Introduction to Machine Learning

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WP3.1 Lead in UDRC 3

Chair in Machine Learning and Computer Vision

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Some slides adopted from: Mike Davies, A. Katsaggelos, S. Theodoridis, A. Ng

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Common questions

Q: Are the slides going to be shared?

A: Yes, a preview version is already in the dropbox link https://www.dropbox.com/s/am2tspic0t0fy2x/Summer_School_Slides_tsaftaris_2021.pptx?dl=0

Updated version is available at the link of the chat!

Q: Will the session be recorded?

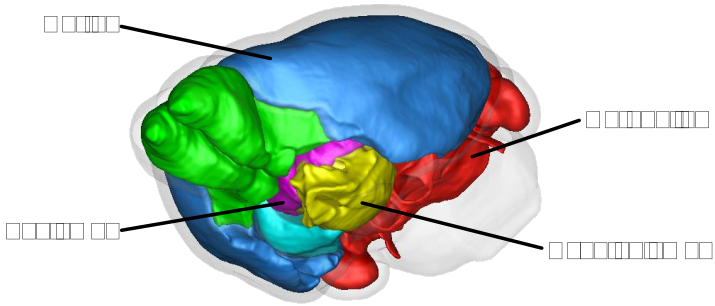
A: Yes and will be shared afterwards.

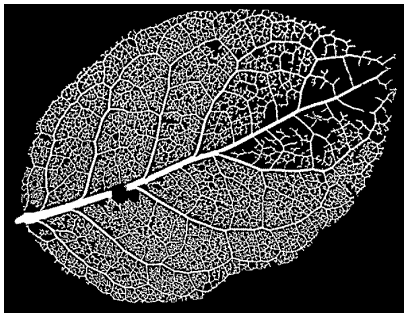
Q: Are you going to show us practical examples?

A: Yes via web-based demos. More hands on follows later in the day.

Our expertise

- **Computer vision & Image Analysis:**
  - Extract information from images
  - Applications: medicine, plants
- **Machine learning & pattern recognition**
  - Shallow or deep representation learning (the process of making sense of data)
  - Learning without lots of data
  - Combining information sources
- Distributed learning





$$z = f\left(\quad \right)$$

We do AI…

Disentangled learning

Weakly supervised learning

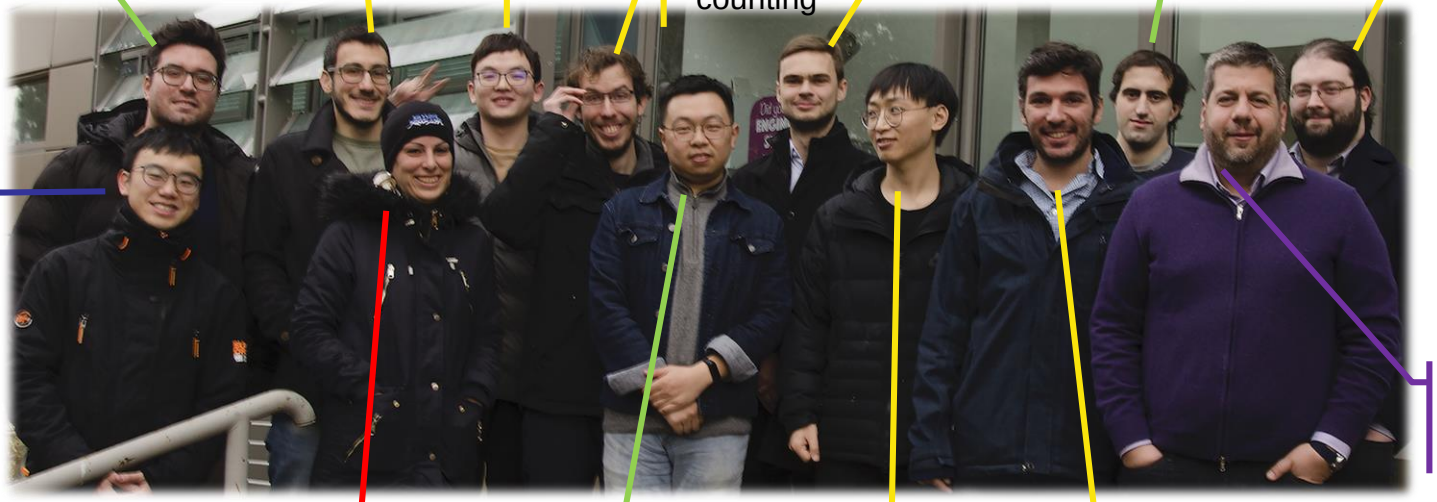
Transfer Disentanglement

Object counting

Conditioning

Generative anomaly detection

DL image compression



+ several MSc students

Privacy Data Leakage

???

Privacy Data Leakage

iCAIRD

Canon Medical AI Team Lead

Canon

CANON MEDICAL

Disentangling Pathology

Xi'an Jiaotong-Liverpool University 西交利物浦大學

Learning to age

Disentangled learning

Causal Machine Learning

PostDoc

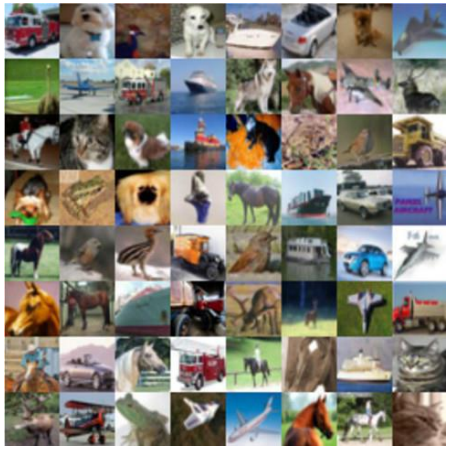
Canon Medical

PhD Student

Intern

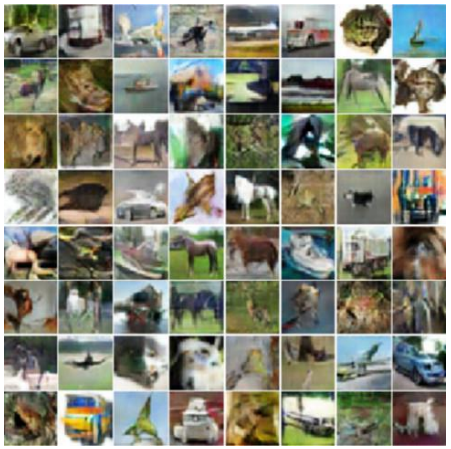
An example of ML in UDRC

- Given data can I learn their distribution?



Real images (CIFAR-10)

- Learn a distribution that can generate that data?



Generated images

Some common applications

- Email spam filtering
- Netflix/Amazon recommendations
- Google suggested queries
- The Google index itself
- Predicting stock prices
- Classifying threats in images
- etc

Extreme (…) applications

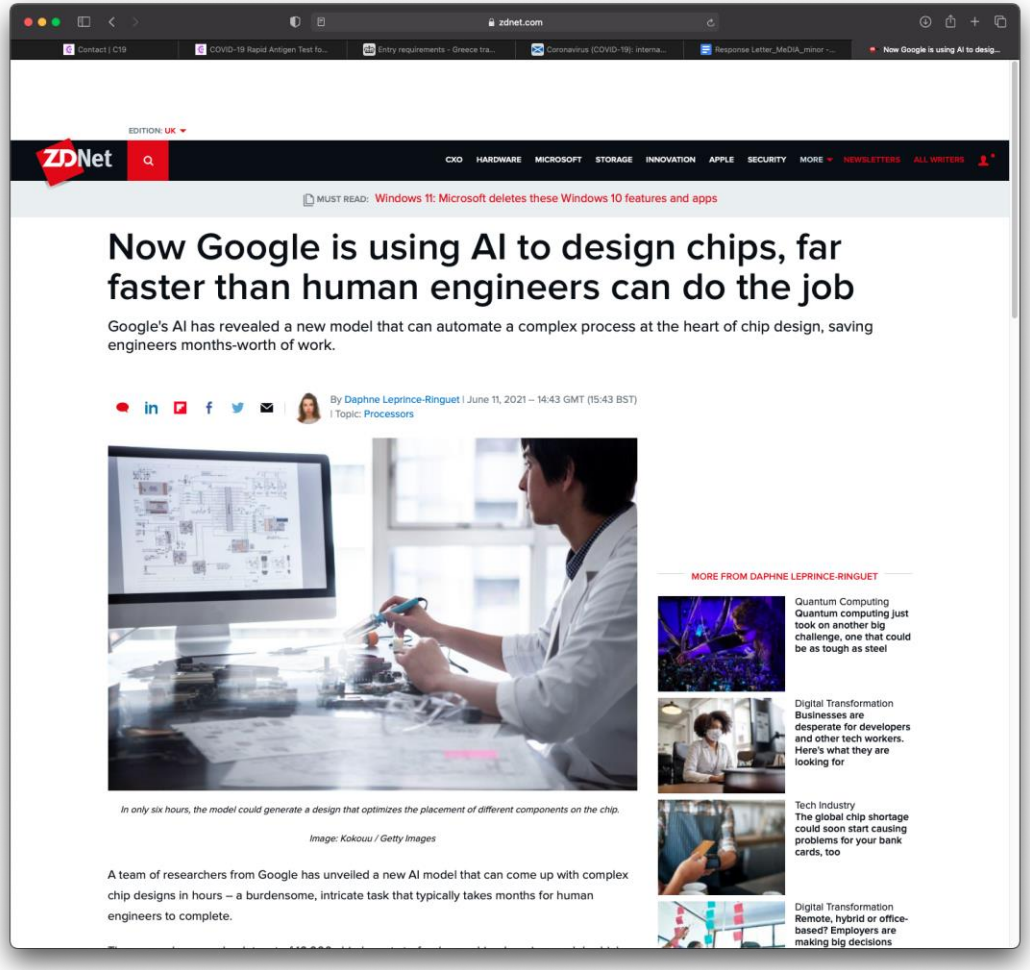
- MIT flight
- http://www.youtube.com/watch?v=aiNX-vpDhMo
- Robot in the dessert
- http://www.youtube.com/watch?v=OIOtOmyySQo
- Google car
- http://www.youtube.com/watch?v=cdgQpa1pUUE

On purpose I leave these "old" extremes to show how quickly ML has advanced in less than 10 years.

Autonomous Drones

https://www.youtube.com/watch?v=2DsJLigMrS0

Use AI to design new chips…



EDITION: UK

ZDNet

CXO HARDWARE MICROSOFT STORAGE INNOVATION APPLE SECURITY MORE NEWSLETTERS ALL WRITERS

MUST READ: Windows 11: Microsoft deletes these Windows 10 features and apps

Now Google is using AI to design chips, far faster than human engineers can do the job

Google's AI has revealed a new model that can automate a complex process at the heart of chip design, saving engineers months-worth of work.

By Daphne Leprince-Ringuet | June 11, 2021 – 14:43 GMT (15:43 BST) | Topic: Processors

In only six hours, the model could generate a design that optimizes the placement of different components on the chip.

Image: Kokouu / Getty Images

A team of researchers from Google has unveiled a new AI model that can come up with complex chip designs in hours – a burdensome, intricate task that typically takes months for human engineers to complete.

MORE FROM DAPHNE LEPRINCE-RINGUET

Quantum Computing
Quantum computing just took on another big challenge, one that could be as tough as steel

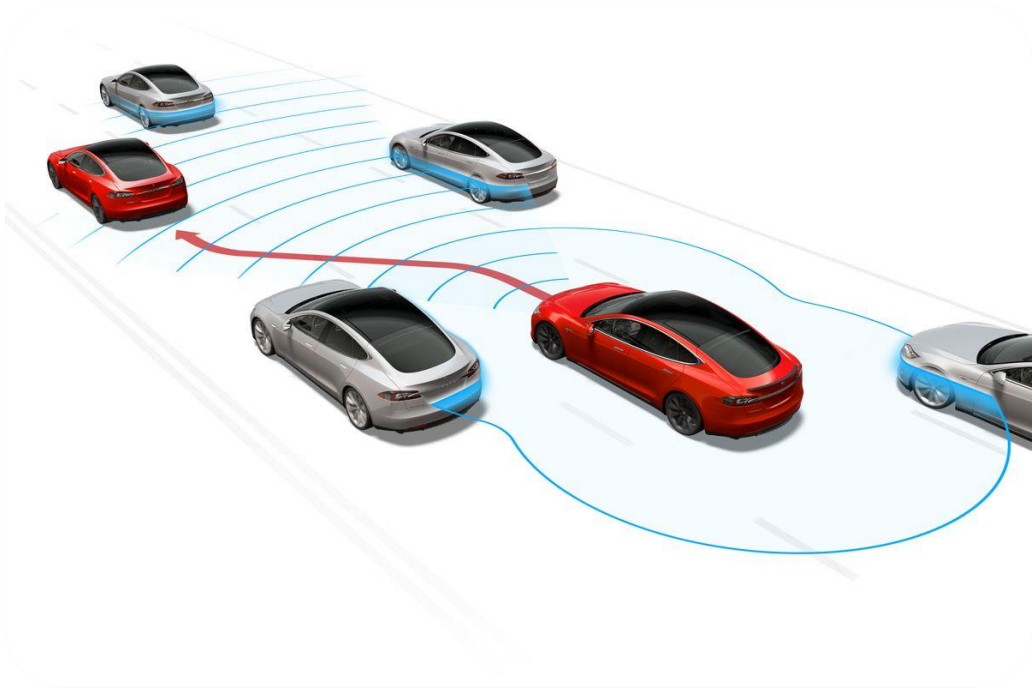
Digital Transformation
Businesses are desperate for developers and other tech workers. Here's what they are looking for

Tech Industry
The global chip shortage could soon start causing problems for your bank cards, too

Digital Transformation
Remote, hybrid or office-based? Employers are making big decisions

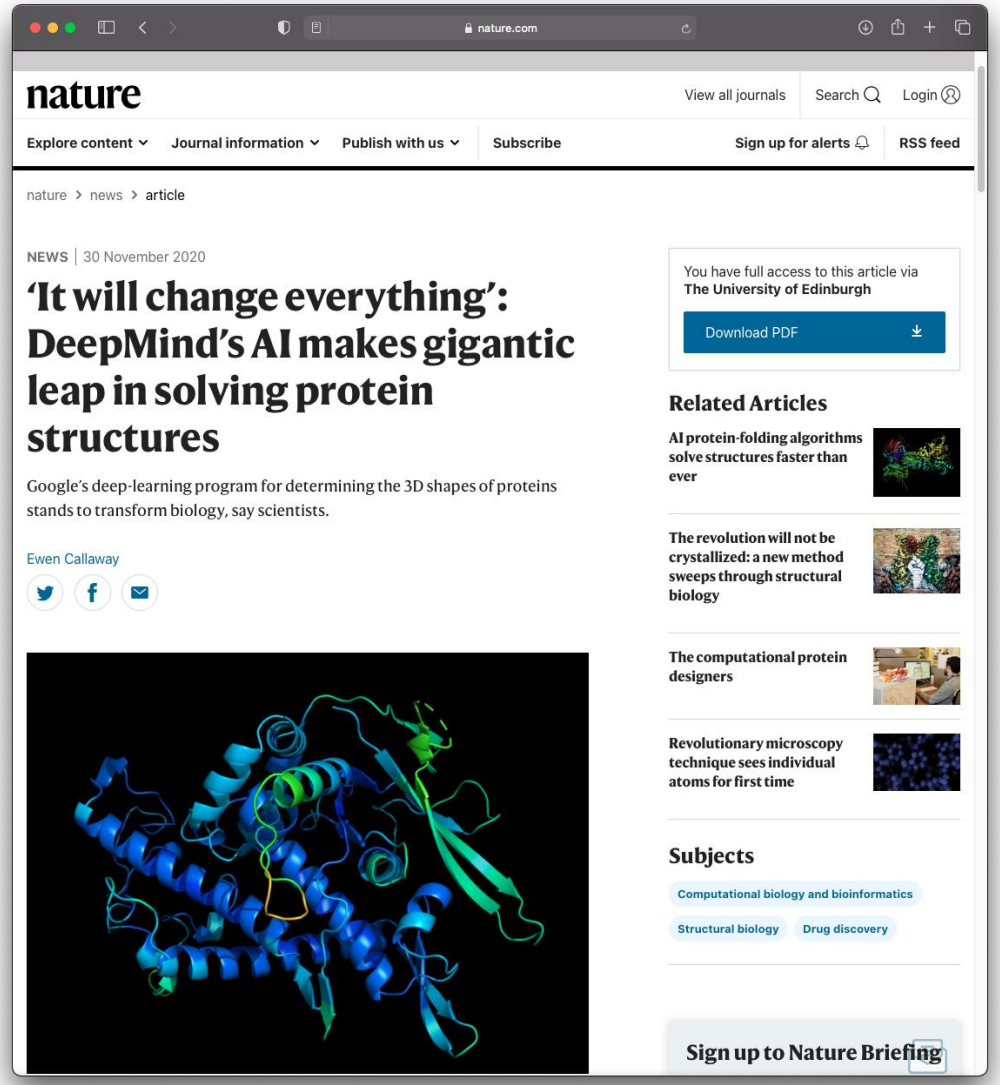
https://www.nature.com/articles/s41586-021-03544-w

Autonomous driving



Source: Andrej Karpathy Director of AI and Autopilot Vision at Tesla,
Multi-Task Learning in the Wilderness
ICML 2019

Protein folding



https://www.nature.com/articles/s41586-019-1923-7.epdf?author_access_token=Z_KaZKDqtKzbE7Wd5HtwI9RgN0jAjWel9jnR3ZoTv0MCcgAwHMgRx9mvLjNQdB2TlQQaa7l420UCtGo8vYQ39gg8lFWR9mAZtvsN_1PrccXfIbc6e-tGSgazNL_XdtQzn1PHfy21qdcxV7Pw-k3htw%3D%3D

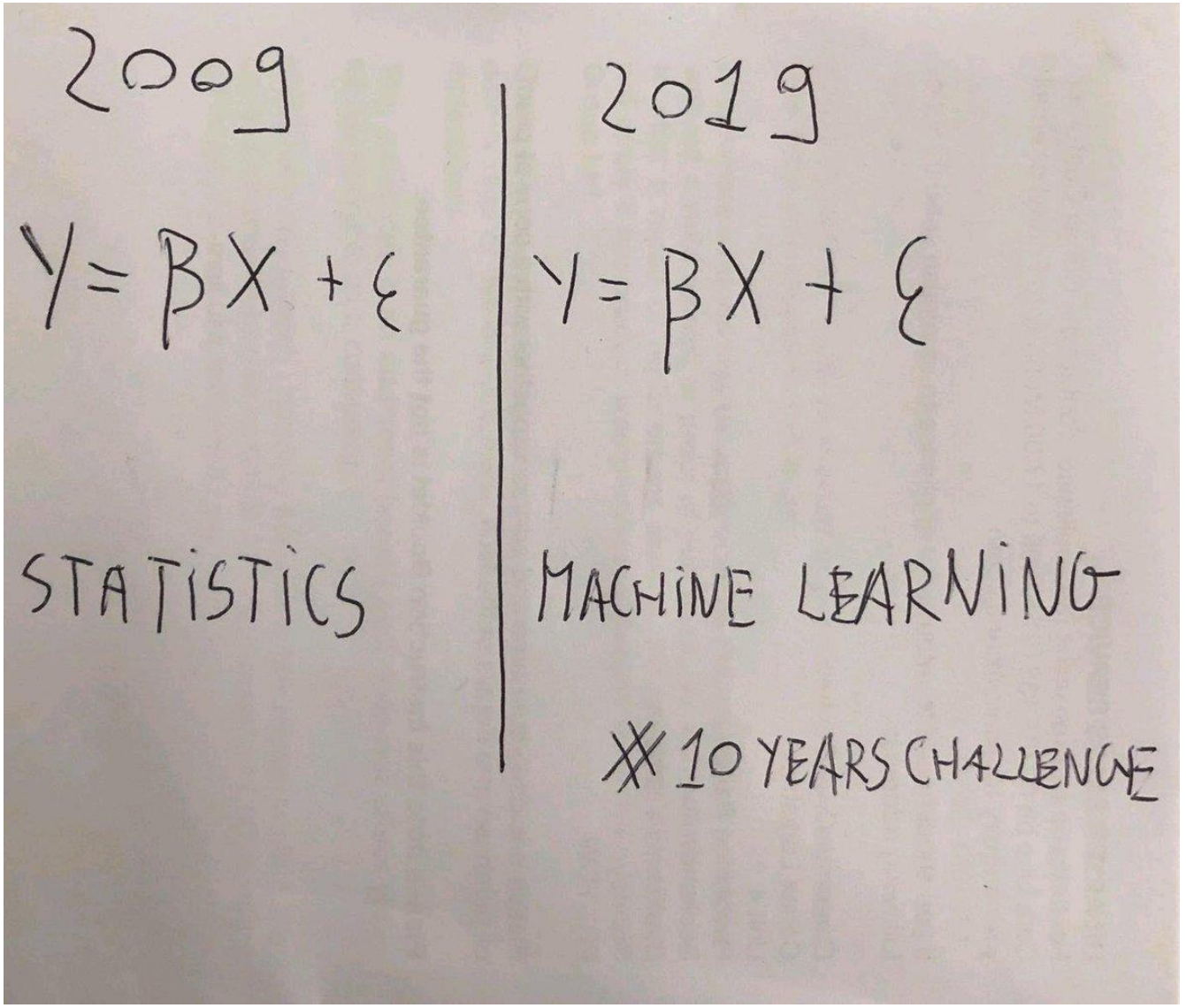
What is machine learning?

- Arthur Samuel [1959] (informal definition) Gives computers ability to learn without being explicitly programmed.

  ➔He built the very first checker's program

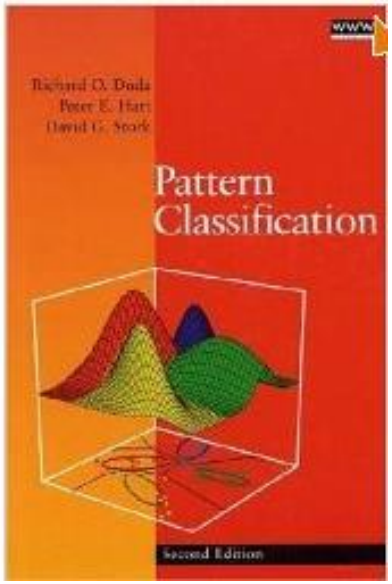
- Tom Mitchell [98] (more formal): A well-posed learning problem is defined as follows:
  - A computer program is set to learn from an **experience E** with respect to some **task T** and some **performance measure P** if its performance on **T** as measured by P **improves** with experience E.

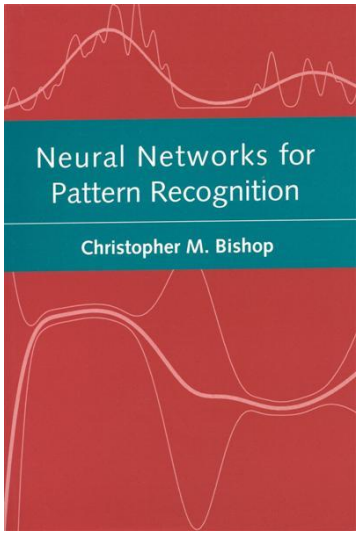
Machine learning the 10 year challenge

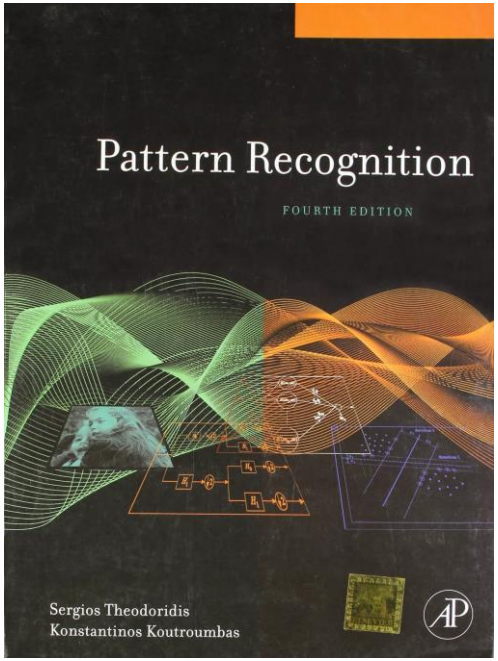


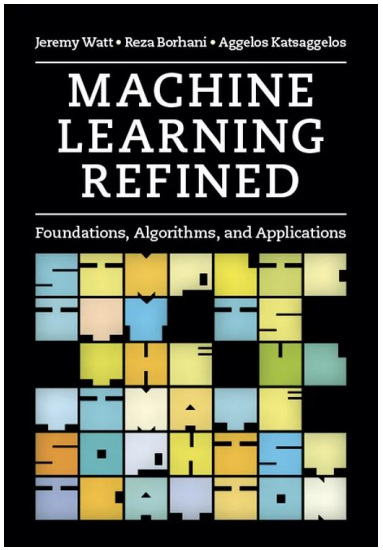
Text Books

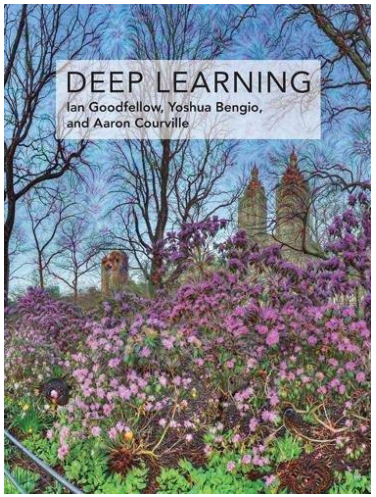
- Useful texts ...











- Most can be found online or libraries: e.g.

https://github.com/jermwatt/machine_learning_refined

https://www.deeplearningbook.org/

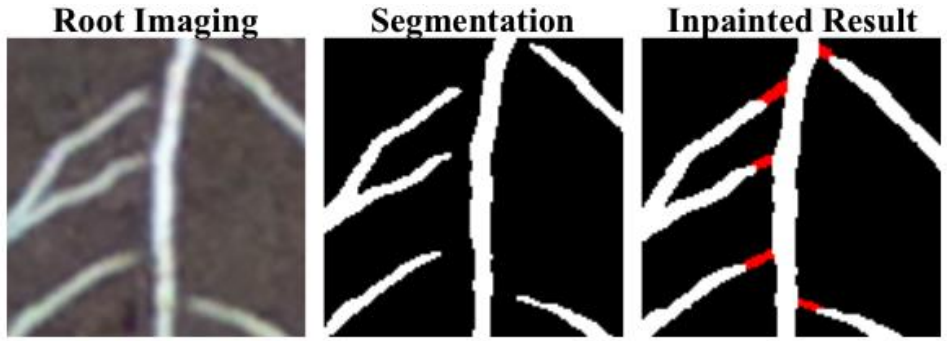
What *we* do with ML…

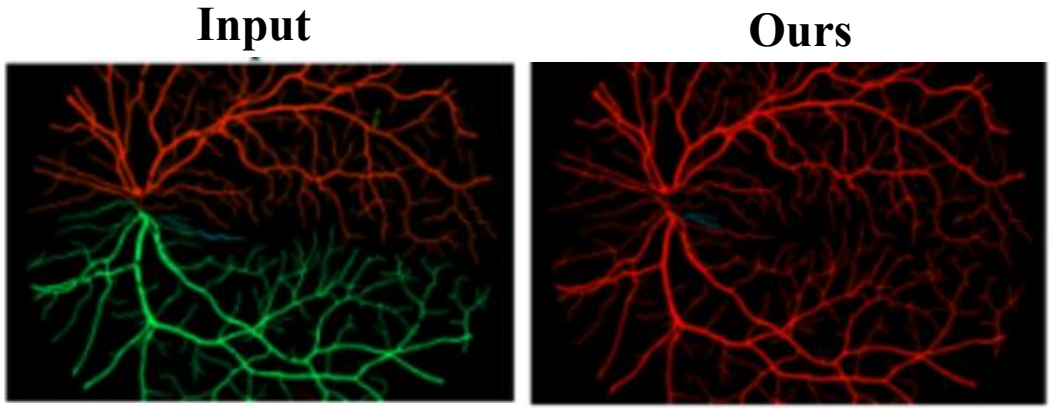
- We build algorithms to analyze **imaging** data (2D, 3D, 2D+t, 3D+t)
- From a **variety** of domains
- Use machine learning throughout

- Some examples…

Restoring faults in images

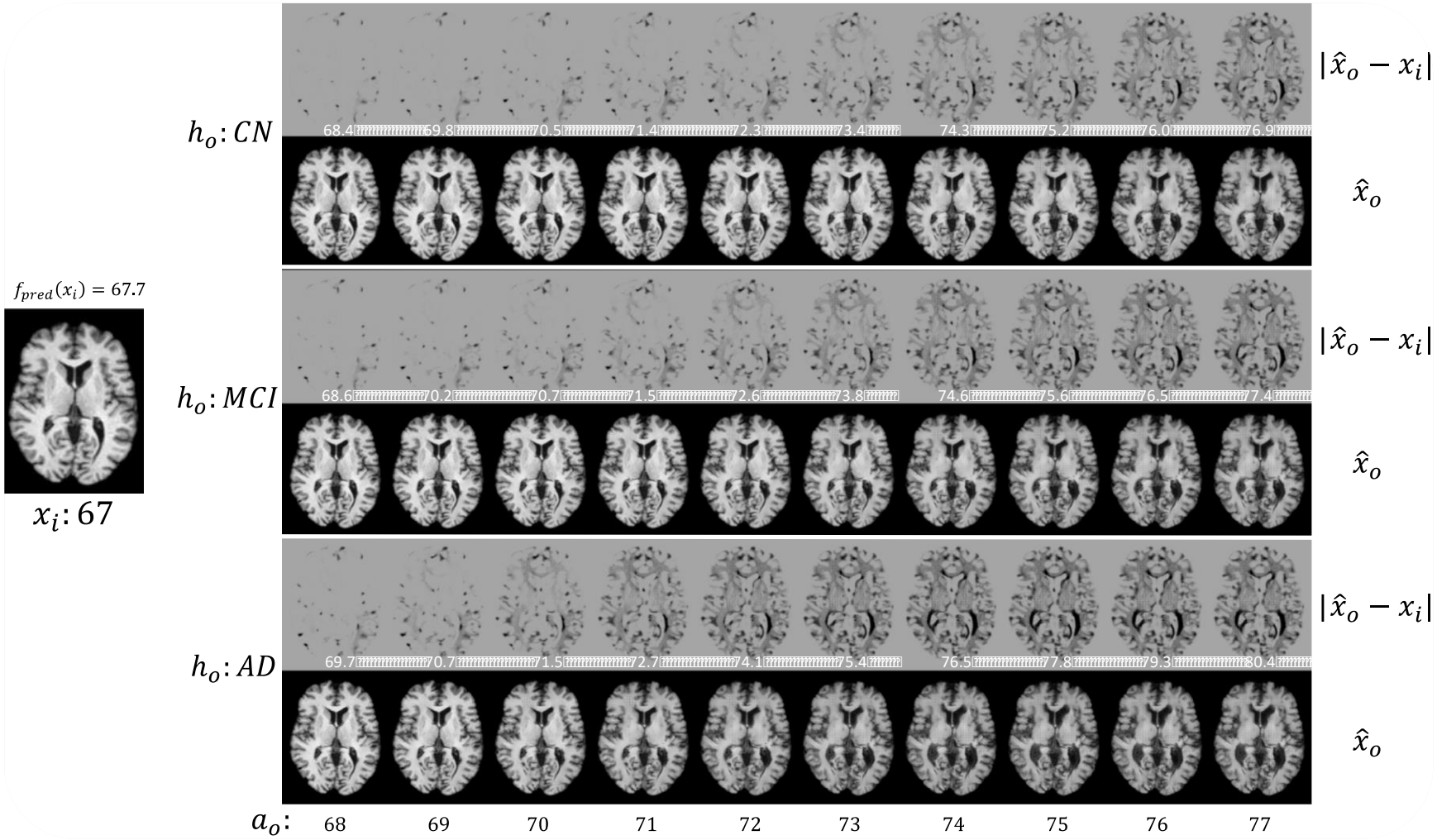
- **Recover gaps** from images of plant roots
- A similar problem is present in medical imaging as well
  ➔Retina fundus





