CS7150 Deep Learning

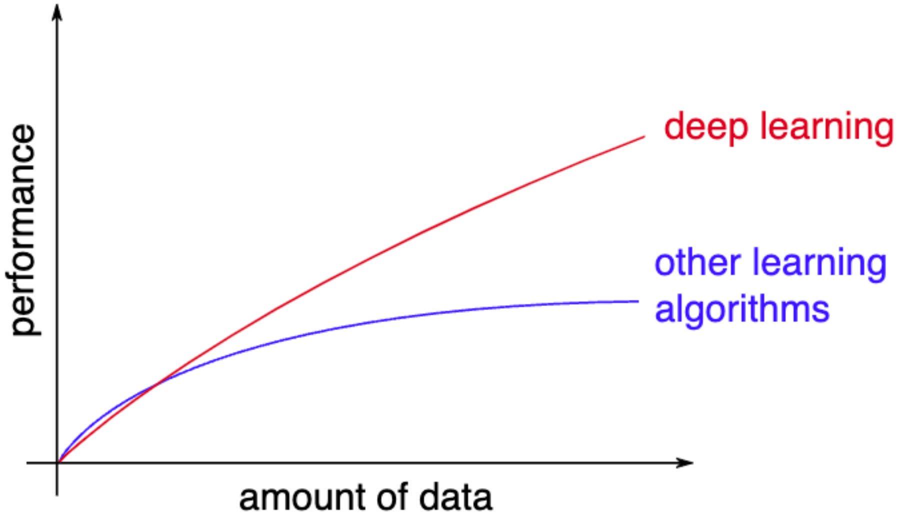
Jiaji Huang

https://jiaji-huang.github.io

01/20/2024

Recap of Last Lecture

- What is DL and why is it useful
- Cool Applications
  - Images, speech, text, robotics, …
- PyTorch
  - Auto-grad
- Linear Algebra, probabilities
  - Linear Least Squares
  - SVD
  - Gradient, Chain rule
  - Gaussian Distribution and its mixture
  - Entropy, Cross Entropy



Agenda

- Machine Learning Paradigms
- Non-Parametric v.s. Parametric Models
- Linear Classifier
- Multi-layer Perceptron (MLP)

Supervised Learning

- Training: learns a model $f: \boldsymbol{x} \longmapsto y$, from data like $\{(\boldsymbol{x}_i, y_i)\}$
- Testing: Use the model to predict y given $\boldsymbol{x}$, i.e. $\hat{y} = f(\boldsymbol{x})$
- Examples:
  - Regression: numeric target

```
data = {
    {4 yr, "Female"} → 3.3 kg,
    {6 yr, "Male"} → 4.5 kg,
    {5 yr 3 mo, "Male"} → 5.1 kg,
    {1 yr 3 mo, "Female"} → 1.7 kg
  };
```

{5 yr, "Female"} →?

Example from this [page]()

Supervised Learning

- Classification: categorical target

( , 0)

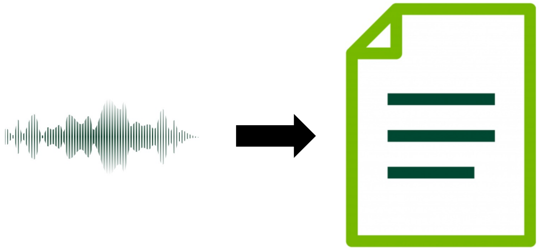
( , 1)

 ?

Supervised Learning

- Classification with structured target

Speech recognition



Translation

We are attending a deep learning class

我们正在参加深度学习课程

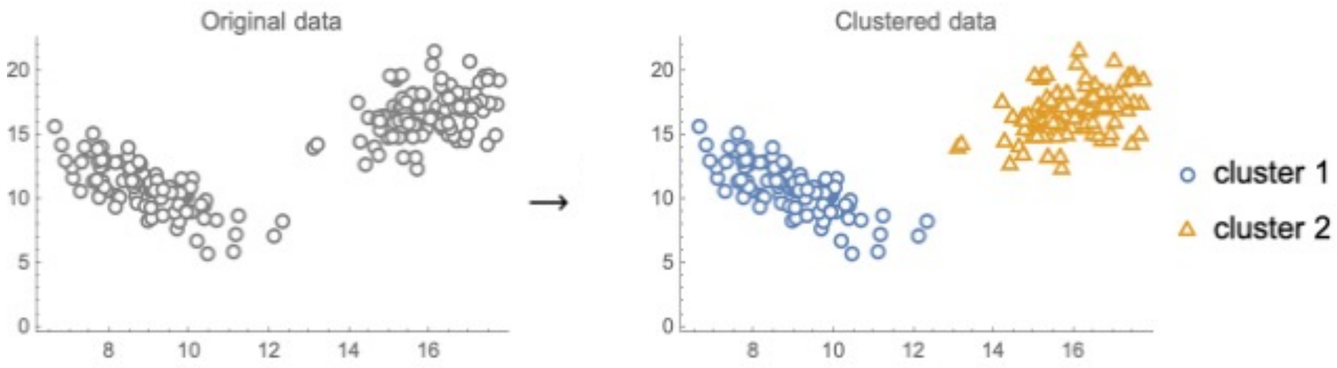
- Classification + regression

Object detection

person → {Rectangle[{0.32, 0.13}, {2.6, 7.8}], ...}
bus → {Rectangle[{7.8, 5.1}, {10, 6.6}], ...}
stoplight → {Rectangle[{1.9, 7.2}, {2.5, 8.9}]}
automobile → {Rectangle[{6.2, 4.5}, {7.2, 5.9}]}
motorcycle → {Rectangle[{9., 1.3}, {9.9, 4.7}]}

Unsupervised Learning

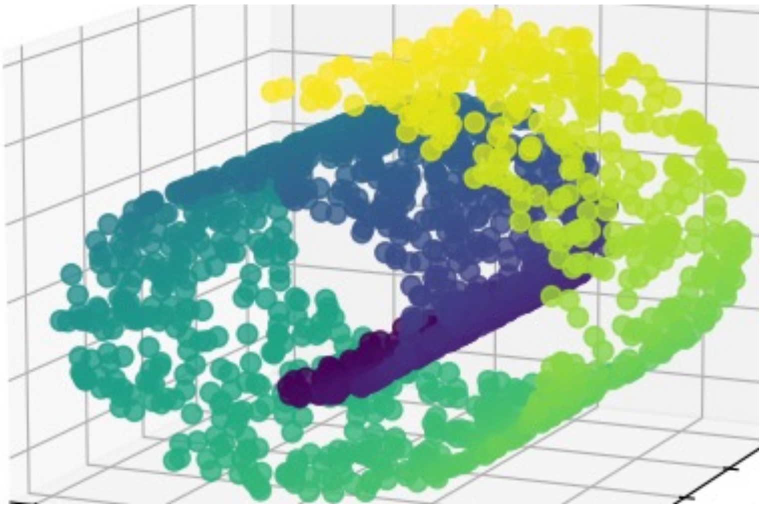
- Given input $\boldsymbol{x}$, learn something about $p_{data}(\boldsymbol{x})$
- Clustering (recap last lecture: infer the latent variable via EM)

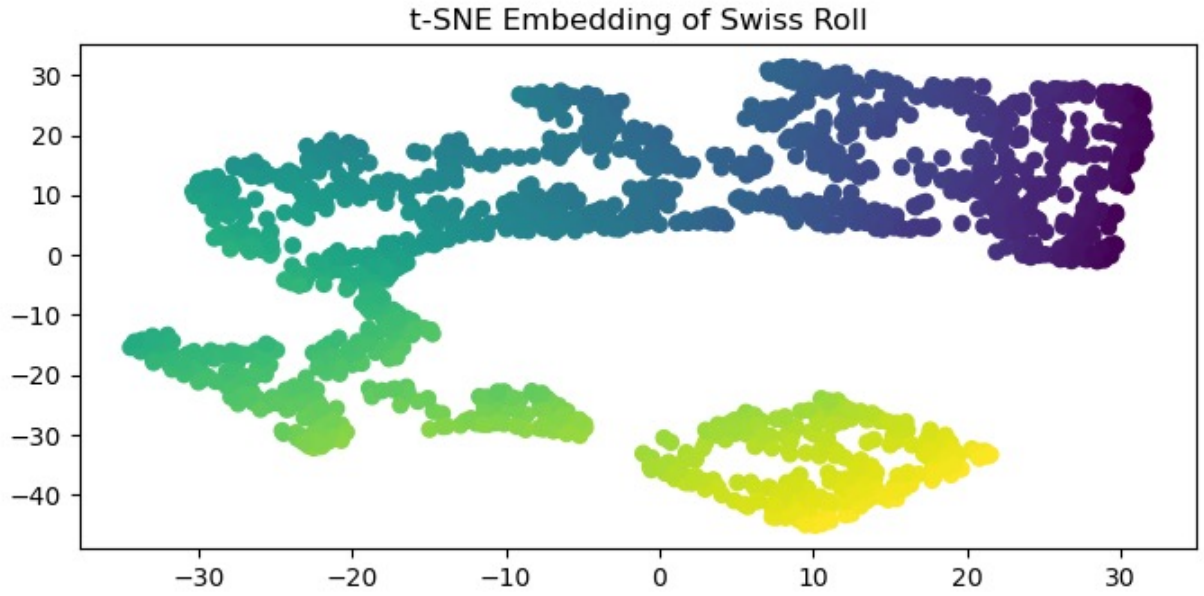


- Generation: sample from $p_{data}(\boldsymbol{x})$

Unsupervised Learning

- Dimension Reduction
  - PCA
  - Non-linear dimension reduction





Example from [sklearn page]

Reinforcement Learning

- Learning by interacting with environment, and
- Maximizing reward

Paradigms can be combined

- Semi-supervised learning
  - Input: $\{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}$ and $\{\boldsymbol{x}_j\}$
  - Output: $\boldsymbol{y}_j$'s
  - Jointly modeling $\{\boldsymbol{x}_i\} + \{\boldsymbol{x}_j\}$

