深度学习

Lecture1 Introduction

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About This Course

- It is
  - An introduction to deep learning methods, from basics to advanced topics.
  - Focused on algorithms and applications, emphasizing the development of strong coding skills. (Math is still important!)
- It isn't
  - Focused on rigorous mathematical definitions and derivations.
  - A comprehensive overview of all topics within deep learning.

About This Course

- Grading Policy
  - Assignments: 3*25%
  - Final Projects: 25%
  - Late policy: 10% off per day late; not accepted after 10 days
- Office hour
  - by appointment
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  - office: 双清综合楼B533

Reference

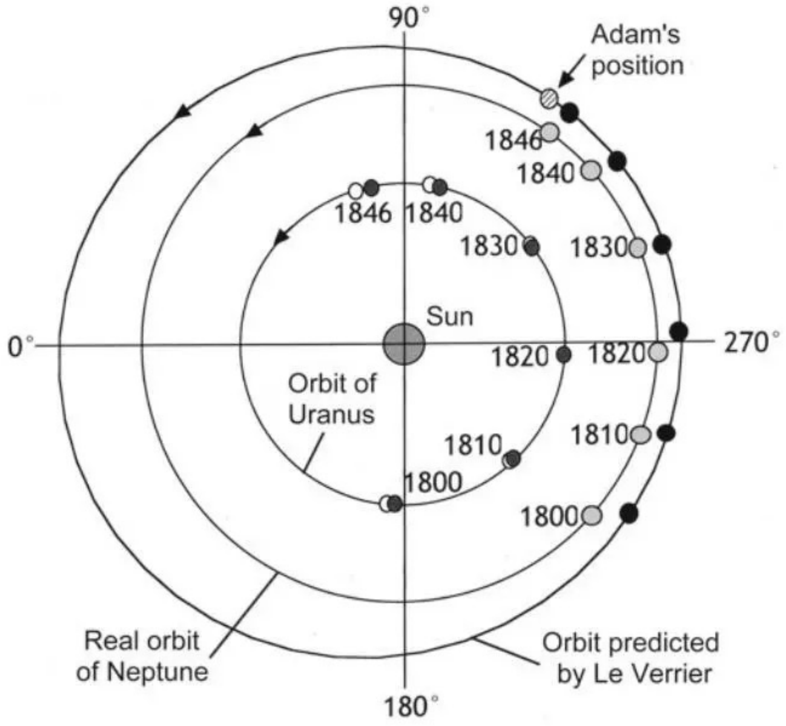
- Books
  - Bishop, Christopher M., and Nasser M. Nasrabadi. **Pattern recognition and machine learning**, Springer, 2006.
  - Bengio, Yoshua, Ian Goodfellow, and Aaron Courville. **Deep learning**, MIT press, 2017.
  - Zhang, Aston and Lipton, Zachary C. and Li, Mu and Smola, Alexander J., **Dive into Deep Learning**, Cambridge University Press, 2023
- Related Courses:
  - 6.8300/6.8301: Advances in Computer Vision, MIT
  - 6.S978: Deep Generative Models, MIT
  - CS231n: Deep Learning for Computer Vision, Stanford
  - Reinforcement Learning, by David Silver, UCL

What is Learning?

Motivating Examples

Year	Housing Price
2021	2
2022	3
2023	4
2024	?

Predict the Housing Price of a City

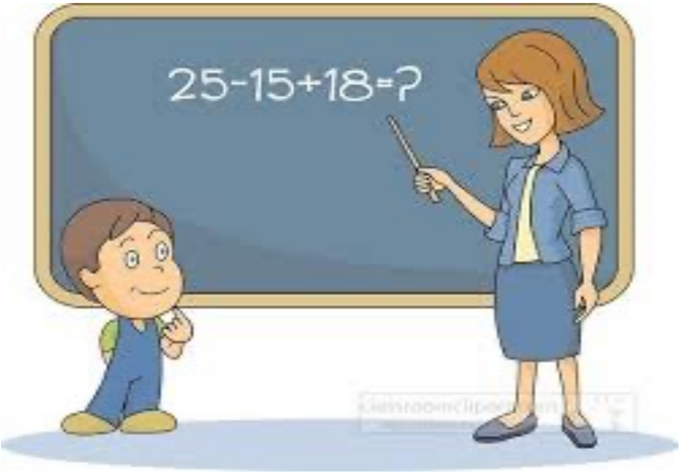


The Discovery of Neptune

Astronomers noticed Uranus' motion differed from predictions and used its trajectory to predict the location and mass of an unknown celestial body.

