Frontiers in deep learning

March 4

Tailin Wu, Westlake University

Website: ai4s.lab.westlake.edu.cn/course

Image from: sdecoret

Project logistics

Choose a **problem related to your research**, and **use AI to solve it.**

Team size: 1-3 people

Timeline:

- By **March 25** (5th class): submit team composition in Feishu
- April 15 & 22 (8th and 9th class): Mid-term course project design (presentation) 30 point
- June 3 & 11 (15th and 16th class): Summary presentation (30 point) and final report (35 point)

Encourage interdisclinary teams: if a team has both **AI** and **non-AI** students (all team members must contribute substantially), the total project score will add 5 points.

How to form teams: Can shout out in the “Random” channel in Feishu

Project guideline

Mid-term course project design

- Give a presentation (10min) that formulates the problem for the **5 questions**, each with one slide:
  1. What is the problem?
  2. Why is it important
  3. Why is it hard?
  4. What is the limitation of the prior method?
  5. What is the main component of the proposed method?

  Then detail the proposed method (3-4 slides) that uses an AI technique to solve the problem

Outline

- Deep learning: fundamentals (Prof. Tailin Wu)
  - Two foundational principles
  - Their realization in neural architecture and learning
- Optimization (SGD) and federative learning (Prof. Tao Lin)
  - Optimization with SGD
  - Federative learning

Previous class: a bird-eye view of deep learning

Tasks		Neural architecture		Learning paradigm
• Classification/ regression • Simulation • Inverse design/ inverse problem • Control/planning	×	• Multilayer perceptron • Graph Neural Networks • Convolutional Neural Networks • Transformers	×	• Supervised learning • Generative modeling • Foundation models • Reinforcement learning • Evolutionary and multi-objective optimization

Application (AI & Science)

- Robotics
- Games (e.g., Go, atari)
- Autonomous Driving
- PDEs
- Life science
- Materials science

Foundational principles in deep learning

What are the most **important insights** from 30 years of deep learning?

Foundational principles in deep learning 1

What are the most **important insights** from 30 years of deep learning?

Method 1: go from A to B in a straight line
(learn a direct mapping from A to B)

Hard to learn due to the complexity of A, B and their difference!

Foundational principles in deep learning 1

What is the most **important insight** from 30 years of deep learning?

Method 2: go from A to B in small, easier steps

Much easier!

(compose step-by-step simple mappings to map A to B)

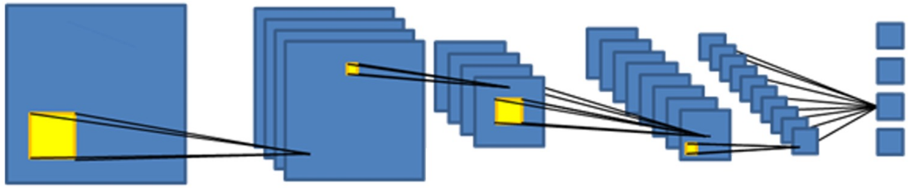
Foundational principles in deep learning 1

Insight: to construct a complex mapping from A to B, it is much easier to compose simple mappings

input

deep neural networks

target



“cat”

Foundational principles in deep learning 1

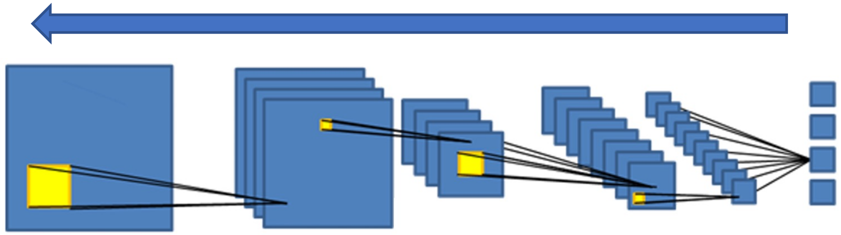
Insight: to construct a complex mapping from A to B, it is much easier to compose simple mappings

gradient w.r.t. parameter

Backpropagation反向传播

loss

$$\frac{\partial L}{\partial \theta}$$

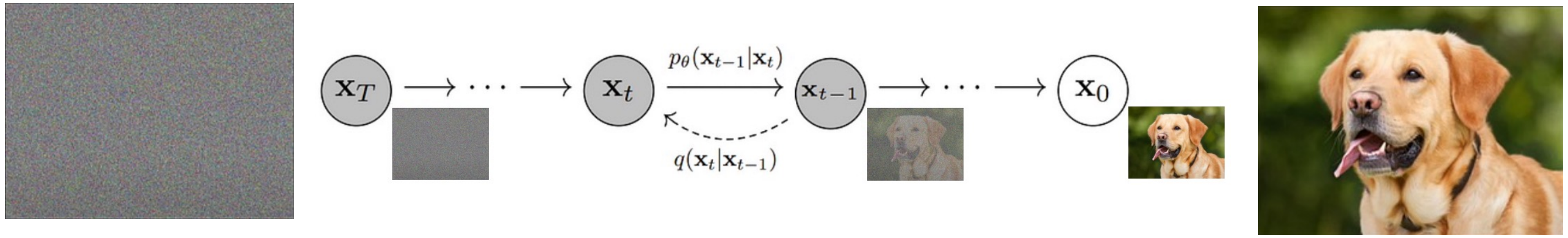


$$L = \mathrm{MSE}(f_\theta(x), y)$$

Foundational principles in deep learning 1

Insight: to construct a complex mapping from A to B, it is much easier to compose simple mappings

Gaussian distribution diffusion model data distribution



Foundational principles in deep learning 1

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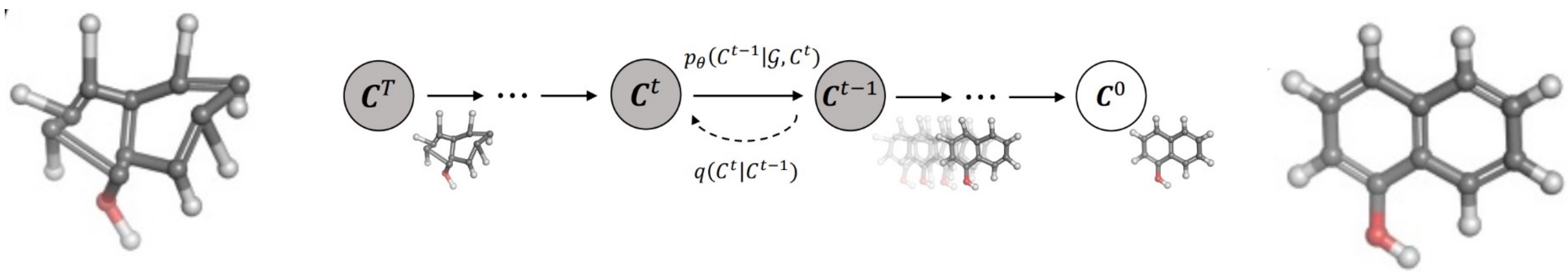
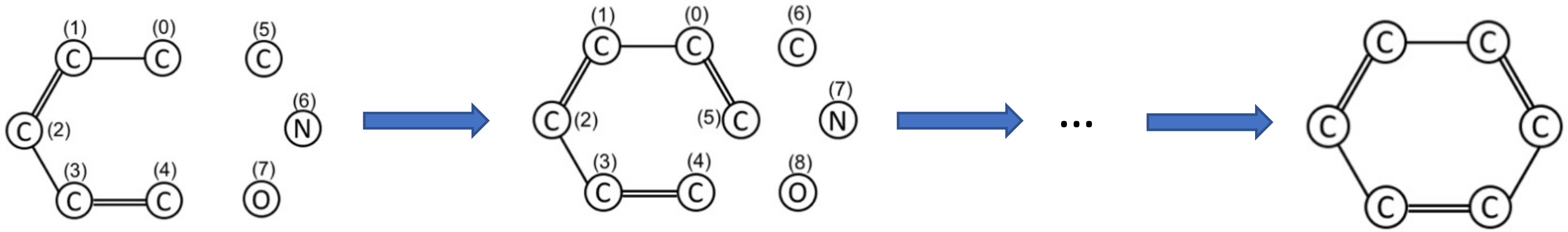
Gaussian distribution diffusion model data distribution



Foundational principles in deep learning 1

Insight: to construct a complex mapping from A to B, it is much easier to compose simple mappings

starting configuration — reinforcement learning — target configuration



Foundational principles in deep learning

What are the most **important insights** from 30 years of deep learning?

1. Model a hard transformation by composing many simple, easy transformations.
   This principle underlies all neural architectures and learning paradigms

2. Directly optimizing the final objective using probability and information theory
   Almost all learning objectives can be reduced to maximum likelihood or minimizing/maximizing information

How to tackle a task using deep learning:

1. Specify the task (including input, target), and define its learning objective;
2. Choose appropriate neural architecture and learning process;
3. Train, evaluate (and iterate)

Foundational principles in deep learning

What are the most **important insights** from 30 years of deep learning?

