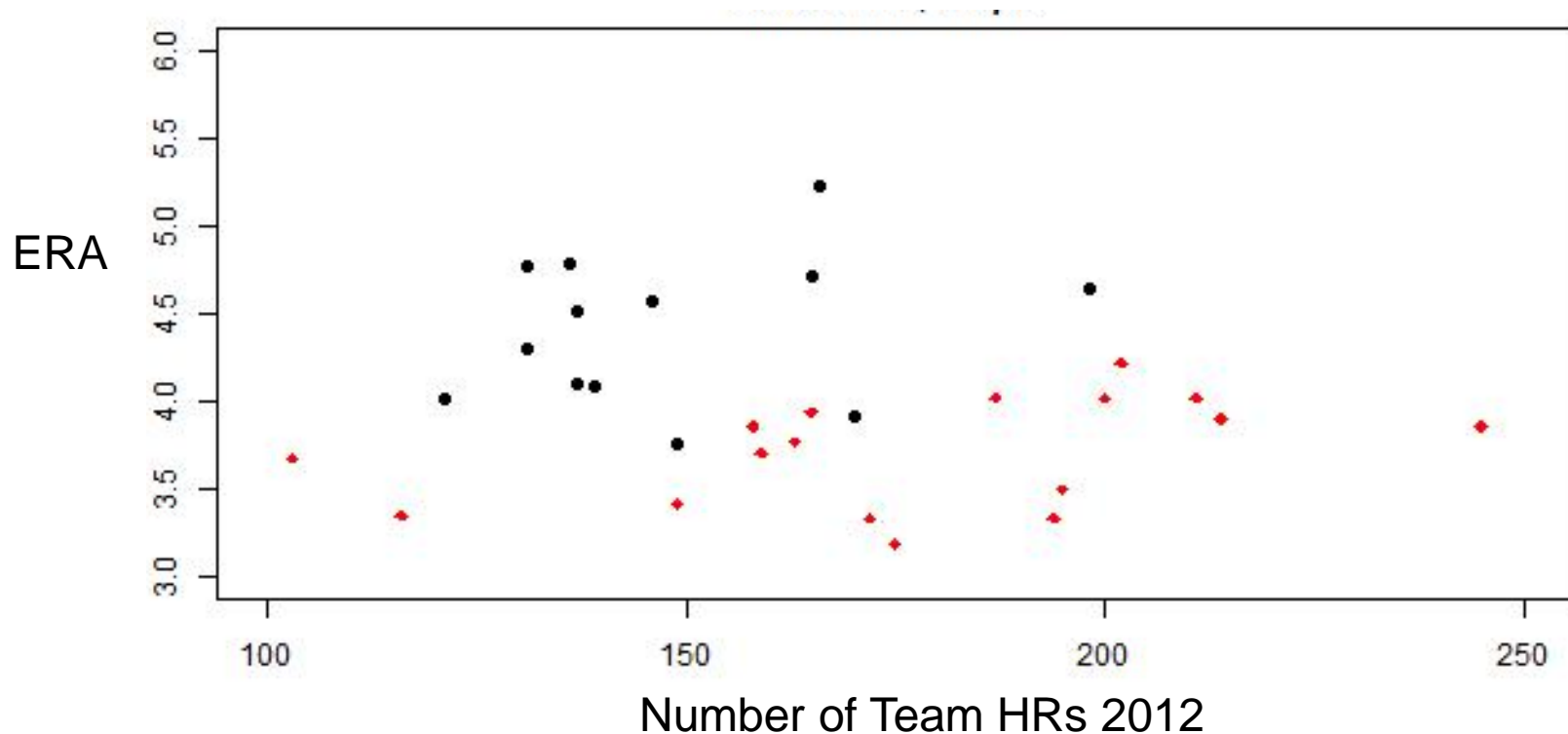
the Model:  $y = f(x, b) = b_0 * 1 + b_1 * x$



# A Model for Classification

- 2 classes: +1=Black (WL% $\geq$ .5) -1=Red (WL% $<$ .5)

*Q: Classify winning records based on HRs and ERA?*

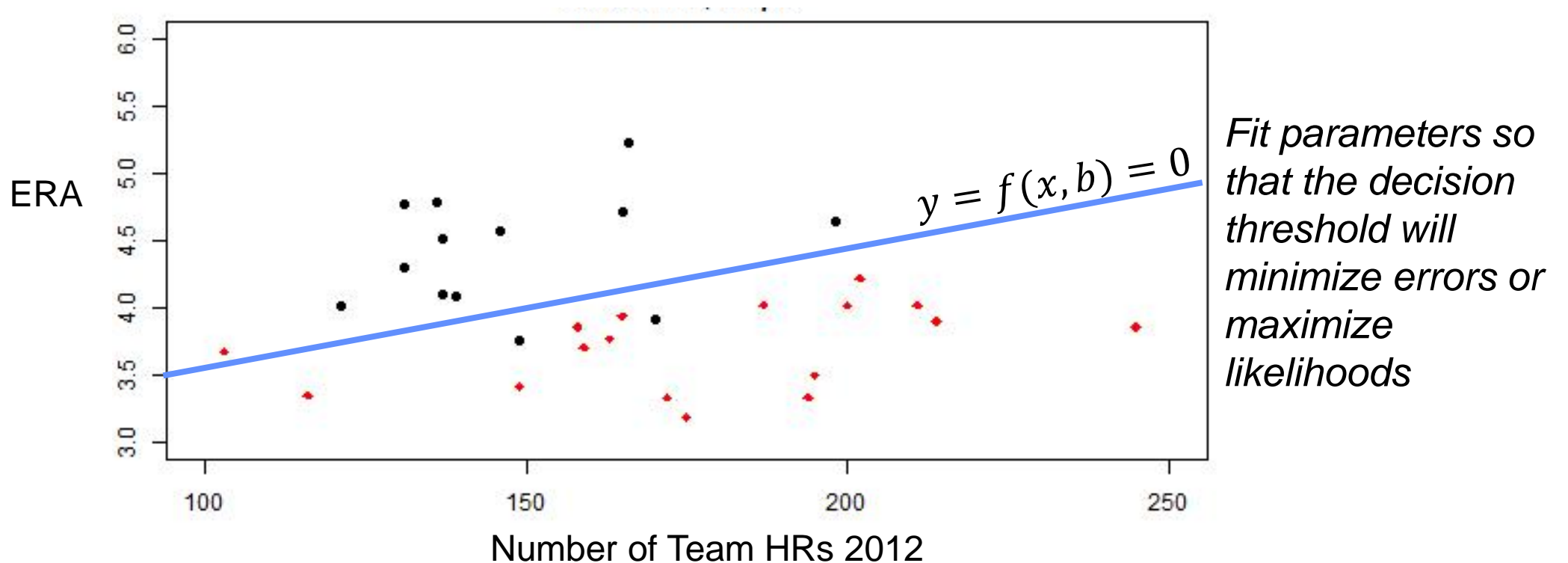




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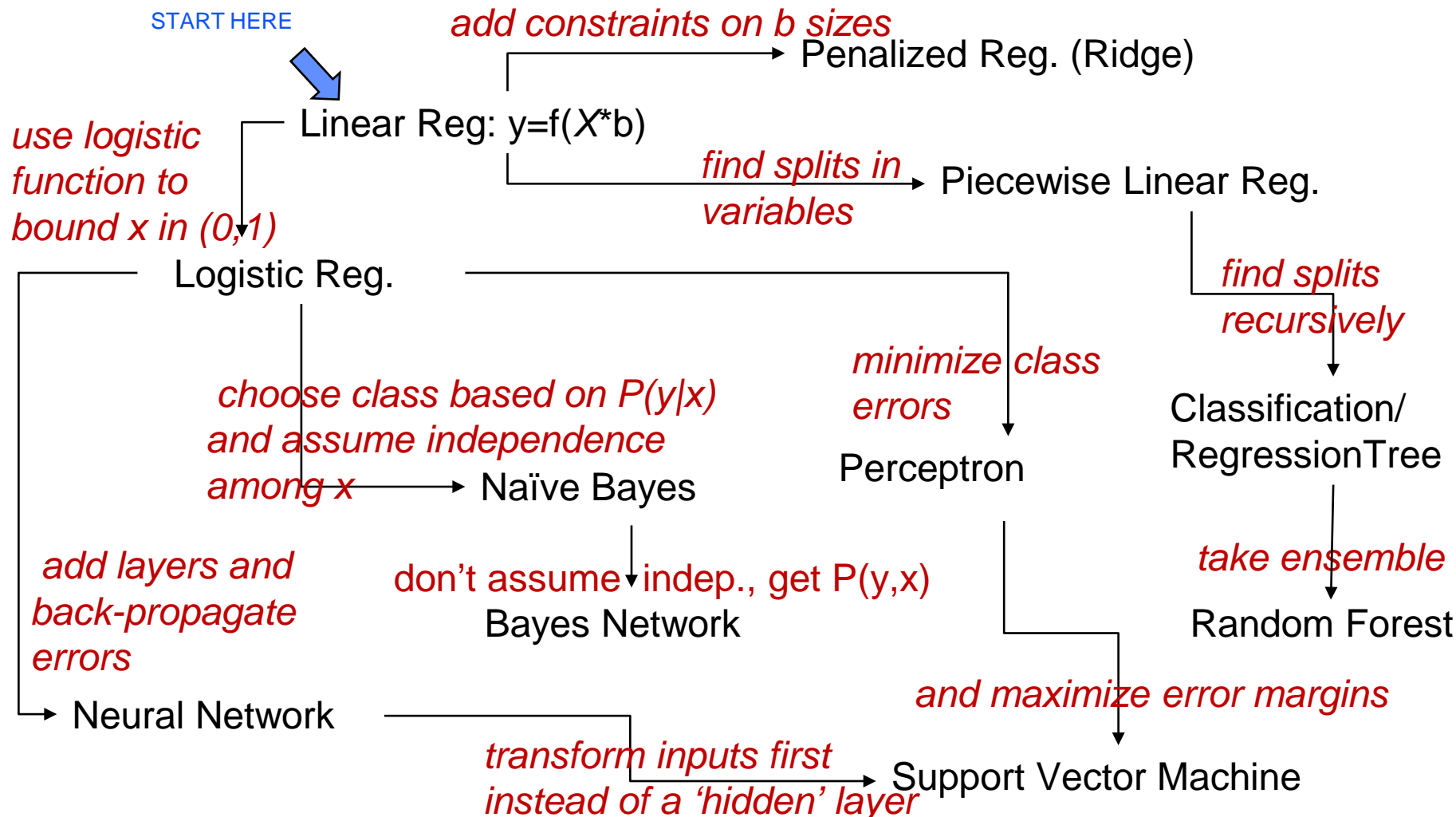
*Q: Classify winning records based on HRs and ERA?*



# Model Choices

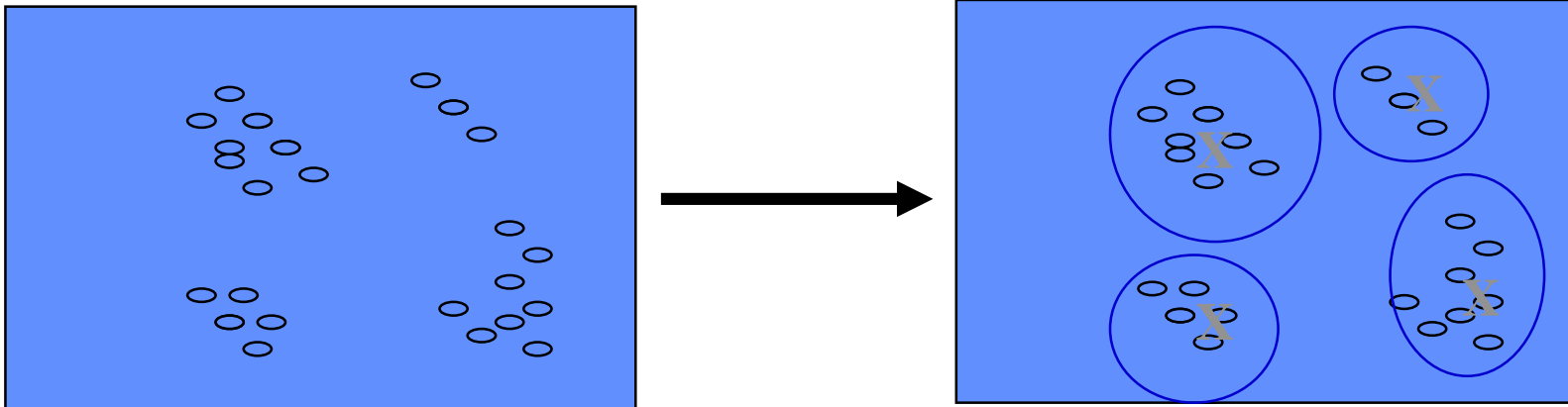
- **What kinds of functions to use**
  - e.g. Linear vs NonLinear
- **What to Optimize**
  - Minimize Sum Squared Error
  - Minimize Classification Errors
  - Maximize Probabilities
- **How to Fit Parameters**
  - Analytically
  - Search parameter space or follow gradients
  - Use Constraints as needed
- **How to avoid overfitting, and generalize well to test data**

# Model Space Map – in a nutshell



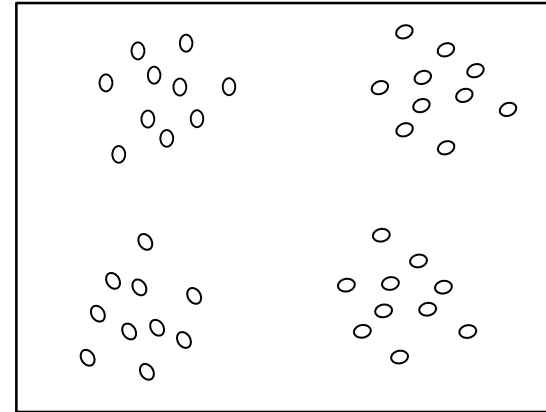
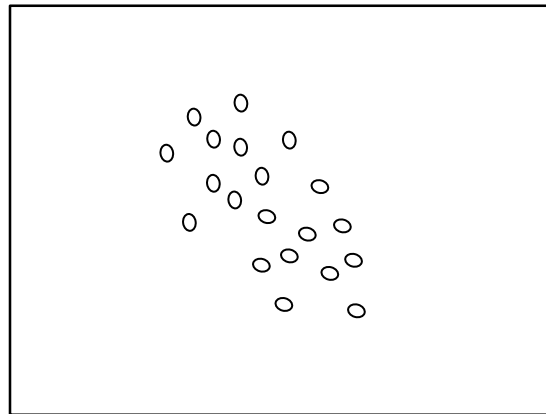
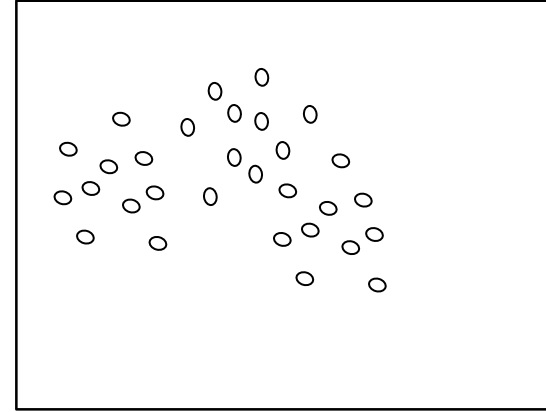
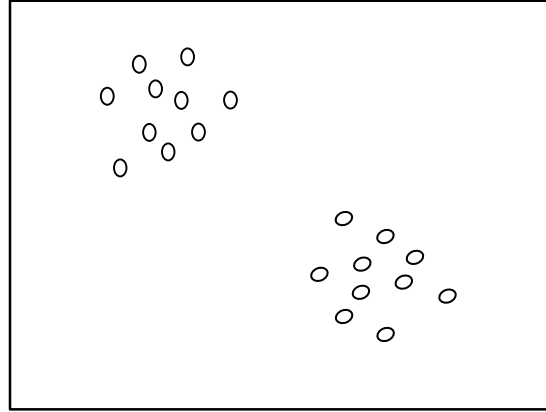
# Clustering

- Basic idea: Group similar things together
- K-means
  - Partitioning instances into  $k$  disjoint clusters
  - Measure of similarity



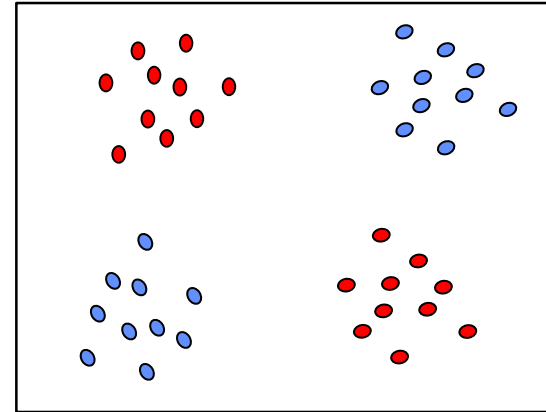
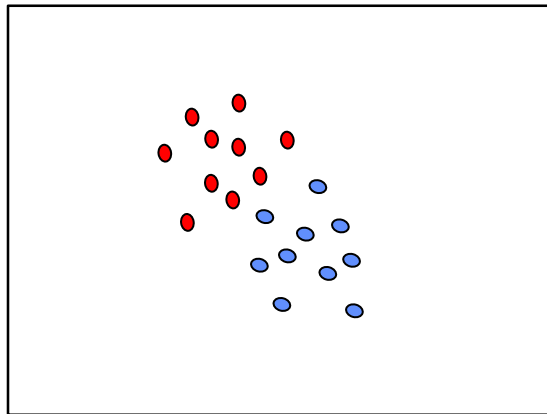
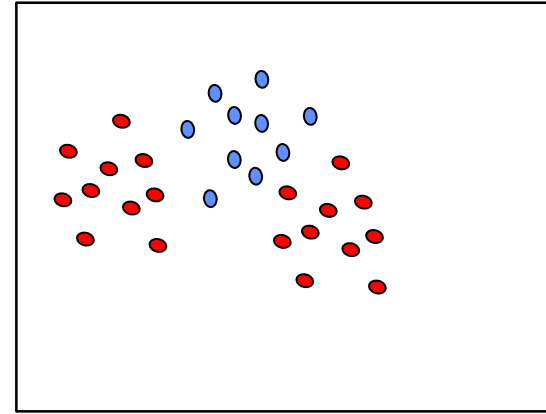
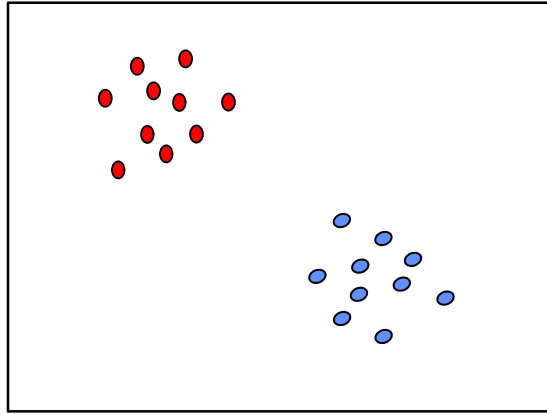
# ***A note about clustering***

Imagine these 2 dimensional input spaces:  
Which of these is easy or hard to cluster?  
(e.g. separate into groups)

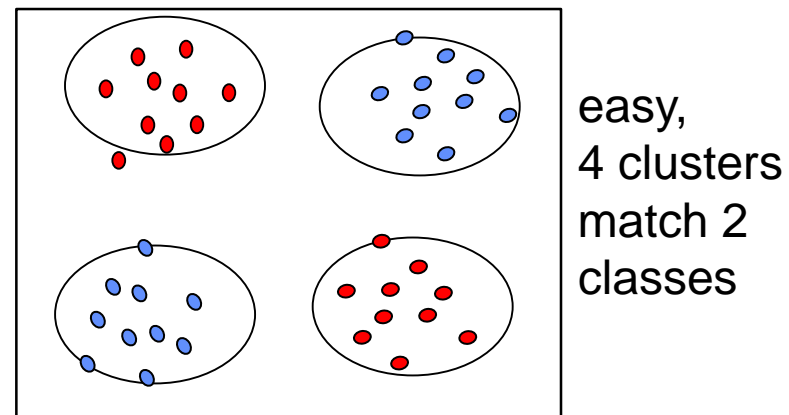
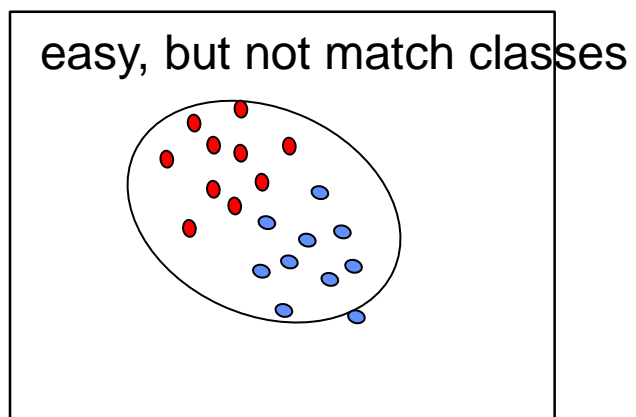
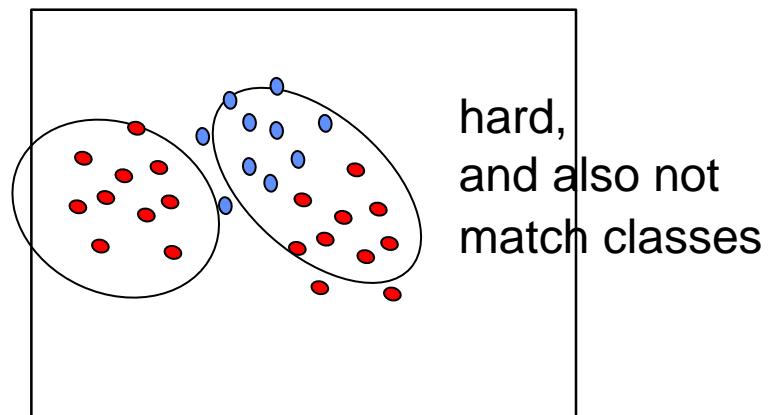
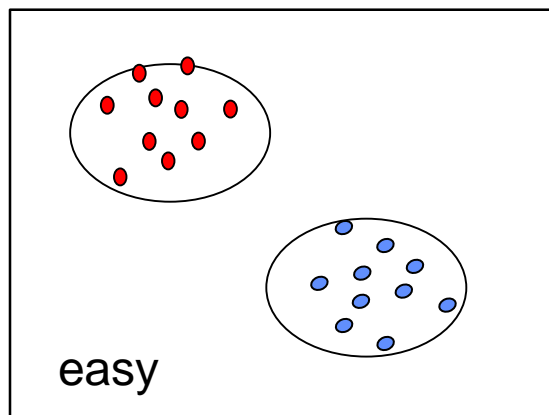