Motivating Examples

A doggie is learning

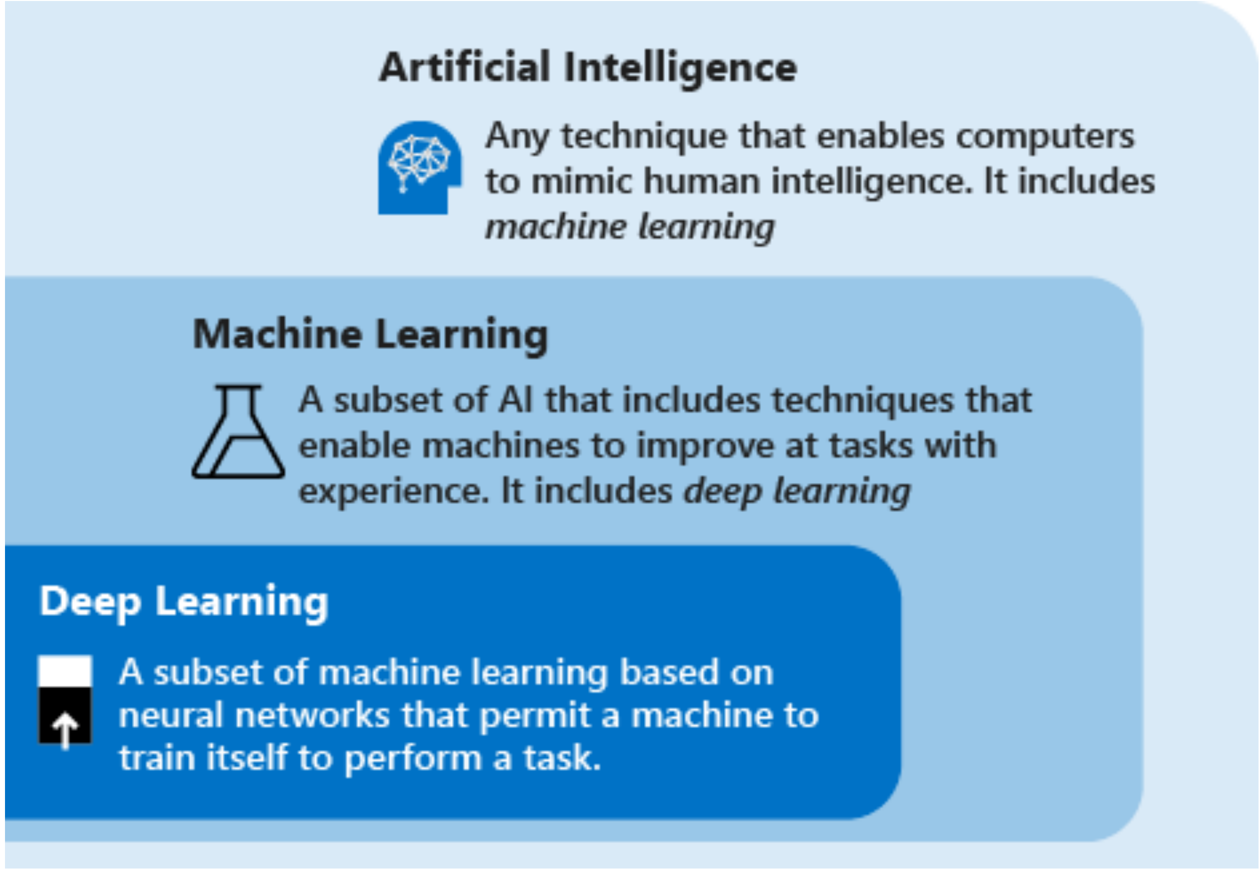


A kid is learning

Also learning……

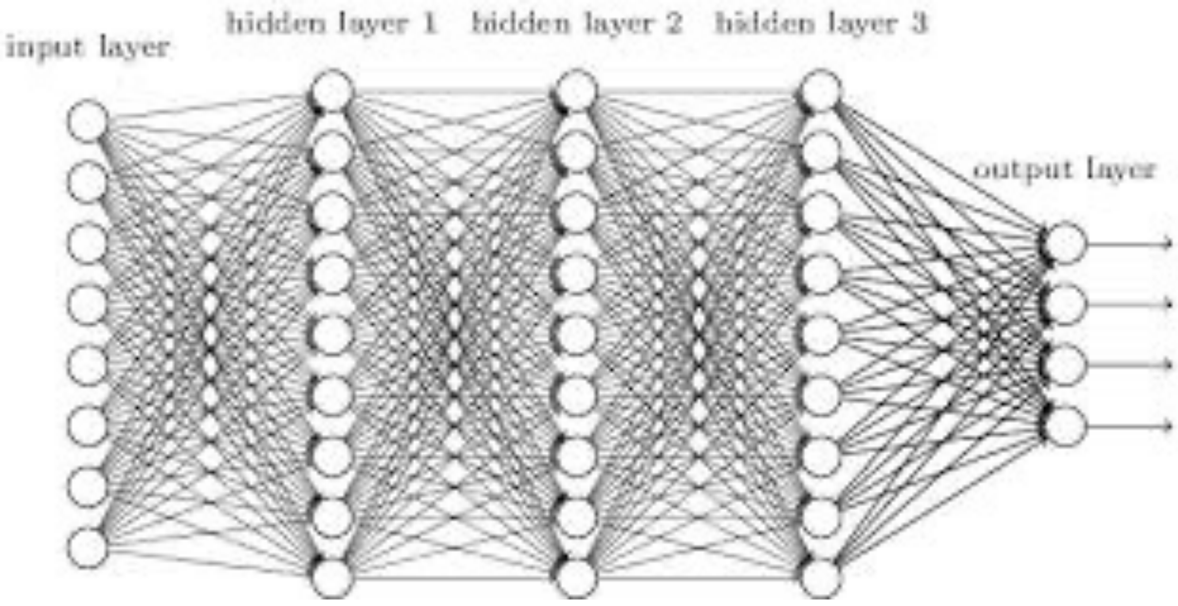
Machine/Deep Learning

- ***Machine learning*** is the study of algorithms that can learn from experience.
- Experience: typically in the form of observational data or interactions with an environment.
- As a machine learning algorithm accumulates more experience, its performance improves.



Deep Learning Methods

- Supervised Learning
- Unsupervised Learning
  - Self-supervised Learning
  - Generative Models
- Reinforcement Learning
- Meta/Transfer Learning
- ……