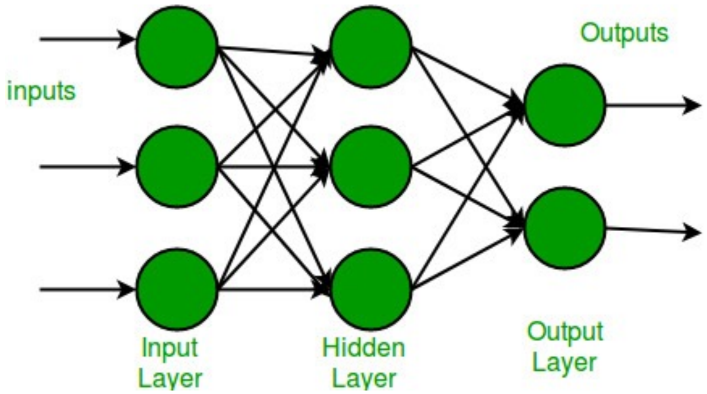
1. Model a hard transformation by composing many simple, easy transformations.
   This principle underlies all neural architectures and learning paradigms
   - Multilayer Perceptron (MLP)
   - Backpropagation
2. Directly optimizing the final objective using probability and information theory
   Almost all learning objectives can be reduced to maximum likelihood or minimizing/maximizing information

Interactive notebook: https://github.com/AI4Science-WestlakeU/frontiers_in_AI_course

Multilayer Perceptron (MLP)

input

f_θ



target

"cat"

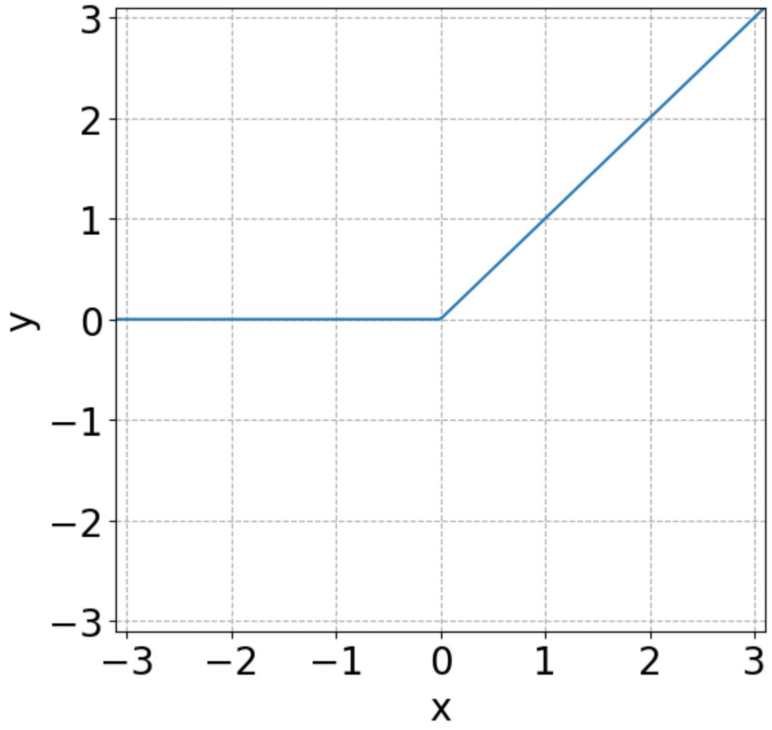
An MLP f_θ with 1 layer: $\sigma(W_1 x + b_1)$: linear transformation with nonlinear activation

An MLP f_θ with n layers: $\sigma(W_n \sigma(\ldots \sigma(W_2 \sigma(W_1 x + b_1) + b_2) \ldots + b_n)$

(Application of the foundational principle 1)

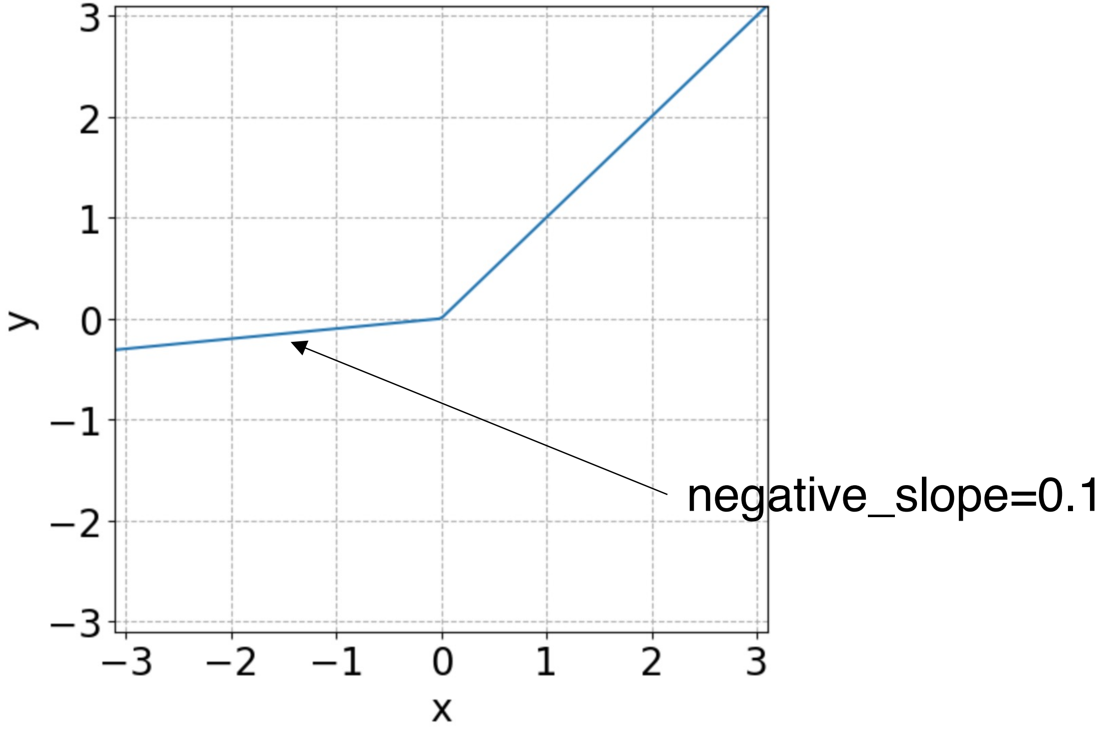
W_i: weight matrix to be learned
b_i: bias vector to be learned
σ: (nonlinear) activation function

Activation function



ReLU (Rectified Linear Unit)

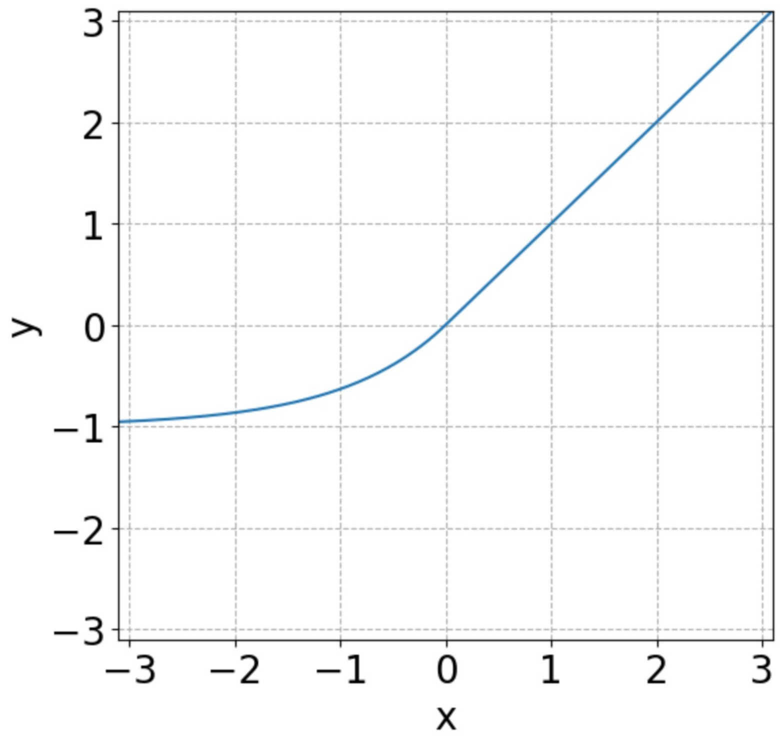
$$\text{ReLU}(x) = \max(0, x)$$



LeakyReLU

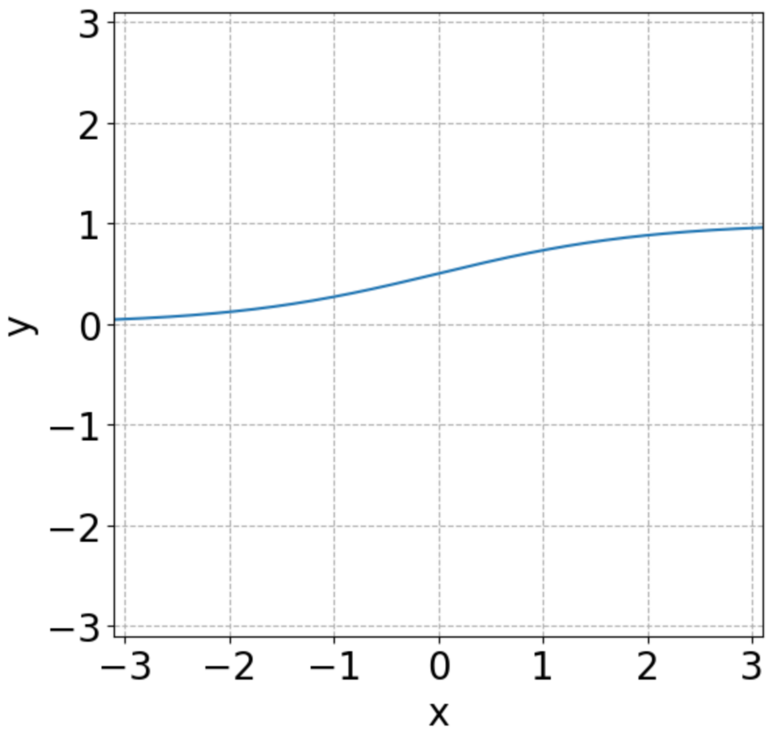
$$\text{LeakyReLU}(x) = \begin{cases} x, & \text{if } x \geq 0 \\ \text{negative\_slope} \times x, & \text{otherwise} \end{cases}$$

Activation function



ELU (Exponential Linear Unit)