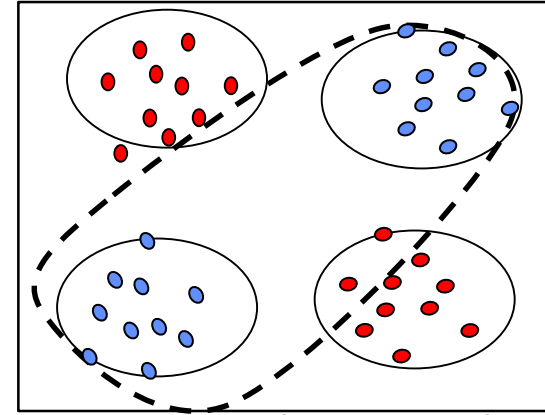
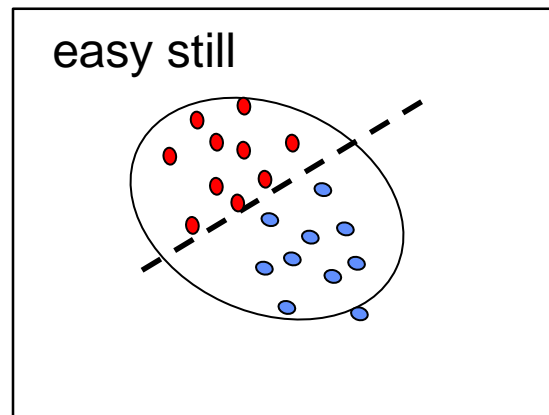
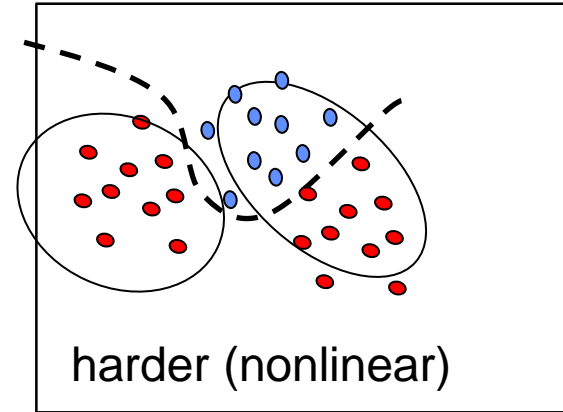
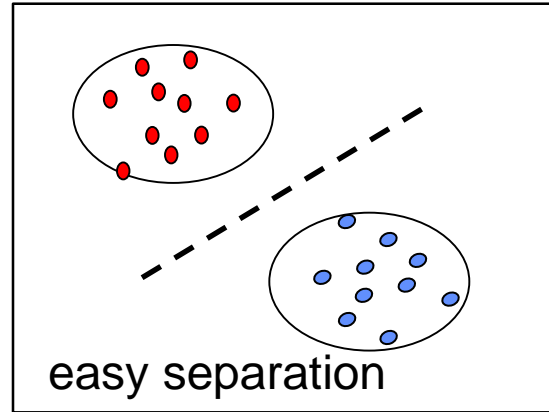
Now imaging there are two classes



# Potential clusters



Which are easy or hard to classify? (ie separate red or blue with lines)



Upshot:  
**No easy  
relationship  
between  
clusters  
and  
classification**

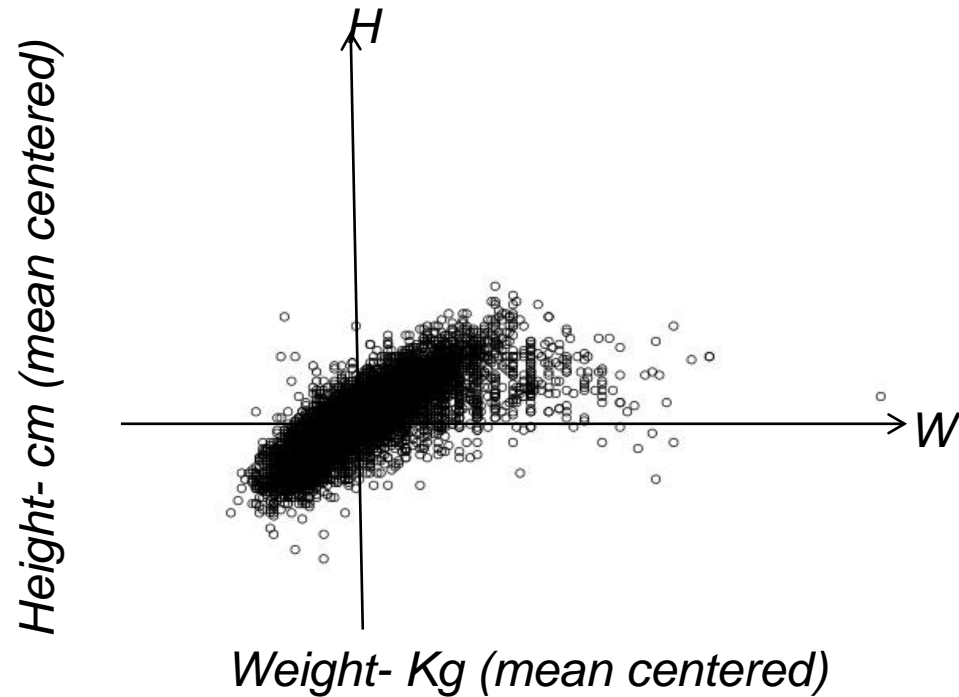
# Matrix Factorization:

*Given a numeric matrix, can we reduce the number of columns?*

- Yes, if features are constant or redundant
- Yes, if features only contribute noise

Conversely, want features that contribute to variations of the data

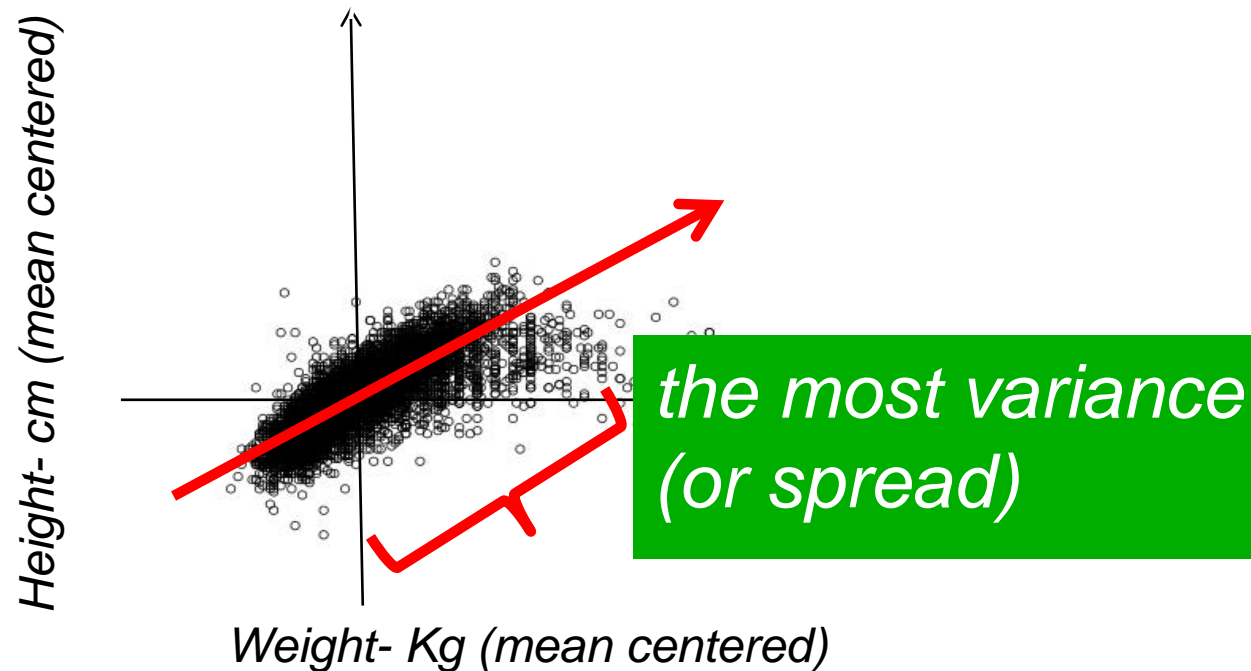
## Example: Athletes' Height by Weight



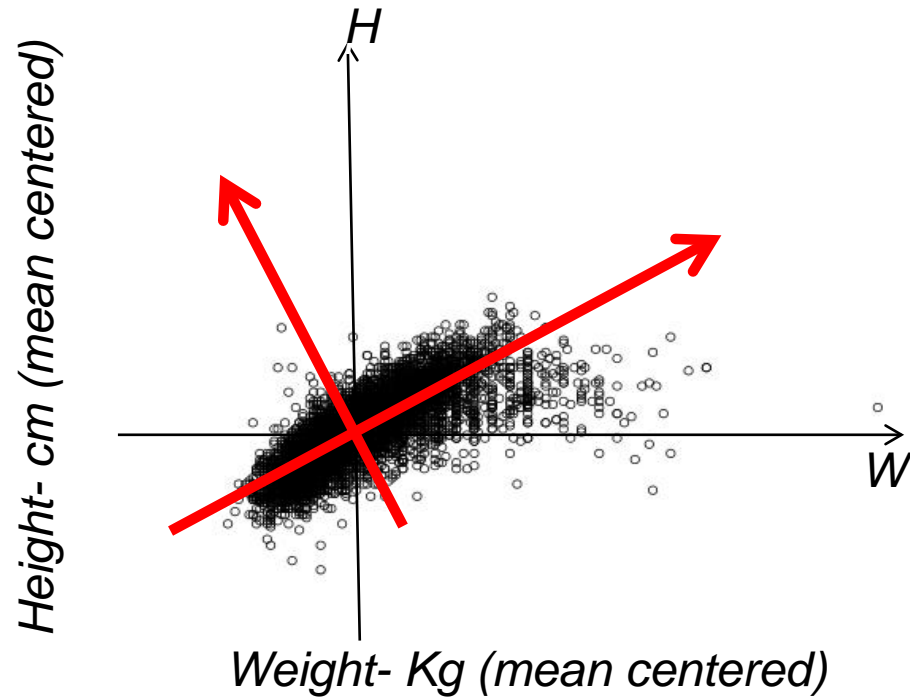
*Find a line that aligns with the data.*



## Example: Athletes' Height by Weight

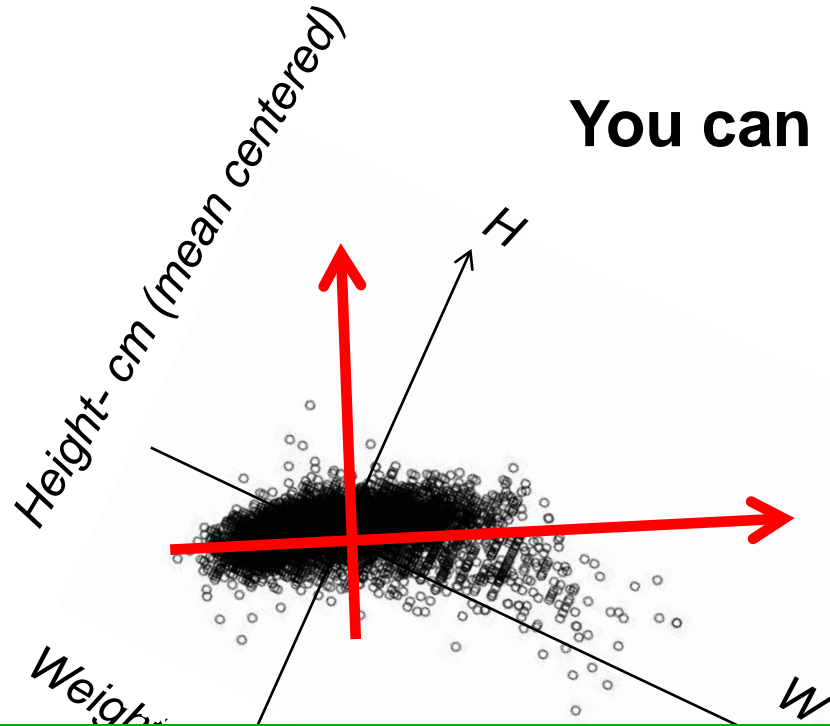


*Find a line that aligns with the data.*

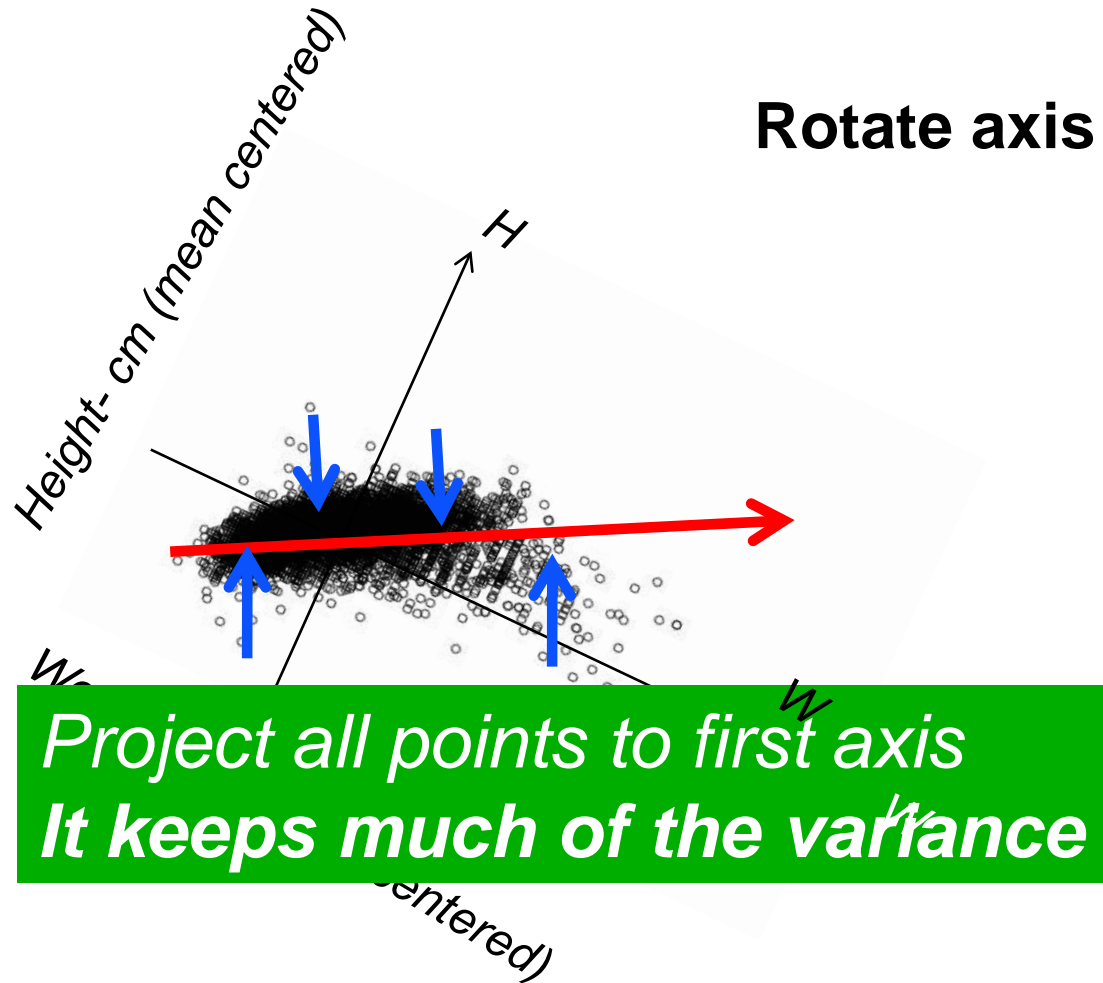


*The next direction of most variance.*

You can rotate the axes



*New axes (i.e., new features or latent factors) are combinations of old axis (i.e., old features or observed factors)*



# Principle Components

- Best Known Factorization Algorithms:
  - SVD (singular value decomposition)
  - PCA (principle component analysis)

*SVD more generally works on non square matrices*

- Can choose  $k$  factors heuristically as approximation improves, or choose  $k$  so that high percent (ie 80-95%) of data variance accounted for
- For higher dimensional data, use factors to visualize data in some 2D subspace



# Exploration and Modeling Recommendations

- Start simple
  - Consider trade off as you go more complex
  - Find what works in your domain
  - Find what works for this model
- 
- R, Python, Matlab: scripting languages with train/predict/test functions
  - Weka, KNIME: GUI tools

**Pause**

# R, Scaling R, Parallel R

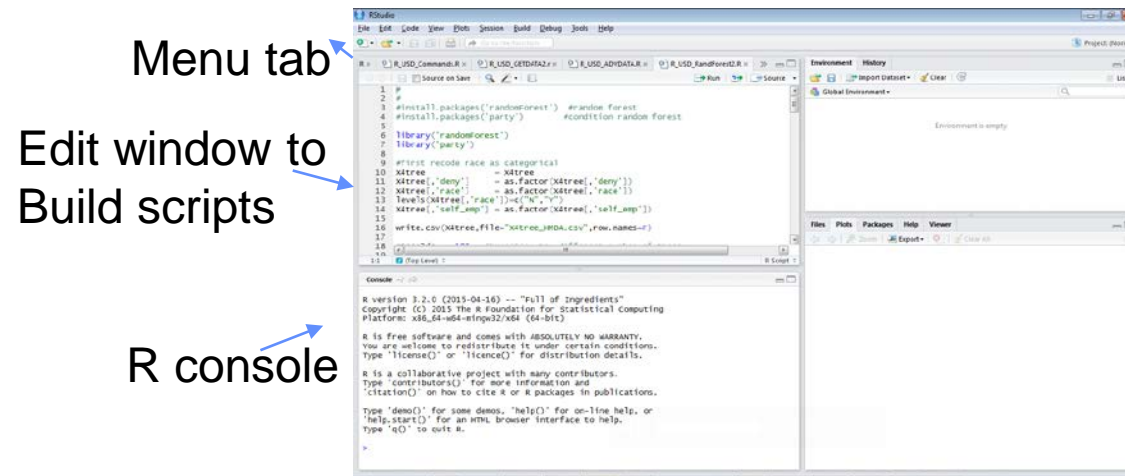
- A Glimpse of R
- R and Scaling
- Parallel options for R
- R on Comet exercise

# The What and Why of R

- **A statistical computing environment**
  - Full set of Statistical/Mathematical functions
  - Programming Language for complete data manipulation
- **Free, Open Source**
- **Extended with user written packages**
- **Widely used in academic and increasingly in industry**

# A typical R development workflow

- R studio: An Integrated development environment for R on your local machine – good for development



Environment  
Information on  
variables and  
command history

Plots, help  
docs,  
package lists



# R commands in brief

- A typical R code workflow:

## **#READ DATA (housing mortgage cases)**

```
X = read.csv('hmda_aer.csv', header=T, stringsAsFactors=T)
```

## **#SUBSET DATA**

```
indices_2keep = which(X[, 's13'] %in% c(3,4,5))
```

```
X = X[unique(indices_2keep),]
```

## **#CREATE/TRANSFORM VARIABLES**

```
pi_rat = as.numeric(X[, 's46']/100) #debt2income ratio
```

```
race = as.numeric(X[, 's13'] %in% c(3,4)) #make race values 1-4 into values 0 or 1
```

```
deny = as.numeric(X[, 's7']==3) #make deny values into 0 or 1,  
# 1 only for deny='3'
```

## **#RUN MODEL and SHOW RESULTS**

```
lm_result = lm(deny~race+pi_rat) #lm is 'linearmodel'
```

```
summary(lm_result)
```

# R strengths for HPC

- **Sampling/bootstrap methods**
- **Data Wrangling**
- **Particular Statistical procedures that you won't find implemented anywhere else, e.g.**
  - Multiple Imputation methods,
  - Instrument Variable (2 stage) Regression
  - Matching subjects for pairwise analysis
  - MCMC routines

# Scaling, practically

- **Scaling (with or without more data):**
  - more complex analysis (ie optimizations)
  - more sampling (ie more trees in Random Forest)
- **Sometimes easy to parallelize (like with sampling)**
- **Sometimes too much communication between parts (matrix inversion)**

# R Scaling In a nutshell

- R takes advantage of math libraries for vector operations
- R packages provide multicore, multimode, or distributed data (SparkR) options
- However, model implementations not necessarily built to use parallel backends
  - Some models more amenable to parallel versions

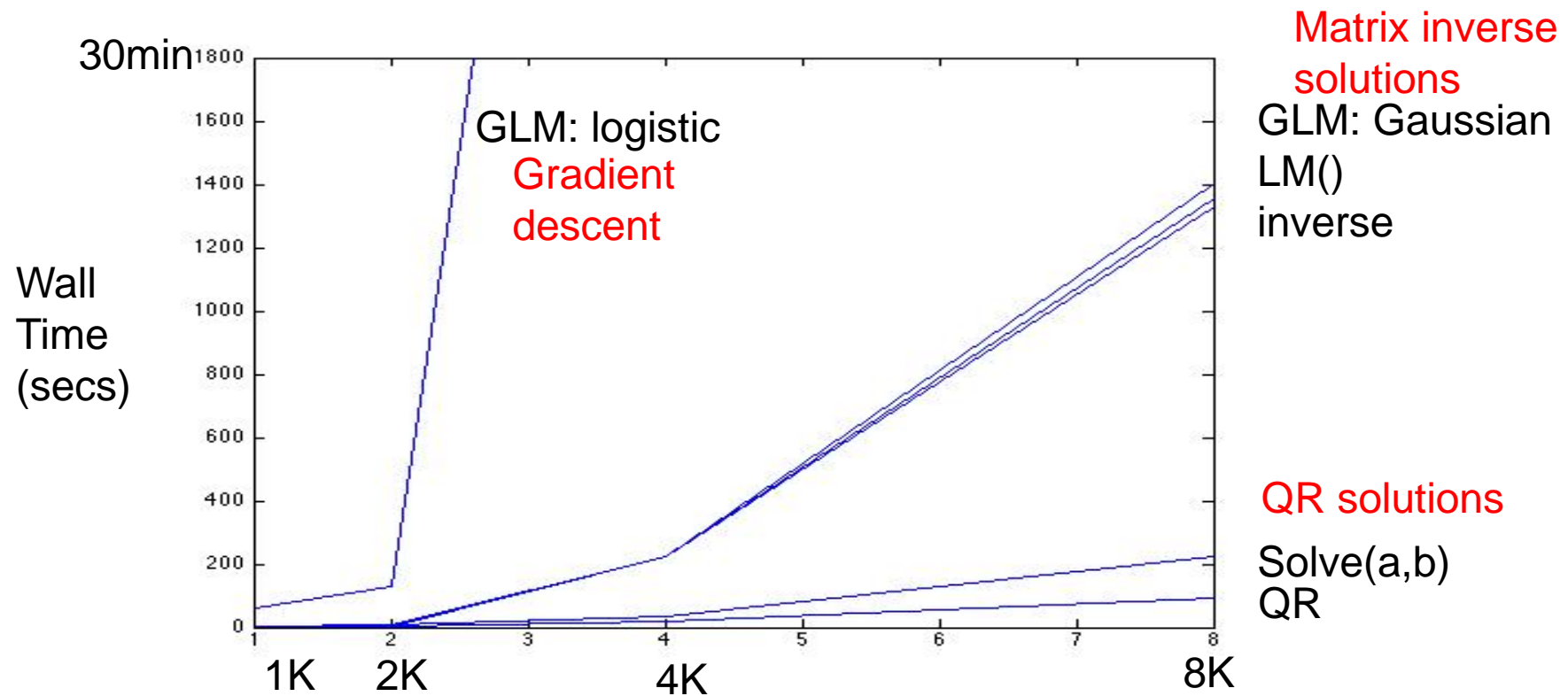
# Solving Linear Systems

## Performance with R, 1 compute node

R:

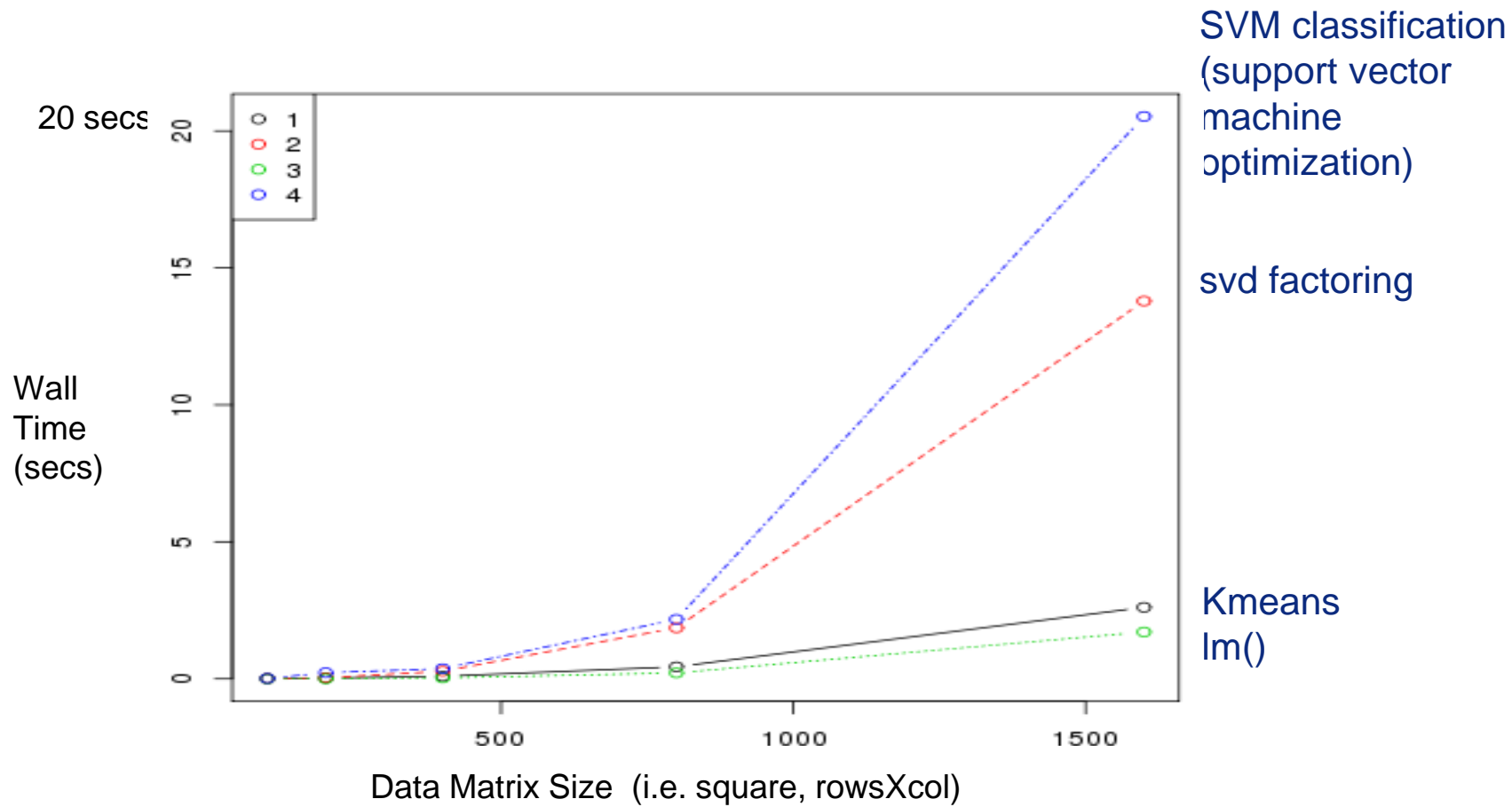
```
glm(Y~X,family=gaussian) #gaussn regrssn (like lm)
```

```
glm(Y~X,family=binomial) # logistic regrssn (Y=0 or 1)
```



Data Matrix Size (i.e. square, rowsXcol)

# Machine learning models: Performance on 1 compute node



# R multicore

- **‘doParallel’ package – provides the back end to the ‘for each’ parallel processing command**
- **uses threads across cpu cores to pass data & commands**
- **Updates and combines the previous ‘snow’ and ‘multicore’ packages, so that it also works for multinode.**

[See https://cran.r-project.org/web/packages/doParallel/vignettes/gettingstartedParallel.pdf](https://cran.r-project.org/web/packages/doParallel/vignettes/gettingstartedParallel.pdf)

# R multicore

- Run loop iterations on separate cores

```
install.packages(doParallel)  
library(doParallel)  
registerDoParallel(cores=24)
```

allocate workers





# R multicore

- Run loop iterations on separate cores

```
install.packages(doParallel)  
library(doParallel)  
registerDoParallel(cores=24)
```

allocate workers



```
my_data_frame = .....
```

```
my_results = foreach(i=1:24,.combine=rbind) %dopar%  
{ ...  
  your code here  
  
  return( a variable or object )  
})
```

%dopar% puts loops  
across cores,  
(loops are independent)  
%do% runs it serially



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%dopar% puts loops across cores, (loops are independent) %do% runs it serially

specify to combine results into array with row bind

returned items 'combined' into list by default

# R multicore

- Run loop iterations on separate cores

**BEWARE:**  
foreach will  
copy data it  
thinks is need to  
every core

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returned items  
'combined'  
by default

```
}
```

specify to combine results into  
array with row bind

# R multinode: parallel backend

- Run loop iterations on separate nodes

```
library(doParallel)
```

```
cl <- makeCluster(48)  
registerDoParallel(cl)
```

allocate cluster as  
parallel backend



# R multinode: parallel backend

- Run loop iterations on separate nodes

```
library(doParallel)

cl <- makeCluster(48)
registerDoParallel(cl)

my_data_frame = .....

results = foreach(i=1:48,.combine=rbind) %dopar%
{ ... your code here

    return( a variable or object )
})
stopCluster(cl)
```

allocate cluster as  
parallel backend

%dopar% puts loops  
across cores and  
nodes

# R multinode: parallel backend

- Run loop iterations on separate nodes

BEWARE:  
foreach will  
copy data it  
thinks is need to  
every node –  
that can take a  
long time!

```
library(doParallel)
```

```
cl <- makeCluster(48)  
registerDoParallel(cl)
```

```
my_data_frame = .....
```

```
results = foreach(i=1:48,.combine=rbind) %dopar%  
{ ... your code here
```

```
return( a variable or object )
```

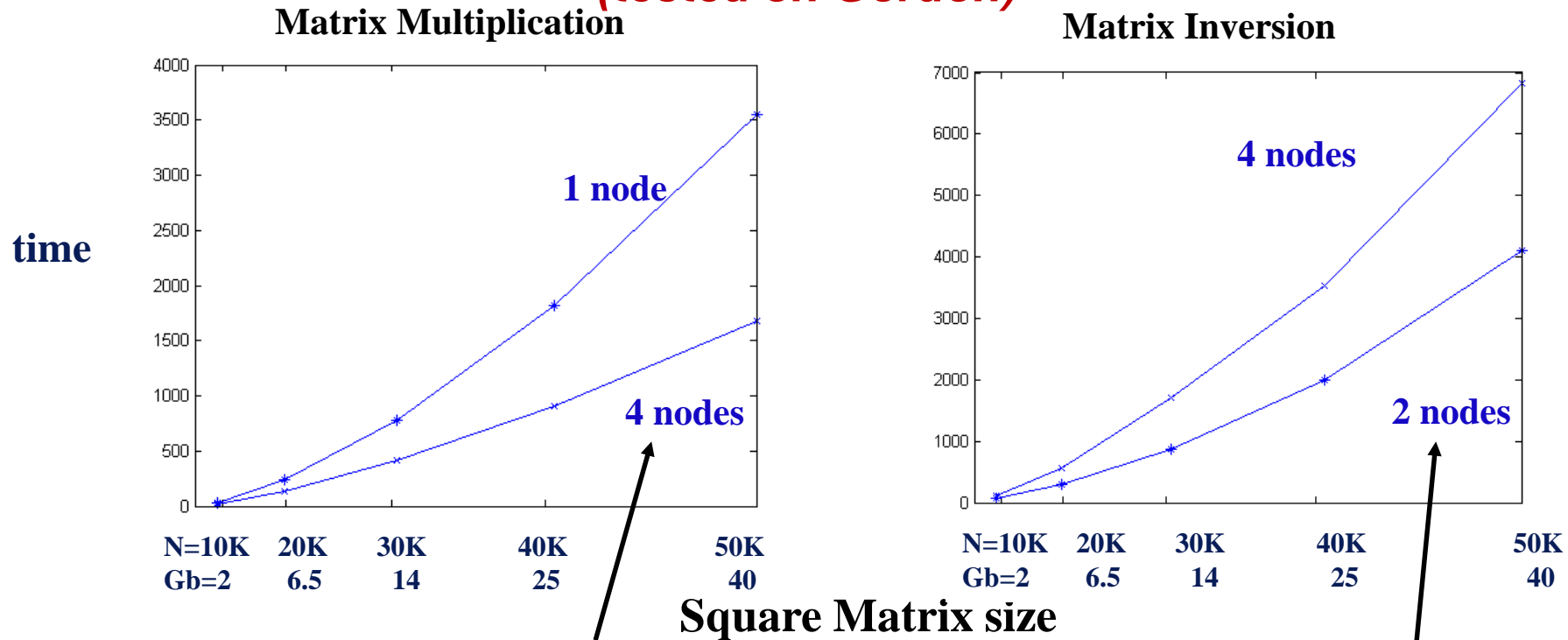
```
})  
stopCluster(cl)
```

allocate cluster as  
parallel backend  
↙

%dopar% puts loops  
across cores and  
nodes  
↙

# Multiple Compute Nodes not always help

(tested on Gordon)

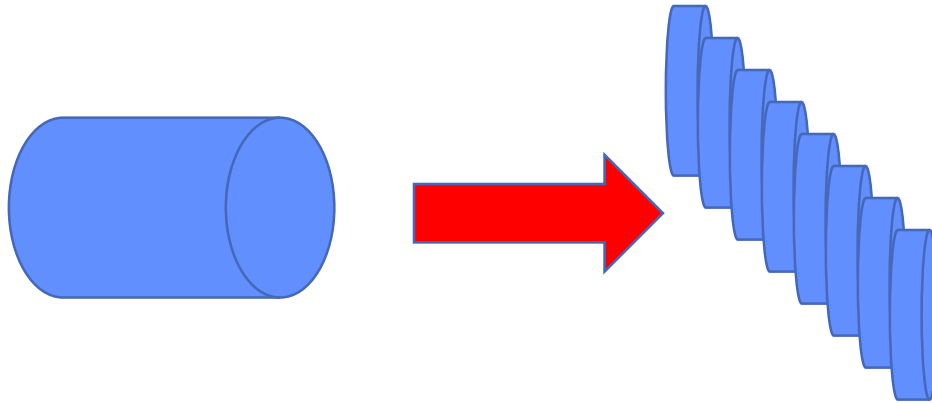


multinodes: more nodes is less time for multiplication,

less nodes is better for inversion

# Another option for (embarrassingly) Parallel R

1. Split up  
data into N  
parts





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1. Split up  
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2. In slurm batch script:

```
ibrun -np processors My-perl-script
```


My-perl-script:  
get cpu-id &  
pass it to R

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Launch MPI  
wraps around  
Perl & R script

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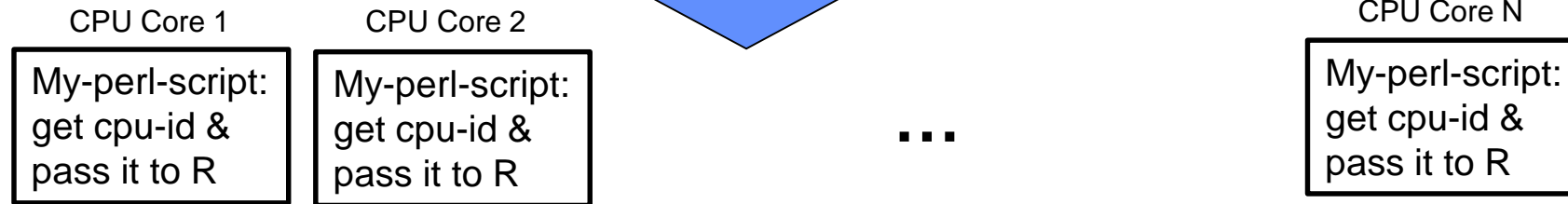
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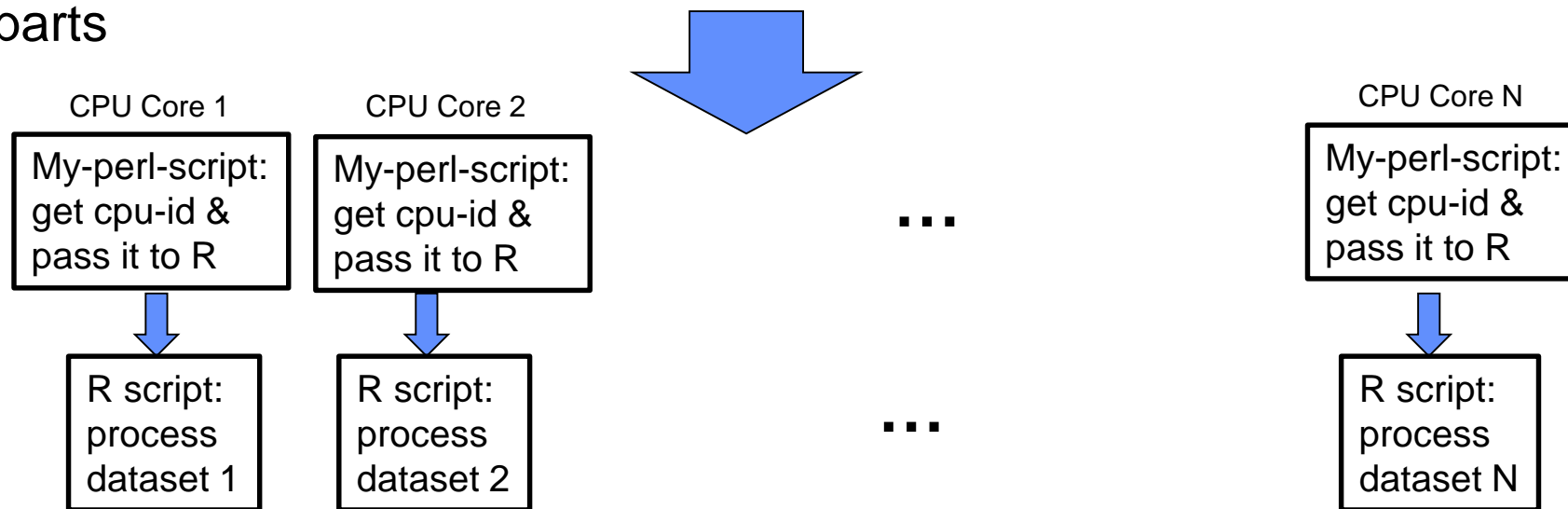


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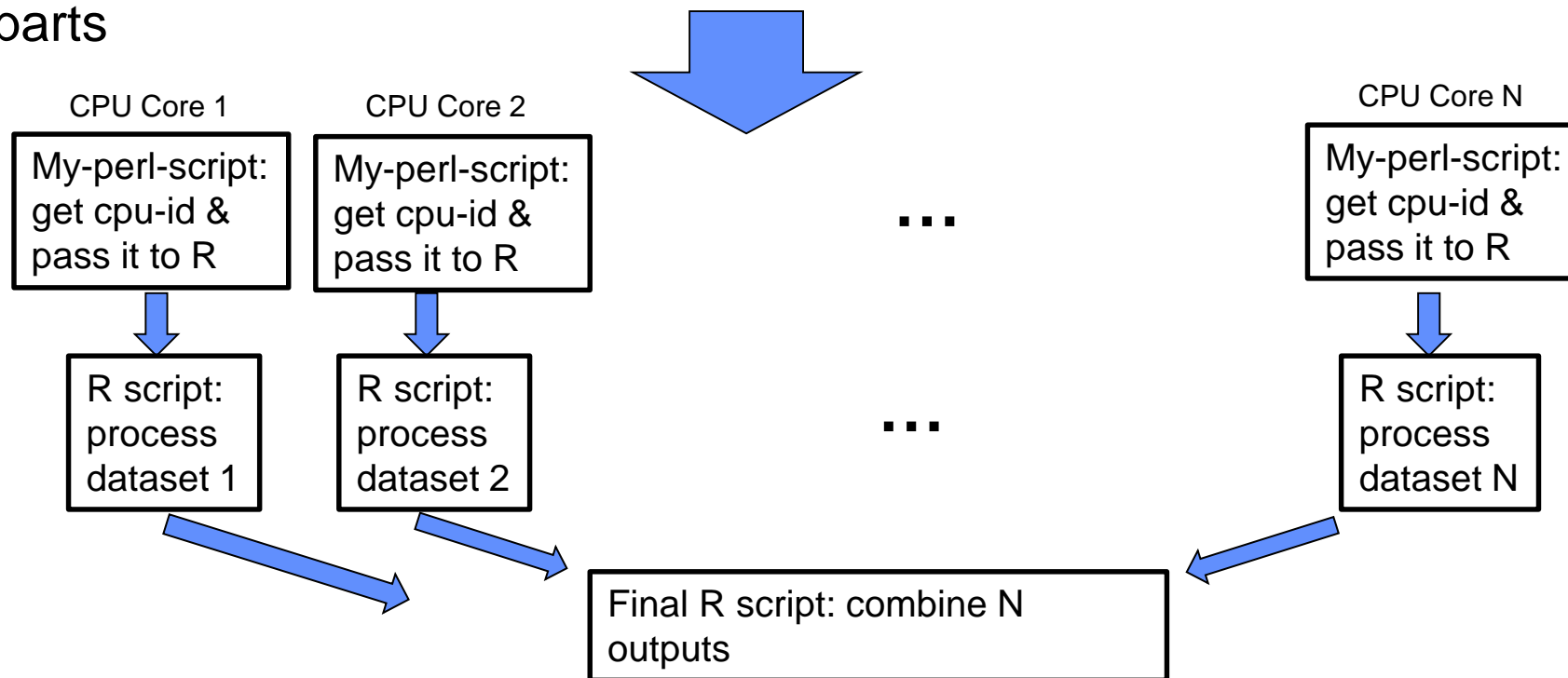


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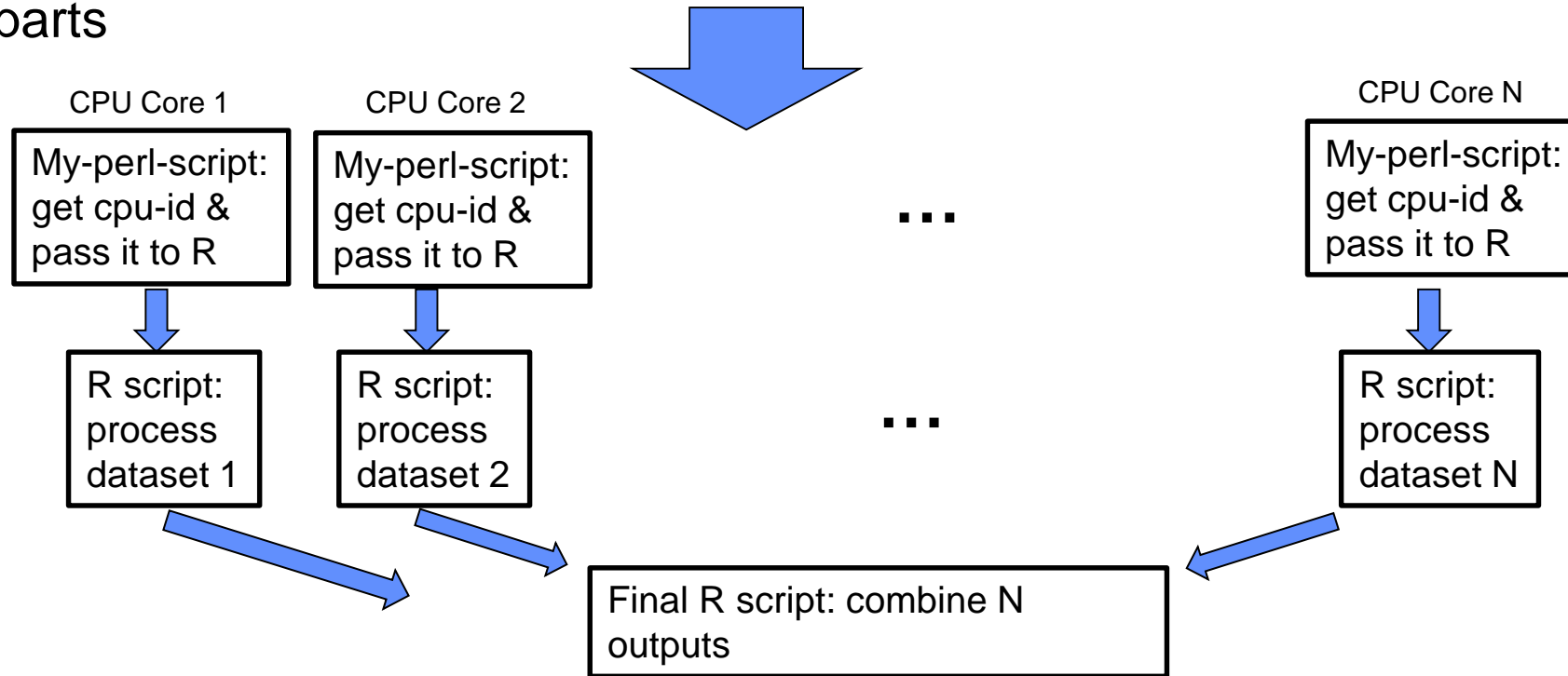


# Another option for (embarrassingly) Parallel R

1. Split up data into N parts

2. In slurm batch script:

`ibrun -np processors My-perl-script`



More programming but more flexible

Normal  
batch  
job info

```
#!/bin/bash
# -----
# slurm script for a batch job on comet
# to run a task on individual cores
# -----
#SBATCH --job-name="packR"
#SBATCH --output="serial-pack.%j.%N.out"
#SBATCH --partition=compute
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=24
#SBATCH --export=ALL
#SBATCH -t 1:00:00
#SBATCH -A sds164

bash

#Generate a hostfile from the slurm node list
export SLURM_NODEFILE=`generate_pbs_nodefile`
module load R
```

ibrun the  
'bundler'  
perl script  
on 24 cores  
per nodes,  
and 1  
thread each

```
#launch 24x2=48 tasks on 48 cores,
# and start this perl script on each task
ibrun --npernode 24 --tpp 1 perl ./bundlerxP.pl

#One can also run hybrid:
# launch 1 process per node, with 24 threads, and
# use doParallel
ibrun --npernode 1 --tpp 24 perl ./bundlerxP.pl
```

the  
'bundler'  
Perl  
script

Get current  
cpu id and  
number of  
processes

```
#!/usr/bin/perl  
use strict;  
use warnings;
```

the backtick  
executes system  
command

```
my ($myid, $numprocs) = split(/\s+/, `./getid`);
```

```
# -----  
# launch an R session for this task  
# -----
```

```
my $task_index = $myid+1;  
`module load R;/opt/R/bin/Rscript Test_PackingR.R  
$task_index >  
Rstd_out.$task_index.txt`;
```

the rank id  
as an  
argument



# Scaling doParallel vs 'Packing' R sessions

- **Packing *independent* R sessions onto cores is more flexible for:**
  - data management
  - large number of separate models
  - large variation in time per model
  - large matrix operations repeated
  - hybrid multimode/multicore scripts