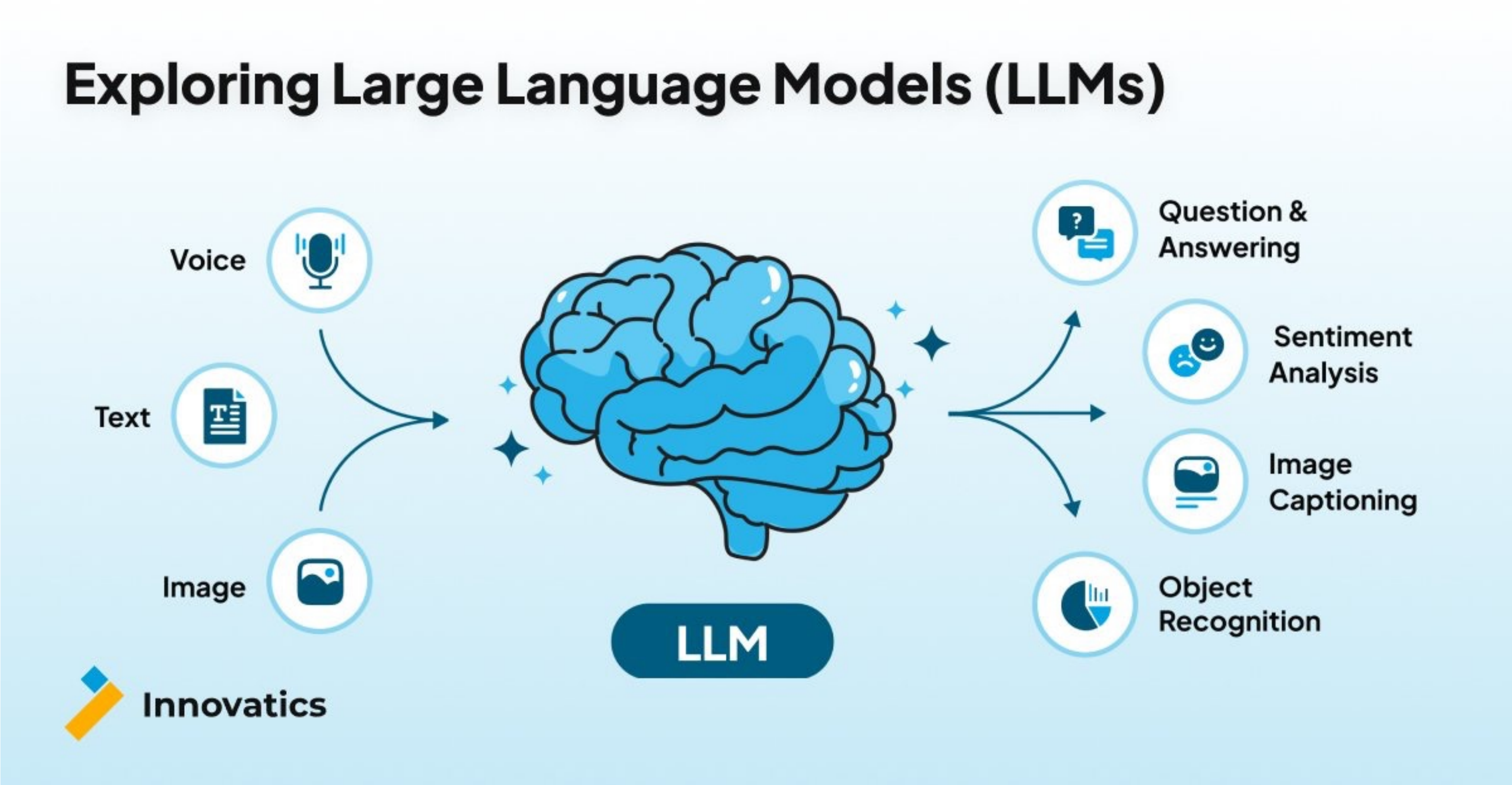


Deep Neural Networks

Applications

Text-to-image Generation

Applications



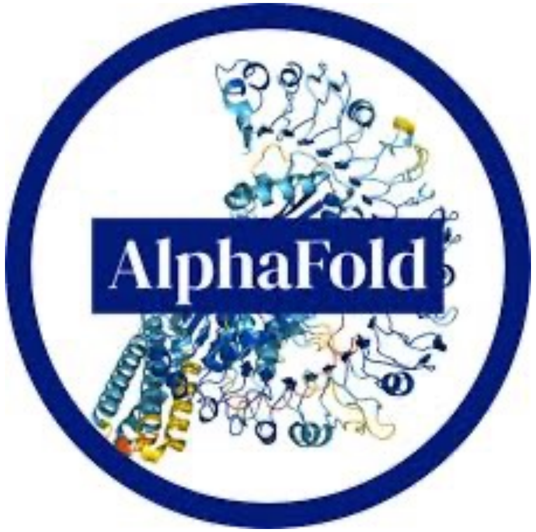
Gemini

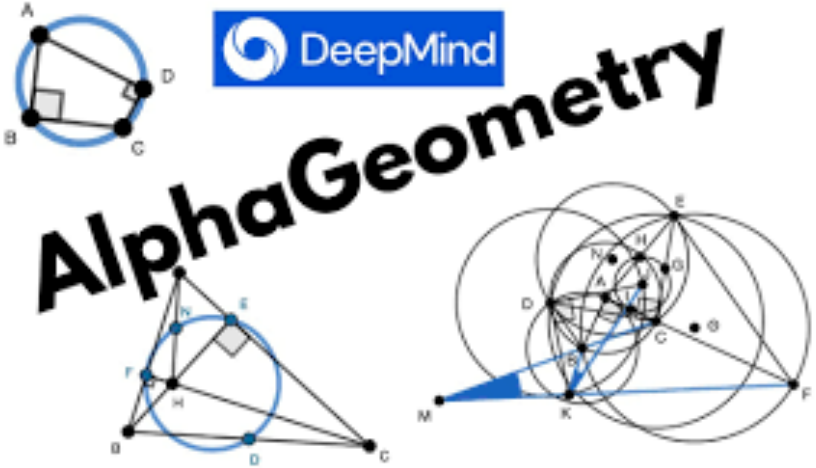
ChatGPT

Claude

deepseek

Applications





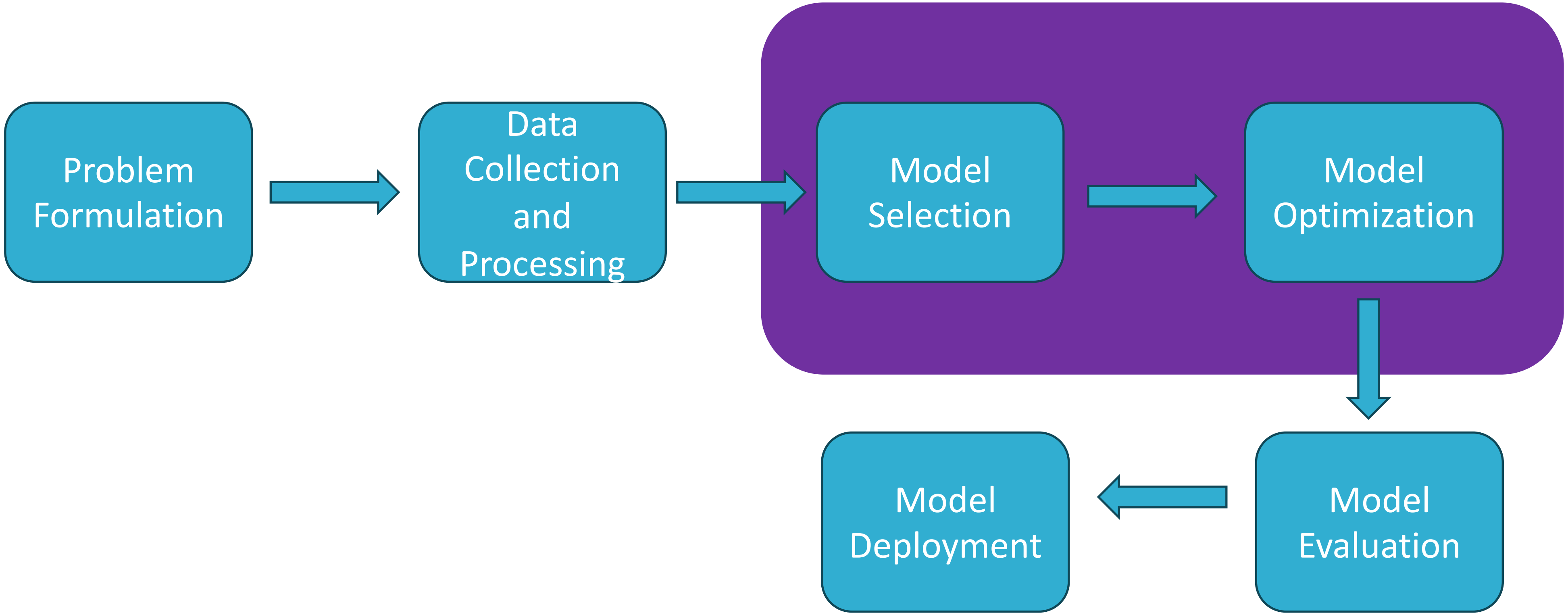
Applications

Embodied Intelligence

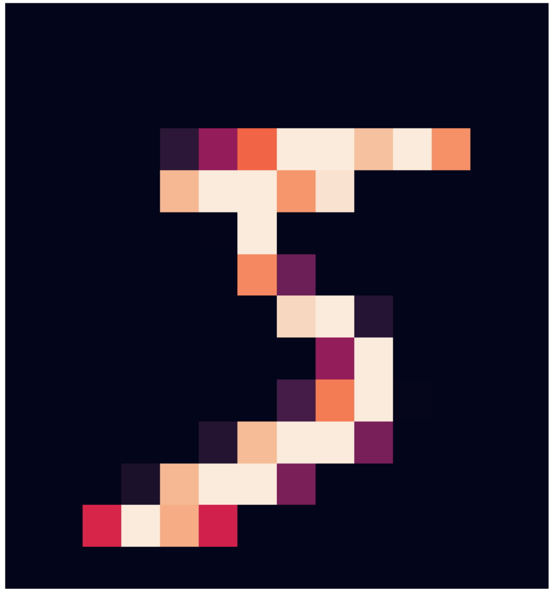
Self-Driving

Start from the very beginning

Typical Process

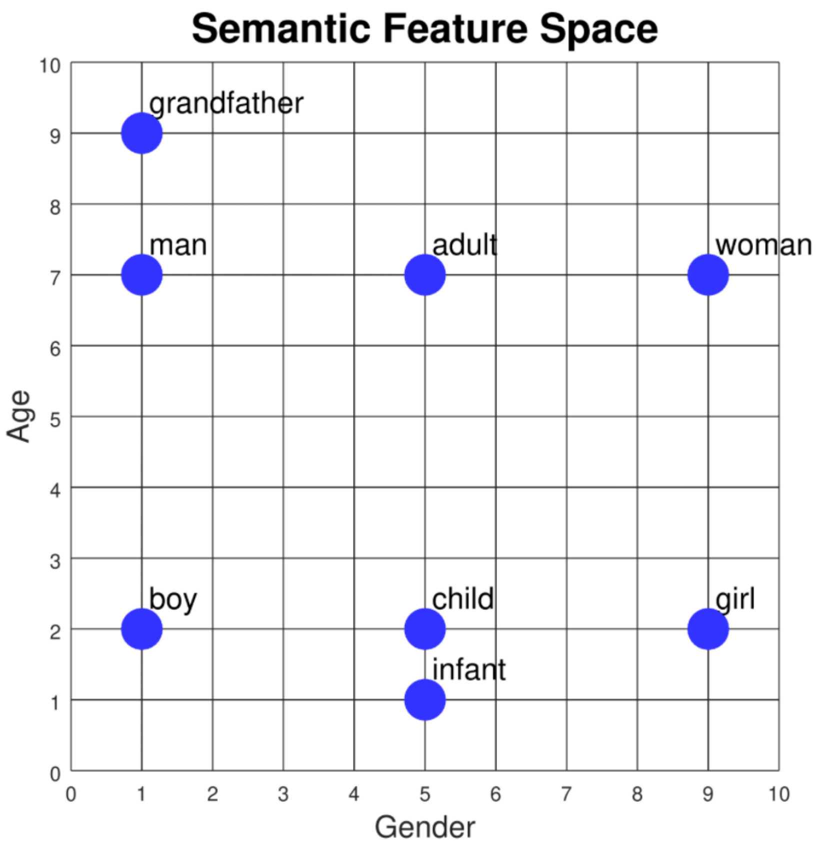


Data Format



0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	30	94	170	253	253	225	253	195	0	0
0	0	0	0	219	253	253	198	247	0	0	0	0	0
0	0	0	0	0	1	253	0	0	0	0	0	0	0
0	0	0	0	0	0	190	70	0	0	0	0	0	0
0	0	0	0	0	0	0	240	253	25	0	0	0	0
0	0	0	0	0	0	0	0	93	253	0	0	0	0
0	0	0	0	0	0	0	46	183	253	2	0	0	0
0	0	0	0	0	24	221	253	253	78	0	0	0	0
0	0	0	18	219	253	253	80	0	0	0	0	0	0
0	0	136	253	212	132	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0

Data Format



Word Coordinates

	Gender	Age
grandfather	[1,	9]
man	[1,	7]
adult	[5,	7]
woman	[9,	7]
boy	[1,	2]
child	[5,	2]
girl	[9,	2]