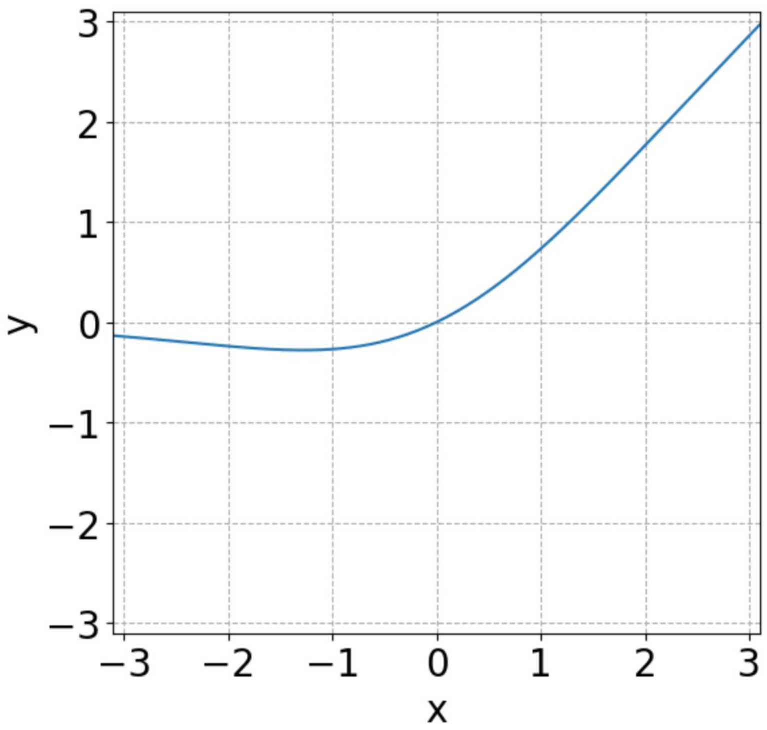
$$\mathrm{ELU}(x) = \begin{cases} x, & x > 0 \\ e^x - 1, & x \leq 0 \end{cases}$$



Sigmoid

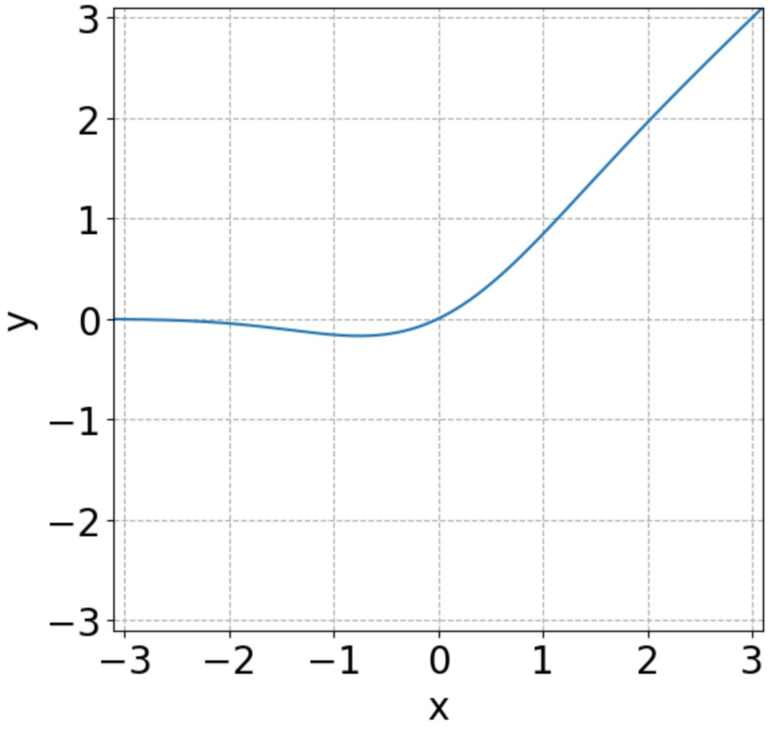
$$\mathrm{Sigmoid}(x) = \frac{1}{1+\exp(-x)}$$

Activation function



SiLU (Sigmoid Linear Unit)

$$\text{SiLU}(x) = x \cdot \text{Sigmoid}(x)$$



GELU (Gaussian Error Linear Unit)

$$\text{SiLU}(x) = x \cdot \Phi(x)$$

$\Phi(x)$ is the cumulative distribution function for Gaussian distribution

Activation function

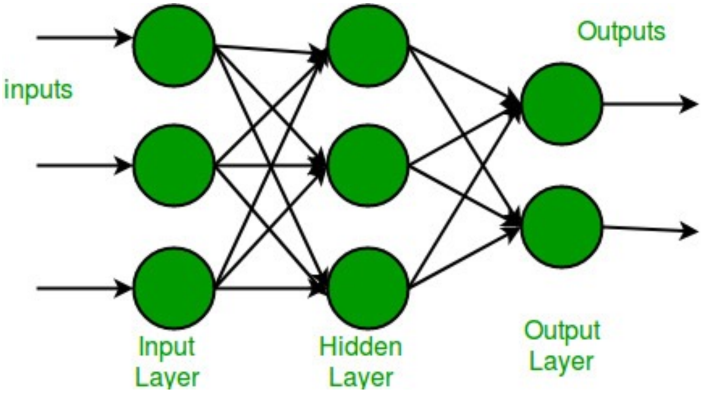
Activation function	Advantages	Drawbacks
ReLU	Simple, suitable for classification	Can have some “dead neurons” The network is piecewise linear
LeakyReLU	Does not have dead neurons	The network is piecewise linear
ELU	Typically useful for regression	
Sigmoid	Output contrained to [0,1]	If input is far from 0, then have saturation (vanishing gradient)
SiLU	Typically useful for regression	
GELU	Typically useful for regression	

Typically try ReLU, LeakyReLU, ELU, and SiLU in hyperparameter search

MLP: universal approximation theorem

input

f_θ



target

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An MLP f_θ that has 1 hidden layer (with arbitrary width) and a nonlinear activation function can approximate any function to arbitrary precision [1][2].

Here $f_\theta(x) = W_2\sigma(W_1 x + b_1)$

- With one hidden layer, may need exponential number of neurons w.r.t. input size
- With more layers, the neurons needed may be polynomial [3]

[1] Funahashi, Ken-Ichi. "On the approximate realization of continuous mappings by neural networks." Neural networks 2.3 (1989): 183-192.
[2] Hornik, Kurt, Maxwell Stinchcombe, and Halbert White. "Multilayer feedforward networks are universal approximators." Neural networks 2.5 (1989): 359-366.
[3] Rolnick, David, and Max Tegmark. "The power of deeper networks for expressing natural functions." ICLR 2018

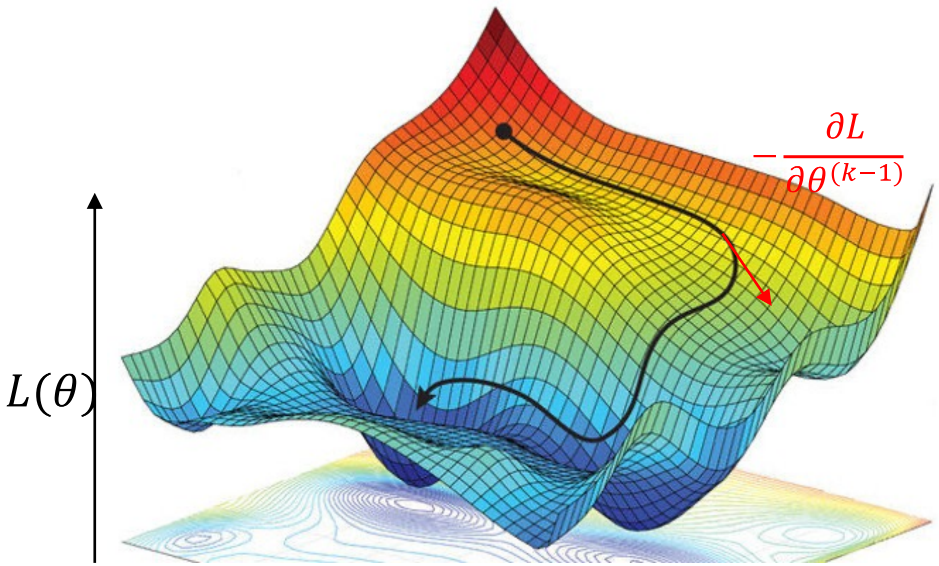
Learning with gradient descent

$$f_\theta(x) = \sigma(W_n\sigma(\dots\sigma(W_2\sigma(W_1x + b_1) + b_2)\dots + b_n)$$

To fit dataset $\{(x_i, y_i)\}, i = 1,2, \dots N$, we can use Mean Squared Error (MSE):

$$L(\theta) = \frac{1}{N}\sum_{i=1}^{N}\left(y_i - f_\theta(x_i)\right)^2$$

How can we optimize the parameter $\theta = (W_1, , \dots W_n, b_1, \dots b_n)$?



