Applied Machine Learning

Maximum Likelihood and Bayesian Reasoning

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Admin

- Add/drop deadline is tomorrow
- Do the quizz before the tomorrow if you are unsure about your math background
- We will solve the issue with study groups later this week
- Office hours for this week: after each class
- Bonus points for lecture notes/summaries

Model fitting

x | input features → **ML algorithm** **with parameters $\boldsymbol{\theta}$** $f(x^{(n)}; \theta)$ → y | output labels

The process of estimating the model parameters θ from given data $\mathcal{D}$, is the core of training ML models which often boils down into optimization of an loss function $\mathcal{L}(\theta)$

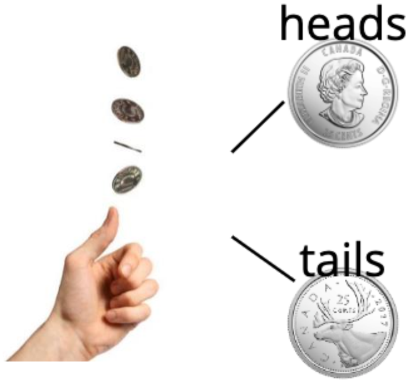
Where do these loss functions come from?

Often from **maximum likelihood** or **Bayesian** methods

Case study

Fundamental machine learning problem that we will study today

You are given observations (e.g. data) of coin flips from a possibly rigged coin



$$\mathcal{D} = \{0, 0, 0, 0, 1\}$$

Coin flip is just one example, could be anything binary:

- Someone purchasing product or not
- Someone getting infected by covid or not
- Bus arrives on time or not
- A penalty kick is scored or not
- Social media post is liked or not
- etc.

What is your **estimate** for the probability of the next throw being head (1) or tail (0)?

Objectives

learn common parameter estimation methods and understand what it means to learn a probabilistic model of the data

- using maximum likelihood principle
- using Bayesian inference
    - prior, posterior, posterior predictive
    - MAP inference
    - Beta-Bernoulli conjugate pairs

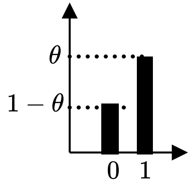
Parameter estimation

we suppose a coin's head/tail outcome has a **Bernoulli distribtion**

$$\text{Bernoulli}(x|\theta) = \theta^x (1-\theta)^{(1-x)}$$

reminder: Bernoulli random variable takes values of 0 or 1, e.g. head/tail in a coin toss

$$p(x|\theta) = \begin{cases} \theta & x = 1 \\ 1-\theta & x = 0 \end{cases}$$



IID is short for *independent and identically distributed*

this is our **probabilistic model** of some head/tail IID data $\mathcal{D} = \{0,0,1,1,0,0,1,0,0,1\}$

Objective: learn the model parameter θ

if we are only interested in the counts, we can also use **Binomial distribution**

$$\text{Binomial}(N, N_h|\theta) = \binom{N}{N_h} \theta^{N_h} (1-\theta)^{N-N_h}$$

N: $|\mathcal{D}|$

N_h: # heads $N_h = \sum_{x \in \mathcal{D}} x$

$N - N_h$: N_t

Maximum likelihood

a coin's head/tail outcome has a **Bernoulli distribtion**

$$\text{Bernoulli}(x|\theta) = \theta^x (1-\theta)^{(1-x)}$$

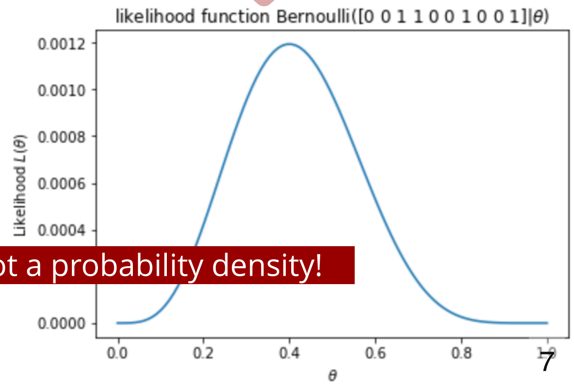
this is our **probabilistic model** of some head/tail IID data $\mathcal{D} = \{0,0,1,1,0,0,1,0,0,1\}$

Objective: **learn** the model parameter θ

Idea: find the parameter θ that maximizes the probability of observing $\mathcal{D}$

Likelihood $L(\theta;\mathcal{D}) = \prod_{x\in\mathcal{D}} \text{Bernoulli}(x|\theta) = \theta^4(1-\theta)^6$ is a function of θ

Max-likelihood assignment



note that this is not a probability density!

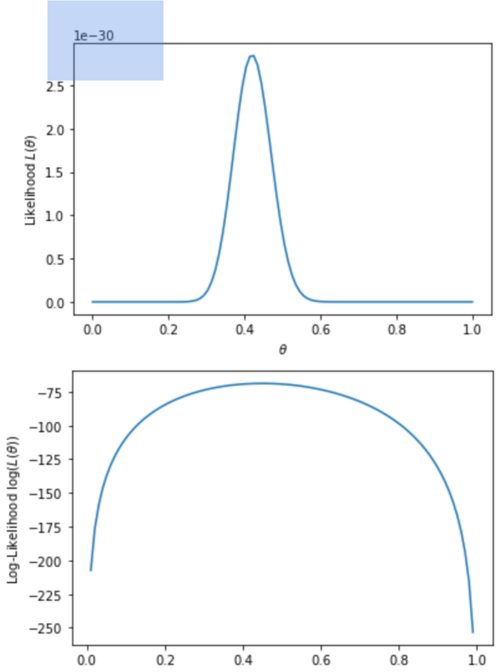
pick the parameters that assign the highest probability to the training data