infant	[5,	1]

--Dave Touretzky

Data Format

One-hot Encoding

apple = [1 0 0 0 0 ......]

bag = [0 1 0 0 0 ......]

cat = [0 0 1 0 0 ......]

dog = [0 0 0 1 0 ......]

elephant = [0 0 0 0 1 ......]

Data Format

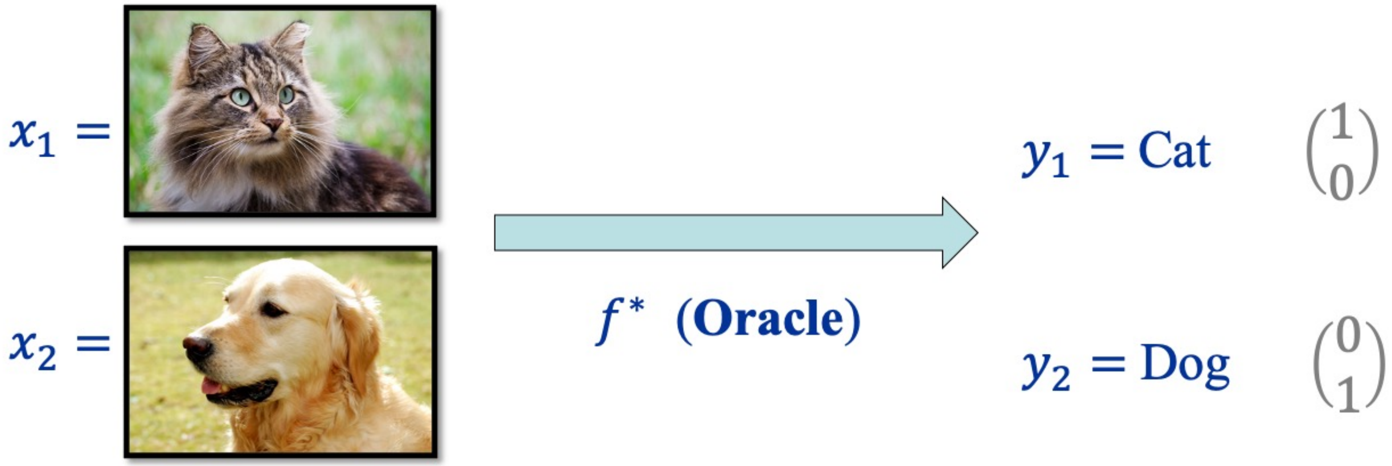
- In deep learning algorithms, most data is in the form of tensors, which can be better utilized for accelerated computation on GPUs.
- Tensor data can still have various structures, such as time series data, graph data, etc.
- Dataset Decomposition

$$\mathcal{D} = \mathcal{D}_{\boldsymbol{train}} \cup \mathcal{D}_{\boldsymbol{test}} \cup \mathcal{D}_{\boldsymbol{validation}}$$

$\mathcal{D}_{\boldsymbol{train}}$: for training; $\mathcal{D}_{\boldsymbol{test}}$: for evaluation; $\mathcal{D}_{\boldsymbol{validation}}$:for selection

Supervised Learning

- Training data with labels: $\mathcal{D} = \{x_i, y_i\}_{i=1}^{N}$, input: x_i , output/label: y_i ,
- Goal: learn the mapping $x_i \to y_i$



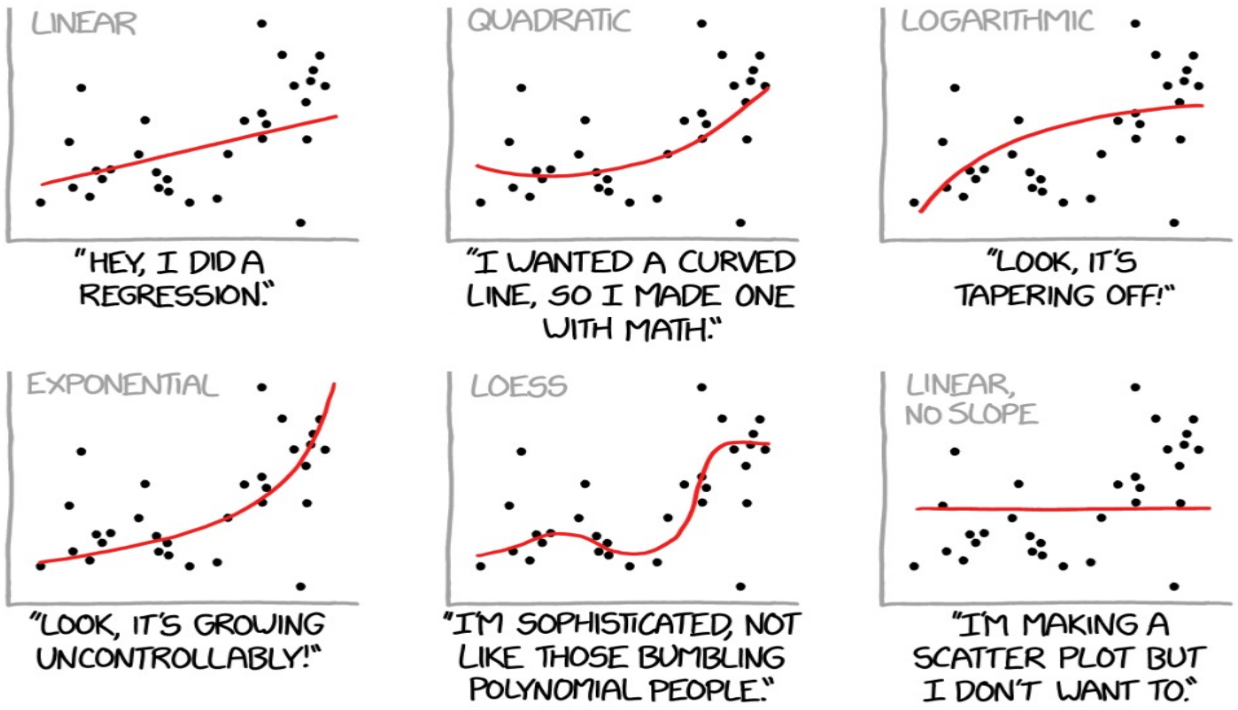
- The oracle f^* is unknown to us, except through the dataset