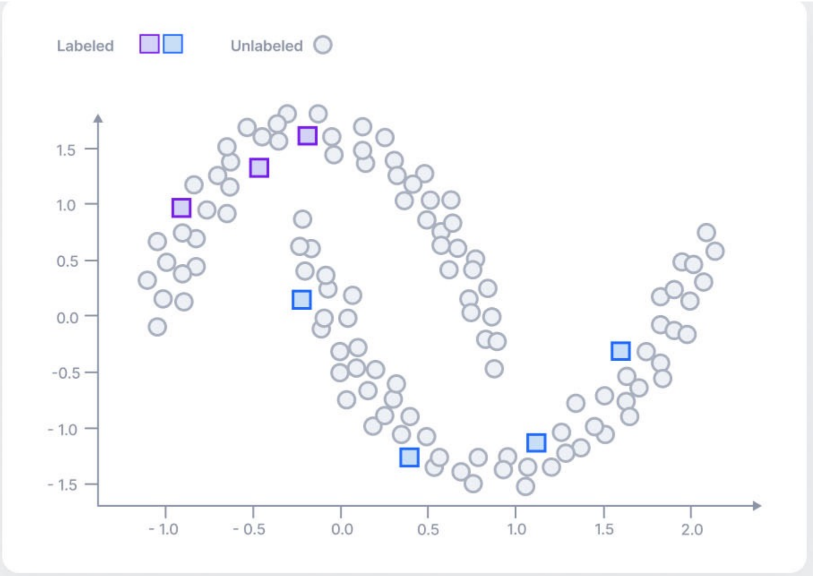
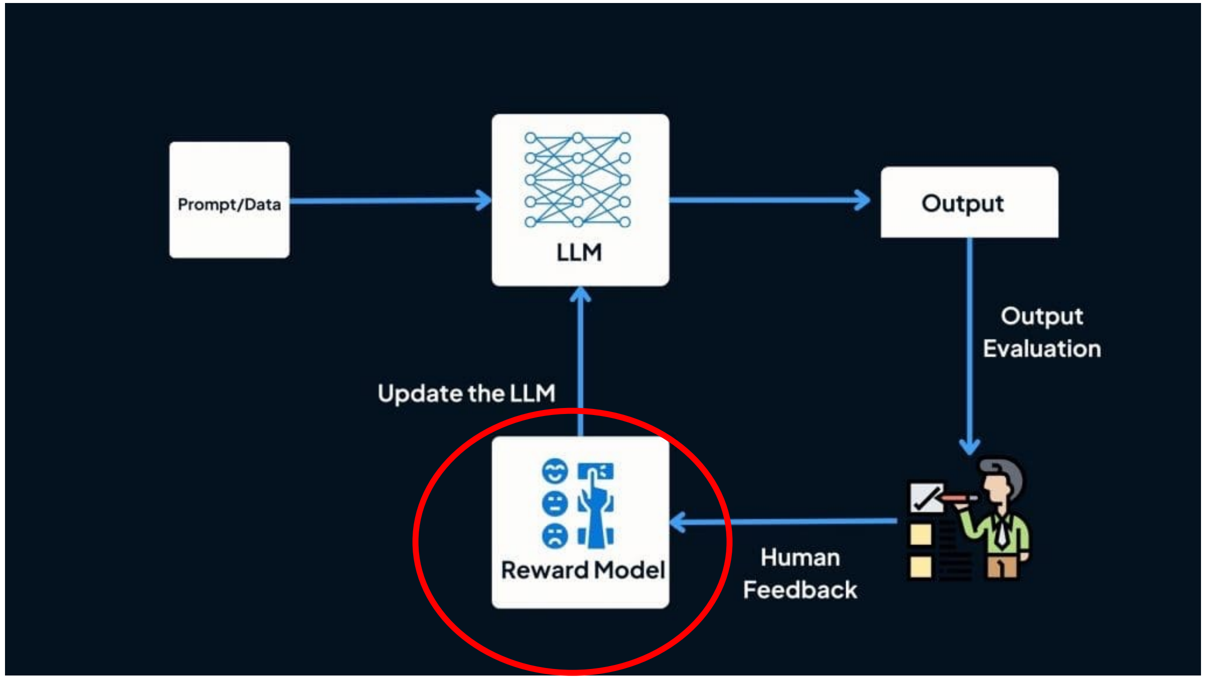


Illustration from [here]() and [here]()

- Reinforcement Learning with Human Feedback (RLHF)



supervised

Agenda

- Machine Learning Paradigms
- Non-Parametric v.s. Parametric Models
- Linear Classifier
- Multi-layer Perceptron (MLP)

Let's focus on Supervised Learning in the following

- Training: learns a model $f: \boldsymbol{x} \longmapsto \boldsymbol{y}$, from data like $\{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}$
- Testing: Use the model to predict $\boldsymbol{y}$ given $\boldsymbol{x}$, i.e. $\hat{y} = f(\boldsymbol{x})$

Non-parametric Model

- Doesn't assume a specific form for $f(\boldsymbol{x})$
- Example: Nearest Neighbor Classifier
  - Stores all training data
  - Take k-nearest neighbors
  - Vote on the label by neighbors' labels
  - Question:
    - How to decide k?
    - What distance to use?

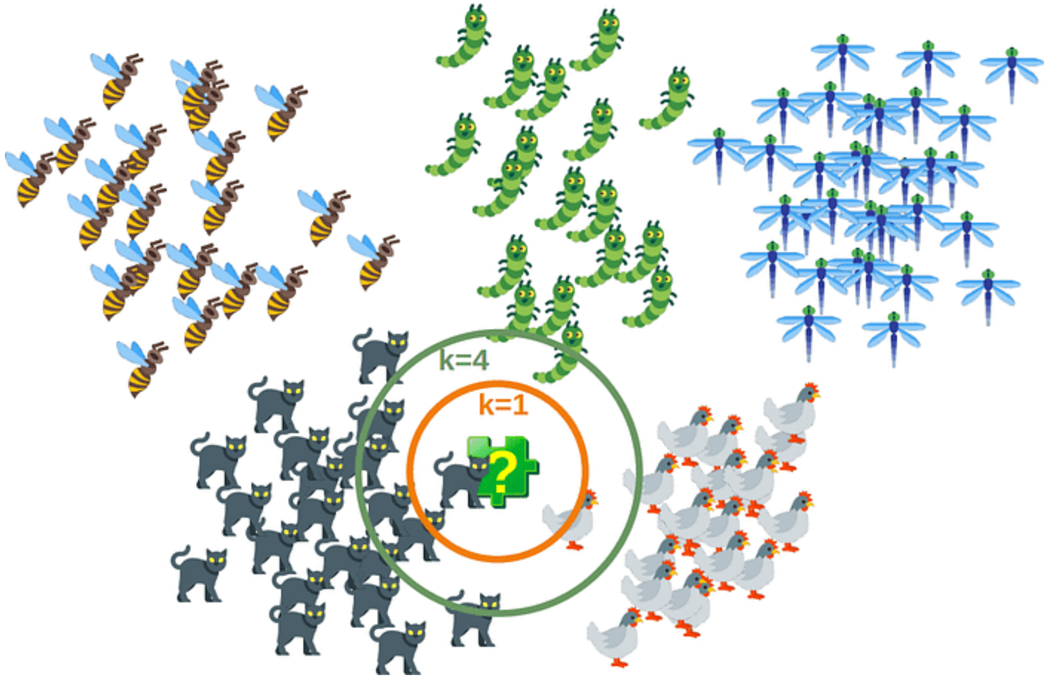


Illustration from here

Hyper-parameters

- The k and choice of distance
- Dangerous idea:
  - Try a bunch, and check which works best for testing
  - As testing data couldn't be access at training
- If we have a validation set, use that
- If not, N-fold cross validation

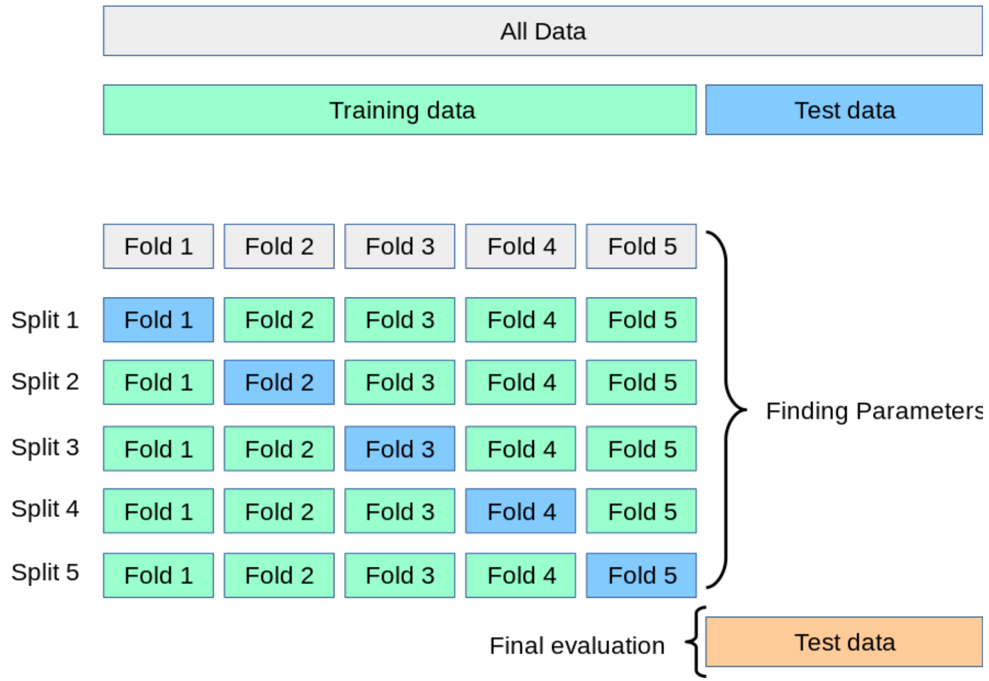


Illustration from [sklearn page]

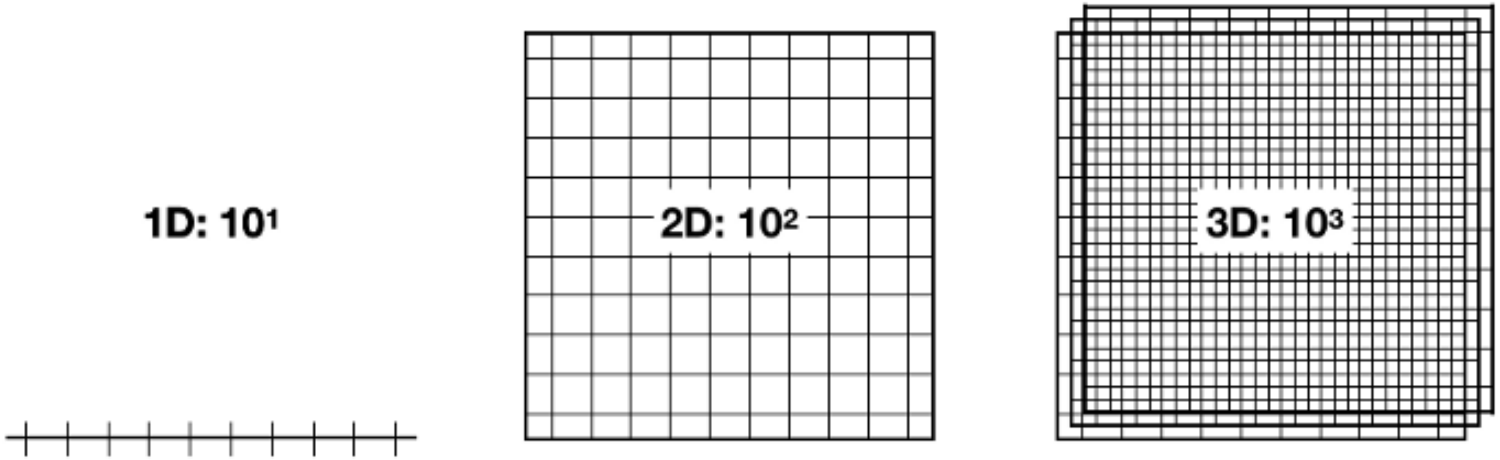
KNN is only for toy problems though

- Consider 128x128 Image classification
  - Flattening the 2D images leads to 16,384 dimensional vector!
- Many irrelevant dimensions
  - E.g.,Background behind the object

Illustration from here and here

KNN is only for toy problems though

- Curse of dimensionality
  - Very sparse point cloud: all distance are big, NN becomes less reliable
  - There are hubs, very popular nearest neighbors



The number of features required to keep average distance constant grows exponentially with the number of dimensions.