Maximizing log-likelihood

likelihood $L(\theta; \mathcal{D}) = \prod_{x \in \mathcal{D}} p(x; \theta)$

using product here creates extreme values

for 100 samples in our example, the likelihood shrinks below 1e-30



log-likelihood has the same maximum but it is well-behaved

$$\ell(\theta; \mathcal{D}) = \log(L(\theta; \mathcal{D})) = \sum_{x \in \mathcal{D}} \log(p(x; \theta))$$

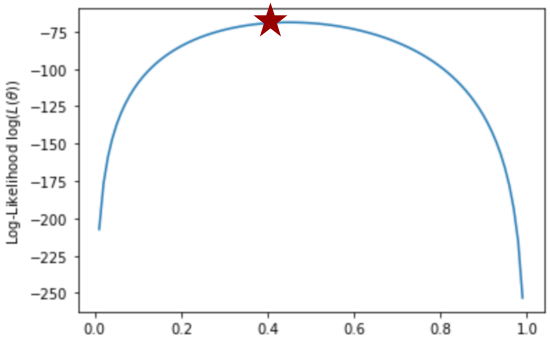
how do we find the max-likelihood parameter? $\theta^* = \arg\max_\theta \ell(\theta; \mathcal{D})$

for some simple models we can get the ***closed form solution***

for complex models we need to use ***numerical optimization***

Maximizing log-likelihood

log-likelihood $\ell(\theta; \mathcal{D}) = \log(L(\theta; \mathcal{D})) = \sum_{x \in \mathcal{D}} \log(\text{Bernoulli}(x; \theta))$

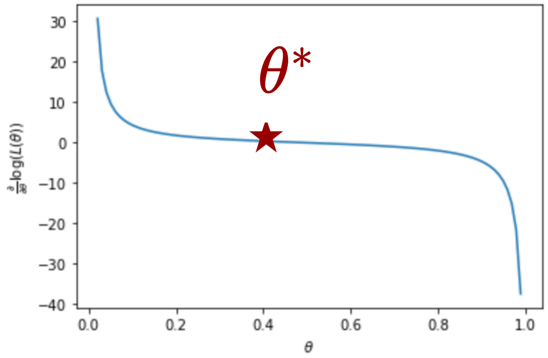


observation: at maximum, the derivative of $\ell(\theta; \mathcal{D})$ is zero

idea: set the the derivative to zero and solve for θ

example max-likelihood for Bernoulli

$$\frac{\partial}{\partial \theta} \ell(\theta; \mathcal{D}) = \frac{\partial}{\partial \theta} \sum_{x \in \mathcal{D}} \log\left(\theta^x (1-\theta)^{(1-x)}\right)$$
$$= \frac{\partial}{\partial \theta} \sum_x x \log \theta + (1-x) \log(1-\theta)$$
$$= \sum_x \frac{x}{\theta} - \frac{1-x}{1-\theta} = 0$$



which gives $\theta^{MLE} = \frac{\sum_{x \in \mathcal{D}} x}{|\mathcal{D}|}$ is simply the portion of heads in our dataset

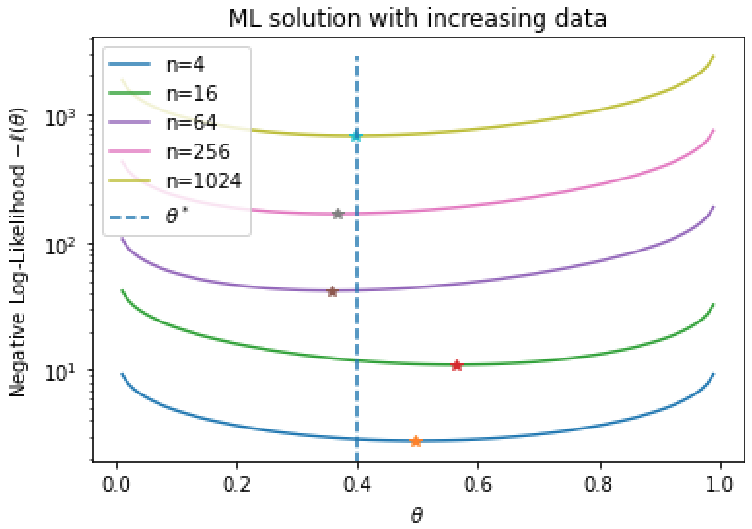
what is θ^{MLE} when $\mathcal{D} = \{0,0,1,1,0,0,1,0,0,1\}$?

Problem with maximum likelihood

max-likelihood estimate does not reflect our uncertainty:

- e.g. for $\mathcal{D} = \{1\}$, $\theta^{MLE} = 1$. If we observe only one head, predicts all future tosses are head!
- e.g., $\theta^{MLE} = .2$ for both 1/5 heads and 1000/5000 heads
  - in which case are we more certain of the predicted θ?

How can we quantify our uncertainty about our prediction?



Bayesian approach

How can we quantify our uncertainty about our prediction?
capture it using a conditional probability distribution instead of a single best guess

Using the Bayesian inference approach

- we maintain a *distribution* over parameters $p(\theta)$ prior — what do we believe about θ before any observation
- after observing $\mathcal{D}$ we update this distribution $p(\theta|\mathcal{D})$ posterior

how to update degree of certainty given data? using **Bayes rule**

$$p(\theta|\mathcal{D}) = \frac{p(\theta)p(\mathcal{D}|\theta)}{p(\mathcal{D})}$$

hidden: θ; observed: $\mathcal{D}$

prior: $p(\theta)$

likelihood of the data: $p(\mathcal{D}|\theta)$
previously denoted by $L(\theta;\mathcal{D})$

evidence: this is a normalization, **marginal likelihood of data**

$$p(\mathcal{D}) = \int p(\theta')p(\mathcal{D}|\theta')\mathrm{d}\theta'$$

We can get a point estimate by collapsing this posterior distribution to a single point, i.e. the best guess

Bayes rule: example reminder

$c = \{\text{yes}, \text{no}\}$ patient having cancer?

