# COMS 4771 Lecture 20

1. Maximum entropy

# Probabilistic modeling

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#### Probabilistic modeling

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- ▶ Is there a general approach for
  - (i) picking a probability model, and
  - (ii) parameter estimation?
- ▶ How do familiar models (as above) fit into this approach?

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Now you observe a random sample  $x_1,x_2,\ldots,x_n$  from  $\mathcal{X}$ , and record some features  $T_1,T_2,\ldots,T_k\colon\mathcal{X}\to\mathbb{R}$ : e.g.,

- $T_1(x) = \mathbb{1}\{x \text{ ends with an 'e'}\}$
- ▶  $T_2(x) = 1\{x \text{ has more than five characters}\}$
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Say you observe

$$\frac{1}{n}\sum_{i=1}^{n}T_1(x_i)=0.22, \quad \frac{1}{n}\sum_{i=1}^{n}T_2(x_i)=0.32, \quad \dots$$

Now what distribution should you pick?

# A NON-COMMITTAL ESTIMATION PRINCIPLE

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Distribution should only be pinned down by the observations, but otherwise should express as much "uncertainty" / be as "random" as possible.

How do we measure how "random" a distribution is?

Let X be a discrete  $\mathcal{X}$ -valued random variable. How "random" is it?

▶ Fair coin toss: one unit of randomness (by definition).

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- ► Fair 32-sided die? This is equivalent to five independent fair coin tosses, so five units of randomness.

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- 5. (Expansibility) If  $X \sim (p_1, p_2, \dots, p_d)$  and  $Y \sim (p_1, p_2, \dots, p_d, 0)$ , then H(X) = H(Y).

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- 5. (Expansibility) If  $X \sim (p_1, p_2, \dots, p_d)$  and  $Y \sim (p_1, p_2, \dots, p_d \mid 0)$ , then H(X) = H(Y).
- 6. (Symmetry) If  $X \sim (p_1, p_2, \dots, p_d)$  and  $Y \sim (p_{\sigma(1)}, p_{\sigma(2)}, \dots, p_{\sigma(d)})$  for some permutation  $\sigma$  on  $\{1, 2, \dots, d\}$ , then

$$H(X) = H(Y).$$

The only measure of randomness that satisfies the desiderata is

$$H(X) = -\sum_{x \in \mathcal{X}} \Pr(X = x) \log_2 \Pr(X = x)$$

which is called (Shannon) entropy. (Note:  $0 \log 0 = 0$  by convention.)

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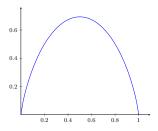
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Also may write this as

$$H(P) = \mathbb{E}_{X \sim P} \left[ -\log_2(P(X)) \right] = \mathbb{E}_{X \sim P} \left[ \log_2 \frac{1}{P(X)} \right].$$

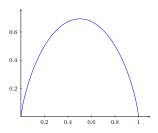
"Bits" = units of entropy with  $\log_2$ . "Nats" = units of entropy with  $\ln$ . Different logarithm bases just change things by constant factors.

# **ENTROPY**



Entropy H(P) is a concave function of P.

#### ENTROPY

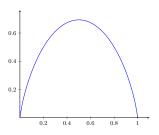


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Distribution over  $\mathcal{X}$  with highest entropy: **uniform distribution** 

$$H(\mathsf{uniform}) \ = \ -\sum_{x \in \mathcal{X}} \frac{1}{|\mathcal{X}|} \log \frac{1}{|\mathcal{X}|} \ = \ \log |\mathcal{X}|.$$

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Distribution over  $\mathcal{X}$  with least entropy: **point mass at any**  $x^* \in \mathcal{X}$ 

$$H(\delta_{x^*}) = -\sum_{x \in \mathcal{X}} \mathbb{1}\{x = x^*\} \log \mathbb{1}\{x = x^*\} = 0.$$

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**Shannon's source coding theorem**: Any lossless compression of an i.i.d. sample from P must use H(P) bits on average.

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Shannon's source coding theorem: Any lossless compression of an i.i.d. sample from P must use  ${\cal H}(P)$  bits on average.

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**Upshot**: Entropy measures the average information content of a RV.

# ASYMPTOTIC EQUIPARTITION PROPERTY

Let  $(X_1, X_2, \dots, X_n)$  be sequence of i.i.d.  $\mathcal{X}$ -valued RVs, with  $X_i \sim P$ .