Illustration from [here]

KNN is only for toy problems though

- Expensive:
  - stores all training data,
  - computational cost $\propto$ #samples $\times$ dimension
  - Resort to approximate NN search
- Dimension Reduction necessary
  - Recall PCA

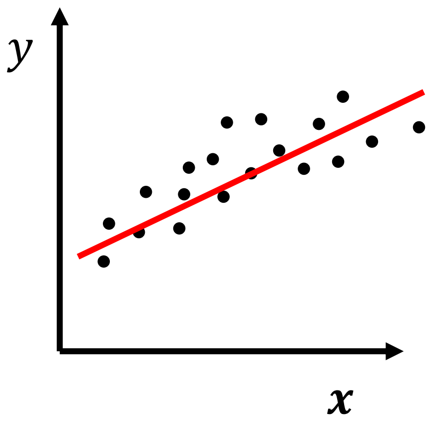
Parametric Model

- Specify explicit form of $f(\boldsymbol{x}; \boldsymbol{\theta})$ with parameter $\boldsymbol{\theta}$
- Example:
  - linear regression $f(\boldsymbol{x}) = \boldsymbol{w}^T\boldsymbol{x} + b$, $\boldsymbol{\theta} = \{\boldsymbol{w}, b\}$
  - Logistic regression
  - Softmax classifier
  - Deep nets

  We will talk about them later this lecture
- Train: learn $\boldsymbol{\theta}$ from training samples $\{(\boldsymbol{x}_i, y_i)\}$
- Test: for testing sample $\boldsymbol{x}$, predict using $f(\boldsymbol{x})$

Linear regression

- Parametric form $f(\boldsymbol{x}) = \boldsymbol{w}^T\boldsymbol{x} + b$
- Learn $\boldsymbol{w}$ and b from samples $\{(\boldsymbol{x}_i, y_i)\}$, by solving



$$\min_{\boldsymbol{w},b} \sum_{i=1}^{n} \|\boldsymbol{w}^T\boldsymbol{x}_i + b - y_i\|^2$$

$$\equiv \left\|\widetilde{\boldsymbol{X}}\widetilde{\boldsymbol{w}} - \boldsymbol{y}\right\|^2$$

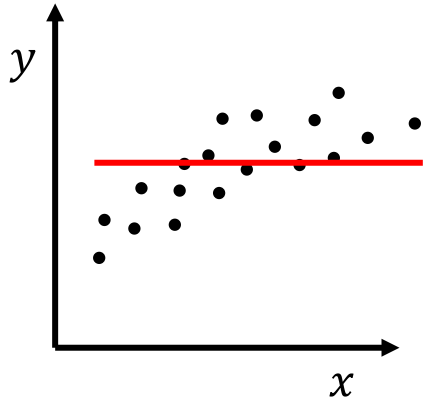
Where $\widetilde{\boldsymbol{X}} = \begin{bmatrix} \boldsymbol{x}_1^T, 1 \\ \vdots \\ \boldsymbol{x}_n^T, 1 \end{bmatrix}, \widetilde{\boldsymbol{w}} = \begin{bmatrix} \boldsymbol{w} \\ b \end{bmatrix}, \boldsymbol{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$

- Revisit last lecture, $\widetilde{\boldsymbol{w}}^* = \widetilde{\boldsymbol{X}}^\dagger\boldsymbol{y}$

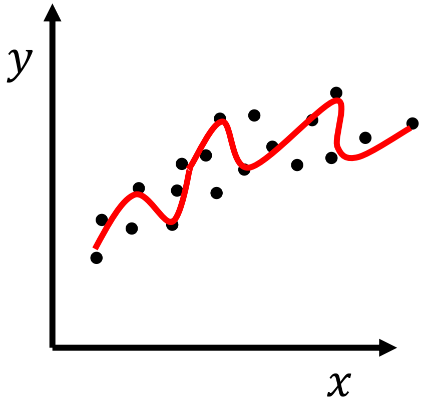
Degree of the polynomial

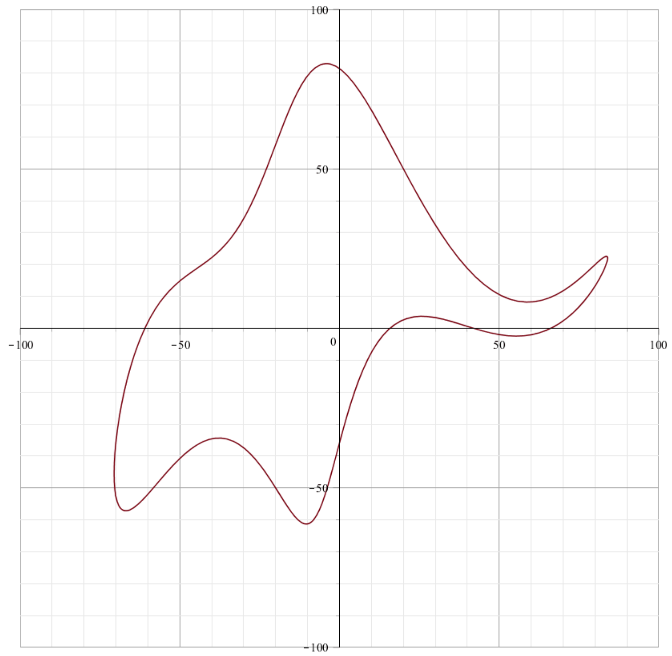
> "With four parameters I can fit an elephant, and with five I can make him wiggle his trunk."
> --- John von Neumann

- Lower degree
  - Pros: avoid overfitting
  - Cons: less powerful



- Higher degree
  - Pros: more powerful
  - Cons: overfits

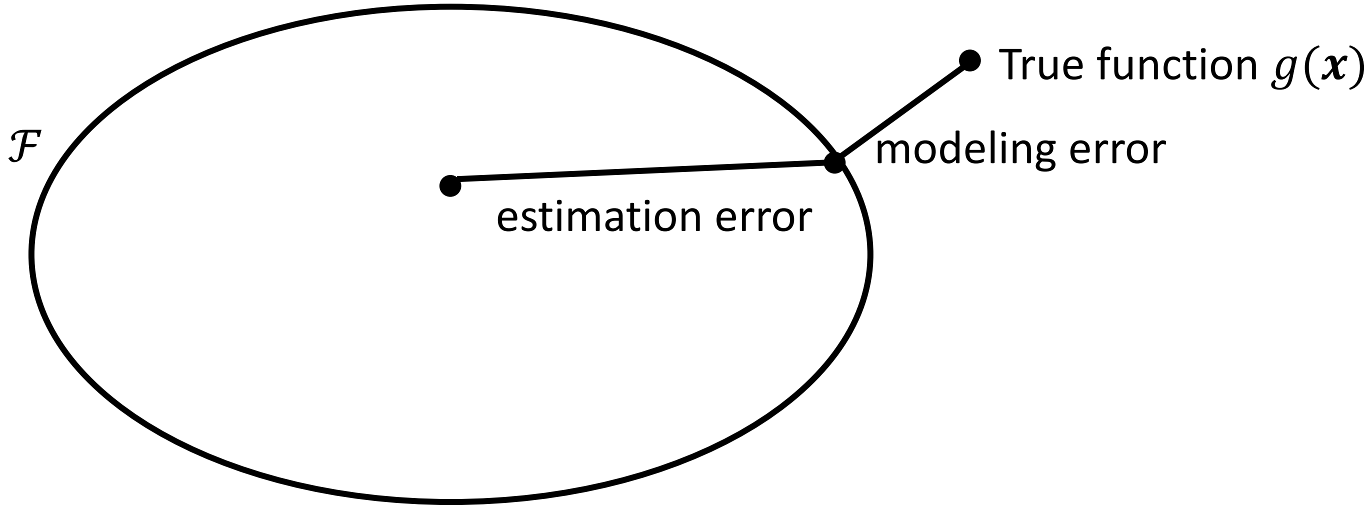




Fermi-Neumann elephant

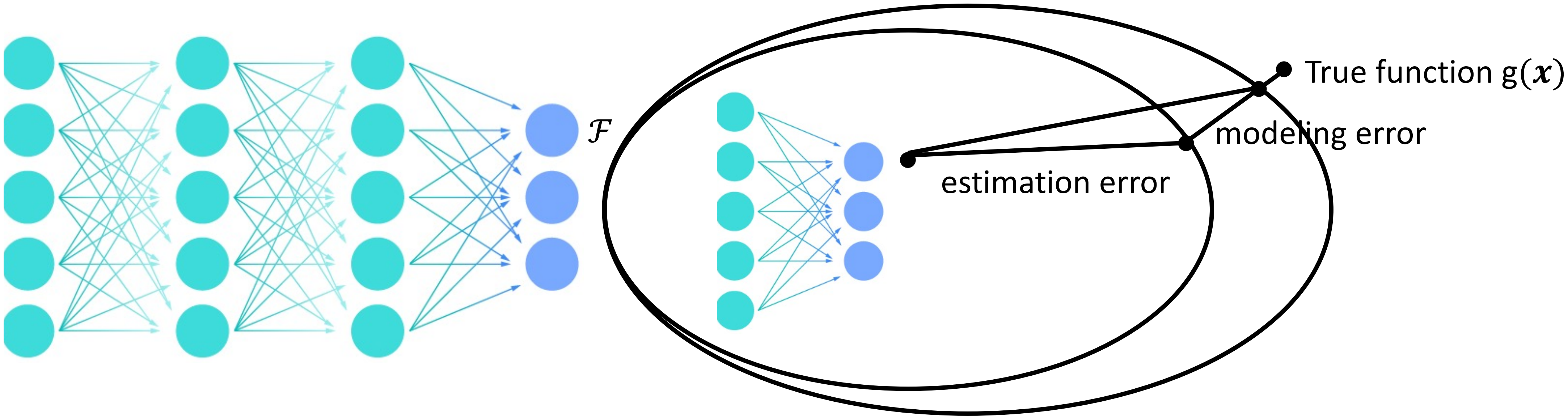
Generalization

- The ability to predict well on unseen samples
- Model family $\mathcal{F} = \{f_{\boldsymbol{\theta}}(\boldsymbol{x})\}$
- Generalization error: expected error/loss on a test input
- $\approx$ modeling error + estimation error



Cartoon adapted from [OMCS lecture slides]

Bias Variance trade-off View



- Modeling error is bias
- Estimation error is variance w.r.t. training data
- bigger $\mathcal{F}$: modeling error↓, but estimation error ↑

Cartoon adapted from [OMCS lecture slides]

Bias Variance trade-off View

- $y = g(\boldsymbol{x}) + \varepsilon$, ε noise with mean=0, std=σ
- Learn a predictor $\hat{y} = f(\boldsymbol{x}; \mathcal{D})$ by minimizing Mean Square Error (MSE) on training set $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}$
- The generalization error is

$$\begin{aligned}
\mathbb{E}_{\mathcal{D},\varepsilon}[(y-\hat{y})^2] &= \mathbb{E}_{\mathcal{D},\varepsilon}[(g(\boldsymbol{x}) - f(\boldsymbol{x};\mathcal{D}) + \varepsilon)^2] \\
&= \mathbb{E}_{\mathcal{D}}\left[[g(\boldsymbol{x}) - f(\boldsymbol{x};\mathcal{D})]^2\right] + \mathbb{E}_{\varepsilon}[\varepsilon^2] \\
&= \mathbb{E}_{\mathcal{D}}\left[[g(\boldsymbol{x}) - \mathbb{E}_{\mathcal{D}} f(\boldsymbol{x};\mathcal{D}) + \mathbb{E}_{\mathcal{D}} f(\boldsymbol{x};\mathcal{D}) - f(\boldsymbol{x};\mathcal{D})]^2\right] + \sigma^2 \\
&= \underbrace{[g(\boldsymbol{x}) - \mathbb{E}_{\mathcal{D}} f(\boldsymbol{x};\mathcal{D})]^2}_{\text{bias}^2} + \underbrace{\mathbb{E}_{\mathcal{D}}[f(\boldsymbol{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}} f(\boldsymbol{x};\mathcal{D})]^2}_{\text{variance}} + \underbrace{\sigma^2}_{\text{Irreducible error}}
\end{aligned}$$

More Interpretations

- How to generalize well?
- Reduce bias: small training loss, rich $\mathcal{F}$
- Reduce variance: small gap between testing and training loss
  - Bigger training set
  - Regularization: constrain to a subset of $\mathcal{F}$

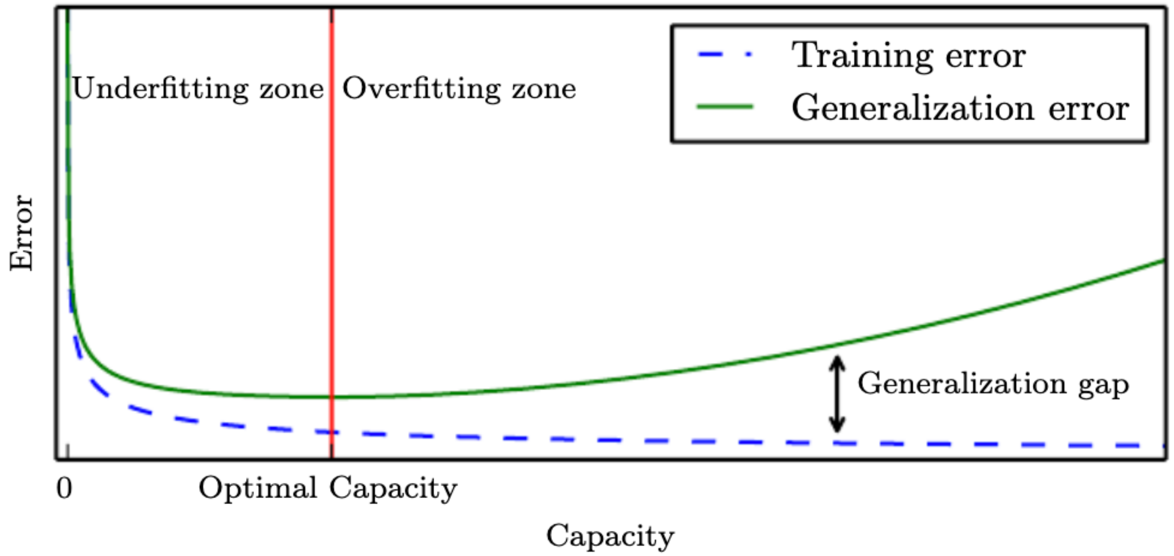


Illustration from textbook chapter 5

20 years of research in Learning Theory oversimplified

If you have:

Enough training data $\mathcal{D}$ and

$\mathcal{F}$ is not too complex

Then:

probably we can generalize to unseen test data

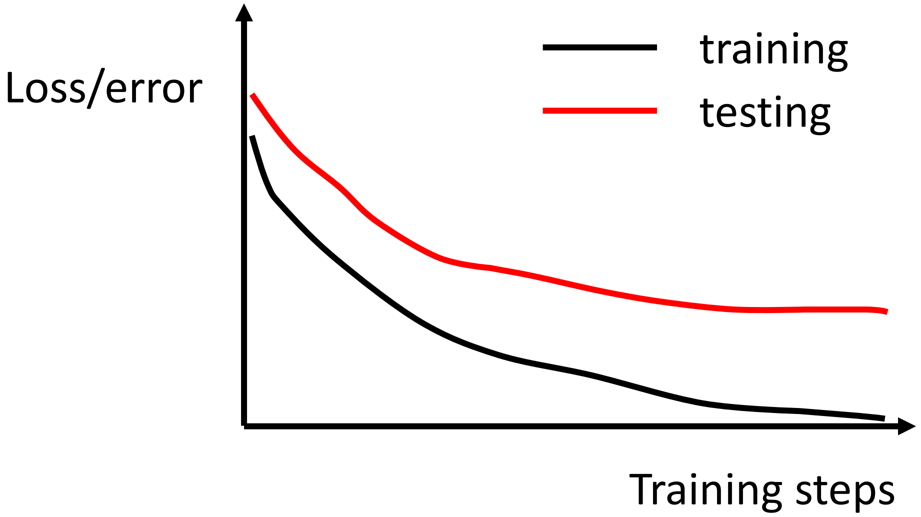
Caveats:

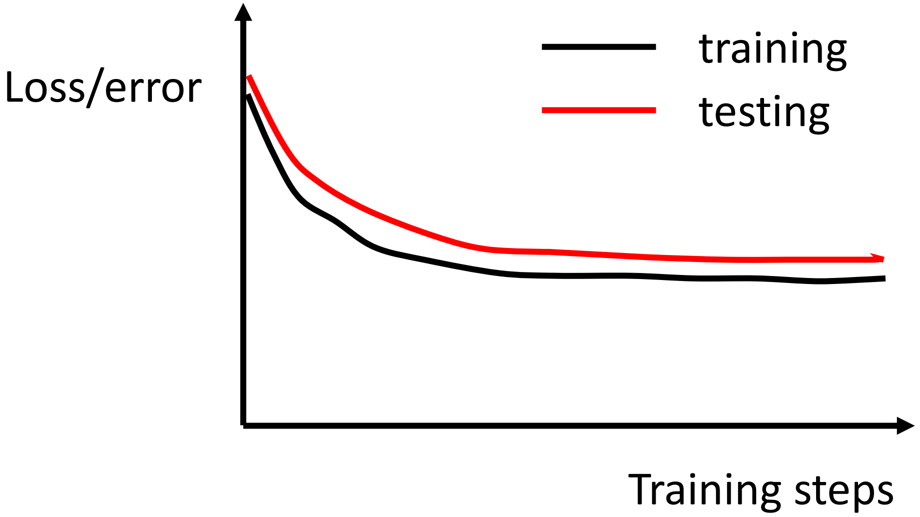
A number of recent empirical results (Zhang et. al) question our intuitions built from this clean separation.

Slides adapted from OMCS lecture slides (page 34)

Exercise

- Judge overfitting/underfitting from learning curves

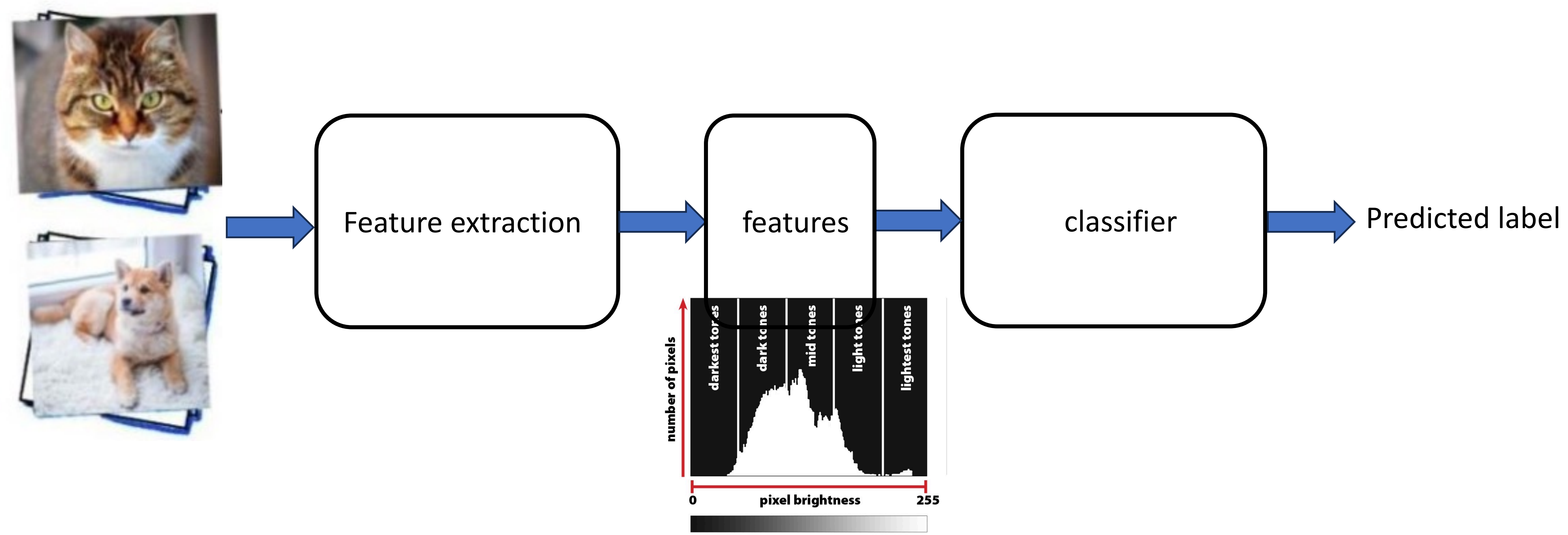




Agenda

- Machine Learning Paradigms
- Non-Parametric v.s. Parametric Models
- Linear Classifier
- Multi-layer Perceptron (MLP)

Classification problem

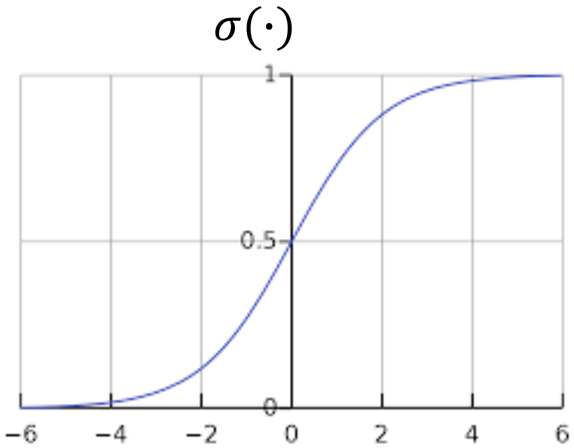


- Before deep learning, we hand-craft the features, e.g., histogram
- With deep learning, we learn the features jointly with classifier

Illustration of histogram from this [page]

Binary classification: Logistic Regression

- Use a hyperplane to separate the two classes
- $p(y=1|\boldsymbol{x}) = \sigma(\boldsymbol{w}^T\boldsymbol{x} + b)$
- $\sigma(z) = \frac{1}{1+e^{-z}}$: sigmoid function
- $\boldsymbol{w}^T\boldsymbol{x} + b$: logit



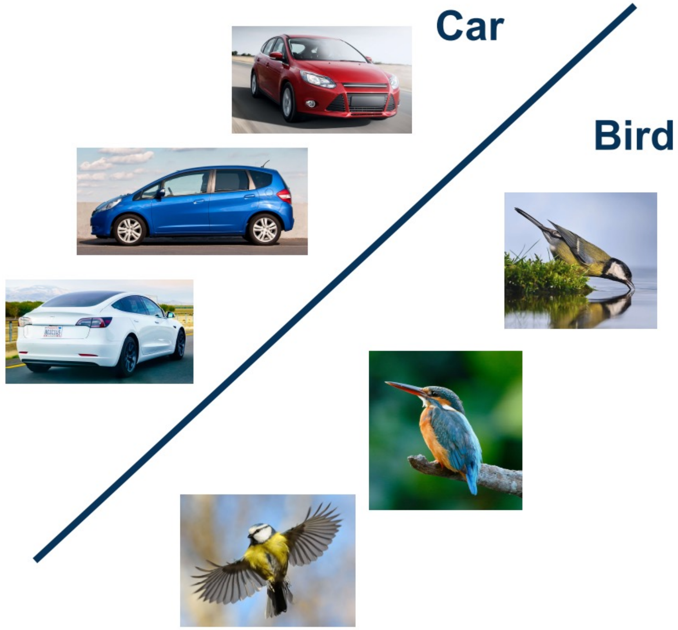


Illustration from [OMCS lecture 2 slides]

Training loss

- Recall Cross-entropy

$$\mathbb{E}_{y\sim p_{data}}[-\log p(y)]$$

- Discretize for each data sample, that's

$$\frac{1}{N}\sum_{i=1}^{N} -p_{data}(y_i = 1)\log p(y_i = 1|\boldsymbol{x}_i)$$
$$-p_{data}(y_i = 0)\log p(y_i = 0|\boldsymbol{x}_i)$$

- Compactly, that's

$$\frac{1}{N}\sum_{i} -y_i \log p(y_i = 1|\boldsymbol{x}_i) + (y_i - 1)\log[1 - p(y_i = 1|\boldsymbol{x}_i)]$$

Gradient

$$\frac{1}{N}\sum_i \{-y_i \log p(y_i = 1|\boldsymbol{x}_i) + (y_i - 1)\log[1 - p(y_i = 1|\boldsymbol{x}_i)] \equiv \ell_i\}$$

- Derive $\frac{\partial \ell_i}{\partial \boldsymbol{w}}$ and $\frac{\partial \ell_i}{\partial b}$ for $i \in \mathfrak{B}$ (some mini-batch)
- Then update

$$\boldsymbol{w} \leftarrow \boldsymbol{w} - \frac{1}{|\mathfrak{B}|}\sum_{i\in\mathfrak{B}} \frac{\partial \ell_i}{\partial \boldsymbol{w}}, \qquad b \leftarrow b - \frac{1}{|\mathfrak{B}|}\sum_{i\in\mathfrak{B}} \frac{\partial \ell_i}{\partial \boldsymbol{b}}$$

- Exercise: derive the gradients
  - Hint: denote $p_i = p(y_i = 1|\boldsymbol{x}_i)$, and invoke chain rule