$x \in \{-, +\}$ observed test results, a single binary feature

prior: .1% of population has cancer $p(\text{yes}) = .01$

likelihood: $p(+|\text{yes}) = .9$ TP rate of the test (90%)

$$p(c = yes \mid x) = \frac{p(c{=}yes)p(x|c{=}yes)}{p(x)}$$

posterior: $p(\text{yes}|+) = .177$

FP rate of the test (5%)

evidence: $p(+) = p(\text{yes})p(+|\text{yes}) + p(\text{no})p(+|\text{no}) = .001 \times .9 + .999 \times .05 = .05$

Beta distribution prior

in our coin example, we know the form of likelihood:

prior $p(\theta)?$

posterior $p(\theta|\mathcal{D})?$

likelihood $p(\mathcal{D}|\theta) = \prod_{x \in \mathcal{D}} \text{Bernoulli}(x;\theta) = \theta^{N_h}(1-\theta)^{N_t}$

proportional

posterior $\propto$ prior $\times$ likelihood

$p(\theta : \alpha') \propto p(\theta : \alpha) \times p(\mathcal{D}|\theta)$

conjugate

A common type of prior is : $p(\theta|a,b) \propto \theta^a(1-\theta)^b$

this means there is a normalization constant that does not depend on θ

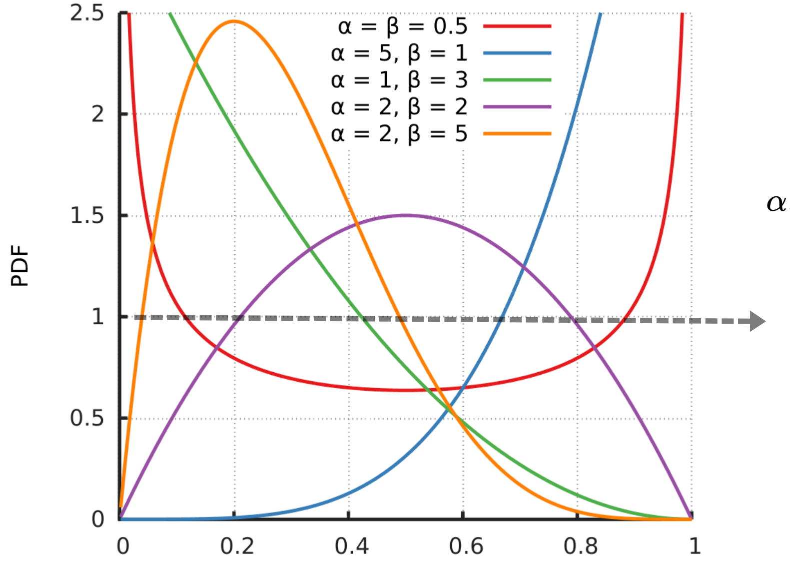
distribution of this form has a name, **Beta** distribution

(so that we can easily update our belief with new observations, i.e. closed under Bayesian updating)

we say Beta distribution is a conjugate prior to the Bernoulli likelihood

Beta distribution

Beta distribution has the following density



$$\text{Beta}(\theta|\alpha,\beta) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}\theta^{\alpha-1}(1-\theta)^{\beta-1}$$

normalization

$\alpha, \beta > 0$

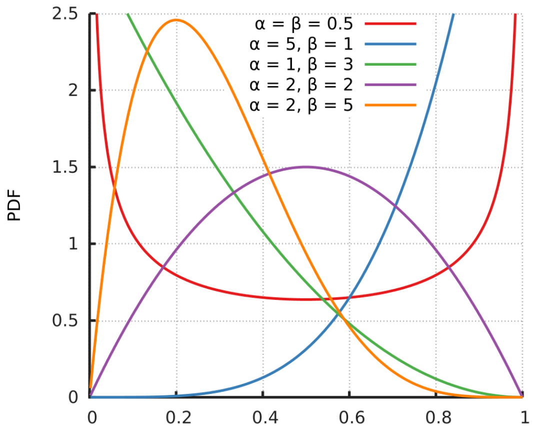
Γ is the generalization of factorial to real number $\Gamma(a+1) = a\Gamma(a)$

