

# Distances and Similarities

## ◆ Distances

- What distances have we used?
- What properties do they have?

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- What similarity measures have we used?
- What properties do they have?

# Distances and Similarities

## ◆ Distances

- What distances have we used?
  - $d_p(x,y) = \|x-y\|_p$
  - What properties do they have?
  - Symmetric, non-negative, triangle inequality

## ◆ Similarities

- What similarity measures have we used?
  - Kernel:  $\exp(-\|x-y\|_p^p)$
- What properties do they have?
  - Haven't covered yet

# Kullback Leibler divergence

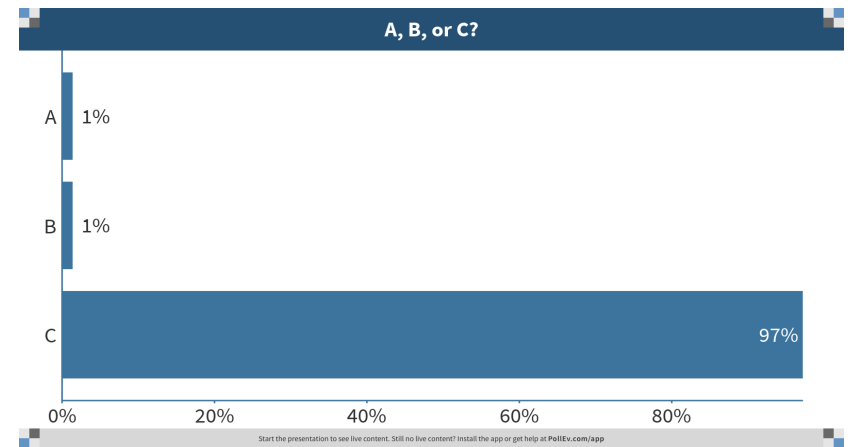
- ◆  $P$  = 'true' distribution
- ◆  $Q$  = alternative distribution that is used to encode data
- ◆ **KL** divergence is the expected extra # of bits per point that must be transmitted using  $Q$  *instead of*  $P$  *if the data comes from*  $P$

$$\begin{aligned} D_{KL}(P \parallel Q) &= \sum_j P(x_j) \log (P(x_j)/Q(x_j)) \\ &= - \sum_i P(x_j) \log Q(x_j) + \sum_i P(x_j) \log P(x_j) \\ &= H(P, Q) \quad - H(P) \\ &= \text{Cross-entropy} - \text{entropy} \end{aligned}$$

- ◆ Measures how different the two distributions are

# KL-Divergence

- A) Distance
- B) Similarity
- C) Neither



$$D_{\text{KL}}(P||Q) = - \sum_i P(i) \log \frac{Q(i)}{P(i)},$$

# KL divergence properties

- ◆ Measures how well a probability distribution  $Q$  approximates a distribution  $P$  (the “truth”)
- ◆ Divergence *is 0* if and only if  $P$  and  $Q$  are equal:
  - $D(P||Q) = 0$  iff  $P = Q$
- ◆ Non-symmetric:  $D(P||Q) \neq D(Q||P)$
- ◆ Non-negative:  $D(P||Q) \geq 0$
- ◆ Does not satisfy triangle inequality
  - $D(P||Q) \leq D(P||R) + D(R||Q)$

**Not a distance metric**

# KL divergence as error

- ◆ Given a label  $y=a$  for a categorical variable which is one of  $k$  outcomes,  $P$  is a unit vector (a “one hot” encoding).
- ◆ The output of a logistic regression or neural net, or any softmax function is a distribution  $Q$  over the  $k$  possible outcomes
- ◆ The KL divergence is a good loss function

$$D_{\text{KL}}(P \parallel Q) = \sum_k P(y=k) \log(P(y=k)/Q(y=k)) = -\log(Q(y=a))$$

What is the loss if  $Q(y=a)=1$ ?

if  $Q(y=a)=0$ ?

# KL divergence as info gain

- ◆ The KL divergence of the posterior measures the information gain expected from query ( $x'$ ):

$$D_{KL}(p(y | x, x') || p(y | x))$$

- ◆ Goal: choose a query that *maximizes* the KL divergence between the updated posterior probability and the current posterior probability
  - This gives the largest expected information gain

# Questions?

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