11-695: AI Engineering
ML Reivews

LTI/SCS

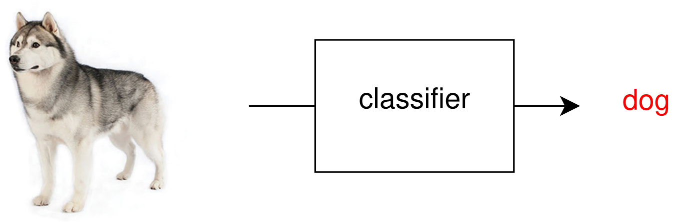
Spring 2020

Outline

1. The Learning Problem
2. Data for Supervised Learning
3. Learning Models
4. Error and Loss Function

Example: Classification

- Find a function $\mathbf{y} = \mathbf{f}(\mathbf{x})$
  - $\mathbf{x}$: an image
  - $\mathbf{y}$: dog, cat, bird, car, etc.



Example: Machine Translation

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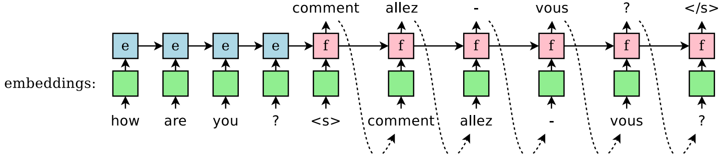
- Find a function $\mathbf{y} = \mathbf{f}(\mathbf{x})$
  - $\mathbf{x}$: an English sentence
  - $\mathbf{y}$: an French sentence



How to Find the Function (or Model) f?

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- An optimization problem: find **f** that minimizes the errors towards a defined an objective function
- Learn from data given
- In many cases, with knowledge/prior/bias about the nature of
  - Data: text, videos, images, ...
  - Expert knowledge: NLP, Medicine, ... For example, to guide the models.
  - ...

How to Model f?

- Parametric:
  - Believe that a fixed param $\mathbf{W} \sim \Omega$ is enough to represent $\mathbf{f}$ in any case
  - The param space Ω is well-defined, *e.g.* $\mathbb{R}^{200\times10}$
  - Choose a learning method, *e.g.* MLE, MAP, ..., to learn $\mathbf{W}$
  - Simple: only estimate params, but we have to inject our bias about data
- Nonparametric:
  - $f \sim \mathbb{F}$, a function space
  - It *has* params, but infinite of them
  - Number of params can change when data change
  - Make no assumption about data, but more complicated because we have to estimate the model, and params of that model
  - More flexible, but a caveat: need to make model assumption

Outline

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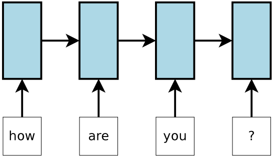
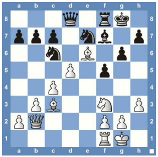
Data for Supervised Learning

- Pairs of $(\mathbf{x}, \mathbf{y})$: $\mathbb{D} = \{(\mathbf{x}^{(1)}, \mathbf{y}^{(1)}), (\mathbf{x}^{(2)}, \mathbf{y}^{(2)}), \ldots, (\mathbf{x}^{(n)}, \mathbf{y}^{(n)})\}$
- Each $\mathbf{x}^{(i)}$ is called a *data point*
- Each $\mathbf{y}^{(i)}$ is called a *label*
- $\mathbf{x}^{(i)}$ and $\mathbf{y}^{(i)}$ can be *anything*





Data Representation

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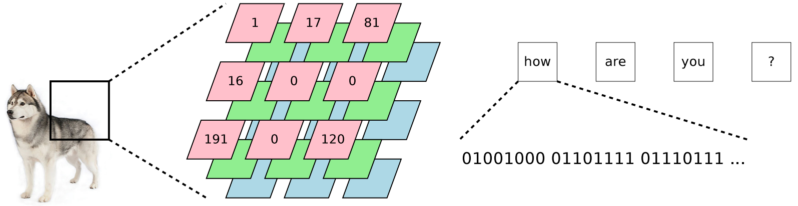
- Computers don't "see" things like we do



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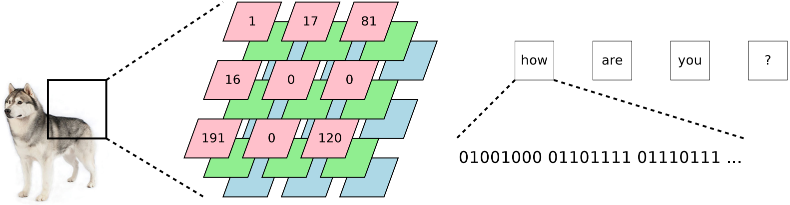

- ... so it's hard to make them think like we do

Some Types of Labels

- Label $\mathbf{y}$ is in a discrete set $\mathcal{C} = \{1, 2, ..., |\mathcal{C}|\}$
  - *Classification* problems

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  - *Structured prediction* problems
- Why learn these?
  - The types of problems you tackle (loosely) tell you how to design the learning models.

