Lecture 1:

Entropy and Information

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Bayesian Data Analysis and Machine Learning for Physical Sciences

Bayesian Data Analysis and Machine Learning for Physical Sciences

Course Map

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Module 2	Naive Bayes, Bayesian Parameter Estimation, MAP
Module 3	Model selection: Comparing Distributions vs Frequentist Methods
Module 4	Model Selection: Bayesian Signal Detection
Module 5	Variational Bayes, Expectation Maximization
Module 6	Stochastic Processes
Module 7	Monte Carlo Methods
Module 8	Markov Models, Graphs
Module 9	Machine Learning Overview, Supervised Methods
Module 10	Unsupervised Methods
Module 11	ANN: Perceptron, Backpropagation
Module 12	ANN: Basic Architecture, Regression vs Classification, Backpropagation again
Module 13	Convolution and Image Classification and Segmentation
Module 14	TBD (GNNs)
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Module 16	TBD (Transformer and LLMs)

Bayesian Data Analysis and Machine Learning for Physical Sciences

<u>Course Map</u>

Outline

Entropy and Information

- definition
- conditional Entropy
- KL divergence
- connection to TD

Maximum Entropy Distributions

- Lagrangian Multiplier
- examples

Bayes Theorem

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Bayes Theorem

idea: gain of information = **"degree of surprise"**

if something happens that we expected already → no surprise

→ no information

$p(x_i)$:   probability of event x_i

$h(x_i)$:   function that measures "information"

$$\log[p(x_i)\,p(x_j)] = \log[p(x_i)] + \log[p(x_j)]$$

1) $h(x_i)$ should be additive

$$h(x_i, x_j) = h(x_i) + h(x_j)$$

2) $h(x_i)$ should be monotonic

3)   if x_i and x_j are independent, then $$p(x_i, x_j) = p(x_i)p(x_j)$$

idea: gain of information = **"degree of surprise"**
              if something happens that we expected already → no surprise
                                                            → no information

$p(x_i)$:   probability of event x_i

$h(x_i)$:   function that measures "information"

1) $h(x_i)$ should be additive $h(x_i, x_j) = h(x_i) + h(x_j)$

2) $h(x_i)$ should be monotonic

3)   if x_i and x_j are independent, then $p(x_i, x_j) = p(x_i)p(x_j)$

$$\log[p(x_i)\,p(x_j)] = \log[p(x_i)] + \log[p(x_j)]$$ $p(x_i) \leq 1$

$h(x_i) = -\log[p(x_i)]$ information is **positive**
                                    low $p(x_i)$ → "great surprise"

idea: gain of information = **"degree of surprise"**
if something happens that we expected already → no surprise
→ no information

$$h(x_i) = -\log[p(x_i)]$$

$p(x_i)$:   **probability of event x_i**

The event x_i is randomly drawn from $p(x_i)$ → **average** amount of information

Entropy S

$$S = -\sum_{i=1}^{I} p(x_i) \log[p(x_i)] \quad \text{(discrete)}$$

$$S = -\int p(x) \log[p(x)] \, dx \quad \text{(continuous or } \textit{differential}\text{)}$$

note: - the **base** of log is **arbitrary** (often 2 or e)

- $\lim_{p \to 0} (p \log p) = 0$

- S is large → no information

- S is zero → all information

- continuous entropy **can** be negative

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Entropy S

$$S = -\sum_{i=1}^{I} p(x_i) \log[p(x_i)] \qquad \text{(discrete)}$$

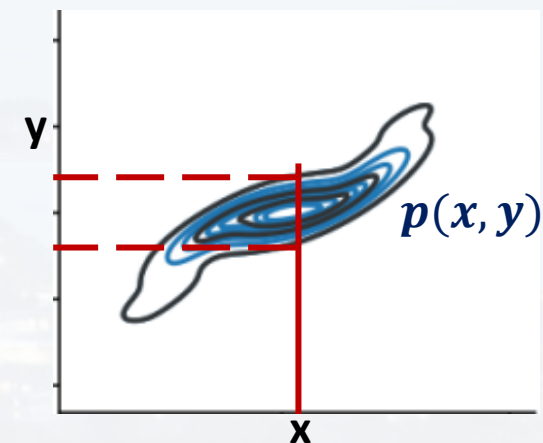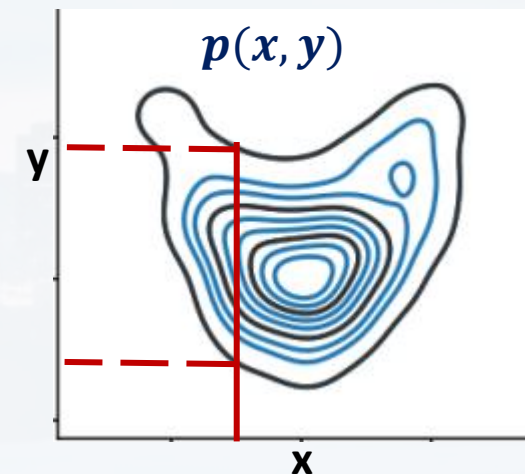$$S = -\int p(x) \log[p(x)] \, dx \qquad \text{(continuous)}$$

definition
conditional Entropy
KL divergence
connection to TD

$p(x_i)$:   **probability of event x_i**

joint distribution $p(x, y)$, what is

$S(y|x)$:   entropy of y, **"given"** x (we know x already)

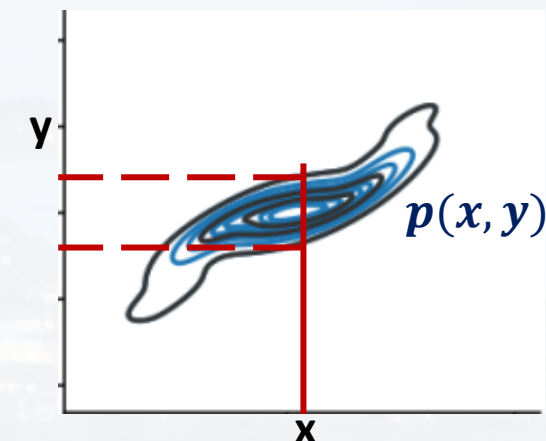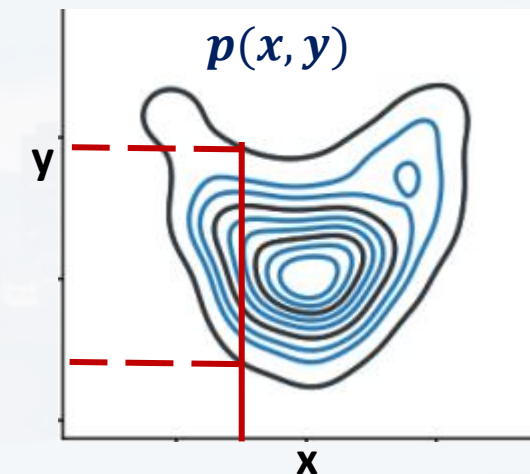**"given"**

Entropy S

$$S = - \int p(x) \log[p(x)]\, dx$$

joint distribution $p(x, y)$, what is

$p(x_i):$ **probability of event x_i**

$S(y|x):$ entropy of *y*, **"given"** *x* (we know *x* already)

$$S[p(x,y)] = - \iint p(x,y) \log[p(x,y)]\, dxdy$$

**conditional probabilities
(see later)**

$$= - \iint p(x,y) \log[\boldsymbol{p(y|x)p(x)}]\, dxdy$$

$$= - \iint p(x,y) \{\log[\boldsymbol{p(y|x)}] + \log[\boldsymbol{p(x)}]\}\, dxdy$$

$$= - \iint p(x,y) \log[\boldsymbol{p(y|x)}]\, dx\, dy - \iint p(x,y) \log[\boldsymbol{p(x)}]\, dxdy$$

we still sample from $p(x,y)$

$p(x,y)$

$p(x,y)$

Entropy S

$$S = - \int p(x) \log[p(x)]\, dx$$

joint distribution $p(x, y)$, what is

$p(x_i)$:   **probability of event x_i**

$S(y|x)$:   entropy of y, **"given"** x (we know x already)

$$S[p(x,y)] = - \iint p(x,y)\, log[\boldsymbol{p(y|x)}]\, dx\, dy \; - \; \iint p(x,y)\, log[\boldsymbol{p(x)}]\; dxdy$$

$$S[p(x,y)] = S[p(y|x)] + S[p(x)]$$

differential   **conditional**   **differential**
entropy of   **entropy**   **entropy of**
$\boldsymbol{p(x, y)}$ $\boldsymbol{p(x)}$