*But requires more programming or preprocessing*

# Example: scaling MCMC

Distributed Markov Chain Monte Carlo for Bayesian Hierarchical Models,  
Frederico Bumbaca, UC Irvine, et al in print

- Probabilities of user web activity interdependent through a hierarchical model
- MCMC search for probabilities made independent through a phased approach.
- Ran on SDSC Comet with '**serial packing**' parallelization

(Using rhierMnIRwMixturefunction in the R package, bayesm)

# Individuals	Cores	Individ per Core	Total Minutes (I/O time)
100 million	1,7282 (max)	~ 58K	206 (38)

# Installing your own R Packages

- **In R:**

*install.packages('package-name')*

(see <https://cran.r-project.org/> for package lists and reviews)

- **on Comet:**

*install.packages('ggmap',  
repos='http://cran.us.r-project.org',dependencies=TRUE)*

If compiling is required and you get an error, call support

## Other R packages:

- **Rspark** - R interface to Spark
- **pdbR** - higher level over R-MPI, distributed matrix support and other  
(better for dense matrices vs Spark)
- **R openMP**  
(e.g. if you want to program your own foreach)
- **Ff, bigmemory – map data to files**  
(can help with foreach)
- **HiPLAR** - GPU and multicore for linear algebra
- **Rgputools – GPU support**

pause

# R on Comet terminal window

1. Get a compute node:

```
[Unix]$ : srun --partition=debug --pty --nodes=1 --ntasks-per-node=24 -t 00:30:00  
--wait=0 --export=ALL -A your-account /bin/bash
```

2. Start R

```
[Unix]$ module load R
```

```
[Unix]$ R          (this gets an interactive R session)
```

```
>quit()           (to exit R)
```

```
[Unix]$ exit      (to exit the compute node)
```

# R multicore exercise

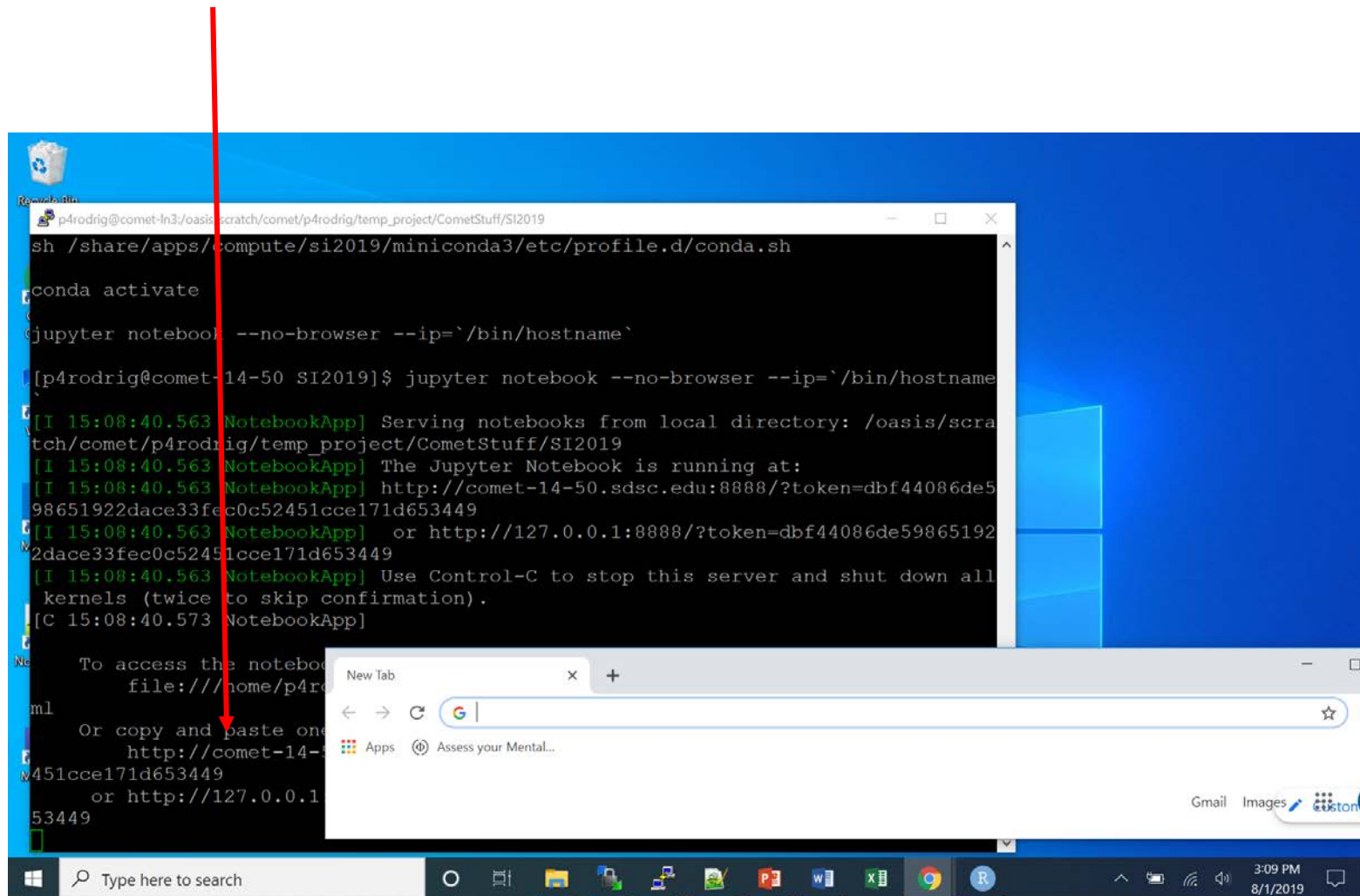
- **Login to comet**
  - cd to this lecture folder
- **Get an interactive compute node session**
- **Start notebook**
  - `jupyter notebook --no-browser --ip="*" &`

# R parallel exercises

- **Open & run TestdoParallel Exercise 1,2,3**
  - remember that foreach assumes independence between loops
  - Start with smallish N,P
- **Look at memory usage in top command**
- **R does not well manage large data frames across cores**
  - N=800000 P=2000, makes ~12Gb data frames, R fails
- **Ex 3 will split up data for large data frames and have each core read a separate data**



Starting jupyter notebook and copy paste URL into browser



The screenshot shows a Windows desktop with a blue background. A terminal window is open, displaying the following commands and output:

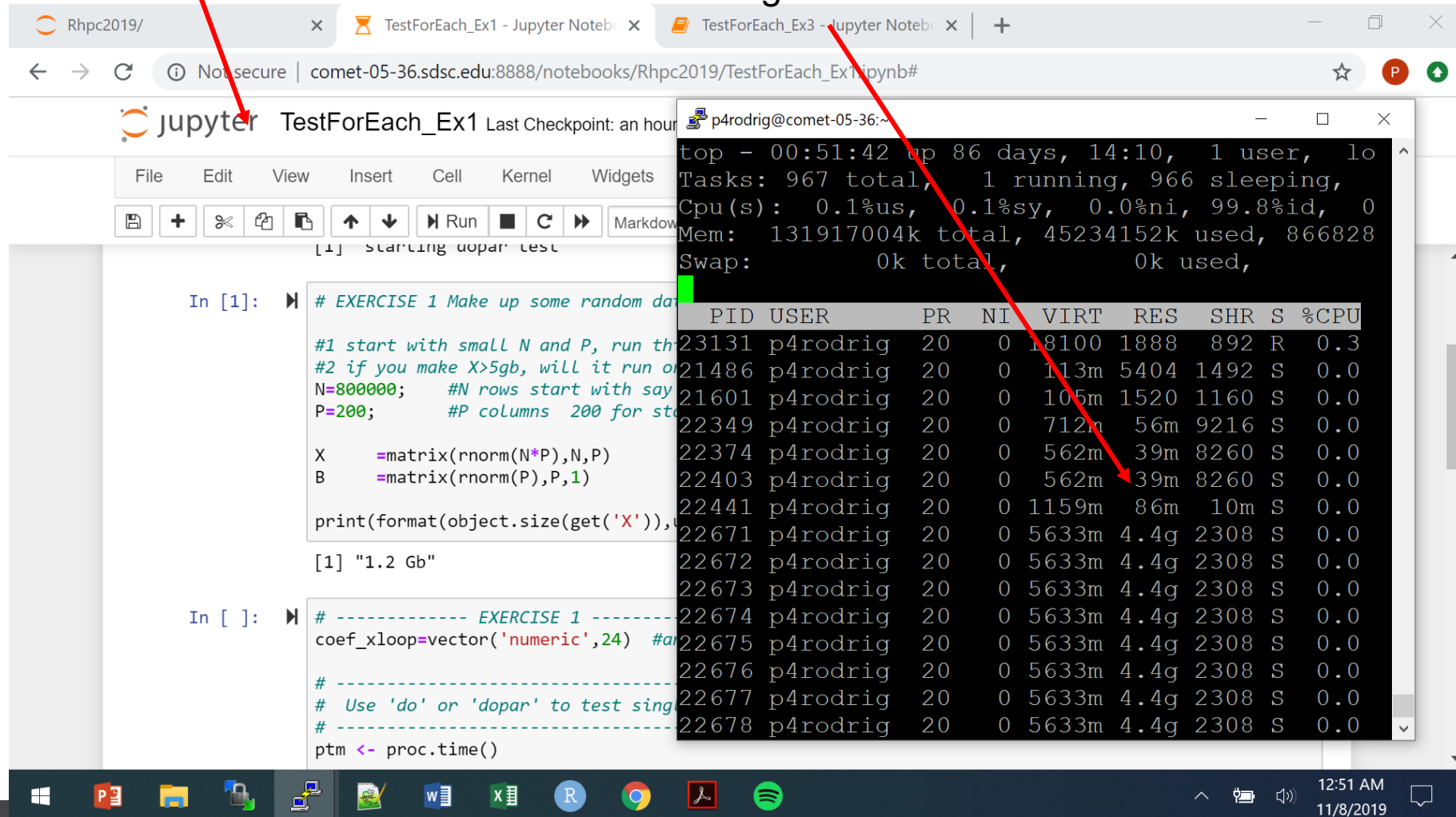
```
p4rodrig@comet-ln3:/oasis/scratch/comet/p4rodrig/temp_project/CometStuff/SI2019$ sh /share/apps/compute/si2019/miniconda3/etc/profile.d/conda.sh
p4rodrig@comet-ln3:/oasis/scratch/comet/p4rodrig/temp_project/CometStuff/SI2019$ conda activate
p4rodrig@comet-ln3:/oasis/scratch/comet/p4rodrig/temp_project/CometStuff/SI2019$ jupyter notebook --no-browser --ip=`/bin/hostname`
[p4rodrig@comet-14-50 SI2019]$ jupyter notebook --no-browser --ip=`/bin/hostname`
[I 15:08:40.563 NotebookApp] Serving notebooks from local directory: /oasis/scratch/comet/p4rodrig/temp_project/CometStuff/SI2019
[I 15:08:40.563 NotebookApp] The Jupyter Notebook is running at:
[I 15:08:40.563 NotebookApp] http://comet-14-50.sdsc.edu:8888/?token=dbf44086de598651922dace33fec0c52451cce171d653449
[I 15:08:40.563 NotebookApp] or http://127.0.0.1:8888/?token=dbf44086de598651922dace33fec0c52451cce171d653449
[I 15:08:40.563 NotebookApp] Use Control-C to stop this server and shut down all kernels (twice to skip confirmation).
[C 15:08:40.573 NotebookApp]
```

Below the terminal window, a web browser is open with a new tab. The address bar is empty, and a red arrow points from the URL in the terminal output to the address bar. The taskbar at the bottom shows various application icons, including the Start button, search bar, and icons for File Explorer, Edge, and several Office applications. The system clock in the bottom right corner shows 3:09 PM on 8/1/2019.

Select Rhpc2019 folder and select  
TestdoParallel exercises

Open 2<sup>nd</sup> terminal window directly in to  
comet-XX-XX.sdsc.edu compute node

Run `top -u $user` (then enter H) to see  
usage



The screenshot shows a Jupyter Notebook interface with a terminal window open. The Jupyter Notebook is titled "TestForEach\_Ex1" and shows the following code:

```
In [1]: # EXERCISE 1 Make up some random data
#1 start with small N and P, run the test
#2 if you make X>5gb, will it run on the node
N=800000; #N rows start with say 1000 columns
P=200; #P columns 200 for storage

X = matrix(rnorm(N*P),N,P)
B = matrix(rnorm(P),P,1)

print(format(object.size(get('X'))), '\n')

[1] "1.2 Gb"

In [ ]: # ----- EXERCISE 1 -----
coef_xloop=vector('numeric',24) #array of coefficients
# -----
# Use 'do' or 'dopar' to test singularity
# -----
ptm <- proc.time()
```

The terminal window shows the output of the `top` command, displaying system statistics and a list of processes. The output is as follows:

```
top - 00:51:42 up 86 days, 14:10, 1 user, load averages: 0.00, 0.01, 0.05
Tasks: 967 total, 1 running, 966 sleeping, 0 stopped, 0 zombie
Cpu(s): 0.1%us, 0.1%sy, 0.0%ni, 99.8%id, 0.0%wa, 0.0%st, 0.0%gn, 0.0%ds, 0.0%dc, 0.0%cc, 0.0%co
Mem: 131917004k total, 45234152k used, 86682888k free, 0k buffers
Swap: 0k total, 0k used, 0k free
```

PID	USER	PR	NI	VIRT	RES	SHR	S	%CPU
23131	p4rodrig	20	0	18100	1888	892	R	0.3
21486	p4rodrig	20	0	113m	5404	1492	S	0.0
21601	p4rodrig	20	0	105m	1520	1160	S	0.0
22349	p4rodrig	20	0	712m	56m	9216	S	0.0
22374	p4rodrig	20	0	562m	39m	8260	S	0.0
22403	p4rodrig	20	0	562m	39m	8260	S	0.0
22441	p4rodrig	20	0	1159m	86m	10m	S	0.0
22671	p4rodrig	20	0	5633m	4.4g	2308	S	0.0
22672	p4rodrig	20	0	5633m	4.4g	2308	S	0.0
22673	p4rodrig	20	0	5633m	4.4g	2308	S	0.0
22674	p4rodrig	20	0	5633m	4.4g	2308	S	0.0
22675	p4rodrig	20	0	5633m	4.4g	2308	S	0.0
22676	p4rodrig	20	0	5633m	4.4g	2308	S	0.0
22677	p4rodrig	20	0	5633m	4.4g	2308	S	0.0
22678	p4rodrig	20	0	5633m	4.4g	2308	S	0.0



- **Pause**

# **pbdR package**

- **API on top of MPI and Scalapack Lin. Algebra library**
- **Sets up virtual grid to handle large matrix multiplication**

[See <https://pbdr.org/packages.html>](https://pbdr.org/packages.html)

# pbdR sample code

```
library(pbdDMAT)
```

```
init.grid()      # <<< ---- pbdR will select grid sizes for you by default
```

```
myr  =comm.rank()  
mys  =comm.size()
```

```
#Simple ways to print information
```

```
comm.print(paste("comm print myrank:",myr, " size:",mys),all=FALSE)
```

```
p=10000
```

```
dx <- ddmatrix(rnorm(p*p*10),p*10,p)  
comm.print(dx,all=F)
```

```
# <<< --- "ddmatrix" - options to indicate global matrix  
dimension, local dimension, and blocking sizes
```

```
....
```

To run: edit Runpbd script and enter: sbatch Runpbd

# Test 1

For 1 node 24 cores:

Using 6x4 for the default grid size

[1] "comm print myrank: 0 size: 24"

[1] " matrix width: 10000"

-----  
orterun noticed that process rank 0 with PID 26491 on  
node comet-18-56 exited on signal 9 (Killed).  
-----

But runs out of memory

(2 nodes 24 cores also runs out of memory)

# Test 2

For 1 node 12 cores:

Using 4x3 for the default grid size

[1] "comm print myrank: 0 size: 12"

[1] " matrix width: 10000"

COMM.RANK = 0

DENSE DISTRIBUTED MATRIX

-----  
Process grid:

4x3

Global dimension:

100000x10000

(max) Local dimension:

25008x3344

Blocking:

16x16

BLACS ICTXT:

0

data split up  
among cores

Runs in about 950 secs  
(for a matrix multiplication)



# Test 3

For 2 node 12 cores:

Using 6x4 for the default grid size

[1] "comm print myrank: 0 size: 24"

[1] " matrix width: 10000"

COMM.RANK = 0

DENSE DISTRIBUTED MATRIX

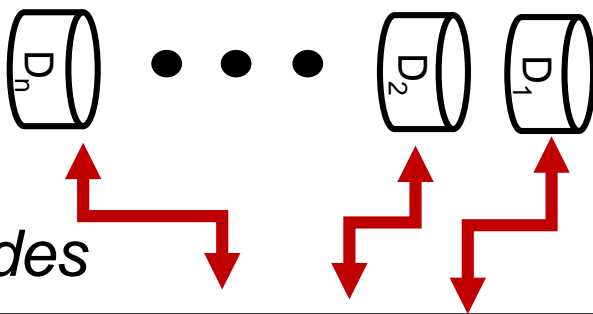
-----  
Process grid: 6x4  
Global dimension: 100000x10000  
(max) Local dimension: 16672x2512  
Blocking: 16x16  
BLACS ICTXT: 0

Runs in about 320 secs  
(for a matrix multiplication)

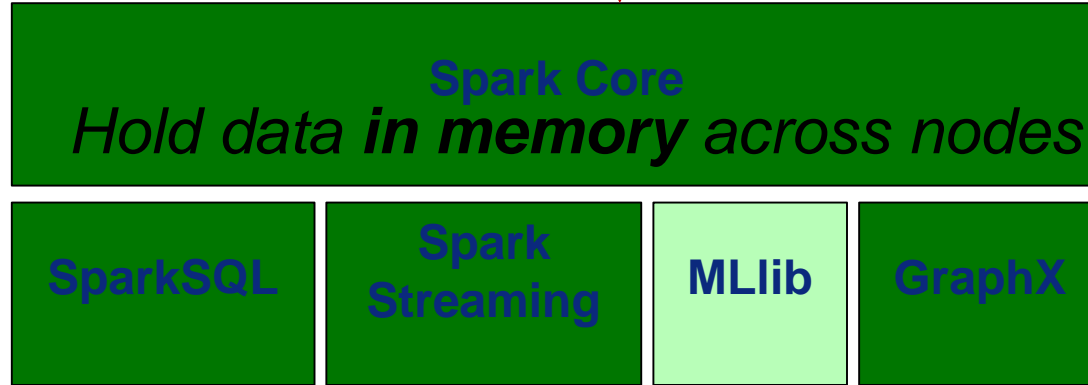
# Spark ML for bigger data:

- **Spark MLlib –**
  - Many standard Machine Learning models that are easiest to parallelize
    - Matrix Factorization
    - Naïve Bayes
    - Linear/NonLinear Regression Models with gradient descent optimization
    - Kmeans
  - Some support for large matrix operations

*distribute  
data  
across nodes*



# Spark MLlib



*Run code on each part and gather as requested*

- Distributed implementations of common ML algorithms and utilities
- APIs for Scala, Java, Python, and R
- Scales well for independent processes

- On to deep learning...

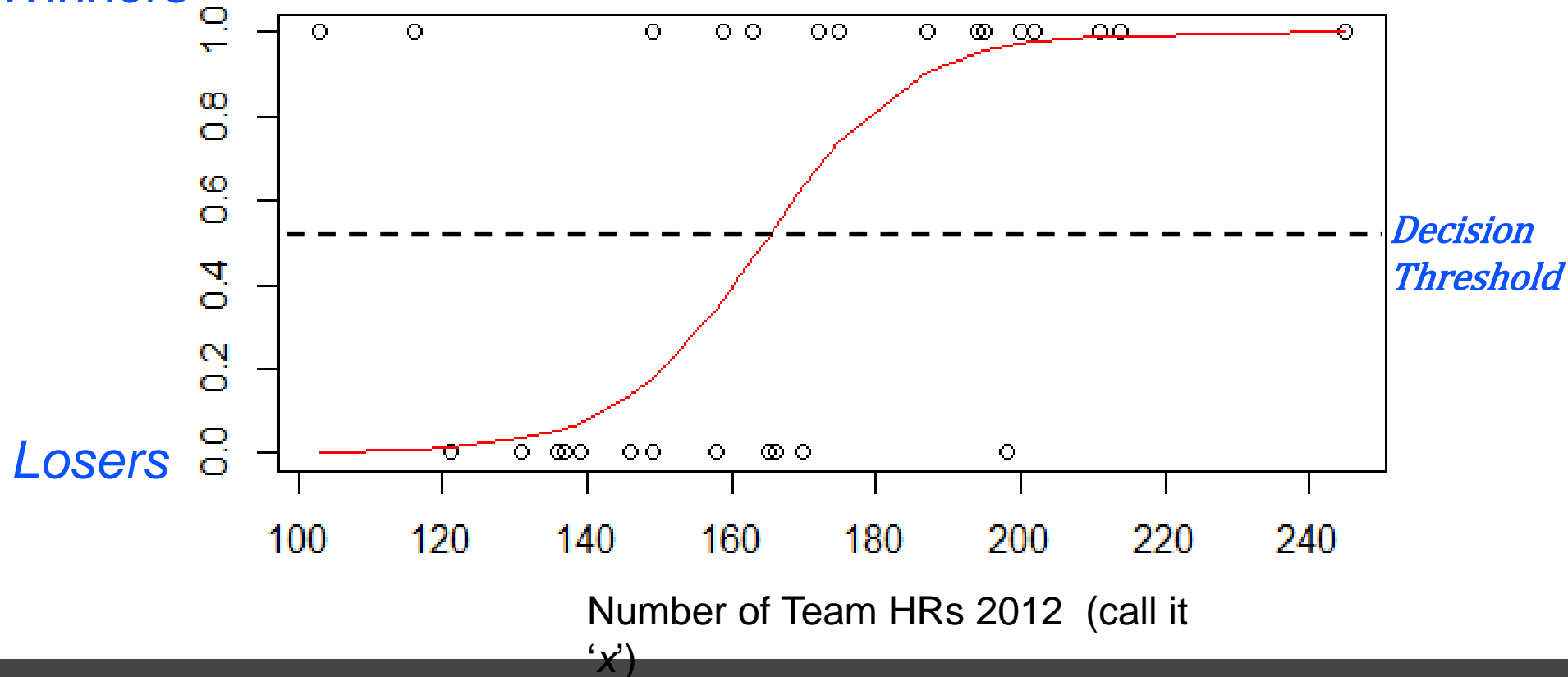
# Deep Learning

- **3 characterizations:**
  1. Learning complicated interactions about input
  2. Discovering complex feature transformations
  3. Using neural networks with many layers