θ (typically high dimensional)

Answer: compute $\frac{\partial L}{\partial \theta}$, then we can perform gradient descent :

$$\theta^{(k)} \leftarrow \theta^{(k-1)} - \eta\frac{\partial L}{\partial \theta^{(k-1)}}$$

η: learning rate

Backpropagation

Consider:

$$z = f(y), y = f(x), x = f(w)$$

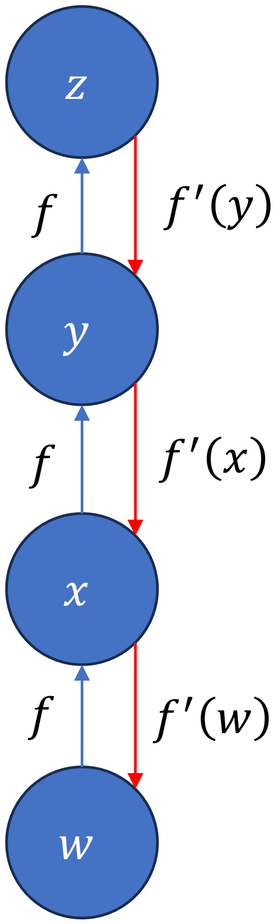
$$z = f\left(f\left(f(w)\right)\right)$$

Chain rule:

$$\frac{\partial z}{\partial w} = \frac{\partial z}{\partial y}\frac{\partial y}{\partial x}\frac{\partial x}{\partial w} = f'(y)f'(x)f'(w)$$

Observation:

1. We need to store intermediate result x, y to avoid recomputing them.
2. Goes layer-by-layer from output to input.



Backpropagation

Let's take a two layer MLP $f_\theta(x) = W_2\sigma(W_1x + b_1)$ as an example:

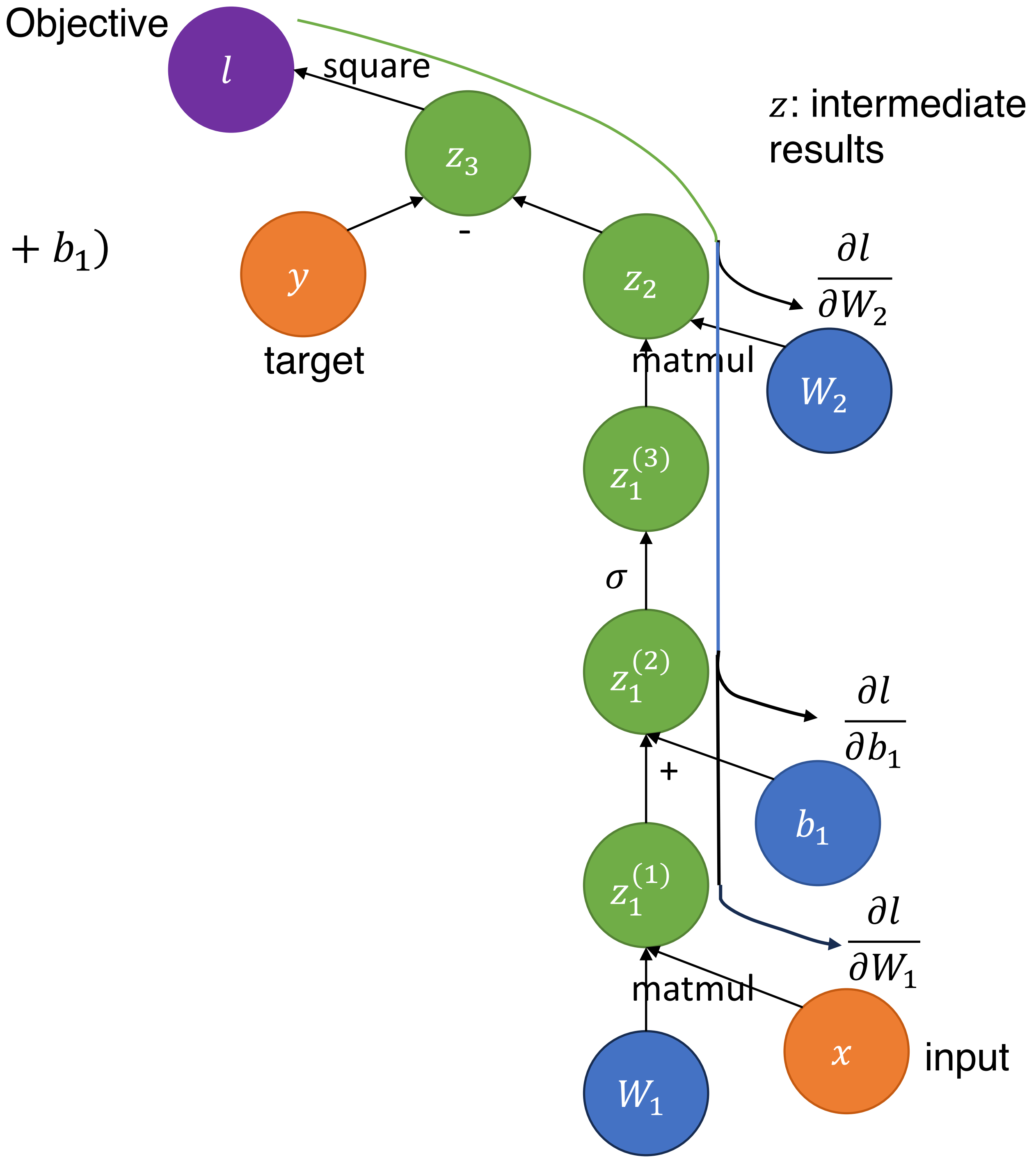
Objective: $l = \left(y - f_\theta(x)\right)^2$

$$\frac{\partial l}{\partial W_2} = \frac{\partial l}{\partial z_3} \cdot \frac{\partial z_3}{\partial z_2} \cdot \frac{\partial z_2}{\partial W_2}$$

$$\frac{\partial l}{\partial b_1} = \frac{\partial l}{\partial z_3} \cdot \frac{\partial z_3}{\partial z_2} \cdot \frac{\partial z_2}{\partial z_1^{(3)}} \cdot \frac{\partial z_1^{(3)}}{\partial z_1^{(2)}} \cdot \frac{\partial z_1^{(2)}}{\partial b_1}$$

$$\frac{\partial l}{\partial W_1} = \frac{\partial l}{\partial z_3} \cdot \frac{\partial z_3}{\partial z_2} \cdot \frac{\partial z_2}{\partial z_1^{(3)}} \cdot \frac{\partial z_1^{(3)}}{\partial z_1^{(2)}} \cdot \frac{\partial z_1^{(2)}}{\partial z_1^{(1)}} \cdot \frac{\partial z_1^{(1)}}{\partial W_1}$$

shared, no need to recompute



Foundational principles in deep learning 1: summary

1. Model a hard transformation by composing many simple, easy transformations.

   This principle underlies all neural architectures and learning paradigms

   - Multilayer Perceptron (MLP)
   - Backpropagation
   - Optimization with gradient descent (Tao Lin will teach in the second half)

Foundational principles in deep learning

2. Directly optimizing the final objective using probability and information theory

   Almost all learning objectives can be reduced to maximum likelihood or minimizing/maximizing information

Maximum likelihood objective underlies:

- **MSE loss**
- **Uncertainty quantification**
- Variational autoencoder (VAE)
- Diffusion model

Information-based objective underlies:

- **Cross-entropy loss**
- **Information Bottleneck**
- GAN, infoGAN
- Contrastive learning
- InfoMax: Deep Graph InfoMax
- Active learning
- Reinforcement learning:
  - Exploration vs. exploitation tradeoff, empowerment

Maximum likelihood

We have data $\{x_i\}, i = 1, \dots N$, and want to use a probability model $p_\theta(x)$ to model it.

Maximizing the likelihood is equivalent to minimizing the negative log-likelihood:

$$-\log P\left(\{x_i\}_{i=1}^{N}\right) = -\log \prod_{i=1}^{N} p_\theta(x_i) = -\sum_{i=1}^{N} \log p_\theta(x_i)$$

Maximum likelihood: deriving MSE

We have data $\{(x_i, y_i)\}, i = 1, \dots N$, and want to use a probability model $p_\theta(y|x)$ to model it.

Here we assume $p_\theta(y|x) \sim \mathcal{N}\left(y; \mu_\theta(x), \sigma_\theta^2(x)\right)$ is a conditional Gaussian:

$$p_\theta(y|x) = \frac{1}{\sqrt{2\pi}\sigma_\theta(x)} e^{-\frac{\left(y-\mu_\theta(x)\right)^2}{2\sigma_\theta^2(x)}}$$

We have

$$-\log P(Y|X) = -\log \prod_{i=1}^{N} p_\theta(y_i|x_i) = -\sum_{i=1}^{N} \log p_\theta(y_i|x_i)$$

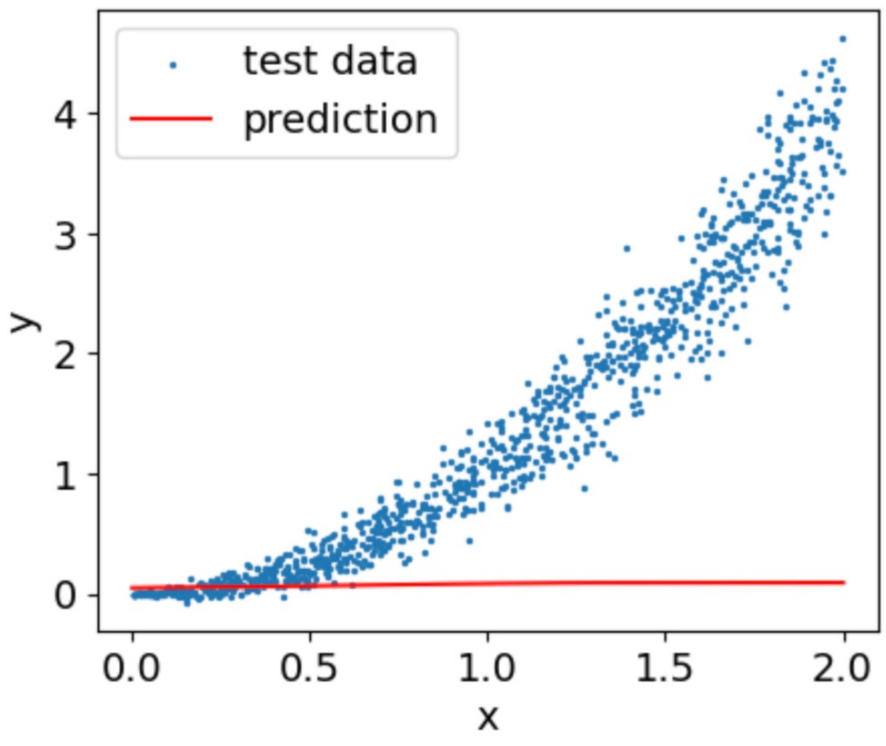
$$X = \{x_i\}_{i=1}^N, Y = \{y_i\}_{i=1}^N$$

$$= \sum_{i=1}^{N} \left[\frac{\left(y-\mu_\theta(x)\right)^2}{2\sigma_\theta^2(x)} + \log \sigma_\theta(x)\right]$$