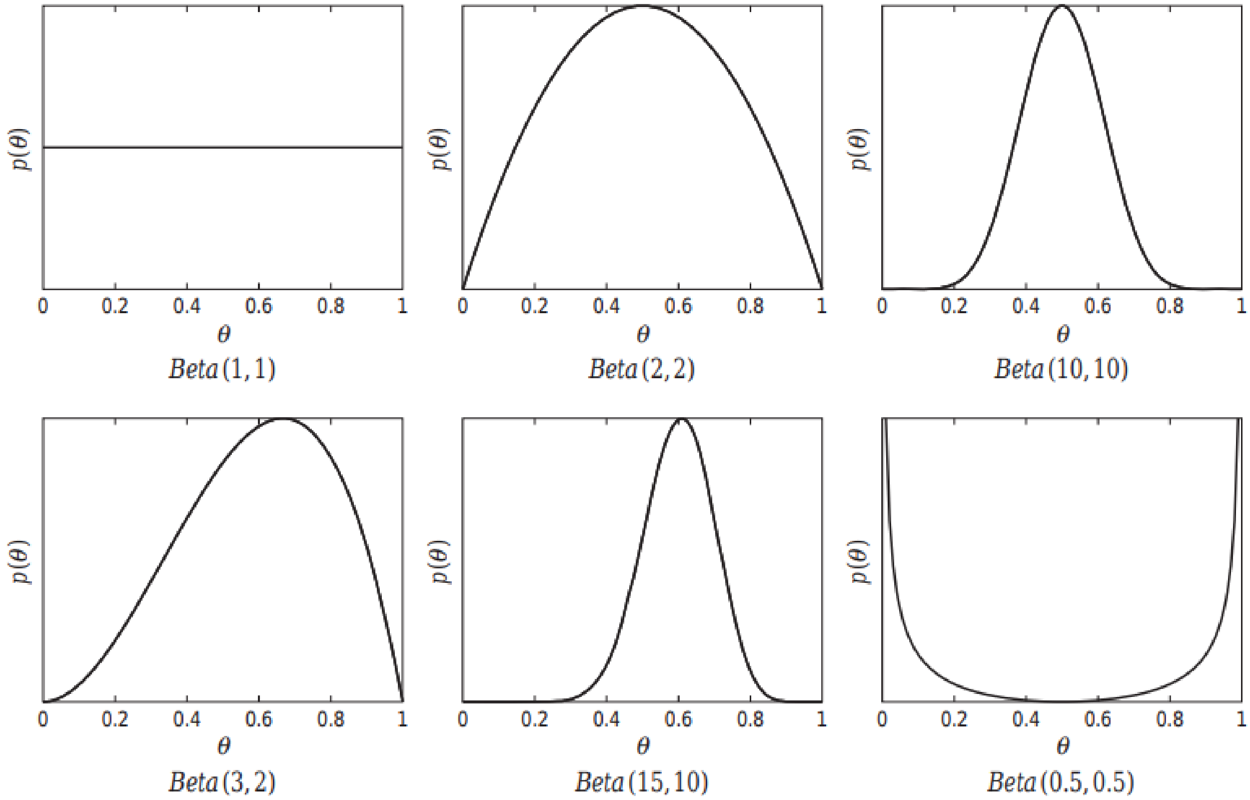
$\text{Beta}(\theta|\alpha=\beta=1)$ is uniform

mean of the distribution is $\mathbb{E}[\theta] = \frac{\alpha}{\alpha+\beta}$

for $\alpha, \beta > 1$ the dist. is unimodal; its mode is $\frac{\alpha-1}{\alpha+\beta-2}$

Beta distribution: more examples





Beta-Bernoulli posterior distribution

how to model probability of heads when we toss a coin N times

proportional

posterior $\propto$ prior $\times$ likelihood

prior $p(\theta) \propto \theta^{\alpha-1}(1-\theta)^{\beta-1}$ $\quad$ $p(\theta) = \text{Beta}(\theta|\alpha, \beta)$

likelihood $p(\mathcal{D}|\theta) = \theta^{N_h}(1-\theta)^{N_t}$ $\quad$ $L(\theta; \mathcal{D}) = \prod \text{Bernoulli}(N_h, N_t|\theta)$

product of Bernoulli likelihoods
equivalent to Binomial likelihood

posterior $p(\theta|\mathcal{D}) \propto \theta^{\alpha+N_h-1}(1-\theta)^{\beta+N_t-1}$ $\quad$ $p(\theta|\mathcal{D}) = \text{Beta}(\theta|\alpha+N_h, \beta+N_t)$

α, β are called *pseudo-counts*

their effect is similar to imaginary observation of heads (α) and tails (β)

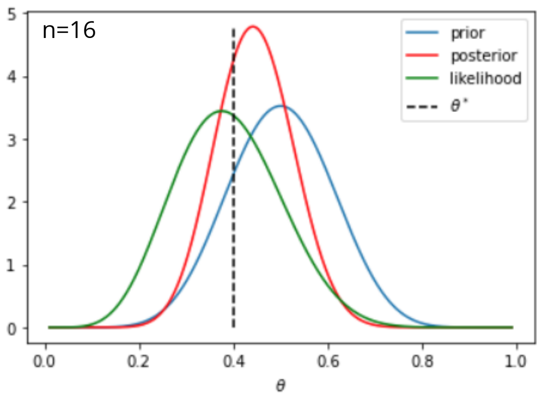
Effect of more data

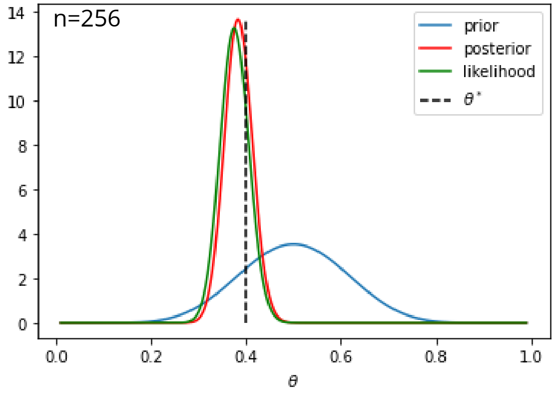
with few observations, prior has a high influence
as we increase the number of observations $N = |\mathcal{D}|$ the effect of prior diminishes
the likelihood term dominates the posterior

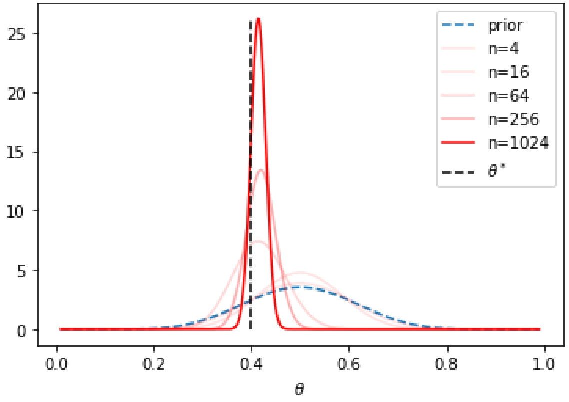
example   prior $\mathrm{Beta}(\theta|10, 10)$

plot of the posterior density with **n** observations

$$p(\theta|\mathcal{D}) \propto \theta^{10+H}(1-\theta)^{10+N-H}$$







Posterior predictive

our goal was to estimate the parameters (θ) so that we can make predictions

what if we use the maximum likelihood estimate for the best parameter, θ^{MLE}, and plug it in the $p(x|\theta)$ to make the prediction?