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Parametric Learning Problem

- Data $\mathbb{D} = \{(\mathbf{x}^{(1)}, \mathbf{y}^{(1)}), (\mathbf{x}^{(2)}, \mathbf{y}^{(2)}), \ldots, (\mathbf{x}^{(n)}, \mathbf{y}^{(n)})\}$
- Objective: find parameter $\mathbf{W}$ that best fits data
- Each model has its own definition of "best fits"

Maximum Likelihood Estimation (MLE)

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- Goal: Maximize probability of data given params $P(\mathbb{D} \mid \theta)$, *a.k.a* likelihood of *the params*
- Normally we deal with log of this likelihood

$$\mathcal{L}(\theta) = \log P(\mathbb{D} \mid \theta) = log \prod_{i=1}^{n} P(\mathbf{x}^{(i)} \mid \theta) = \sum_{i=1}^{n} log P(\mathbf{x}^{(i)} \mid \theta)$$

- MLE estimator is:

$$\hat{\theta}_{\mathrm{MLE}} = \underset{\theta}{\operatorname{argmax}}\, \mathcal{L}(\theta) = \underset{\theta}{\operatorname{argmax}} \sum_{i=1}^{n} log P(\mathbf{x}^{(i)} \mid \theta)$$

Maximum-A-Posteriori (MAP)

- Goal: Maximize probability of posterior of params given data

$$\underbrace{P(\theta \mid \mathbb{D})}_{\text{posterior}} = \frac{P(\theta) \times P(\mathbb{D} \mid \theta)}{P(\mathbb{D})} \propto \underbrace{P(\theta)}_{\text{prior}} \times \underbrace{P(\mathbb{D} \mid \theta)}_{\text{likelihood}}$$

- Same as MLE, normally we deal with log of this posterior

$$\log P(\theta \mid \mathbb{D}) \propto \log P(\theta) + \log P(\mathbb{D} \mid \theta)$$

- MAP estimator is:

$$\hat{\theta}_{\text{MAP}} = \underset{\theta}{\operatorname{argmax}} \log P(\theta \mid \mathbb{D}) = \underset{\theta}{\operatorname{argmax}} \Big(\log P(\theta) + \underbrace{\log P(\mathbb{D} \mid \theta)}_{\text{loglikelihood}} \Big)$$

A Classic Linear Regression Example

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- Linear Regression model: $\mathbf{y} = \mathbf{f}(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + \epsilon$ where $\epsilon \sim \mathbf{N}(\mathbf{0}, \sigma^2)$
- Each $i.i.d$ sample:

$$\begin{aligned} P(y^{(i)} \mid x^{(i)}, \mathbf{w}) &= \mathbf{N}(y^{(i)} \mid \mathbf{w}^T x^{(i)}, \sigma^2) \\ &= \frac{1}{\sigma\sqrt{2\pi}} \exp\Big(-\frac{(y^{(i)} - \mathbf{w}^T x^{(i)})^2}{2\sigma^2}\Big) \end{aligned}$$

- Log Likelihood

$$\mathcal{L}(\mathbf{w}) = \sum_{i=1}^{n} \Big(-\frac{1}{2}\log(2\pi\sigma^2) - \frac{(y^{(i)} - \mathbf{w}^T x^{(i)})^2}{2\sigma^2}\Big)$$

A Classic Linear Regression Example

Carnegie Mellon

- MLE estimator

$$\hat{\mathbf{w}}_{MLE} = \operatorname*{argmin}_{\mathbf{w}} \frac{1}{2\sigma^2} \sum_{i=1}^{n} (y^{(i)} - \mathbf{w}^T x^{(i)})^2$$

- With prior $\mathbf{w} \sim \mathbf{N}(\mathbf{0}, \lambda^{-1}\mathbf{I}) = \frac{1}{(2\pi)^{D/2}} \exp(-\frac{\lambda}{2}\mathbf{w}^T\mathbf{w})$ then MAP estimator

$$\hat{\mathbf{w}}_{MAP} = \operatorname*{argmin}_{\mathbf{w}} \frac{1}{2\sigma^2} \sum_{i=1}^{n} (y^{(i)} - \mathbf{w}^T x^{(i)})^2 + \frac{\lambda}{2}\mathbf{w}^T\mathbf{w}$$