Chen et al. “Adversarial Large-scale Root Gap Inpainting ”, CVPRW - CVPPP 2019

Learning to age

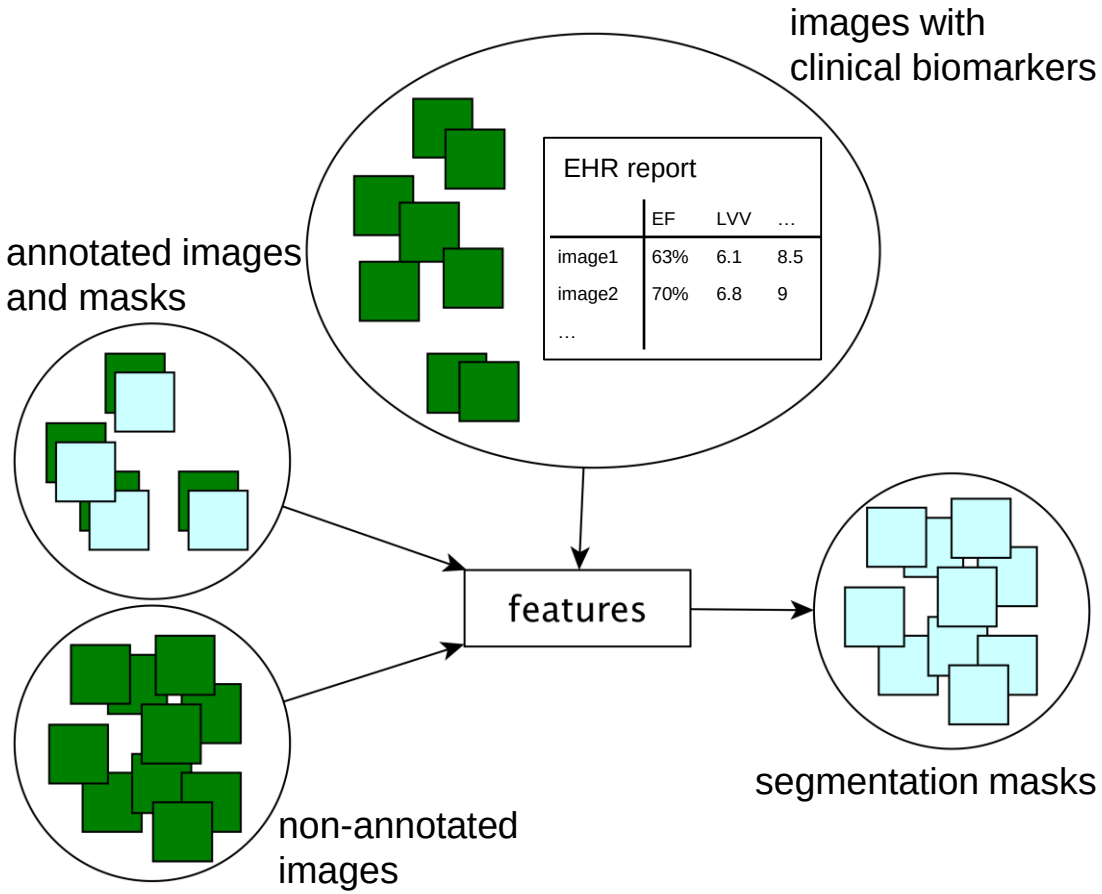


Xia, Chartsias, Wang, & Tsaftaris (2019) Learning to synthesise the ageing brain without longitudinal data. arXiv 1912.02620

Xia, Chartsias & Tsaftaris (2019) Consistent Brain Ageing Synthesis. MICCAI

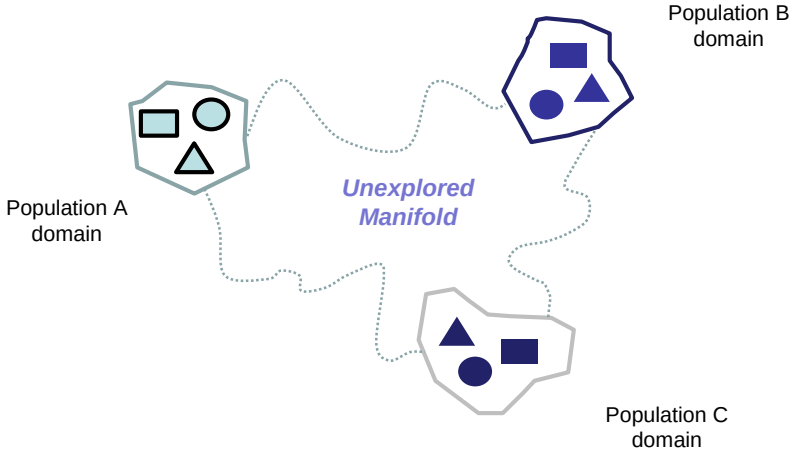
Doing more with less

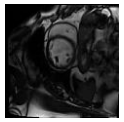
- Build systems that learn from few data, few annotations
  - Understand the world
  - Build intuition about the world



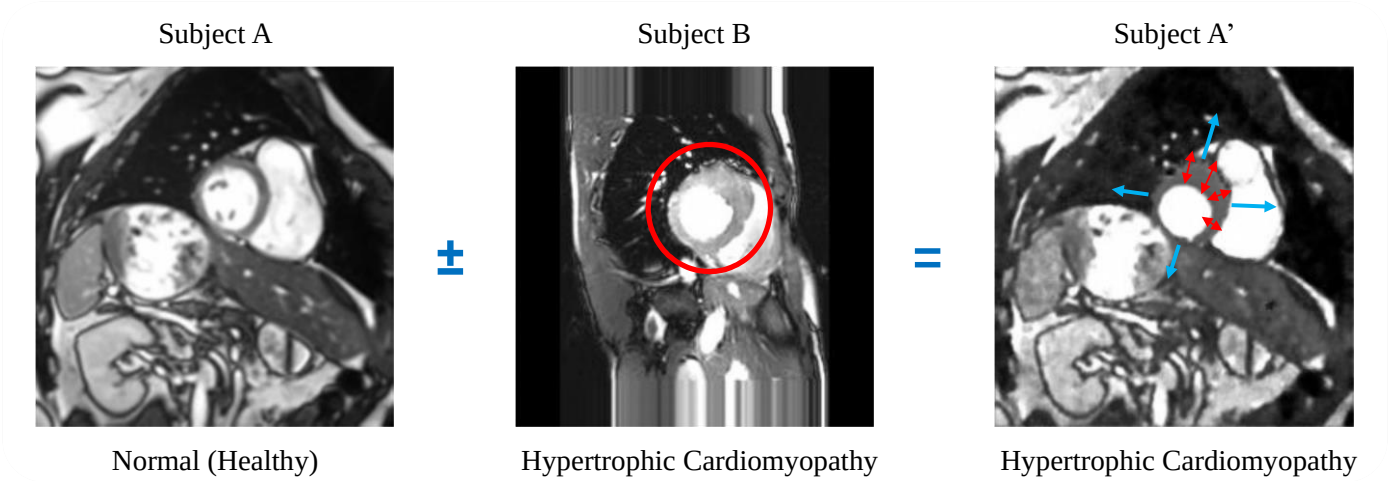
Chartsias, Joyce, Papanastasiou, Semple, Williams, Newby, Dharmakumar & Tsaftaris (2018 and 2019) Disentangled Representation Learning in Cardiac Image Analysis. Medical Image Analysis 2019 and MICCAI 2018 Code: https://github.com/agis85/anatomy_modality_decomposition

Generate high quality synthetic data





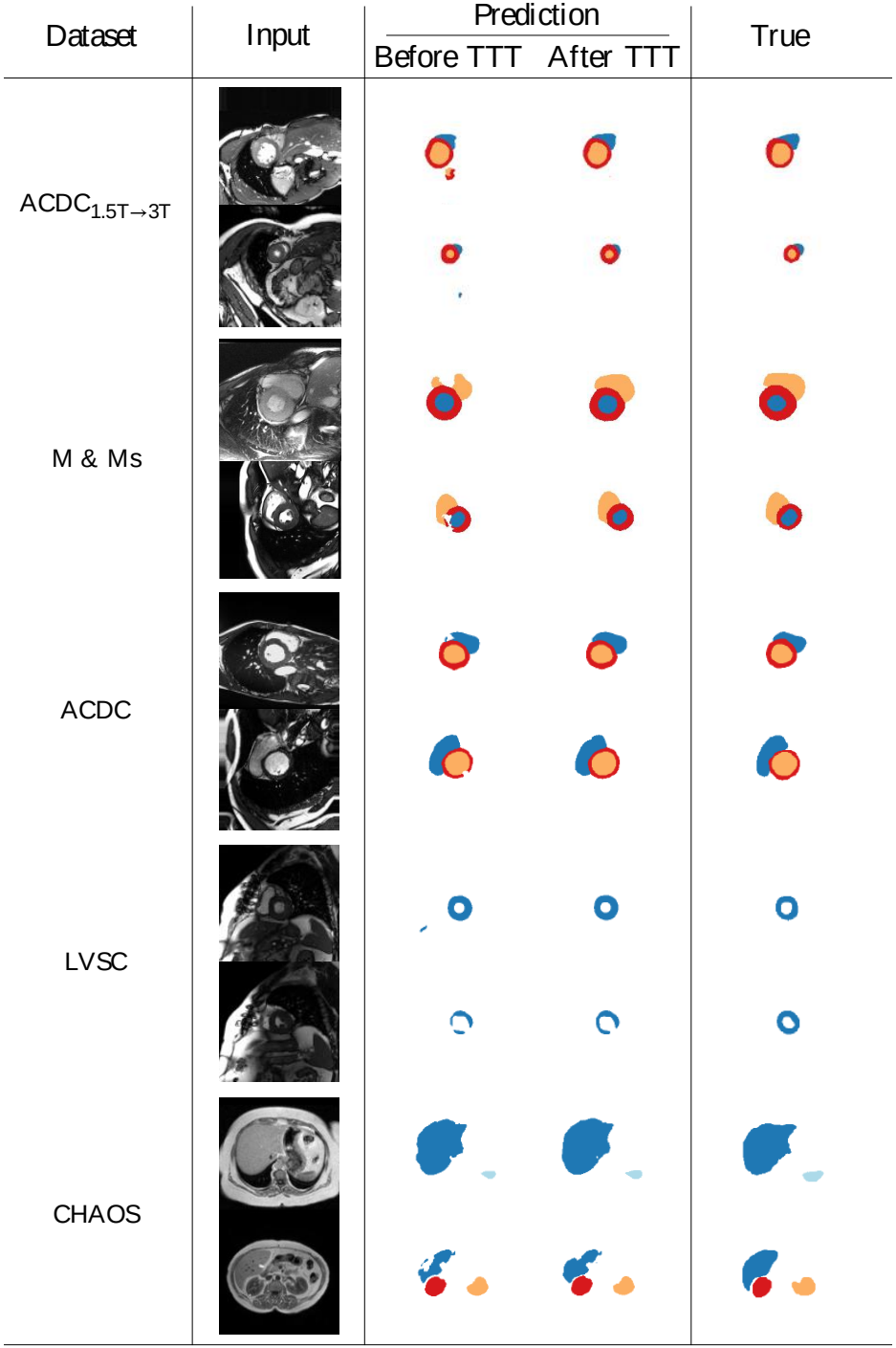
Create **high quality** synthetic images combining data



Thermos, Liu, O'Neil, & Tsaftaris (2021) Controllable cardiac synthesis via disentangled anatomy arithmetic. To appear MICCAI 2021

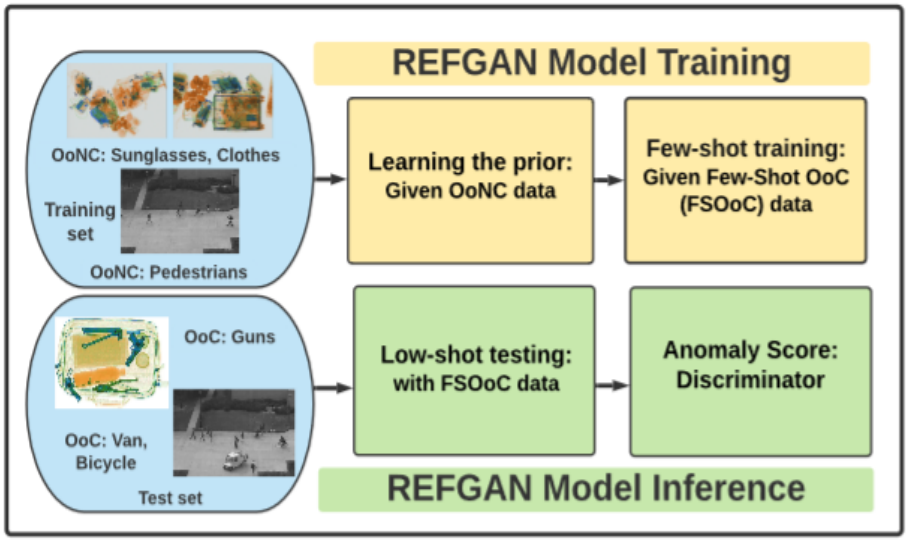
Test-time adaptation

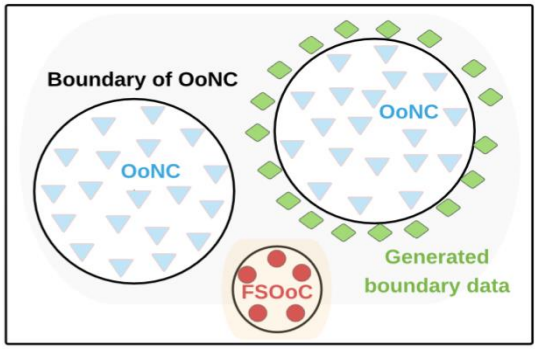
- Encoders, decoders, discriminators capture priors
- At test time we throw them away.
- Can we reuse them and adapt networks during testing?



G. Valvano, A. Leo and S. A. Tsaftaris, Stop Throwing Away Discriminators! Re-using Adversaries for Test-Time Training, Work in progress

Anomaly detection



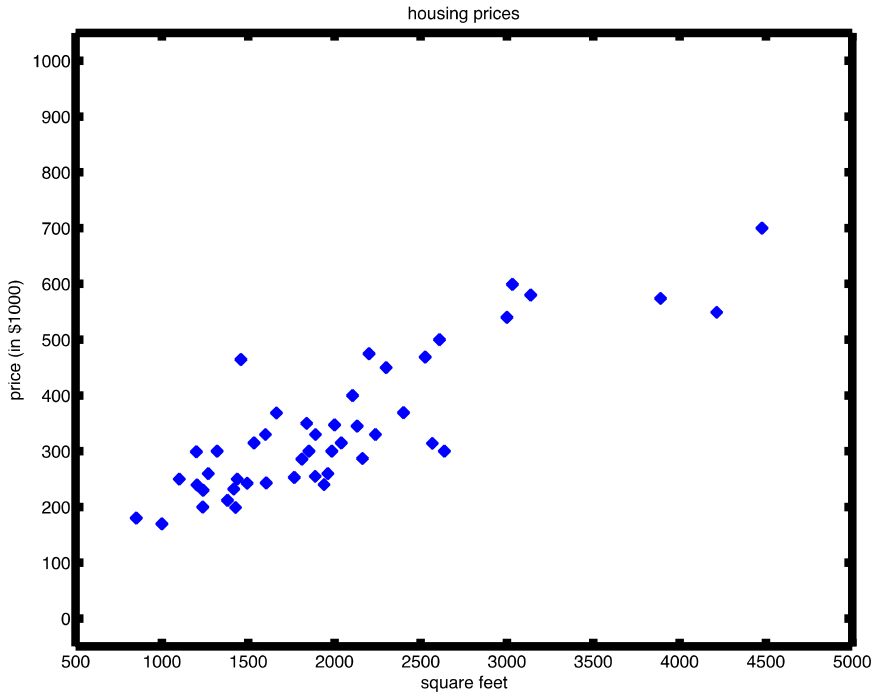


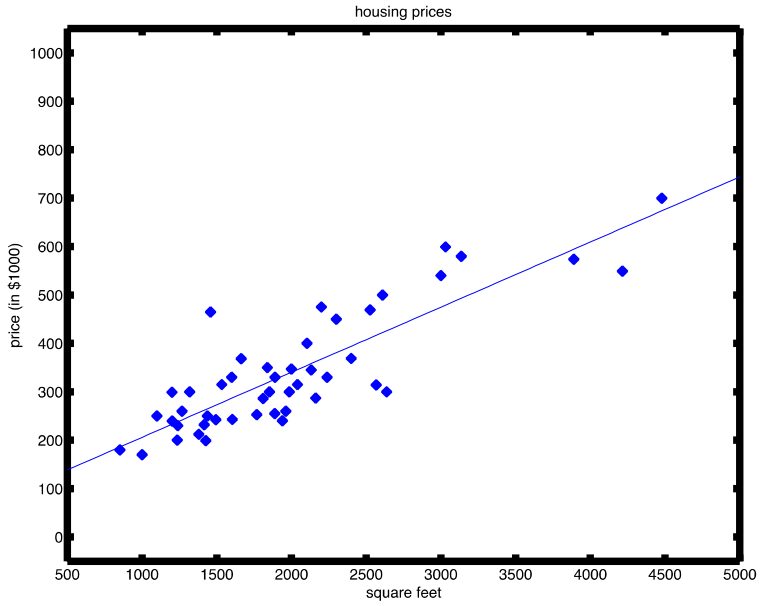
1. N. Dionelis, M. Yaghoobi, S. A. Tsaftaris, “Boundary of Distribution Support Generator (BDSG): Sample Generation on the Boundary,” *IEEE ICIP* 2020.
2. N. Dionelis, M. Yaghoobi, S. A. Tsaftaris, “Tail of Distribution GAN: GAN-Based Boundary of Distribution Formation,” *SSPD* 2020.
3. N. Dionelis, M. Yaghoobi, S. A. Tsaftaris, “Few-Shot Adaptive Detection of Objects of Concern Using Generative Models with Negative Retraining (REFGAN model)”, Work in Progress, 2021.

- The major directions of learning are:
  - **Supervised**: Patterns whose class is known a-priori are used for training.
  - **Unsupervised**: The number of classes/groups is (in general) unknown and no training patterns are available.
  - **Semisupervised:** A mixed type of patterns is available. For some of them, their corresponding class is known and for the rest is not.

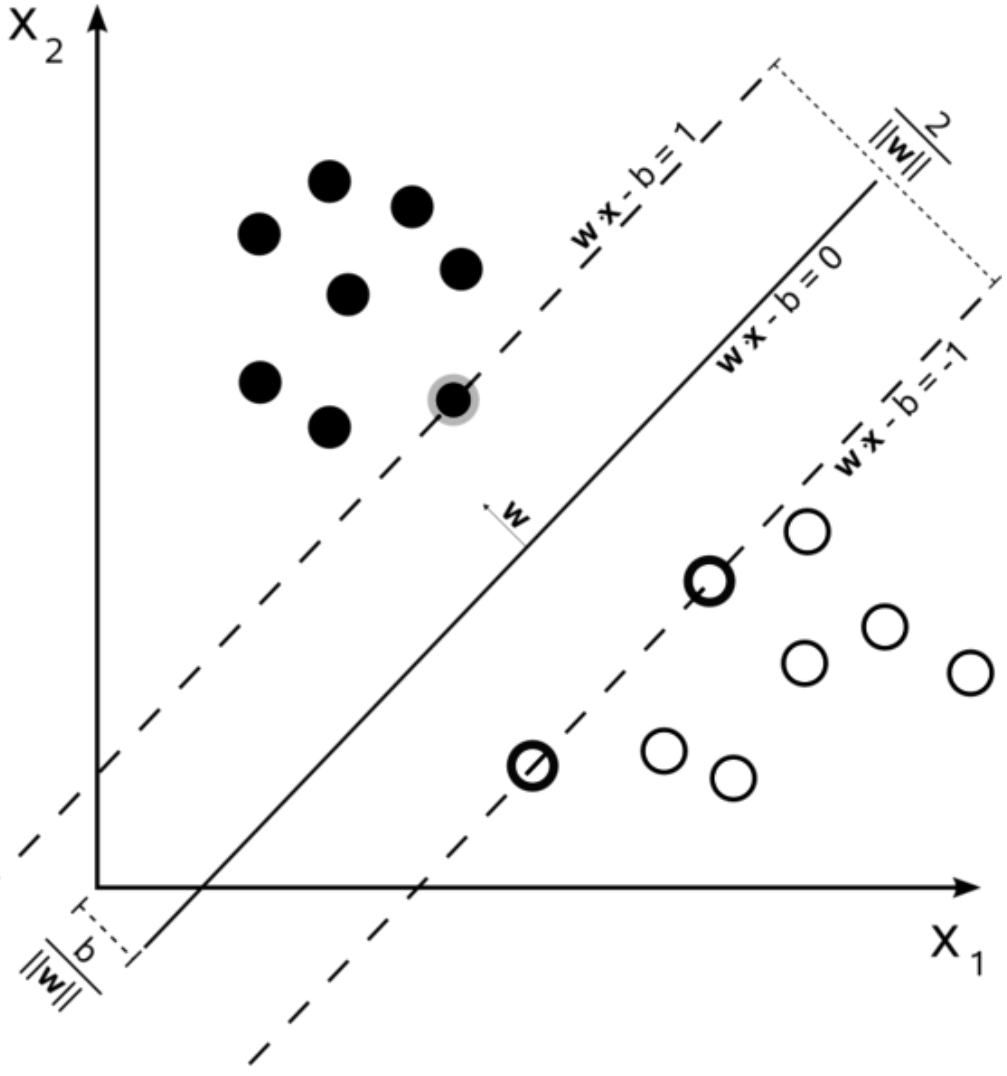
Supervised example

Living area (feet^2)	Price (1000$s)
2104	400
1600	330
2400	369
1416	232
3000	540
⋮	⋮



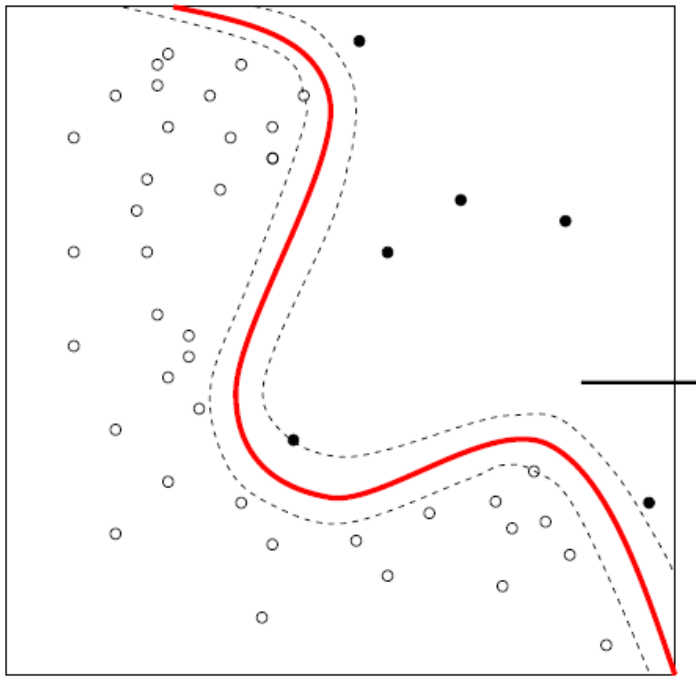


A classification example



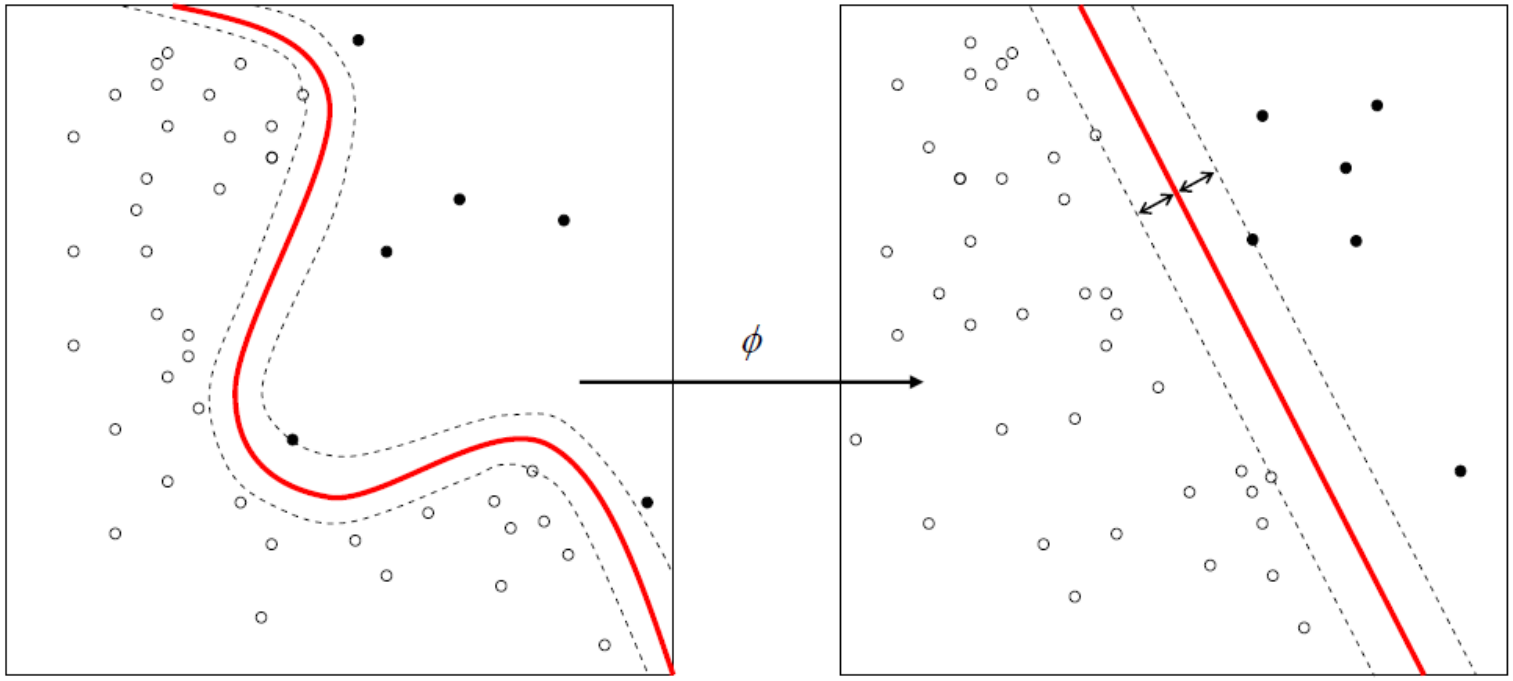
Goal find a “line” to separate the two classes