$$\mathcal{D} = \{x_i, y_i = f^*(x_i)\}_{i=1}^{N}$$

Hypothesis Space

Supervised Learning:

1. Define a **hypothesis space** $\mathcal{H}$ consisting of a set of candidate functions, e.g.
$\mathcal{H} = \{f: f(x) = w_0 + w_1 x\}$
2. Find the "**best**" function $\hat{f}$ in $\mathcal{H}$ that **approximates** f^*



What you get depends on $\mathcal{H}$!

https://xkcd.com/2048/

Optimization

- Define a **loss function** to measure the distance between the model solution and the oracle solution. Then, we can find the best approximation by an optimization problem

$$\min_{f \in \mathcal{H}} R_{emp}(f) = \frac{1}{N} \sum_{i=1}^{N} L(f(x_i), f^*(x_i))$$

The empirical loss

- Optimization algorithms to be explored in the following lectures……

Generalization

- **Generalization ability:** to do well on new, unseen data.

What we **can** solve

Empirical risk minimization

$$\min_{f \in \mathcal{H}} R_{emp}(f) = \frac{1}{N} \sum_{i=1}^{N} L(f(x_i), f^*(x_i)) \quad \Longrightarrow \quad \hat{f}$$

$$x_i \sim \mu$$

Population risk minimization

$$\min_{f \in \mathcal{H}} R_{pop}(f) = \mathbb{E}_{x \sim \mu}[L(f(x), f^*(x))] \quad \Longrightarrow \quad \tilde{f}$$

What we **really** want to solve

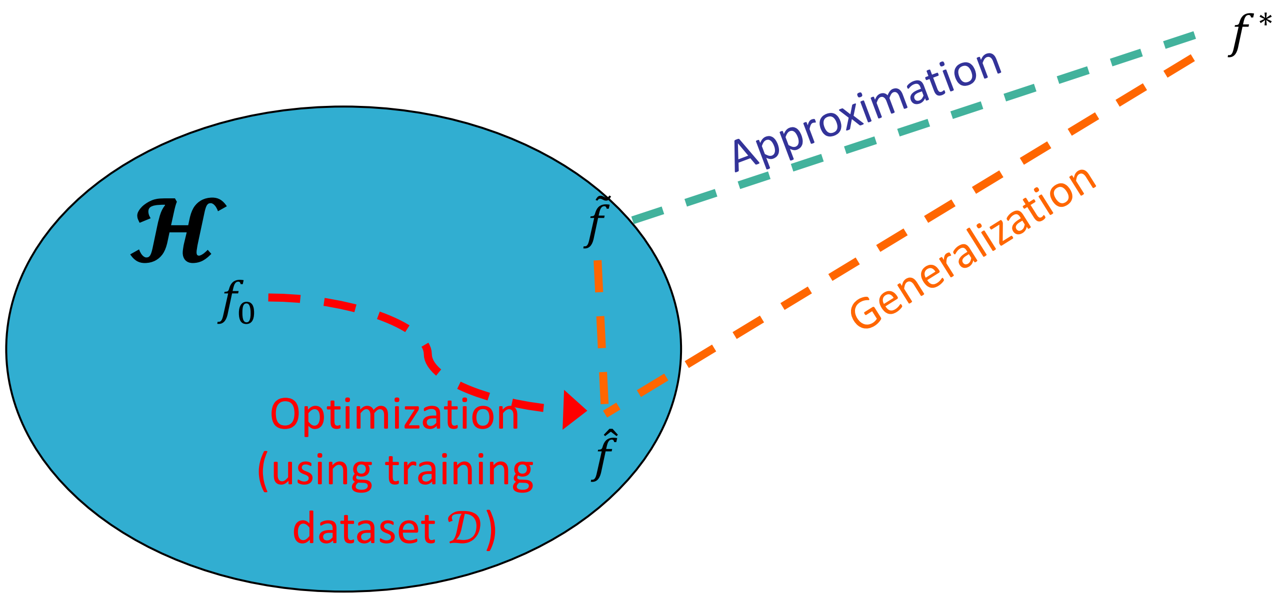
Generalization Gap

$$\hat{f} \neq \tilde{f}$$

Generalization error depends on the training dataset, hypothesis spaces, and optimization algorithms etc.

Paradigms of Supervised Learning

- **Approximation**: the distance between the hypothesis space and the oracle solution.
- **Optimization**: Seeks the best solution within the hypothesis space based on training data.
- **Generalization**: Examines the difference between the optimized solution and the true solution on unseen data.



Linear Regression

Linear Regression

- Linear Model with Continuous Output
- Step 1: Define the hypothesis space as the set of linear models.

$$\mathcal{H} = \{f : f(x) = w_0 + w_1 x, w_0 \in \mathbb{R}, w_1 \in \mathbb{R}\}$$

- Step 2: Find the best approximation.

First, define the loss function, for example:

$$L(f_1, f_2) = \int p(x) ||f_1 - f_2||_2^2 d\mu$$

Minimize the empirical loss over the training dataset $\mathcal{D} = \{x_i, y_i\}_{i=1}^{N}$

$$\min_{f \in \mathcal{H}} R_{emp}(f) = \min_{w_0, w_1} \frac{1}{2N} \sum_{i=1}^{N} (w_0 + w_1 x_i - y_i)^2$$

Solution:

$$\frac{\partial R_{emp}}{\partial w_0}(\widehat{w}_0, \widehat{w}_1) = 0 \text{ and } \frac{\partial R_{emp}}{\partial w_1}(\widehat{w}_0, \widehat{w}_1) = 0$$

$$\widehat{w}_0 = \bar{y} - \widehat{w}_1 \bar{x} \qquad \widehat{w}_1 = \frac{\sum_i (x_i - \bar{x})(y_i - \bar{y})}{\sum_i (x_i - \bar{x})^2} \qquad \bar{x} = \frac{1}{N} \sum_i x_i \qquad \bar{y} = \frac{1}{N} \sum_i y_i$$