A Classic Logistic Regression Example

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- Binary classification with labels $\mathbf{y} \in \{-1, 1\}$ and logistic classification function: $\text{sigmoid}(x) = 1/(1 + \exp(-x))$
- Log Likelihood

$$\mathcal{L}(\mathbf{w}) = \sum_{i=1}^{n} - \log \left(1 + \exp(-y^{(i)} \mathbf{w}^T x^{(i)}\right)$$

- MLE estimator

$$\hat{\mathbf{w}}_{MLE} = \operatorname*{argmin}_{\mathbf{w}} \sum_{i=1}^{n} \log \left(1 + \exp(-y^{(i)} \mathbf{w}^T x^{(i)}\right)$$

- With the same prior for $\mathbf{w}$, MAP estimator:

$$\hat{\mathbf{w}}_{MAP} = \operatorname*{argmin}_{\mathbf{w}} \sum_{i=1}^{n} \log \left(1 + \exp(-y^{(i)} \mathbf{w}^T x^{(i)}\right) + \frac{\lambda}{2} \mathbf{w}^T \mathbf{w}$$

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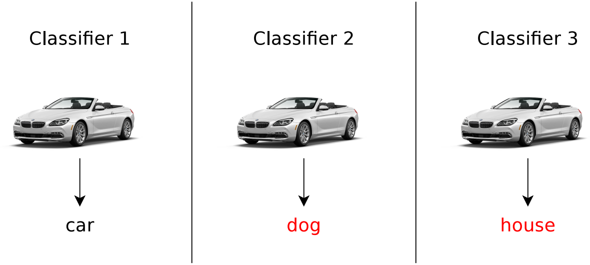
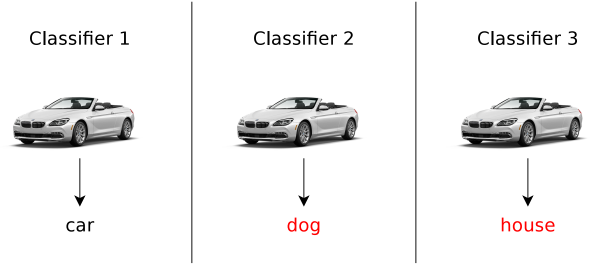
Loss Function



- Notations:
  - $\mathbf{x}$ is your data; $\mathbf{y}$ is your label;
  - $\mathbf{f}$ is your model; θ is your parameter;
  - $\hat{\mathbf{y}} = \mathbf{f}(\mathbf{x}; \theta)$ is your *empirical prediction.*

Loss Function



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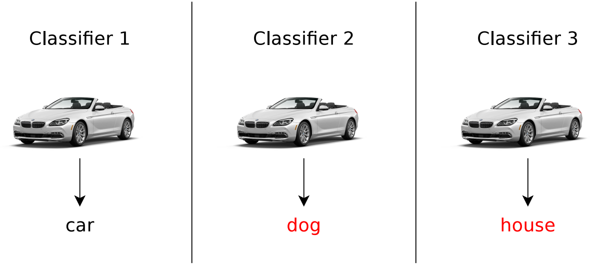

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- Loss function: $\mathcal{L}(\mathbf{y}, \hat{\mathbf{y}}) = \mathcal{L}(\mathbf{y}, \mathbf{f}(\mathbf{x}, \theta))$
  - How "off" is $\mathbf{y}$ from $\hat{\mathbf{y}} = \mathbf{f}(\mathbf{x}; \theta)$

Case Study: Car prize prediction

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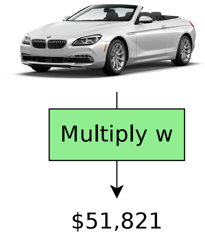
- Data: image of a car $\mathbf{x} \in \mathbb{R}^{3 \times 512 \times 512}$
- Label: cost of the car $\mathbf{x}$, namely $\mathbf{y} \in \mathbb{R}$
- Linear regression:
  - Parameters: $\theta = \{\mathbf{w} \in \mathbb{R}^{786432 \times 1}\}$, where $786432 = 3 \times 512 \times 512$.
  - $\mathbf{x}_1 = \text{reshape}(\mathbf{x}, [1, 786432])$
  - $\hat{\mathbf{y}} = \mathbf{x}_1 \cdot \mathbf{w}$



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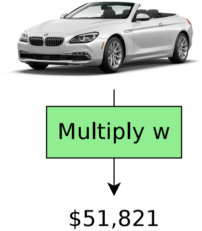