Multi-class: softmax Classifier

- Multiple hyper-planes
- Defined by $\{(\boldsymbol{w}_c, b_c)\}, c = 1, \dots, C$
- Logits: $\{\boldsymbol{w}_c^T \boldsymbol{x} + b_c\}$
- $p(y = c|\boldsymbol{x})$ =softmax$_c(\{\boldsymbol{w}_c^T \boldsymbol{x} + b_c\})$
- Softmax$_c(\{z_c\}) = \frac{e^{z_c}}{\sum_{i=1}^{N} e^{z_i}}$

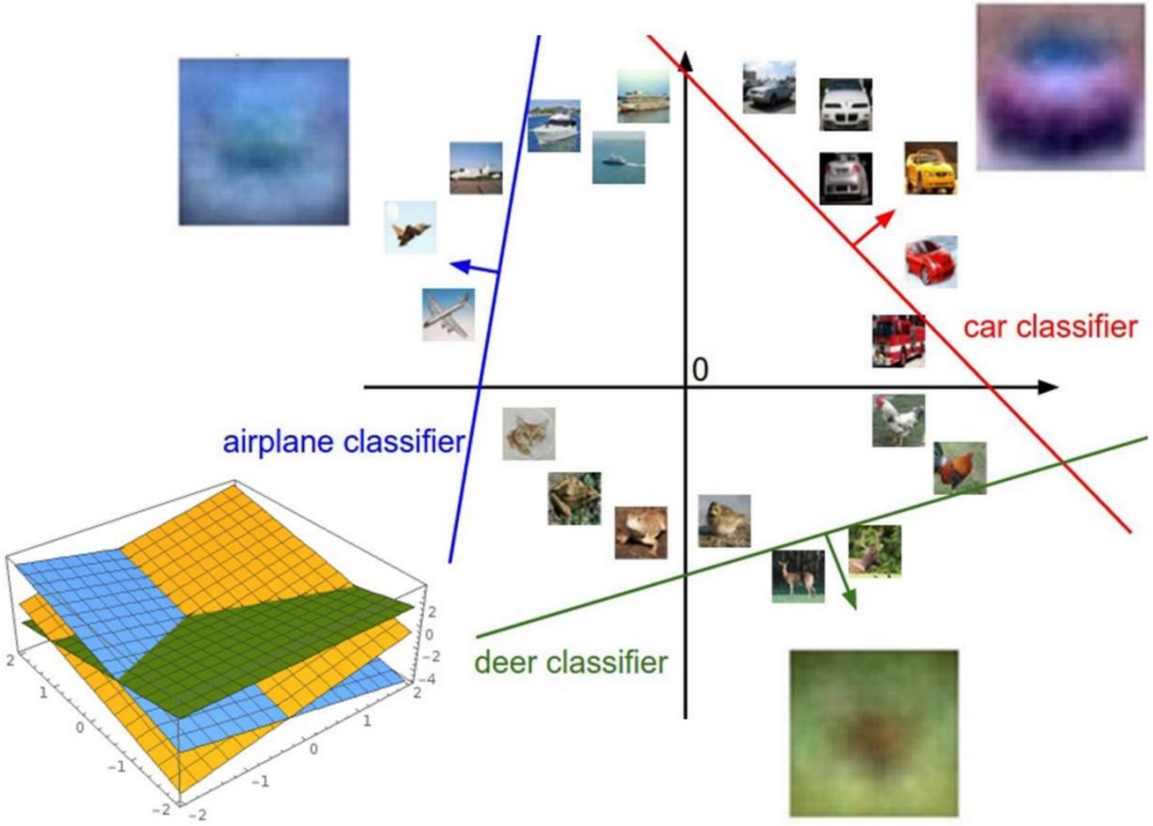


Illustration adapted from [OMCS lecture 2 slides]

Softmax

- E.g., C=3
- Logits {-1, 0, 1} corresponding to class ID: 0, 1, 2
- P(y=0)=$\frac{e^{-1}}{e^{-1}+e^{0}+e^{1}} = 0.090$
- P(y=1)=$\frac{e^{0}}{e^{-1}+e^{0}+e^{1}} = 0.245$
- P(y=2)=$\frac{e^{1}}{e^{-1}+e^{0}+e^{1}} = 0.665$

Training Softmax Classifier

- Cross Entropy

$$\mathbb{E}_{y\sim p_{data}}[-\log p(y)]$$

- Discretize for each data sample, that's

$$\frac{1}{N}\sum_{i=1}^{N} -\log p(y = y_i|\boldsymbol{x}_i)$$

- The minimum loss? 0
- The maximum loss? $+\infty$
- Loss at initialization? $\log C$

Derive the Gradient

- Denote logits $z_c = \boldsymbol{w}_c^T x + b$
- And $p_c = softmax_c(\{z_c\})$
- $\ell = -\log p(y|\boldsymbol{x}) = \log \sum_{c=1}^{C} e^{z_c} - z_y$
- $\frac{\partial \ell}{\partial \boldsymbol{w}_c} = \begin{cases} (p_y - 1) \cdot \boldsymbol{x}, & c = y \\ p_c \cdot \boldsymbol{x}, & c \neq y \end{cases}$
- Practically
  - moves $\boldsymbol{w}_c$ closer to $\boldsymbol{x}$ if it's label $y = c$
  - Otherwise, move away from $\boldsymbol{x}$

Discussion

- Does initialization matter?

  No, the function is convex

- What if the number of classes is very big?

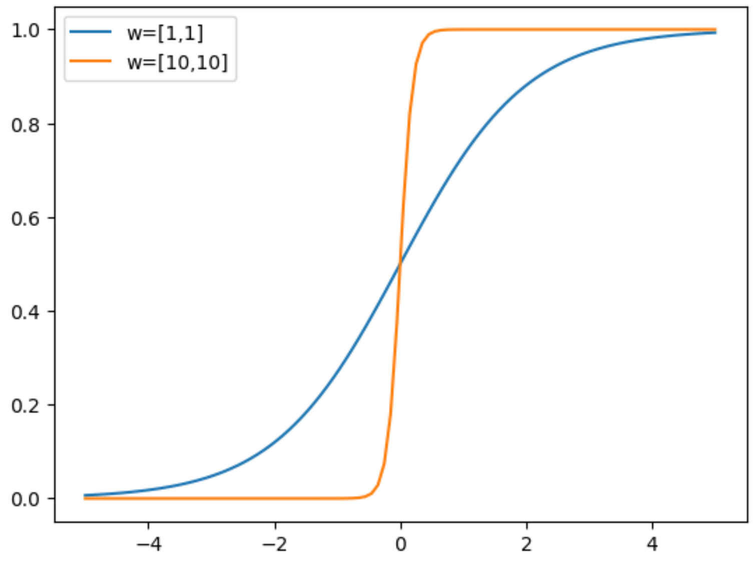
  Hierarchical softmax, sampled softmax

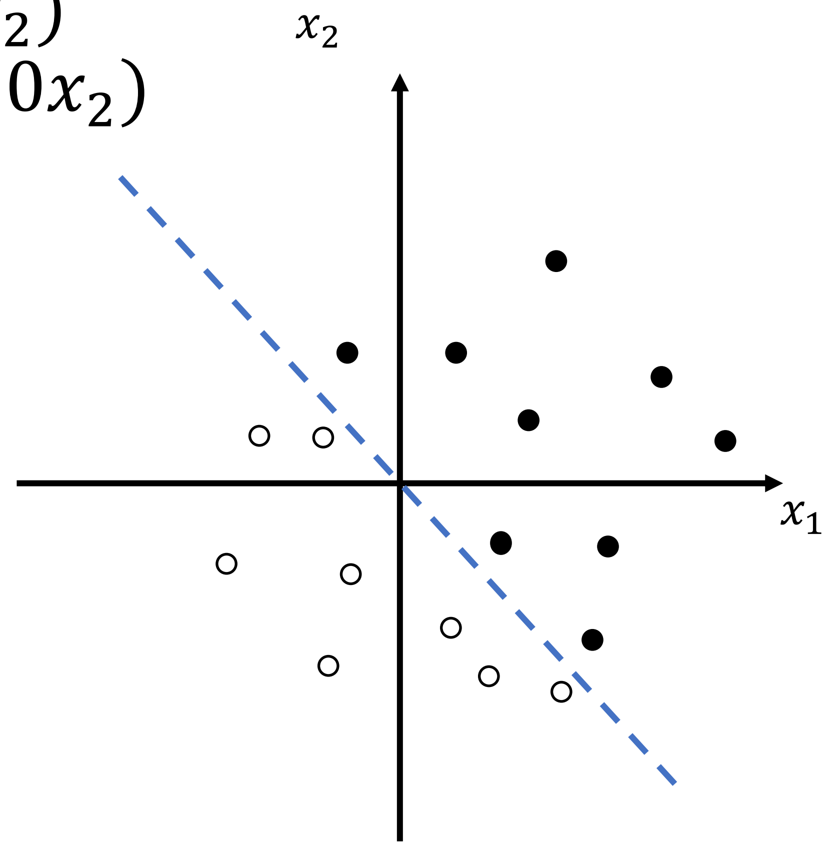
Reduce Overfitting in Linear classifiers

- Consider two logistic regression models

$$\mathcal{M}_1: p(y=1|\boldsymbol{x}) = \sigma(x_1 + x_2)$$
$$\mathcal{M}_2: p(y=1|\boldsymbol{x}) = \sigma(10x_1 + 10x_2)$$

- Training data is better distinguished by $\mathcal{M}_2$

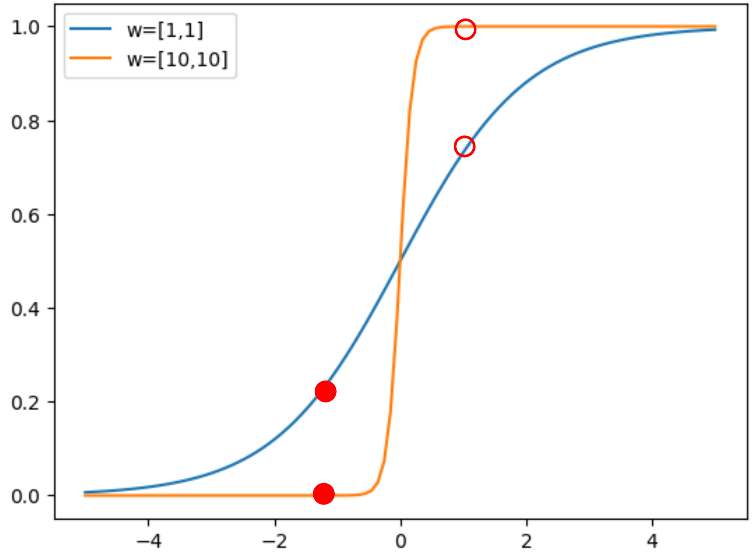


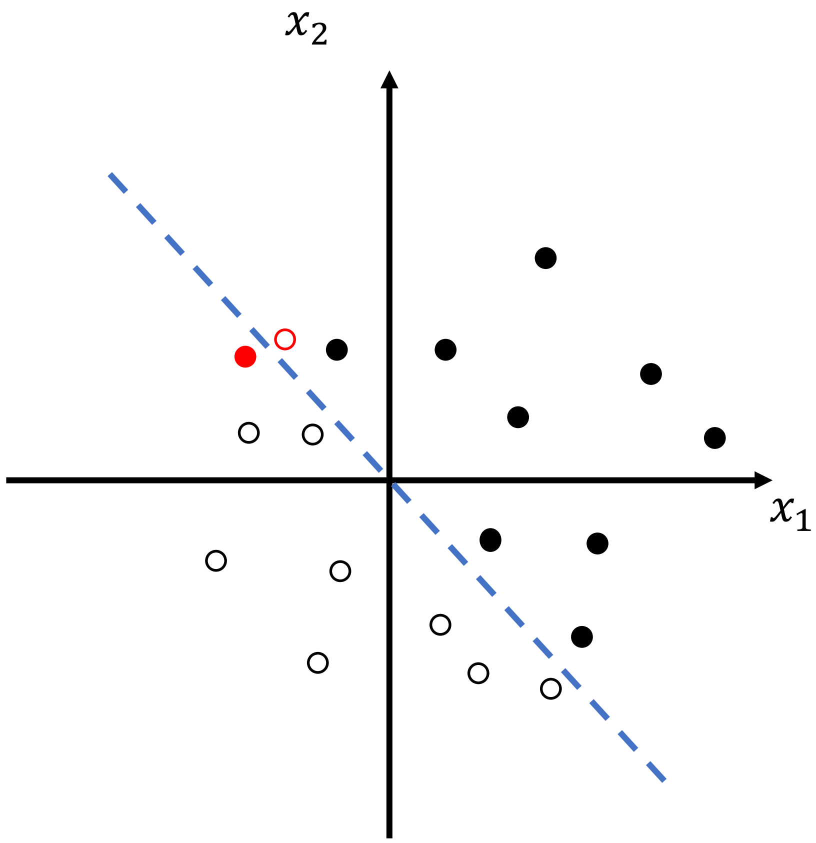


Example from [Quora page]()