We can learn about $p(x, y)$ when we have information about x first
and then y, given x
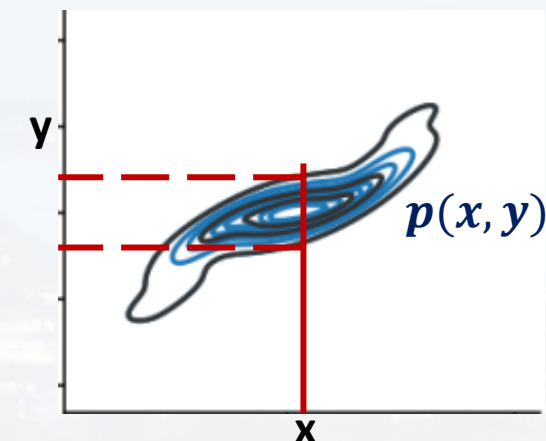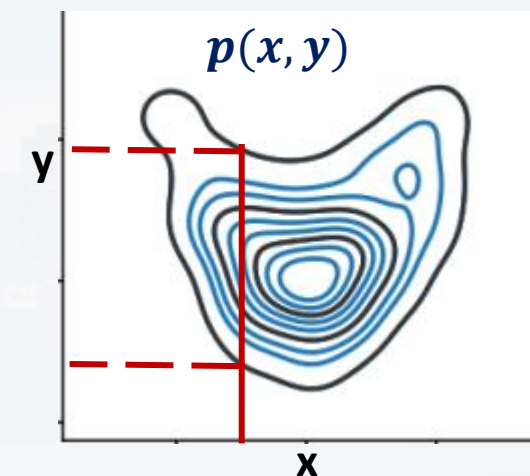
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Maximum Entropy Distributions

- Lagrangian Multiplier
- examples

Bayes Theorem

often, we (need to) approximate $p(x)$ by some other distribution $q(x)$

How much is our information "off" if we work with the approximation $q(x)$?

$$-\int p(x)\log[q(x)]\,dx - \left[-\int p(x)\log[p(x)]\,dx\right] = -\int p(x)\log\left[\frac{q(x)}{p(x)}\right]dx = KL(p||q)$$

KL or *Kullback-Leiber divergence*

It is **not** a distance! $KL(p||q) \neq KL(q||p)$

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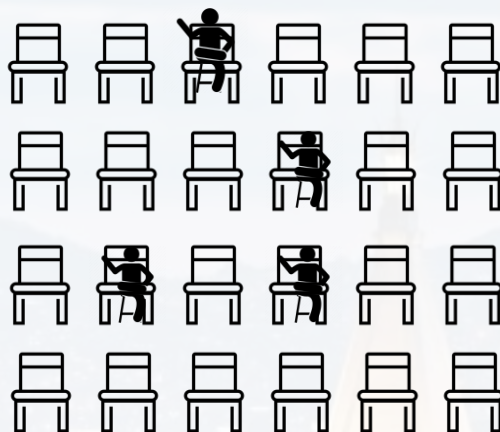Maximum Entropy Distributions

- Lagrangian Multiplier
- examples

Bayes Theorem

"Shannon" Entropy S

$$S = -\sum_{i=1}^{I} p(x_i) \log[p(x_i)]$$

definition
conditional Entropy
KL divergence
connection to TD

I = 2 states

N:	number of **indistinguishable** particles
n_i:	number of particles in micro state i
I:	number of states

multiplicity Ω : number of macro states

$$\Omega = \frac{N!}{n_1!\,(N - n_1)!} = \frac{N!}{n_1!\,n_2!}$$

for I states $\Omega = \dfrac{N!}{\prod_{i=1}^{I} n_i}$ for large N: $\displaystyle\lim_{N \to \infty} \left(\frac{n_i}{N}\right) = p_i$ p_i: probability of a particle being in micro state i

"Shannon" Entropy S
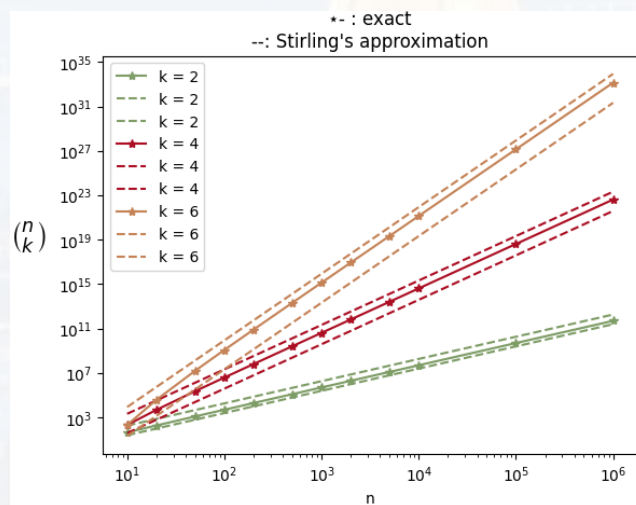
$$S = -\sum_{i=1}^{I} p(x_i) \log[p(x_i)]$$

$$\Omega = \frac{N!}{\prod_{i=1}^{I} n_i} \qquad \text{for large } N: \lim_{N \to \infty} \left(\frac{n_i}{N}\right) = p_i$$

N:	number of indistinguishable particles
n_i:	number of particles in micro state i
I:	number of states
p_i:	probability of a particle being in micro state i

Stirling's approximation

$$\left(\frac{n}{k}\right)^k \leq \binom{n}{k} \leq \left(\frac{en}{k}\right)^k$$

$$N! \approx \left(\frac{N}{e}\right)^N$$

*-- : exact
-- : Stirling's approximation

$$\Omega = \frac{N!}{n_1! \, n_2! \dots n_I!} \approx \frac{N^N}{n_1^{n_1} n_2^{n_2} \dots n_I^{n_I}} \underbrace{\frac{e^{n_1} e^{n_2} \dots e^{n_I}}{e^N}}_{}$$

$$\frac{e^{\sum_i^I n_i}}{e^N} = \frac{e^N}{e^N} = 1$$

$$\Omega = \frac{N^N}{(Np_1)^{n_1} (Np_2)^{n_2} \dots (Np_I)^{n_I}} = \frac{N^N}{N^{\sum_i^I n_i}} \frac{1}{p_1^{n_1} p_2^{n_2} \dots p_I^{n_I}}$$

"Shannon" Entropy S
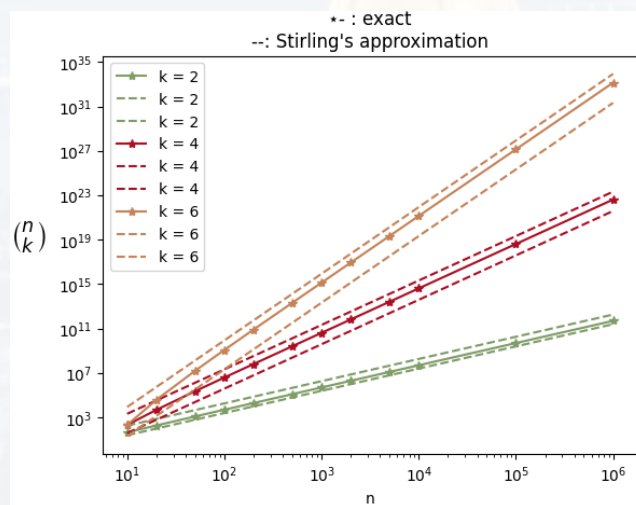
$$S = -\sum_{i=1}^{I} p(x_i) \log[p(x_i)]$$

$$\Omega = \frac{N!}{\prod_{i=1}^{I} n_i} \qquad \text{for large } N: \lim_{N \to \infty} \left(\frac{n_i}{N}\right) = p_i$$

N:	number of **indistinguishable** particles
n_i:	number of particles in micro state i
I:	number of states
p_i:	probability of a particle being in micro state i

Stirling's approximation

$$\left(\frac{n}{k}\right)^k \leq \binom{n}{k} \leq \left(\frac{en}{k}\right)^k$$

$$N! \approx \left(\frac{N}{e}\right)^N$$

*-- : exact
--: Stirling's approximation

$$\Omega = \frac{N^N}{(Np_1)^{n_1}(Np_2)^{n_2} \dots (Np_I)^{n_I}} = \frac{N^N}{N^{\sum_i^I n_i}} \frac{1}{p_1^{n_1} p_2^{n_2} \dots p_I^{n_I}}$$

$$log\Omega = -\sum_i^I n_i \, log(p_i) \qquad \frac{log\Omega}{N} = -\sum_i^I p_i \, log(p_i)$$

"Shannon" Entropy S

$$S = -\sum_{i=1}^{I} p(x_i) \log[p(x_i)]$$

definition
conditional Entropy
KL divergence
connection to TD

$$\frac{\log\Omega}{N} = -\sum_{i}^{I} p_i \log(p_i)$$ entropy per particle

N:	number of **indistinguishable** particles
n_i:	number of particles in micro state i
I:	number of states
p_i:	probability of a particle being in micro state i

$$S = -N \sum_{i}^{I} p_i \log(p_i)$$ total entropy

note: - using $\log\Omega$ vs Ω is **arbitrary**, but more **convenient** when calculating TD potentials

- We used $\lim_{N \to \infty} \left(\frac{n_i}{N}\right) = p_i$ and Stirling's approximation for large N. Therefore, $\lim_{t \to \infty} S(t) = S_{max}$

does **not** hold for small N in closed systems!   **see HW assignment**

- interpreting S as order/disorder is **not** a good concept

Often people explain entropy with an ordered vs messy office…

…and then say, that entropy (disorder)
grows with time (in closed systems).