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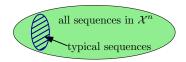
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1. "Typical sequences":

$$(x_1, x_2, \ldots, x_n) \in \mathcal{X}^n$$
 with

$$P(x_1, x_2, \dots, x_n) \approx 2^{-n(H(P) \pm \varepsilon)}$$
.



2. All other sequences.

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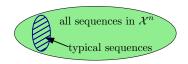
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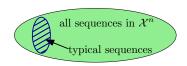
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  - ► Number of typical sequences:

Between 
$$(1-\varepsilon)2^{n(H(P)-\varepsilon)}$$
 and  $2^{n(H(P)+\varepsilon)}$ .

Far fewer than  $|\mathcal{X}|^n$  when  $H(P) \ll \log_2 |\mathcal{X}|$ .

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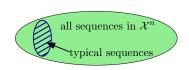
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**Upshot**: H(P) characterizes the number of typical i.i.d. sequences from P.

### ENTROPY: RECAP

- ▶ Entropy is a fundamental measure of the
  - randomness
  - uncertainty
  - ▶ information content

in a probability distribution.

- ▶ Quantifies achievable rates for data compression.
- ▶ Quantifies number of typical i.i.d. sequences.
- **.** . . .

Maximum entropy principle

## MAXIMUM ENTROPY PRINCIPLE

Observe a random sample  $x_1, x_2, \ldots, x_n$  of words from  $\mathcal{X}$ , and record some features  $T_1, T_2, \ldots, T_k \colon \mathcal{X} \to \mathbb{R}$ : e.g.,

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#### Observations:

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more general way in depict whether a sample meets certain condition

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Maximum entropy principle (Jaynes, 1957):

Pick the distribution that agrees with the empirical observations, but is otherwise as "random" as possible.

Our empirical observations from sample  $x_1, x_2, \ldots, x_n \in \mathcal{X}$ :

Text

$$b_i := \frac{1}{n} \sum_{i=1}^n T_i(x_i) = \widehat{\mathbb{E}}[T_i(X)] \text{ for } i = 1, 2, \dots, k$$

where  $\widehat{\mathbb{E}}[\,\cdot\,]$  is expectation w.r.t. empirical distribution based on the sample.

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#### Maximum entropy optimization problem:

$$\label{eq:max} \max_{P \in \Delta(\mathcal{X})} \qquad H(P)$$
 s.t. 
$$\mathbb{E}_{X \sim P}[T_i(X)] \ = \ b_i \quad \text{for all } i = 1, 2, \dots, k$$

(where  $\Delta(\mathcal{X})$  is the space of probability distributions over  $\mathcal{X}$ ).

just for constrain purpose, has nothing to do with entropy, which is the target!!

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Maximum entropy optimization problem: through all possible distributions

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 s.t. 
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expirical distribution

Without the constraints (i.e., before observations are made),  $\max_{P \in \Delta(\mathcal{X})} H(P)$  is achieved by the *uniform distribution* over  $\mathcal{X}$ .

## Non-uniform base distributions

If  $\mathcal X$  is discrete but infinite (e.g.,  $\mathcal X=\mathbb N$ ), no uniform distribution over  $\mathcal X.$ 

## NON-UNIFORM BASE DISTRIBUTIONS

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How do we measure how close two probability distributions are?

### RELATIVE ENTROPY

**Entropy**: expected information content measured by P, where expectation is w.r.t. random draw from P.

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Relative entropy: expected information content measured by Q, where expectation is w.r.t. random draw from  ${\it P}$ 

$$\operatorname{RE}(P||Q) := \mathbb{E}_{X \sim P} \left[ \ln \frac{1}{Q(X)} \right] - H(P).$$

(and we subtract off H(P) so it is zero when P=Q).