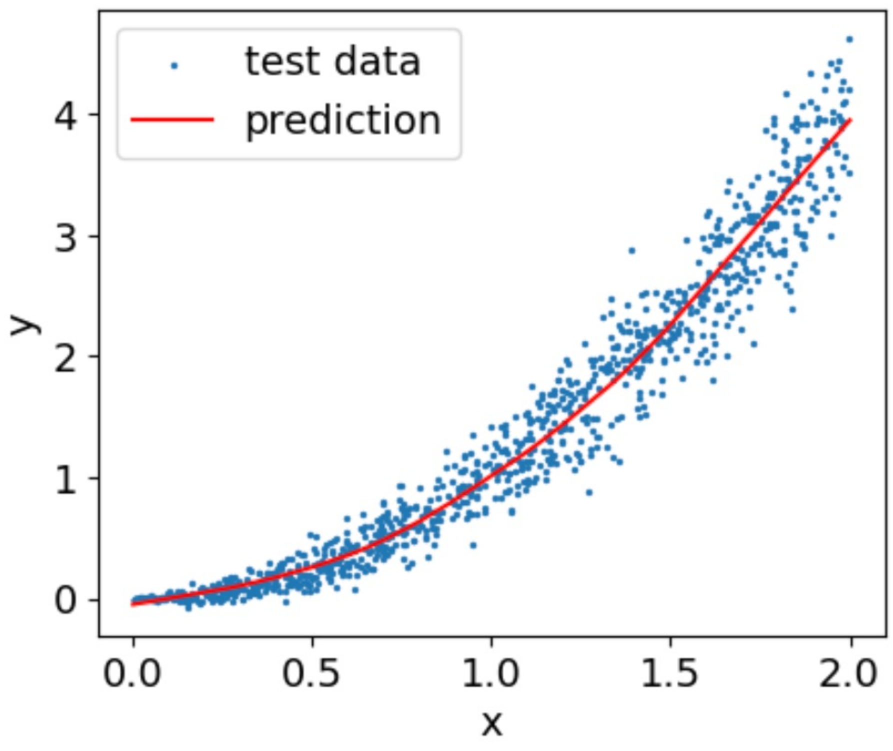
Assuming $\sigma_\theta(x) \equiv 1$, we have $-\log P(Y|X) = \frac{1}{2}\sum_{i=1}^{N}\left(y-\mu_\theta(x)\right)^2$ MSE loss

Maximum likelihood: deriving MSE

Prediction by initial model f_θ:



Prediction after training f_θ:

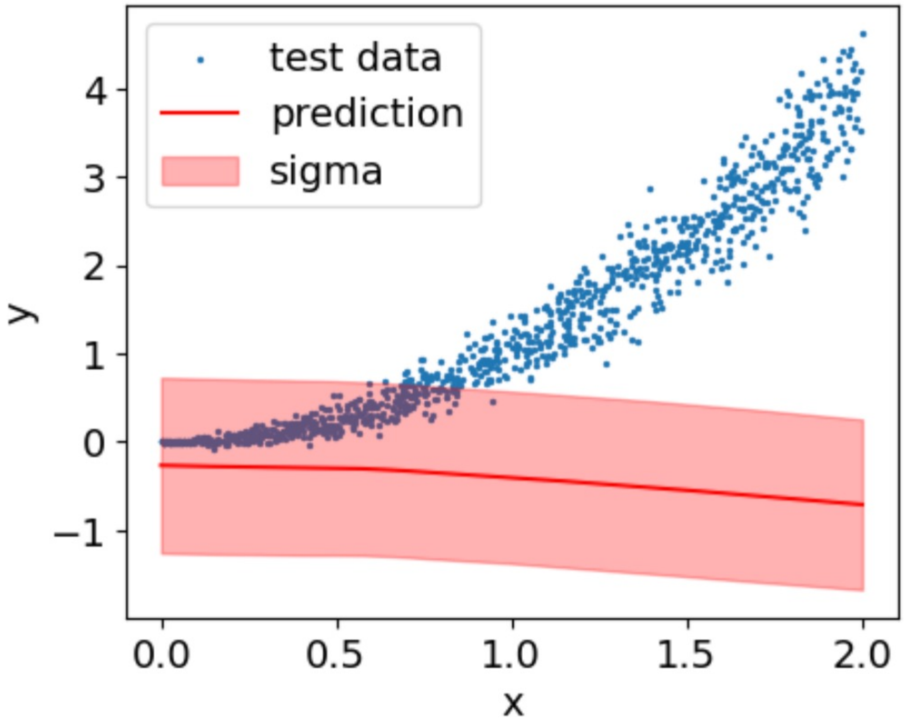


Maximum likelihood: estimating uncertainty

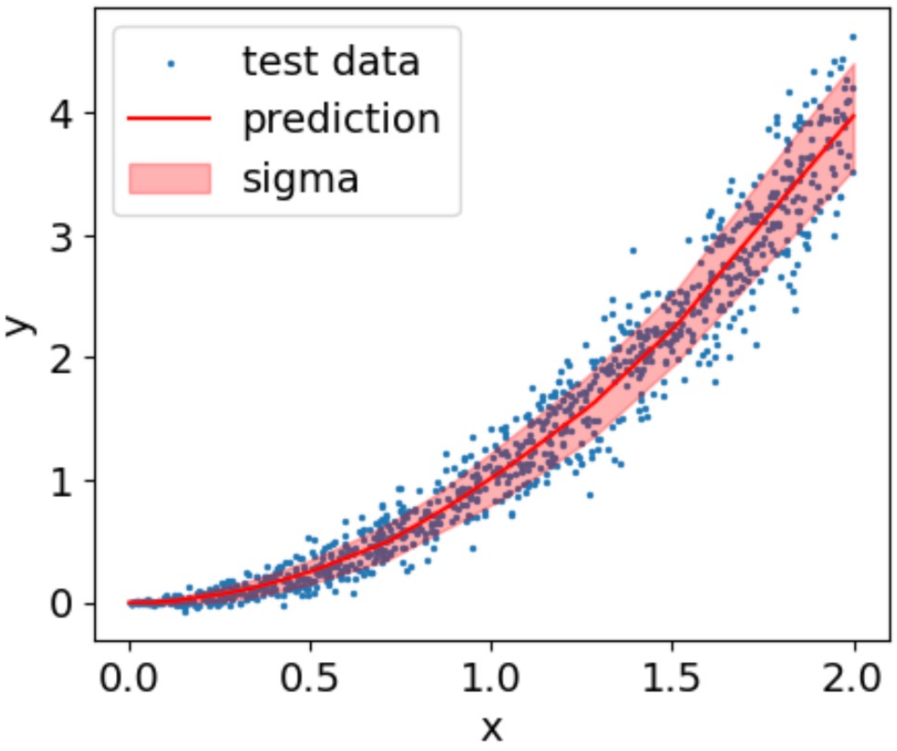
If $\sigma_\theta(x)$ can be learned, we can also estimate uncertainty [1]:

$$-\log P(Y|X) = \sum_{i=1}^{N} \left[\frac{\left(y - \mu_\theta(x)\right)^2}{2\sigma_\theta^2(x)} + \log \sigma_\theta(x) \right]$$

Prediction by initial model f_θ:



Prediction by trained model f_θ:



Foundational principles in deep learning

2. Directly optimizing the final objective using probability and information theory

Almost all learning objectives can be reduced to maximum likelihood or minimizing/maximizing information

Maximum likelihood objective underlies:

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- InfoMax: Deep Graph InfoMax
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- Reinforcement learning:
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Information diagram

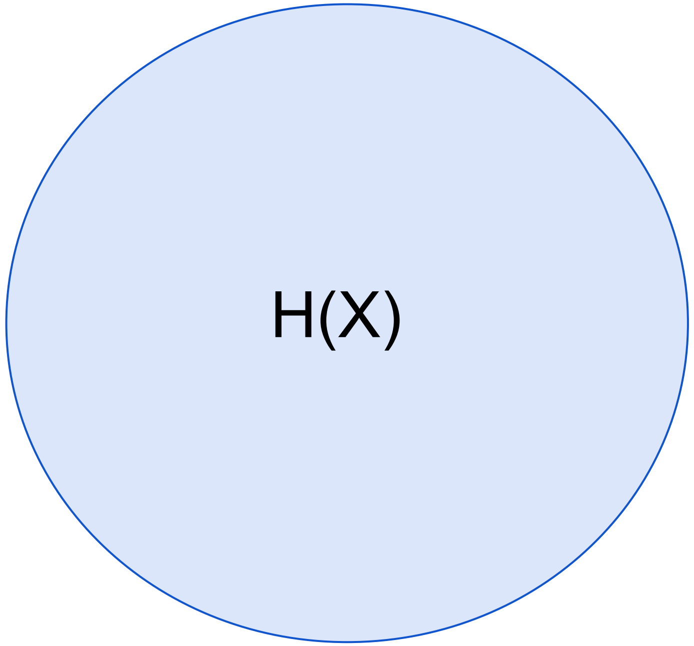
A type of Venn diagram to illustrate relationships among Shannon's basic measures of information for (multiple) variables.

H(X): entropy of variable X, means the expected amount of information conveyed by identifying the outcome of a random sampling.

E.g. if X is a categorical variable taking values in X \in {1,2,3} with probability of {¼,¼, ½}.

When we draw a sample, and get e.g. X=1, the probability of it happening is P(X=1)=¼, this event gains us $\log_2 \frac{1}{P(X=1)} = 2\,(\mathrm{bits})$ of information.

Entropy: $H(X) = \sum_x P(X=x) \log_2 \frac{1}{P(X=x)}$



Alternatively, we can understand it as the amount of information needed to deterministically specify a random variable.