Hmm this looks harder

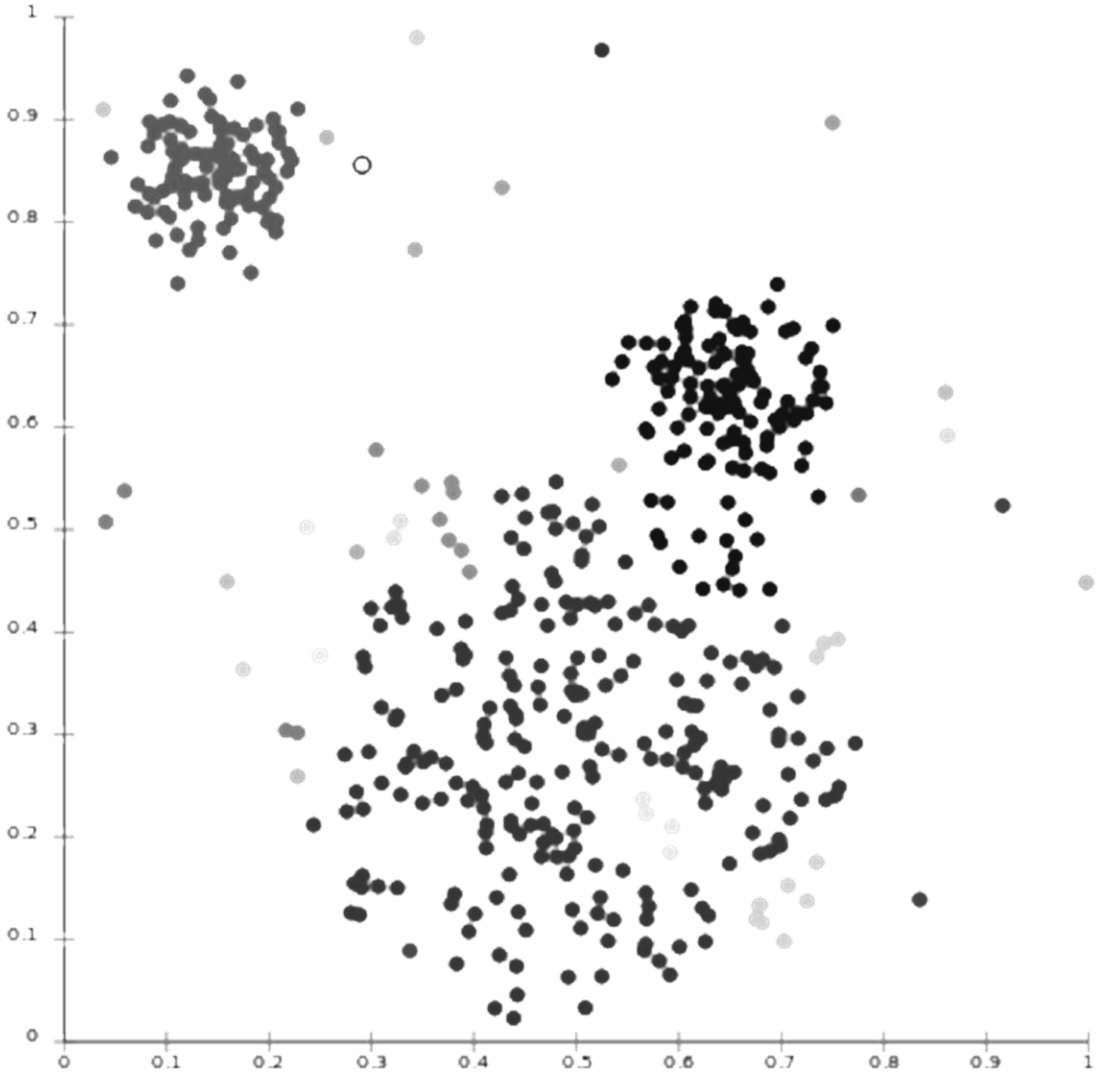


Looks like separating the data needs a more “complex” line

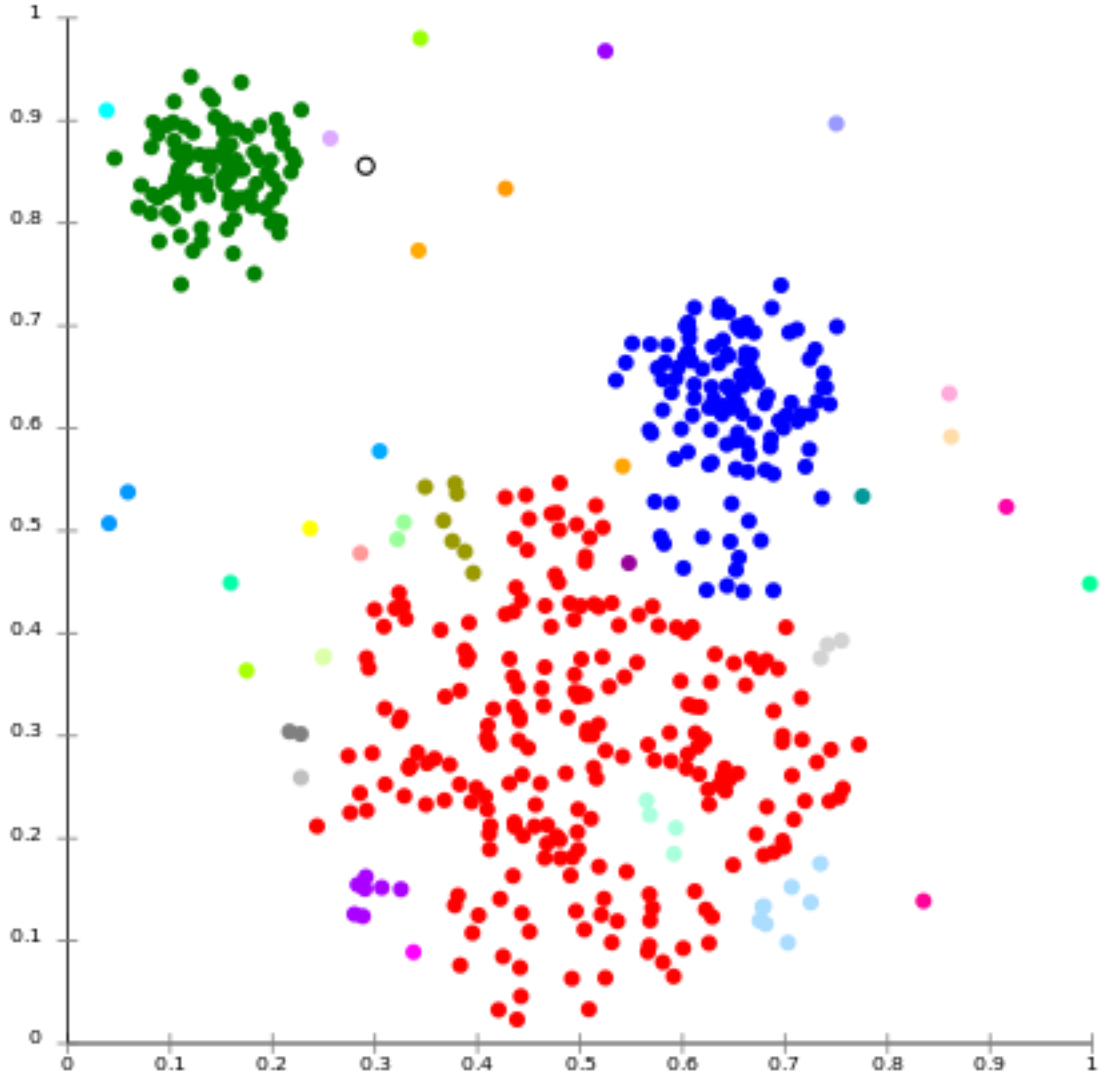
Hmm this looks harder



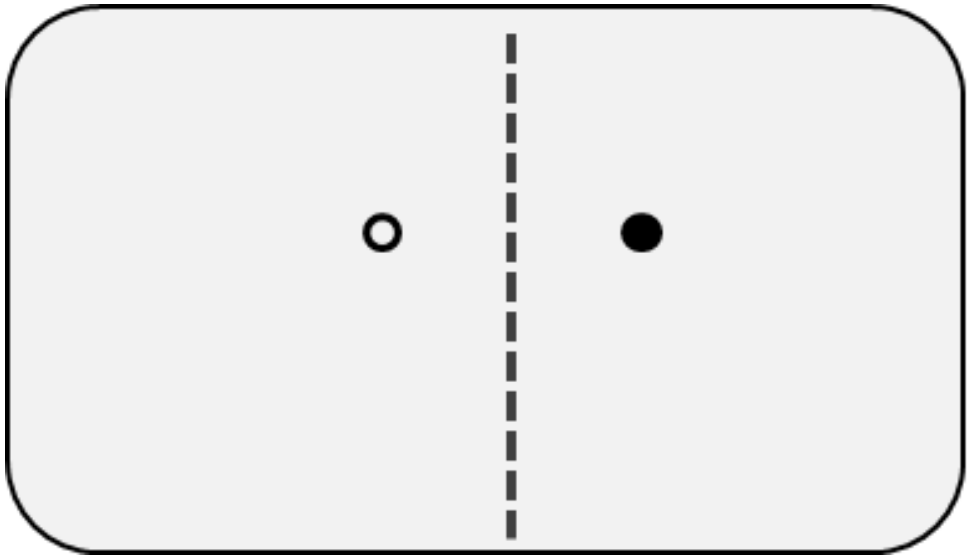
Unsupervised clustering



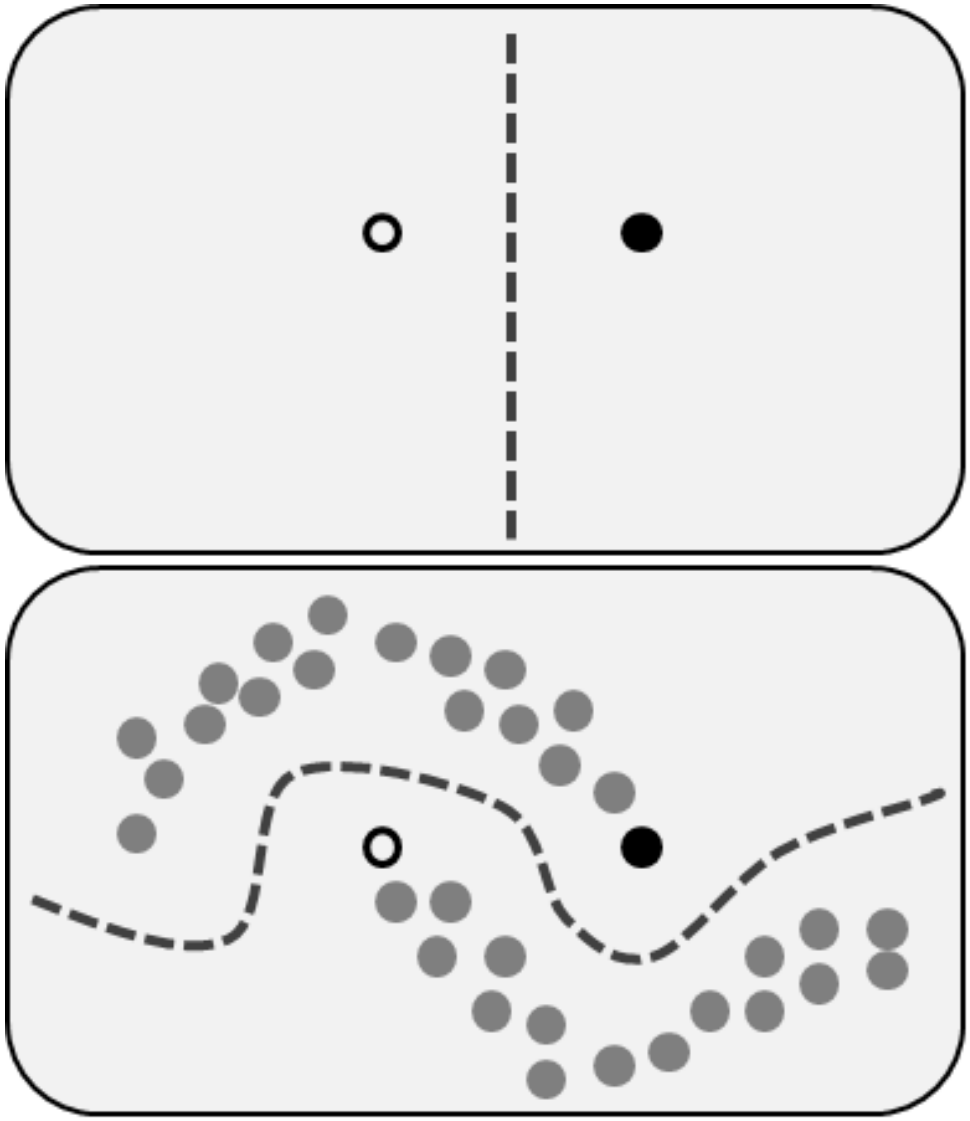
Unsupervised clustering



Semi-supervised learning



Semi-supervised learning



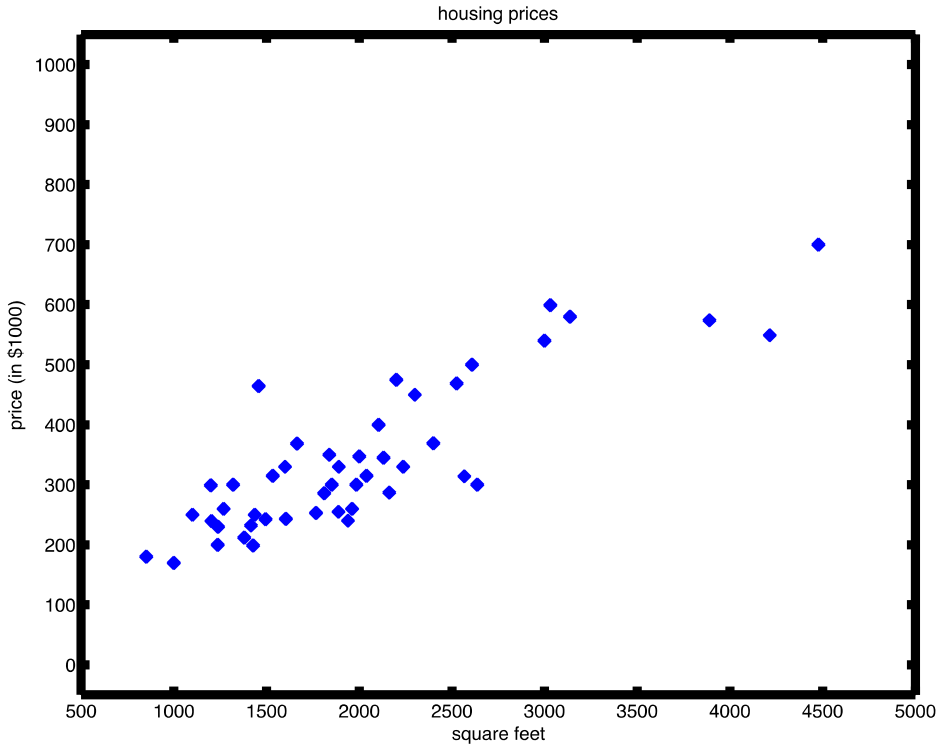
Topics that we will try to cover

- **Supervised** methods
  - Linear regression
  - Logistic regression
  - ~~Support vector machines (briefly)~~
  - Perceptron Classifier
- **Unsupervised** (and dimensionality reduction)
  - PCA, ~~kernel PCA~~
- **Learning theory** (simple view)
- Introduction; simple feed forward neural network architecture; how to train a neural network; backpropagation (briefly); ~~introduction to convolutional neural networks.~~

PART 1: INTRO TO ML

Supervised learning

Living area (feet^2)	Price (1000$s)
2104	400
1600	330
2400	369
1416	232
3000	540
⋮	⋮



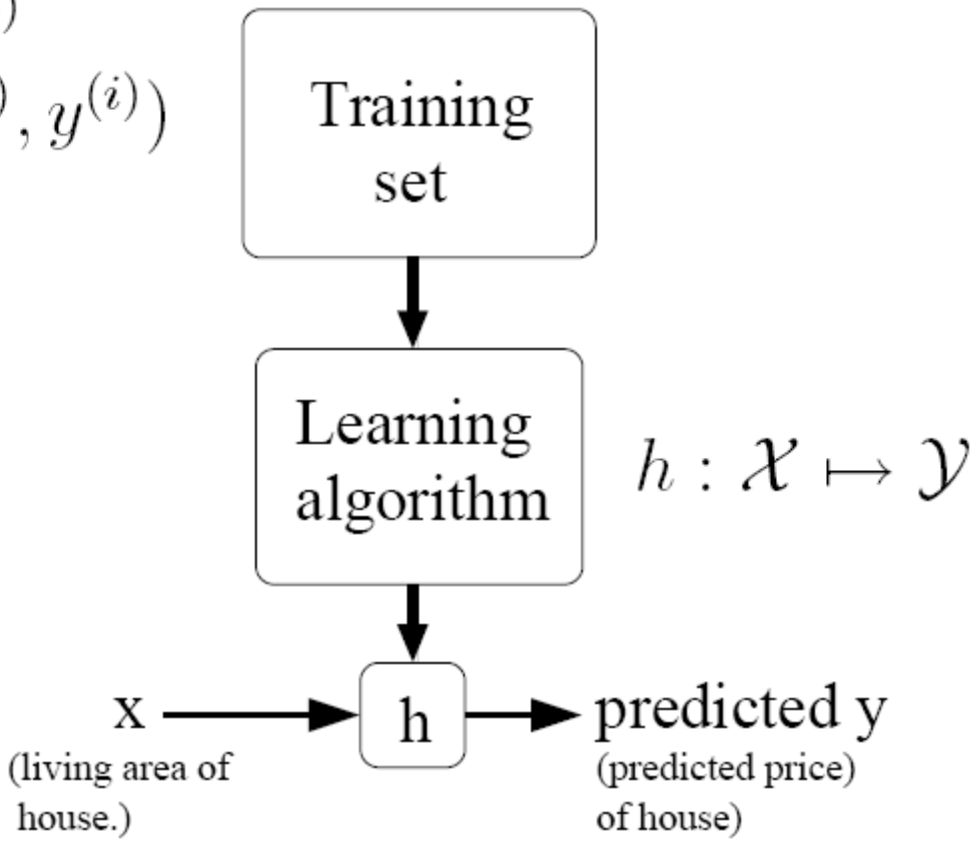
A typical formulation

- Input or features: $x^{(i)}$
- Output or target: $y^{(i)}$
- Training example: $(x^{(i)}, y^{(i)})$
- Training set==
  List of m examples:

$$\{(x^{(i)}, y^{(i)}); i = 1, \ldots, m\}$$

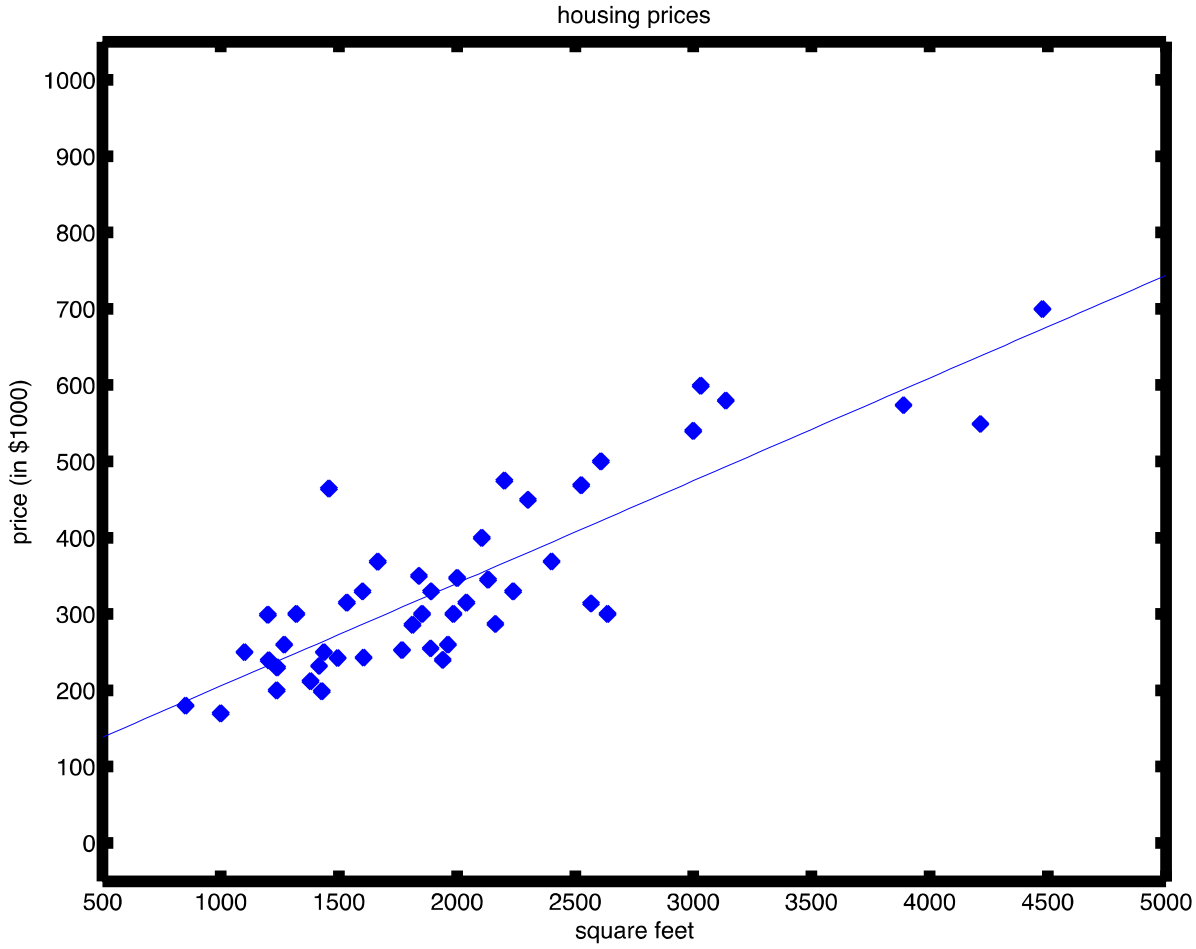
- Space:

$\mathcal{X}$ $\mathcal{Y}$



Living area (feet^2)	#bedrooms	Price (1000$s)
2104	3	400
1600	3	330
2400	3	369
1416	2	232
3000	4	540
$\vdots$	$\vdots$	$\vdots$

Linear fit



Objective function:
How do we find the solution to this problem?

We are given some data.
We are given a desired form of the line, but we want to find the *best* line.

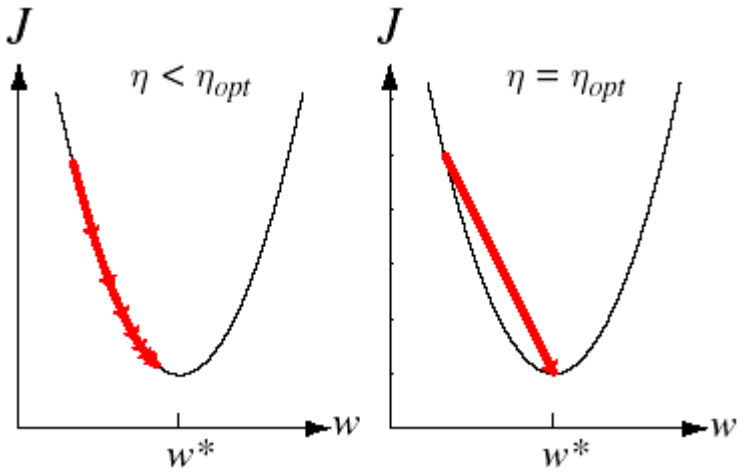
We need an objective function = training cost
=*measure of performance*
that we can **optimize**.

Optimization

Many ML techniques need *optimization*, e.g.

- Minimizing error in a neural network/adaptive system
- Maximizing probability in Bayesian inference

From simple “steepest descent” to more advanced techniques (Newton, conjugate gradient,…)



Solving the linear regression problem

- The LMS algorithm

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 \qquad h(x) = \sum_{i=0}^{n} \theta_i x_i = \theta^T x,$$

- Define a cost: $J(\theta) = \frac{1}{2} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2.$

- Optimise for the cost $\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta).$

$$\begin{aligned}
\frac{\partial}{\partial \theta_j} J(\theta) &= \frac{\partial}{\partial \theta_j} \frac{1}{2} (h_\theta(x) - y)^2 \\
&= 2 \cdot \frac{1}{2} (h_\theta(x) - y) \cdot \frac{\partial}{\partial \theta_j} (h_\theta(x) - y) \\
&= (h_\theta(x) - y) \cdot \frac{\partial}{\partial \theta_j} \left(\sum_{i=0}^{n} \theta_i x_i - y \right) \\
&= (h_\theta(x) - y)\, x_j
\end{aligned}$$

$$\theta_j := \theta_j + \alpha \left(y^{(i)} - h_\theta(x^{(i)}) \right) x_j^{(i)}$$

For a dataset of size 1

Batch vs stochastic

- Batch

Repeat until convergence {

$$\theta_j := \theta_j + \alpha \sum_{i=1}^{m} \left(y^{(i)} - h_\theta(x^{(i)})\right) x_j^{(i)} \qquad \text{(for every } j\text{)}$$

}

- Stochastic

Loop {

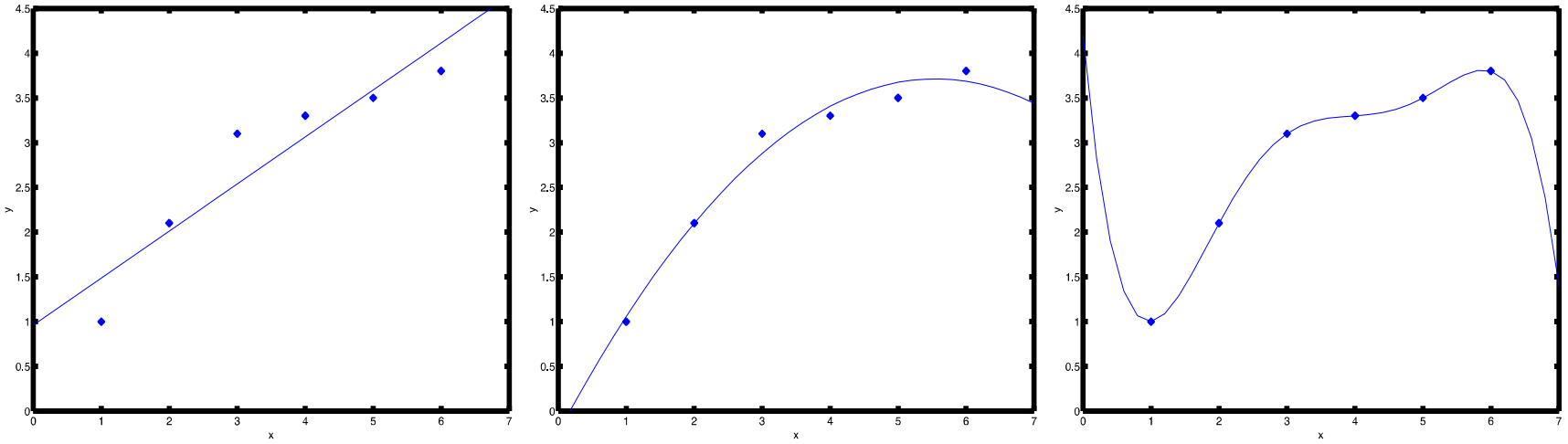
for i=1 to m, {

$$\theta_j := \theta_j + \alpha \left(y^{(i)} - h_\theta(x^{(i)})\right) x_j^{(i)} \qquad \text{(for every } j\text{)}$$

}

}

Higher model complexity



Model choice:
How do we tell what is the right choice?
Theoretical background: the bias variance dilemma
The practical solution: cross validation

Coming later…

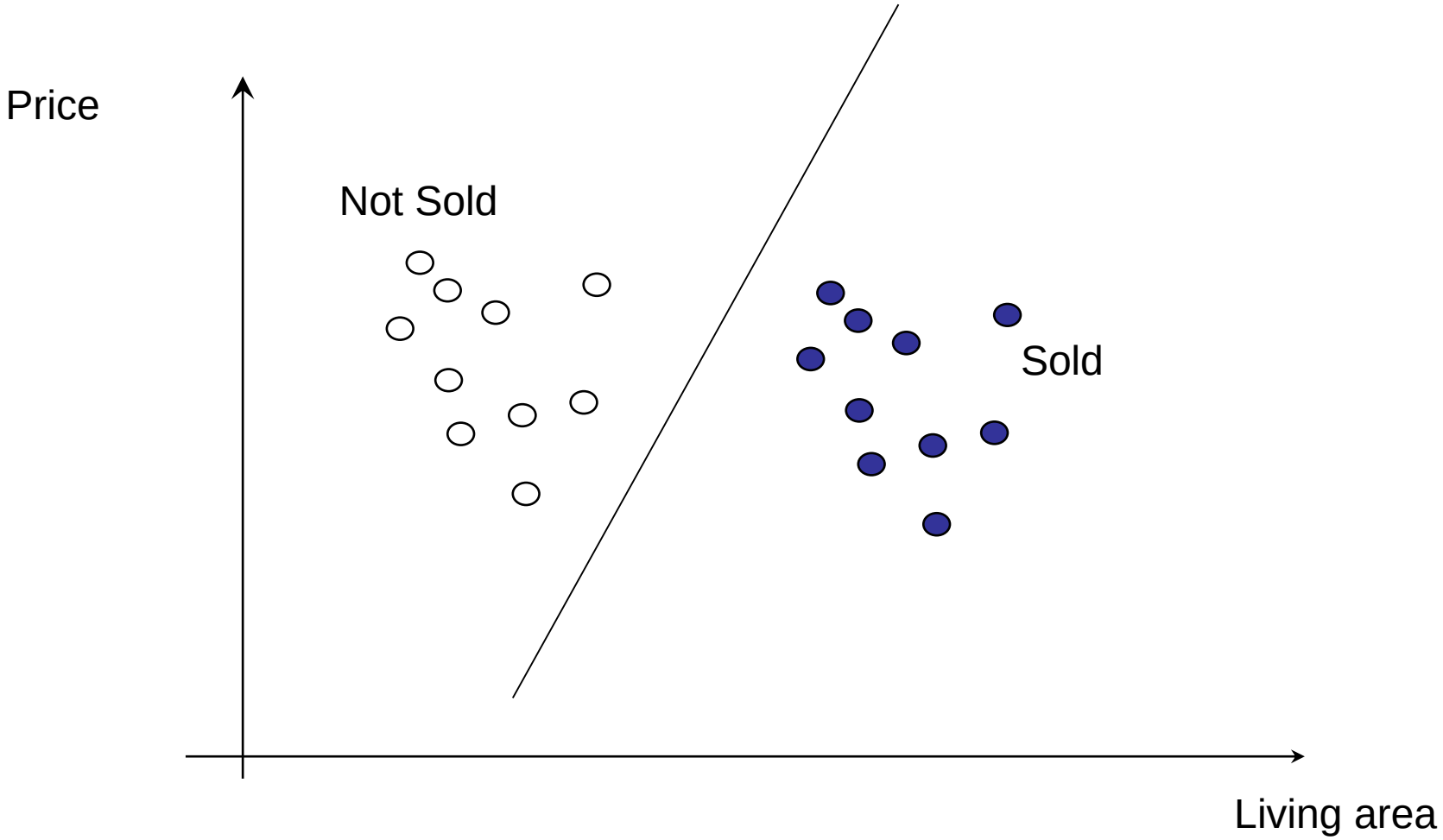
Logistic Regression

- Suppose now that we don't have a regression problem but classification
  - Decide whether a house will sell (1) or not (0)

Living area (feet^2)	#bedrooms	Price (1000$s)
2104	3	400
1600	3	330

- y, our output variable, is now a binary number
- We can encode this as:
  - 0 or 1
  - -1 , 1
  - Or anything else according to convenience (which will be obvious)

Visualizing a classification problem



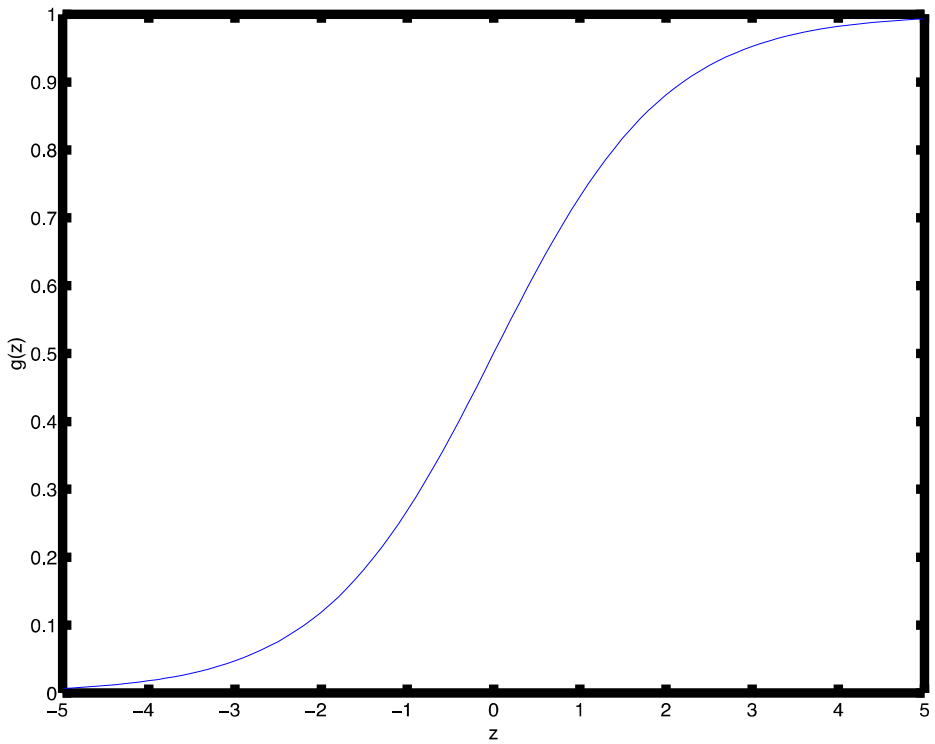
Logistic Regression

- Can we solve a binary classification problem 0 or 1 as linear regression?

$$h_\theta(x) = g(\theta^T x) = \frac{1}{1 + e^{-\theta^T x}},$$

- The logistic function (sigmoid function) ➔

$$g(z) = \frac{1}{1 + e^{-z}}$$



Self-learning

Why?

- It has some nice property

$$
\begin{aligned}
g'(z) &= \frac{d}{dz}\frac{1}{1+e^{-z}} \\
&= \frac{1}{(1+e^{-z})^2}(e^{-z}) \\
&= \frac{1}{(1+e^{-z})} \cdot \left(1 - \frac{1}{(1+e^{-z})}\right) \\
&= g(z)(1-g(z)).
\end{aligned}
$$

How to solve the problem (find the theta's)?

- A maximum likelihood view
- Assume

$$P(y = 1 \mid x; \theta) = h_\theta(x)$$
$$P(y = 0 \mid x; \theta) = 1 - h_\theta(x)$$

- Or…

$$p(y \mid x; \theta) = (h_\theta(x))^y \, (1 - h_\theta(x))^{1-y}$$

- Assuming the training examples were generated independently

$$\begin{aligned} L(\theta) &= p(\vec{y} \mid X; \theta) \\ &= \prod_{i=1}^{m} p(y^{(i)} \mid x^{(i)}; \theta) \\ &= \prod_{i=1}^{m} \left(h_\theta(x^{(i)})\right)^{y^{(i)}} \left(1 - h_\theta(x^{(i)})\right)^{1-y^{(i)}} \end{aligned}$$

Objective function

$$\begin{aligned} \ell(\theta) &= \log L(\theta) \\ &= \sum_{i=1}^{m} y^{(i)} \log h(x^{(i)}) + (1 - y^{(i)}) \log(1 - h(x^{(i)})) \end{aligned}$$

Contd…

- Lets use gradient ascent $\theta := \theta + \alpha \nabla_\theta \ell(\theta)$

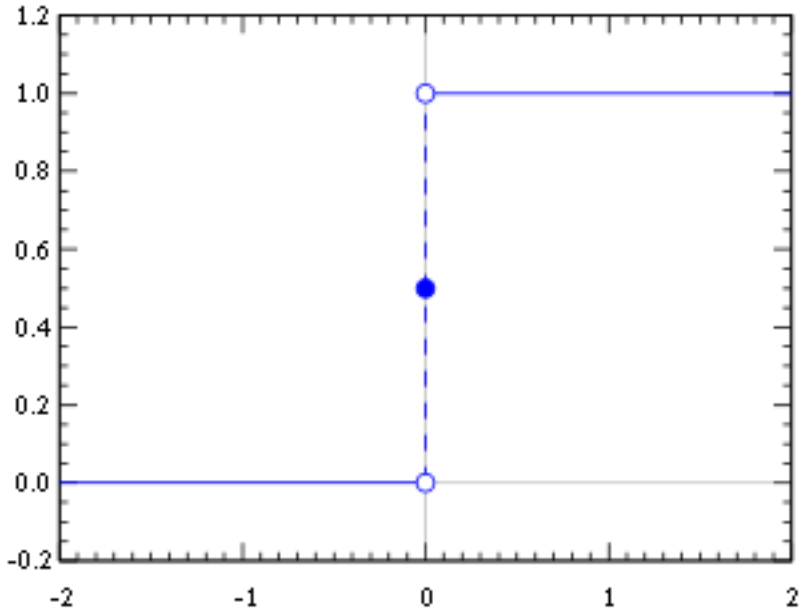
$$
\begin{aligned}
\frac{\partial}{\partial \theta_j} \ell(\theta) &= \left(y \frac{1}{g(\theta^T x)} - (1-y) \frac{1}{1 - g(\theta^T x)} \right) \frac{\partial}{\partial \theta_j} g(\theta^T x) \\
&= \left(y \frac{1}{g(\theta^T x)} - (1-y) \frac{1}{1 - g(\theta^T x)} \right) g(\theta^T x)(1 - g(\theta^T x) \frac{\partial}{\partial \theta_j} \theta^T x \\
&= \left(y(1 - g(\theta^T x)) - (1-y) g(\theta^T x) \right) x_j \\
&= \left(y - h_\theta(x) \right) x_j
\end{aligned}
$$

$$\theta_j := \theta_j + \alpha \left(y^{(i)} - h_\theta(x^{(i)}) \right) x_j^{(i)}$$

PART 2: INTRO TO PERCEPTRONS

What if we take an extreme sigmoidal

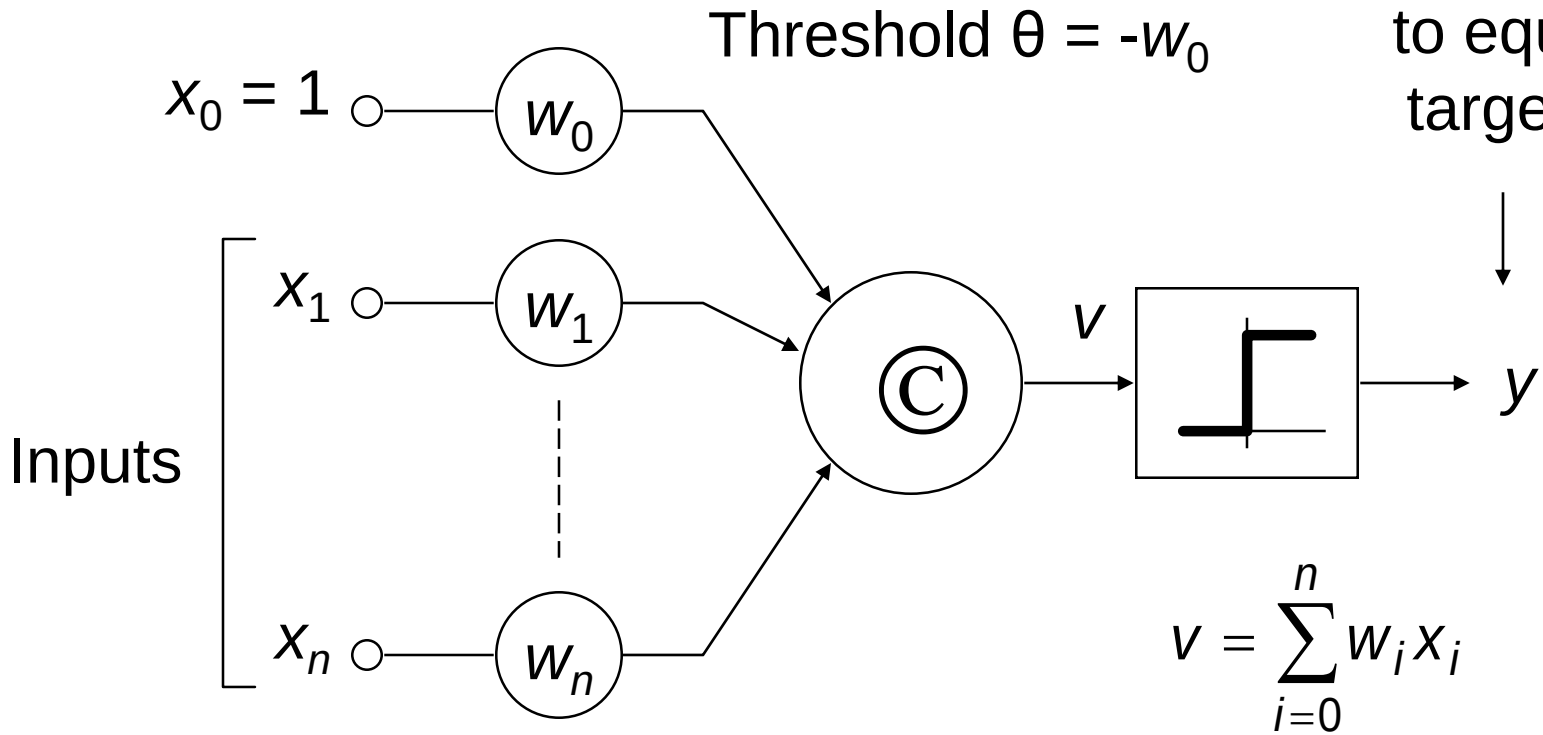
$$g(z) = \begin{cases} 1 & \text{if } z \geq 0 \\ 0 & \text{if } z < 0 \end{cases}$$