### Relative entropy

More typical form:

**Entropy**: expected information content measured by P, where expectation is w.r.t. random draw from P.

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 $\operatorname{RE}(P\|Q) = \sum_{x \in \mathcal{X}} P(x) \ln \frac{P(x)}{Q(x)} \cdot \frac{\text{note the}}{\text{expansion}}$ 

## PROPERTIES OF RELATIVE ENTROPY

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- ▶  $RE(Q||P) \neq RE(P||Q)$  in general, and triangle inequality does not hold. So RE is **not** a metric.
- $RE(P||uniform) = \ln |\mathcal{X}| H(P).$
- ▶ RE(P||Q) is a convex function of (P,Q) (and hence also a convex function of P, by itself, and also of Q).

$$RE(P||Q) = \sum_{x \in \mathcal{X}} P(x) \ln \frac{P(x)}{Q(x)}.$$

- ►  $RE(P||Q) \ge 0$  for all P and Q. RE(P||Q) = 0 if and only if P = Q.
- ▶ RE $(Q||P) \neq$  RE(P||Q) in general, and triangle inequality does not hold. So RE is **not** a metric. the larger the less randomness. we don't care about constrain at this time
- ▶  $RE(P||uniform) = ln |\mathcal{X}| H(P)$ .
- ▶ RE(P||Q) is a *convex function* of (P,Q) (and hence also a convex function of P, by itself, and also of Q).
- Also called "Kullback-Leibler divergence".

#### Maximum entropy optimization problem with base distribution $\pi$ :

$$\begin{aligned} & \min_{P \in \Delta(\mathcal{X})} & & \text{RE}(P \| \pi) \\ & \text{s.t.} & & \mathbb{E}_{X \sim P}[T_i(X)] \ = \ b_i & \text{for all} \ i = 1, 2, \dots, k. \end{aligned}$$

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### Maximum entropy optimization problem

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 (If  $\pi = \text{uniform}$ , then objective is  $\operatorname{RE}(P \| \pi) = \ln |\mathcal{X}| - H(P)$ .) More explicitly, with  $\boldsymbol{T}(x) := (T_1(x), T_2(x), \dots, T_k(x))$  and  $\boldsymbol{b} := (b_1, b_2, \dots, b_k)$ , 
$$\min_{P \in \mathbb{R}^{\mathcal{X}}} \quad \sum_{x \in \mathcal{X}} P(x) \ln \frac{P(x)}{\pi(x)}$$
 s.t. 
$$\sum_{x \in \mathcal{X}} P(x) \boldsymbol{T}(x) = \boldsymbol{b}$$
 
$$P(x) \geq 0 \quad \text{for all } x \in \mathcal{X}$$
 
$$\sum_{x \in \mathcal{X}} P(x) = 1.$$

### Maximum entropy optimization problem with base distribution $\pi$ :

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$$\min_{P \in \mathbb{R}^{\mathcal{X}}} \quad \sum_{x \in \mathcal{X}} P(x) \ln \frac{P(x)}{\pi(x)} \quad \text{for given x, each of its}$$
 T(x) is meet with related

both P(x) and Q(x) are kinds of

s.t. 
$$\sum_{x \in \mathcal{X}} P(x)T(x) = \mathbf{b}$$
 b. (a list of b, with imposed feature requirement) 
$$\sum_{x \in \mathcal{X}} P(x) = 1.$$

Convex objective function, with linear (in)equality constraints.

minimize

## ENTROPY PROJECTION

Note that  $\emph{any}$  feasible solution P must satisfy

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These constraints define an affine hyperplane in  $\mathbb{R}^{\mathcal{X}}$ .

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$$\left\{ P : \sum_{x} P(x) \mathbf{T}(x) = \mathbf{b} \right\}$$

#### Entropy projection

Note that any feasible solution P must satisfy

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project the base into the constrain plane

These constraints define an affine hyperplane in  $\mathbb{R}^{\mathcal{X}}$ .

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Similar to the Euclidean projection of  $\pi$  onto an affine hyperplane, except we use relative entropy instead of Euclidean distance: an entropy projection.

# SOLUTION FORM

Maximum entropy optimization problem:

$$\begin{aligned} \min_{P \in \Delta(\mathcal{X})} & & \text{RE}(P \| \pi) \\ \text{s.t.} & & \sum_{x \in \mathcal{X}} P(x) \boldsymbol{T}(x) \ = \ \boldsymbol{b}. \end{aligned}$$

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**Claim**: A solution  $P_{\star}$  to the optimization problem must have the form

$$P_{\star}(x) = \frac{1}{Z(\eta)} \cdot \exp\{\langle \eta, T(x) \rangle\} \cdot \pi(x)$$

for some  $\eta \in \mathbb{R}^k$ , where

$$Z(\boldsymbol{\eta}) = \sum_{x \in \mathcal{X}} \exp \left\{ \langle \boldsymbol{\eta}, \boldsymbol{T}(x) \rangle \right\} \cdot \pi(x)$$

is the normalizing constant that makes  $P_{\star}$  a probability distribution.