Example:

if we see four heads in a row, what is the probability of seeing a tail next?

if $\mathcal{D} = \{1, 1, 1, 1\}$, what is θ^{MLE}? 1.0

$$p(0|\theta) = \theta^0(1-\theta)^{(1-0)} = 1-\theta$$

$$\Rightarrow 1 - \theta^{MLE} = 0.0$$

Next, let's use the posterior distribution we learn through Bayesian inference

Posterior predictive

our goal was to estimate the parameters (θ) so that we can make predictions

now we have a (posterior) **distribution** over parameters, $p(\theta|\mathcal{D})$, rather than a single θ^{MLE}

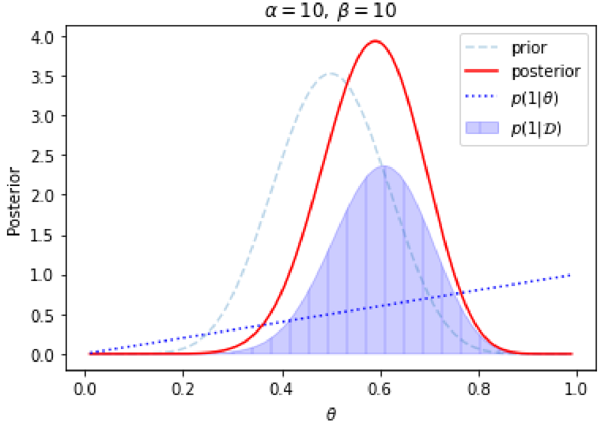
θ^{MLE} only gives a single best guess based on that parameter, $p(x|\theta)$

To make predictions, we calculate the average prediction over all possible values of θ

$$p(x|\mathcal{D}) = \int_\theta p(\theta|\mathcal{D})p(x|\theta)\mathrm{d}\theta$$

for each possible θ, weight the prediction by the posterior probability of that parameter being true

posterior predictive



Posterior predictive

our goal was to estimate the parameters (θ) so that we can make predictions

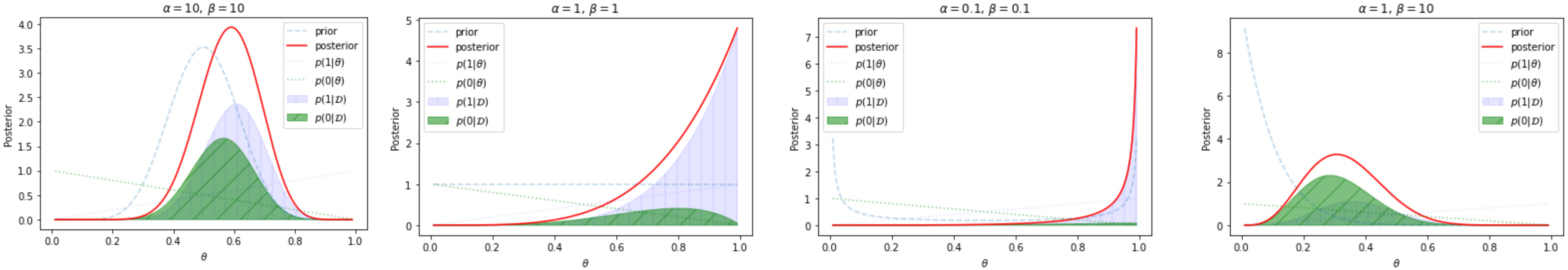
now we have a (posterior) **distribution** over parameters, $p(\theta|\mathcal{D})$

To make predictions, we calculate the average prediction over all possible values of θ

Example

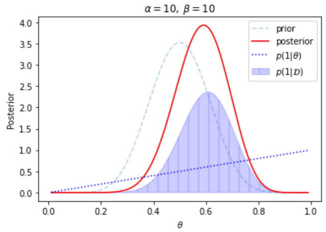
if we see four heads in a row, what is the probability of seeing a tail next?

if $\mathcal{D} = \{1, 1, 1, 1\}$, what is $p(0|\mathcal{D})$? depends on our prior belief



when the strenght of prior gets close to zero the prediction becomes similar to MLE

Posterior predictive for Beta-Bernoulli



start from a Beta prior $p(\theta) = \mathrm{Beta}(\theta|\alpha, \beta)$

observe N_h heads and N_t tails, the posterior is $p(\theta|\mathcal{D}) = \mathrm{Beta}(\theta|\alpha + N_h, \beta + N_t)$

Given this estimate of the parameters from training data,
how can we predict the future?

what is the probability that the next coin flip is head?

marginalize over θ

$$p(x=1|\mathcal{D}) = \int_\theta \mathrm{Bernoulli}(x=1|\theta)\mathrm{Beta}(\theta|\alpha + N_h, \beta + N_t)\mathrm{d}\theta$$

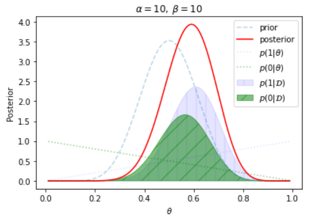
$$= \int_\theta \theta\, \mathrm{Beta}(\theta|\alpha + N_h, \beta + N_t) d\theta = \frac{\alpha + N_h}{\alpha+\beta+N}$$

mean of Beta dist.