Reduce Overfitting in Linear classifiers

- But $\mathcal{M}_2$ is too certain
- $\mathcal{M}_2$ can be very wrong for some test samples





Example from [Quora page]

Reduce Overfitting in Linear classifiers

- Use smaller weights
- Weight decay

$$\text{Cross-entropy loss} + \lambda\|\boldsymbol{w}\|^2$$

- Sparsity

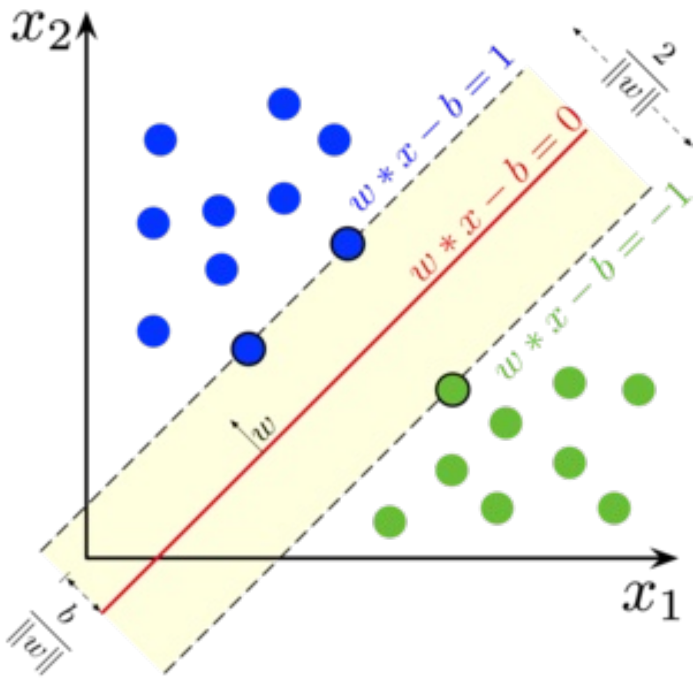
$$\text{Cross-entropy loss} + \lambda\|\boldsymbol{w}\|_1$$

Recap of SVM

- Instead of modeling $p(y|x)$,
- Learn a hyperplane to separate the classes with maximum margin
- Samples on the margin are called **support vectors**
- Learn $\boldsymbol{w}$ by solving:

$$\min \frac{1}{2}||\boldsymbol{w}||^2$$
$$s.t.\,(2y_i - 1)(\boldsymbol{w}^T\boldsymbol{x}_i + b) \geq 1$$

- Predict by $\hat{y} = 1$ if $\boldsymbol{w}^T\boldsymbol{x} + b \geq 0$, 0 otherwise



Source: wikipedia

Connect SVM to Logistic Regression

- SVM only asks for good separation
- i.e., if data label $y = 1$, SVM ask

$$\frac{p(y=1|x)}{p(y=0|x)} \geq c$$

- Adopting $p(y=1|x) = \sigma(\boldsymbol{w}^T\boldsymbol{x} + b)$, that's

$$\boldsymbol{w}^T\boldsymbol{x} + b \geq \log c$$

- Non-unique solution, so we put a penalty $||\boldsymbol{w}||^2$

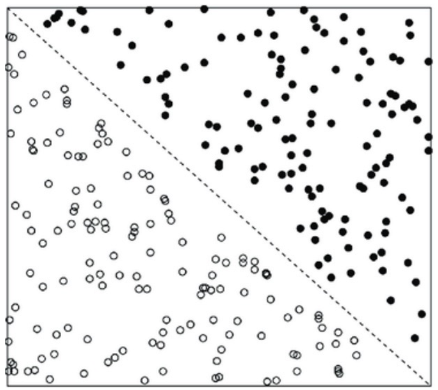
Adapted from CSC2515 slides

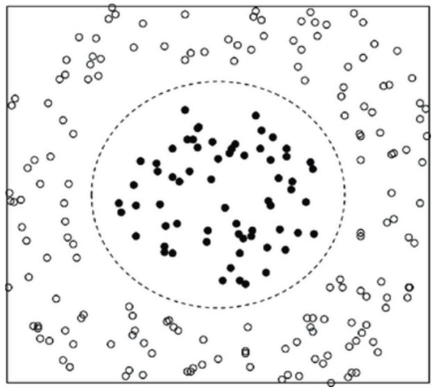
Agenda

- Machine Learning Paradigms
- Non-Parametric v.s. Parametric Models
- Linear Classifier
- Multi-layer Perceptron (MLP)

linearly Separable vs Non-separable

- linearly separable (left) and nonlinear separable (middle)

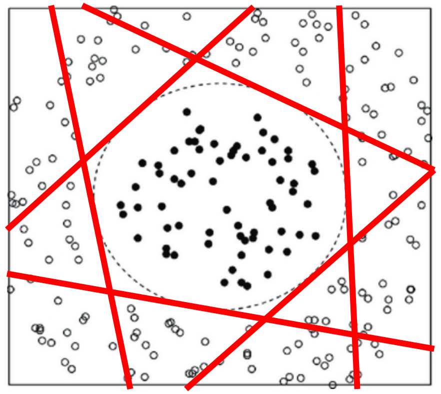




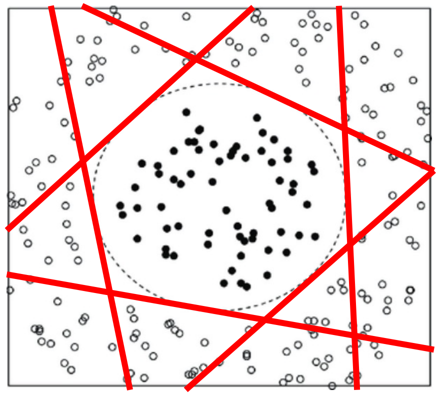
- Logistic regression fails for the right case
  - Huge modeling error (bias)

Multi-layer Perceptron (MLP)

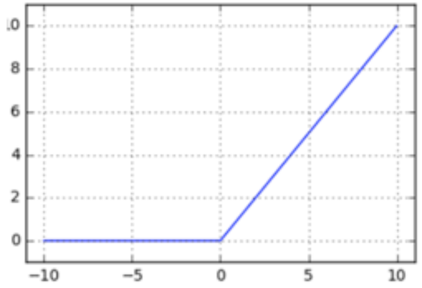
- We could use multiple lines to segregate the classes
- For each line,
  - assign 0 for the side with dots
  - assign 1 for the side with circle
- So the center region get an all-0 coding
- All other regions get at least one coding of 1
- Adding the 6 codings suffice to distinguish



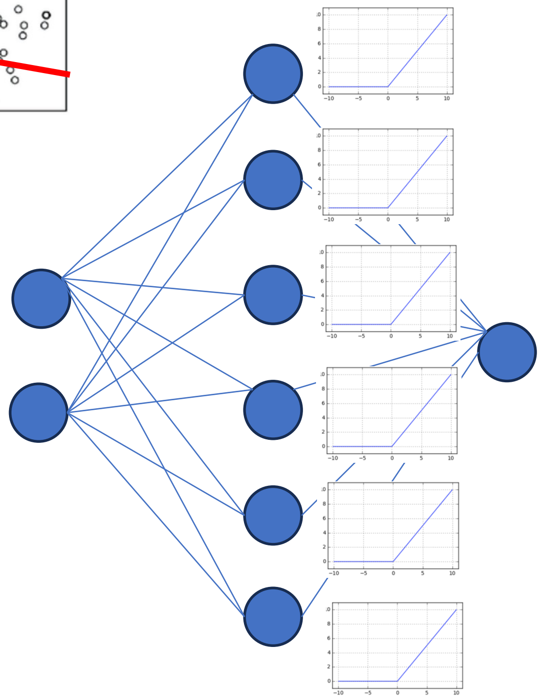
Multi-layer Perceptron (MLP)



- How do we assign the 1’s and 0’s?
- Need a (nonlinear) activation function
- Rectifier, i.e.,ReLU
- More terminologies:
  - The network is also called feedforward network
  - The linear layer is also called as fully connected layer

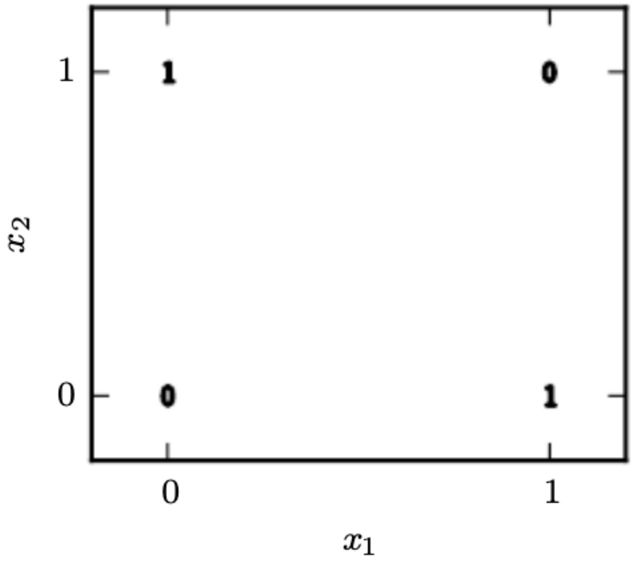


$$ReLU(x) = \max(x, 0)$$



Another example: modeling XOR

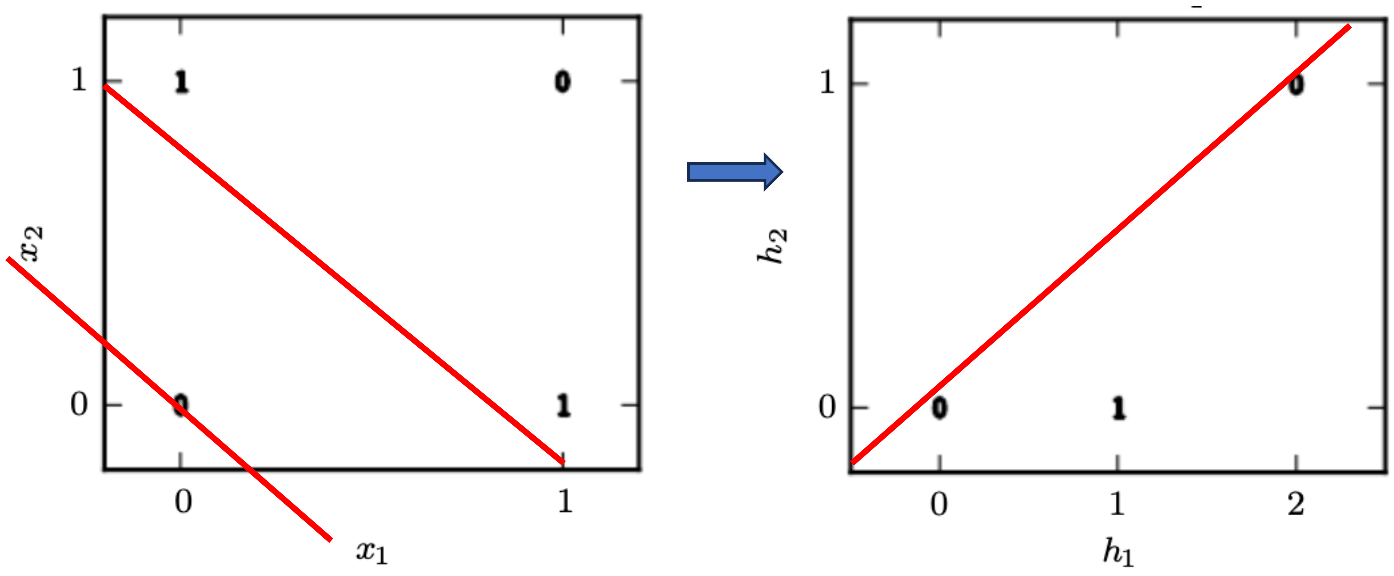
- Find a model space $\mathcal{F}$ that capture this setup
- i.e., no modeling error
- $\mathcal{F}$ cannot be a space of linear models
- As a single line cannot separate the two classes