# Logistic regression

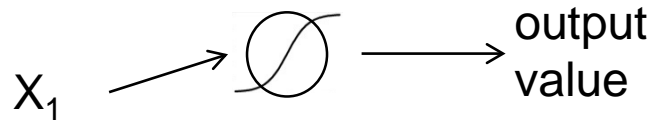
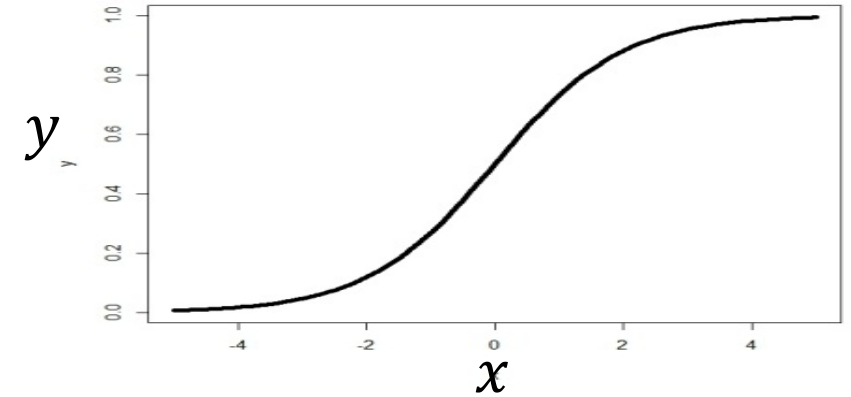
**the Model:**  $y = f(x, b) = 1 / (1 + \exp[-(b_0 * 1 + b_1 * x)])$

Winners



# Logistic to Neural Network model

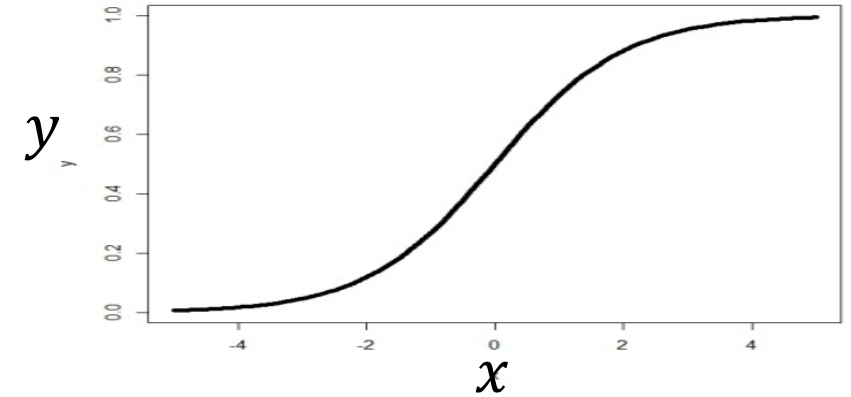
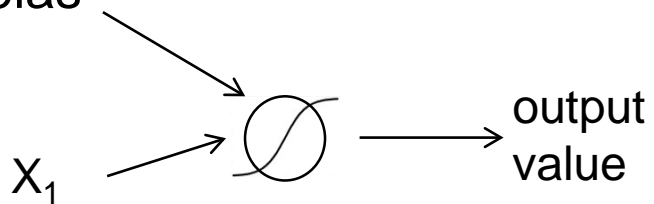
- In other words –
  - Squash ( $b_0 * 1 + b_1 * x$ ) to 0,1 range using logistic function
  - *And use graphical depiction:*



# Logistic to Neural Network model

- In other words –
  - Squash ( $b_0 * 1 + b_1 * x$ ) to 0,1 range using logistic function
  - *And use graphical depiction:*

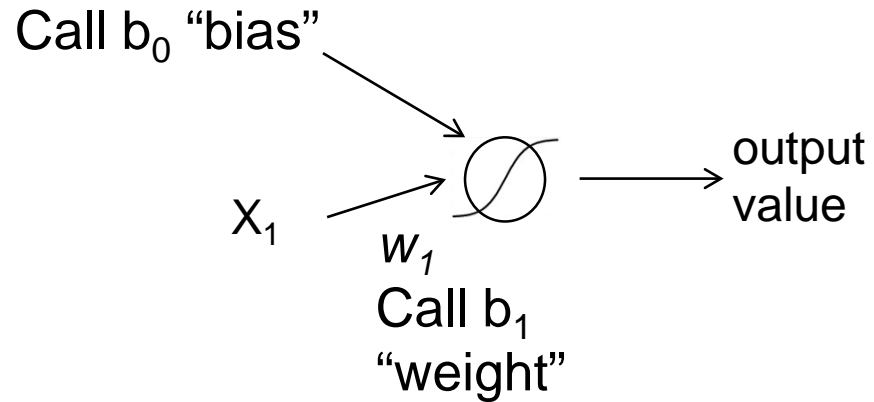
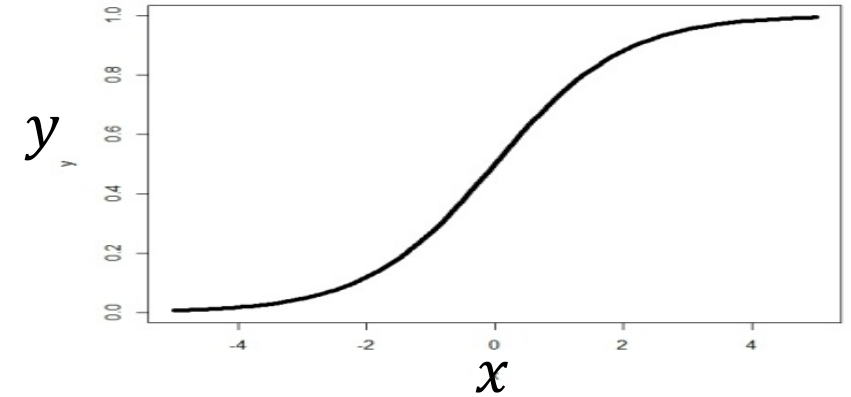
Call  $b_0$  “bias”





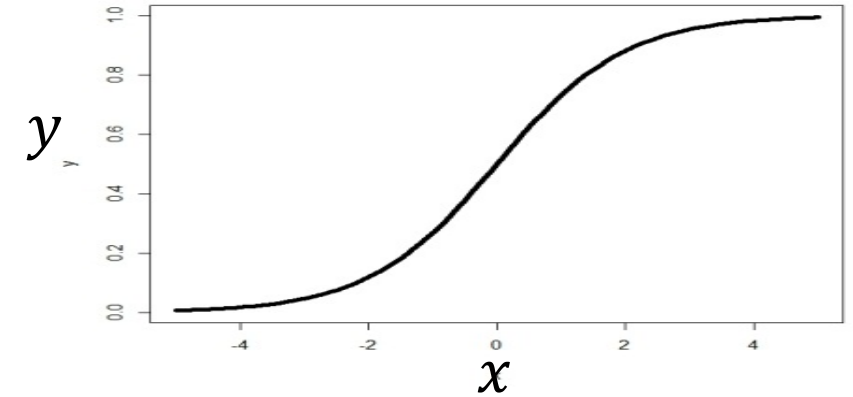
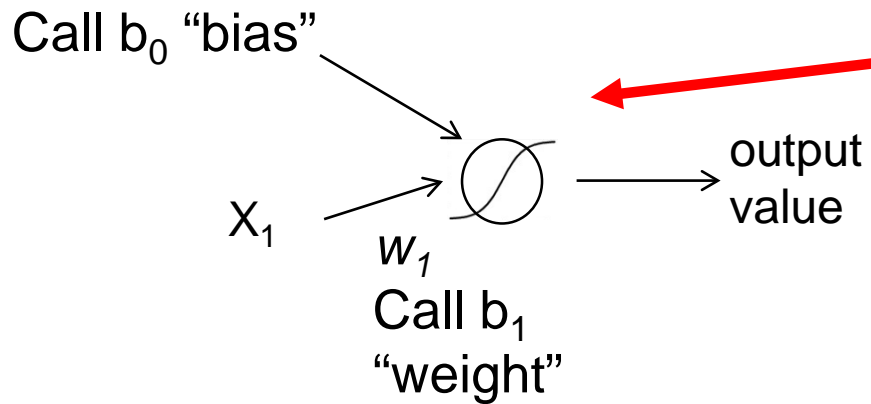
# Logistic to Neural Network model

- In other words –
  - Squash  $(b_0 * 1 + b_1 * x)$  to 0,1 range using logistic function
  - *And use graphical depiction:*



# Logistic to Neural Network model

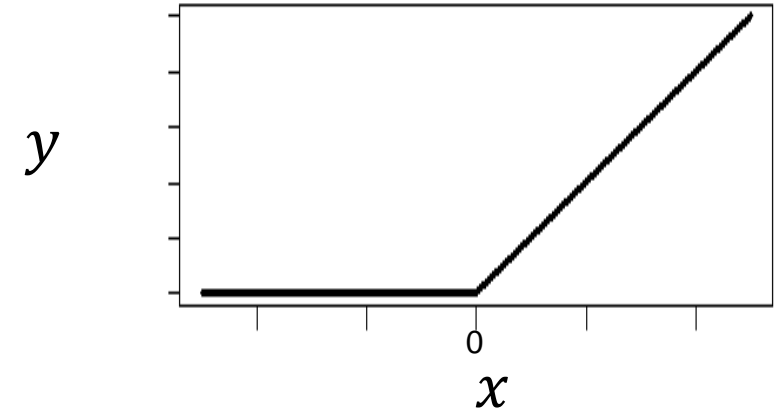
- In other words –
  - Squash ( $b_0 * 1 + b_1 * x$ ) to 0,1 range using logistic function
  - *And use graphical depiction:*



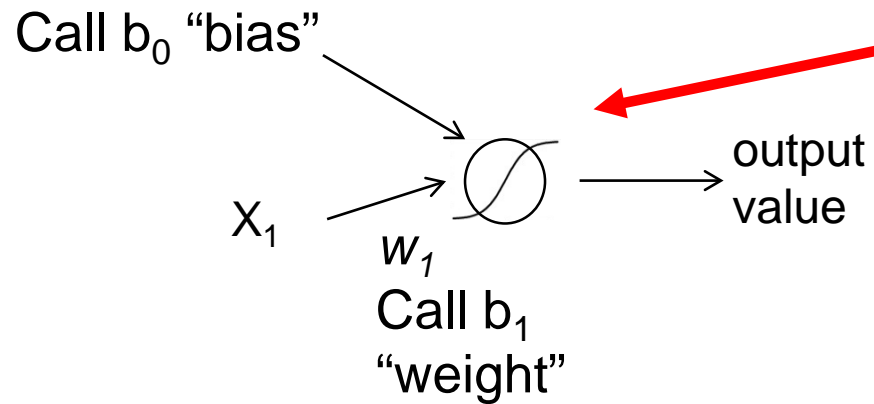
logistic function will transform input to output – call it the 'activation' function

# Logistic to Neural Network model

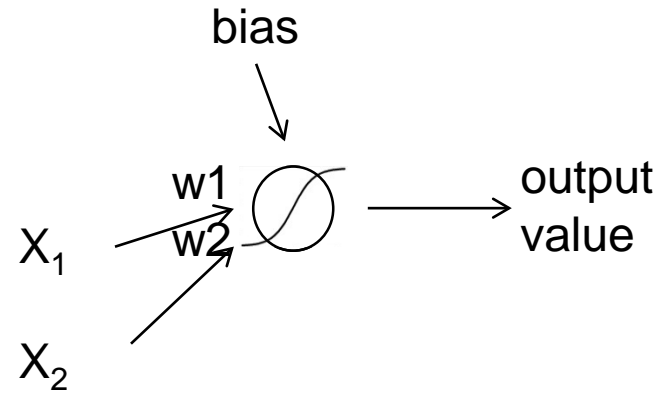
- **RELU activation function**
  - If  $(b_0 * 1 + b_1 * x) < 0$  set to 0
  - *And use graphical depiction:*



RELU (rectified linear unit)



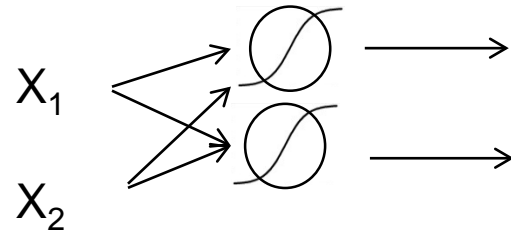
## Next step: More general networks



*Add input variables*

# More general networks

(assume bias present)

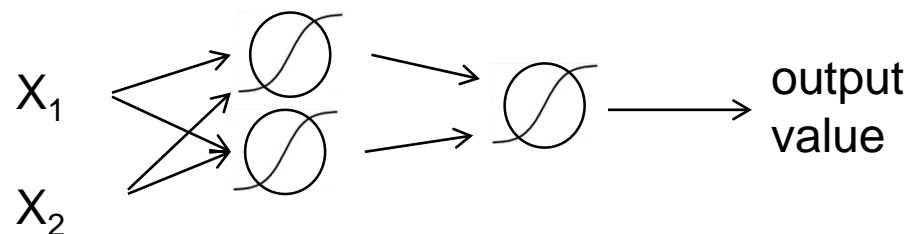


*Add input variables*

*Add logistic transformations ...*

# More general networks

(assume bias)



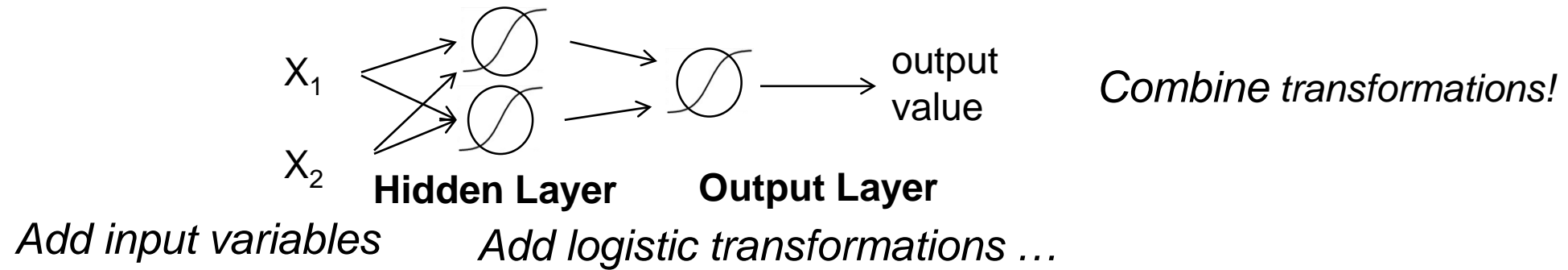
*Combine transformations!*

*Add input variables*

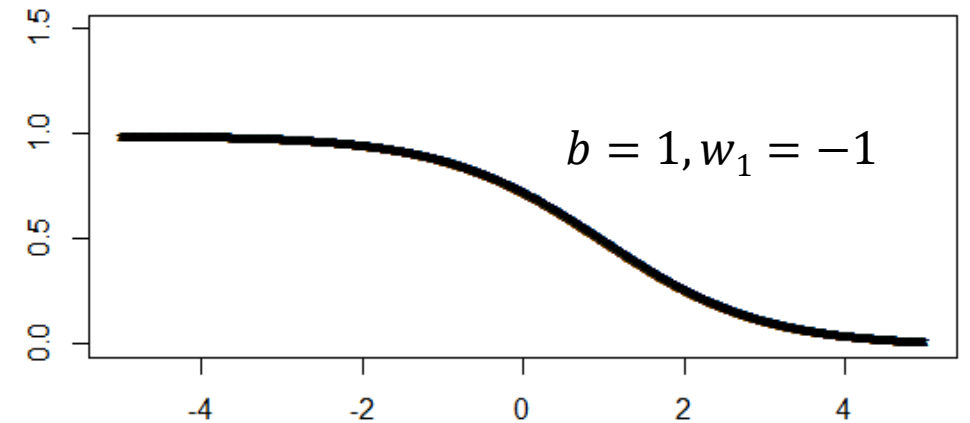
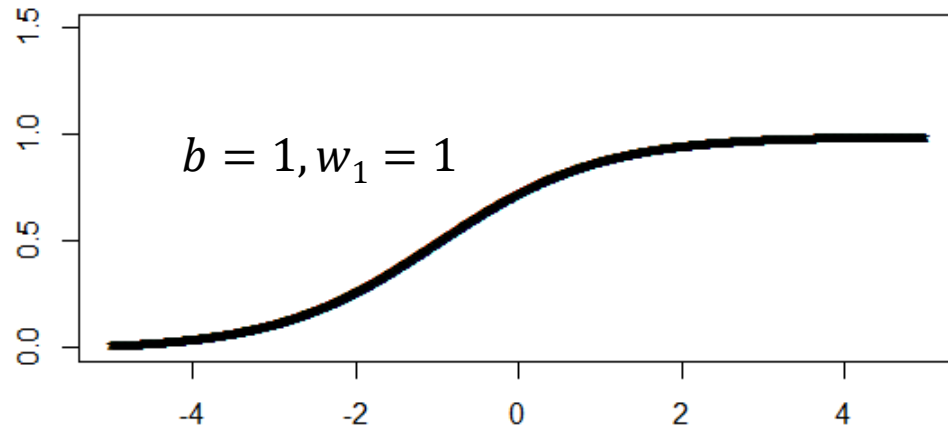
*Add logistic transformations ...*

# More general networks

(assume bias)

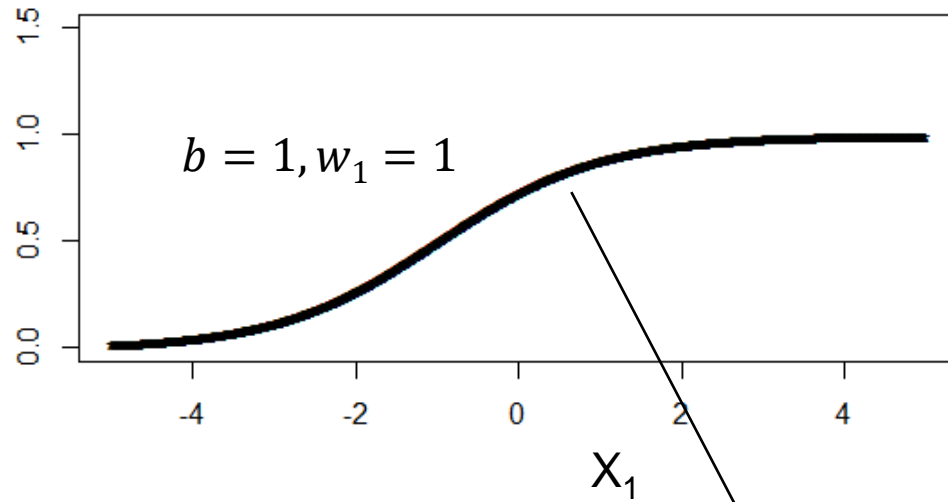


# So combinations are highly flexible and nonlinear

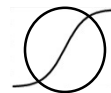
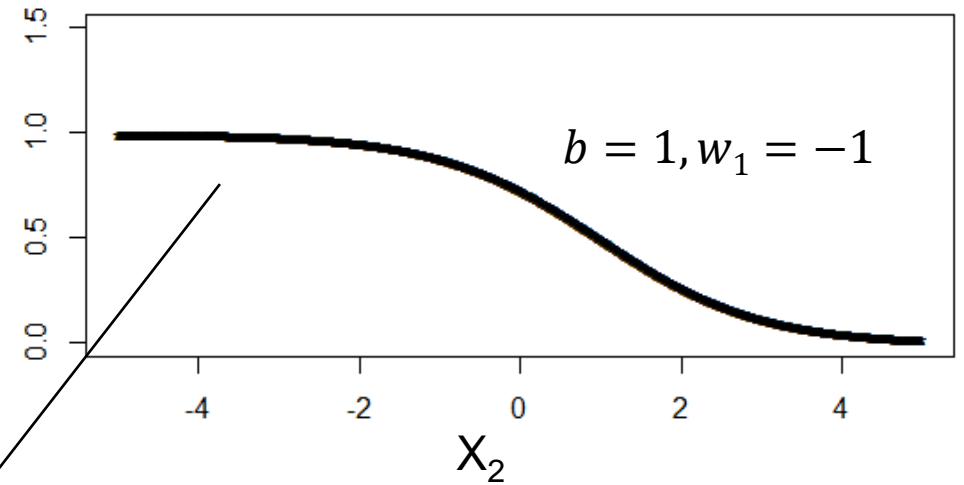
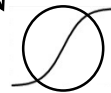




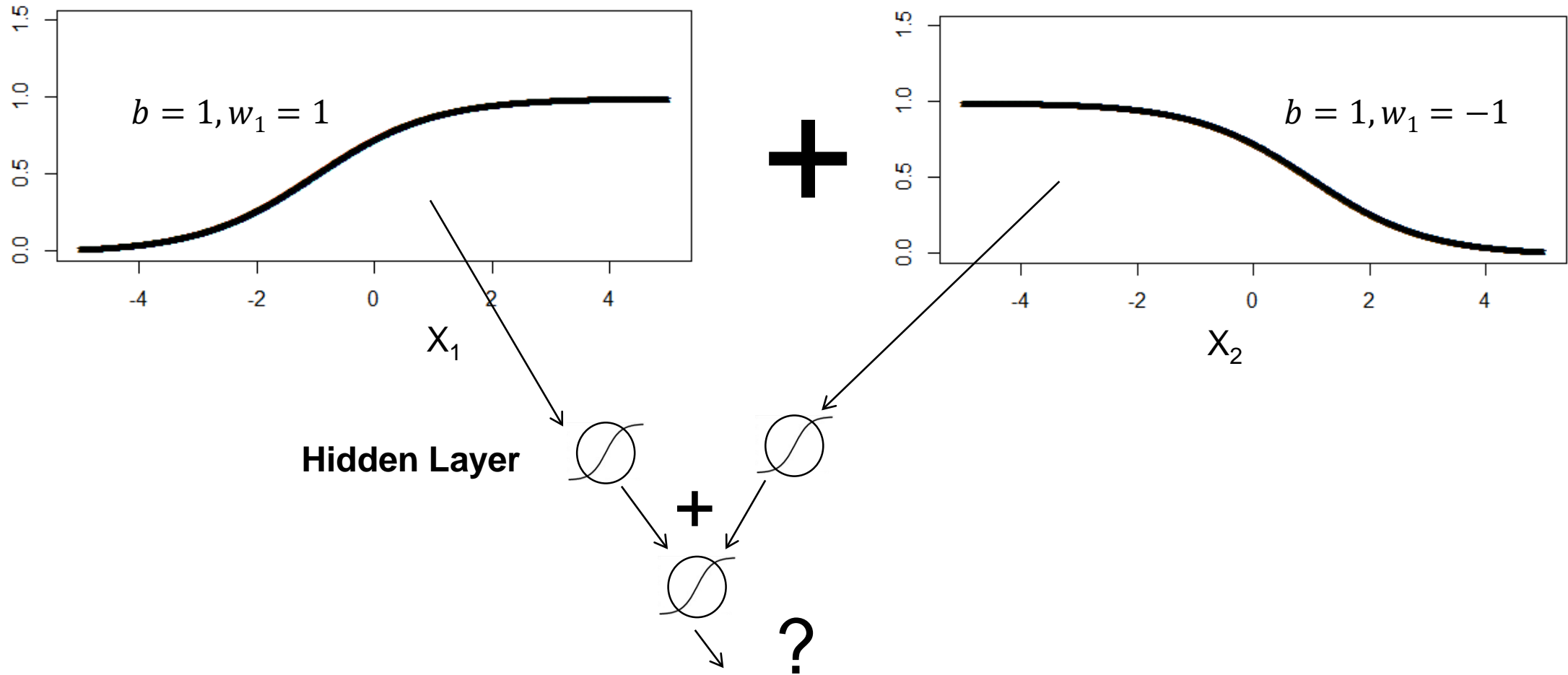
# So combinations are highly flexible and nonlinear