The Perceptron: A Simple Learning Neuron

Rosenblatt (1958)

We want output y to equal target t



$$v = \sum_{i=0}^{n} w_i x_i$$

$$y = f(v)$$

Inputs may be from {-1, +1} or {0, +1}

Perceptron Learning Algorithm

One example of a learning algorithm (presents samples one at a time)

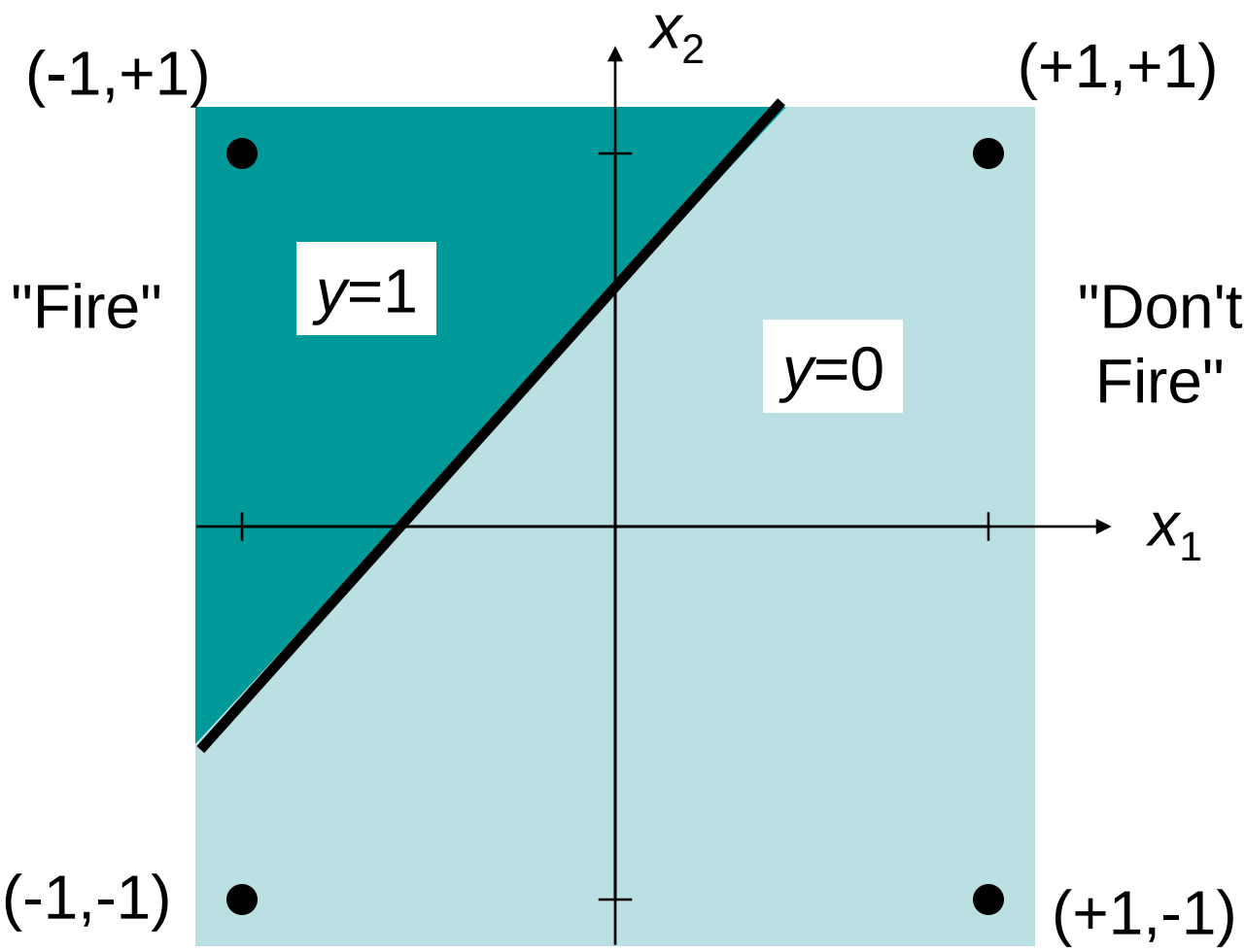
For all input vectors in training set:

1) Present input vector x
2) Calculate y=1 if $w^T x \geq 0$, y=0 if $w^T x < 0$
3) Compare y with target output t
   a) If t=1 but y=0, set new w = old w + ηx [punish]
   b) If t=0 but y=1, set new w = old w − ηx [punish]
   c) Otherwise (If y=t), do nothing [reward]

Repeat until correct for all input vectors.

Factor η is called the *learning rate*

Decision Boundary Example



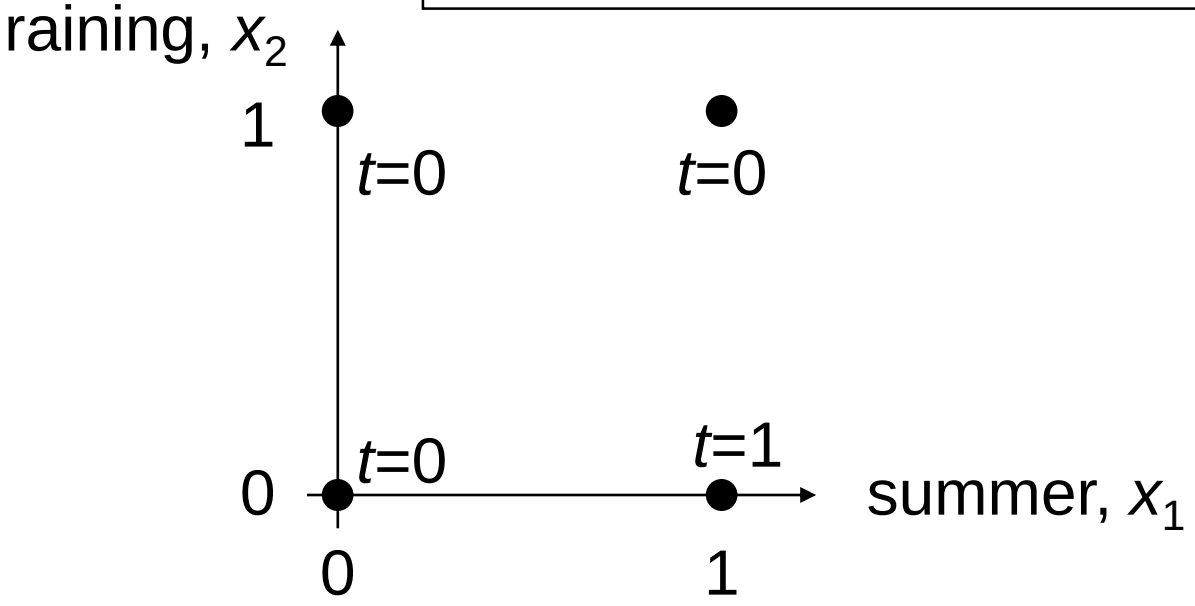
Self-learning

Simple Example

"If summer and not raining, play tennis"

Training set.
Specifies target *t*
for different inputs

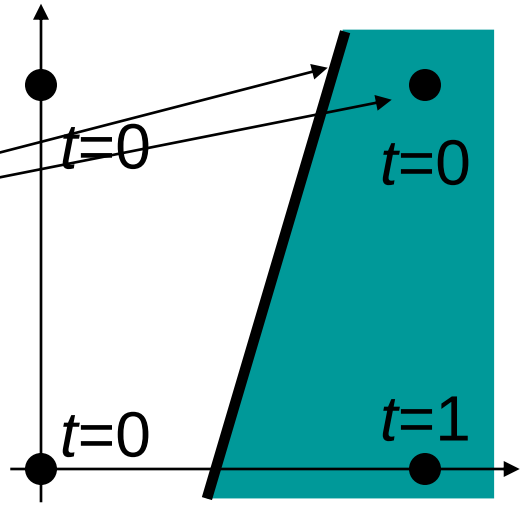
(threshold, x_0	1	1	1	1)
summer, x_1	0	0	1	1
raining, x_2	0	1	0	1
play tennis, t	0	0	1	0



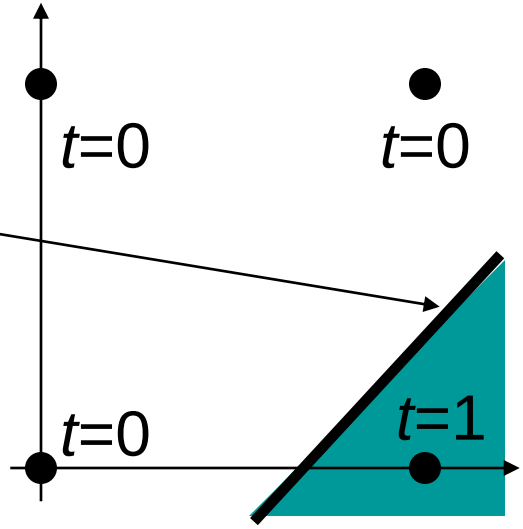
Self-learning

Simple Example (cont)

Suppose initially
$\mathbf{w} = (w_0, w_1, w_2) = (-0.5, +2.5, -1.5)$
Try input $\mathbf{x} = (1,1,1)$:
$\mathbf{w}^T\mathbf{x} = -0.5+2.5-1.5>0$
so y=1: Wrong



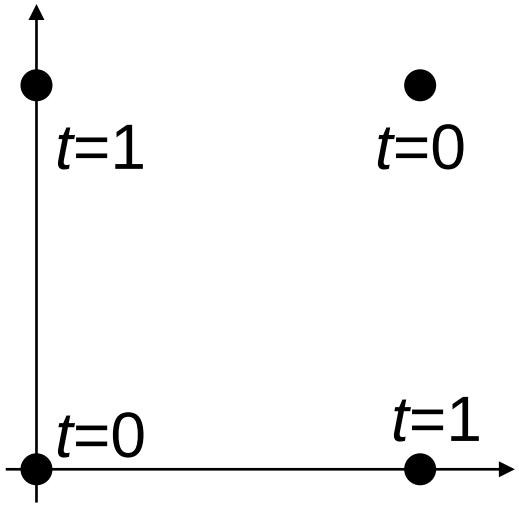
Using η=0.5,
subtract η**x** from **w** to give us
w = (-1.0, +2.0, -2.0)



Perceptron decision boundary is now correct for all inputs.

Perceptron Limitations

- Problem must be *linearly separable*
- Classic non-linearly separable problem: *XOR problem*



- Minsky & Pappert (1969) - conjectured this limitation would *not* be overcome.
- But it was…

From linear discriminants to more complex decision surfaces

Linear Discriminant Functions

Suppose we wished to decide whether some data

$$\mathbf{x} = (x_1, x_2, \ldots, x_d)$$

belonged to one of two categories

One way to do this is to construct a *Discriminant function.* Let g(**x**) define the categories as:

$$\omega(\mathbf{x}) = \begin{cases} \omega_1, g(\mathbf{x}) > 0 \\ \omega_2, g(\mathbf{x}) \leq 0 \end{cases}$$

If g(x) is linear we can write:

$$g(\mathbf{x}) = \mathbf{w}^t\mathbf{x} + w_0 = \sum_{i=1}^{d} w_i x_i + w_0$$

where **w** = {w_1, … , w_d} are called the weights and w_0 is called the bias or threshold weight.

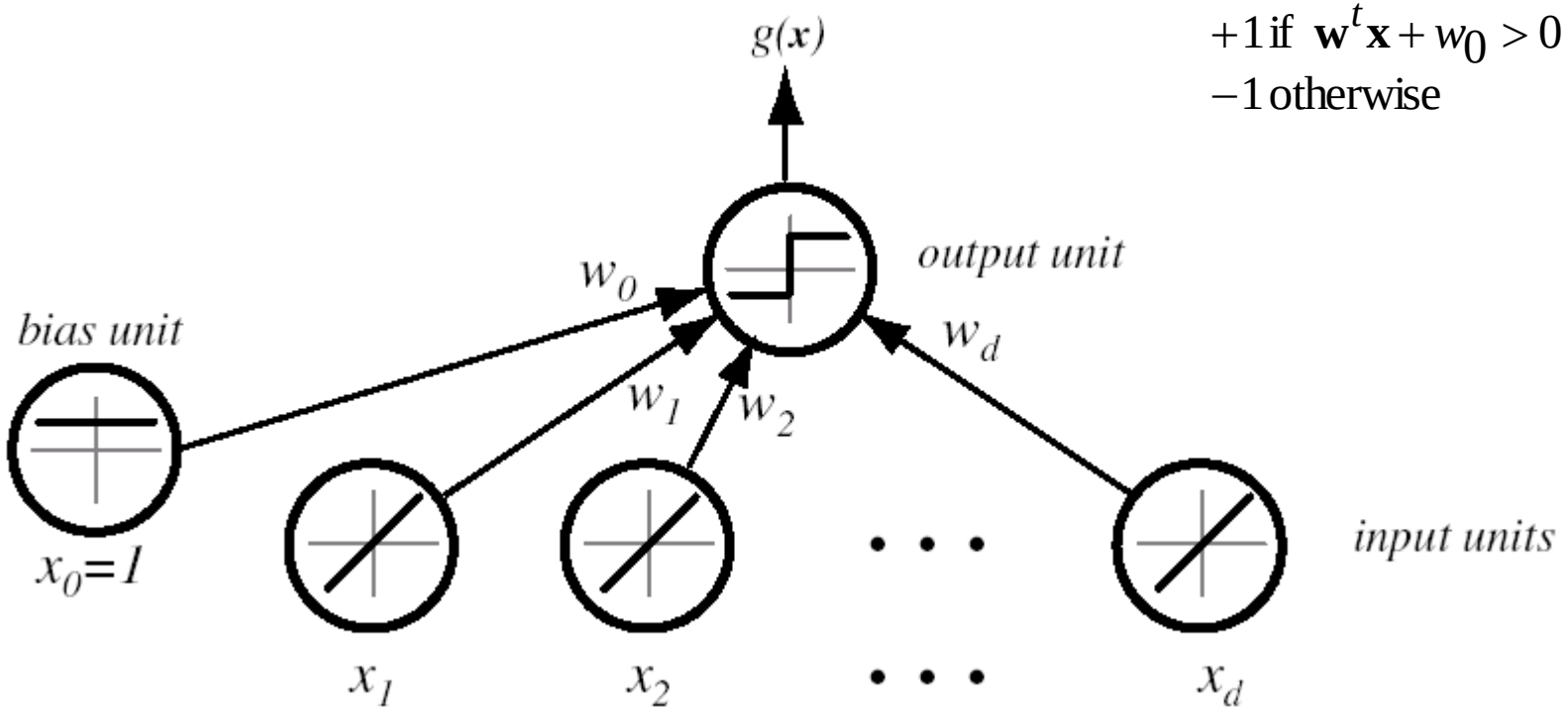
See ch 5.2 Linear Discriminant Functions
Duda Hart

Simple Linear Classifier

Output emits

$+1$ if $\mathbf{w}^t\mathbf{x} + w_0 > 0$

-1 otherwise



Each unit shows its effective input-output function.

Decision surface

g(**x**) = 0 defines a *decision surface* which separates points into ω_1 and ω_2. If g(**x**) is linear, this decision surface is a *hyperplane*.

The hyperplane divides the space into two regions:

R_1 : g(**x**) > 0, hence **x** is in ω_1 and

R_2 : g(**x**) ≤ 0, hence **x** is in ω_2

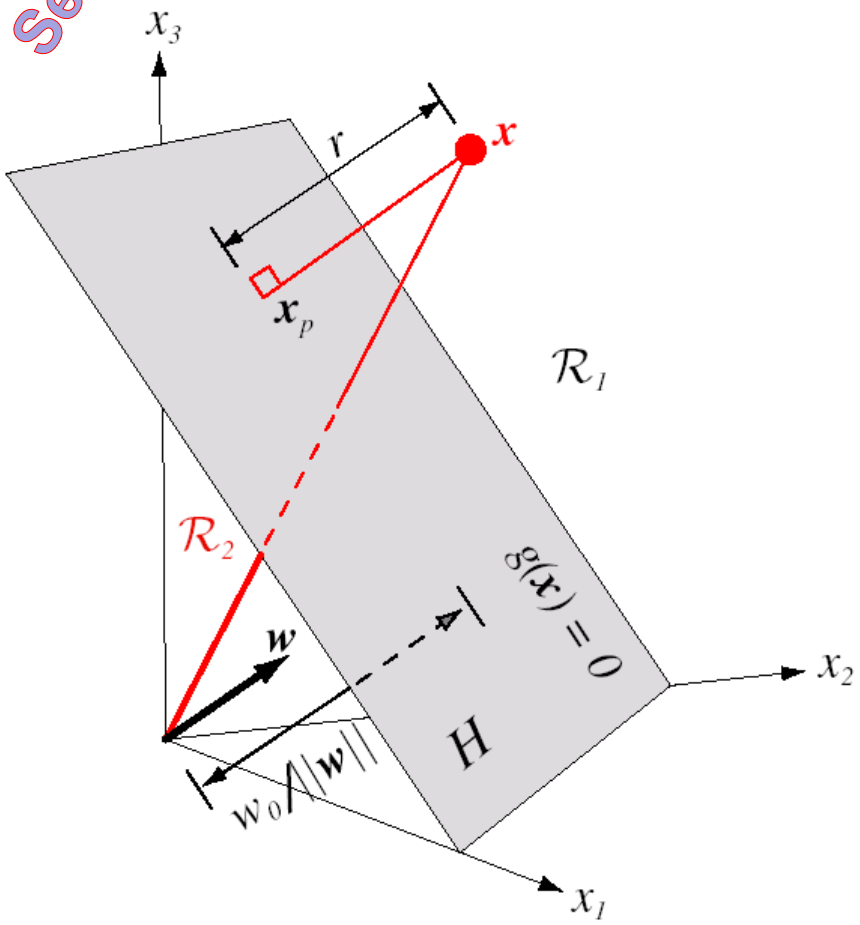
Suppose x_1 and x_2 are both on the decision surface. Then:

$$\mathbf{w}^t\mathbf{x}_1 + w_0 = \mathbf{w}^t\mathbf{x}_2 + w_0 \qquad \text{i.e.} \qquad \mathbf{w}^t(\mathbf{x}_1 - \mathbf{x}_2) = 0.$$

Therefore **w** is normal (orthogonal) to the hyperplane.

Self-learning

Hyperplane decision surface



Let us write

$$\mathbf{x} = \mathbf{x}_p + r\frac{\mathbf{w}}{\|\mathbf{w}\|}$$

where $\mathbf{x}_p$ is normal projection

of $\mathbf{x} \rightarrow H$ and r is distance from H

($r > 0$ on $+$ ve side, $r < 0$ on -ve)

Since $g(\mathbf{x}_p) = 0$,

$$g(\mathbf{x}) = \mathbf{w}^t\mathbf{x} + w_0 = \mathbf{w}^t(\mathbf{x}_p + r\frac{\mathbf{w}}{\|\mathbf{w}\|}) + w_0 =$$

$$= \ldots = r\|\mathbf{w}\|$$

$$\Rightarrow\ r = g(\mathbf{x})/\|\mathbf{w}\|$$

$g(\mathbf{x})$ measures dist from $\mathbf{x}$ to H.

Self-learning

Generalized Linear Discriminants

We can generalize g(**x**) by adding terms $x_i x_j$ to give a quadratic (nonlinear) discriminant function:

$$g(\mathbf{x}) = w_0 + \sum_{i=1}^{d} w_i x_i + \sum_{i=1}^{d}\sum_{j=1}^{d} w_{ij} x_i x_j$$

Can generalize to cubic, etc.

We can view this as a linear discriminant function in a **new space**.

Let $y_i(\mathbf{x})$ define a new variable as a (nonlinear) function of **x**.

$$g(\mathbf{x}) = \sum_{i=1}^{\hat{d}} a_i y_i(\mathbf{x})$$

Note we have absorbed the bias weight in this formulation - A process called *augmentation*.

See ch 5.3 Generalized Linear Discriminant Functions
Duda Hart

Quadratic discriminant: 1-d example

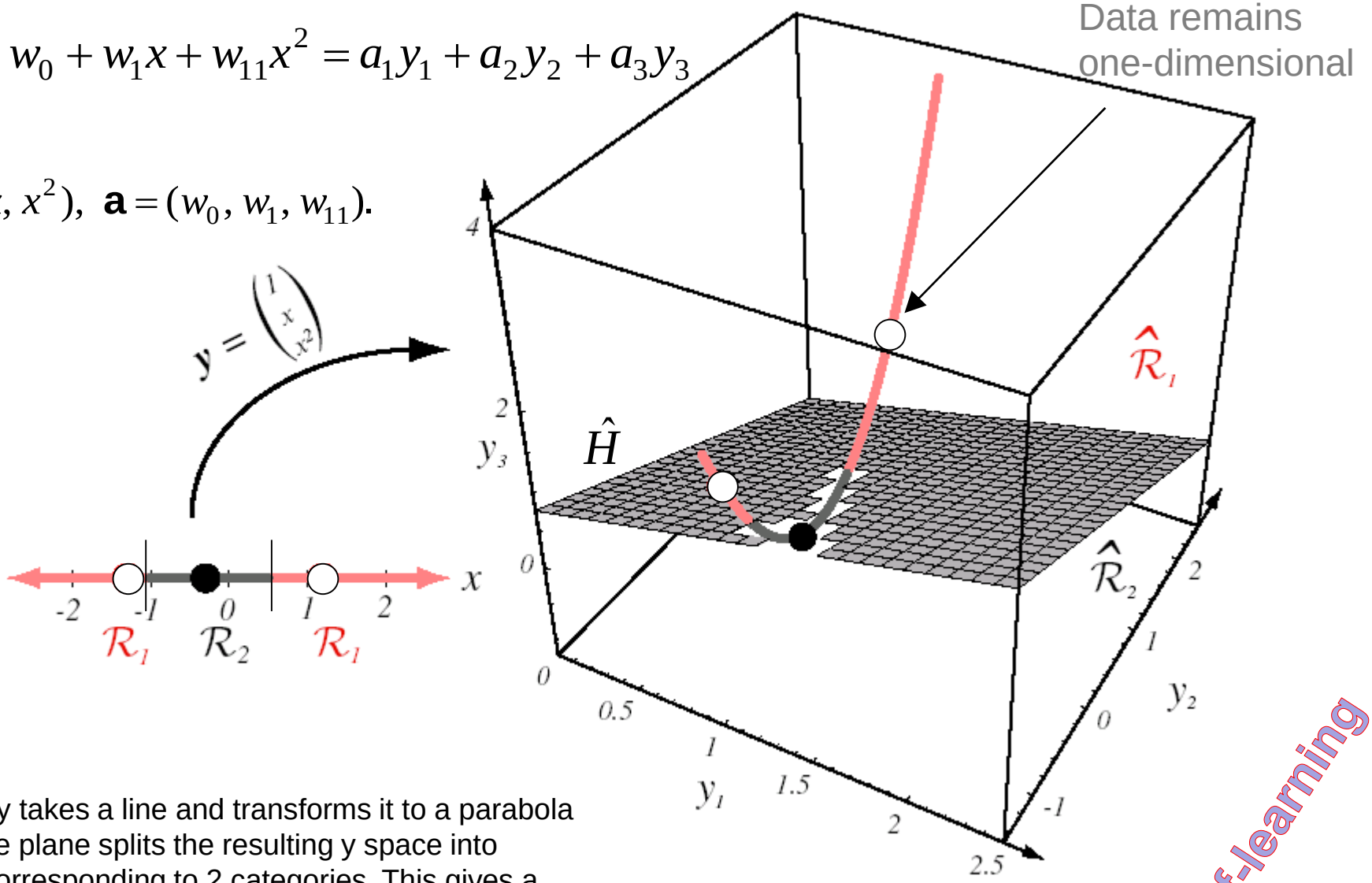
e.g.

$$g(\mathbf{x}) = w_0 + w_1 x + w_{11} x^2 = a_1 y_1 + a_2 y_2 + a_3 y_3$$

with

$$\mathbf{y} = (1, x, x^2), \quad \mathbf{a} = (w_0, w_1, w_{11}).$$

Data remains one-dimensional



Mapping y takes a line and transforms it to a parabola in 3D. The plane splits the resulting y space into regions corresponding to 2 categories. This gives a non-simply connected decision region in the 1D x space. Decision in y is **convex**, but not in x.

Self-learning

Linearly Separable Case (2 category)

Suppose we have n samples $y_1,\ldots y_n$, each labelled either ω_1 or ω_2 and we wish to *learn* a discriminant function $g(\mathbf{y}) = \mathbf{a}^T\mathbf{y}$, that correctly classifies the data.

Sample $\mathbf{y}_i$ is correctly classified if

$$\mathbf{a}^T\mathbf{y}_i > 0 \text{ when } \mathbf{y}_i \text{ is labelled } \omega_1$$

or

$$\mathbf{a}^T\mathbf{y}_i < 0 \text{ when } \mathbf{y}_i \text{ is labelled } \omega_2$$

A data set is called *linearly separable* if there exists a vector a which correctly classifies all samples. This is called a *separating vector* or *solution vector.*

[The case of $g(\mathbf{y}) = \mathbf{a}^T\mathbf{y}+a_0$ with augmentation: $\mathbf{y}' \equiv [\mathbf{y},1]^T, \mathbf{a}' \equiv [\mathbf{a}, a_0]^T$]

See Ch 5.4 The Two-Category Linearly-Separable Case Duda Hart

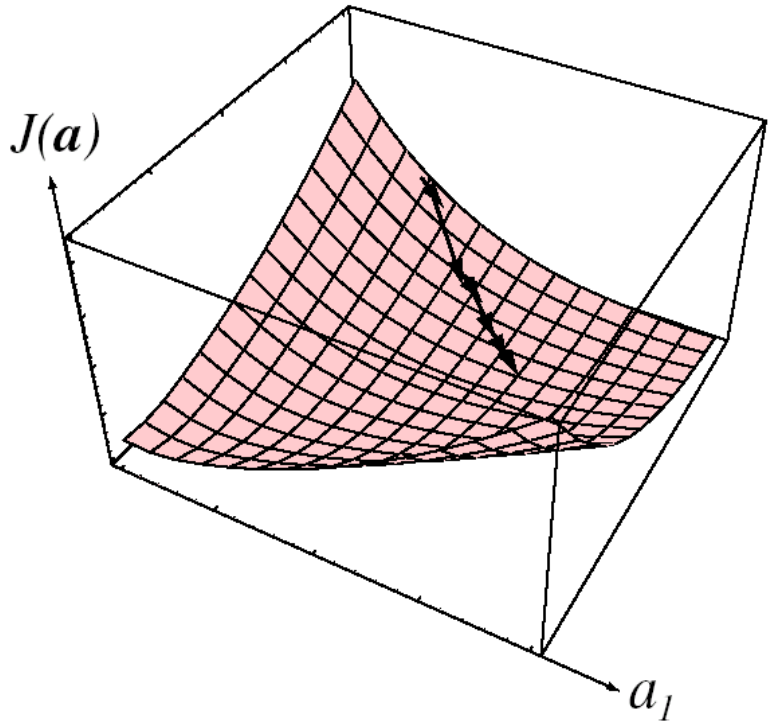
How to find **a**

- Great now we have understood what the **a** must satisfy (linear inequalities) and some properties.
- **However, we still do not know how to find a**
- We are given some data and their labels and we need a procedure to find a
- We need to find a criterion that when optimized we have a solution vector **a**.
  - Lets call this criterion **J(a)**. Observe it is a scalar function of **a : returns a value** pending on **a**
  - If we make good choices of J() we can use **optimization** theory. [We will talk about this a lot later in the class.]
  - Learning a classifier is then reduced to an optimization problem
  - We will consider for now a simple approach: Gradient Descent

Gradient Descent

Simple concept: Consider I am at some point in my function $\mathbf{J(a_k)}$. I need to move to a new point $\mathbf{a_{k+1}}$. **What is a good point?**

Gradient: Gradient points in the direction of the greatest rate of increase of the function. (Generalization of derivative in multivariate functions)

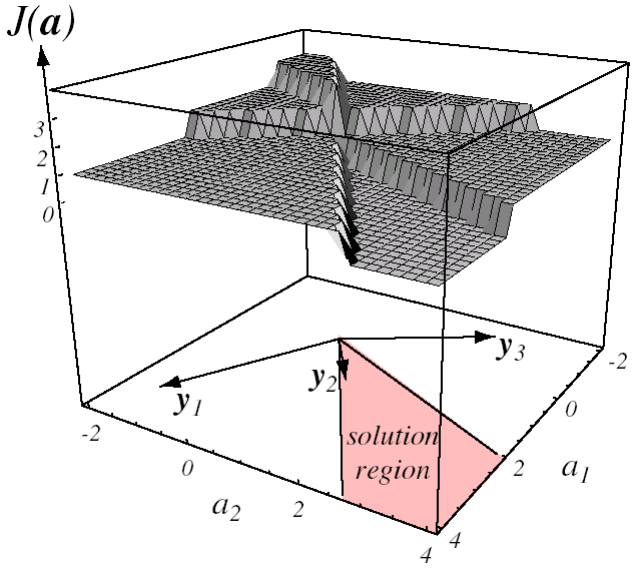


Update : $\mathbf{a}(k+1) = \mathbf{a}(k) - \eta(k)\nabla J(\mathbf{a}(k))$
Learning rate $\eta(k)$
Gradient vector $\nabla J(\cdot)$

Basic gradient descent algorithm :
1. Initialize $k \leftarrow 0, \mathbf{a}(1), \theta, \eta(.)$
2. $k \leftarrow k+1$
3. $\mathbf{a} \leftarrow \mathbf{a} - \eta(k)\nabla J(\mathbf{a})$
4. If $|\eta(k)\nabla J(\mathbf{a})| > \theta$, repeat from 2.

Perceptron Revisited

Could J = number of samples misclassified?
No – the function is piecewise constant.
Why is this bad? The cost function has 0 gradient at most points and wherever non-zero has discontinuities. We need a better cost.



The Perceptron

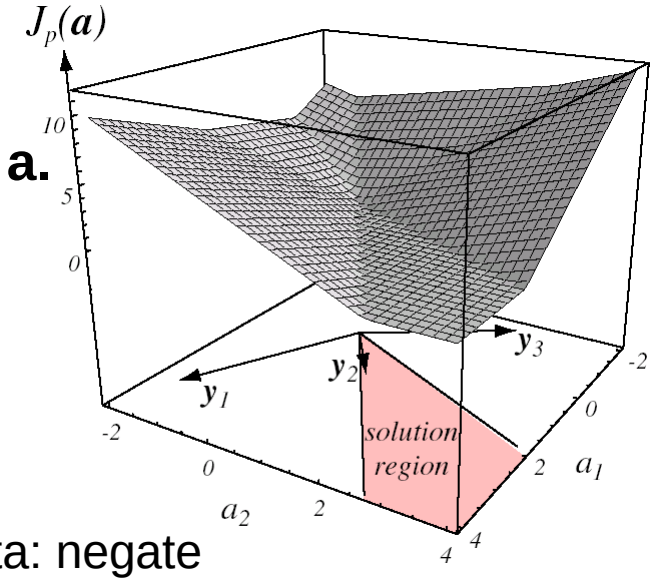
$$J_p(\mathbf{a}) = \sum_{\mathbf{y} \in Y_m} (-\mathbf{a}^T \mathbf{y})$$

warning: Data are assumed normalized

where Y_m is the set of samples misclassified by **a.**

When is $J_p(a)=0$?

Is $J_p(a)$ always positive?



In the 2-category problem it is possible to *normalize* the data: negate all $\mathbf{y}_i$ labelled as ω_2. Then we require: $\mathbf{a}^T \mathbf{y}_i > 0$ for all samples.