- But how is it possible, that an office can do that,
  just by itself?

- What if my office just *looks* messy,
  but I can still pull any file you are asking me for?

order/disorder is not a physical quantity!

Those examples have nothing to do with entropy
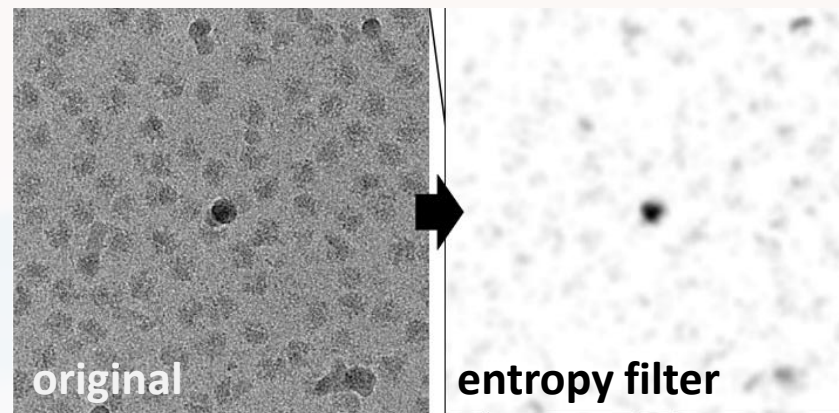conceptionally!

actually, the idea of entropy is more like that:

data analysis:
- image processing
- noise reduction
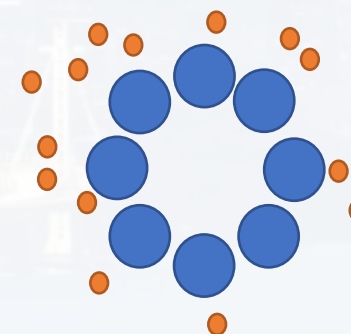- feature detection

Cryo-EM image of ribosomes

original → entropy filter

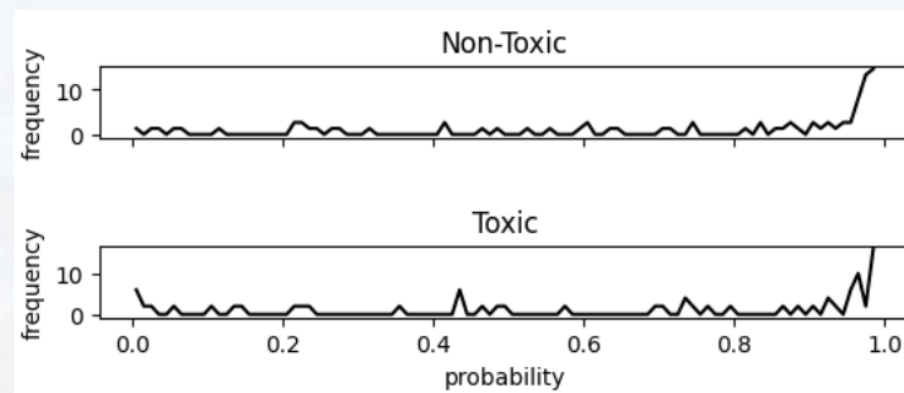definition
conditional Entropy
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biophysics:
- molecular driving forces
- formation of macromolecules
- "*ordering forces*"

AI:
- optimization
- cross entropy

Non-Toxic

Toxic

entropy S is a **measure of information** we have **about a system**

$$S = - \sum_{i=1}^{I} p_i \, ln(p_i)$$

two states   ↑ or   ↓

and three entities → system

possible states of the system

all three up	two up	one up	all three down
↑↑↑	↑↑↓	↑↓↓	↓↓↓
	↑↓↑	↓↑↓	
	↓↑↑	↓↓↑	

eight possible states

no idea (before the experiment) $S = - \sum_{i=1}^{8} \frac{1}{8} \, ln\left(\frac{1}{8}\right) = \sum_{i=1}^{8} \frac{1}{8} \, ln(8) \; = ln(8) \approx \mathbf{2.08}$

entropy S is a **measure of information** we have **about a system**

$$S = -\sum_{i=1}^{I} p_i \, ln(p_i)$$

two states ↑ or ↓

and three entities → system

possible states of the system

all three up	two up	one up	all three down
↑↑↑	↑↑↓	↑↓↓	~~↓↓↓~~
	↑↓↑	↓↑↓	
	↓↑↑	↓↓↑	

one measurement
→ at least one arrow up

seven possible states

$$S = \sum_{i=1}^{7} \frac{1}{7} \, ln(7) + 0 \ln(0) = ln(7) \approx \mathbf{1.95}$$

entropy S is a **measure of information** we have **about a system**

$$S = -\sum_{i=1}^{I} p_i \, ln(p_i)$$

two states $\uparrow$ or $\downarrow$

and three entities $\rightarrow$ system

possible states of the system

all three up	two up	one up	all three down

second measurement
$\rightarrow$ another arrow up

four possible states

$$S = \sum_{i=1}^{4} \frac{1}{4} \, ln(4) \ = ln(4) \approx \mathbf{1.39}$$

entropy S is a **measure of information** we have **about a system**

$$S = -\sum_{i=1}^{I} p_i \, ln(p_i)$$

two states $\uparrow$ or $\downarrow$

and three entities $\rightarrow$ system

possible states of the system

all three up   two up   one up   all three down

third measurement
$\rightarrow$ one arrow down

three possible states

$$S = ln(3) \approx \mathbf{1.10}$$

The lower the entropy, the more information!

entropy S is a **measure of information** we have **about a system**

$$S = -\sum_{i=1}^{I} p_i \, ln(p_i)$$

two states ↑ or ↓

and three entities → system

note: - since the base is **arbitrary**, we use **base two** if there are only **two** micro states

- unit is one **bit** (**bi**nary digi**t**)