Information diagram

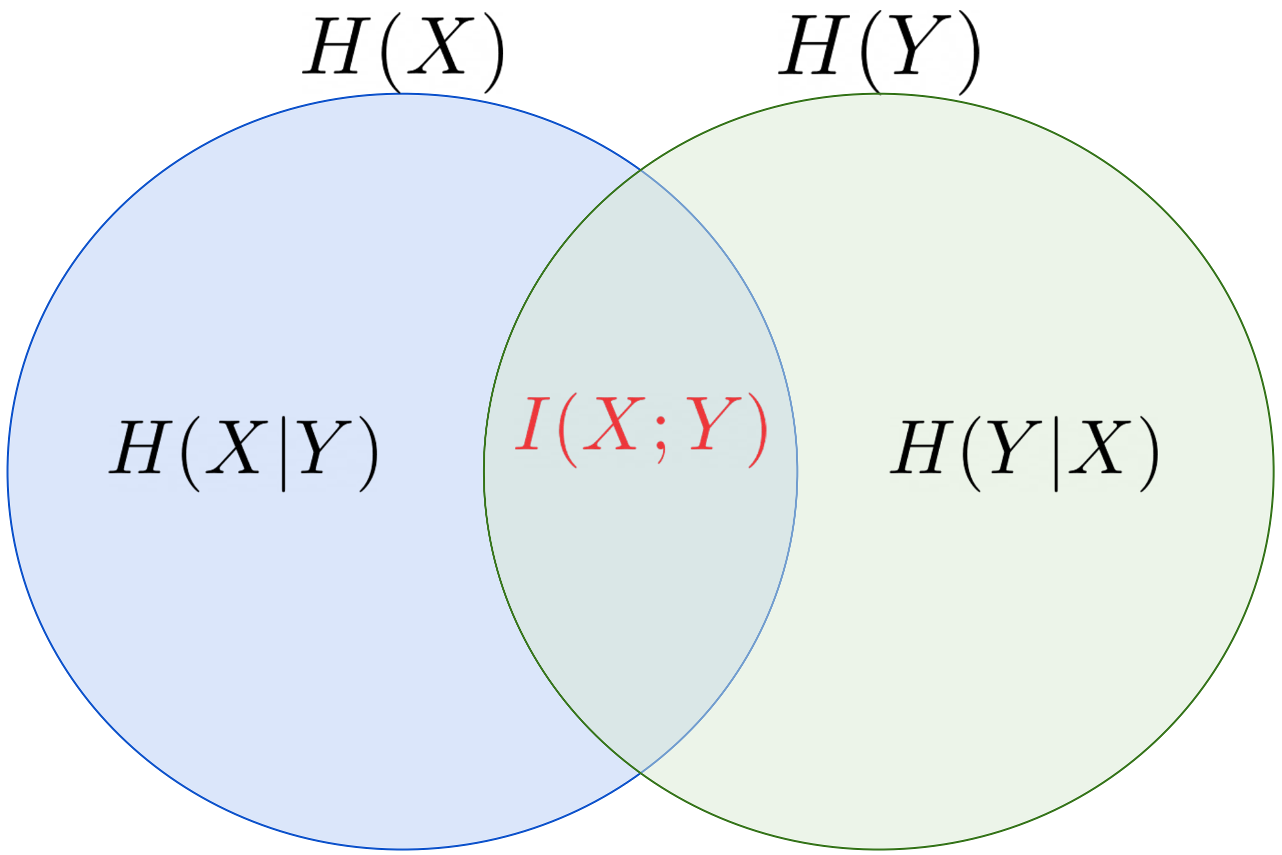
For multiple variables, we can treat each circle as a "set".

$H(X|Y)$: entropy of X conditioned on Y

Meaning: given Y, how much more information needed to fully specify X.

$I(X;Y)$: mutual information between X and Y

Meaning: how much information obtained about X by observing Y



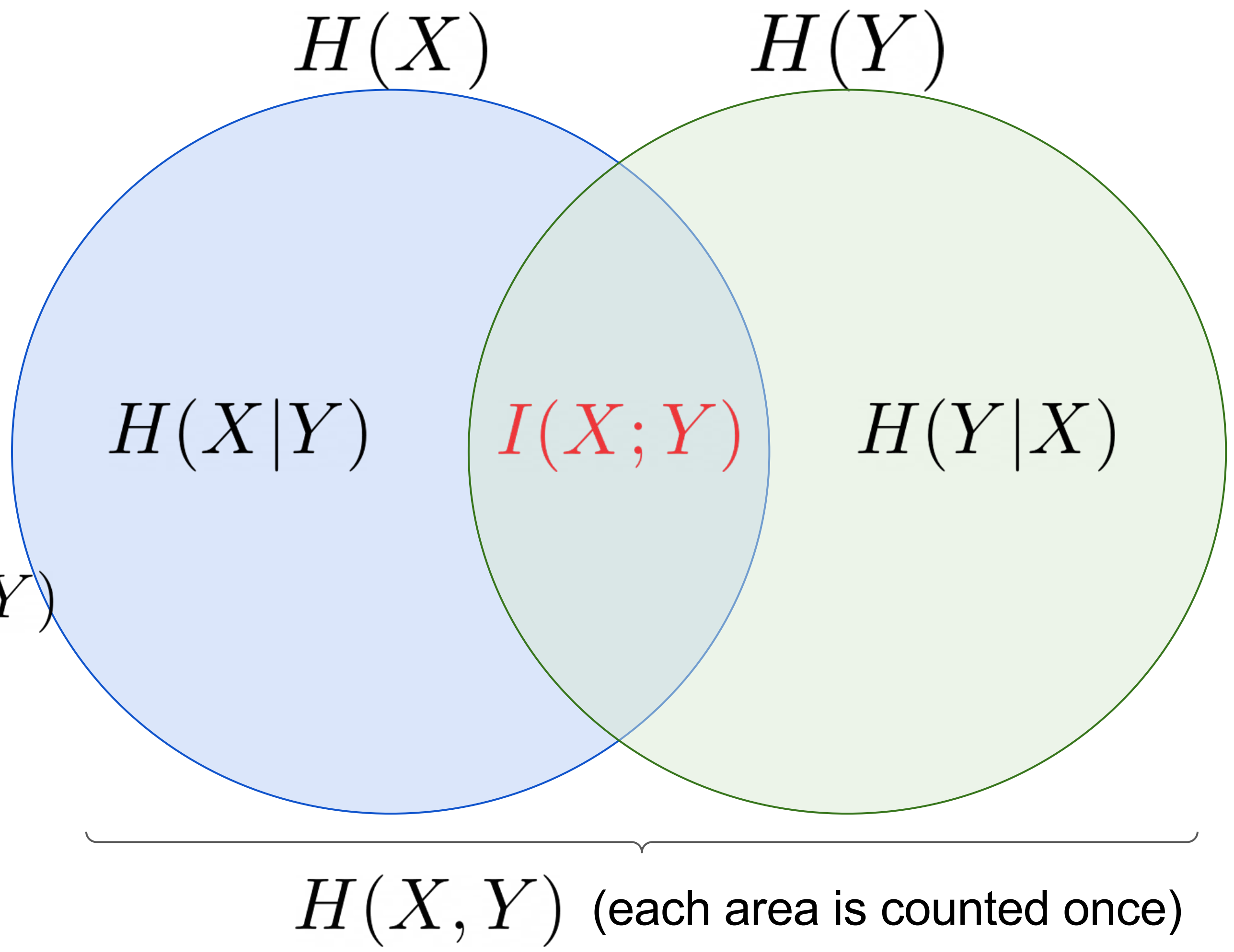
Information diagram

For multiple variables, we can treat each circle as a "set".

Using set operations in the Venn diagram, we can easily derive:

$$H(X|Y) = H(X,Y) - H(Y)$$

$$\begin{aligned} I(X;Y) &= H(X) - H(X|Y) \\ &= H(Y) - H(Y|X) \\ &= H(X) + H(Y) - H(X,Y) \end{aligned}$$



(each area is counted once)

Information diagram: quiz

If Y is a deterministic function of X, how does the information diagram look like?

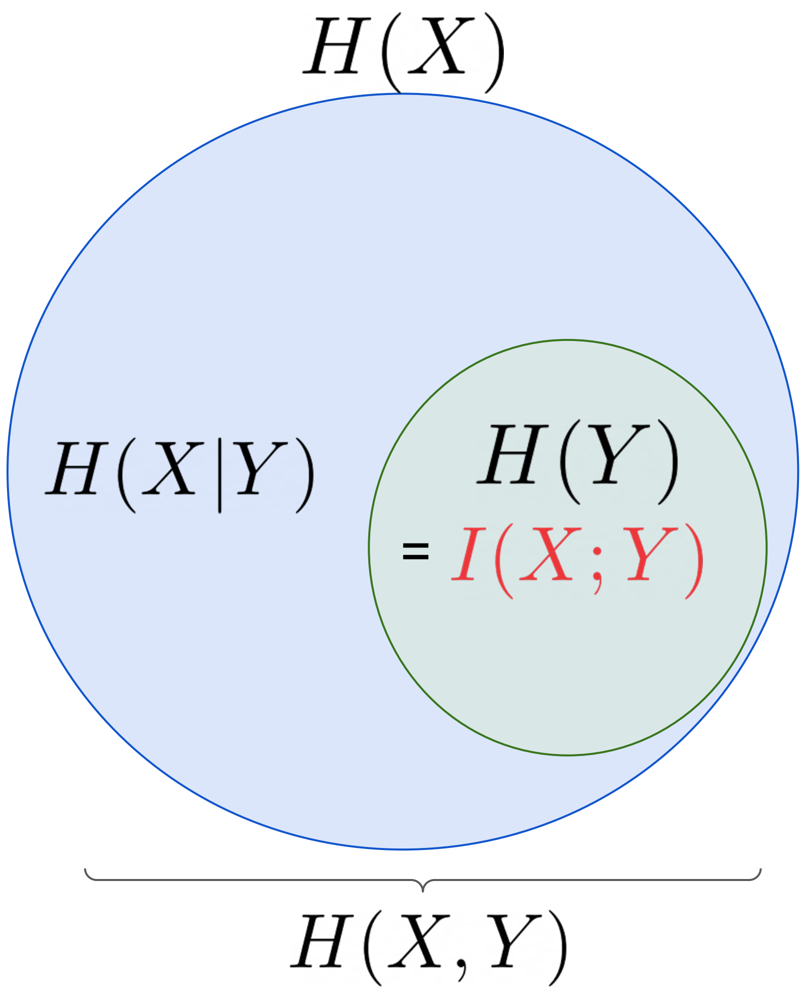
$$H(Y|X) = 0$$

Given X, the amount of information needed to specify Y is 0.