Plot from deep learning textbook [chapter 5]

Modeling XOR

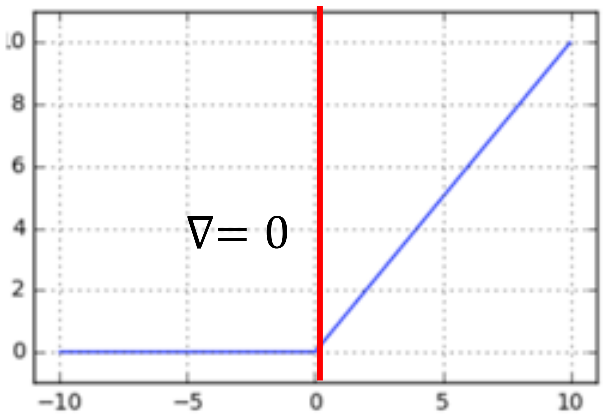
- $f(x) = \boldsymbol{w}^T ReLU(\boldsymbol{W}^T \boldsymbol{x} + c)$
- $\boldsymbol{W} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$
- $c = \begin{bmatrix} 0 \\ -1 \end{bmatrix}$
- $\boldsymbol{w} = \begin{bmatrix} 1 \\ -2 \end{bmatrix}$

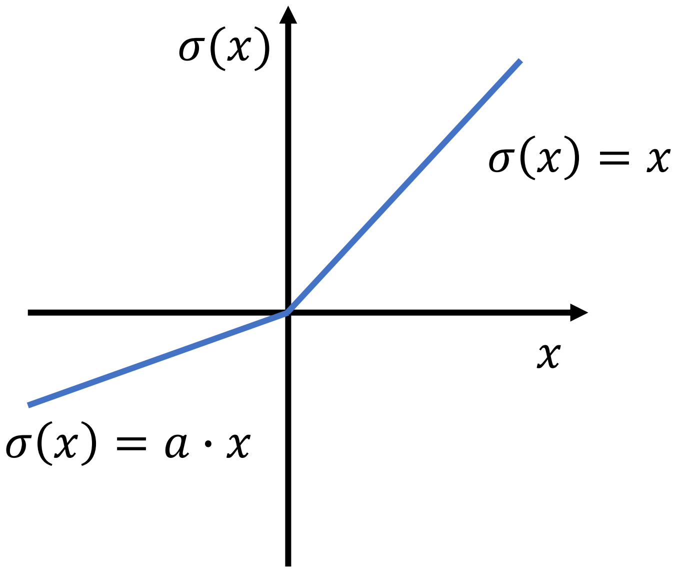


Plots from deep learning textbook chapter 5

Generalize ReLU

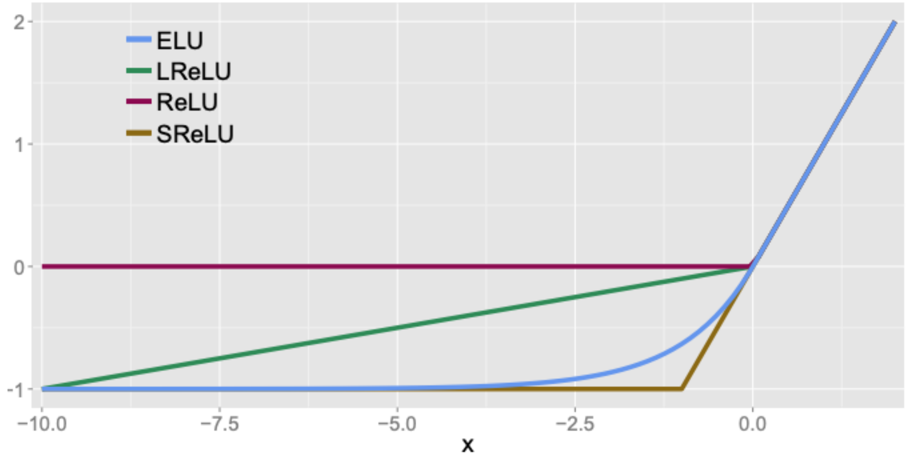
- Drawback of ReLU
- Zero gradient when not activated
  - No learning happens
- Leaky ReLU, fix a small $a > 0$
- Parametric ReLU (PReLU), learn a





Generalize ReLU

- Exponential Linear Units (**ELU**)
- $\sigma(x) = \begin{cases} x, & x > 0 \\ \alpha(e^x - 1), & x \leq 0 \end{cases} \quad (\alpha > 0)$
- push mean unit activations closer to zero
- Shown to speed up learning

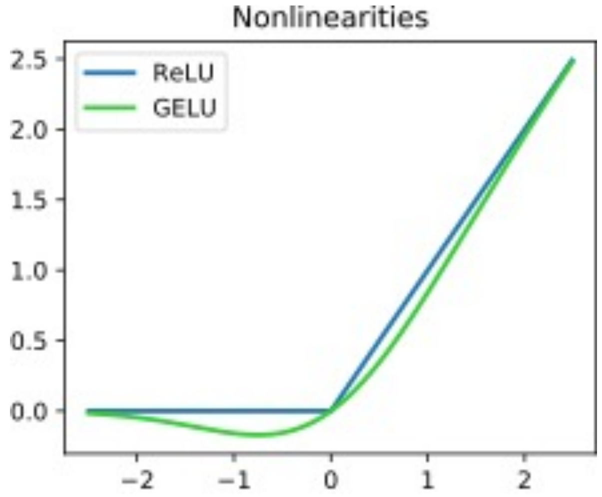


Clevert et. al 2016

Generalize ReLU

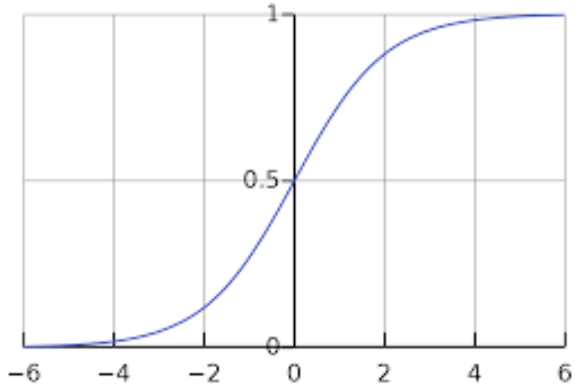
- But still it's non-differentiable at zero
- Gaussian-error Linear Unit (**GELU**): $\sigma(x) = x \cdot \Phi(x)$

  $\Phi(x)$ is the CDF of standard Gaussian distribution
- Used in BERT

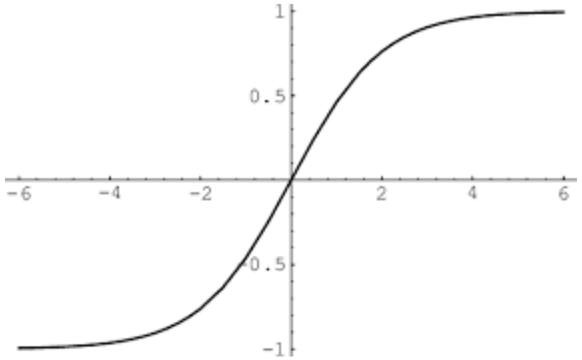


Plot from [wikipage]

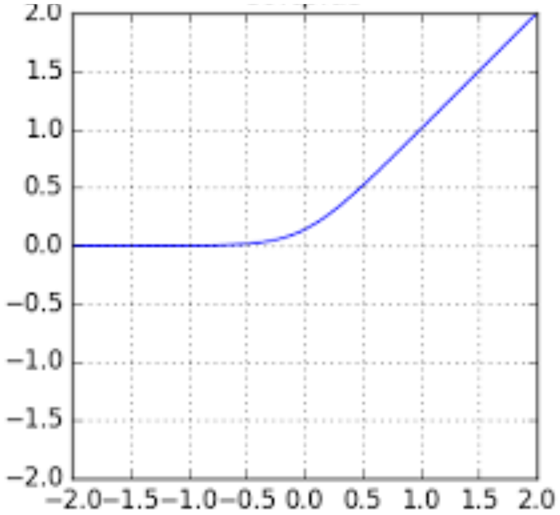
Other activation functions



$$sigmoid(x) = \frac{1}{1 + e^{-x}}$$



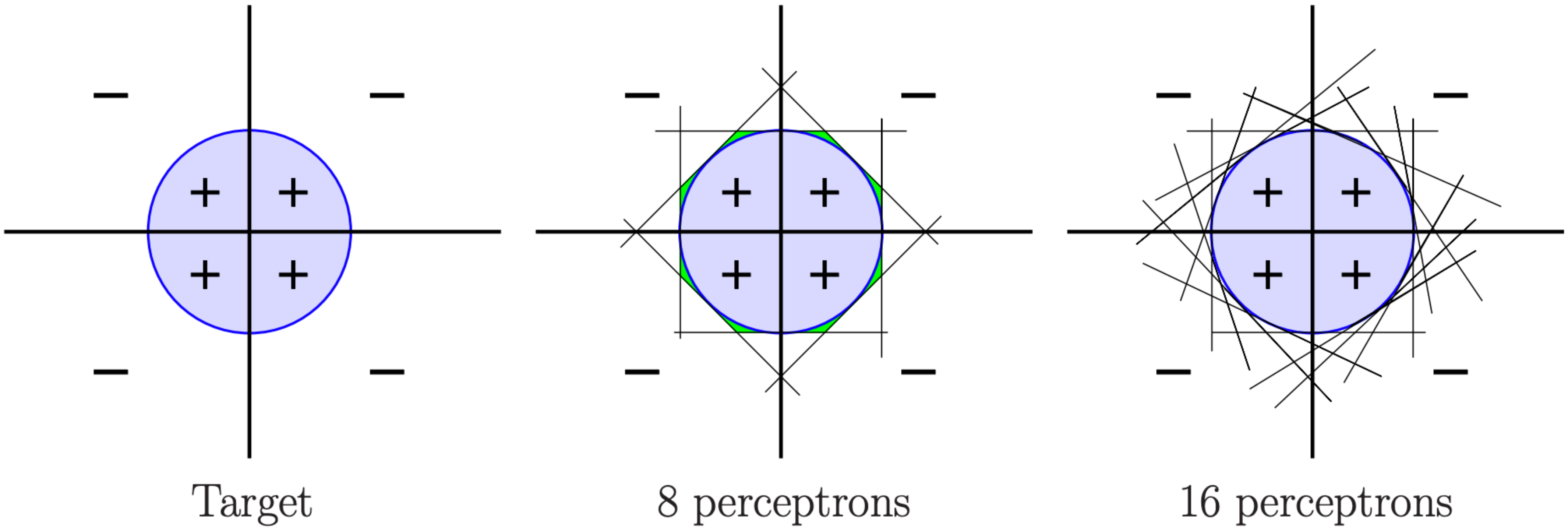
$$tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$



$$softplus(x) = \ln(1 + e^x)$$

Note: sigmoid and tanh are called **squashing function** as their output range is bounded

Universal Approximation Theorem



Slide page from [here]

Universal Approximation Theorem (Simplified)