- $S = -\sum_{i=1}^{8} \frac{1}{8} \, lg\left(\frac{1}{8}\right) = lg(8) = 3$
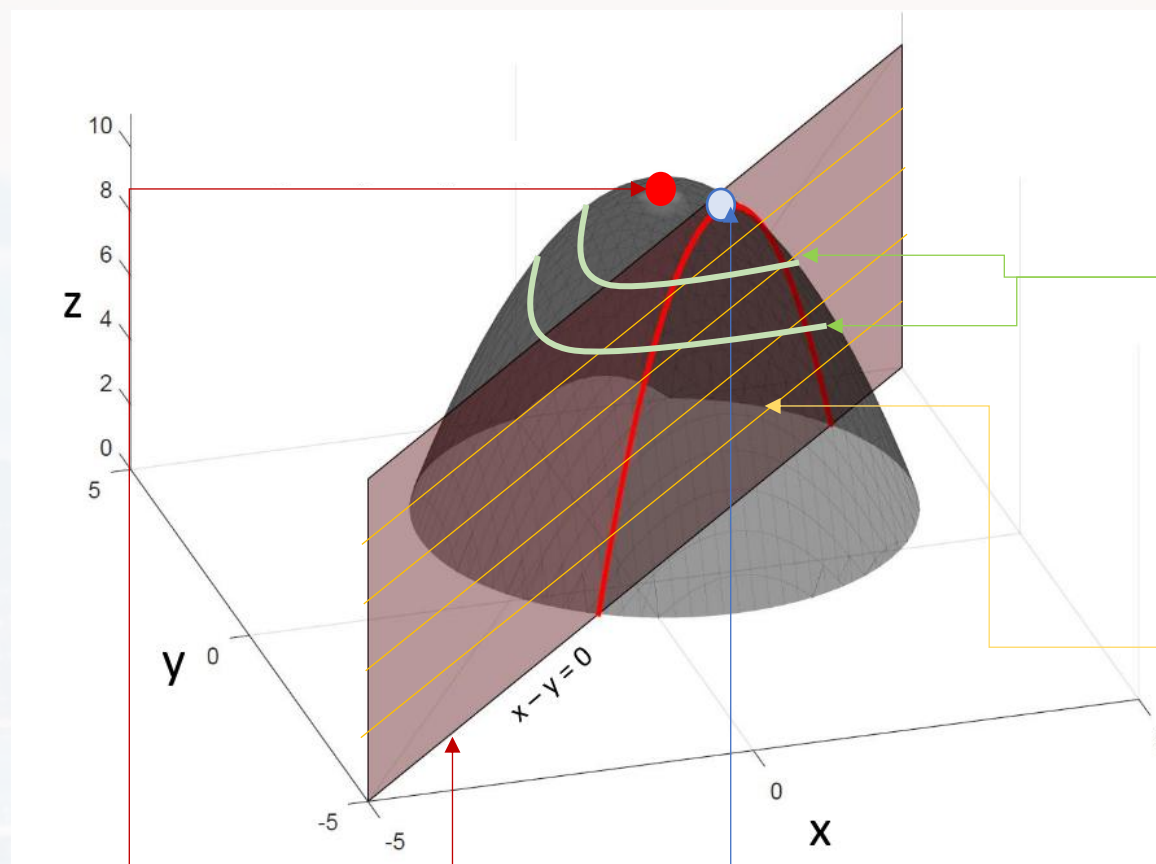
maximum of the function

$$f(x,y) = z = -(x-2)^2 - (y-1)^2 + 10$$

level lines $f(x,y) = const$

$$df(x,y) = \frac{\partial f(x,y)}{\partial x} dx + \frac{\partial f(x,y)}{\partial y} dy = 0$$

$$= grad f \, d\vec{r} = 0$$

level lines $g(x,y) = const$

$$dg(x,y) = \frac{\partial g(x,y)}{\partial x} dx + \frac{\partial g(x,y)}{\partial y} dy = 0$$

$$= grad g \, d\vec{r} = 0$$

$z = 10$ at
$x = 2$
$y = 1$

constrain $g(x,y) = x - y = 0$

maximum of the function, subject to $g(x,y)$

constrain $g(x, y) = x - y = 0$

level lines $f(x, y) = const$

$gradg$

$gradf$

$z = 10$ at
$x = 2$
$y = 1$

maximum of the function, subject to $g(x, y)$
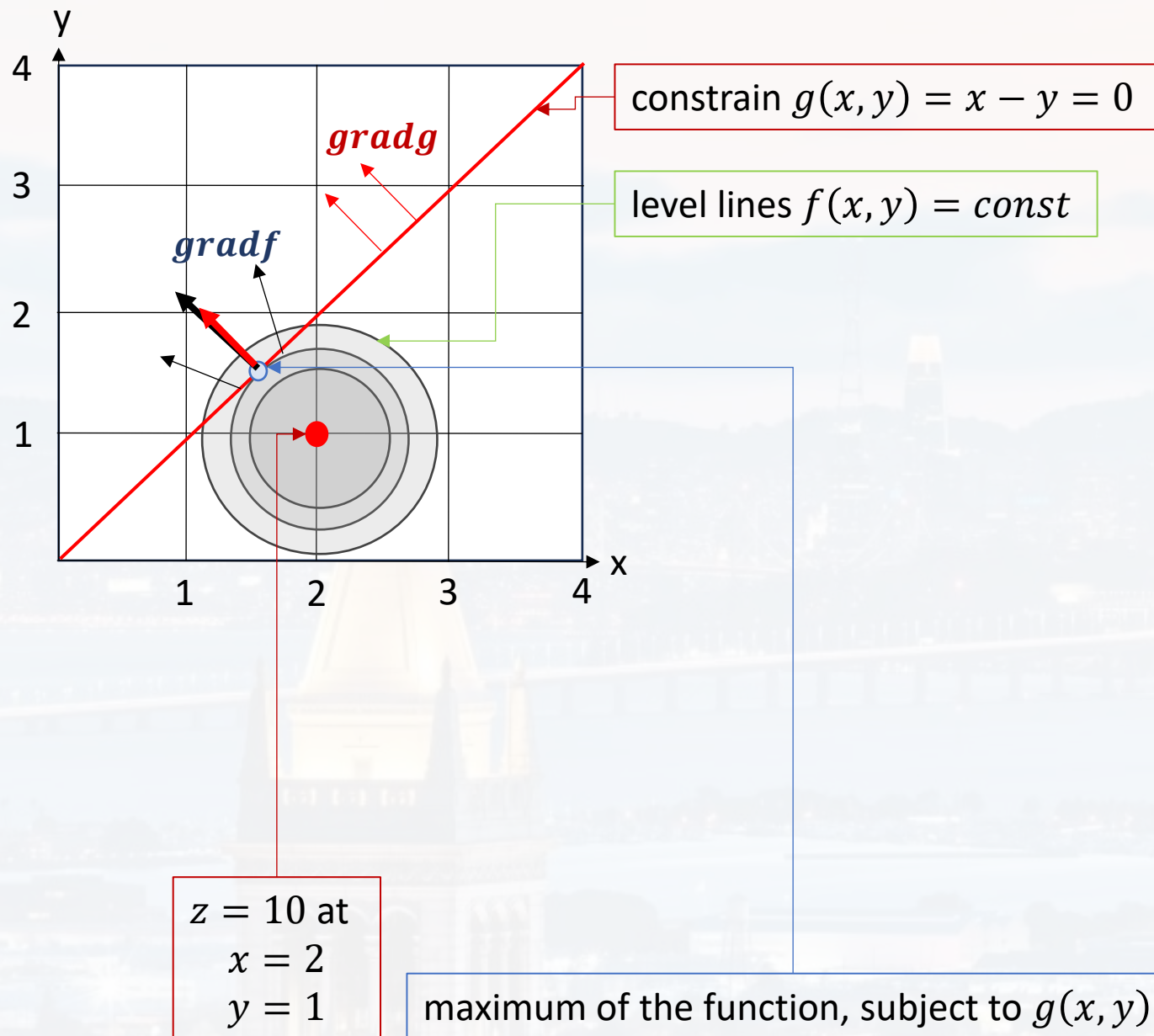
the maximum of $f(x, y)$
subject to $g(x, y)$ located
where:

$$df(x, y) \quad = dg(x, y)$$

$$gradf \; d\vec{r} = gradg \; d\vec{r}$$

$$gradf \quad = gradg$$

Both gradients need to point
in the same direction
**(hence, can be multiplied with a constant,
say λ)!**

$$gradf \quad = \lambda \, gradg$$

λ　**Lagrangian Multiplier**

the maximum of $f(x, y)$ subject to $g(x, y)$

$$grad f = \lambda \, grad g$$

$$f(x, y) - \lambda g(x, y) = const$$

the Lagrangian
$L(x, y, \lambda)$

more general:

$$L(x_1, x_2, \ldots, x_i, x_N, \lambda_1, \lambda_2, \ldots, \lambda_k, \lambda_K) = f(x_1, x_2, \ldots, x_i, x_N) - \sum_{k=1}^{K} \lambda_k \, g_k(x_1, x_2, \ldots, x_i, x_N)$$

note: - **N dimensions and $K \leq N$ constrains**

     - we need to solve N (from the gradient) + K equations by using the constrains

     - optimization: more robust results (most common L1 and L2 regularization, see later)