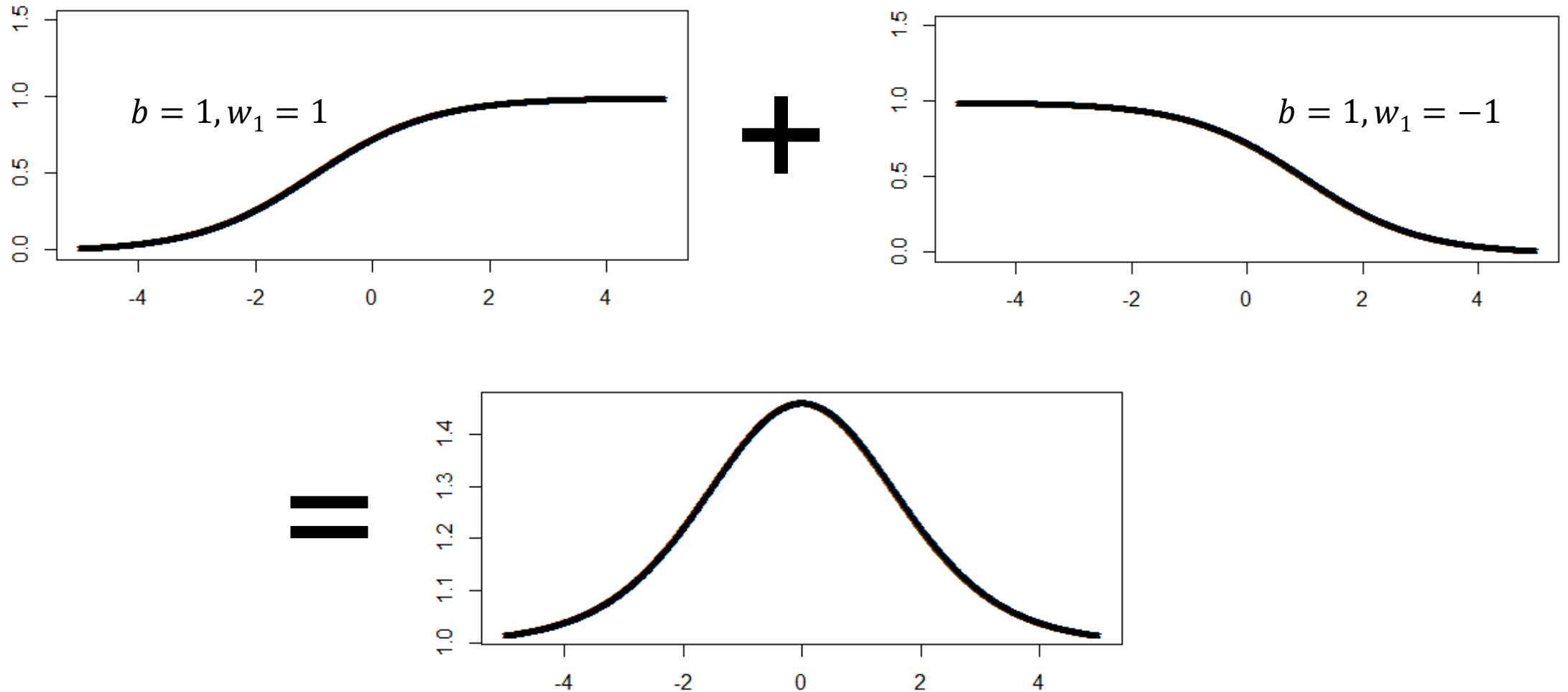
Hidden Layer



# So combinations are highly flexible and nonlinear

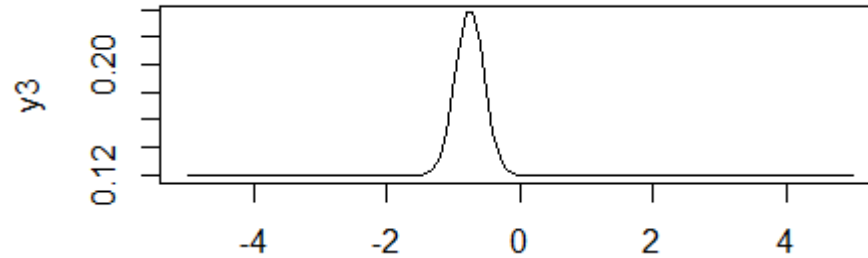


# So combinations are highly flexible and nonlinear

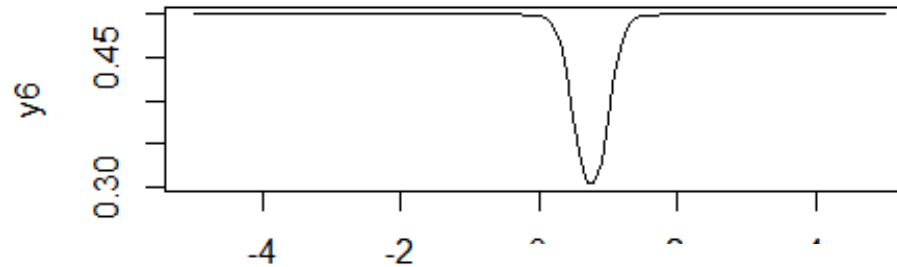


# Higher level function combinations

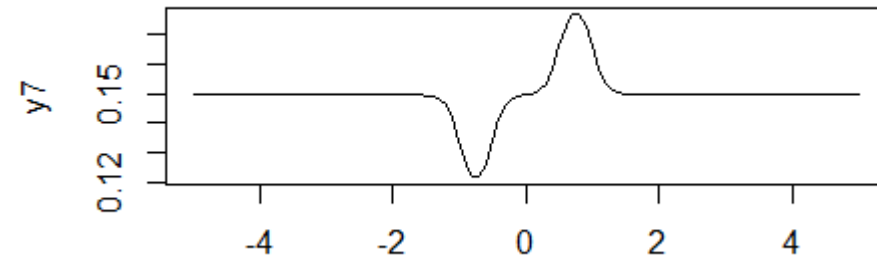
```
x=seq(-5,5,.1)
y1=1/(1+exp(10+ 10*x))
y2=1/(1+exp(-5+(-10)*x))
y3=1/(1+exp(1+1*y1+1*y2))
plot(x,y3,type="l")
```



```
y4=1/(1+exp(10+ (-10)*x))
y5=1/(1+exp(-5+(10)*x))
y6=1/(1+exp(1-1*y4-1*y5))
plot(x,y6,type="l")
```

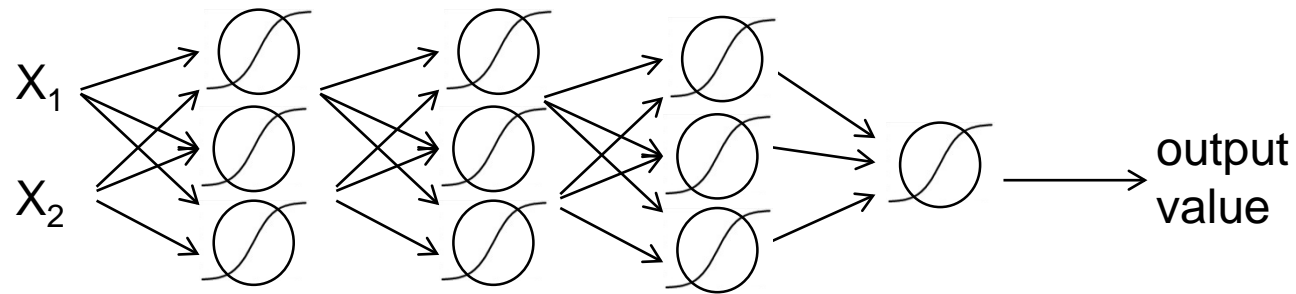


```
y7=1/(1+exp(1+2*y3+1*y6))
plot(x,y7,type="l")
```

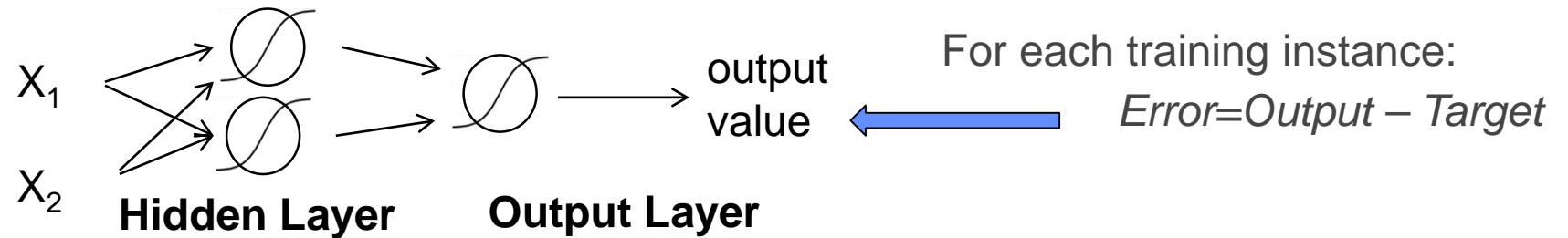


# Why stop at 1 hidden layer?

More hidden layers => More varied features and transformation



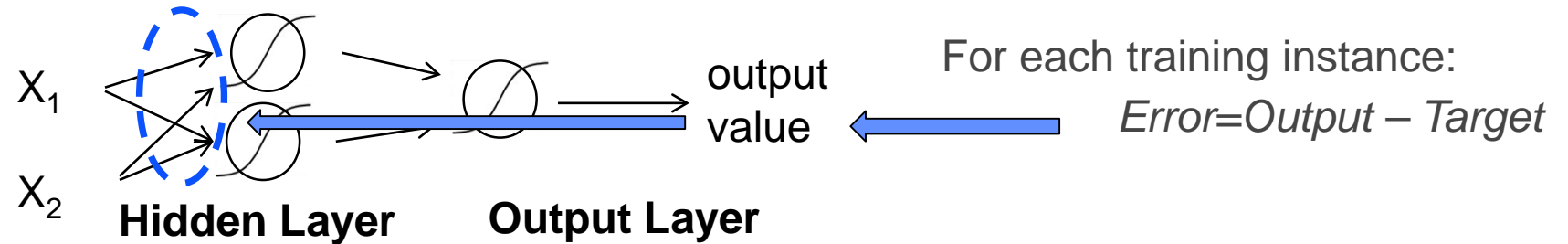
# But parameter fitting is harder too



Calculate a **Loss function** of the **Error**

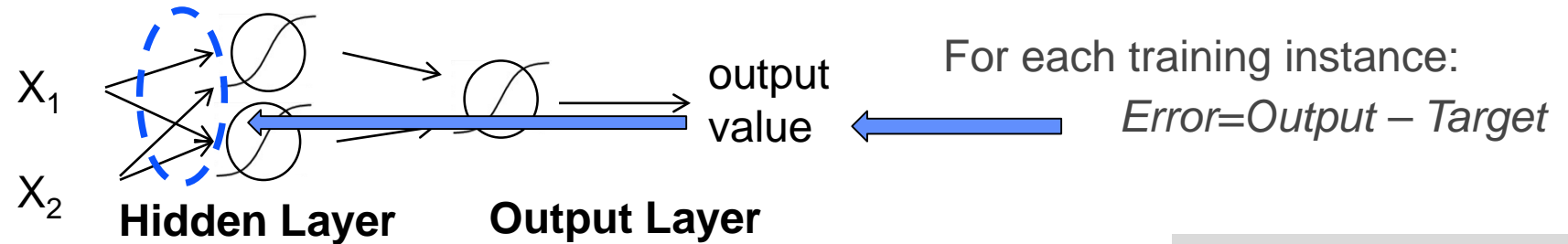
- cross-entropy for binary classification
- soft-max for multi-classification
- root MSE for regression

# But parameter fitting is harder too



*use derivative chains to ‘back-propagate’ errors*

# But parameter fitting is harder too



*use derivative chains to 'back-propagate' errors*

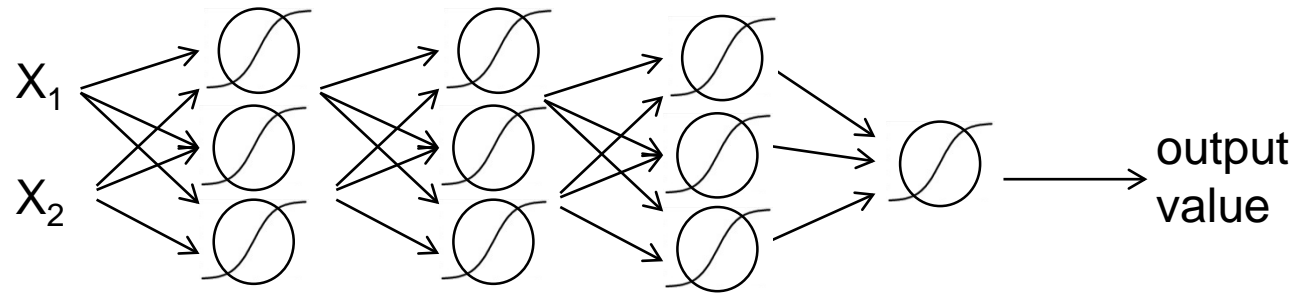
Also, take batches and iterate over whole training set

The method is called:  
**Stochastic  
Gradient Descent  
(sgd)**



# Train with Care

More hidden layers => More varied features and transformations

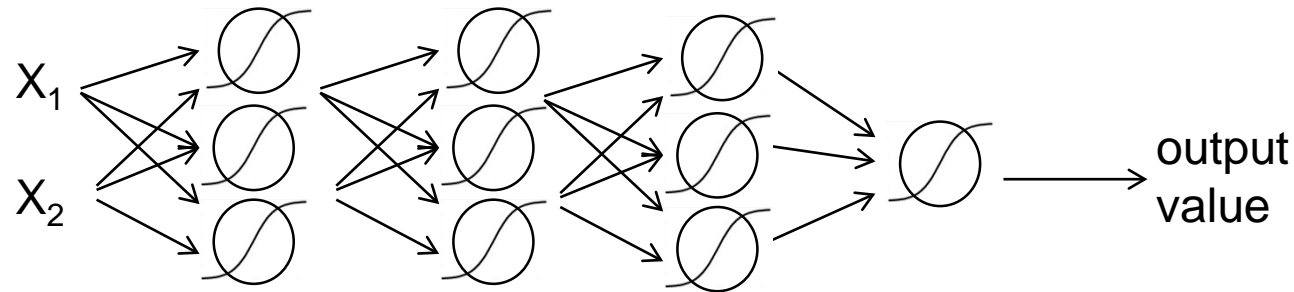


But:

More layers => more parameters

# Train with Care

More hidden layers => More varied features and transformations

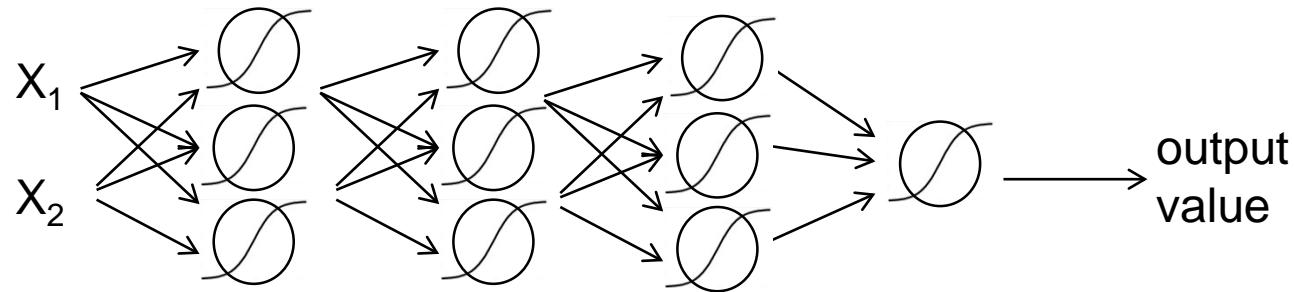


But:

More layers => more parameters => Smaller error for each  
*especially* at lower layers

# Train with Care

More hidden layers => More varied features and transformations



But:

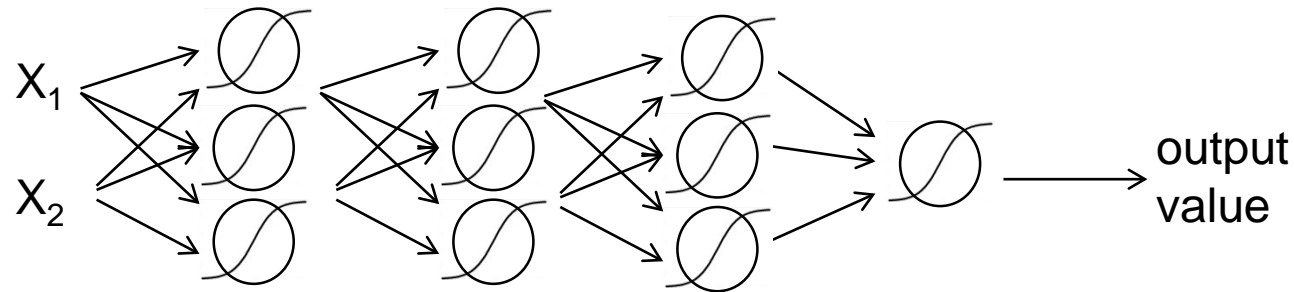
More layers => more parameters => Smaller error for each  
*especially* at lower layers

Need:

More data and computing power (gpu)

# Train with Care

More hidden layers => More varied features and transformations



But:

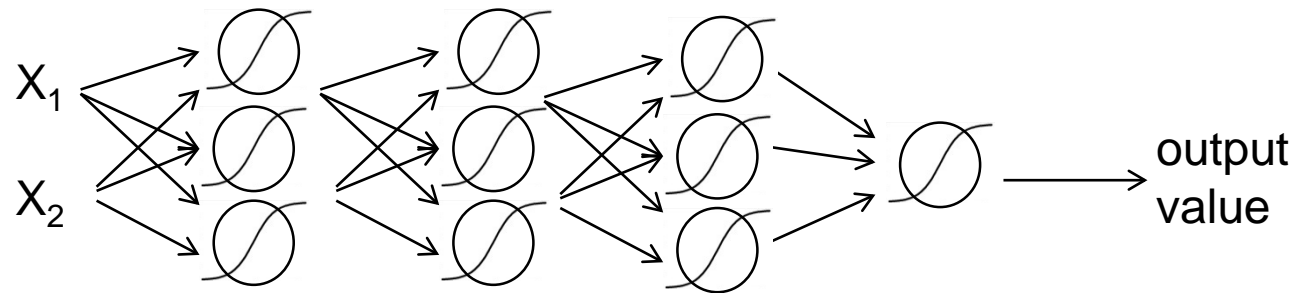
More layers => more parameters => Smaller error for each  
*especially* at lower layers

Need:

More data and computing power (gpu), functions that don't saturate(RELU)

# Train with Care

More hidden layers => More varied features and transformations



But:

More layers => more parameters => Smaller error for each  
*especially* at lower layers

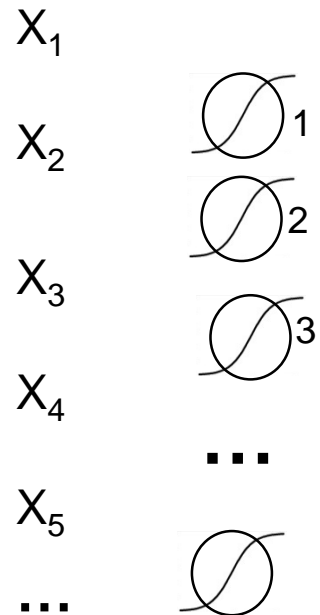
Need:

More data and computing power (gpu), functions that don't saturate(RELU), and ways to avoid over fitting (random node "dropout" or weight penalties)

# Feature Transformations, Projections, and Convolutions

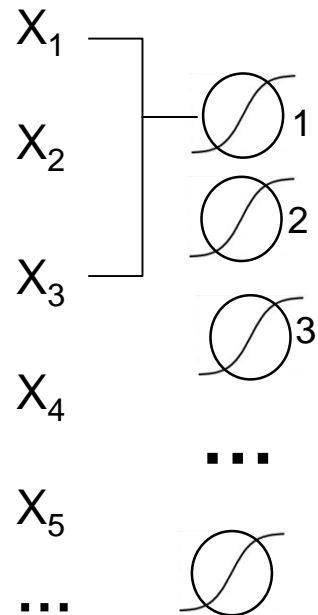
# A Filter

Many X input, many hidden nodes, ...