Perceptron Algorithm

$$[\nabla J_p(\mathbf{a})]_i = \partial J_p(\mathbf{a})/\partial a_i = \sum_{\mathbf{y}\in Y_m}(-y_i)$$

warning: Data are assumed normalized

i.e. $\nabla J_p(\mathbf{a}) = \sum_{\mathbf{y}\in Y_m}(-\mathbf{y})$ so gradient descent rule is:

$$\mathbf{a}(k+1) = \mathbf{a}(k) - \eta(k)\sum_{\mathbf{y}\in Y_m}(-\mathbf{y})$$

where Y_m is set of samples misclassified by $\mathbf{a}(k)$.

Batch Perceptron Algorithm

1. Initialize $\mathbf{a}, \eta(\cdot)$, stopping criterion $\theta, k \leftarrow 0$
2. $k \leftarrow k+1$
3. $\mathbf{a} \leftarrow \mathbf{a} + \eta(k)\sum_{\mathbf{y}\in Y_m}\mathbf{y}$
4. If $|\eta(k)\sum_{\mathbf{y}\in Y_m}\mathbf{y}| > \theta$, repeat from 2.

η(k) is the learning rate or step size

PART 3: INTRO TO NEURAL NETS

Multilayer Neural Networks

Linear discriminants are good for many problems but not **general** enough for demanding applications.

We can get more complex decision surfaces with nonlinear pre-processing,

$$y_i = \varphi_i(\mathbf{x})$$

Where $\varphi_i(.)$, is, for example, a polynomial expansion to some order k.

But **too many free** parameters, so we may not have enough data points to fix them. ➔ *learn* which nonlinearities to use.

The best-known method is based on gradient descent: the so-called *backpropagation* algorithm.

Three-Layer Network

Network has:

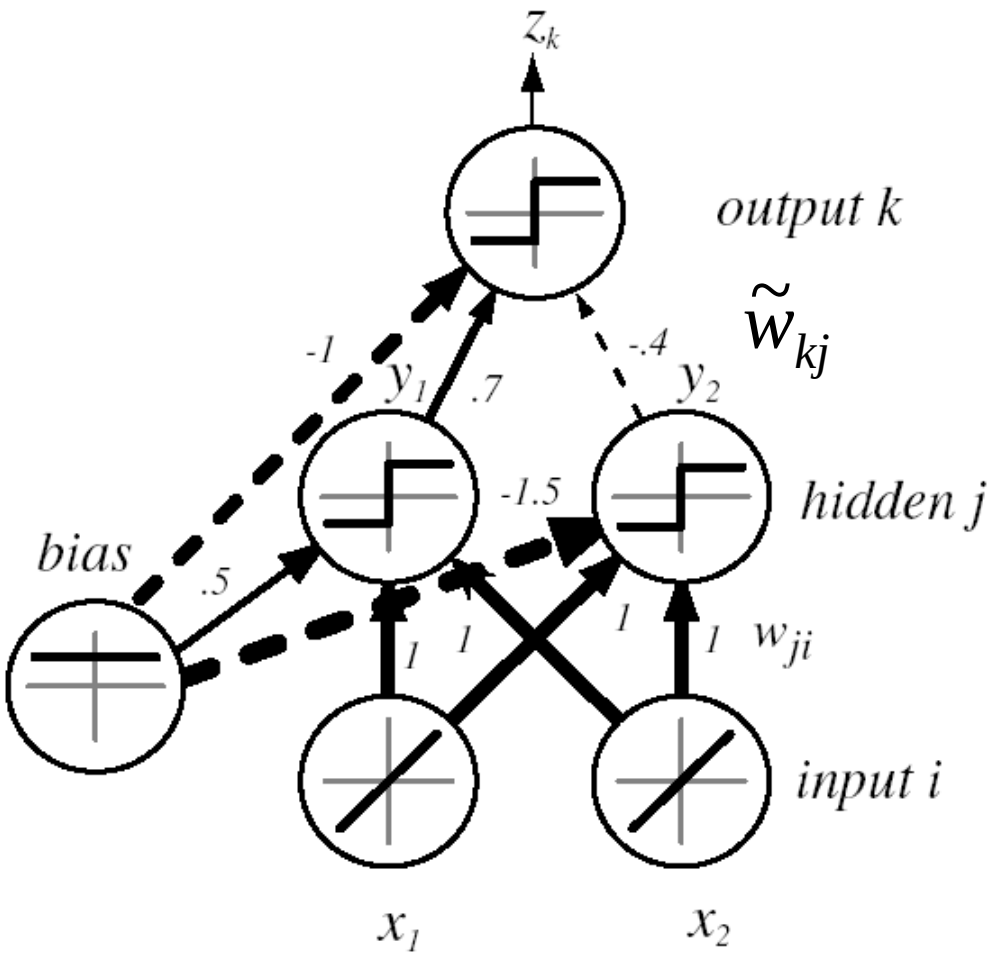
- Input layer
- Hidden layer
- Output layer

with adjustable weights between layers

Also:

- Bias unit

with weights to all hidden and output units.



Biological terms sometimes used:
“neuron” = unit; “synapses” = connection; “synaptic weight” = weight.

Operation

Step 1: each d-dimensional input vector $(x_1, \ldots, x_d)$ is presented to input layer of the network and augmented with a bias term $x_0 = 1$ to give $x = (x_0, x_1, \ldots, x_d)$

'old school' term for input vector was input pattern.

Step 2: at each hidden layer we calculate the weighted sum of inputs to give the net activation:

$$net_j = \sum_{i=1}^{d} x_i w_{ji} + w_{j0} = \sum_{i=0}^{d} x_i w_{ji} = \mathbf{w}_j^T \mathbf{x}$$

where w_{ji} is the weight from the input unit i to the hidden unit j

Step 3: The hidden unit emits the output: $y_j = f\left(net_j\right)$ where $f(.)$ is some nonlinear activation function

Operation (cont)

Step 4: At each output unit we calculate the weighted sum of the hidden layer units it is connected to giving:

$$n\tilde{e}t_k = \sum_{j=1}^{n_H} y_j \tilde{w}_{kj} + \tilde{w}_{k0} = \sum_{j=0}^{n_H} y_j \tilde{w}_{kj} = \tilde{\mathbf{w}}_k^T \mathbf{y}$$

where $\tilde{w}_{kj}$ is the weight from the hidden unit j to the output unit k

Step 5: each output unit emits $z_k = f\left(n\tilde{e}t_k\right)$
where $f(.)$ is again the nonlinear activation function.

We can therefore think of the network as calculating c discriminant functions:

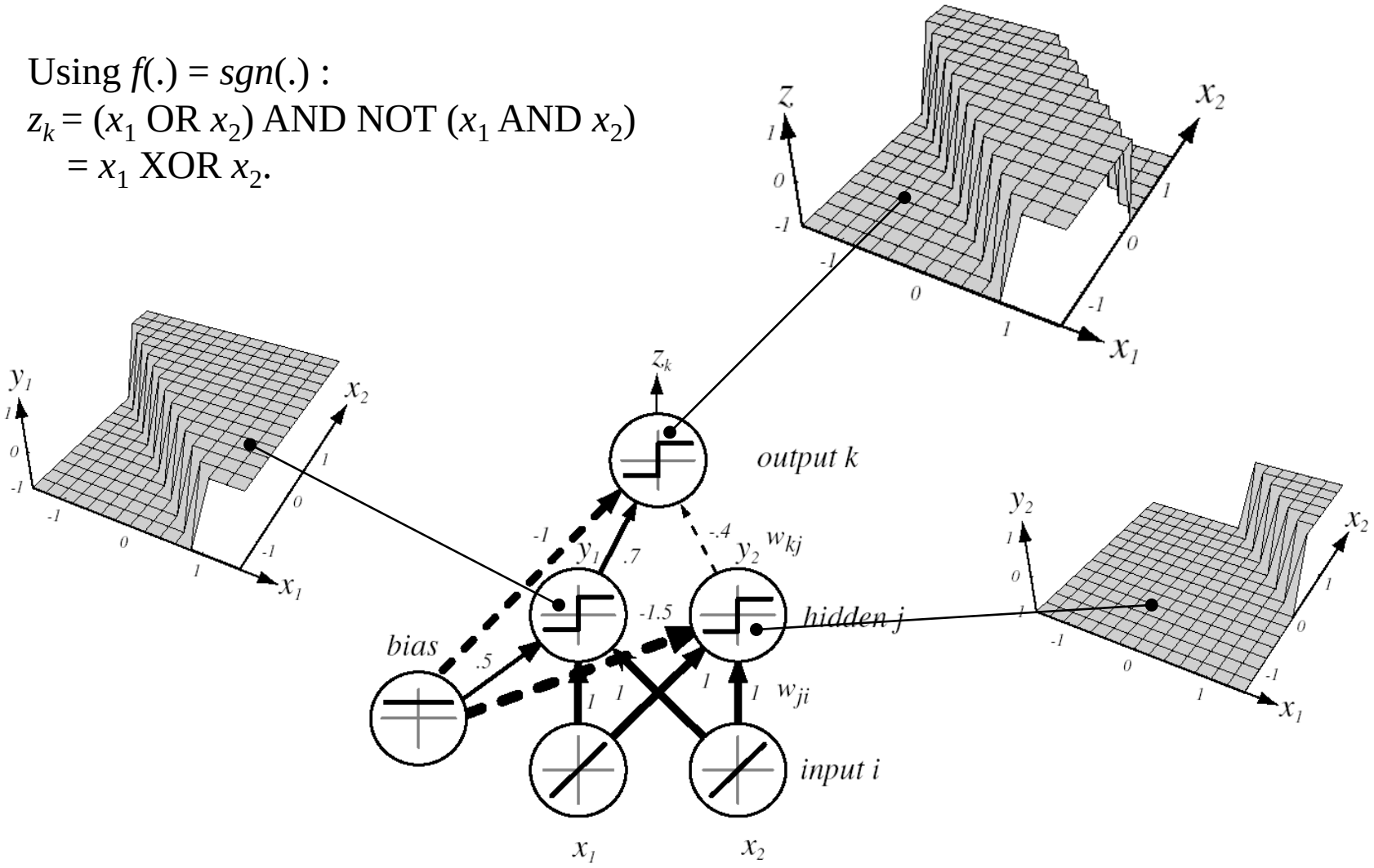
$$z_k = g_k(\mathbf{x})$$

Example: XOR Problem

Using $f(.) = sgn(.)$:

$z_k = (x_1 \text{ OR } x_2) \text{ AND NOT } (x_1 \text{ AND } x_2)$

$= x_1 \text{ XOR } x_2$.



General Feedfoward Operation

General form of output discriminant functions:

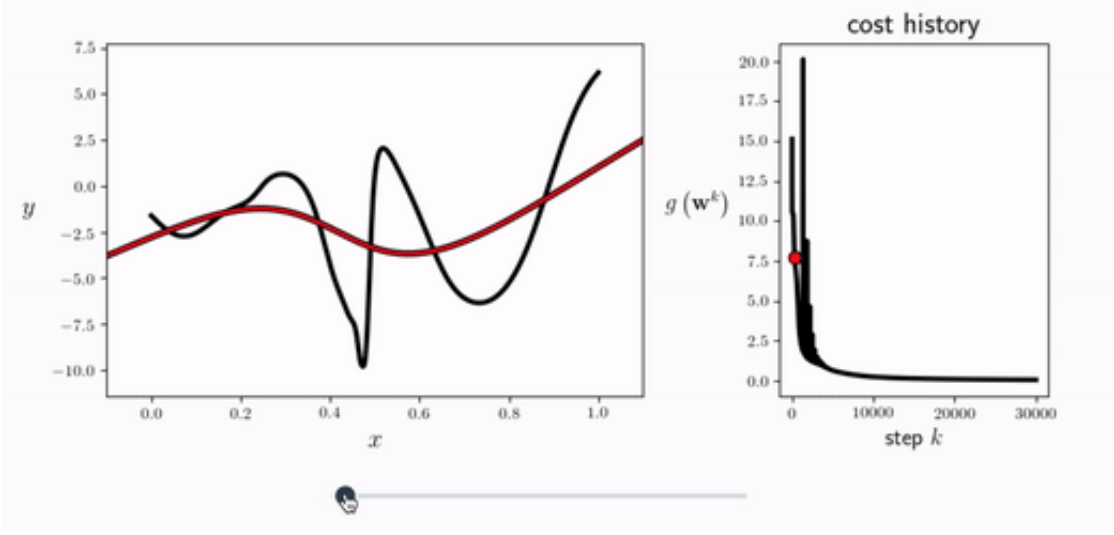
$$g_k(\mathbf{x}) \equiv z_k = f\left(\sum_{j=1}^{n_H} \tilde{w}_{kj} f\left(\sum_{i=1}^{d} w_{ji} x_i + w_{j0}\right) + \tilde{w}_{k0}\right)$$

[Note that the $\tilde{w}_{kj}$s are different from the w_{ji}s.]

Question: can every decision be implemented with a 3-layer network?

Answer [Kolmogorov + others]: (in theory) Yes.

Typically needs very nasty functions at each layer.



See 6.2 and onwards
Duda Hart

Backpropagation

We have seen that we can *approximate* any function but how do we ***learn*** functions?

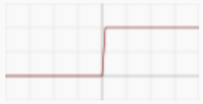
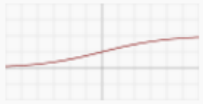
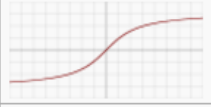
Perceptrons (single layer network): each input affects the output via its weight: so we know which weight to change to reduce errors.

Multilayer networks (a.k.a *multilayer perceptron*, *MLP*): hidden units have no “teacher” – so how reduce the error?

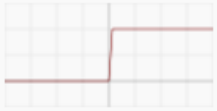
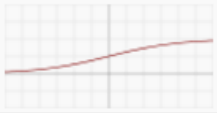
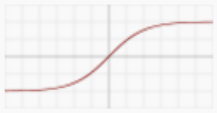
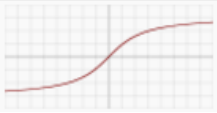
This is known as the *credit assignment problem*.

Backpropagation solves the credit assignment problem using a smooth activation function *f(.)* and gradient descent.

Some known non-linearities (activation functions)

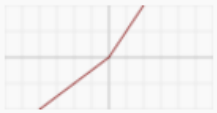
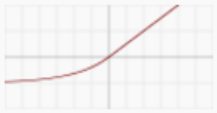
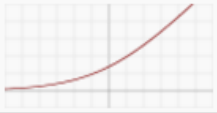
Name	Plot	Equation	Derivative
Identity		$f(x) = x$	$f'(x) = 1$
Binary step		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x \neq 0 \\ ? & \text{for } x = 0 \end{cases}$
Logistic (a.k.a Soft step)		$f(x) = \frac{1}{1+e^{-x}}$	$f'(x) = f(x)(1-f(x))$
TanH		$f(x) = \tanh(x) = \frac{2}{1+e^{-2x}} - 1$	$f'(x) = 1 - f(x)^2$
ArcTan		$f(x) = \tan^{-1}(x)$	$f'(x) = \frac{1}{x^2+1}$
Rectified Linear Unit (ReLU)		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
Parameteric Rectified Linear Unit (PReLU) [2]		$f(x) = \begin{cases} \alpha x & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} \alpha & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
Exponential Linear Unit (ELU) [3]		$f(x) = \begin{cases} \alpha(e^x - 1) & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} f(x) + \alpha & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
SoftPlus		$f(x) = \log_e(1+e^x)$	$f'(x) = \frac{1}{1+e^{-x}}$

Some known non-linearities (activation functions)

Name	Plot	Equation	Derivative
Identity		$f(x) = x$	$f'(x) = 1$
Binary step		$f(x) = \begin{cases} 0 & \text{for} \quad x < 0 \\ 1 & \text{for} \quad x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for} \quad x \neq 0 \\ ? & \text{for} \quad x = 0 \end{cases}$
Logistic (a.k.a Soft step)		$f(x) = \frac{1}{1+e^{-x}}$	$f'(x) = f(x)(1-f(x))$
TanH		$f(x) = \tanh(x) = \frac{2}{1+e^{-2x}} - 1$	$f'(x) = 1 - f(x)^2$
ArcTan		$f(x) = \tan^{-1}(x)$	$f'(x) = \frac{1}{x^2+1}$

These were the “classical ones”.

Some known non-linearities (activation functions)

Rectified Linear Unit (ReLU)		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
Parameteric Rectified Linear Unit (PReLU) [2]		$f(x) = \begin{cases} \alpha x & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} \alpha & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
Exponential Linear Unit (ELU) [3]		$f(x) = \begin{cases} \alpha(e^x - 1) & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} f(x) + \alpha & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
SoftPlus		$f(x) = \log_e(1 + e^x)$	$f'(x) = \frac{1}{1 + e^{-x}}$

The newer ones. Some have contributed to the new AI revolution.

Backpropagation: why needed?

We have seen that we can *approximate* any function but how do we ***learn*** functions?

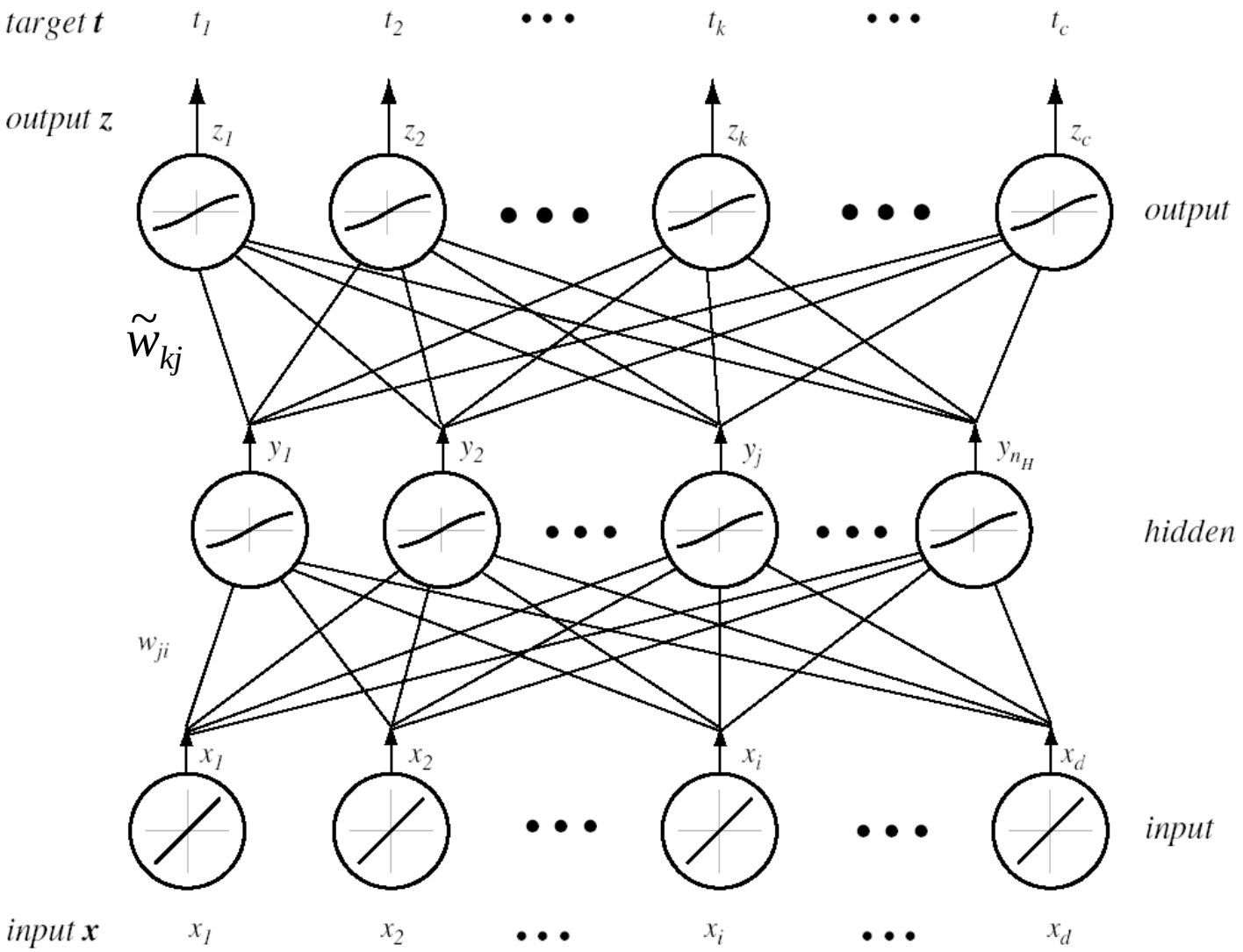
Perceptrons (single layer network): each input affects the output via its weight: so we know *which* weight to change to reduce errors.

Multilayer networks (a.k.a *multilayer perceptron*, *MLP*): hidden units have no “teacher” – so how can we reduce the error?

This is known as the *credit assignment problem*.

Backpropagation solves the credit assignment problem using a smooth activation function *f*(.), gradient descent and the chain rule.

Backpropagation Network



Backpropagation: Outline

Step 1: start with an untrained network (random weights)

Step 2: present training data to network and calculate outputs: $\mathbf{z}(\mathrm{n}) = g(\mathbf{x}(\mathrm{n}))$ This generates a training error:

$$J(\mathbf{w}) = \frac{1}{2}\sum_{n}\sum_{k=1}^{c}\left(t_k(n) - z_k(n)\right)^2 = \frac{1}{2}\sum_{n}\|\mathbf{t}(n) - \mathbf{z}(n)\|^2$$

where $\mathbf{w}$ represents the set of all weights in the network and $\mathbf{t}(n)$ are the target outputs

Step 3: change the weights in the direction of the negative gradient:

$$\Delta\mathbf{w} = -\eta\frac{\partial J}{\partial \mathbf{w}} \quad \text{or} \quad \Delta w_{pq} = -\eta\frac{\partial J}{\partial w_{pq}}$$

where η is the learning rate (step size).

Step 4: iterate until convergence

But I know things…

I just need to be able to calculate

$$\frac{\partial J}{\partial w_{pq}}$$

Indeed. For example, if we need to find:

$$\frac{\partial J}{\partial \tilde{w}_{kj}}$$

we can use the *chain rule* to differentiate the training error, and then use general form of the forward pass, and use the chain rule again.

$$g_k(\mathbf{x}) \equiv z_k = f\left(\sum_{j=1}^{n_H} \tilde{w}_{kj} f\left(\sum_{i=1}^{d} w_{ji} x_i + w_{j0}\right) + \tilde{w}_{k0}\right)$$

True…but there is a more ”elegant” way.

See 6.2 and onwards
Duda Hart

Self-learning

Backpropagation: hidden-to-output

Let us calculate the gradient for a 3-layer network. We work backwards, starting at the **hidden-to-output** weights. The *chain rule* gives:

$$\frac{\partial J}{\partial \widetilde{w}_{kj}} = \sum_n \frac{\partial J}{\partial n\tilde{e}t_k(n)} \frac{\partial n\tilde{e}t_k(n)}{\partial \widetilde{w}_{kj}} = -\sum_n \tilde{\delta}_k(n) \frac{\partial n\tilde{e}t_k(n)}{\partial \widetilde{w}_{kj}}$$

where $\tilde{\delta}_k(n) = -\frac{\partial J}{\partial n\tilde{e}t_k(n)}$ is termed the *sensitivity* of J to the net activation of k. Applying the chain rule again:

$$\tilde{\delta}_k(n) = -\frac{\partial J}{\partial n\tilde{e}t_k(n)} = -\frac{\partial J}{\partial z_k(n)} \frac{\partial z_k(n)}{\partial n\tilde{e}t_k(n)} = \underbrace{(t_k(n) - z_k(n))}_{\text{error}} f'\left(n\tilde{e}t_k(n)\right)$$

where $f'(.)$ is the *derivative* of $f(.)$.

Self-learning

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where $f'(.)$ is the *derivative* of $f(.)$.

$$\text{Since} \quad n\tilde{e}t_k(n) = \sum_j \tilde{w}_{kj} y_j(n) \quad \Rightarrow \quad \frac{\partial n\tilde{e}t_k(n)}{\partial \widetilde{w}_{kj}} = y_j(n)$$

Hence:

$$\Delta \widetilde{w}_{kj} = -\eta \partial J / \partial \widetilde{w}_{kj} = \eta \sum_n \tilde{\delta}_k(n) y_j(n) = \eta \sum_n \left(t_k(n) - z_k(n)\right) f'\left(n\tilde{e}t_k(n)\right) y_j(n)$$

Self-learning

Backpropagation: input-to-hidden

Again using the chain rule for **input-to-hidden** units we have:

$$\frac{\partial J}{\partial w_{ji}} = \sum_n \frac{\partial J}{\partial y_j(n)} \frac{\partial y_j(n)}{\partial net_j(n)} \frac{\partial net_j(n)}{\partial w_{ji}}$$

(Note that $\frac{\partial J}{\partial y_j(n)}$ involves all outputs $k = 1, ..., c$.)

$$\frac{\partial J}{\partial y_j(n)} = \frac{\partial}{\partial y_j(n)} \left[\frac{1}{2} \sum_{k=1}^{c} (t_k(n) - z_k(n))^2 \right] = -\sum_{k=1}^{c} (t_k(n) - z_k(n)) \frac{\partial z_k(n)}{\partial y_j(n)}$$

$$= -\sum_{k=1}^{c} (t_k(n) - z_k(n)) \frac{\partial z_k(n)}{\partial net_k(n)} \frac{\partial net_k(n)}{\partial y_j(n)} = -\sum_{k=1}^{c} (t_k(n) - z_k(n)) f'(net_k(n)) w_{kj}$$

$$= -\sum_{k=1}^{c} \delta_k(n) w_{kj}(n)$$

since $\delta_k(n) = (t_k(n) - z_k(n)) f'(net_k(n))$

Hidden Units (cont)

We also have

$$\frac{\partial y_j(n)}{\partial net_j(n)} = f'(net_j(n)),$$

thus we can define

$$\delta_j(n) \equiv -\frac{\partial J}{\partial net_j(n)} = -\frac{\partial J}{\partial y_j(n)}\frac{\partial y_j(n)}{\partial net_j(n)} = f'\left(net_j(n)\right)\sum_{k=1}^{c}\tilde{w}_{kj}\tilde{\delta}_k(n)$$

as the *hidden unit sensitivities*. Note that the output sensitivities are propagated back to the hidden unit sensitivities; hence the name "**back-propagation of errors**".

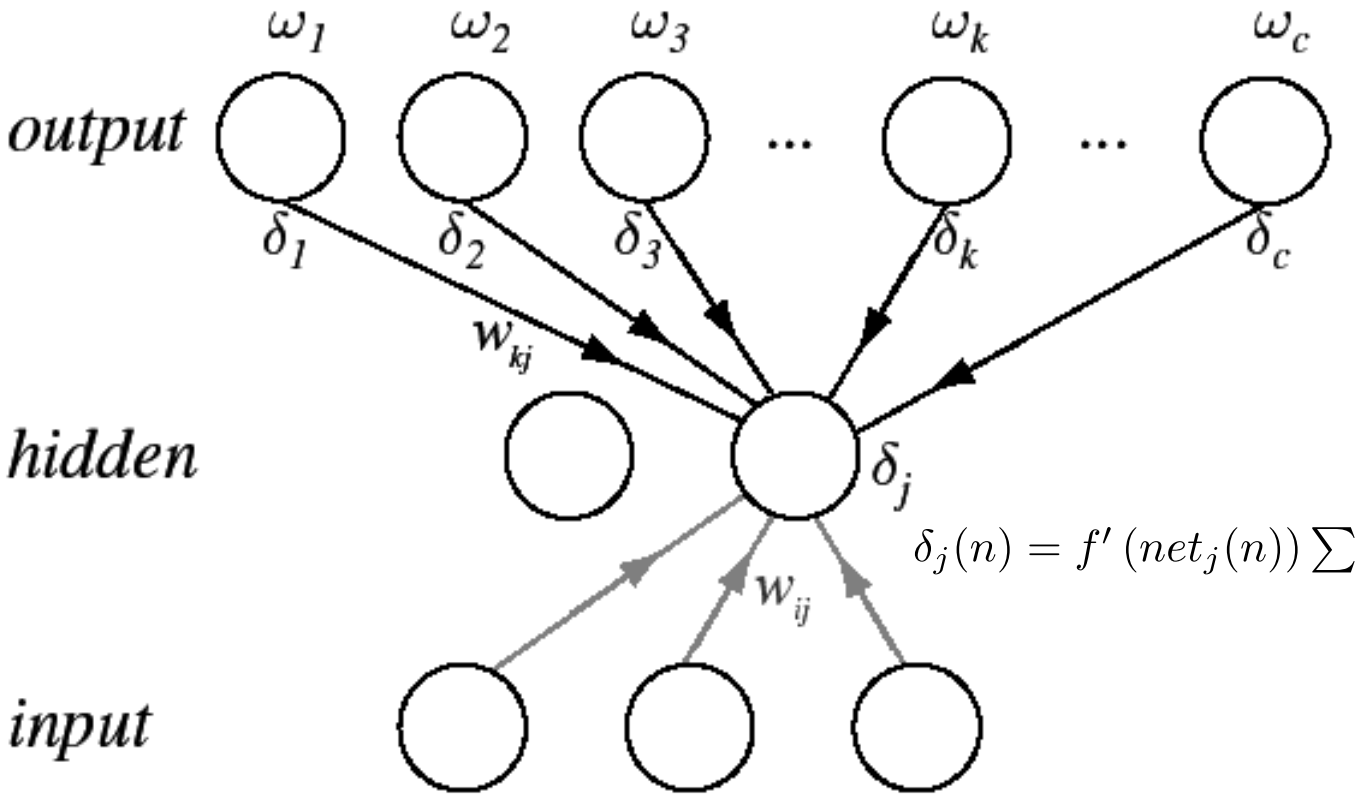
Finally we have:

$$\frac{\partial net_j(n)}{\partial w_{ji}} = x_i(n)$$

So the update rule for the input-to-hidden weights is:

$$\Delta w_{ji} = -\eta\frac{\partial J}{\partial w_{ji}} = \eta\sum_n x_i(n)\delta_j(n) = \eta\sum_n\left[\sum_{k=1}^{c}\tilde{w}_{kj}\tilde{\delta}_k(n)\right]f'\left(net_j(n)\right)x_i(n)$$

Backwards propagation



$$\delta_j(n) = f'\left(net_j(n)\right) \sum_{k=1}^{c} \tilde{w}_{kj} \tilde{\delta}_k(n)$$

The backpropagation algorithm can be easily generalized to any network with feed-forward connections, e.g. more layers, different nonlinearities in different layers, etc.

Criticisms of MLPs

MLPs provide one way to achieve the required expressive power needed to build general classifiers. However they do have their weaknesses:

- Possibility of multiple (local) minima
- g(**x**) is nonlinear in terms of the weights: this makes training slow.
- *ad hoc* solution (how many units, hidden layers, etc?)

Other popular discriminant learning structures:

- Support Vector Machines (SVMs), left as “self-learning”
- Convolutional Networks (CNNs), Sen Wang will cover these

TensorFlow Demo

- https://playground.tensorflow.org/
- Start with the bottom left (linear activation)
  - Observations: linearly separable
  - Start with a very simple net 1 layer 1 node (linear activations)
- Move to upper right still separable but not linear in input space
  - Options to fix: change layer size, add layers, change activation, change inputs?

Self-learning

PART 4: SUPPORT VECTOR MACHINES

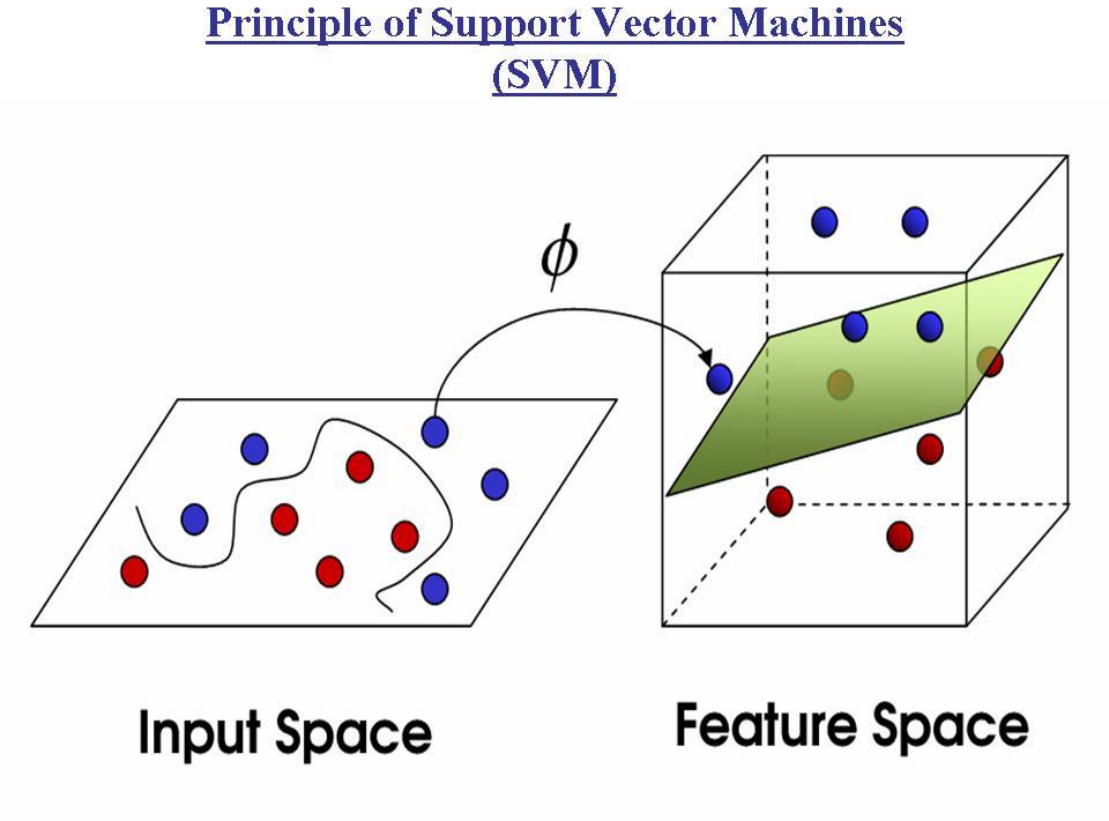
Self-learning

Support Vector Machines

Self-learning

Support Vector Machines

- SVMs solve a problem in linear or non-linear space by projecting the input space into a new (possibly infinite) space.