     - machine learning: including constrains in loss function (see later)

the maximum of $f(x, y)$ subject to $g(x, y)$
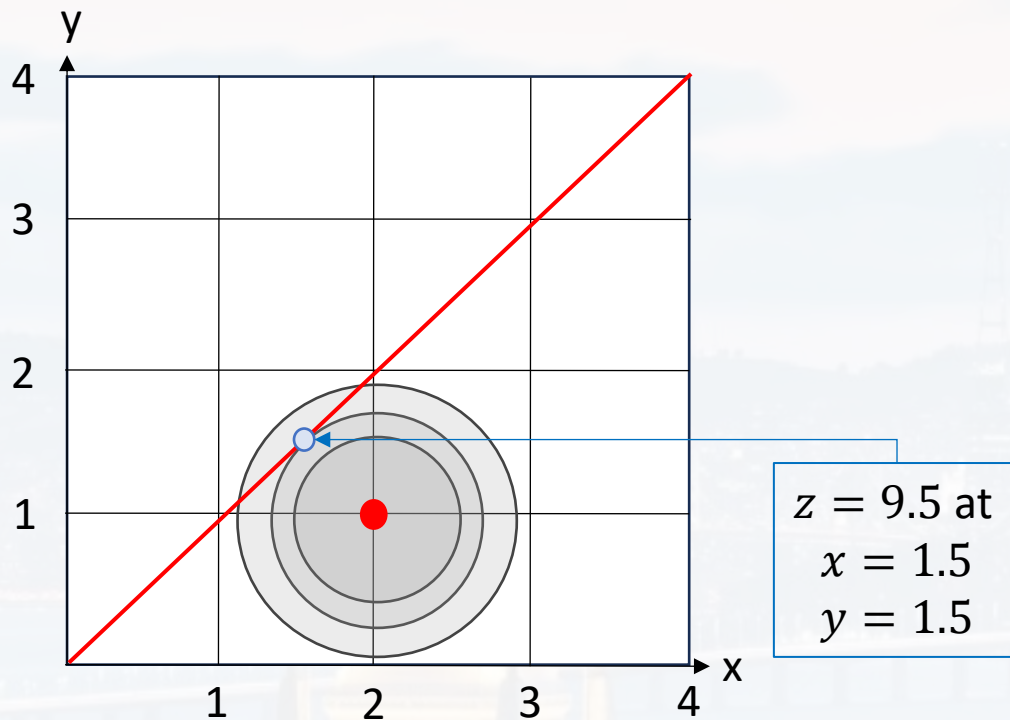
$$f(x, y) = z = -(x - 2)^2 - (y - 1)^2 + 10$$

constrain $g(x, y) = x - y = 0$

constrain $x = y$ $\quad\quad x = 1.5$
$\quad\quad\quad\quad\quad\quad\quad\quad y = 1.5$

$$f(1.5, 1.5) = 9.5$$

$z = 9.5$ at
$x = 1.5$
$y = 1.5$

$grad f = \lambda \, grad g$ $\qquad \dfrac{\partial f(x,y)}{\partial x} = \lambda \dfrac{\partial g(x,y)}{\partial x}$ $\qquad -2(x - 2) = \lambda$

$$y = -x + 3$$

$$\dfrac{\partial f(x,y)}{\partial y} = \lambda \dfrac{\partial g(x,y)}{\partial y} \qquad -2(y - 1) = -\lambda$$

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Bayes Theorem

maximum entropy of flipping a coin:

$$f(p_1, p_2) = -p_1 \ln p_1 - p_2 \ln p_2$$

subject to

$$g(p_1, p_2) = p_1 + p_2 = 1$$

absolute maximum:

$$\frac{\partial f(p_1, p_2)}{\partial p_1} = 0 \qquad\qquad \frac{\partial f(p_1, p_2)}{\partial p_2} = 0$$

$$-\ln p_1 - 1 = 0 \qquad\qquad -\ln p_2 - 1 = 0$$

$$p_1 = p_2 = \frac{1}{e}$$

$$f\left(\frac{1}{e}, \frac{1}{e}\right) = \frac{2}{e} \approx 0.74$$
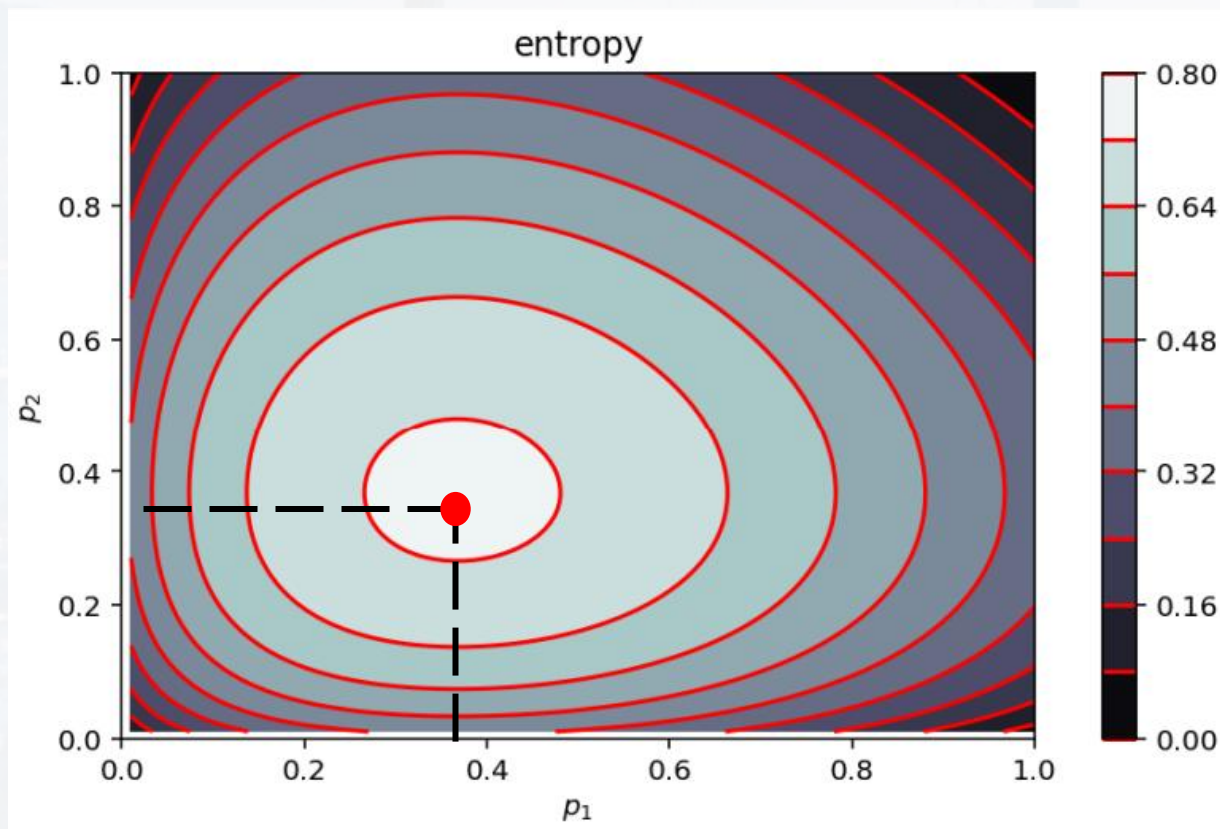
maximum entropy of flipping a coin:

$$f(p_1, p_2) = -p_1 \ln p_1 - p_2 \ln p_2$$

subject to

$$g(p_1, p_2) = p_1 + p_2 = 1$$

maximum subject to $g(p_1, p_2)$:

$$\frac{\partial f(p_1, p_2)}{\partial p_1} = \lambda \frac{\partial g(p_1, p_2)}{\partial p_1}$$

$$\frac{\partial f(p_1, p_2)}{\partial p_2} = \lambda \frac{\partial g(p_1, p_2)}{\partial p_2}$$