# A Filter

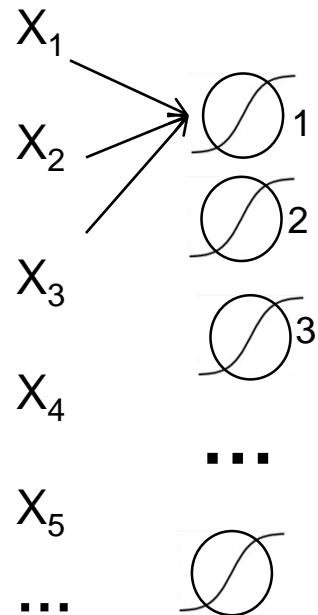
Many X input, many hidden nodes, but only local connectivity:





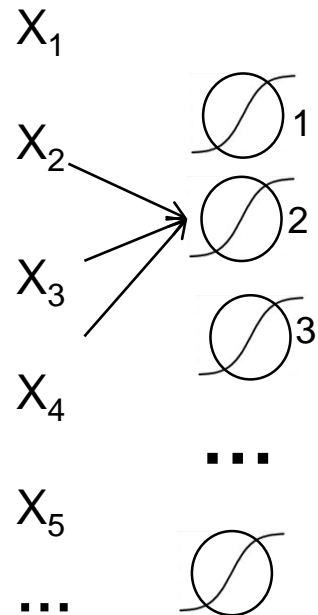
# A Filter

Many  $X$  input, but only 3 connections to each hidden node  
(a *local connectivity pattern*, aka *receptive field*)



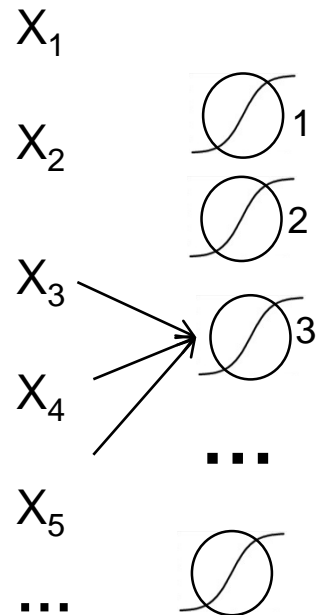
# A Filter

Many  $X$  input, but only 3 connections to each hidden node  
(a *local connectivity pattern*, aka *receptive field*)



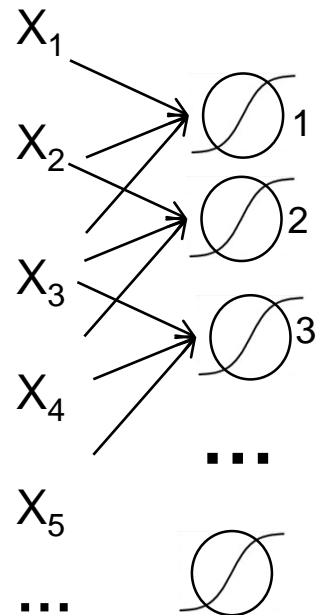
# A Filter

Many X input, but only 3 connections to each hidden node  
(a *local connectivity pattern*, aka *receptive field*)



# A Filter

Many  $X$  input, but only 3 connections to each hidden node  
(a *local connectivity pattern*, aka *receptive field*)

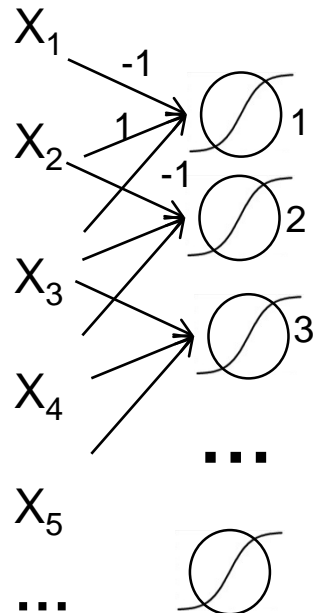


# A Filter

Many X input, but only 3 connections to each hidden node  
(a *local connectivity pattern*, aka *receptive field*)

For node 1 let  $W = [w_1 \ w_2 \ w_3] = [-1 \ 1 \ -1]$

*What is the node 1 doing?*

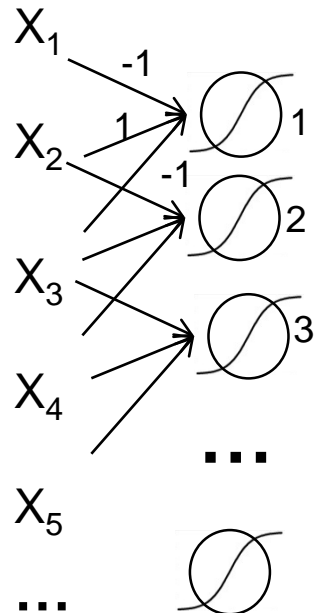


# A Filter

Many X input, but only 3 connections to each hidden node  
(a *local connectivity pattern*, aka *receptive field*)

For node 1 let  $W = [w_1 \ w_2 \ w_3] = [-1 \ 1 \ -1]$

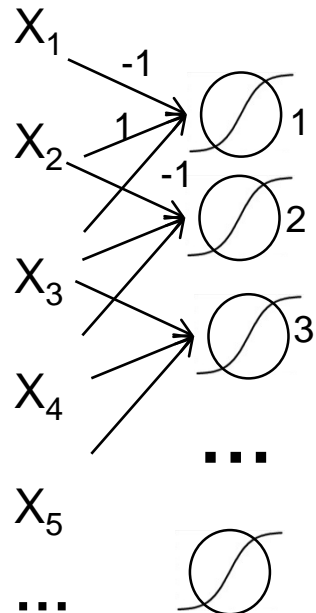
*What is the node 1 doing?*



Informally, node 1 has max activation for a ‘spike’, e.g. when  $X_2$  is positive and  $X_1, X_3$  are negative

# A Filter

Many X input, but only 3 connections to each hidden node  
(a *local connectivity pattern*, aka *receptive field*)



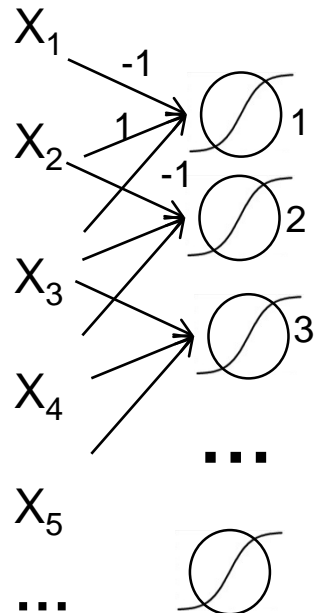
For node 1 let  $W = [w_1 \ w_2 \ w_3] = [-1 \ 1 \ -1]$

For node 2,3, etc... copy  $W$  for node 1 so that node 2 and 3 are looking for spikes in their “receptive” field

*What is the hidden layer doing?*

# A Filter

Many X input, but only 3 connections to each hidden node  
(a *local connectivity pattern*, aka *receptive field*)



For node 1 let  $W=[w_1 \ w_2 \ w_3] = [-1 \ 1 \ -1]$

For node 2,3, etc... copy  $W$  for node 1 so that node 2 and 3 are looking for spikes in their “receptive” field

*What is the hidden layer doing?*

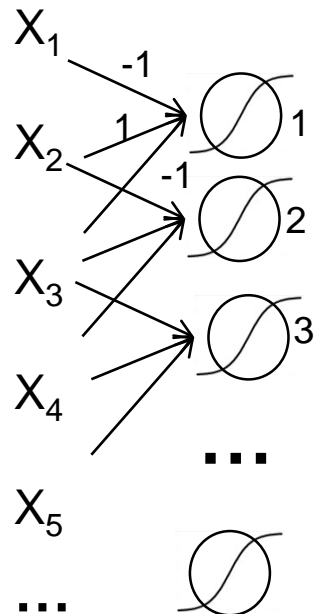
Informally, looking for a spike everywhere.

This is essentially a convolution operator,  
where  $W$  is the kernel.



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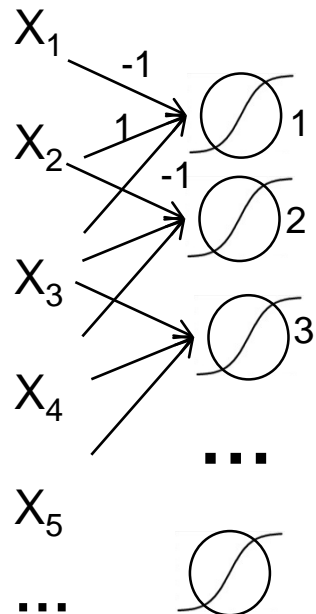
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Note: copying weights is like *sliding*  $W$  across input

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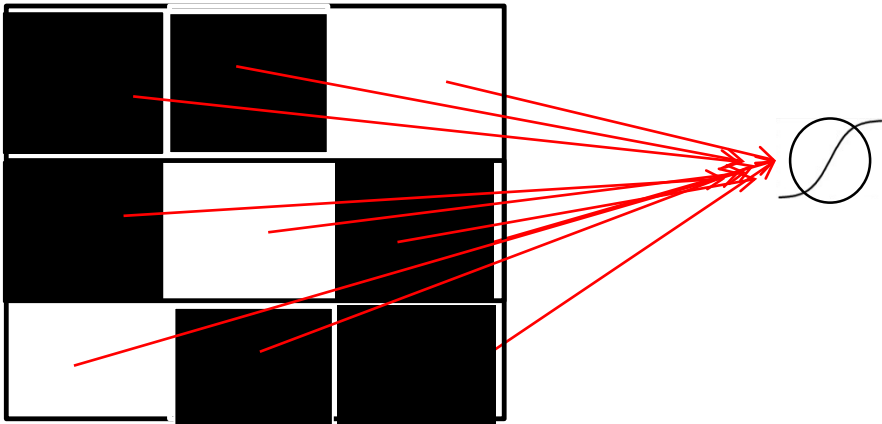
Note: copying weights is like *sliding*  $W$  across input

This is essentially a convolution operator, where  $W$  is the kernel

Note: if we take max activation across nodes (‘Max Pool’) then it’s like looking for a spike *anywhere*.

# 2D Convolution

Now let input be a 2D binary matrix, e.g. a binary image, fully connected to 1 node

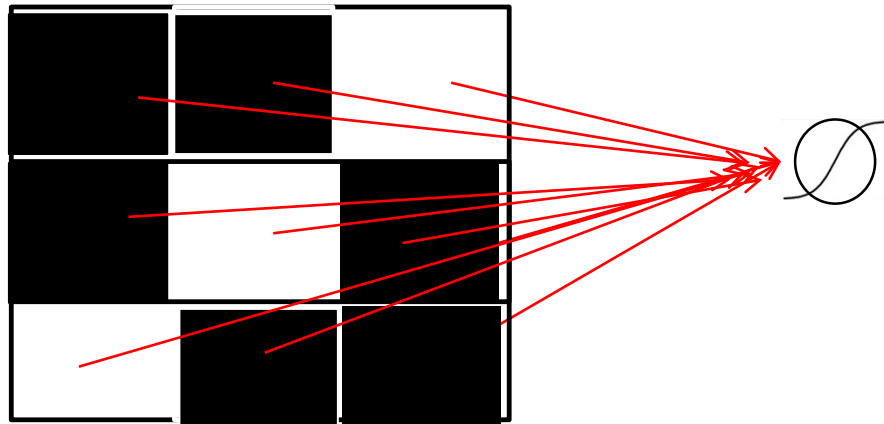


(black= -1 white=1)

*What  $W$  matrix would 'activate' for a upward-toward-left diagonal line?*

# 2D Convolution

Now let input be a 2D binarized 3x3 matrix fully connected to 1 node



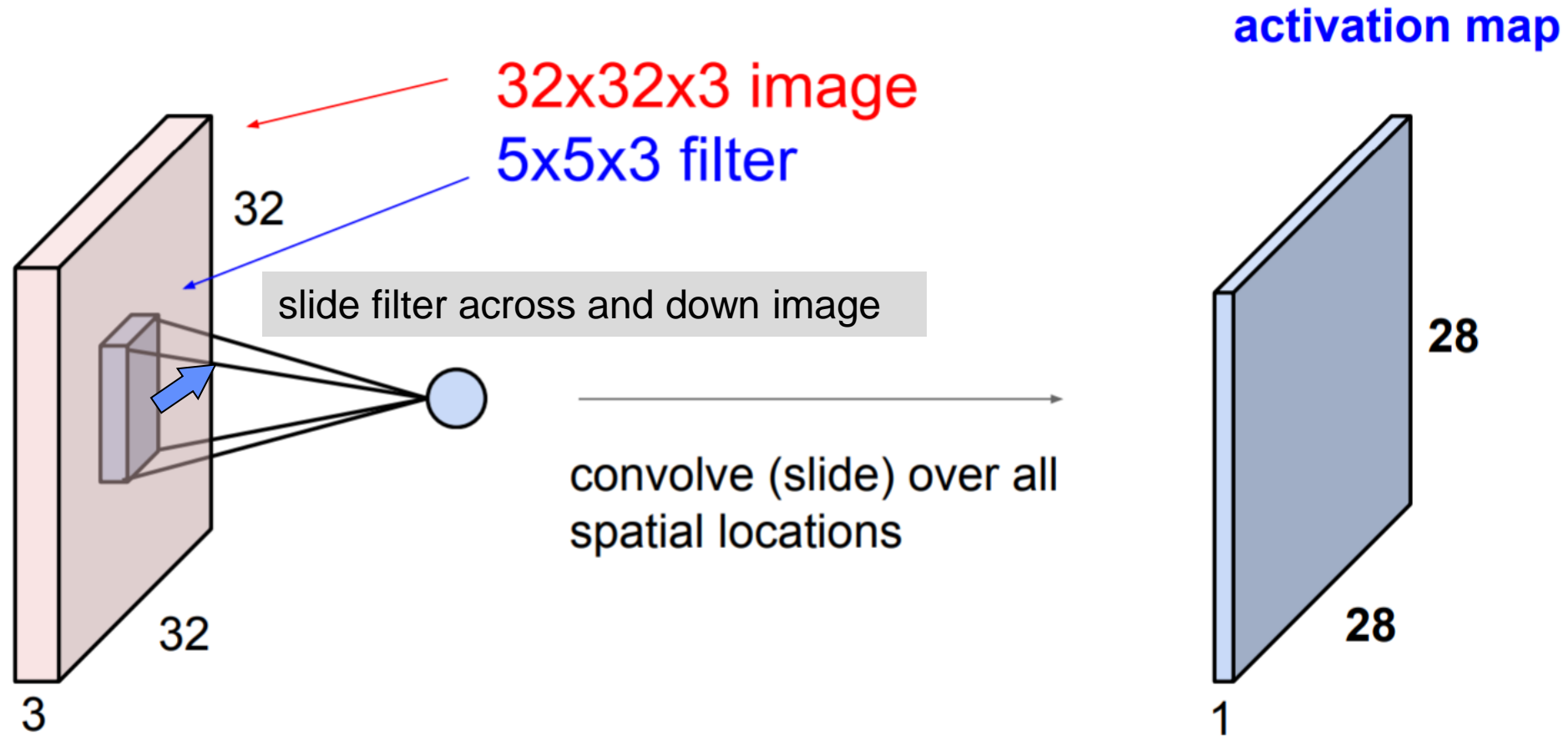
(black= -1 white=1)

*What  $W$  matrix would 'activate' for a upward-toward-left diagonal line?*

How about:

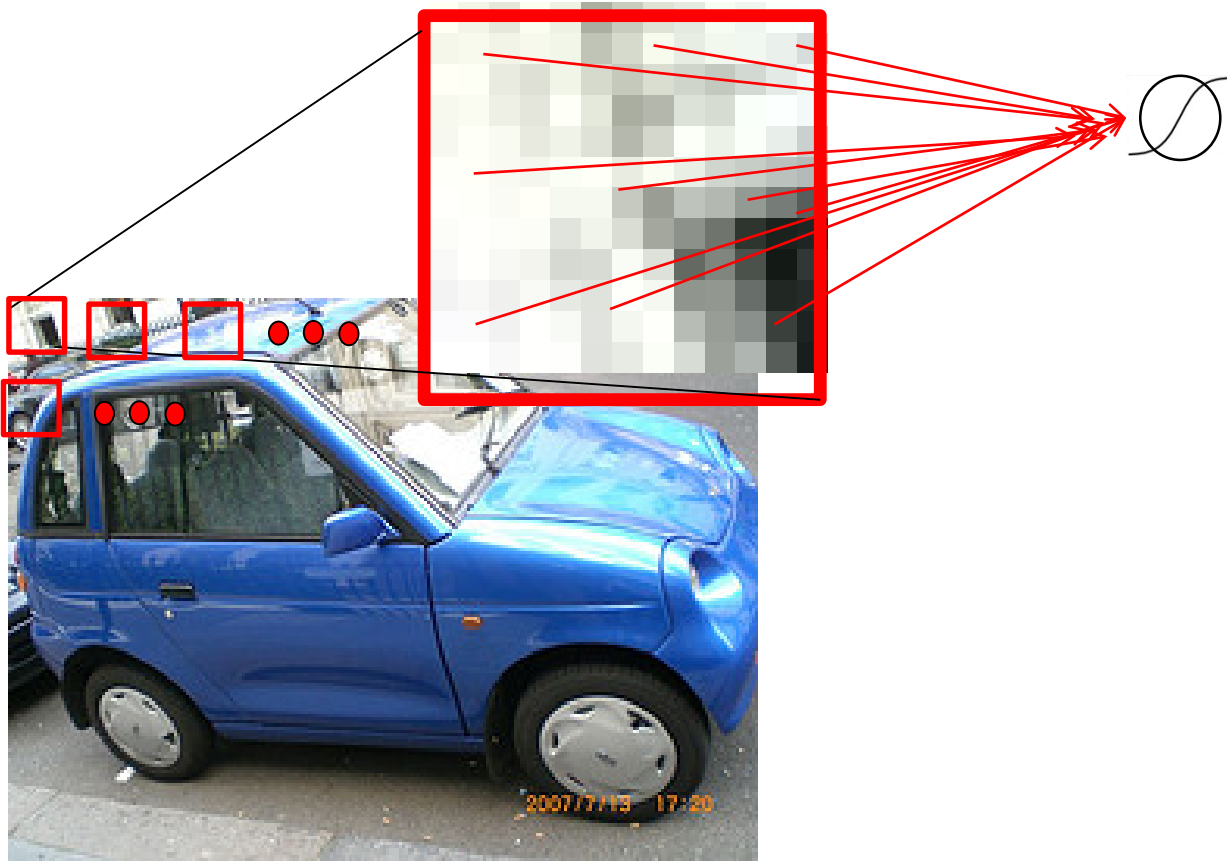
$$W = \begin{bmatrix} -1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & -1 \end{bmatrix}$$

# 2D Convolution of Image to Feature map



# 2D Convolution

For full image, 1 filter is applied to 1 region in 1 color channel at a time, and then slid across regions (or done in parallel with shared weights) and produces 1 new 2D image (hidden) layer



Convolution Layer parameters:

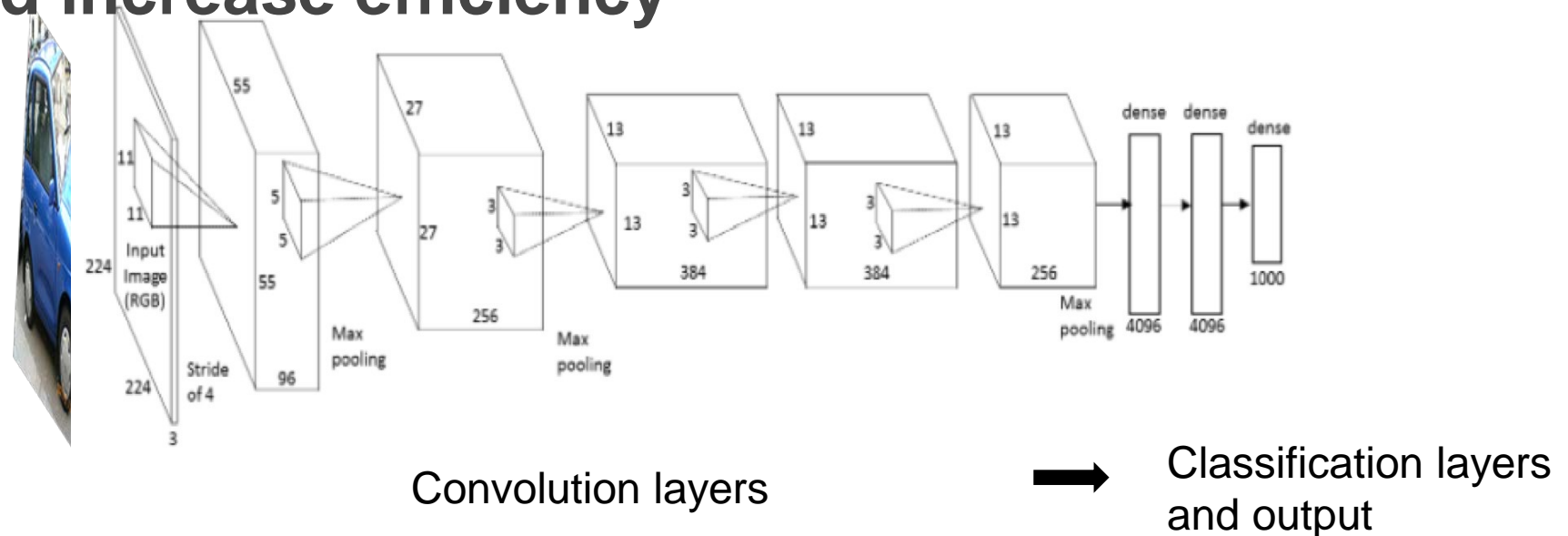
- filter size depends on input:  
smaller filters for smaller details  
2 layers of 3x3 ~ 1 layer of 5x5
- sliding amount  
smaller better but less efficient
- number of filters  
depends on task  
each filter is a new 2D layer

Convolution Network :

many layers and architecture options

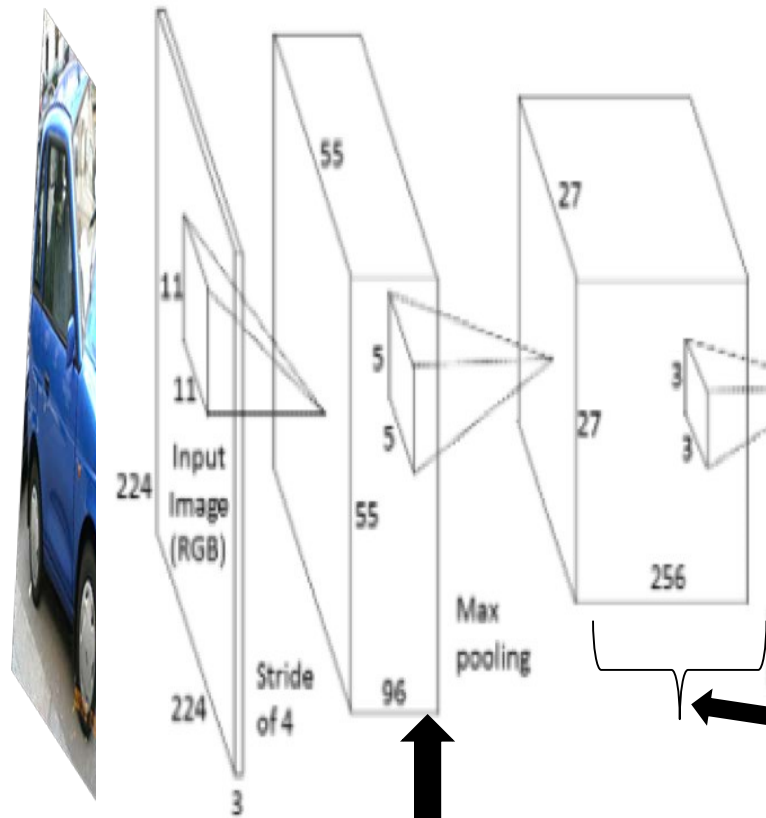
# Large Scale Versions

- Large (deep) Convolution Networks are turning out to be feasible with GPUs (some are 100+ layers)
- Need large amounts of data and many heuristics to avoid overfitting and increase efficiency



# Large Scale Versions

- Zooming in:  
Convolution  
layers



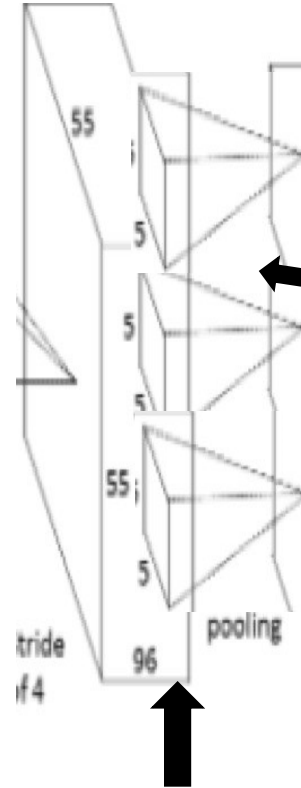
The thickness is the number of different convolutions, i.e. different transformations, sometimes called “channels”

Each convolution layer uses RELU (rectified linear activation units instead of logistic function) and is followed by Max Pooling layer (over 2D regions with sliding)



# Large Scale Versions

- Zooming in:  
Max pooling



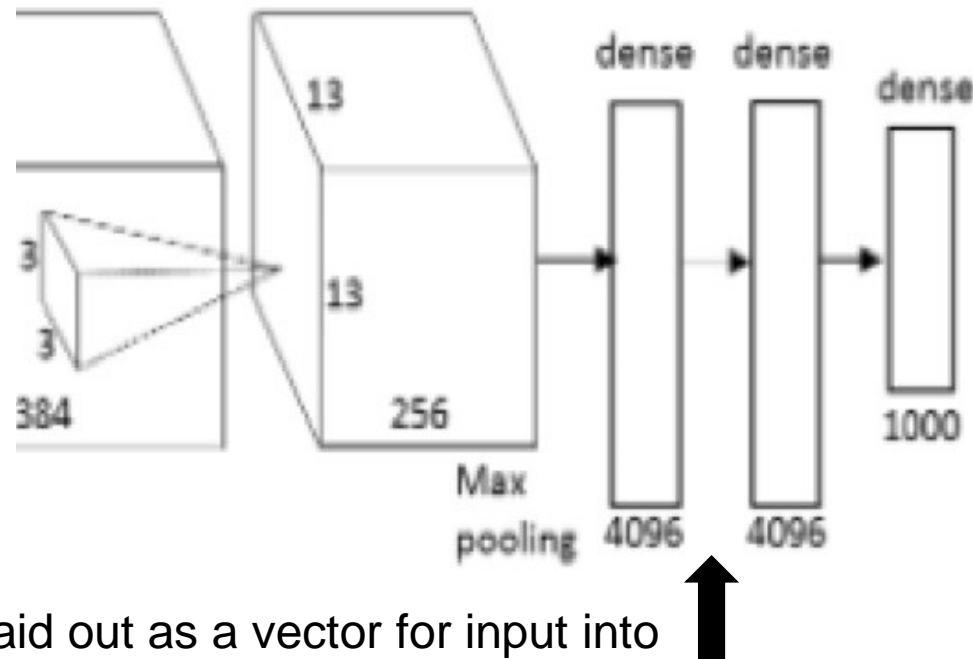
Max pooling: take the maximum over a region and slide the region.