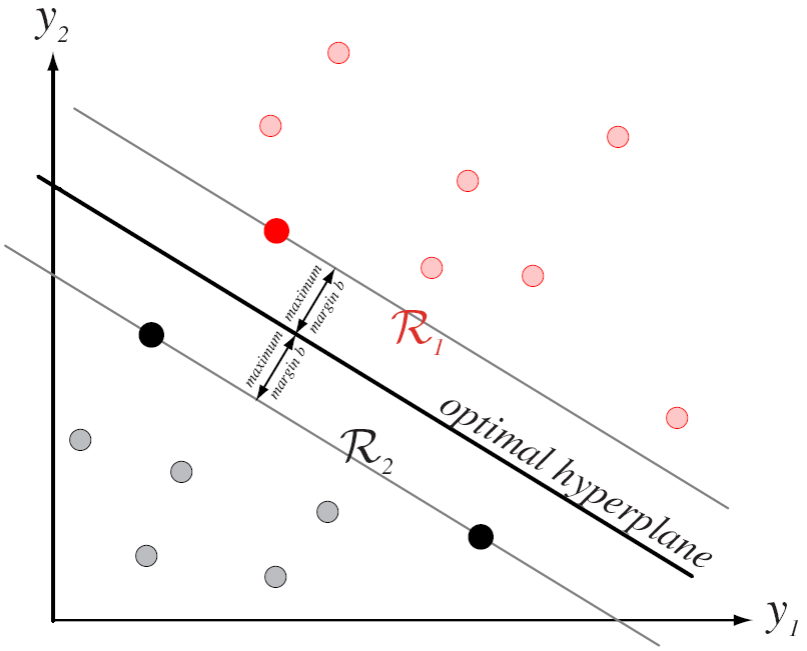
Ch 5.11 Duda

Self-learning

Support Vector Machines

SVMs aim to solve the linearly separable problem. First map feature space into high (possibly $\infty-$) dimensional space.

Then find separating hyperplane with **maximal margin**. Recall, intuitively we are more confident in classifying point far away from the decision boundary.



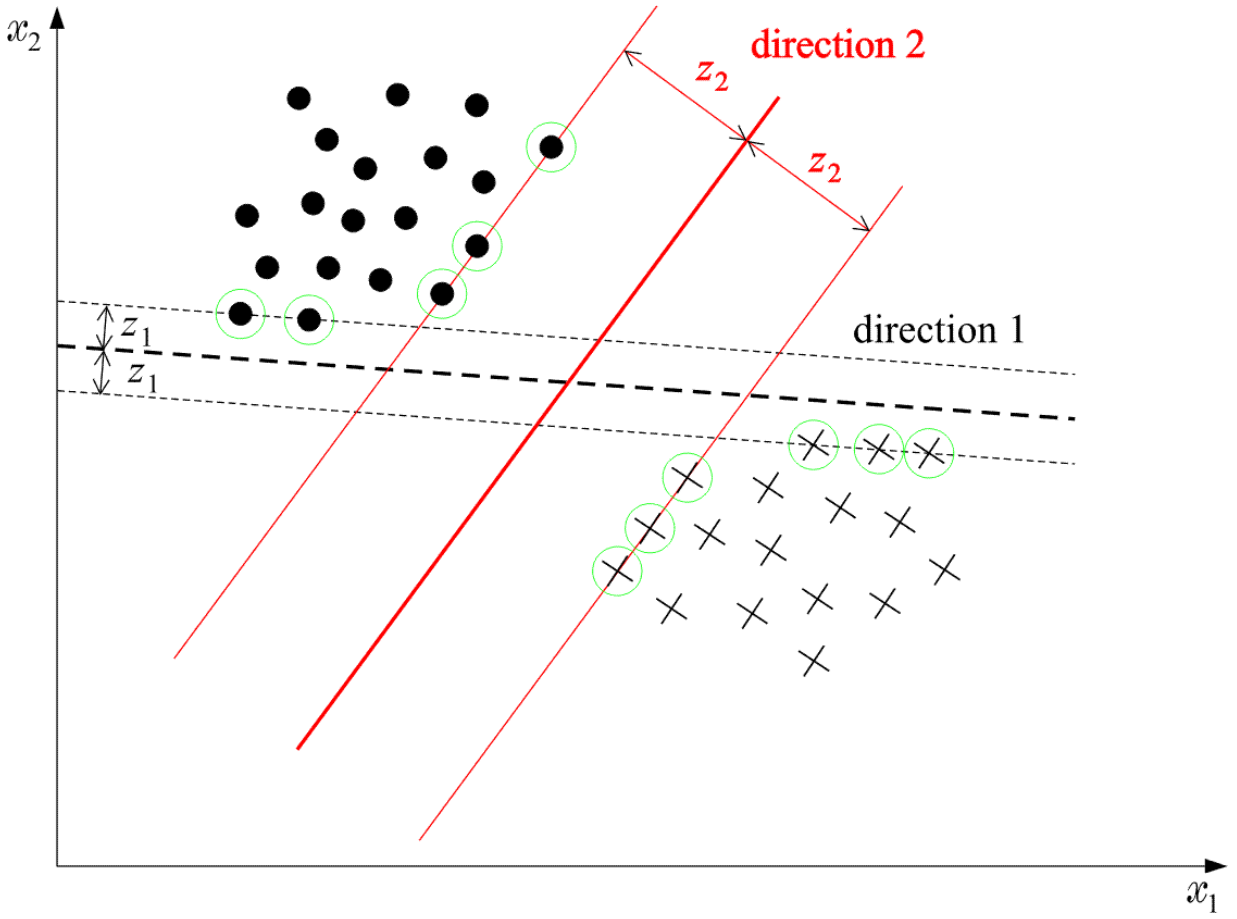
Learning takes the form of a constrained optimization scheme.

Ch 5.11 Duda

Self-learning

Why max margin

- For example these possible hyperplanes. Which one you will choose?
- "Direction 1" has a narrow margin thus on unseen (test) data it has higher likelihood of error.
- Clearly 'direction 2' is preferred



Ch 5.11 Duda

Self-learning

SVMs: Maximizing the Margin

Suppose that we have a margin γ, such that $\omega^{(i)} a^T y_i \geq \gamma$ for all points, $i = 1, 2, \ldots, n$. We therefore want to solve the following:

$$\max \gamma, \text{such that: } \omega^{(i)} a^T y_i \geq \gamma$$
$$\text{and: } \|a\| = 1$$

This is a messy optimization problem. However, equivalently we can solve:

$$\min \|a\|^2, \text{such that: } \omega^{(i)} a^T y_i \geq 1$$

That is, we search for the minimum size weight vector that is able to separate the data with a margin of $\gamma = 1$.

This form of the problem is a constrained quadratic optimization problem. It is convex and (relatively) easy to solve.

Ch 5.11 Duda

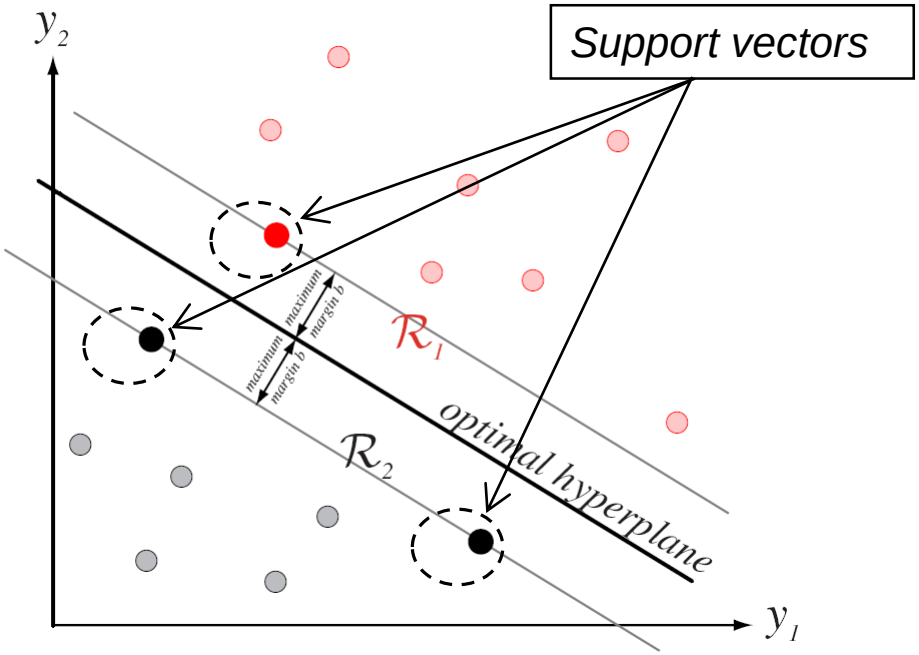
Self-learning

The Support Vectors

Interestingly the Max margin solution only depends on a subset of the training data – those that lie exactly on the margin (why?). These are called the **support vectors** (SVs).

Also

- the support vectors also define the equation of the optimal hyperplane:
  a ~ weighted sum of $\omega^{(i)}y_i$
- The hyperplane is unique the SVs are not unique. Why?



Ch 5.11 Duda

Self-learning

SVM Generalization Error

- **Cross Validation (CV)** – Break the data into a *training set* and a *testing set*. Use the training data to learn the classifier then evaluate on the test data
- **Leave-one-out CV**: choose one data point at random as the testing set.

$$\{x_1, x_2, \ldots, x_p, x_{p+1}, \ldots x_n\}$$

- Note the LOOCV error will be unaffected unless x_p is a support vector. Therefore we have:

$$error_{LOOCV} \leq \frac{\#\text{ of SVs}}{n}$$

- Therefore the number of SVs tells us how confident we are in the SVM.

Ch 5.11 Duda

PART 5: FEATURE ENGINEERING

Principal Component Analysis

MLP can learn “functions” of data but with high dimensional inputs they need some help!

This topic concerns decomposing signals into useful low dimensional subsets:

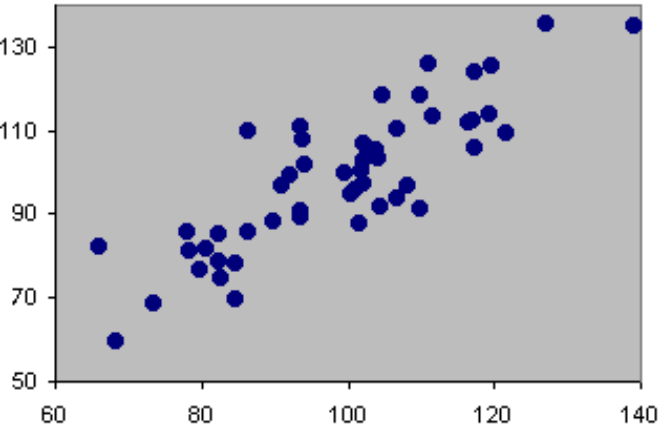
- For feature space selection in classification
- For redundancy reduction
- To avoid overfitting
- For signal separation

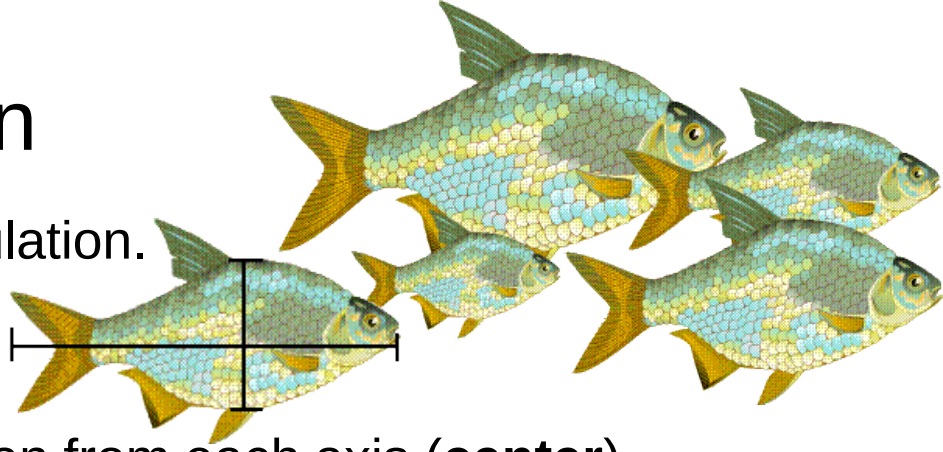
The key aim is to find a linear transform of the data that better represents the underlying information

e.g. Fourier transform of an image concentrates information into low frequencies

PCA – Graphical Intuition

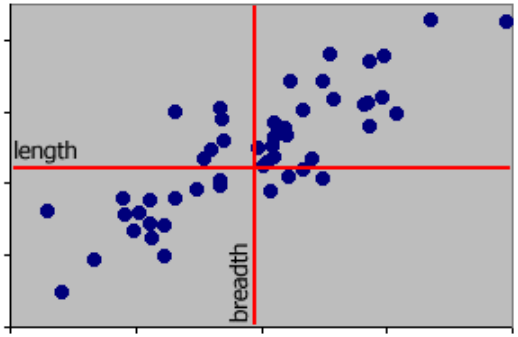
Suppose I want to characterize fish population.
Measure length/breadth and plot.





Subtract mean from each axis (**center**)

Note relationship between data matters only**.**



Inspired by http://www.cmbi.ru.nl/edu/bioinf4/prac-microarray/stats/PCA%20graphical%20explanation.htm

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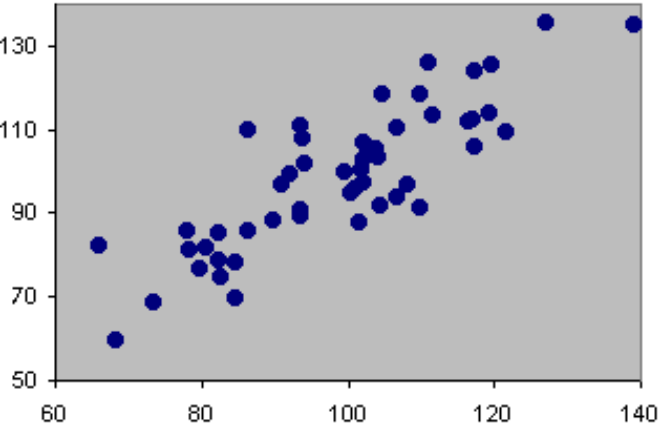

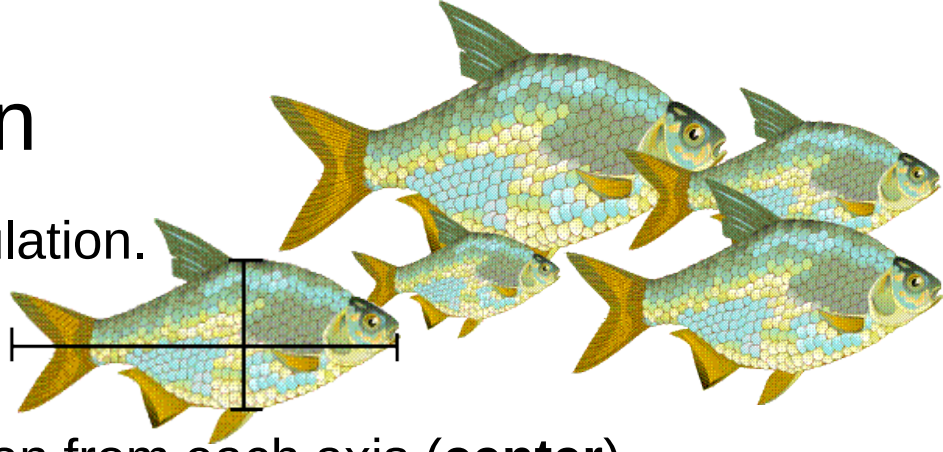

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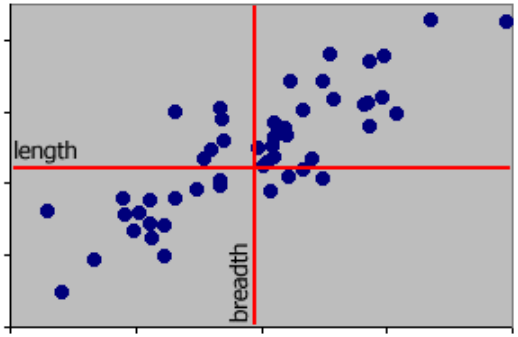

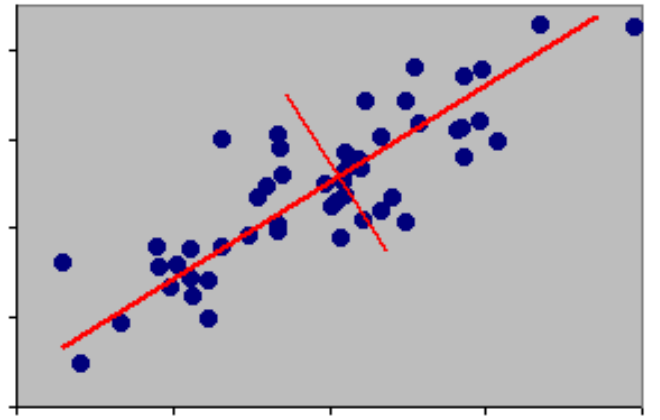

I can **move the axis!** But how to chose them? **I can rotate them.**

What is my objective: position one axis in such a way that it accounts for the largest proportion of the data's **variance**.

Inspired by http://www.cmbi.ru.nl/edu/bioinf4/prac-microarray/stats/PCA%20graphical%20explanation.htm

PCA – Graphical Intuition

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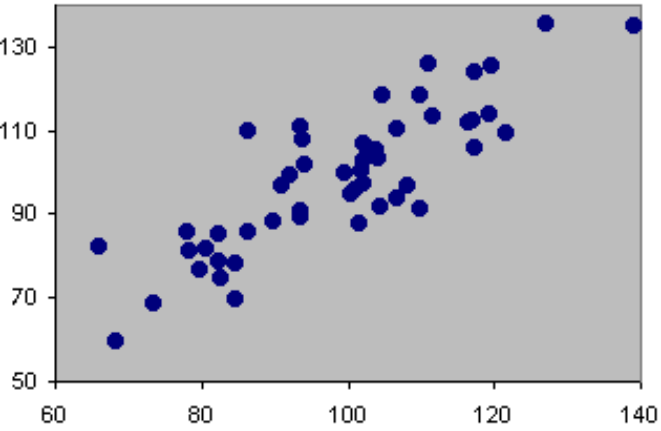

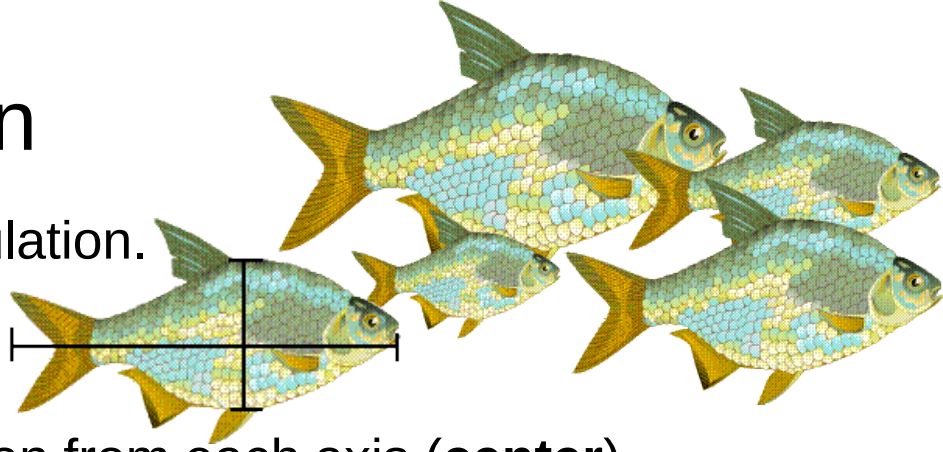

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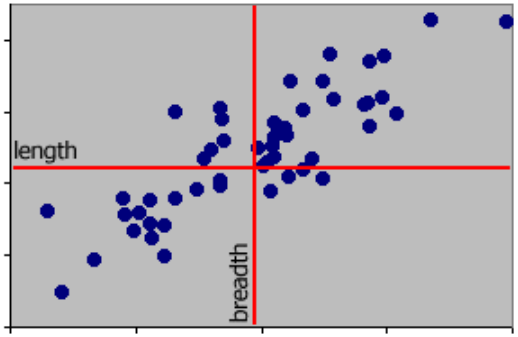
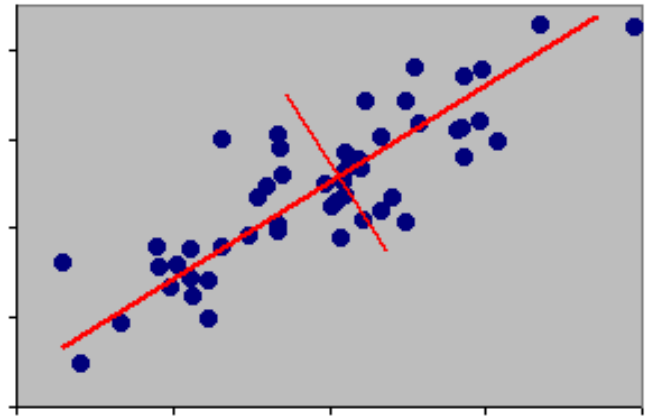
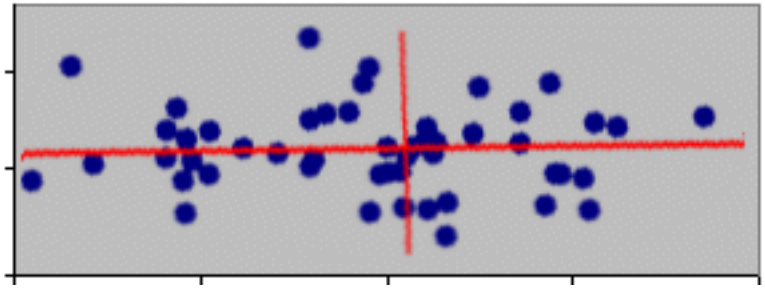


I can **move the axis!** But how to chose them? **I can rotate them.**





What is my objective: position one “new” axis in such a way that it accounts for the largest proportion of the data's **variance**.

Inspired by http://www.cmbi.ru.nl/edu/bioinf4/prac-microarray/stats/PCA%20graphical%20explanation.htm

PCA – Graphical Intuition

What might you **call** this new axis? **size = length + breadth**

However, we could make one of the **variables** more important.

size = 0.75 x length + 0.25 x breadth

[these are weights and are important! They tell us the "significance" of each of the original variables.

What about the second axis of the ellipse?

Objective: account for as much of the remaining variation as possible but must also be uncorrelated (**orthogonal**) with the first. [trivial in 2D]

Apart from size, how else do the above fish differ?

Not much, minor differences in shape. If we ignore 2nd axis (after rotation) we would lose information about the different shapes, but since they are all very similar in shape we wouldn't lose much information at all.

Thus, in the above example we can reduce the data's dimensionality from two (length and breadth) to one (size), with little information loss.

Self-learning

PCA & Subspace Projections

Introduced by Pearson in 1901 "*On lines and planes of closest fit to a system of points in space.*" (a.k.a. Karhunen-Loéve transform (KLT), or the Hotelling transform,…).

Suppose our data consists of d-dimensional vectors $x^{(n)} \in R^d$ and we want a low-dimensional approximation for the data.

Let $\boldsymbol{u}_i$ be an **orthonormal** basis for R^d (i.e. $U^T U = I$) then we can approximate x by:

$$\tilde{\mathbf{x}} = \sum_{i=1}^{M} (\mathbf{u}_i^T \mathbf{x}) \mathbf{u}_i + \sum_{j=M+1}^{d} b_j \mathbf{u}_j$$

Each b_j is a constant

let $z_i = \mathbf{u_i}^T \mathbf{x}$

Self-learning

Subspace Projections

x has d degrees of freedom while $\tilde{\mathbf{x}}$ has M deg. of freedom.

Principal Component Analysis – choose $\boldsymbol{u}_i$ and b_j to best approximate x in the LSE sense, ie., minimize E_M:

$$E_M = \frac{1}{2}\sum_{n=1}^{N}\left\|\mathbf{x}^{(n)} - \tilde{\mathbf{x}}^{(n)}\right\|^2 = \frac{1}{2}\sum_{n=1}^{N}\left\|\mathbf{U}^T\mathbf{x}^{(n)} - \mathbf{U}^T\tilde{\mathbf{x}}^{(n)}\right\|^2 = \frac{1}{2}\sum_{n=1}^{N}\sum_{j=M+1}^{d}\left(z_j^{(n)} - b_j\right)^2$$

Taking the derivative with respect to b_j *gives:*

$$\sum_{n=1}^{N}\left(z_j^{(n)} - b_j\right) = 0 \quad \Rightarrow \quad b_j = \frac{1}{N}\sum_{n=1}^{N} z_j^{(n)} = \frac{1}{N}\sum_{n=1}^{N}\mathbf{u}_j^T\mathbf{x}^{(n)} = \mathbf{u}_j^T\bar{\mathbf{x}}$$

Self-learning

Subspace Projections (cont.)

So we can write:

$$E_M = \frac{1}{2}\sum_{n=1}^{N}\sum_{j=M+1}^{d}\left(\mathbf{u}_j^T\left(\mathbf{x}^{(n)}-\bar{\mathbf{x}}\right)\right)^2$$

$$= \frac{1}{2}\sum_{j=M+1}^{d}\sum_{n=1}^{N}\mathbf{u}_j^T\left(\mathbf{x}^{(n)}-\bar{\mathbf{x}}\right)\left(\mathbf{x}^{(n)}-\bar{\mathbf{x}}\right)^T\mathbf{u}_j = \frac{1}{2}\sum_{j=M+1}^{d}\mathbf{u}_j^T\mathbf{R}_{\mathbf{x}}\mathbf{u}_j$$

where $\mathbf{R}_{\mathbf{x}}$ is the sample covariance matrix for $\{\mathbf{x}^{(n)}\}$

Minimizing E_M with respect to $\boldsymbol{u}_j$ is satisfied by:

$$\mathbf{R}_{\mathbf{x}}\,\mathbf{u}_j = \lambda\mathbf{u}_j, \text{ for } \mathrm{j} = 1,...,\mathrm{M}$$

i.e. the M basis vectors are the principal eigenvectors of the sample covariance matrix.

PCA Algorithm and Projection on Principal Directions

The PCA algorithm is summarized as follows:

1. subtract mean $\bar{\mathbf{x}}$ from data
2. Calculate sample covariance matrix, $\mathbf{R}_{\mathbf{x}}$ for $\{\mathbf{x}_n - \bar{\mathbf{x}}\}$
3. Perform eigenvalue decomposition: $\mathbf{R}_x = \mathbf{U}\Lambda\mathbf{U}^T$
4. Approximate data by the first M components that have the largest eigenvalue:

$$\mathbf{x}_n \approx \bar{\mathbf{x}} + \sum_{i=1}^{m} (\mathbf{u}_i^T (\mathbf{x}_n - \bar{\mathbf{x}}))\mathbf{u}_i$$

Recall by design eigenvectors are **ORTHOGONAL** with each other $\mathbf{u_i}^T\mathbf{u_j}=0$ (i # j) and have length 1 ($\mathbf{u_i}^T\mathbf{u_i}=1$).

PCA example: eigenfaces

In face recognition a common practice is to first project data (after alignment) onto a low dimensional PCA space,

e.g. images from images AT&T Laboratories Cambridge.

u_1 u_2 u_3 u_4

Eigenfaces capture appearance and lighting conditions quite well.

An interactive demo

- http://setosa.io/ev/principal-component-analysis/

Kernel PCA

(linear) PCA method is built upon the eigenanalysis of (n number of data points)

$$R_X = \frac{1}{n} X^T X = \frac{1}{n} \sum_{i=1}^{n} \underline{x}_i \underline{x}_i^T$$

There is an equivalent built upon the eigenanalysis of

$$K = XX^T = \begin{bmatrix} \underline{x}_1^T \underline{x}_1 & \cdots & \underline{x}_1^T \underline{x}_n \\ \vdots & \ddots & \vdots \\ \underline{x}_n^T \underline{x}_1 & \cdots & \underline{x}_n^T \underline{x}_n \end{bmatrix}$$

known as the Gram matrix.

The kernel PCA method is the kernelized version of this, where inner products are replaced by kernel operations.

Kernels

- Achieve projections in higher dimensions as we saw in GLD without actually explicitly defining the projection
- Examples of kernels
  - Radial basis Functions:

$$K(\underline{x},\underline{z}) = \exp\left(-\frac{\|\underline{x}-\underline{z}\|^2}{\sigma^2}\right)$$

  - Polynomial:

$$K(\underline{x},\underline{z}) = (\underline{x}^T\underline{z}+1)^q,\ \ q>0$$

  - Hyperbolic Tangent:

$$K(\underline{x},\underline{z}) = \tanh(\beta\underline{x}^T\underline{z}+\gamma)$$

for appropriate values of β, γ.

Self-learning

Kernel PCA: The algorithm

- Compute the Gram matrix.

$$K(i,j)=K(\underline{x}_i,\underline{x}_j)\ ,\quad i,j=1,2,...,n$$

- Compute the m dominant eigenvalues / eigenvectors.

$$\lambda_k\ ,\underline{a}_k\ ,\ k=1,2,...,m$$

- Perform normalization to unity.

$$1=n\lambda_k\underline{a}_k^T\underline{a}_k\ ,\ k=1,2,...,m$$

- Given a vector $\underline{x}$, perform the following "nonlinear mapping".

$$y(k)=\sum_{i=1}^{n}a_k(i)K(\underline{x}_i,\underline{x})\ ,\ k=1,2,...,m$$

Self-learning

Remark

- The kernel PCA is equivalent with performing a (linear) PCA in a Reproducing kernel Hilbert space (RKHS) H, after a mapping

$$\underline{x} \to \phi(\underline{x}) \in H$$

- It can be shown that the dominant eigenvectors of

$$\frac{1}{n}\sum_{i=1}^{n}\phi(\underline{x}_i)\phi^T(\underline{x}_i)$$

are given in terms of the dominant eigenvectors of the Gram matrix, i.e.,

$$\underline{v}_k = \sum_{i=1}^{n} a_k(i)\phi(\underline{x}_i), \quad k = 1,2,\ldots,m$$

Hence the projection of $\underline{\phi}(\underline{x})$ on $\underline{v}_k$ is given by:

$$\left\langle \underline{v}_k, \phi(\underline{x}) \right\rangle = \sum_{i=1}^{n} a_k(i)\left\langle \phi(\underline{x}_i), \phi(\underline{x}) \right\rangle = \sum_{i=1}^{n} a_k(i)K(\underline{x}_i, \underline{x}),$$

using the properties of the RKHS.

PART 6: BIAS AND VARIANCE DILEMMA

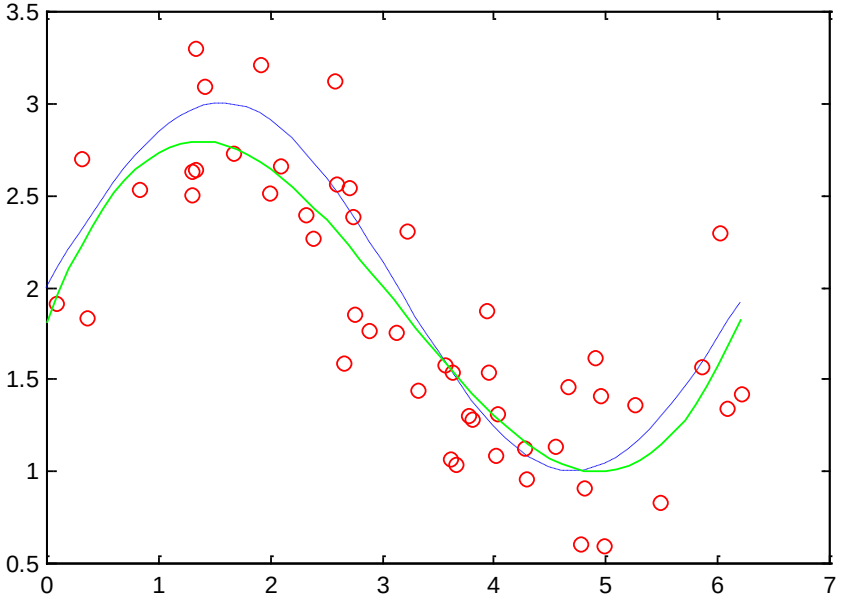
Why we care about generalisation?