$$-\ln p_1 - 1 = \lambda \qquad\qquad -\ln p_2 - 1 = \lambda$$

$$p_1 = p_2$$

constrain: $\qquad\qquad p_1 + p_2 = 1$

$$p_1 = p_2 = \frac{1}{2}$$

$$f\left(\frac{1}{2}, \frac{1}{2}\right) = ln2 \approx 0.69$$
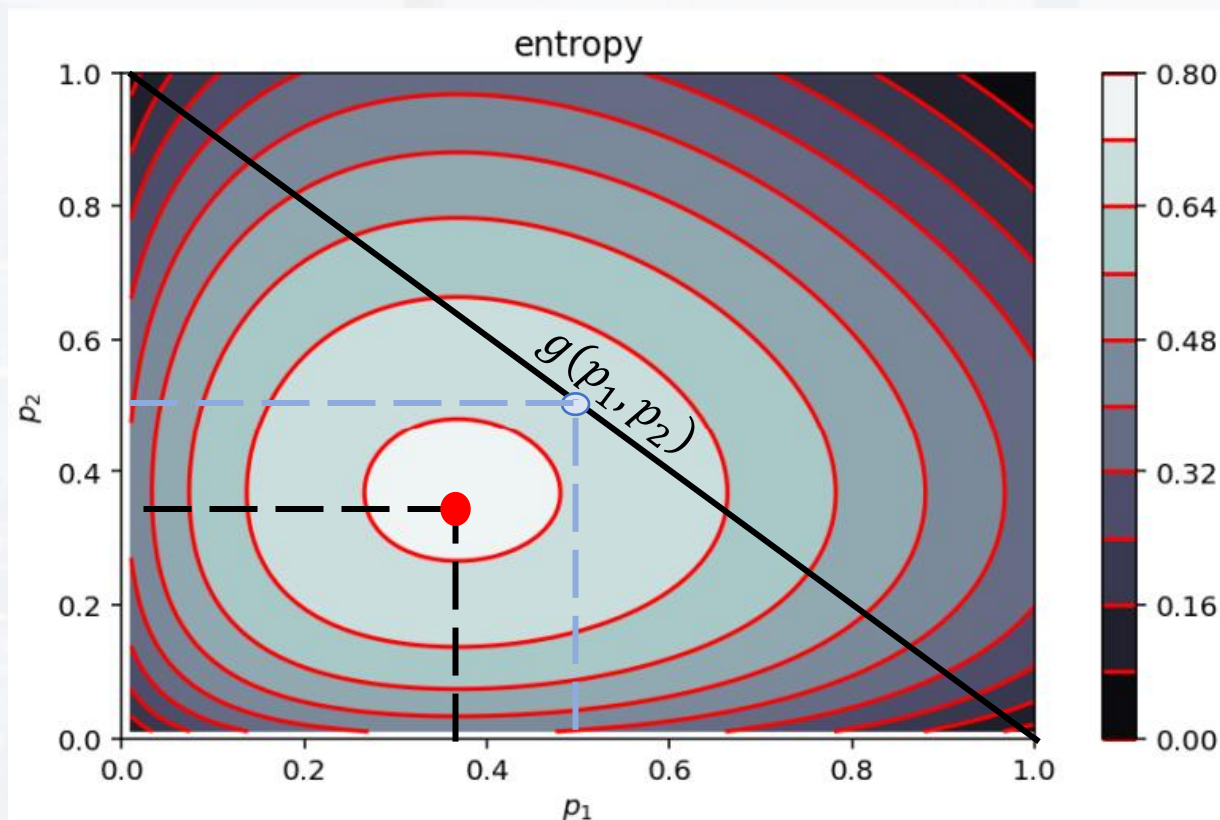
maximum entropy for I states:

$$f(p_1,..,p_i,...p_I) = -\sum_{i=1}^{I} p_i \, lnp_i$$

subject to

$$g(p_1,..,p_i,...p_I) = \sum_{i=1}^{I} p_i = 1$$

maximum subject to $g(p_1,..,p_i,...p_I)$:

$$\frac{\partial f(p_1,..,p_i,...p_I)}{\partial p_i} = \lambda \frac{\partial g(p_1,..,p_i,...p_I)}{\partial p_i}$$

$$-\ln p_i - 1 = \lambda \qquad p_i = e^{-(1+\lambda)}$$

constrain:

$$\sum_{i=1}^{I} e^{-(1+\lambda)} = 1$$

$$I e^{-(1+\lambda)} = 1$$

$$e^{-(1+\lambda)} = \frac{1}{I}$$

probabilities are constant!
→ flat distribution!

$$\boxed{p_i = \frac{1}{I}}$$
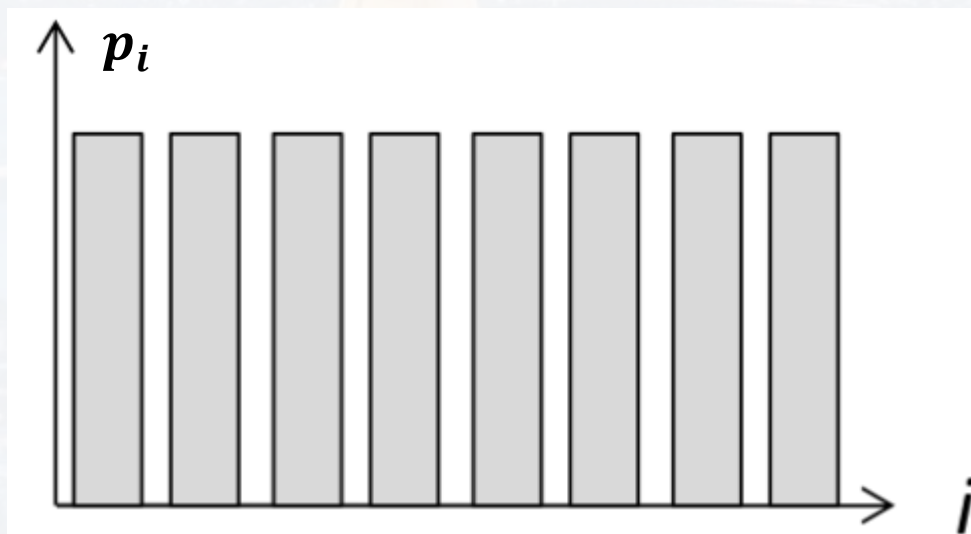
maximum entropy for I states:

$$f(p_1, \ldots, p_i, \ldots p_I) = - \sum_{i=1}^{I} p_i \, ln p_i$$

subject to

$$g_1(p_1, \ldots, p_i, \ldots p_I) = \sum_{i=1}^{I} p_i = 1$$

if N <u>and</u> ***total energy*** is conserved

$$g_2(p_1, \ldots, p_i, \ldots p_I) = \sum_{i=1}^{I} p_i \varepsilon_i = \frac{E_{tot}}{N} = \frac{1}{N} \sum_{i=1}^{I} n_i \varepsilon_i$$

$$\frac{\partial f(p_1, \ldots, p_i, \ldots p_I)}{\partial p_i} = \lambda_1 \frac{\partial g_1(p_1, \ldots, p_i, \ldots p_I)}{\partial p_i} + \lambda_2 \frac{\partial g_2(p_1, \ldots, p_i, \ldots p_I)}{\partial p_i}$$

$$-\ln p_i - 1 = \lambda_1 + \lambda_2 \frac{\partial \sum_{i=1}^{I} p_i \varepsilon_i}{\partial p_i}$$

Lagrangian Multiplier
Examples

N:	number of **indistinguishable** particles
n_i:	number of particles in micro state i
I:	number of states
p_i:	probability of a particle being in micro state I
ε_i:	energy in state i

maximum entropy for I states:

$$f(p_1, .., p_i, ... p_I) = -\sum_{i=1}^{I} p_i \, ln p_i$$

subject to

$$g_1(p_1, .., p_i, ... p_I) = \sum_{i=1}^{I} p_i = 1$$

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if N <u>and</u> **total energy** is conserved

$$g_2(p_1, .., p_i, ... p_I) = \sum_{i=1}^{I} p_i \varepsilon_i$$

from g_1: $p_i = \dfrac{1}{\sum_{i=1}^{I} e^{-\lambda_2 \varepsilon_i}} \, e^{-\lambda_2 \varepsilon_i}$

$$-\ln p_i - 1 = \lambda_1 + \lambda_2 \frac{\partial \sum_{i=1}^{I} p_i \varepsilon_i}{\partial p_i}$$

partition function Z $Z = \sum_{i=1}^{I} e^{-\lambda_2 \varepsilon_i}$

$$-\ln p_i - 1 = \lambda_1 + \lambda_2 \varepsilon_i$$

Boltzmann distribution $p_i = \dfrac{1}{Z} e^{-\lambda_2 \varepsilon_i}$

$$p_i = e^{-(1+\lambda_1)} e^{-\lambda_2 \varepsilon_i}$$

Maximum Entropy and Information, Bayes Theorem:

partition function Z

$$Z = \sum_{i=1}^{I} e^{-\lambda_2 \varepsilon_i}$$

Boltzmann distribution

$$p_i = \frac{1}{Z} e^{-\lambda_2 \varepsilon_i}$$

one can show: $\lambda_2 = \frac{1}{kT}$

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note: - for $T \rightarrow \infty$, $Z \rightarrow I$, i. e. higher states become more accessible and $p_i \rightarrow \frac{1}{I}$