Test process: $y_{test} = \widehat{w}_0 + \widehat{w}_1 x_{test}$

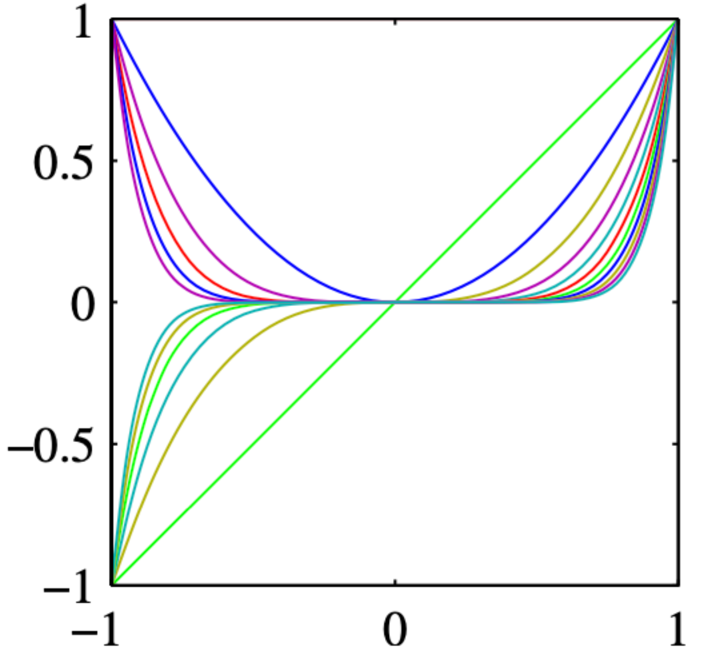
Linear Basis Models

- Q: Can linear models only represent linear relationships between x and y?
- No! Introduce basis functions or feature mappings can extend its ability to model more complex relationships.

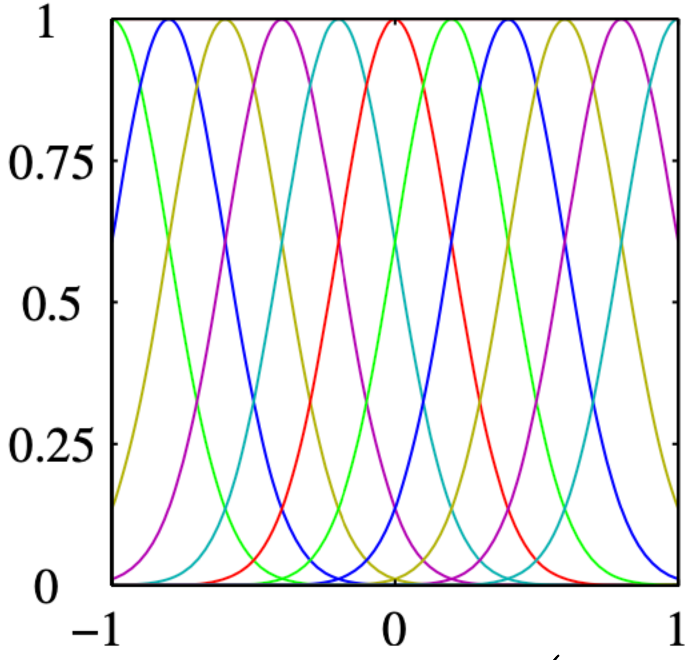
$$\mathcal{H}_M = \left\{ f : f(x) = \sum_{j=0}^{M-1} w_j \phi_j(x) \right\}$$

$\mathcal{H} = \{f : f(x) = w_0 + w_1 x, w_0 \in \mathbb{R}, w_1 \in \mathbb{R}\}$ corresponds to $d = 1, M = 2, \phi_0(x) = 1, \phi_1(x) = x$

Example of Basis Functions



Polynomials: $\phi_j(x) = x^j$



Gaussian: $\phi_j(x) = \exp\left(-\frac{(x-m_j)^2}{2s^2}\right)$

-- Bishop

Linear Basis Models

- Optimization:

$$\min_{f \in \mathcal{H}_M} R_{emp}(f) = \min_{w \in \mathbb{R}^M} R_{emp}(w)$$

$$= \min_{w \in \mathbb{R}^M} \frac{1}{2N} \sum_{i=1}^{N} \left(f(x_i) - y_i\right)^2$$

$$= \min_{w \in \mathbb{R}^M} \frac{1}{2N} \sum_{i=1}^{N} \left(\sum_{j=0}^{M-1} w_j \, \phi_j(x_i) - y_i \right)^2$$

$$\Longleftrightarrow$$

$$\min_{w \in \mathbb{R}^M} \frac{1}{2N} \|\Phi w - y\|^2$$

where

$$\Phi = \begin{pmatrix} \phi_0(x_1) & \cdots & \phi_{M-1}(x_1) \\ \phi_0(x_2) & \cdots & \phi_{M-1}(x_2) \\ \vdots & \ddots & \vdots \\ \phi_0(x_N) & \cdots & \phi_{M-1}(x_N) \end{pmatrix}$$

$$w = \begin{pmatrix} w_0 \\ w_1 \\ \vdots \\ w_{M-1} \end{pmatrix} \quad y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix}$$

Linear Regression

- To solve $\min_{w \in \mathbb{R}^M} \frac{1}{2N} ||\Phi w - y||^2$,

we can do this by setting $\nabla R_{emp}(\hat{w}) = 0 \Leftrightarrow \Phi^{\mathrm{T}}(\Phi \hat{w} - y) = 0$

Solve the linear equation systems:

- When $\Phi^{\mathrm{T}}\Phi$ is invertible, there is an unique solution $\hat{w} = \left(\Phi^{\mathrm{T}}\Phi\right)^{-1}\Phi^{\mathrm{T}}y$
- When $\Phi^{\mathrm{T}}\Phi$ is not invertible, there are many solutions

$$\hat{w}(u) = \Phi^{\dagger}y + \left(I - \Phi^{\dagger}\Phi\right)u \,, \forall\, u \in \mathbb{R}^M, \Phi^{\dagger} = \left(\Phi^{\mathrm{T}}\Phi\right)^{-1}\Phi^{\mathrm{T}}$$

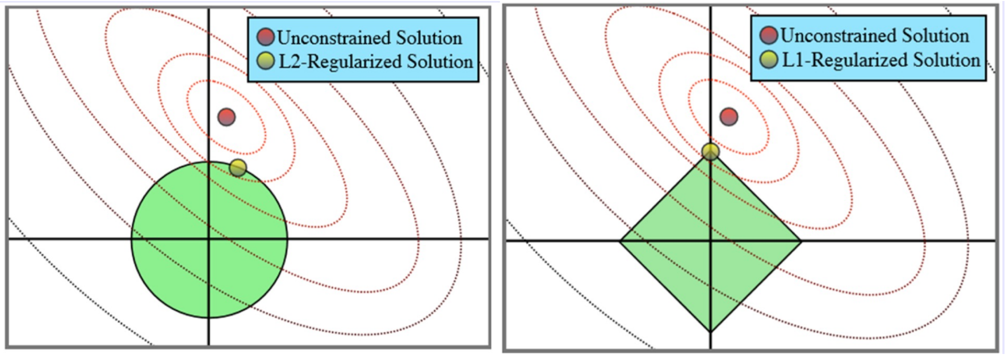
Q: how to select the desirable one?