- We can always train an algorithm to zero "training" error.
  - e.g. neural networks can approximate any function
  - Does this really matter?
- What matters is how the algorithm will perform on **new unseen data** that are NOT the same as the training data
  - How will the algorithm then behave?
  - If the algorithm has understood the underlying structure ➔ then it should do well
- We say then that the algorithm "generalizes well" (we now formalize this using the bias and variance dilemma)

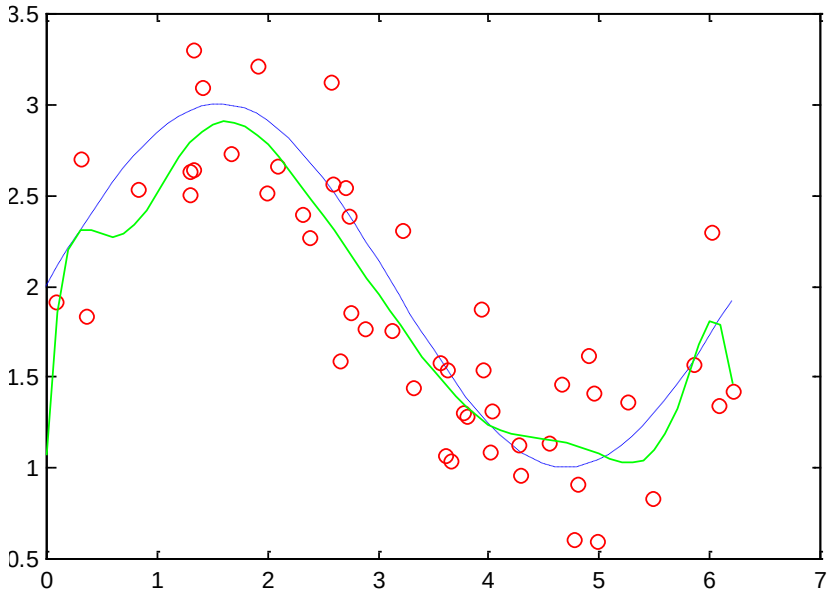



Overfitting in ML

Given a limited data set maximising the likelihood L(**w**) may lead to *overfitting.* If the model order (dimensions of **w**) is large enough we can 'exactly' fit model to data.



3rd order polynomial fit



10th order polynomial fit

Ch 9.3.1 Duda

Self-learning

Overfitting in ML

Overfitting relates to *Model Order Selection.* As with estimating power spectra the problem comes from a *bias - variance* trade-off. Consider the expected error between an optimal estimator $F(x)$ (ie. the true function) and an empirical estimator $g(x)$.

[We use a trick.]

$$\mathbb{E}_x\left\{(F(x)-g(x))^2\right\} = \mathbb{E}_x\left\{\left(\ F(x)-\mathbb{E}_x\{g(x)\}+\mathbb{E}_x\{g(x)\}-g(x)\ \right)^2\right\}$$

$$= \underbrace{\mathbb{E}_x\left\{\left(F(x)-\mathbb{E}_x\{g(x)\}\right)^2\right\}}_{\text{bias}^2} + \underbrace{\mathbb{E}_x\left\{\left(\mathbb{E}_x\{g(x)\}-g(x)\right)^2\right\}}_{\text{variance}}$$

$$+ \underbrace{2\,\mathbb{E}_x\left\{\left(F(x)-\mathbb{E}_x\{g(x)\}\right)\left(\mathbb{E}_x\{g(x)\}-g(x)\right)\right\}}_{=0}$$

The expectation over all possible different training sets (also known as the ensemble average). It is **not** the E we used to denote as the cost function thus far.

To show why this is 0 do the multiplication and then recall properties of the Expectation of constants!

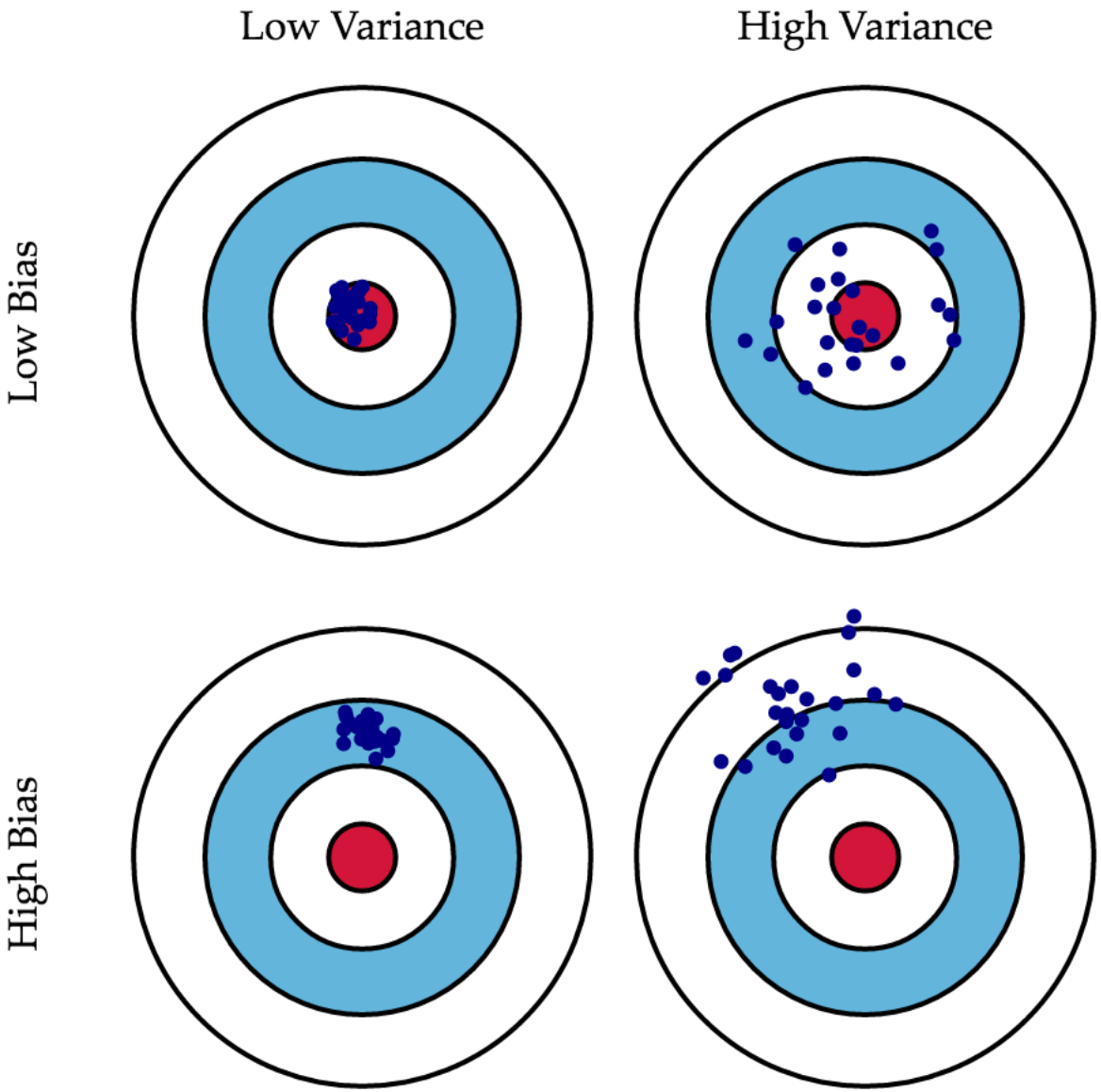
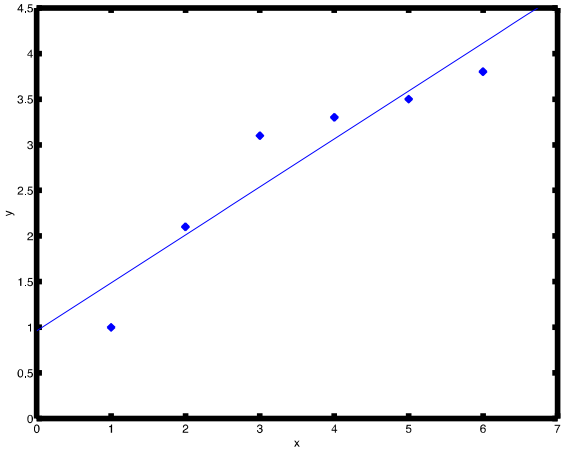


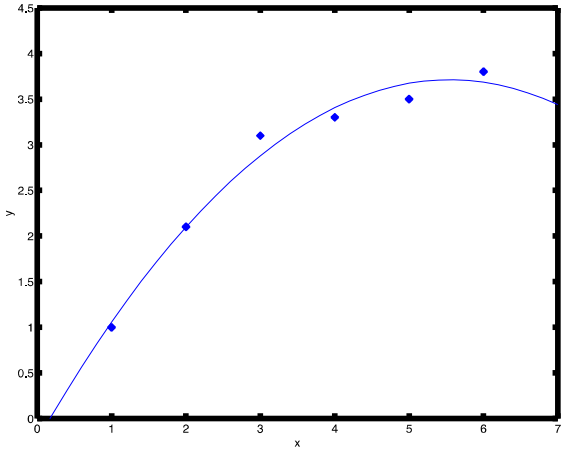
Fig. 1 Graphical illustration of bias and variance.

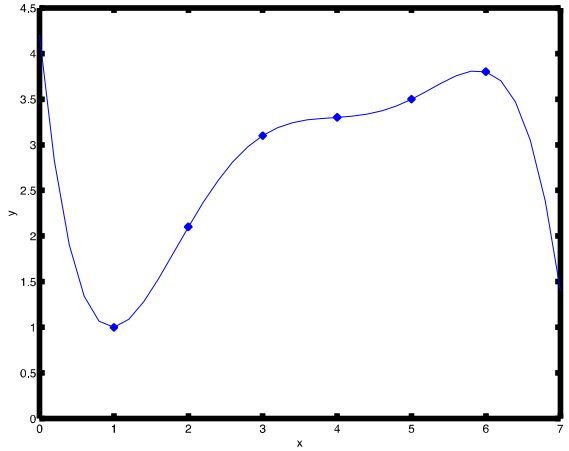
Source: http://scott.fortmann-roe.com/docs/BiasVariance.html

Example in regression

- Identify high bias / variance cases:







Ignore the data ➔

* Big approximation errors (high bias)
* No variation between data sets (no variance)

Use all data ➔

* No approximation errors (zero bias)
* Variation between data sets (high variance)

Overfitting in ML

These examples tell us:

- Too **complex** a model → **high variance**.
- Too **simple** a model → **high bias** (the simplest model is the fixed value).

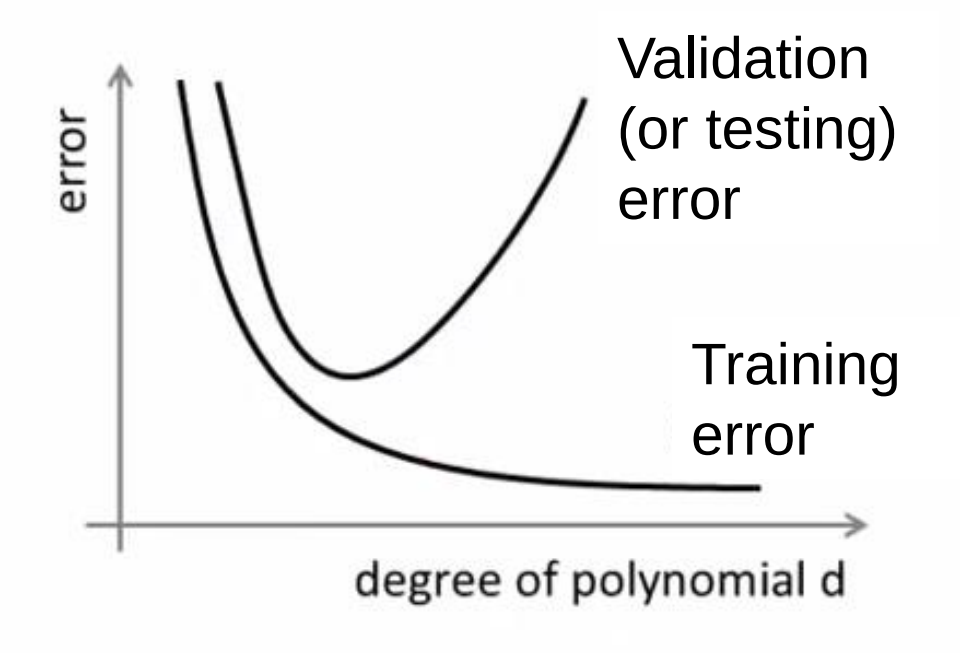
Possible solution on diagnosis for models and data (size)
Cross-validation: Break the data into **3 pieces**: *training*, *validation* and *testing* sets. Set the testing set apart, do not touch it, till the end.

Use the training data to learn the model parameters.
But identify the best model order (and other parameters such as step size, regularizers, type of activation function etc) using the validation ("out-of-sample") set.

If you are happy with the performance on the validation set, then you can now take the testing set and run the algorithm on the testing set.
Then report results on the training and testing sets.

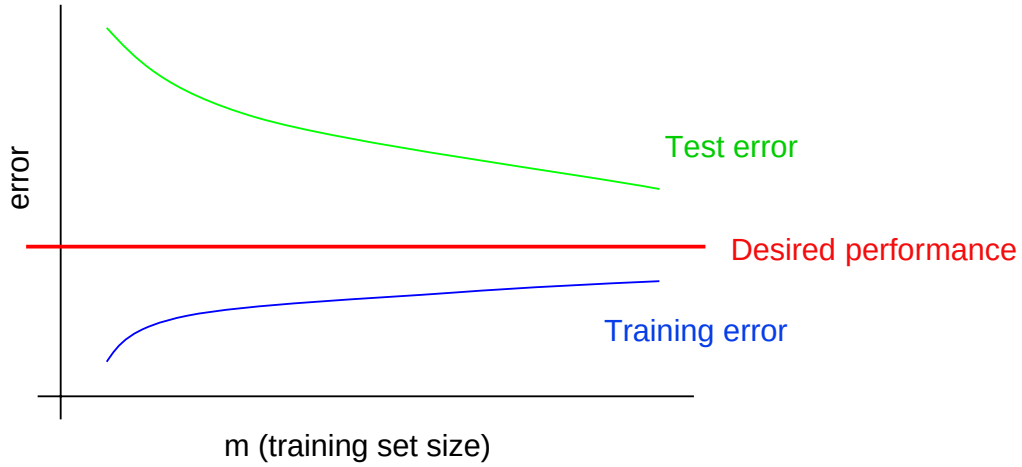
Diagnosing bias/variance: the practical picture

- Finding a good model size



Bias vs variance: on data size

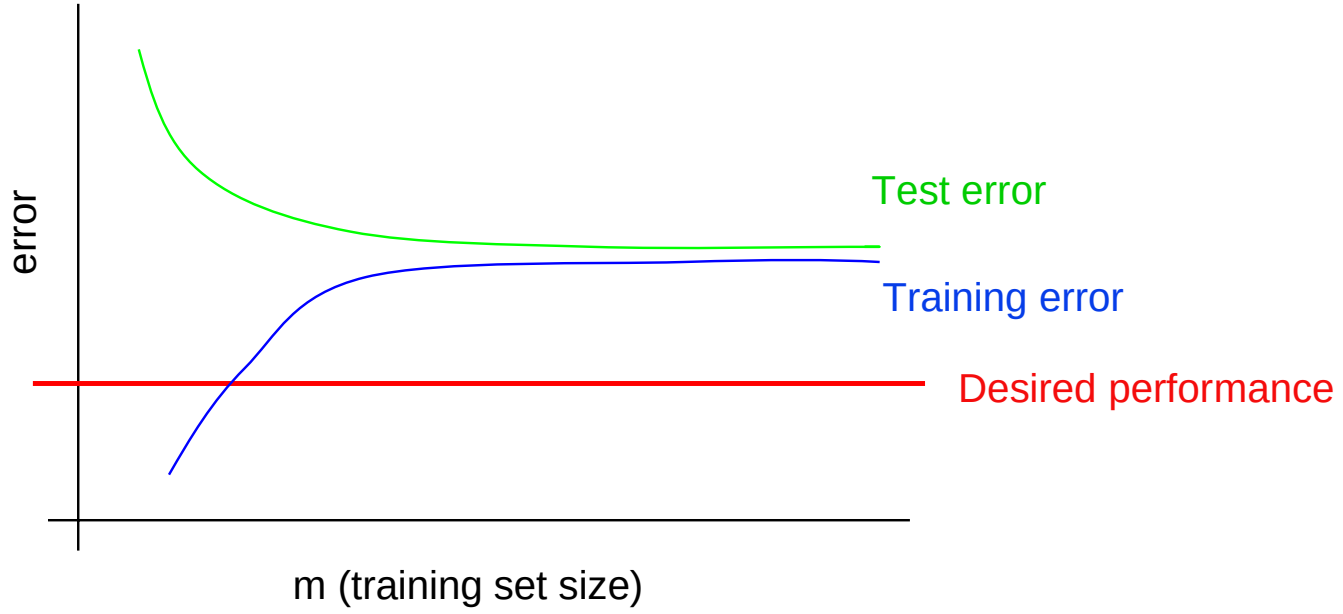
- Typical curve with high variance



- Test error decreases as m increases ➔ larger training set may help
- There is a gap between training & test error

Bias vs. variance: on data size

- Typical curve with high bias



- We are in trouble: training error is high too
- Small gap between the two errors

Take away messages

- Supervised learning relies on examples to learn
  - Unsupervised does not
    - Semi-supervised combines them
- It is easier to classify when data are **linearly** separable
- We can always **project** to new features to solve linear problems
  - By **design** (e.g. via polynomial functions)
  - Or we can **summarise** them statistically (e.g. PCA)
  - Or we can **learn** them (via NNs)
- We cannot create **magic**
  - It is not training error we care for but **generalization** to unseen data and hence testing error
    - We have **theoretical** tools (bias and variance dilemma) and **practical** tools to assess this

Thank you

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- Web: https://vios.science

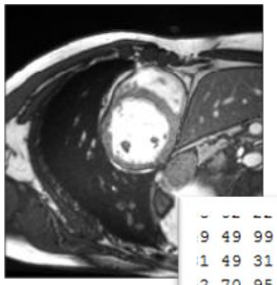
- Additional slides on machine learning and deep learning and particularly in augmentation are here: https://edin.ac/2vSP6T3 (Tutorial at ICASSP 2019 on Data augmentation techniques for deep learning)

PART 7: Convolutional Neural Networks & Deep Learning

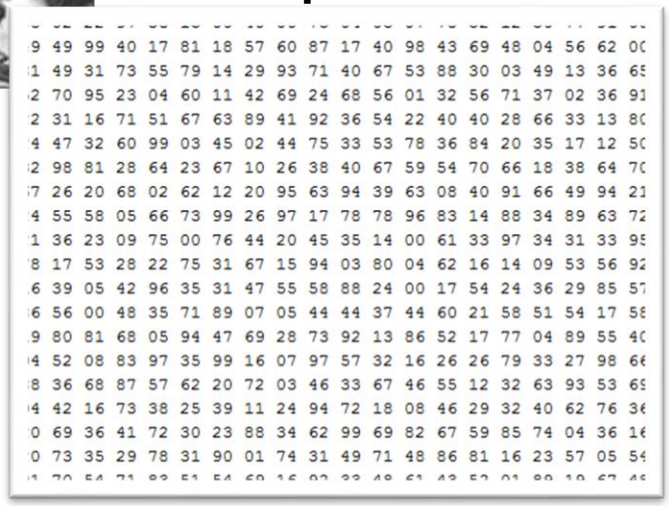
Convolutional Neural Networks & Deep Learning

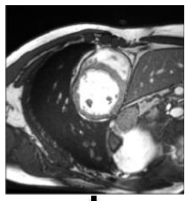
From “hand-designed” feature spaces to data-driven ones…

We see



Computer sees





Extract features

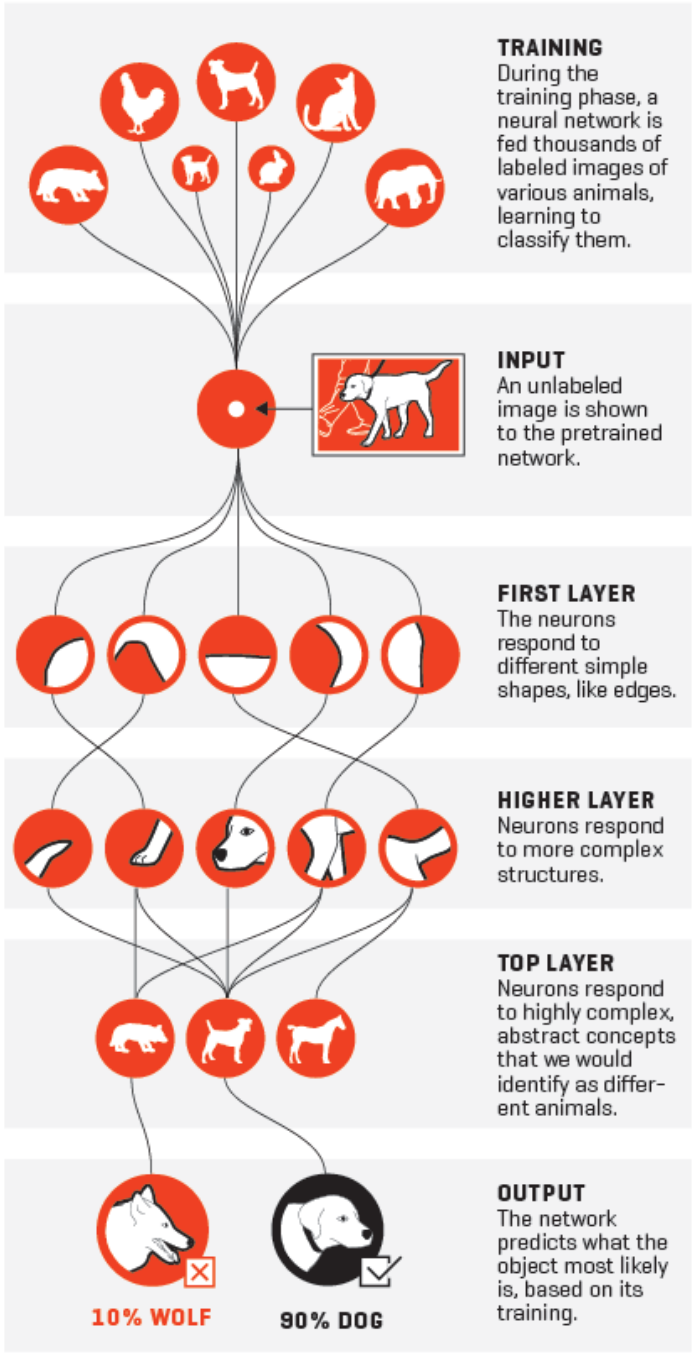
Human engineering
(e.g. input x and x^2)

Decision function

decision

e.g. SVM, GLD, MLP

What if we could “extract” automatically good features….



http://fortune.com/ai-artificial-intelligence-deep-machine-learning/

Convolutional Networks (CNNs)

Consider the problem of building a classifier that is insensitive to translation (or scale, rotation, etc.). A Convolutional Network encodes the invariance within the MLP structure [LeCun 1998].

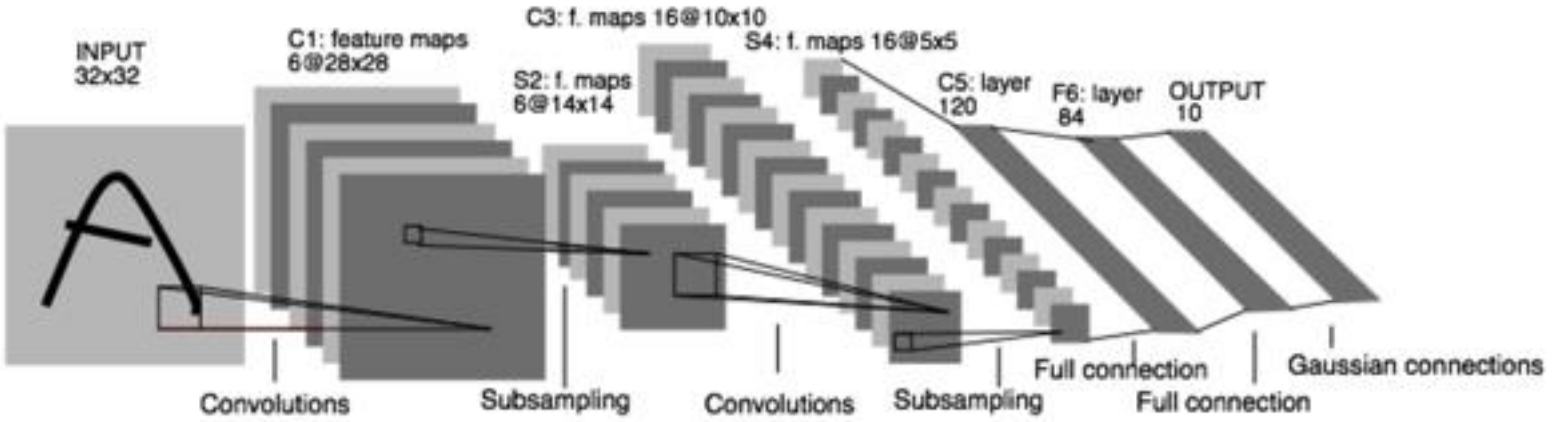


Figure from: LeCun, Boser, Denker, Henderson, Howard, Hubbard, Jackel. (December 1989). "Backpropagation Applied to Handwritten Zip Code Recognition". Neural Computation. ***1*** *(4): 541-51.*

Convolutional Networks (CNNs)

Consider the problem of building a classifier that is insensitive to translation (or scale, rotation, etc.). A Convolutional Network encodes the invariance within the MLP structure [LeCun 1998].

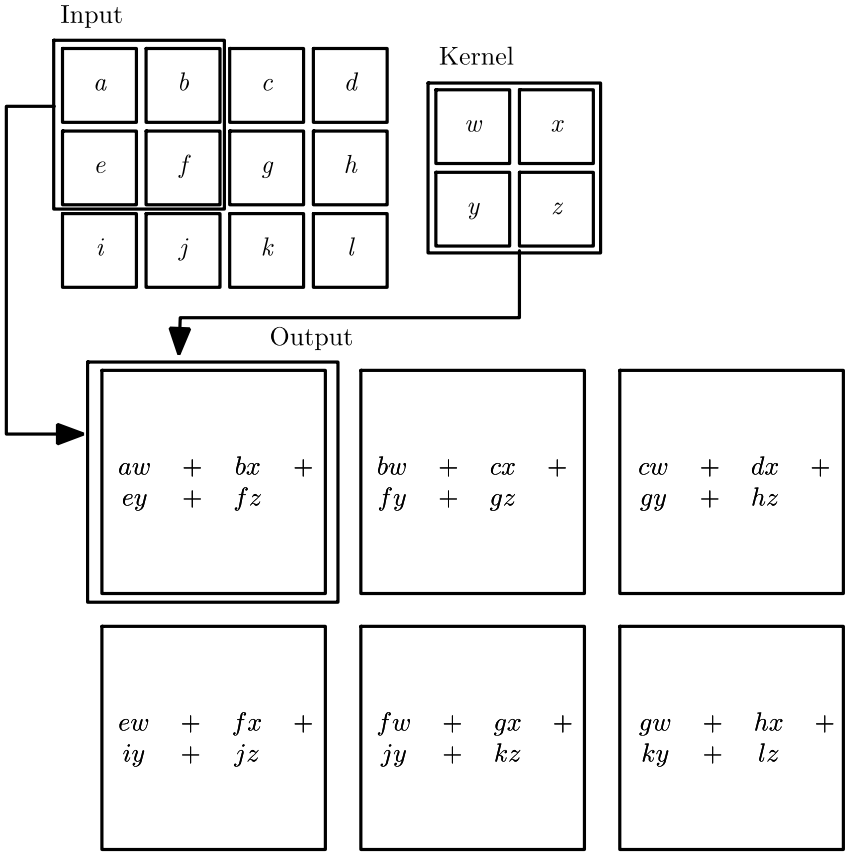
Let us first review 2D convolution ➔

Can I write *w conv I* as a matrix multiplication?

Next layer O = W*I

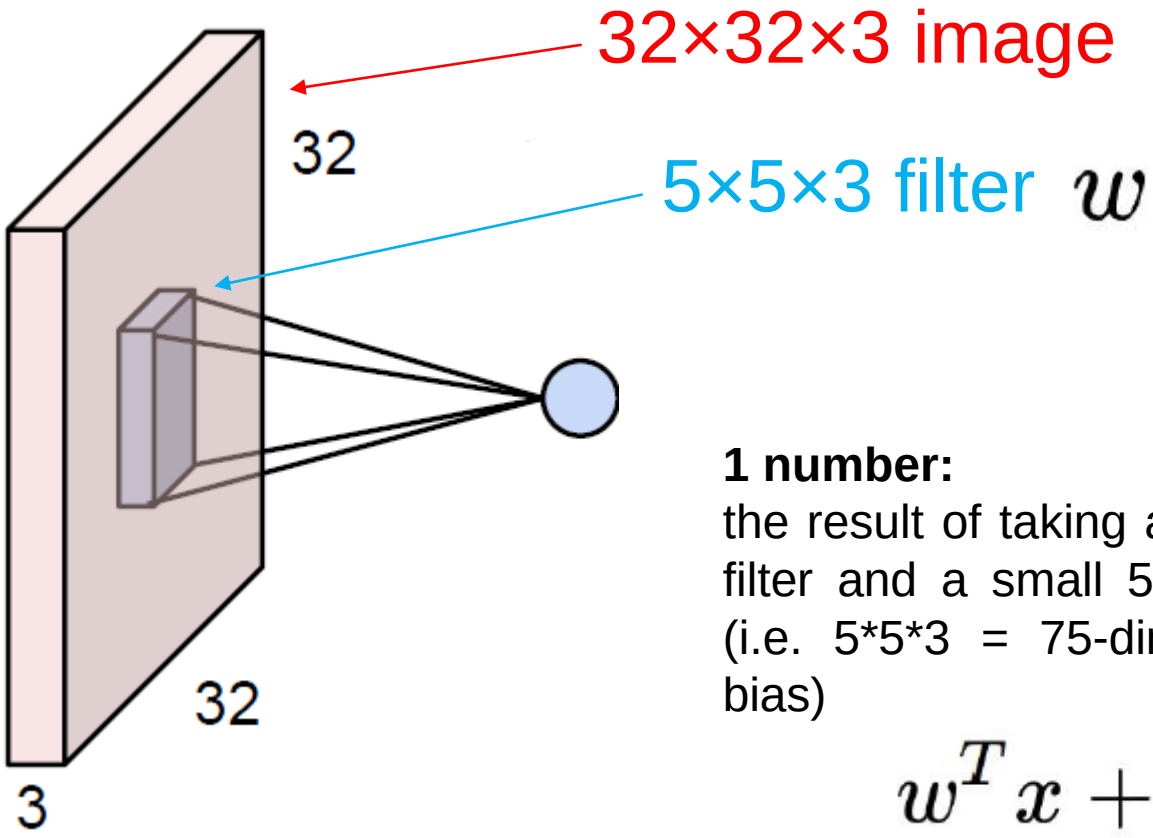
W must have a correct shape and

I: a vector (input layer)!