A feedforward network with

- a linear output layer, and
- at least one hidden layer, with enough hidden units

can approximate any function from one finite-dimensional space to another

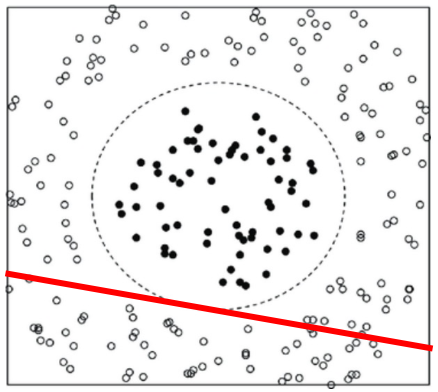
Caveats:

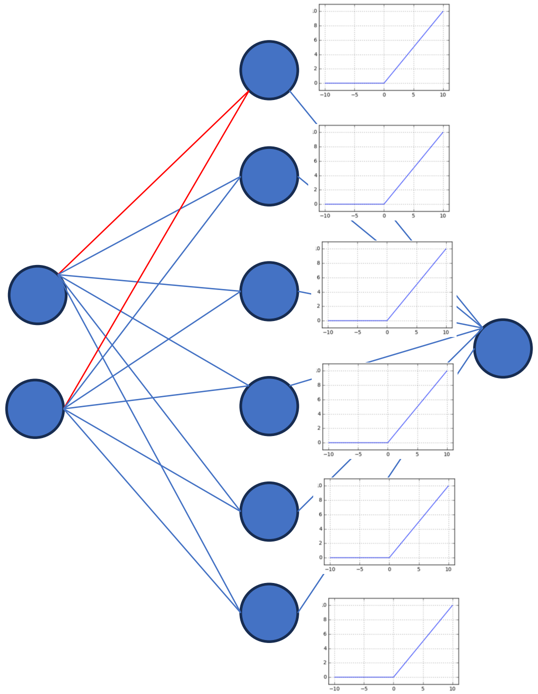
1. Although modeling error is 0, there may still be estimation error
2. Optimizer may fail to find the correct parameter values

Counting (linear) regions

Consider one layer:

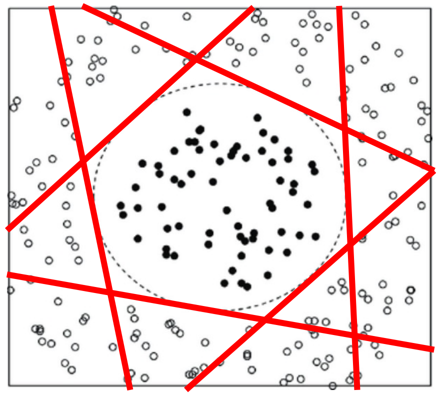
- $ReLU(\boldsymbol{w}^T\boldsymbol{x} + b)$ defines a hyper plane
- One side deactivated (all 0)
- The other side activated: computes $\boldsymbol{w}^T\boldsymbol{x} + b$





Counting (linear) regions

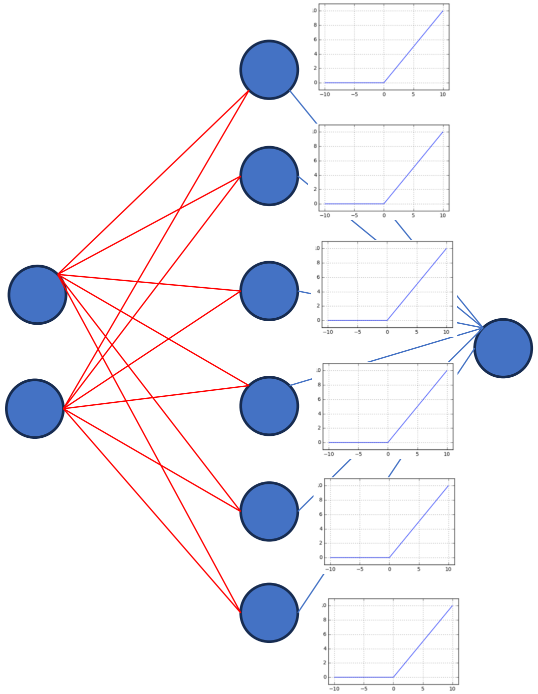
- n $\boldsymbol{w}$'s: separate the space into multiple regions



- More generally, $\boldsymbol{x} \in \mathbb{R}^d$, at most

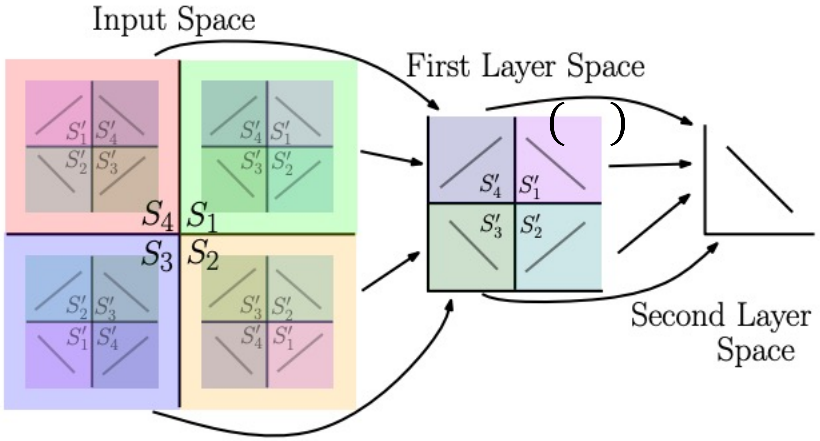
$$\sum_{i=1}^{d} \binom{n}{i}$$

regions



The effect of more layers

- The 2nd layer works on each of the regions defined by the first layer

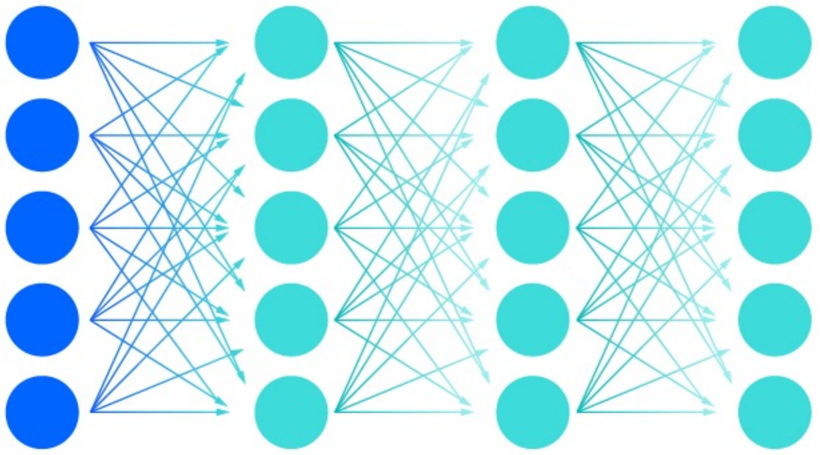


- L layer, each n hidden units: Number of regions $O\left(\binom{n}{d}^{d(L-1)} n^d\right)$

[Montufar et. al, 2014](#)

Recap end-to-end pipeline

Feature extraction → features → classifier → Predicted label

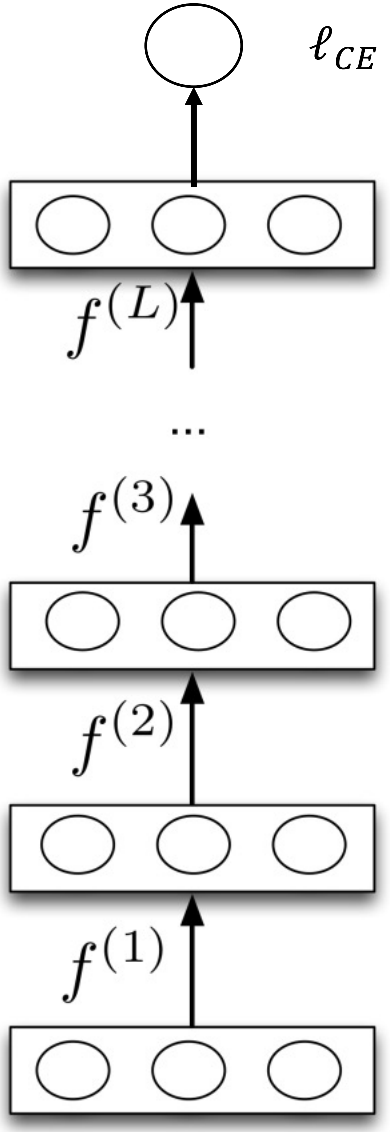


Logistic regression
softmax classifier
SVM
…

Illustration of histogram from this [page]

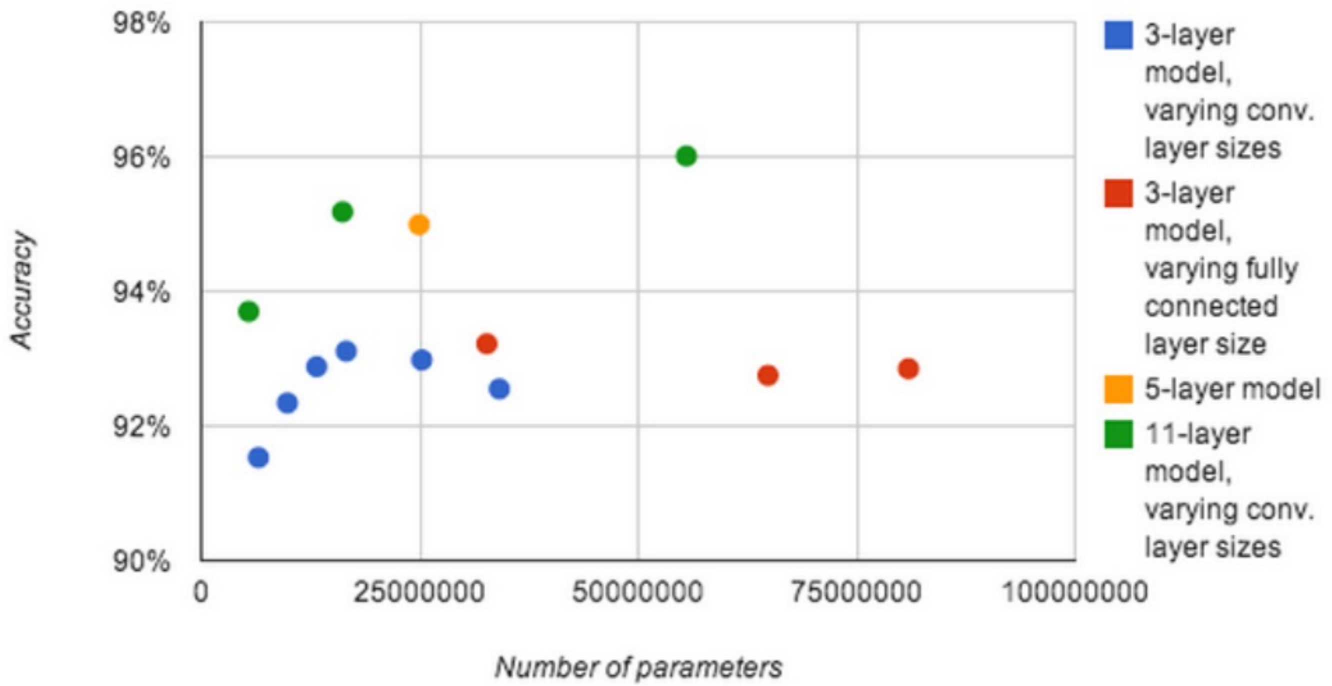
As composite function

- Each layer compute
$$\boldsymbol{x}^{(l)} = f^{(l)}(\boldsymbol{x}^{(l-1)}) = \sigma(\boldsymbol{W}^{(l)}\boldsymbol{x}^{(l-1)})$$
- Over all layers, a composite function
$$f^{(L)} \circ f^{(L-1)} \circ \cdots \circ f^{(1)}(\boldsymbol{x})$$
- Last layer is your favorite classifier with a loss
- Trained by back-propagation



Cartoon from [CSC lecture 5 slides]

Shallow vs Deep



Increasing the number of parameters in shallower models does not allow such models to reach the same level of performance as deep models, primarily due to overfitting.

- (linear) Regions grows exponentially w.r.t depth
- Deeper model use fewer parameter to achieve necessary number of (linear) regions

Plot from [Goodfellow et. al, 2014]