Linear Regression

- Add regularization

$$\min_{w \in \mathbb{R}^M} \frac{1}{2N} \|\Phi w - y\|^2 + \lambda \underbrace{C(w)}_{\text{the regularization term}}$$

  - ℓ_2 regularization (ridge regression): $C(w) = ||w||_2^2$.
  - ℓ_1 regularization (**lasso**): $C(w) = ||w||_1$, pursuit sparsity
  - ……



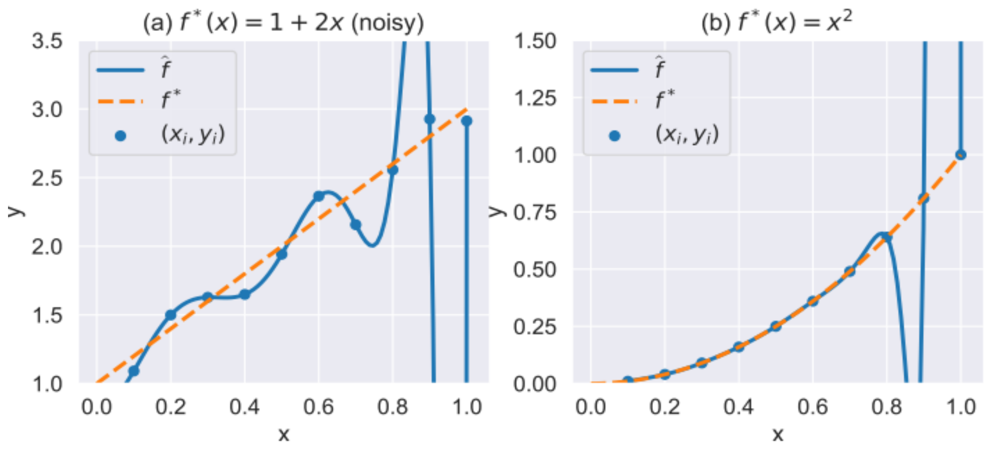
-- Mark Schmidt

Regularization and generalization

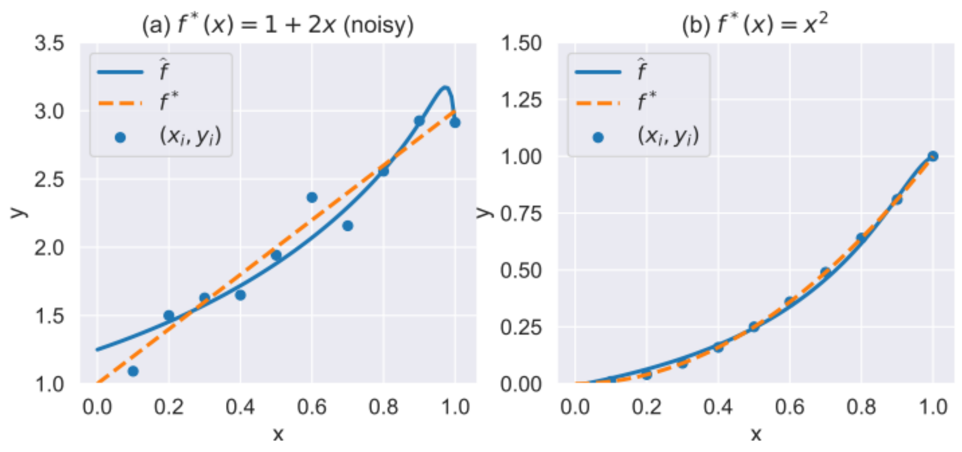
- We apply ℓ^2 regularization on the over-fitting examples
- Consider

$$\mathcal{H}_M = \left\{ f : f(x) = \sum_{i=0}^{99} w_j x^j \right\} \text{ so } M = 100 \text{ , but } N = 10$$

<u>Without regularization</u>



<u>With regularization</u>



Linear Regression

- Ridge regression

$$\min_{w\in\mathbb{R}^M} \frac{1}{2N} \|\Phi w - y\|^2 + \lambda ||w||_2^2$$

$$\hat{w} = \left(\Phi^{\mathrm{T}}\Phi + 2N\lambda I\right)^{-1} \Phi^{\mathrm{T}} y$$

- Lasso: no analytical solution

$$\min_{w\in\mathbb{R}^M} \frac{1}{2N} \|\Phi w - y\|^2 + \lambda ||w||_1$$

Optimization Algorithms

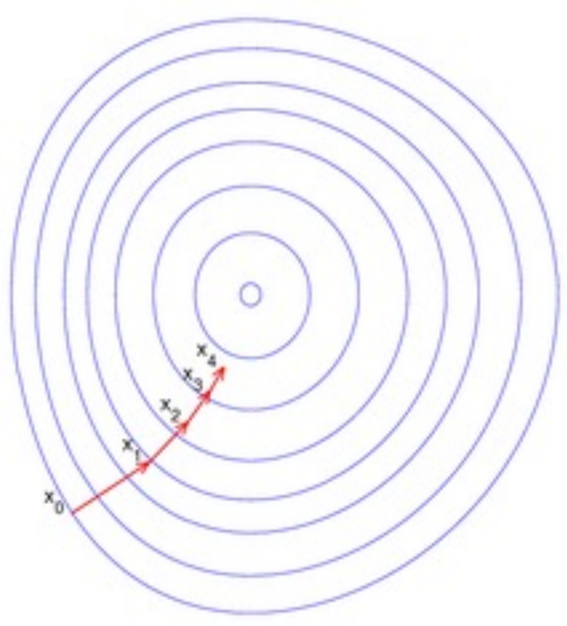
- A necessary first-order optimality condition for $\min f(x)$

$$\nabla f(x^*) = 0$$

- Solve it iteratively:

Gradient Descent : $x_{n+1} = x_n - \gamma \nabla f(x_n)$

- Provided $\gamma < ||\nabla^2 f||$, it can be shown that $||\nabla f(x_n)|| \to 0$

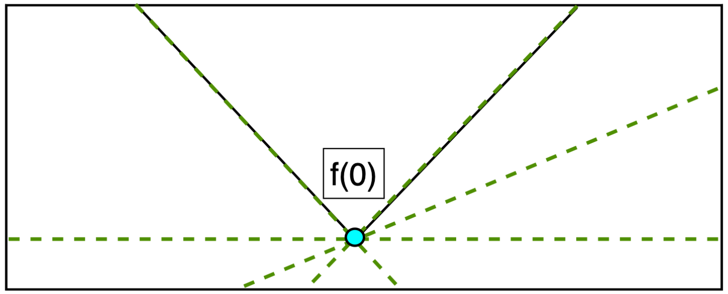


Optimization Algorithms

- $||\cdot||_1$ is not differentiable at 0. Consider subgradient

$$\partial f(x_0) = \{g | f(x) \geq f(x_0) + g^T(x - x_0)\}$$

$$\partial |x| = \begin{cases} 1, & x > 0 \\ -1, & x < 0 \\ [-1,1], & x = 0 \end{cases}$$



- Subgradient methods: $w_{k+1} = w_k - \gamma_k g_k,\ g_k \in \partial f(w_k)$
- Due to the slow convergence rate of subgradient methods, many advanced algorithms have been proposed to solve Lasso, e.g. ADMM, proximal gradient descent.