- we used maximum entropy:

  equilibrium state for large N

- N **and** E_{tot} are constant

- ANN: **softmax layer** for classification

probabilities (see later)

$$f(x) = \int_{-\infty}^{+\infty} p(x)\ln[p(x)]\,dx$$

continuous distribution with support $(-\infty, +\infty)$

$$g_1(x) = \int_{-\infty}^{+\infty} p(x)dx = 1$$

$$g_2(x) = \int_{-\infty}^{+\infty} x\,p(x)dx = \mu$$

mean μ

$$g_3(x) = \int_{-\infty}^{+\infty} (x-\mu)^2\,p(x)dx = \sigma^2$$

standard deviation σ^2

$$\int_{-\infty}^{+\infty} p(x)\ln[p(x)]\,dx = \lambda_1 \int_{-\infty}^{+\infty} p(x)dx + \lambda_2 \int_{-\infty}^{+\infty} x\,p(x)dx + \lambda_3 \int_{-\infty}^{+\infty} (x-\mu)^2\,p(x)dx$$

$$p(x) = \exp[-\lambda_1 - \lambda_2 x - \lambda_3 (x-\mu)^2 - 1]$$

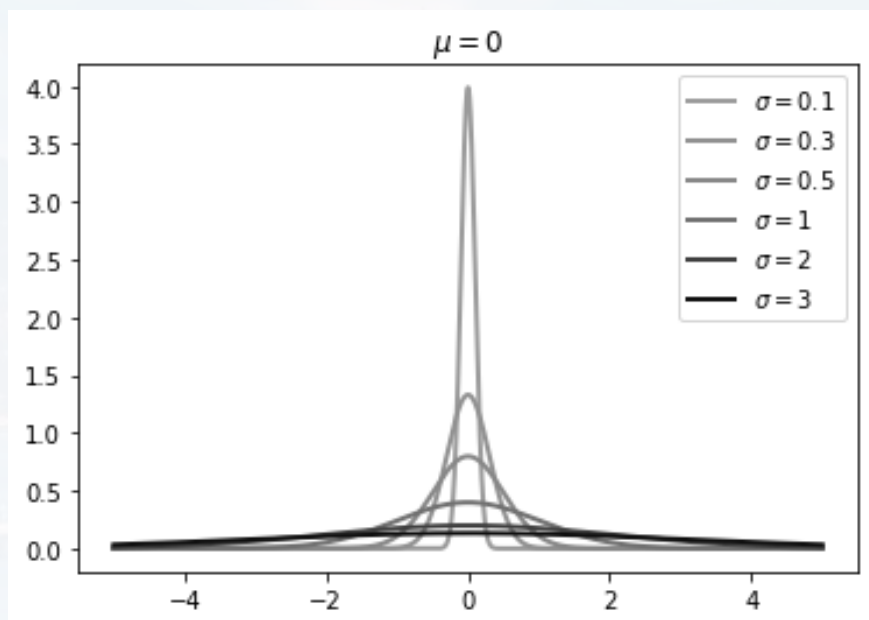Normal (Gauss) distribution

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x-\mu)^2}$$

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note: - $S[p(x)] = \ln(2\pi\sigma) + 1/2$ **(which can be negative)**

- constrains where very generic → normal distribution is **often a good approximation**

- often: $N(\mu, \sigma^2)$

maximum entropy distributions

Distribution name	Probability density / mass function	Maximum entropy constraint	Support
Uniform (discrete)	$f(k) = \dfrac{1}{b-a+1}$	None	$\{a, a+1, \ldots, b-1, b\}$
Uniform (continuous)	$f(x) = \dfrac{1}{b-a}$	None	$[a, b]$
Bernoulli	$f(k) = p^k(1-p)^{1-k}$	$\mathrm{E}[K] = p$	$\{0, 1\}$
Normal	$f(x) = \dfrac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\dfrac{(x-\mu)^2}{2\sigma^2}\right)$	$\mathrm{E}[X] = \mu,$ $\mathrm{E}[X^2] = \sigma^2 + \mu^2$	$\mathbb{R}$
Gamma	$f(x) = \dfrac{x^{k-1}e^{-x/\theta}}{\theta^k \Gamma(k)}$	$\mathrm{E}[X] = k\theta,$ $\mathrm{E}[\ln X] = \psi(k) + \ln\theta$	$[0, \infty)$
Binomial	$f(k) = \dbinom{n}{k} p^k(1-p)^{n-k}$	$\mathrm{E}[X] = \mu,$ $f \in$ n-generalized binomial distribution[11]	$\{0, \ldots, n\}$
Poisson	$f(k) = \dfrac{\lambda^k e^{-\lambda}}{k!}$	$\mathrm{E}[X] = \lambda,$ $f \in \infty$-generalized binomial distribution[11]	$\mathbb{N} = \{0, 1, \ldots\}$
Logistic	$f(x) = \dfrac{e^{-x}}{(1+e^{-x})^2} = \dfrac{e^{+x}}{(e^{+x}+1)^2}$	$\mathrm{E}[X] = 0,$ $\mathrm{E}\left[\ln\left(1 + e^{-X}\right)\right] = 1$	$\{-\infty, \infty\}$

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Bernoulli	$f(k) = p^k(1-p)^{1-k}$	$E[K] = p$	$\{0, 1\}$
Multivariate normal	$f_X(\mathbf{x}) = \dfrac{\exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathsf{T}}\Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu})\right]}{\sqrt{(2\pi)^N |\Sigma|}}$	$E[\mathbf{x}] = \boldsymbol{\mu},$ $E\left[(\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^{\mathsf{T}}\right] = \Sigma$	$\mathbb{R}^n$
Gamma	$f(x) = \dfrac{x^{k-1}e^{-x/\theta}}{\theta^k \Gamma(k)}$	$E[X] = k\theta,$ $E[\ln X] = \psi(k) + \ln\theta$	$[0, \infty)$
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Outline

Entropy and Information

- definition
- conditional Entropy
- KL divergence
- connection to TD

Maximum Entropy Distributions

- Lagrangian Multiplier
- examples

Bayes Theorem

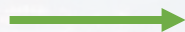P(A $\cap B$)   probability **P** that the events **A** **and** **B** occur

so far: A and B were independent   P(A $\cap B$) = P(A)P(B) = P(B)P(A)

Thomas Bayes
(1701 - 1761)

now: **conditional probabilities** | "given" or "under the condition"

P(A$\cap B$) = P(A|B)P(B)
              = P(B|A)P(A)

$$P(A|B)P(B) = P(B|A)P(A)$$

Bayes Theorem

posterior $$\boldsymbol{P(A|B)} = \frac{P(B|A)\boldsymbol{P(A)}}{P(B)}$$ **prior**

Maximum Entropy and Information, Bayes Theorem:

posterior $\quad P(A|B) = \dfrac{P(B|A)P(A)}{P(B)} \quad$ prior $\qquad$ **Bayes Theorem**
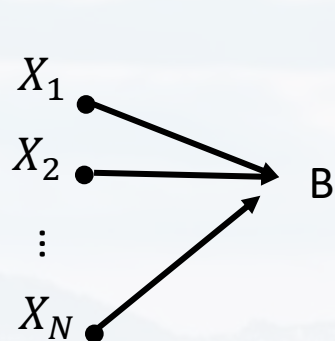
$$P(B) = \sum_{n=1}^{N} P(B|X_n)P(X_n)$$

$$P(B) = \int P(B|X)P(X)\, dX$$

marginalization

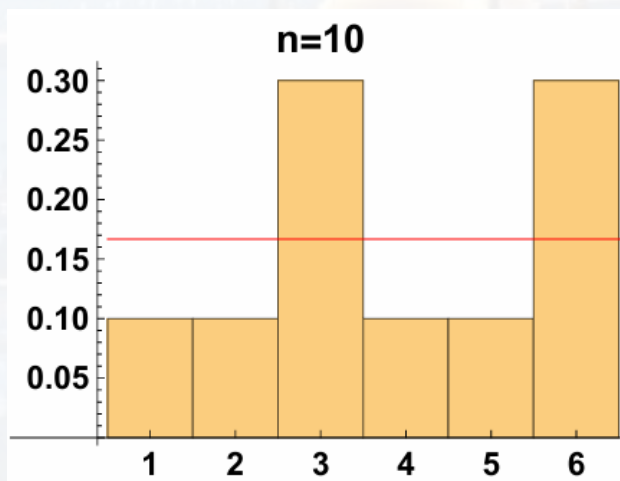**Thomas Bayes
(1701 - 1761)**

for a normal distribution $M = \mathcal{N}(\mu, \sigma)$

$$P(D|\mathcal{N}) = \int P(D|\mathcal{N}(\mu, \sigma))\, P(\mu, \sigma | \mathcal{N}(\mu, \sigma))\, d\Omega_{\mu,\sigma}$$

model: M
data: D

n=10

σ = 2, μ = 3.5

σ = 2, μ = 5.0

σ = 1.5, μ = 3.5

σ = 7.0, μ = 1.0

....and so on

Maximum Entropy and Information, Bayes Theorem:

example: cancer diagnosis from blood test

+ : positive test result
D : diseased
H : health

Bayes Theorem

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

Marginalization

$$P(B) = \sum_{n=1}^{N} P(B|X_n)P(X_n)$$

example: cancer diagnosis from blood test

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Bayes Theorem $P(A|B) = \dfrac{P(B|A)P(A)}{P(B)}$

Marginalization $P(B) = \sum\limits_{n=1}^{N} P(B|X_n)P(X_n)$

statement 1: If a person is **diseased**, there is a **95% probability** that the test is **positive.**

statement 2: The **prevalence** for the disease in the average **population** is **0.001%** .

statement 3: **5% of healthy** patients have **a positive result** (aka p-value).