We can then easily derive:

$$H(X,Y) = H(X)$$

$$I(X;Y) = H(Y)$$



Information diagram: more variables

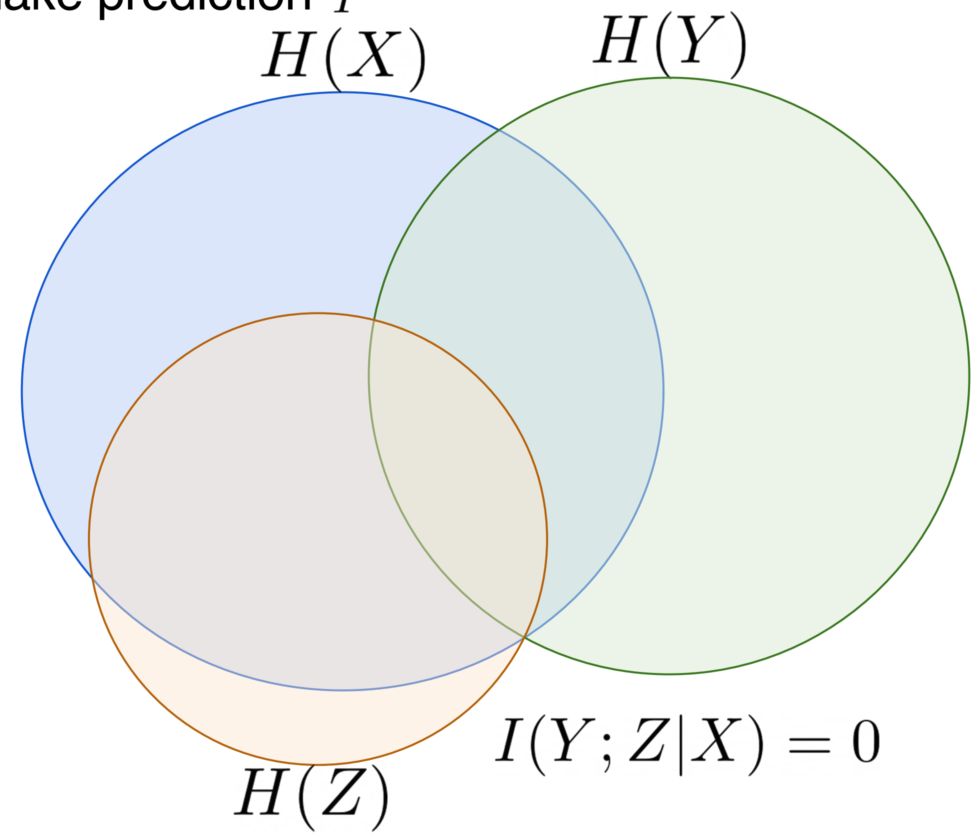
Procedure: (1) Specify dependence between variables; (2) Draw information diagram

Scenario: we have variables of X (images) and Y (labels). We also have a neural network that maps X to latent representation Z, based on which we make prediction $\hat{Y}$

Dependence: $\hat{Y} - Z - X - Y$

Since Z is a function of X, we have:
conditioned on X, Z is <u>independent</u> of Y:

$$I(Y; Z|X) = 0$$



How to optimize the information-based objective?

To maximize some quantity Q that is hard to optimize, we can maximize a learnable quantity $\tilde{Q}$ that is less than Q (similar goes for minimizing)

Example: Evidence Lower Bound (ELBO) in variational autoencoder (VAE) [1], which is a lower bound for the log-likelihood of data.

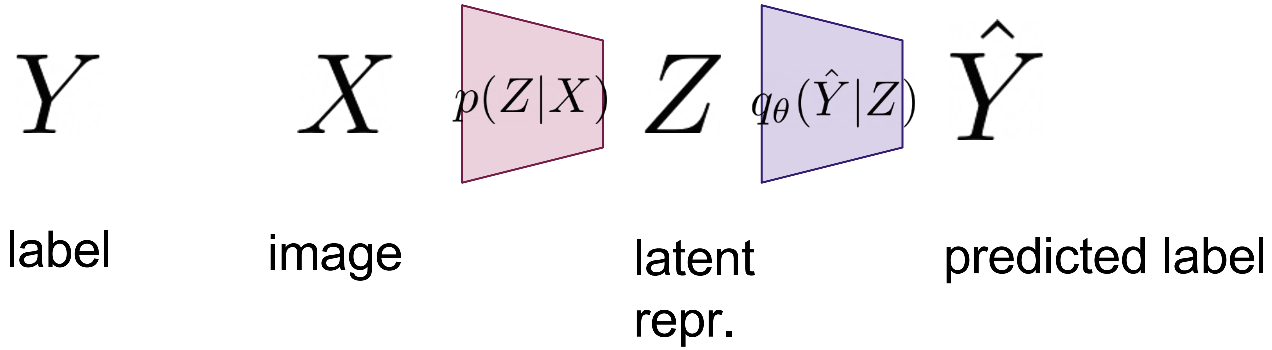
[1] Kingma, Diederik P., and Max Welling. "Auto-encoding variational bayes." arXiv preprint arXiv:1312.6114 (2013).

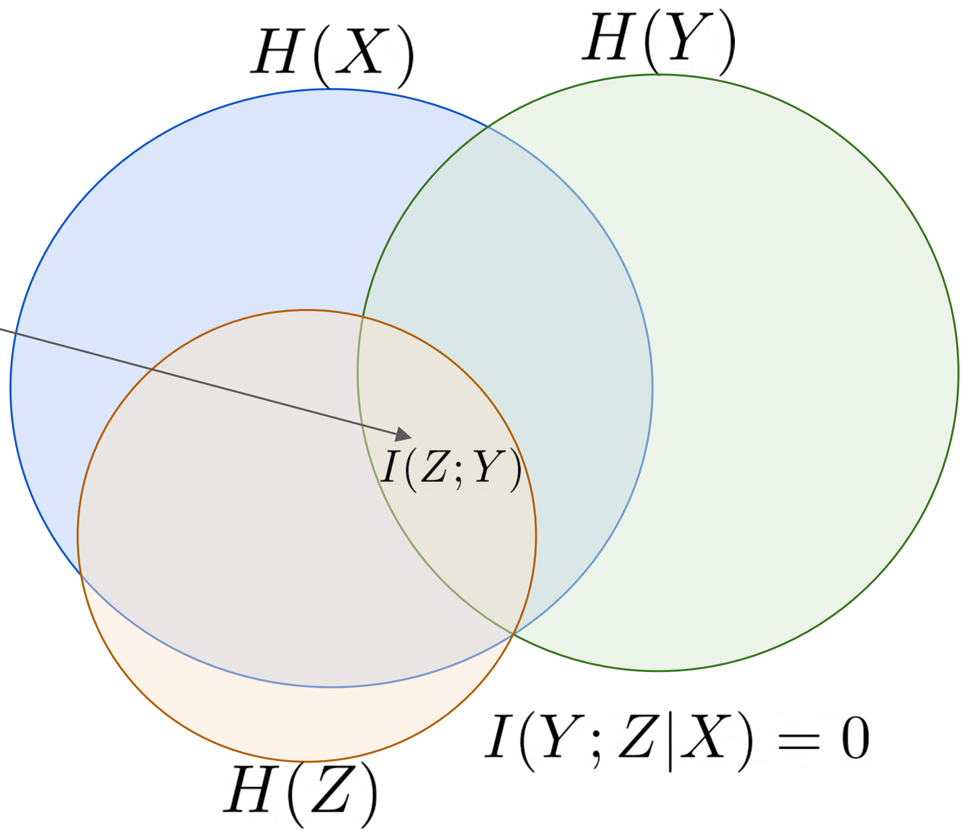
Maximizing mutual information

X are images, Y are corresponding labels. We have an encoder that takes as input X and outputs representation Z, which then predict label $\hat{Y}$

Dependence: $Y - X - Z - \hat{Y}$

Objective: $\max_Z I(Z;Y)$





Maximizing mutual information: cross-entropy

X are images, Y are corresponding labels. We have an encoder that takes as input X and outputs representation Z, which then predict label $\hat{Y}$

$$
\begin{aligned}
I(Y;Z) &:= \int dydz\, p(y,z) \log \frac{p(y|z)}{p(y)} \quad \text{(definition)} \\
&= \int dydz\, p(y,z) \log \frac{q_\theta(y|z)}{p(y)} + \underbrace{\int dydz\, p(y,z) \log \frac{p(y|z)}{q_\theta(y|z)}}_{= KL[p(y|z);\, q_\theta(y|z)] \geq 0} \\
&\geq \int dydz\, p(y,z) \log \frac{q_\theta(y|z)}{p(y)} \\
&= \int dydz\, p(y,z) \log q_\theta(y|z) + H(Y) \\
&= \int dydz\, dx\, p(x)p(y|x)p(z|x) \log q_\theta(y|z) + H(Y)
\end{aligned}
$$

(negative of cross-entropy!)