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$$= \sum_{x} P(x) \ln \frac{P(x)}{\pi(x)} - \sum_{x} P_{\star}(x) \ln \frac{P_{\star}(x)}{\pi(x)}$$

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#### Proof

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$$= \sum_{x} P(x) \ln \frac{P(x)}{\pi(x)}$$

#### Proof

Consider any other feasible solution P—i.e., P is a valid probability distribution and (like  $P_{\star}$ ) satisfies

$$\sum_{x} P(x) T(x) = b.$$

$$\begin{split} \operatorname{RE}(P\|\pi) - \operatorname{RE}(P_{\star}\|\pi) \\ &= \sum_{x} P(x) \ln \frac{P(x)}{\pi(x)} - \sum_{x} P_{\star}(x) \ln \frac{P_{\star}(x)}{\pi(x)} \\ &= \sum_{x} P(x) \ln \frac{P(x)}{\pi(x)} - \sum_{x} P_{\star}(x) \Big\{ \langle \boldsymbol{\eta}, \boldsymbol{T}(x) \rangle - \ln Z(\boldsymbol{\eta}) \Big\} \\ &= \sum_{x} P(x) \ln \frac{P(x)}{\pi(x)} - \sum_{x} P(x) \Big\{ \langle \boldsymbol{\eta}, \boldsymbol{T}(x) \rangle - \ln Z(\boldsymbol{\eta}) \Big\} & \text{the minimization is} \\ &= \sum_{x} P(x) \ln \frac{P(x)}{\pi(x)} - \sum_{x} P(x) \ln \frac{P_{\star}(x)}{\pi(x)} & \text{sachieved when} \\ &= \sum_{x} P(x) \ln \frac{P(x)}{\pi(x)} = \operatorname{RE}(P\|P_{\star}) \geq 0 & \text{with equality iff } P = P_{\star}. \end{split}$$

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#### Interpretation of the solution form

#### From our earlier example:

- $ightharpoonup T_1(x) = \mathbb{1}\{x \text{ ends with an 'e'}\}$
- ▶  $T_2(x) = 1\{x \text{ has more than five characters}\}$

Maximum entropy solution is of the form

$$P_{\star}(x) = \frac{1}{Z(\eta)} \cdot \exp\left\{\eta_1 T_1(x) + \eta_2 T_2(x) + \cdots\right\} \cdot \pi(x).$$

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How do we get these  $\eta$  parameters?

## EXPONENTIAL FAMILIES

The  $\eta$  parameters for distributions of the form

$$P_{\eta}(x) = \frac{1}{Z(\eta)} \cdot \exp\{\langle \eta, T(x) \rangle\} \cdot \pi(x)$$

are strongly related to a different parameterization of the distributions called the **expectation parameters**, which are easily estimated.

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This relationship is revealed through the study of these distribution families, called **exponential families**.

#### EXPONENTIAL FAMILIES

The  $\eta$  parameters for distributions of the form

#### Zn is the normalizer!

$$P_{\boldsymbol{\eta}}(x) = \frac{1}{Z(\boldsymbol{\eta})} \cdot \exp\left\{ \langle \boldsymbol{\eta}, \boldsymbol{T}(x) \rangle \right\} \cdot \pi(x)$$

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This relationship is revealed through the study of these distribution families, called **exponential families**.

Many familiar probability models are exponential families:

Bernoulli, binomial, Poisson, exponential, Gaussian, gamma, categorical, multinomial, Dirichlet, . . .

#### RECAP

- Maximum entropy approach to probabilistic modeling: choose the most non-committal distribution that agrees with the empirical observation.
- Solution must have the form

$$P_{\eta}(x) = \frac{1}{Z(\eta)} \cdot \exp\{\langle \eta, T(x) \rangle\} \cdot \pi(x),$$

corresponds to the entropy projection of the base distribution  $\pi$  onto an affine hyperplane.

ightharpoonup Extracting the  $\eta$  parameters: next time, via study of exponential families.