Inspired by Goodfellow et al Deep learning book

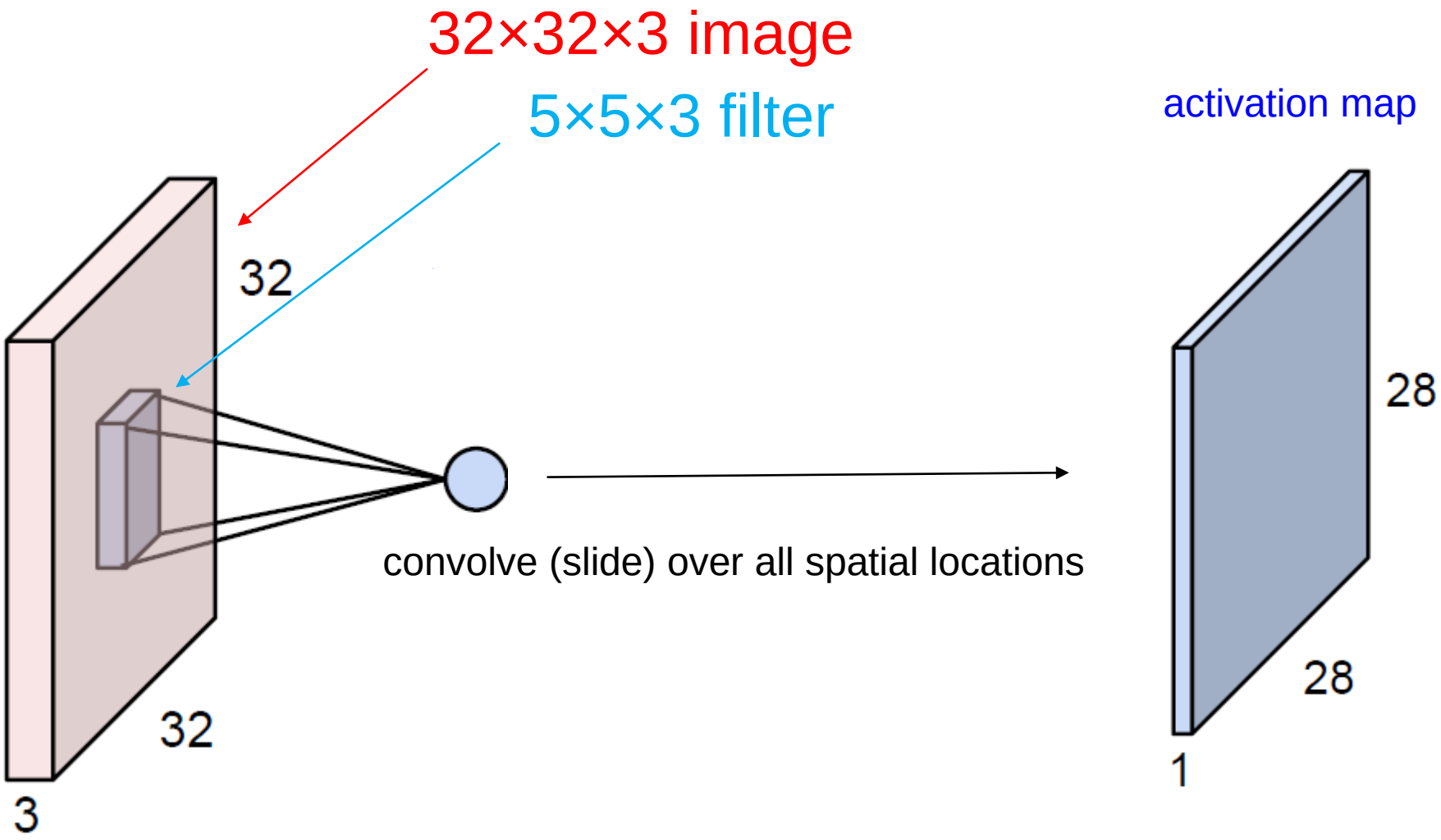
Convolution Layer



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)

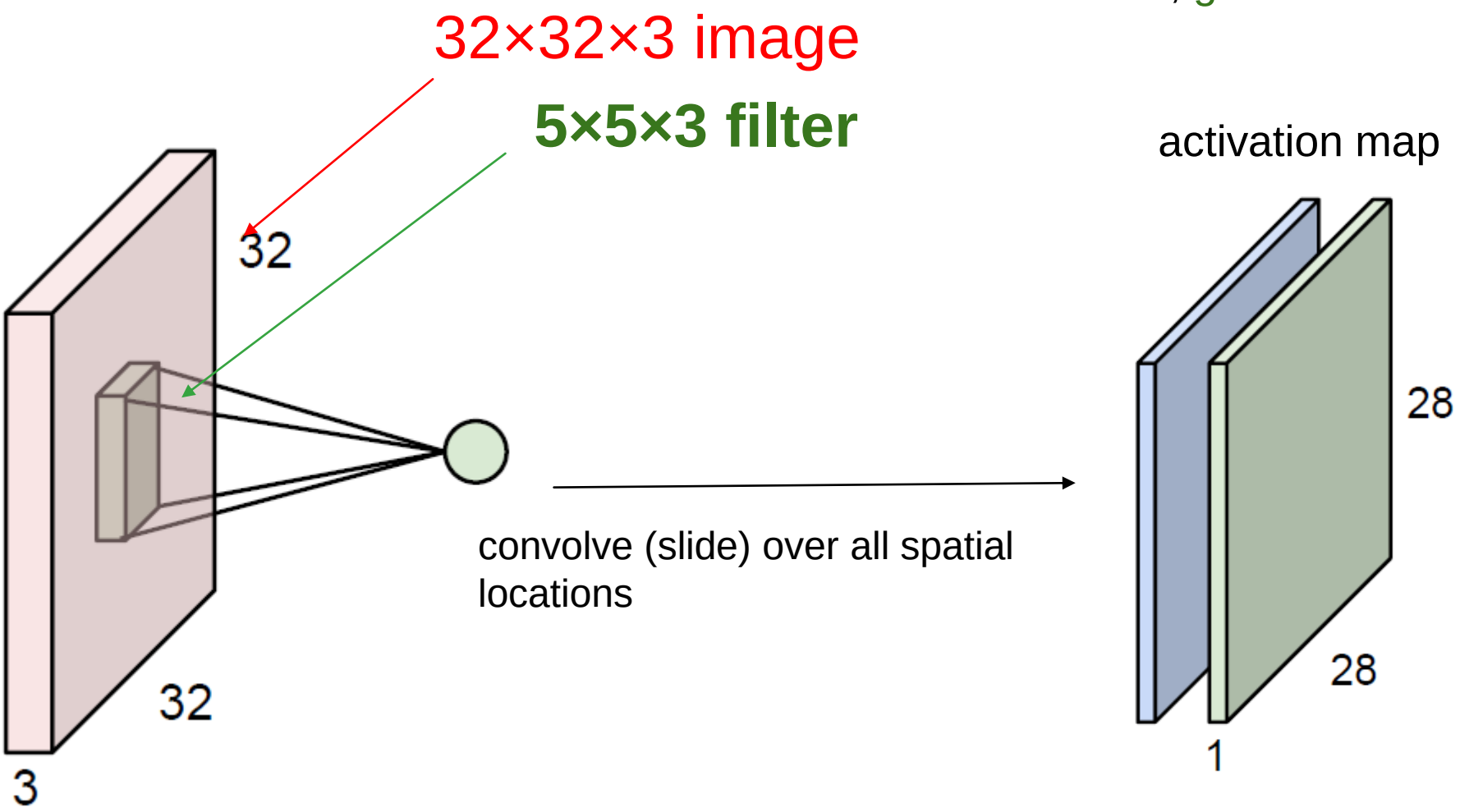
$$w^T x + b$$

Convolution Layer



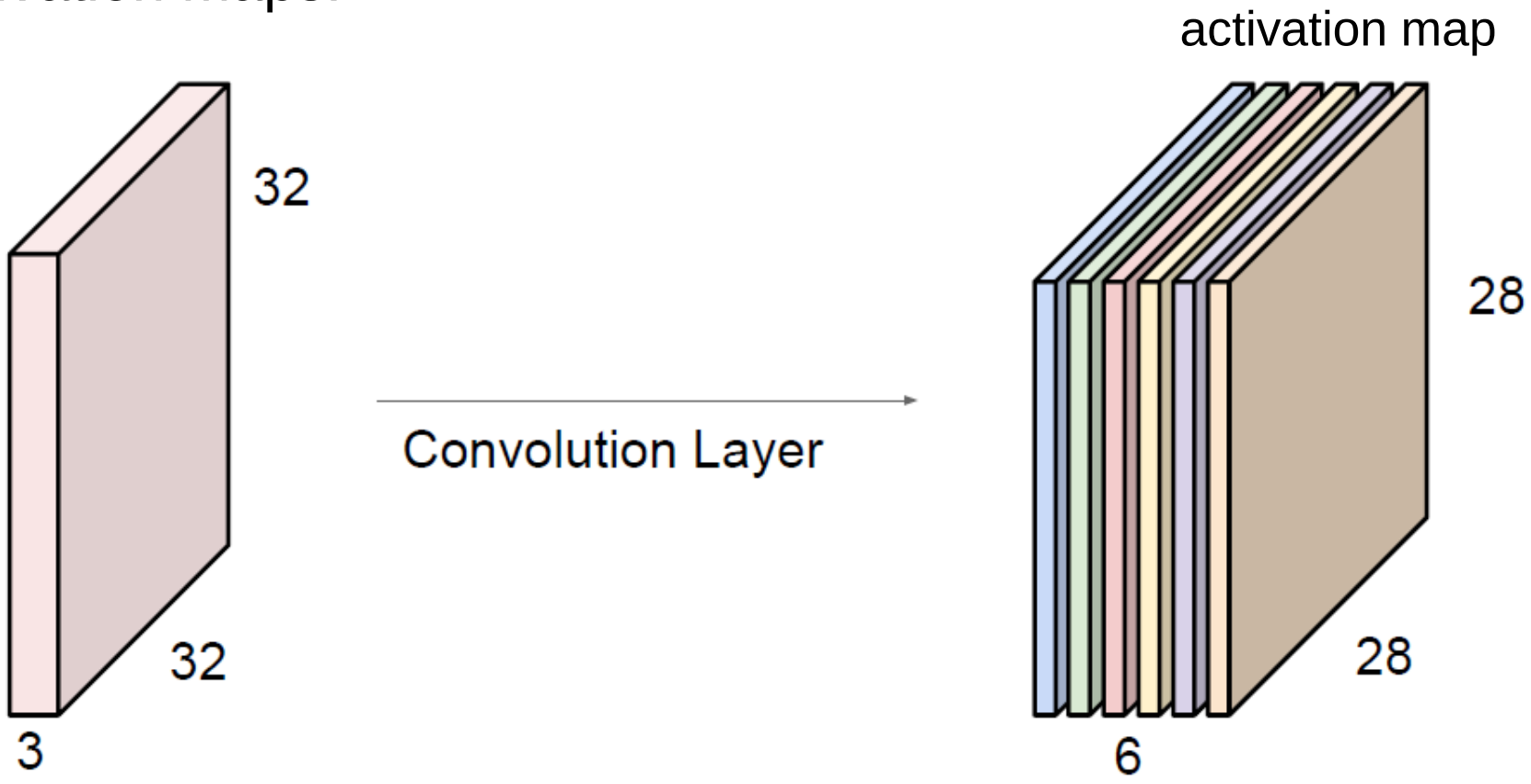
Convolution Layer

consider a second, green filter



Convolution Layer

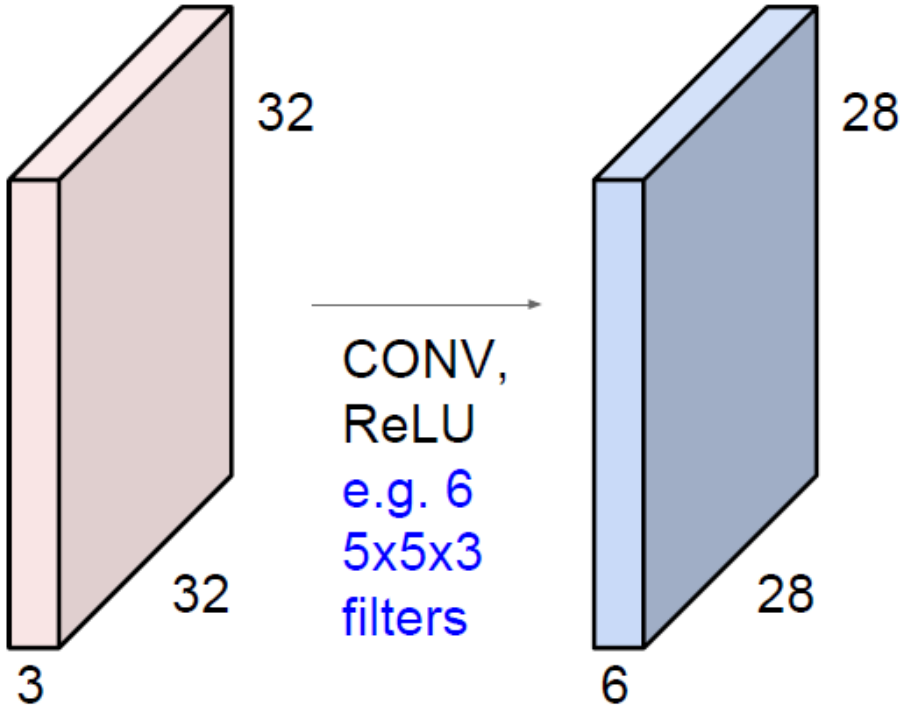
For example, if we had 6 5x5 filters, we'll get 6 separate activation maps:



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

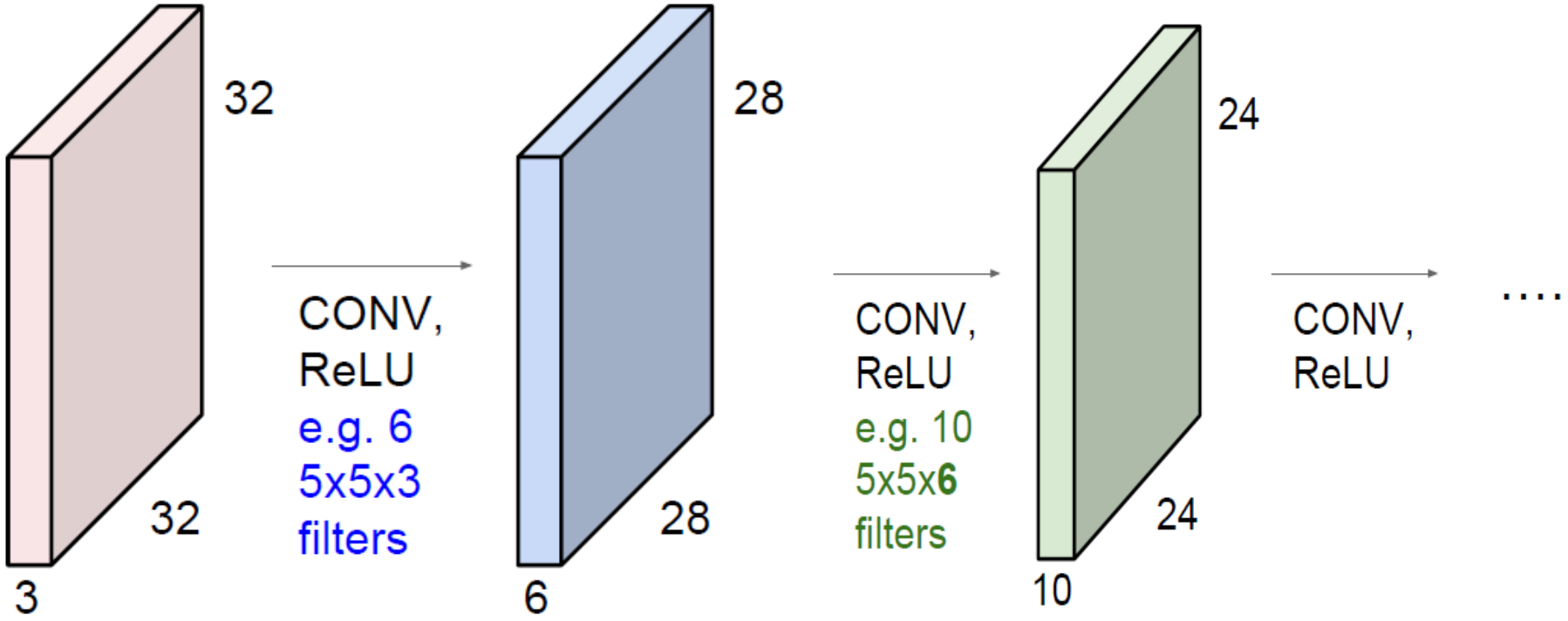
Convolutional Layers

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



Convolutional Layers

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



Convolutional Networks (CNNs)

- Connections are **restricted**: hidden units are connected identically to neighbours to encode shift/delays
- Training using back prop. but with ties weights across shifted units (***weight sharing***)
- The resulting MLP has much fewer weights to train than a traditional MLP

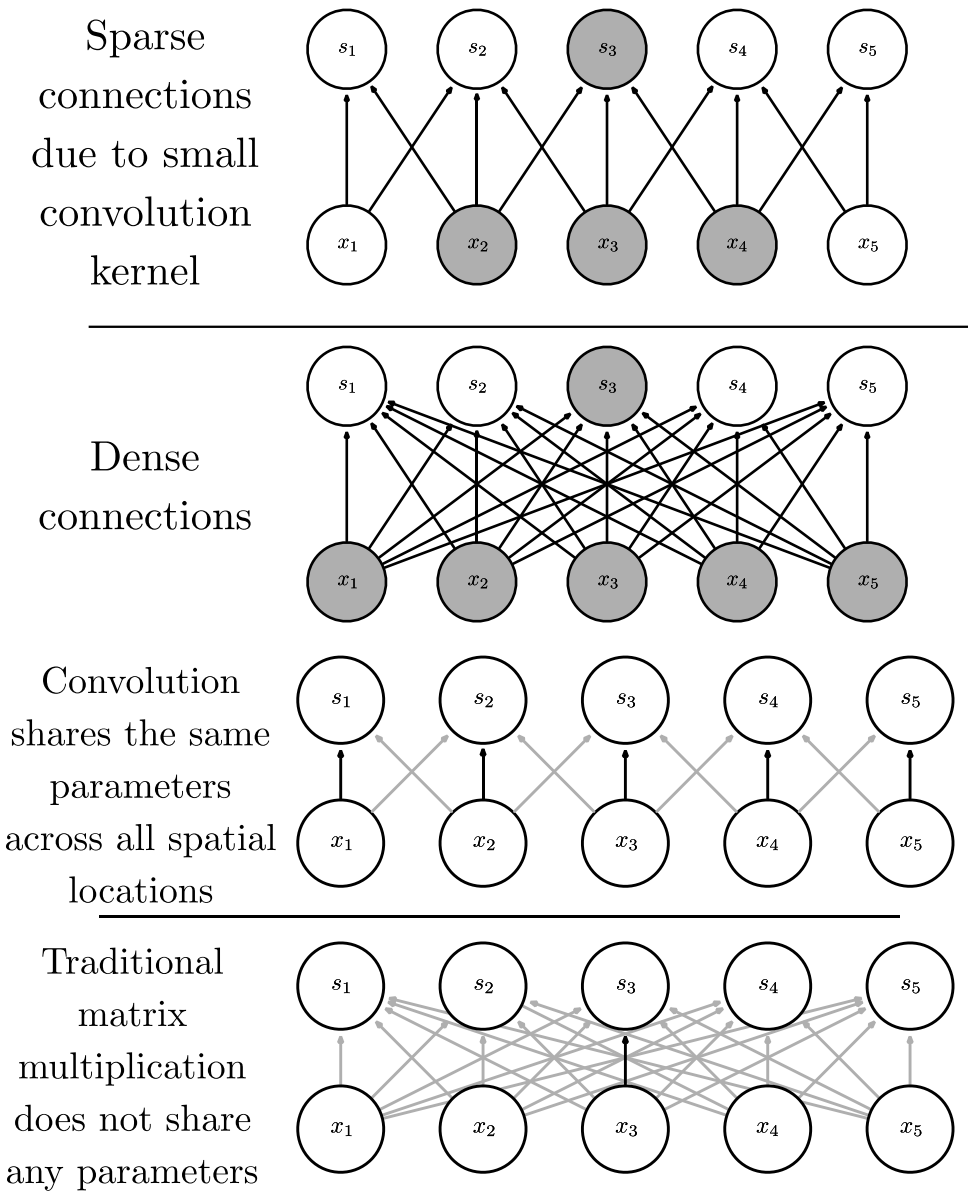


Figure from Goodfellow, Bengio and Courville, Deep Learning, MIT Press, 2016

Convolutional Networks (CNNs)

- Growing "*influence*" with depth ➔
  (the top layer is influenced by a large span of inputs despite only connected to 3 previous units)

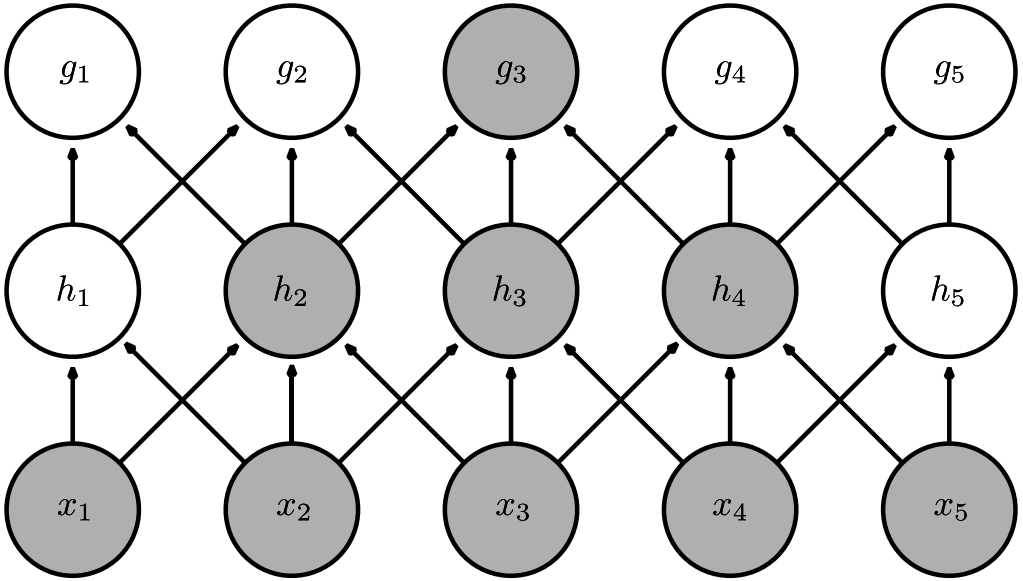
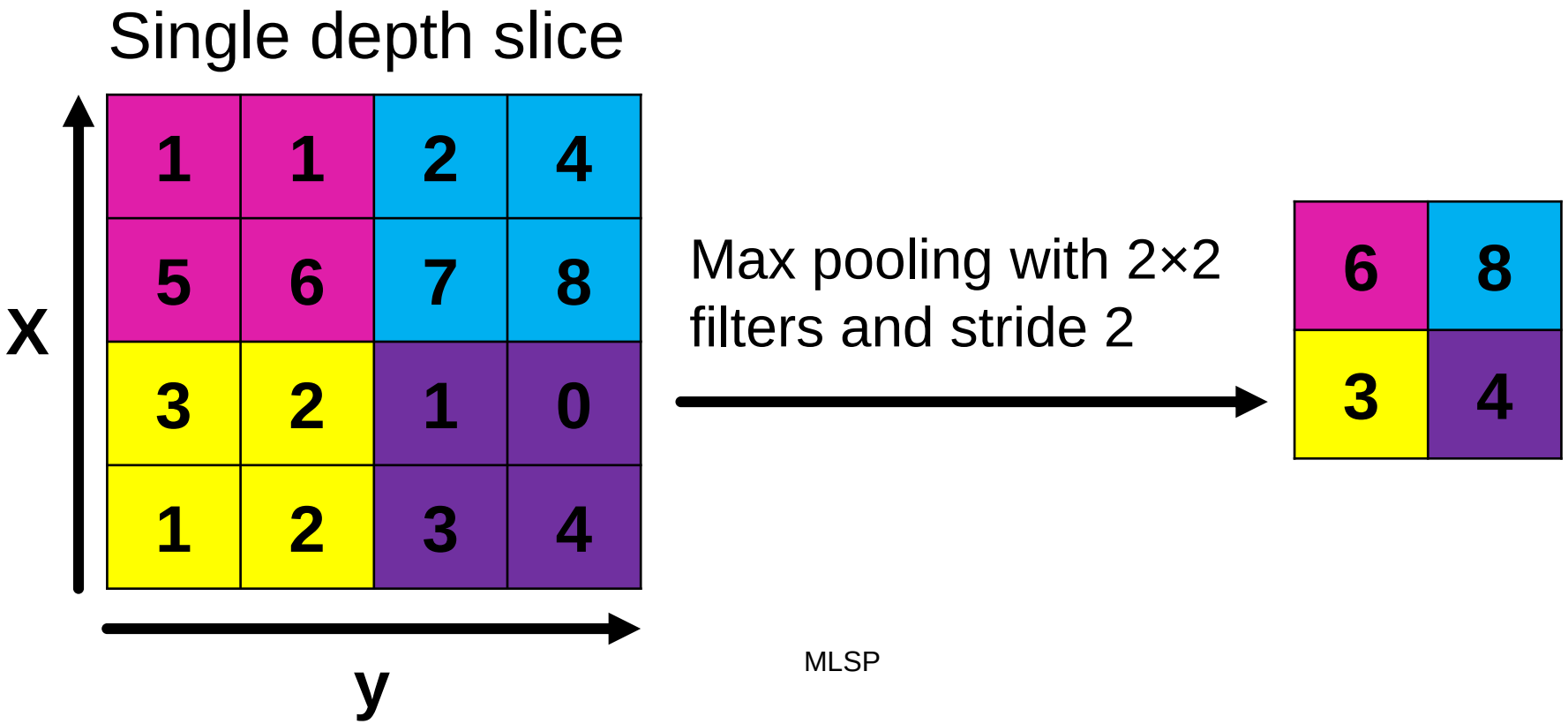


Figure from Goodfellow, Bengio and Courville, Deep Learning, MIT Press, 2016

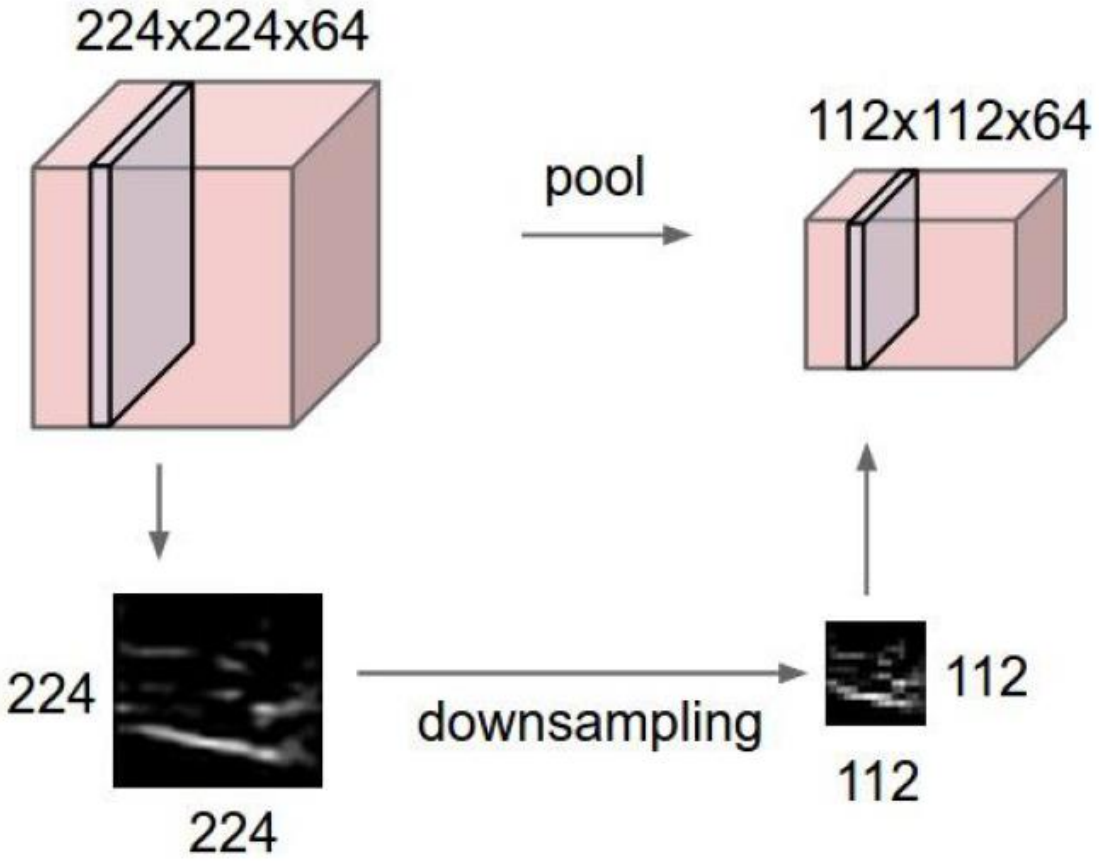
Pooling

- *Max pooling* helps with invariance and *down sampling* reduces number of parameters
  - Reduces dimensionality of representations



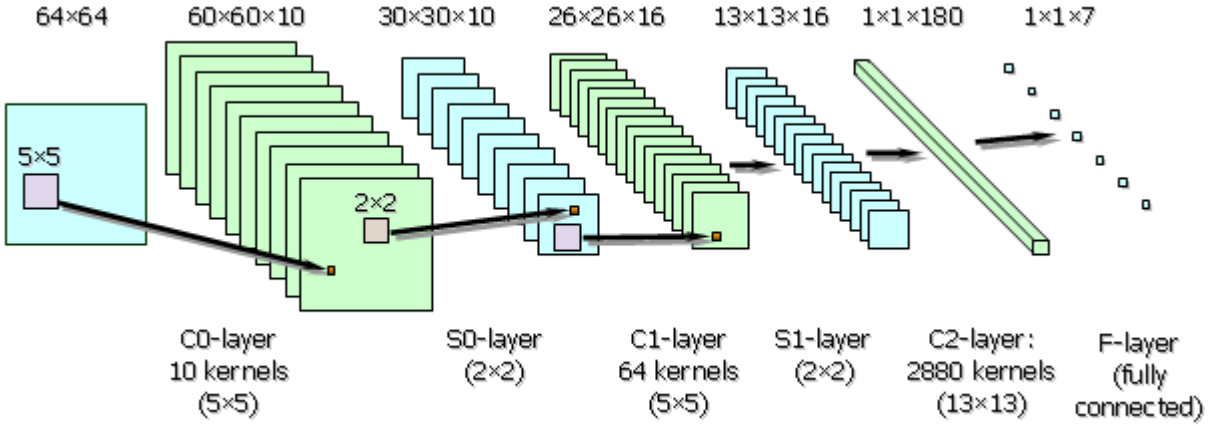
Pooling on the layers

- Important to remember that pooling operates on each activation map independently



CNNs & Deep Learning

- CNNs are often considered the ancestors of Deep Learning.
- The idea is to use MLP with many (≥ 3) hidden layers. This involves lots of 'tricks' to make training work: convolution, subsampling, pooling of outputs,…, pretraining (helps to start the weights with good initial values)



Application to face detection and pose estimation

but exhibit state-of-the-art performance…

e.g. see - http://www.cs.nyu.edu/~yann/research

Deep learning has many hyperparameters

- Network design
- Activation function
- Optimisation choices
- **Lots of 'tricks' to make training work**: convolution, subsampling, pooling of outputs,…, good initialisation, pretraining (helps to start the weights with good initial values), batch normalisation, learning rate schedules, Adam, RMSprop, SELu, PreLu, noise injection, label smoothing,…, …, …, …, …, …, …, …, …, …, …, …

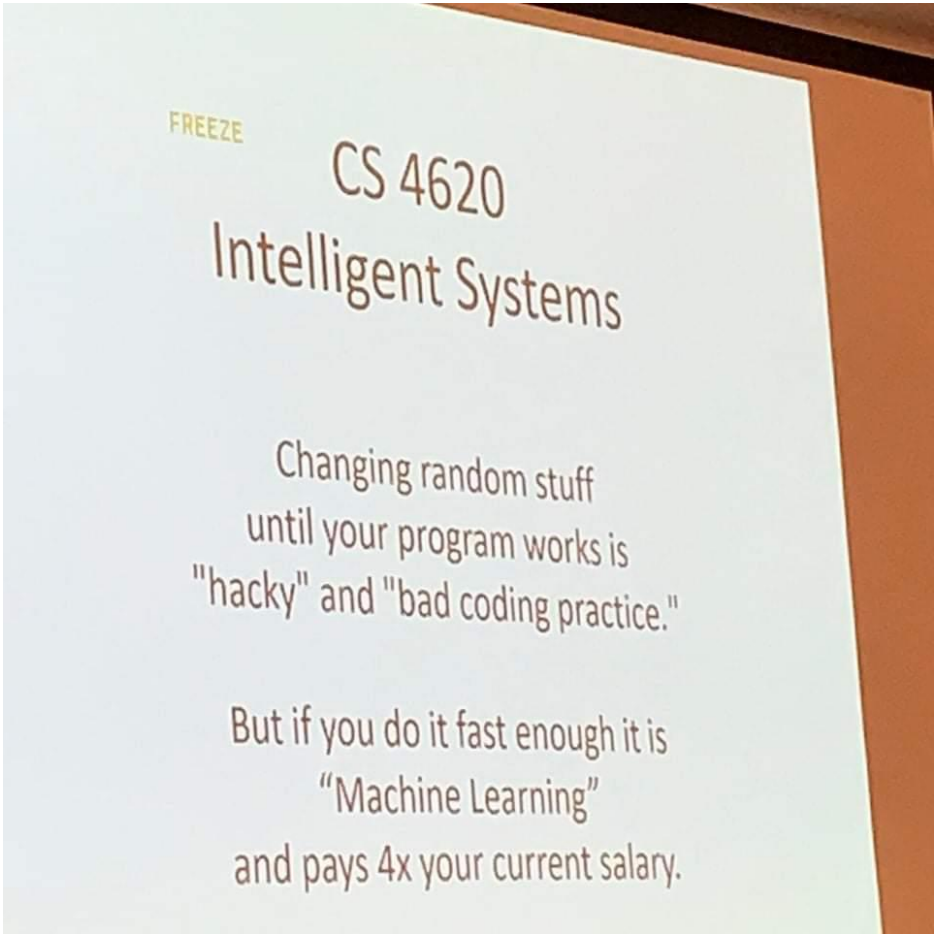


Image source: I saw it on https://www.reddit.com/r/MachineLearning/, but supposedly it is taken from a course at CS 4620. No copyright claimed. Original source unknown.

More Demos

- http://cs.stanford.edu/people/karpathy/convnetjs/

Some additional info

- Additional slides on machine learning and deep learning and particularly in augmentation are here: https://edin.ac/2vSP6T3 (Tutorial at ICASSP 2019 on Data augmentation techniques for deep learning)