Ignoring the constant $H(Y)$, we are maximizing $\mathbb{E}_{x,y\sim p(x,y),z\sim p(z|x)}[\log q_\theta(y|z)]$

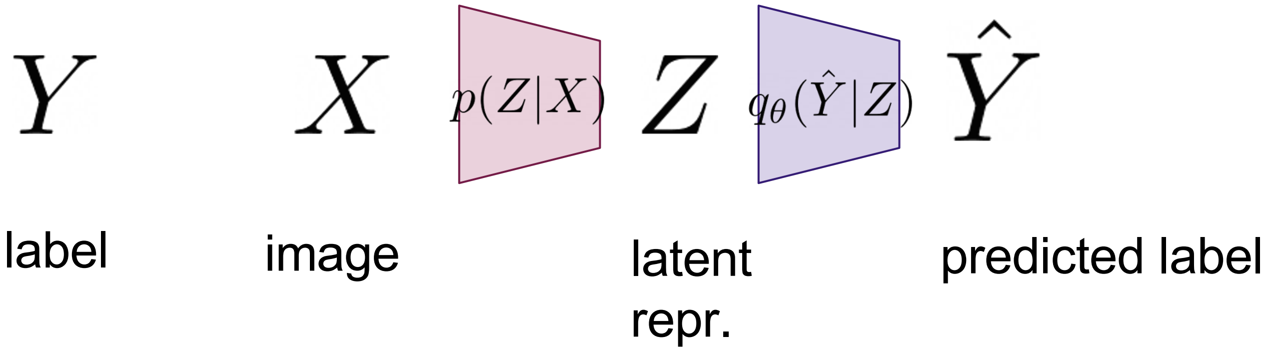
Minimizing mutual information

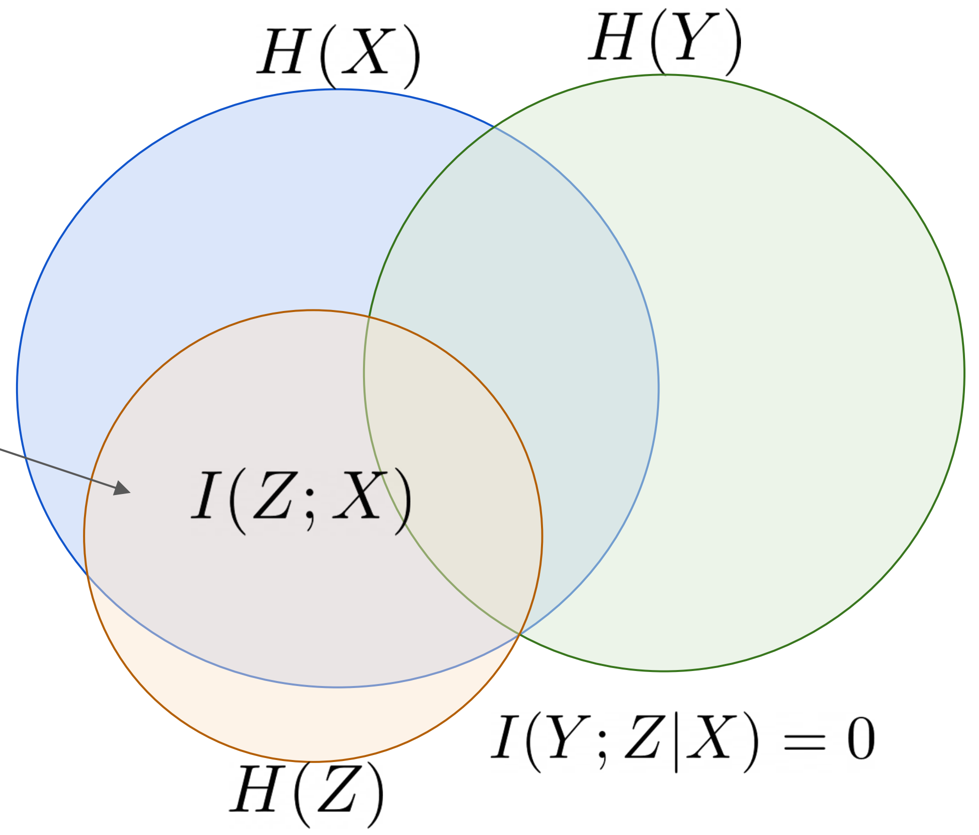
X are images, Y are corresponding labels. We have an encoder that takes as input X and outputs representation Z, which then predict label $\hat{Y}$

Dependence: $Y - X - Z - \hat{Y}$

Objective: $\min_Z I(Z;X)$

so that Z contains *less* information that is not relevant to predict Y: improving robustness and generalization





Minimizing mutual information

X are images, Y are corresponding labels. We have an encoder that takes as input X and outputs representation Z, which then predict label $\hat{Y}$

$$I(Z;X) := \int dxdz\, p(x,z) \log \frac{p(z|x)}{p(z)}$$ (definition)

$$= \int dxdz\, p(x,z) \log \frac{p(z|x)}{r(z)} - \underbrace{\int dxdz\, p(x,z) \log \frac{p(z)}{r(z)}}_{= KL[p(z);r(z)] \geq 0}$$

$$\leq \int dxdz\, p(x,z) \log \frac{p(z|x)}{r(z)}$$

$$\simeq \frac{1}{N} \sum_{i=1}^{N} p(z|x_n) \log \frac{p(z|x_n)}{r(z)}$$ (Monte Carlo estimation of the integral)

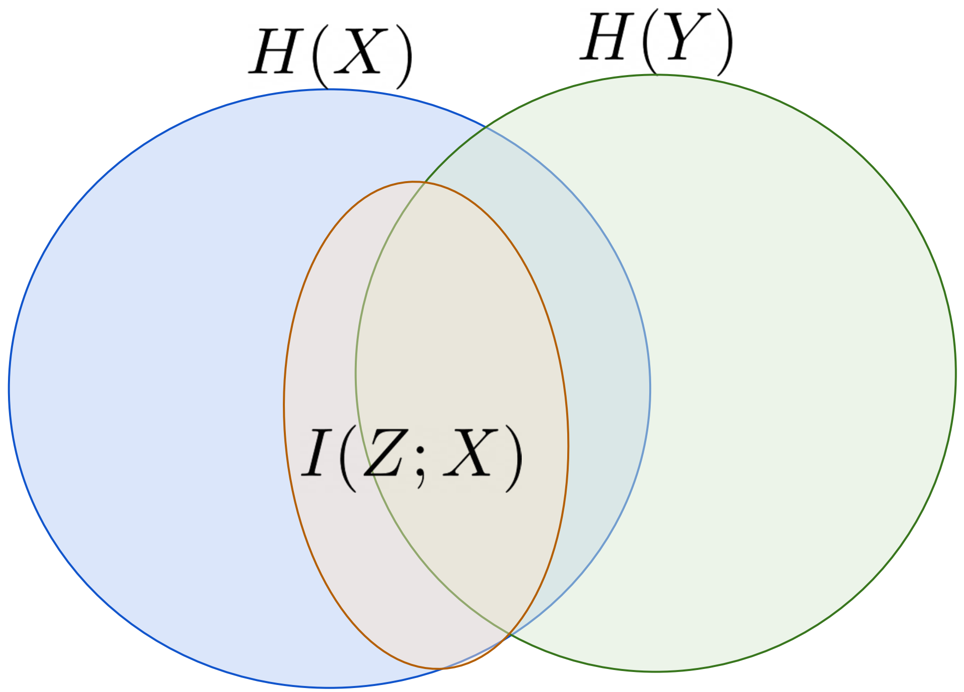
$r(z)$ can be approximated by a Gaussian or mixture of Gaussian, similar to the prior term in VAE

Information Bottleneck [1][2]

[1] Tishby, Naftali, Fernando C. Pereira, and William Bialek. "The information bottleneck method." *arXiv preprint physics/0004057* (2000).
[2] Alemi, Alexander A., et al. "Deep variational information bottleneck." ICLR 2017.
[3] Wu, Tailin, et al. "Graph information bottleneck." *NeurIPS 2020*.
[4] Achille, Alessandro, and Stefano Soatto. "Emergence of invariance and disentanglement in deep representations." *JMLR* 19.1 (2018): 1947-1980.
[5] Lu, Xingyu, et al. "Dynamics generalization via information bottleneck in deep reinforcement learning." *arXiv preprint arXiv:2008.00614* (2020).
[6] Sharma, Archit, et al. "Dynamics-aware unsupervised discovery of skills." *arXiv preprint arXiv:1907.01657* (2019).
[7] Goyal, Anirudh, et al. "Infobot: Transfer and exploration via the information bottleneck." *arXiv preprint arXiv:1901.10902* (2019).

$$\min L = I(Z;X) - \beta \cdot I(Y;Z)$$

$$\simeq \frac{1}{N}\sum_{i=1}^{N} \mathbb{E}_{z\sim p(z|x_i)}\left[\log q_\theta(y_i|z) - \beta \cdot p_\theta(z|x_i)\log\frac{p_\theta(z|x_i)}{r_\theta(z)}\right]$$



Application of Information Bottleneck:

- Robust against adversarial attacks [2][3]
- Learning invariant and disentangled representations [4]
- RL:
  - Improving generalization [5]
  - Facilitating skill discovery [6]
  - Learning goal-conditioned policy [7]

Foundational principles in deep learning

2. Directly optimizing the final objective using probability and information theory

   Almost all learning objectives can be reduced to maximum likelihood or minimizing/maximizing information

Maximum likelihood objective underlies:

- **MSE loss**
- **Uncertainty quantification**
- Variational autoencoder (VAE)
- Diffusion model

Information-based objective underlies:

- **Cross-entropy loss**
- **Information Bottleneck**
- GAN, infoGAN
- Contrastive learning
- InfoMax: Deep Graph InfoMax
- Active learning
- Reinforcement learning:
  - Exploration vs. exploitation tradeoff, empowerment

Foundational principles in deep learning: Summary

1. Model a hard transformation by composing many simple, easy transformations.
   - Multilayer Perceptron (MLP)
   - Backpropagation
2. Directly optimizing the final objective using probability and information theory
   - Maximum likelihood: MSE, uncertainty estimation
   - Information: cross-entropy, Information Bottleneck

Interactive notebook: https://github.com/AI4Science-WestlakeU/frontiers_in_AI_course