Example if we see four heads in a row, what is the probability of seeing a tail next?

if $\mathcal{D} = \{1,1,1,1\}$, what is $p(1|\mathcal{D})$? $\frac{14}{24}$, $p(0|\mathcal{D})$? $\frac{10}{24}$

when we assume the prior is $\mathrm{Beta}(\alpha = 10, \beta = 10)$



compare with prediction of maximum-likelihood: $p(x=1|\mathcal{D}) = \frac{N_h}{N} = 1,\ p(x=1|\mathcal{D}) = 1$

Posterior predictive for Beta-Bernoulli

start from a Beta prior $p(\theta) = \mathrm{Beta}(\theta|\alpha, \beta)$

observe N_h heads and N_t tails, the posterior is $p(\theta|\mathcal{D}) = \mathrm{Beta}(\theta|\alpha + N_h, \beta + N_t)$

Given this estimate of the parameters from training data, how can we predict the future?

$$p(x=1|\mathcal{D}) = \int_\theta \mathrm{Bernoulli}(x=1|\theta)\mathrm{Beta}(\theta|\alpha+N_h, \beta+N_t)\mathrm{d}\theta = \frac{\alpha+N_h}{\alpha+\beta+N}$$

compare with prediction of maximum-likelihood: $p(x=1|\mathcal{D}) = \frac{N_h}{N}$

if we assume a uniform prior, the posterior predictive is $p(x=1|\mathcal{D}) = \frac{N_h+1}{N+2}$

Laplace smoothing

a.k.a. add-one smoothing

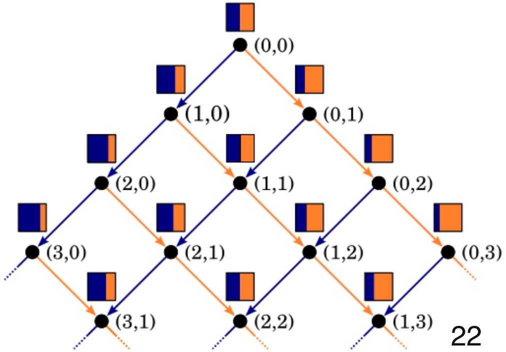
to avoid ruling out unseen cases with zero counts

Example:

sequential Baysian updating

with uniform prior

(N_h, N_t)

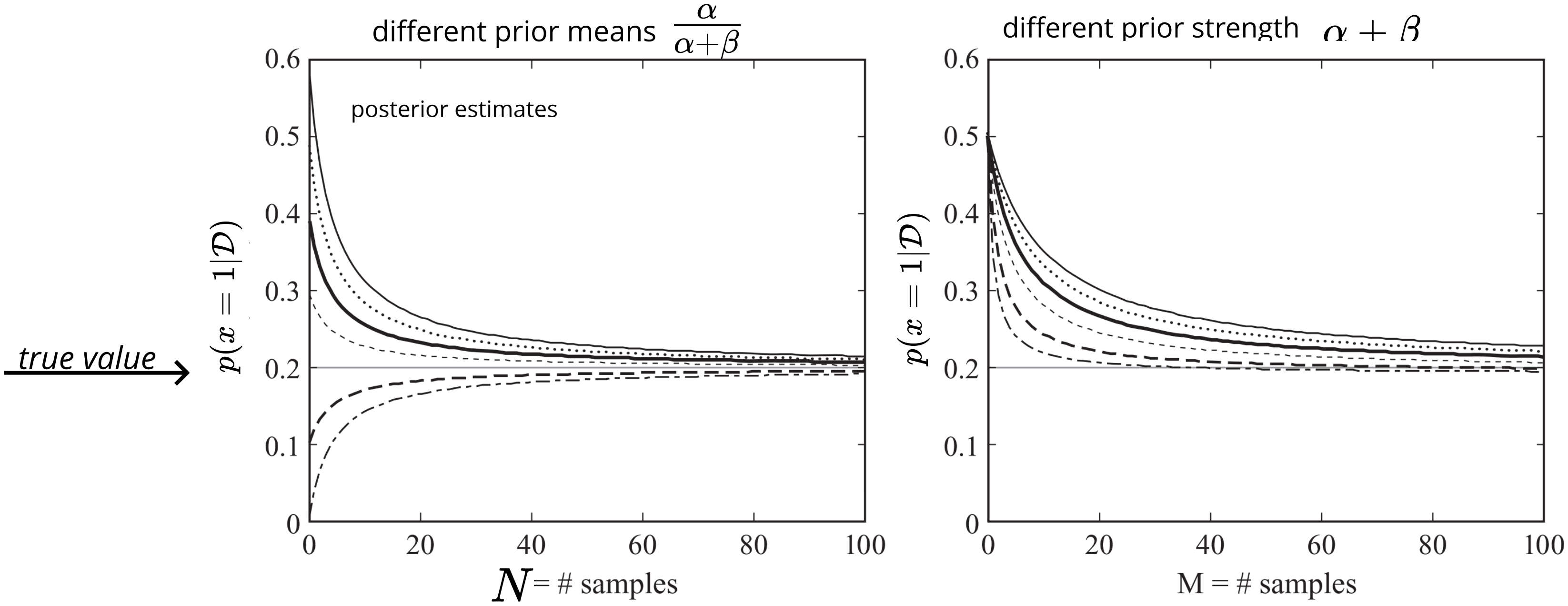


Strength of the prior

with a **strong prior** we need many samples to really change the posterior

for Beta distribution $\alpha + \beta$ decides how strong the prior is: how confident we are in our prior

example as our dataset grows our estimate becomes more accurate



example: PGM book by Koller & Friedman, figure 17.5

Maximum a Posteriori (MAP)

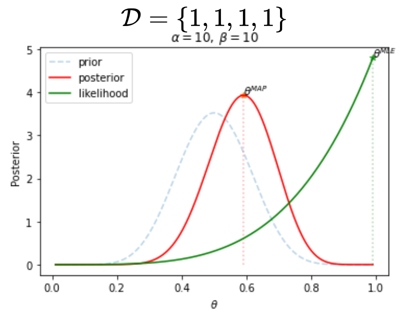
sometimes it is difficult to work with the posterior dist. over parameters

alternative: use the parameter with the highest posterior probability $p(\theta|\mathcal{D})$