*The larger the slide, the more down sampling occurs (which helps compute time)*

Each convolution layer uses RELU (rectified linear activation units instead of logistic function) and is followed by Max Pooling layer (over 2D regions with sliding)

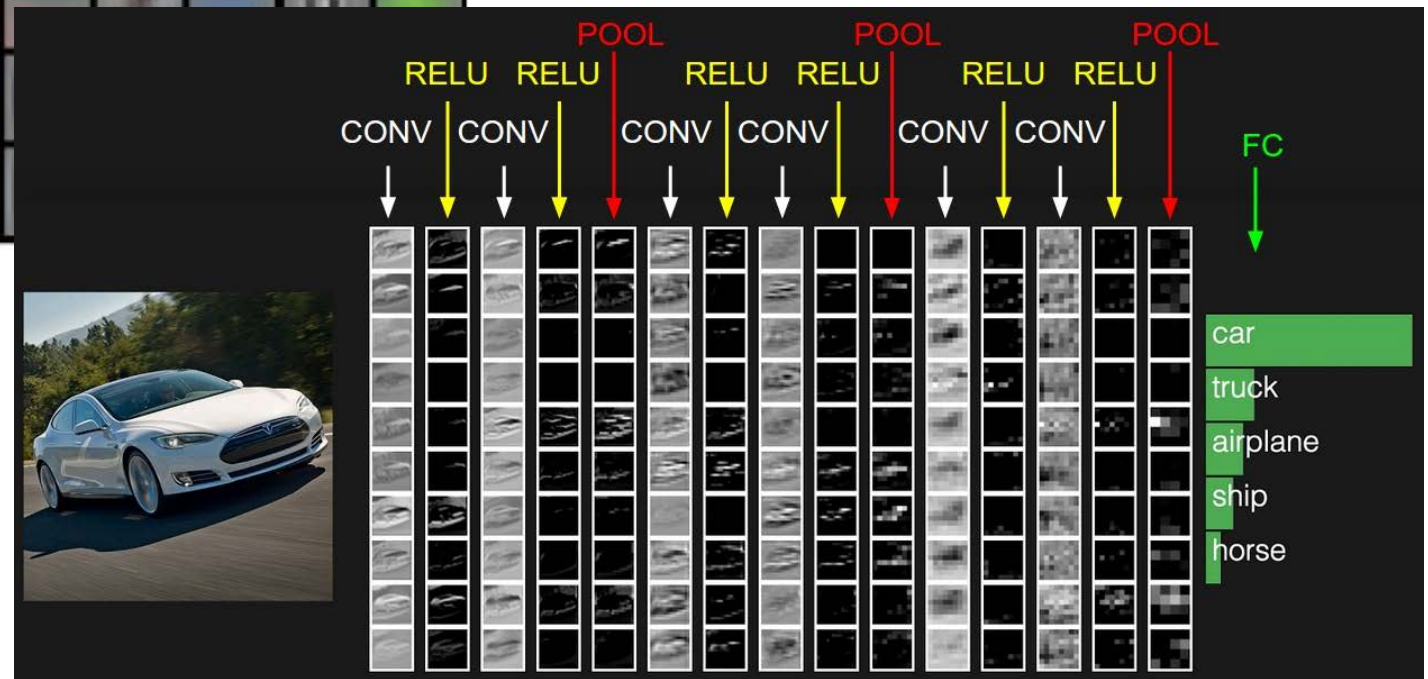
# Large Scale Versions

- Zooming in:  
Classification layers



Last convolution layer is laid out as a vector for input into classification layers.  
Classification uses dense, i.e. fully connected, hidden layers and output layer.

# What Learned Convolutions Look Like



# Summarizing Deep Layers

- **Hidden layers transform input into new features:**
  - Feature can be highly nonlinear
  - Features as a new space of input data
  - Features as projection onto lower dimensions (compression)
  - Features as filters, which can be used for convolution
- **But also:**
  - Many algorithm parameters
  - Many weight parameters
  - Many options for stacking layers

# Feature Coding vs Discovery

- Edge detection with Support Vector Machine  
OR  
Convolution Neural Network?
- With small datasets and reasonable features, SVMs can work well
- Large classification problems can benefit from common features that CNNs can discover

**Pause**

# What is Transfer Learning?

- **To overcome challenges of training model from scratch:**
  - Insufficient data
  - Very long training time
- **Use pre-trained model**
  - Trained on another dataset
  - This serves as starting point for model
  - Then train model on current dataset for current task

# Transfer Learning Approaches

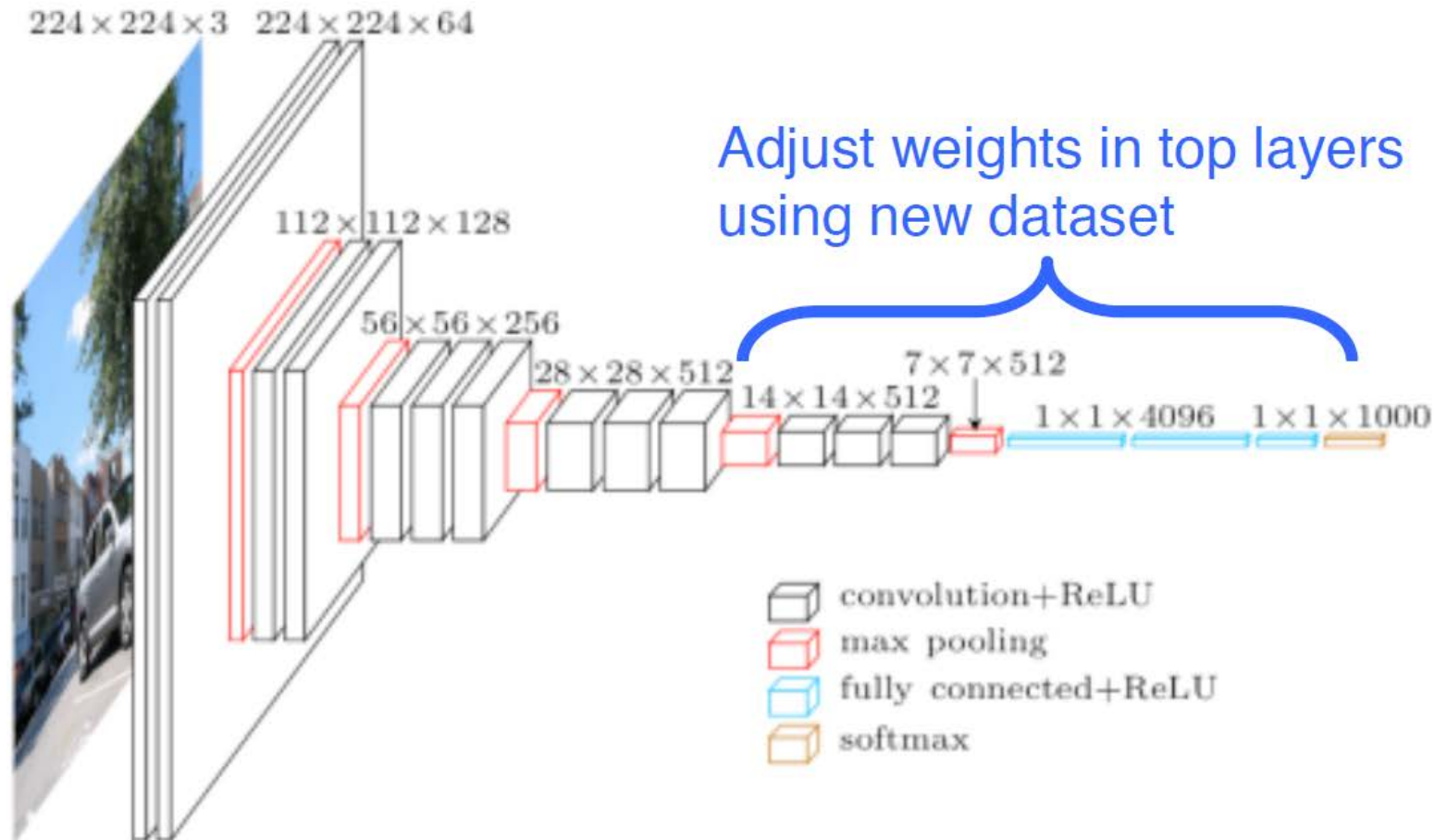
- **Feature extraction**
  - Remove last fully connected layer from pre-trained model
  - Treat rest of network as feature extractor
  - Use features to train new classifier (“top model”)
- **Fine tuning**
  - Tune weights in some layers of original model (along with weights of top model)
  - Train model for current task using new dataset



# CNNs for Transfer Learning

- **Popular architectures**
  - AlexNet
  - GoogLeNet
  - VGGNet
  - ResNet
- **All winners of ILSVRC**
  - ImageNet Large Scale Visual Recognition Challenge
  - Annual competition on vision tasks on ImageNet data

# Transfer Learning – Fine Tuning



Works best when new data is similar to original data, else use lower layers and more retraining.

Source: <https://www.cs.toronto.edu/~frossard/post/vaa16/>

# The Zoo

- Machine learning/convolution network frameworks:

Tensorflow, pyTorch (libraries and API to build graphs of networks and processing)

Keras - higher level CNN library with tensorflow (best for learning)

Caffe – C/C++ library with many pretrained models

Caffe2 – Facebook takeover Caffe, Pytorch (has a good model for people detection)

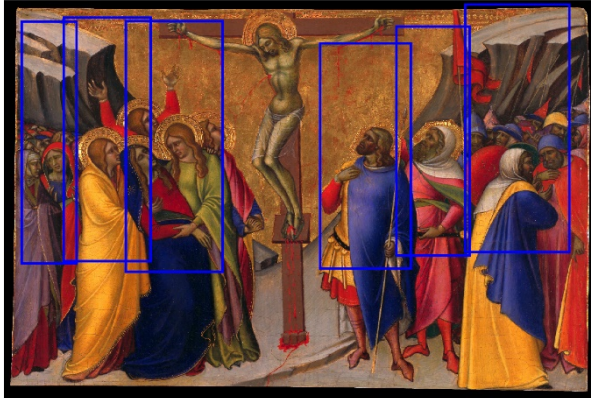
YOLO/Darknet – A C++ library, with object detection

Matlab – CNN functions, and pretrained networks

- Many networks pretrained on large or particular object classes are available:  
AlexNet, VGG19, Googlenet, Detectron
- Training CNNs require GPUs; CPUs are fine running pretrained CNNs
- Big Tech have online services (see next page)

# Caffe2, Facebook “Detectron” networks

Object Detection  
ie getting a region  
bounding box  
(rcnn)



Object  
Segmentation  
ie getting a mask  
(mask-rcnn)



Object Parts  
ie getting keypoints  
(keypoint-rcnn)



# Caffe2 Detectron on Comet

- **git clone *<https://github.com/facebookresearch/Detectron>***  
*You will get folders of tools, utilities, etc..*
- **On Comet compute node, run:**  
module purge  
module load singularity  
singularity shell /share/apps/gpu/singularity/images/pytorch/pytorch-v1.0.0-gpu-20190110.simg

# Google tool for objects, faces, text

- Google Vision api – object recognition network

fails on “Soldier”

gets “Musician”

groundbreaking.jpg

Label	Confidence
White	94%
Black And White	93%
Photograph	93%
Black	93%
People	88%
Monochrome Photography	78%
Monochrome	78%
Musician	75%

fsa1997023652#soldier\_81;military\_62;recreation\_59.jpg

Label	Confidence
Black And White	93%
Soldier	86%
Monochrome Photography	84%
Photography	82%
Monochrome	72%
Military	69%
Recreation	58%
Stock Photography	58%
Grass	52%

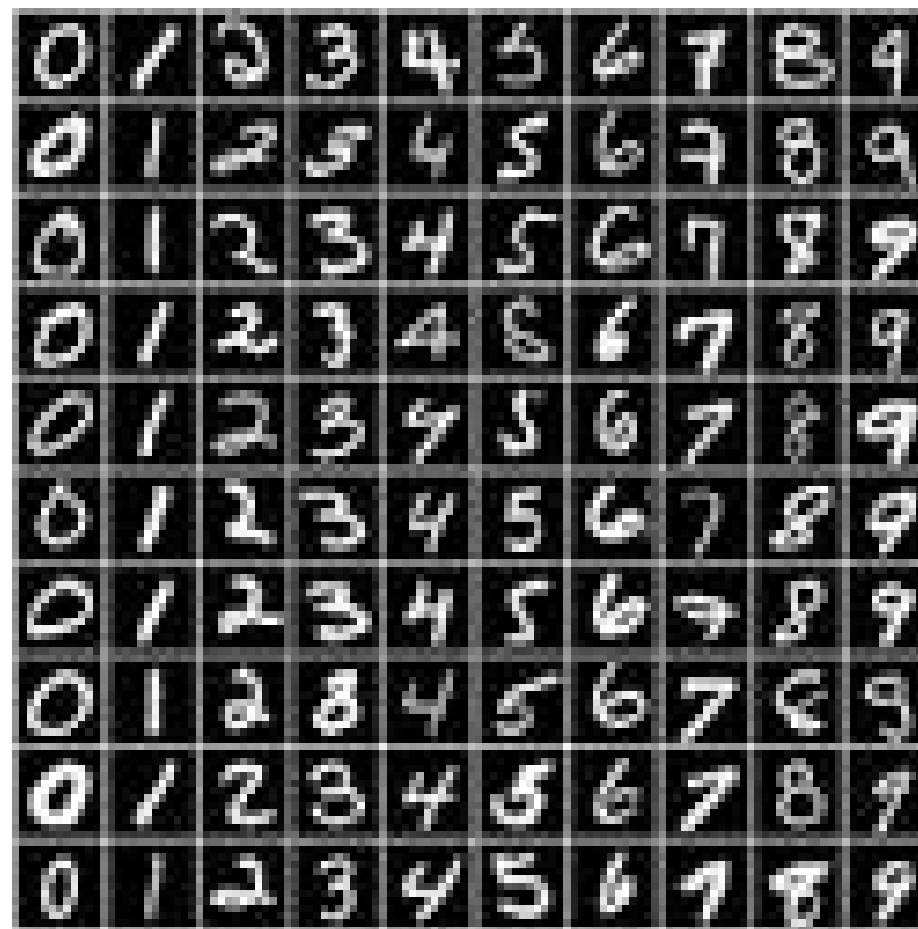


# References

- **Book:** <https://mitpress.mit.edu/books/deep-learning>
- **F. Chollet “Deep Learning with Python”**
- **Documentation:** <https://keras.io/>
- **Tutorials I used (borrowed):**
  - <http://cs231n.github.io/convolutional-networks/>
  - <https://hackernoon.com/visualizing-parts-of-convolutional-neural-networks-using-keras-and-cats-5cc01b214e59>
  - [https://github.com/julienr/ipynb\\_playground/blob/master/keras/convmnist/keras\\_cnn\\_mnist.ipynb](https://github.com/julienr/ipynb_playground/blob/master/keras/convmnist/keras_cnn_mnist.ipynb)

# Tutorial

- MNIST database of handwritten printed digits
- The 'hello world' of Conv. Neural Networks
- Use Keras front end (high level neural functions) to Tensorflow engine (neural math operations)
- Works with GPU or CPUs





# MNIST on Comet

- **Login and get an interactive compute node session**
- **Start up conda python environment**
  - . /share/apps/compute/si2019/miniconda3/etc/profile.d/conda.sh  
(^ yes, it's a 'dot' followed by space)
  - conda activate
  - jupyter notebook --no-browser --ip="\*" &

Cut and paste http address, edit localhost, look in DeepLearningTutorial for notebook

Home x LabMNIST\_Final x

comet-18-14.sdsc.edu:8888/notebooks/LabMNIST\_Final.ipynb

jupyter LabMNIST\_Final Last Checkpoint: 7 minutes ago (autosaved) Logout

File Edit View Insert Cell Kernel Help Not Trusted Python 3

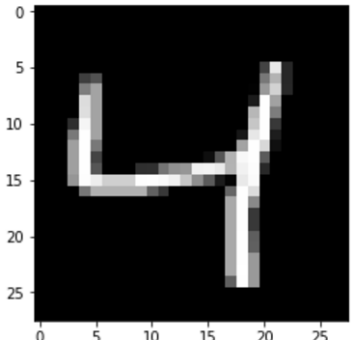
```
for i in range(0,3):
    im = Image.fromarray(X_train[i,:,:])
    im.save("Xtrain_num"+str(i)+"_cat_"+str(Y_train[i])+".jpeg")

plt.figure()
plt.imshow(im,'gray')
plt.show()

print('img load done')
print (time.strftime("%H:%M:%S"))
```

(5000, 28, 28)

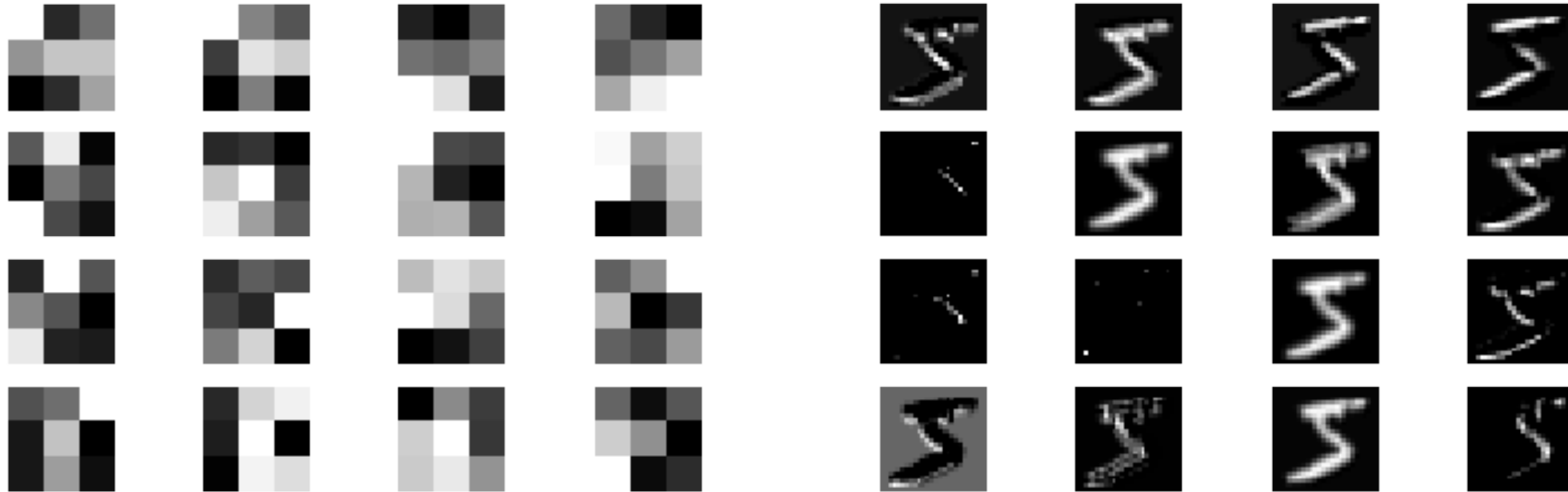
<matplotlib.figure.Figure at 0x2ad45d04f2e8>



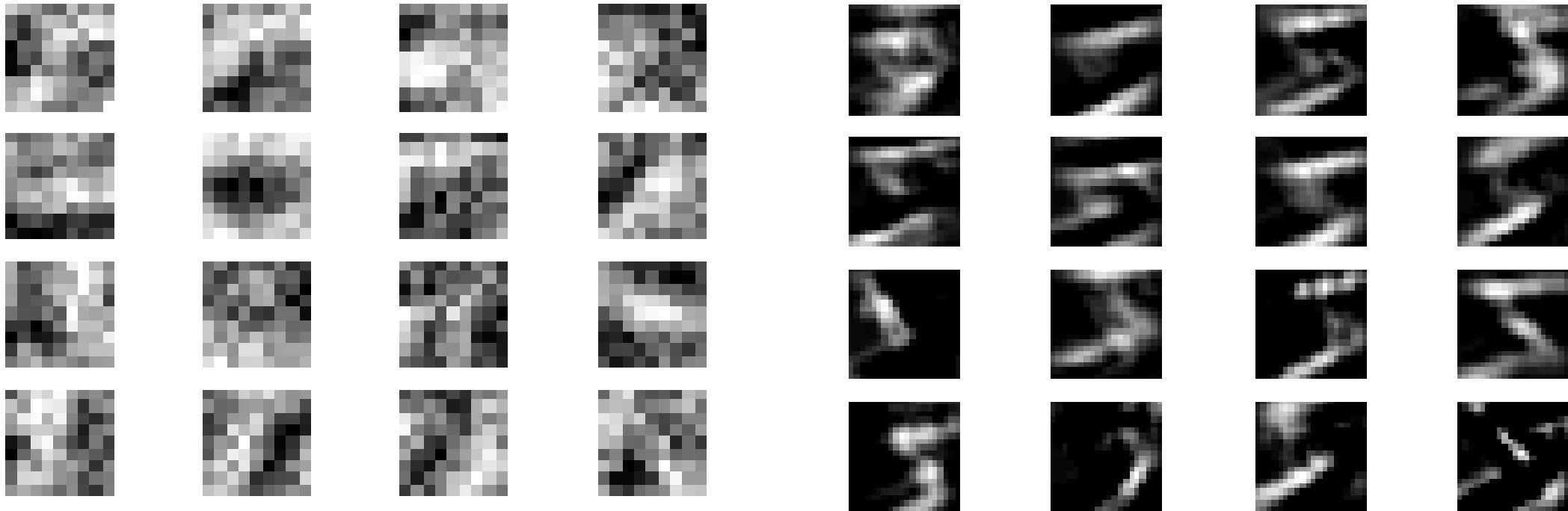
img load done

Windows taskbar: 10:09 PM 7/31/2017

# 3x3 first convolution layer filter and activation



# 9x9 first convolution layer filter and activation



Pause