A person takes the test and gets a positive test result. **What is the probability that the person is sick?**

$$P(D|+) = \frac{P(+|D)P(D)}{P(+)} = \frac{0.95\,P(D)}{P(+)} = \frac{0.95 \cdot 0.00001}{P(+)} = \frac{0.95 \cdot 0.00001}{P(+|D)P(D) + P(+|H)P(H)}$$

                         statement 1   statement 2   marginalization

example: cancer diagnosis from blood test

+	**: positive test result**
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Bayes Theorem

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Marginalization

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statement 1   statement 2   marginalization

$$= \frac{0.95 \cdot 0.00001}{P(+|D)P(D) + P(+|H)[1 - P(D)]}$$

complement probability

example: cancer diagnosis from blood test

Bayes Theorem	$P(A\|B) = \dfrac{P(B\|A)P(A)}{P(B)}$

+ : positive test result
D : diseased
H : health

Marginalization $P(B) = \sum\limits_{n=1}^{N} P(B\|X_n)P(X_n)$

statement 1: If a person is **diseased**, there is a **95% probability** that the test is **positive.**
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$$P(D|+) = \frac{P(+|D)P(D)}{P(+|D)P(D) + P(+|H)[1 - P(D)]}$$

$$= \frac{1}{1 + \dfrac{P(+|H)[1 - P(D)]}{P(+|D)P(D)}} = \frac{1}{1 + \dfrac{0.05\,[1 - 0.00001]}{0.95 \cdot 0.00001}} = 1/5000$$

Maximum Entropy and Information, Bayes Theorem:

example: cancer diagnosis from blood test

+ : positive test result
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H : health

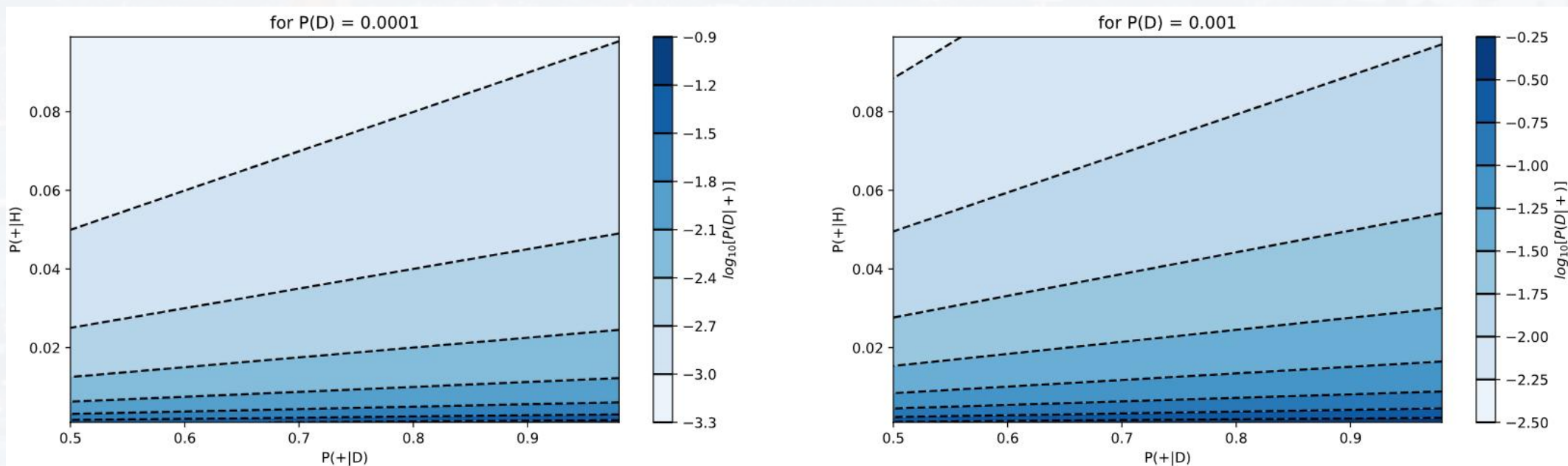| statement 1: | sensitivity | P(D|+) = 95% |
| statement 2: | prior | P(D) = 0.001% |
| statement 3: | p-value or false positive rate | P(+|H) = 5% |

$$P(D|+) = \frac{1}{1 + \dfrac{P(+|H)[1 - P(D)]}{P(+|D)P(D)}}$$

check: **PlotPD_Plus.py**

Maximum Entropy and Information, Bayes Theorem:

example: cancer diagnosis from blood test

+   : **positive test result**
D   : **diseased**
H   : **health**

statement 1:	sensitivity	**P(D	+) = 95%**
statement 2:	prior	**P(D) = 0.001%**
statement 3:	p-value or false positive rate	**P(+	H) = 5%**

$$P(D|+) = \frac{1}{1 + \dfrac{P(+|H)[1 - P(D)]}{P(+|D)P(D)}}$$

check: `PlotPD_Plus.py`

for P(D) = 0.01

statement 1:	sensitivity	$P(D	+) = 95\%$
statement 2:	prior	$P(D) = 0.001\%$
statement 3:	p-value or false positive rate	$P(+	H) = 5\%$

odds ratios:

$$\rho_1 = \frac{P(+|H)}{P(+|D)}$$

$$\rho_2 = \frac{1 - P(D)}{P(D)}$$

$$P(D|+) = \cfrac{1}{1 + \cfrac{P(+|H)[1 - P(D)]}{P(+|D)P(D)}}$$

log odds ratios:

$$r_1 = \log\left[\frac{P(+|H)}{P(+|D)}\right]$$

$$r_2 = \log\left[\frac{1 - P(D)}{P(D)}\right]$$
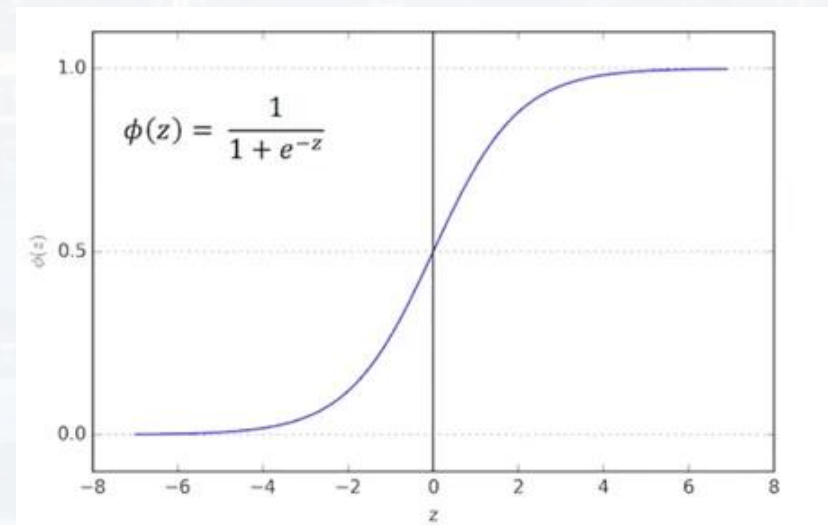
$$P(D|+) = \frac{1}{1 + e^{r_1} e^{r_2}}$$

log odds ratios: $\quad r_1 = \log\left[\dfrac{P(+|H)}{P(+|D)}\right]$

$$P(D|+) = \dfrac{1}{1 + \dfrac{P(+|H)[1 - P(D)]}{P(+|D)P(D)}}$$

$$r_2 = \log\left[\dfrac{1 - P(D)}{P(D)}\right]$$

$$\boxed{P(D|+) = \dfrac{1}{1 + e^{r_1}e^{r_2}}}$$

note: - **logistic (or logit or sigmoid) function**

        - transfer function ANN (see later)

        - bound growth (Verhulst equation)

$$\phi(z) = \frac{1}{1 + e^{-z}}$$

Thank you very much for your attention!