MAP estimate $\theta^{MAP} = \arg\max_\theta p(\theta|\mathcal{D}) = \arg\max_\theta p(\theta)p(\mathcal{D}|\theta)$

compare with max-likelihood estimate *(the only difference is in the prior term)*

$$\theta^{MLE} = \arg\max_\theta p(\mathcal{D}|\theta)$$

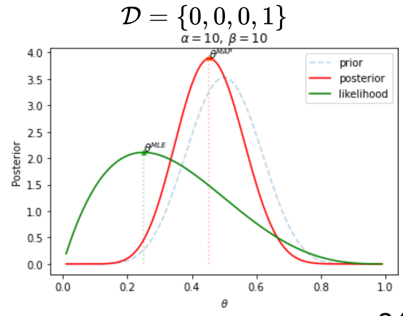


example for the posterior $p(\theta|\mathcal{D}) = \mathrm{Beta}(\theta|\alpha + N_h, \beta + N_t)$

MAP estimate is the **mode** of posterior $\theta^{MAP} = \frac{\alpha+N_h-1}{\alpha+\beta+N_h+N_t-2}$

compare with MLE $\theta^{MLE} = \frac{N_h}{N_h+N_t}$

they are equal for uniform prior $\alpha = \beta = 1$



Categorical distribution

what if we have more than two categories (e.g., loaded dice instead of coin)

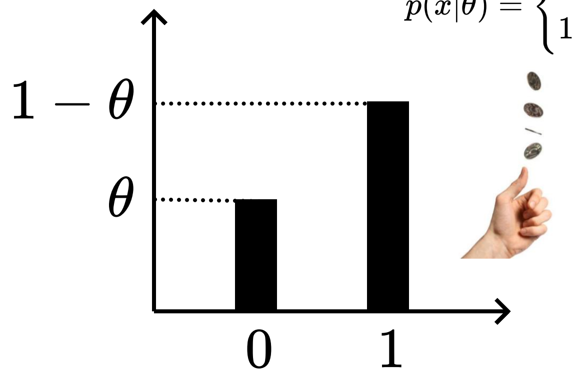
instead of Bernoulli we have multinoulli or **categorical** dist.

$$\text{Bernoulli}(x|\theta) = \theta^{x}(1-\theta)^{(1-x)}$$

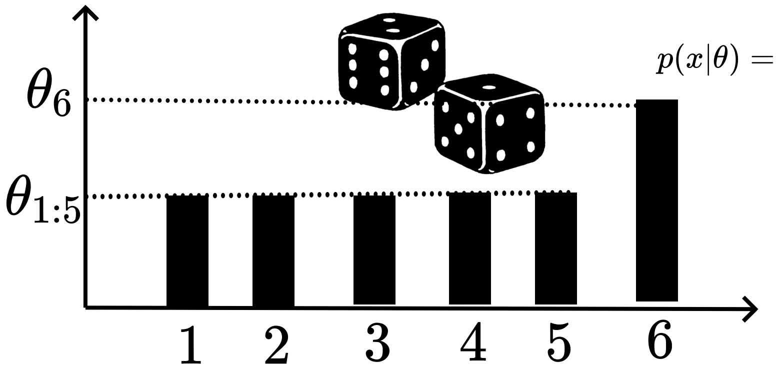
categories

$$\text{Cat}(x|\theta) = \prod_{k=1}^{K} \theta_k^{\mathbb{I}(x=k)}$$

$$p(x|\theta) = \begin{cases} \theta & x = 1 \\ 1-\theta & x = 0 \end{cases}$$



$$p(x|\theta) = \begin{cases} \theta_1 & x = 1 \\ \theta_2 & x = 2 \\ \theta_3 & x = 3 \\ \theta_4 & x = 4 \\ \theta_5 & x = 5 \\ \theta_6 & x = 6 \end{cases}$$



once:	Bernoulli distribution	categorical distribution
n times:	binomial distribution	multinomial distribution

Categorical distribution

what if we have more than two categories (e.g., loaded dice instead of coin)
instead of Bernoulli we have multinoulli or **categorical** dist.

\# categories

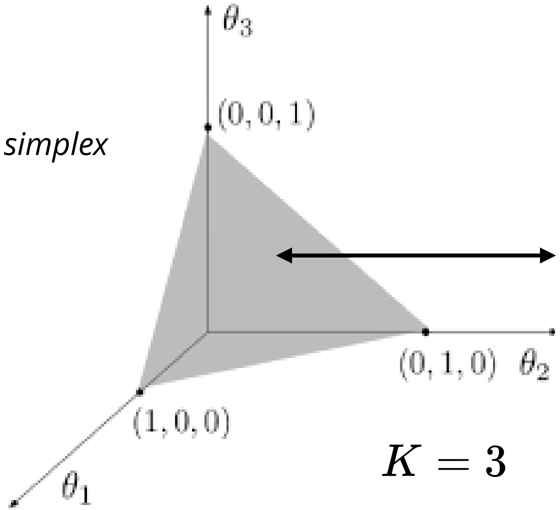
$$\mathrm{Cat}(x|\theta) = \prod_{k=1}^{K} \theta_k^{\mathbb{I}(x=k)}$$

where $\sum_k \theta_k = 1$

$$p(x|\theta) = \begin{cases} \theta_1 & x = 1 \\ \theta_2 & x = 2 \\ \theta_3 & x = 3 \\ \theta_4 & x = 4 \\ \theta_5 & x = 5 \\ \theta_6 & x = 6 \end{cases}$$

$\sum_k^6 \theta_k = 1$

θ *belongs to probability simplex*



$\theta_1 + \theta_2 + \theta_3 = 1$

$K = 3$

Maximum likelihood for categorical dist.