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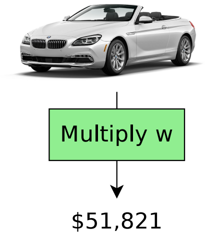

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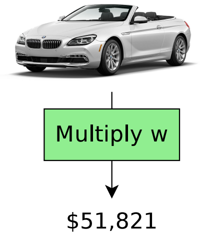
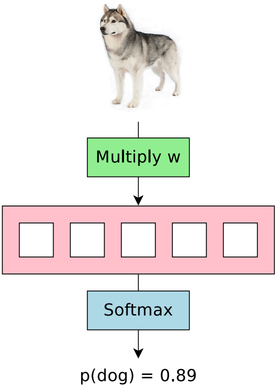
  - $\mathcal{L}(\mathbf{y}, \hat{\mathbf{y}}) = |\hat{\mathbf{y}} - \mathbf{y}|$ is called the ℓ_1-*loss*
- Do we have other options of losses?



Case Study 2: Image classification

- Data: $\mathbf{x} \in \mathbb{R}^{3\times 32\times 32}$
- Label: $\mathbf{y} \in \{\text{dog}, \text{cat}, \text{house}, \text{car}, \text{flower}\}$
  - For ease: $\mathbf{y} \in \{1, 2, 3, 4, 5\}$
- Softmax classification:
  - Parameters: $\theta = \{\mathbf{w} \in \mathbb{R}^{3072\times 10}\}$.
  - $\mathbf{x}_1 = \text{reshape}(\mathbf{x}, [1, 3072])$
  - $\ell = \mathbf{x}_1 \cdot \mathbf{w}$
  - $\hat{p} = \mathbf{Prob}\left[\mathbf{y} = i\right] = \underbrace{\frac{\exp\{\ell_i\}}{\sum_{j=1}^{5} \exp\{\ell_j\}}}_{\text{soft-max}}$ l



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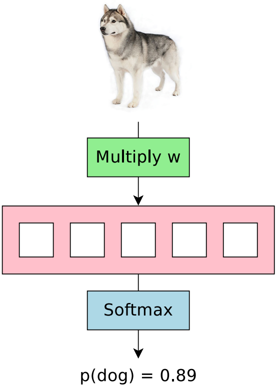
  - Cross-entropy loss: $\mathcal{L}(\hat{p}, \mathbf{y}) = -\mathbf{y} \log \hat{p}_{\mathbf{y}}$.



Review: Information Theory

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- Let $X \sim P(X)$ be a random variable
- (Shannon) information content of an outcome x is $h(x) = -\log_2 P(x)$

Image credit: David Mackay

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- Measure the "uncertainty" of an outcome
- Entropy of a set S is the average information content:

$$\mathrm{H}(X) = \sum_{x \in S} -P(x) \log P(x)$$
$$= -\mathbb{E}_{x \sim P}[logP(x)]$$

i	a_i	p_i	$h(p_i)$
1	a	.0575	4.1
2	b	.0128	6.3
3	c	.0263	5.2
4	d	.0285	5.1
5	e	.0913	3.5
6	f	.0173	5.9
7	g	.0133	6.2
8	h	.0313	5.0
9	i	.0599	4.1
10	j	.0006	10.7
11	k	.0084	6.9
12	l	.0335	4.9
13	m	.0235	5.4
14	n	.0596	4.1
15	o	.0689	3.9
16	p	.0192	5.7
17	q	.0008	10.3
18	r	.0508	4.3
19	s	.0567	4.1
20	t	.0706	3.8
21	u	.0334	4.9
22	v	.0069	7.2
23	w	.0119	6.4
24	x	.0073	7.1
25	y	.0164	5.9
26	z	.0007	10.4
27	-	.1928	2.4
$\sum_i p_i \log_2 \frac{1}{p_i}$			4.1

Image credit: David Mackay

Review: Information Theory

- Joint Entropy of X, Y is

$$\mathrm{H}(X, Y) = -\sum_{x,y} P(x, y) \log P(x, y)$$

- Conditional entropy

$$\mathrm{H}(X|Y) = -\sum_{y} \mathrm{H}(X|Y = y) P(Y = y) = -\sum_{x,y} P(x, y) \log P(x|y)$$