Classification

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

→ cat

(Discrete output)

Logistic Regression

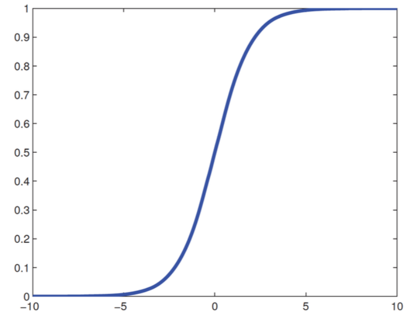
- Binary classification problem:

$$\text{one-hot encoding for the output } \left\{\begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}\right\}$$

This two-dimensional vector can be understood as the probability for each class and can take continuous values.

- A linear hypothesis space: $\{u(x): u = w^T x, x \in \mathbb{R}^n, \mathrm{w} \in \mathbb{R}^n\}$.
- Softmax: Map the extracted feature u to the space of one-hot codes

$$\mu = \frac{1}{1+e^{-u}}, 1-\mu = \frac{e^{-u}}{1+e^{-u}}$$



Logistic Regression

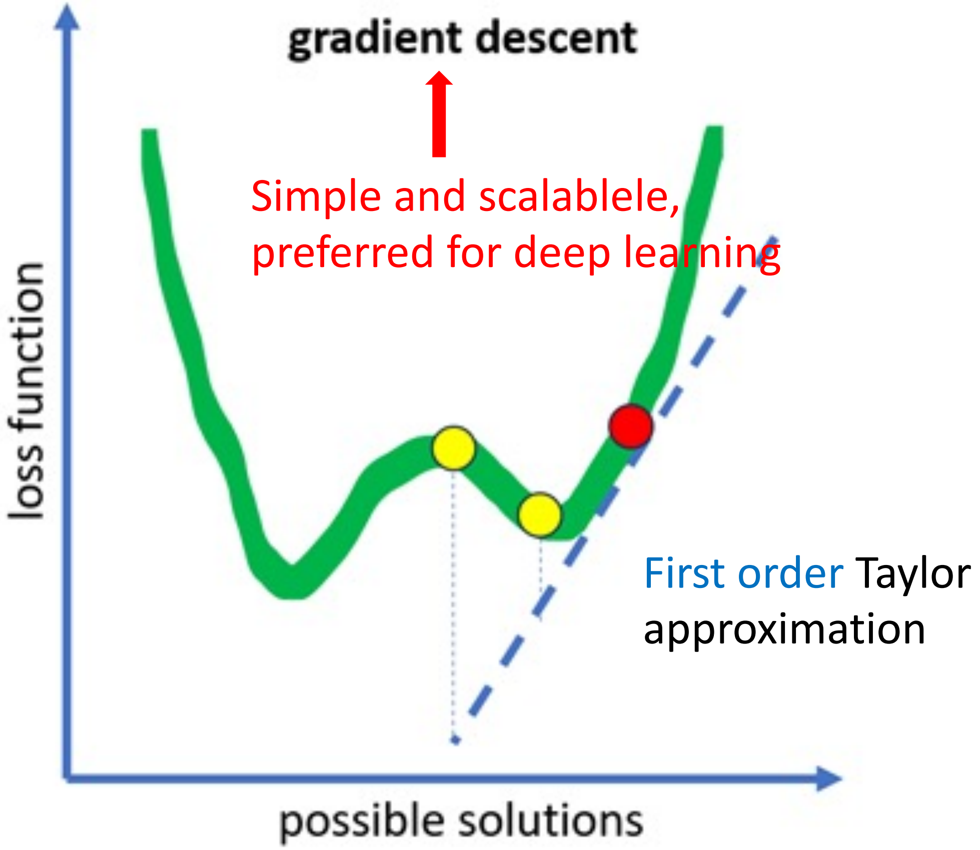
- Loss function
  - ℓ_2-loss
  - Maximum likelihood (KL divergence)

$$\max \Pi_{i=1}^{N} p(y_i|x_i,w) \Leftrightarrow \min -\sum_{i=1}^{N} \log p(y_i|x_i,w) \ \ (\textit{cross entropy})$$

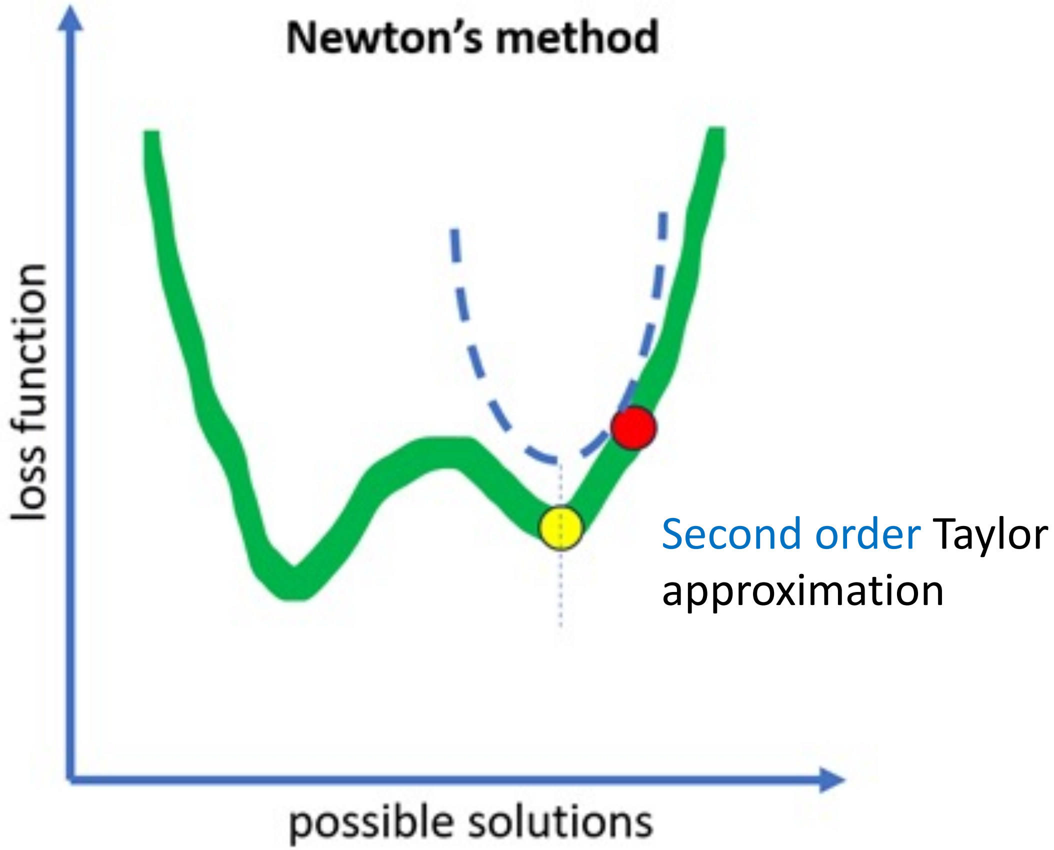
$$-\sum_{i=1}^{N} \log p(y_i|x_i,w) = \sum_{i=1}^{N} -y_i \log \mu_i - (1-y_i)\log(1-\mu_i)\,,\mu_i = \frac{1}{1+e^{-w^T x}}$$

- Optimization: smooth and convex loss function; gradient descent, newton methods…

Optimization



lower convergence, low memory
requirements and computational cost



faster convergence, high memory
requirements and computational cost

Summary

- Machine Learning: learning from experience (or data).
- Supervised learning is to learn the mapping from x to y given paired training dataset $\{(x_i, y_i)\}$. Key steps include
  1. Define the hypothesis space
  2. Define the empirical loss
  3. Find the best approximation under the given empirical loss