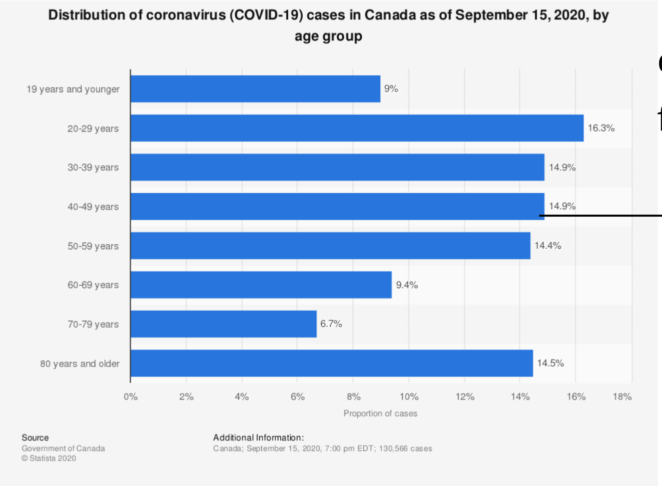
likelihood $p(\mathcal{D}|\theta) = \prod_{x \in \mathcal{D}} \mathrm{Cat}(x|\theta) = \prod_{x \in \mathcal{D}} \prod_{k=1}^{K} \theta_k^{\mathbb{I}(x=k)} = \prod_{k=1}^{K} \theta_k^{N_k}$, $N_k = \sum_{x \in \mathcal{D}} \mathbb{I}(x = k)$

log-likelihood $\ell(\theta, \mathcal{D}) = \sum_{x \in \mathcal{D}} \sum_k \mathbb{I}(x = k) \log(\theta_k) = \sum_k N_k \log(\theta_k)$

we need to solve $\frac{\partial}{\partial \theta_k} \ell(\theta, \mathcal{D}) = 0$ subject to $\sum_k \theta_k = 1$ using Lagrange multipliers

similar to the binary case, max-likelihood estimate is given by data-frequencies $\theta_k{}^{MLE} = \frac{N_k}{N}$

example



categorical distribution with K=8

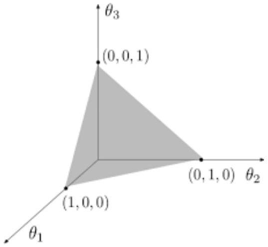
frequencies are max-likelihood parameter estimates

$\theta_5^{MLE} = .149$

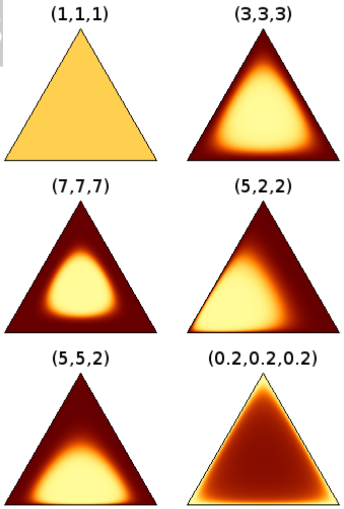
optional

Dirichlet distribution

$\alpha =$



$K = 3$



$\mathrm{Dir}(\theta, [.2, .2, .2])$

is a distribution over the parameters θ of a Categorical dist.

is a generalization of Beta distribution to K categories

this should be a dist. over prob. simplex $\sum_k \theta_k = 1$

$$\mathrm{Dir}(\theta|\alpha) = \frac{\Gamma(\sum_k \alpha_k)}{\prod_k \Gamma(\alpha_k)} \prod_k \theta_k^{\alpha_k - 1}$$

normalization constant

vector of psedo-counts for K categories *(aka concentration parameters)*

$\alpha_k > 0 \ \forall k$

for $\alpha = [1, \ldots, 1]$, we get uniform distribution

for K=2, it reduces to Beta distribution optional

Dirichlet-Categorical conjugate pair

Dirichlet dist. $\mathrm{Dir}(\theta|\alpha) = \frac{\Gamma(\sum_k \alpha_k)}{\prod_k \Gamma(\alpha_k)} \prod_k \theta_k^{\alpha_k - 1}$ is a conjugate prior for Categorical dist. $\mathrm{Cat}(x|\theta) = \prod_k \theta_k^{\mathbb{I}(x=k)}$

posterior $\propto$ prior $\times$ likelihood

prior $p(\theta) = \mathrm{Dir}(\theta|\alpha) \propto \prod_k \theta_k^{\alpha_k - 1}$

likelihood $p(\mathcal{D}|\theta) = \prod_k \theta_k^{N_k}$ we observe $\underbrace{N_1, \ldots, N_K}_{\eta}$ values from each category

posterior $p(\theta|\mathcal{D}) = \mathrm{Dir}(\theta|\alpha + \eta) \propto \prod_k \theta_k^{N_k + \alpha_k - 1}$ again, we add the real counts to pseudo-counts

posterior predictive $p(x = k|\mathcal{D}) = \frac{\alpha_k + N_k}{\sum_{k'} \alpha_{k'} + N_{k'}}$

MAP $\theta_k^{MAP} = \frac{\alpha_k + N_k - 1}{(\sum_{k'} \alpha_{k'} + N_{k'}) - K}$

Summary

in ML we often build a probabilistic model of the data $p(x;\theta)$

learning a good model could mean **maximizing the likelihood** of the data

$\max_\theta \log p(\mathcal{D}|\theta)$ | sometimes closed form solution
for more complex p, we use numerical methods

an alternative is a **Bayesian approach**:

- maintain a **distribution** over model parameters
- can specify our **prior** knowledge $p(\theta)$
- we can use **Bayes rule** to update our belief after new oabservation $p(\theta|\mathcal{D})$
- we can make predictions using **posterior predictive** $p(x|\mathcal{D})$
- can be computationally **expensive** *(not in our examples so far)*

a middle path is **MAP estimate**: $\max_\theta \log p(\mathcal{D}|\theta)p(\theta)$

- models our **prior** belief
- use a single point estimate and picks the model with highest posterior probability