- Chain rule:

$$\mathrm{H}(X|Y) = \mathrm{H}(X, Y) - \mathrm{H}(Y)$$

- Bayes' rule:

$$\mathrm{H}(Y|X) = \mathrm{H}(X|Y) - \mathrm{H}(X) + \mathrm{H}(Y)$$

Review: Information Theory

- Mutual Information (Information gain) of X and Y:

$$\mathrm{I}(X,Y) = \sum_{x,y} P(x,y) \log \frac{P(x,y)}{P(x)P(y)}$$

- Relation to conditional entropy:

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

- If X, Y are independent, we have:

$$\mathrm{I}(X,Y) = 0$$

$$\mathrm{H}(X|Y) = H(X)$$

$$\mathrm{H}(X,Y) = \mathrm{H}(X) + \mathrm{H}(Y)$$

Review: Information Theory

- Relative Entropy or Kullback-Leibler (KL) divergence of 2 distributions P(x) and Q(x) over the same set is:

$$\mathbf{D}_{KL}(P \,\|\, Q) = \sum_x P(x) \log \frac{P(x)}{Q(x)} = \mathbb{E}_{x \sim P}[P(x)] - \mathbb{E}_{x \sim P}[Q(x)]$$

- Is Asymmetric:

$$\mathbf{D}_{KL}(P \,\|\, Q) \neq \mathbf{D}_{KL}(Q \,\|\, P)$$

- Satisfy Gibbs inequality: $\mathbf{D}_{KL}(P \,\|\, Q) \geq 0$, with equality happens iff $P \equiv Q$

Review: Information Theory

- Cross-Entropy of P and Q over the same set:

$$\mathrm{H}(P, Q) = -\sum_{x \sim P} P(x) \log Q(x) = -\mathbb{E}_{x \sim P}[\log Q(x)]$$

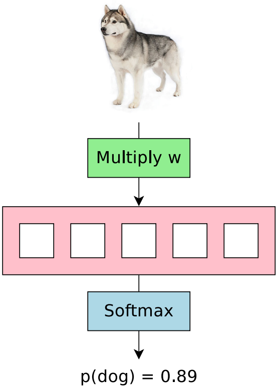
- Relation to relative entropy:

$$\mathrm{H}(P, Q) = \mathrm{H}(P) + \mathbf{D}_{KL}(P \,\|\, Q)$$

- Let P be the ground-truth distribution, and Q be the predicted distribution

Cross-Entropy Loss

- $\mathcal{L}(\hat{p}, \mathbf{y}) = \mathrm{H}(y, \hat{p}_{\mathbf{y}}) = -\mathbf{y} \log \hat{p}_{\mathbf{y}}$
  - One of the most important loss functions of deep learning, and classification in general.



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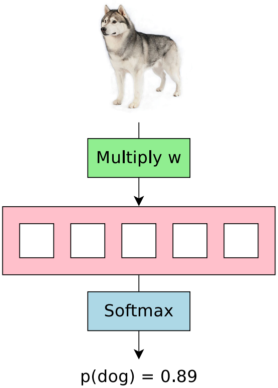
  - $\mathcal{L}$ is mall when $\hat{p}_{\mathbf{y}}$ is large, i.e. model is more confident



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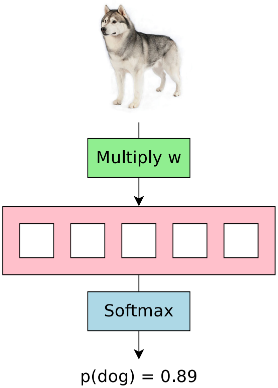
  - But $\mathcal{L}$ is *always positive*



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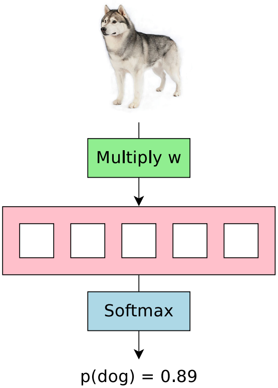

Cross-Entropy Loss

- $\mathcal{L}(\hat{p}, \mathbf{y}) = \mathrm{H}(y, \hat{p}_{\mathbf{y}}) = -\mathbf{y} \log \hat{p}_{\mathbf{y}}$
  - One of the most important loss functions of deep learning, and classification in general.
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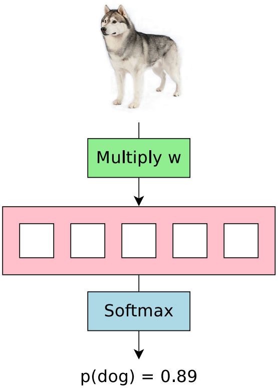

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  - Differentiable. Recall $\hat{p}_i = \exp\{\ell_i\} / \sum_j \exp\{\ell_j\}$
    - Important for learning.