Lecture 2:

Naïve Bayes and Parameter Estimation

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Bayesian Data Analysis and Machine Learning for Physical Sciences

Course Map

Outline

Naïve Bayes

- Idea
- Example

Parameter Estimation

- Idea
- Sharing new Information
- Laplace Approximation and MAP

Naive Bayes, Bayesian Parameter Estimation, MAP

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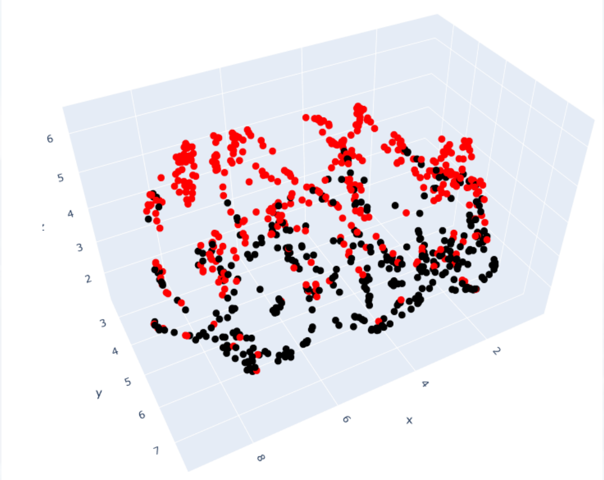
Naive Bayes, Bayesian Parameter Estimation, MAP:

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

UMAP projection
(**toxic**, **non-toxic**)



$\vec{x}$: vector with all model parameters (or features)

Index	molecular_weight	electronegativity	bond_lengths	num_hydrogen_bonds	logP	label
0	413.228	2.94416	3.41991	1	10.4335	Toxic
1	447.945	3.55371	3.66831	7	10.3475	Toxic
2	309.199	3.19761	2.84841	0	7.88825	Non-Toxic
3	382.554	3.8653	3.46237	8	9.59041	Toxic
4	310.904	3.18141	2.87774	6	7.85477	Non-Toxic
5	353.857	3.12105	3.32724	6	8.58887	Non-Toxic

K different classes
(here K = 2)

Naive Bayes, Bayesian Parameter Estimation, MAP:

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

$P(C_k|\vec{x})$: **probability that datapoint belongs to class C_k, given $\vec{x}$**

$P(\vec{x}|C_k)$: **probability that datapoint has features $\vec{x}$, given class C_k**

goal: predicting class C_k of a new datum, given $\vec{x}$

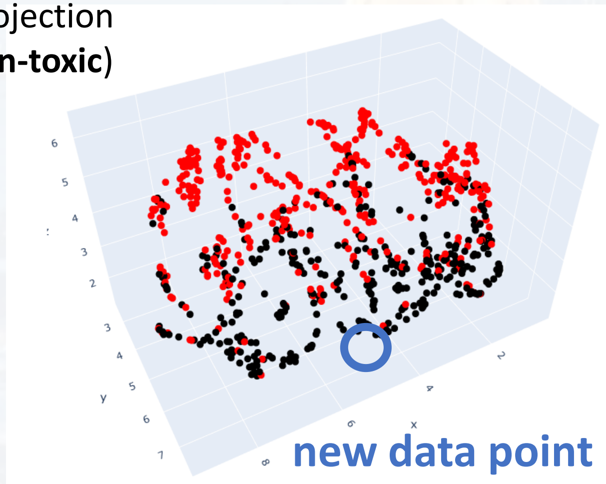
$$P(C_k|\vec{x}) = \frac{\boxed{P(\vec{x}|C_k)}P(C_k)}{P(\vec{x})} = \frac{P(C_k)}{P(\vec{x})}\boxed{\prod_{i=1}^{I} P(x_i|C_k)} \sim P(C_k)\prod_{i=1}^{I} P(x_i|C_k)$$

$$\sum_{k=1}^{K} P(C_k|\vec{x}) = 1$$

Naïve Bayes:

- all features are **mutually independent**
- i. e.: no **correlation** between features
- features can be factorized

UMAP projection
(**toxic**, **non-toxic**)



$$k_{new} = \underset{k}{argmax}\left\{P(C_k)\prod_{i=1}^{I}\boxed{P(x_i|C_k)}\right\}$$

from the training data → supervised learning (see later)

Naive Bayes, Bayesian Parameter Estimation, MAP:

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

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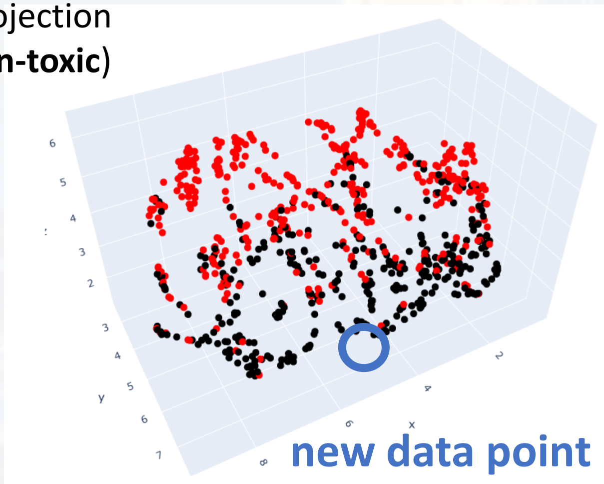
$$\sum_{k=1}^{K} P(C_k|\vec{x}) = 1$$

UMAP projection
(**toxic**, **non-toxic**)



$$k_{new} = \underset{k}{argmax}\left\{P(C_k)\prod_{i=1}^{I}\boxed{P(x_i|C_k)}\right\}$$

from the training data → supervised learning (see later)

different models for $P(x_i|C_k)$

- multinomial
- Gaussian
- …

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Naive Bayes, Bayesian Parameter Estimation, MAP:

from the training data → supervised learning

1) creating the model:

```
my_model = library.method(argument1 = 'arg1', … )
```

2) training the model

```
out = my_model.fit(xtrain, ytrain)
```

3) evaluation

```
ypred = out.predict(xeval)
accur = (ypred == yeval).sum()/len(yeval)
```

4) prediction (actual application)

```
ypred = out.predict(xnew)
```

Naive Bayes, Bayesian Parameter Estimation, MAP:

Python:

```
from sklearn.naive_bayes import *
from sklearn.preprocessing import MinMaxScaler
```

importing methods for naïve bayes

scaling/normalizing data

```
Train = pd.read_csv('molecular_train_gbc_cat.csv')
Test  = pd.read_csv('molecular_test_gbc_cat.csv')

XTrain = Train.drop('label', axis = 1).values
YTrain = Train['label']

XTest = Test.drop('label', axis = 1).values
YTest = Test['label']
```

```
print(YTrain[:10])
```

```
0        Toxic
1        Toxic
2    Non-Toxic
3    Non-Toxic
4    Non-Toxic
5        Toxic
6    Non-Toxic
7    Non-Toxic
8        Toxic
9    Non-Toxic
Name: label, dtype: object
```

Naive Bayes, Bayesian Parameter Estimation, MAP:


```
scaler   = MinMaxScaler(feature_range = (0, 1))
XTrainS  = scaler.fit_transform(XTrain)
```

scaling the data to mean = 0 and std = 1

```
gnb = GaussianNB()
Fit = gnb.fit(XTrainS, YTrain)
```

the actual fit

applying the model to the test data set

```
XTestS  = scaler.transform(XTest)
```

scaling the test set **without** fitting

```
Ypred   = Fit.predict(XTestS)
Probs   = Fit.predict_proba(XTestS)
```

predicting the class C_k and calculating the probabilities

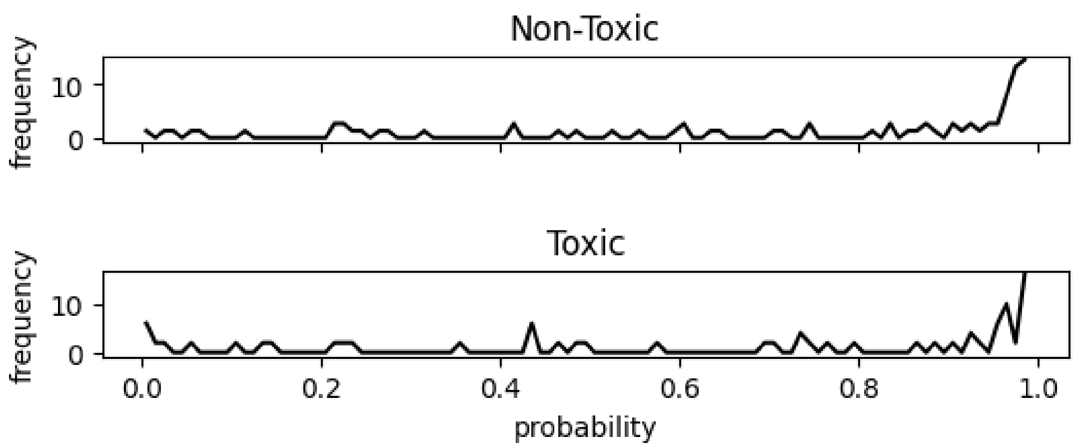
Naive Bayes, Bayesian Parameter Estimation, MAP:

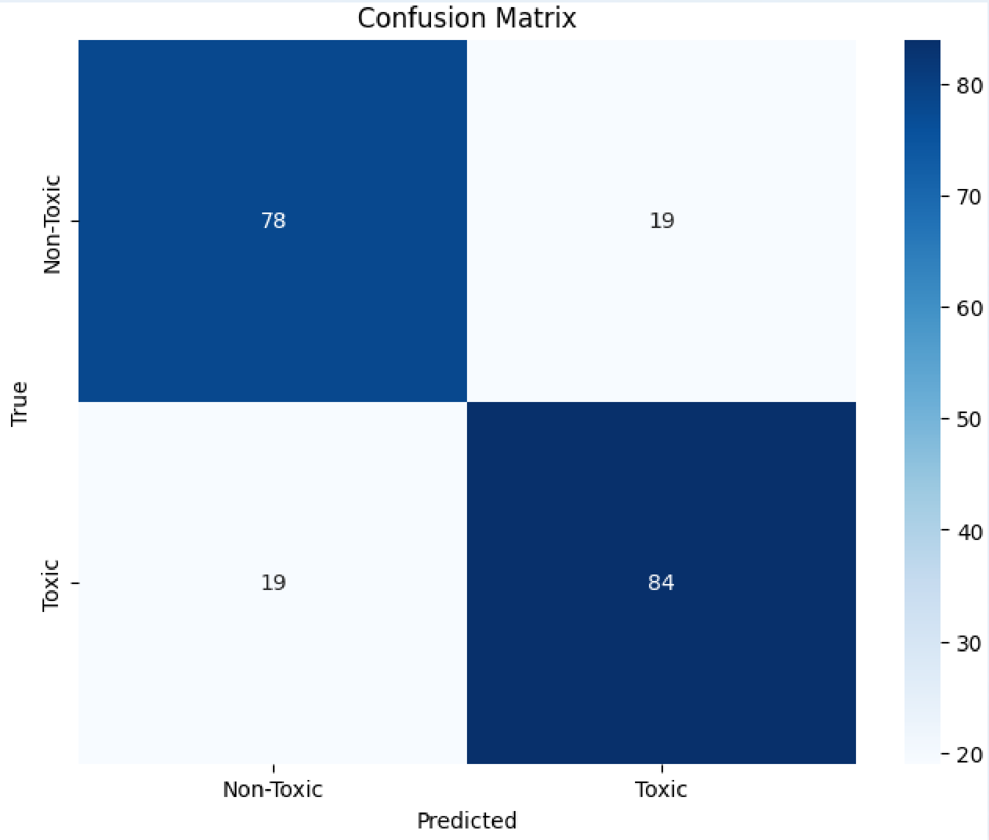
Idea
Example

```
XTestS = scaler.transform(XTest)

Ypred  = Fit.predict(XTestS)
Probs  = Fit.predict_proba(XTestS)
```

evaluation





see
`Walk_Through_NaiveBayes.ipynb`

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Naive Bayes, Bayesian Parameter Estimation, MAP:

D:	data set
q:	parameter
L=L(D|q):	**known** likelihood function

goal: finding the parameter *q* as *P(q|D)* such that
- entropy of *P(q|D)* **decreases** for **increasing** amount of *D*
- we derive the actual *P(q|D)*

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

likelihood function **(eg: binomial)**

$$P(q|D) = \frac{\boxed{P(D|q)}\boxed{P(q)}}{\boxed{P(D)}}$$

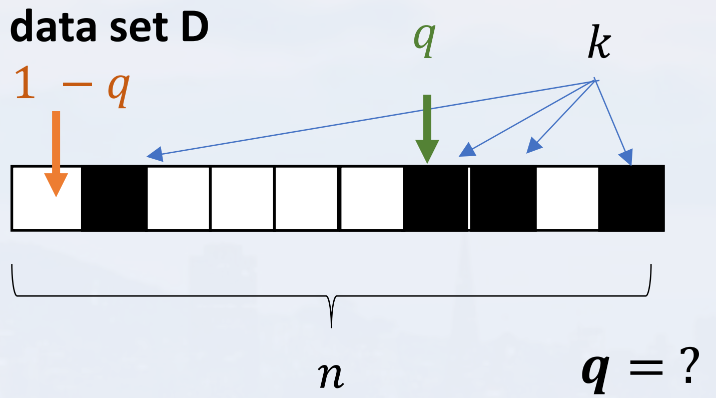
prior

evidence **(const wrt q)**

$$\int P(q|D)\ dq = 1$$

Naive Bayes, Bayesian Parameter Estimation, MAP:

D: data set
q: parameter
$L = L(D|q)$: **known** likelihood function



likelihood function **(eg: binomial)**

$$P(q|D) = \frac{\boxed{P(D|q)}\,\boxed{P(q)}}{\boxed{P(D)}}$$

prior

evidence **(const wrt q)**

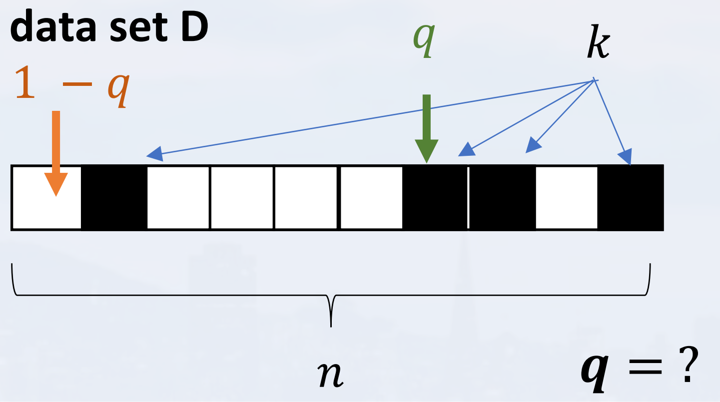
in **this** example: $P(k,n|q) = \binom{n}{k} q^k (1-q)^{n-k}$

$$P(q|D) = \frac{\binom{n}{k}\; q^k (1-q)^{n-k}}{P(D)} P(q)$$

$P(D)$ and $\binom{n}{k}$ are no functions of q

$$\sim q^k (1-q)^{n-k}\; P(q)$$

D:	data set
q:	parameter
$L=L(D\|q)$:	**known** likelihood function



in **this** example: $P(k|n,q) = \binom{n}{k} q^k (1-q)^{n-k}$

$$P(q|D) = \frac{\binom{n}{k} q^k (1-q)^{n-k}}{P(D)} P(q)$$

$$\sim q^k (1-q)^{n-k}\, P(q)$$

max. entropy: $\mathrm{P}(q) = const$
if no prior information about q

$$\sim q^k (1-q)^{n-k}$$

$$\boxed{P(q|D) = \frac{q^k (1-q)^{n-k}}{\int_0^1 q^k (1-q)^{n-k}\, dq}}$$

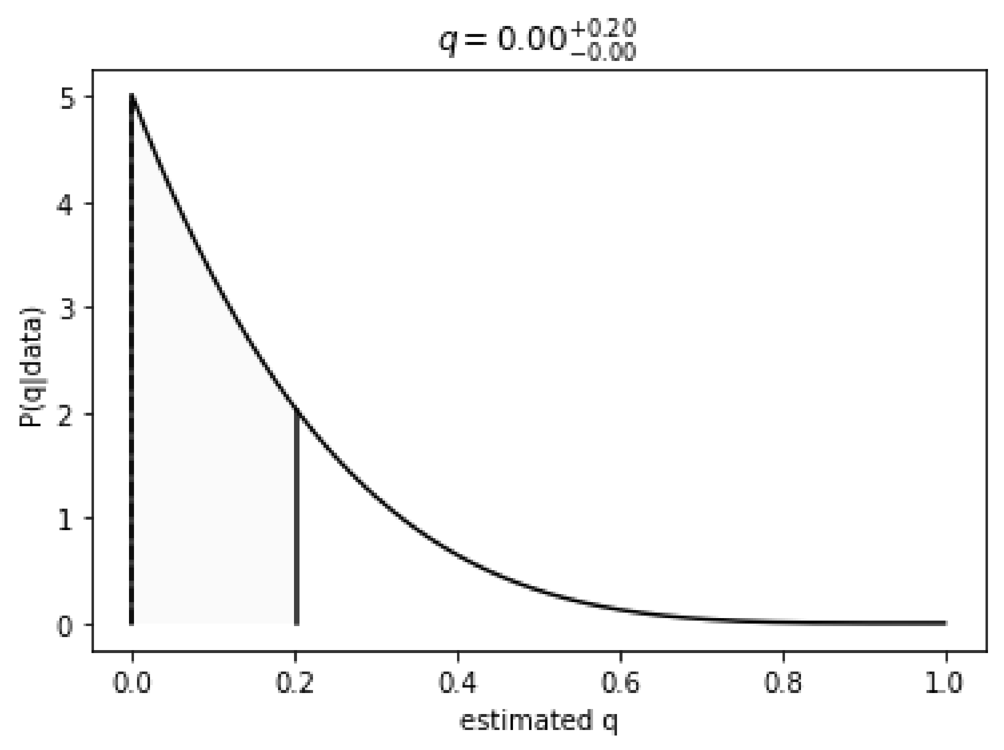
check out `bayesian_bino.py`

```
n1 = 4
k1 = np.random.binomial(n1, 0.25)
```

creating artificial data set
note: in reality ***q*** is unknown!

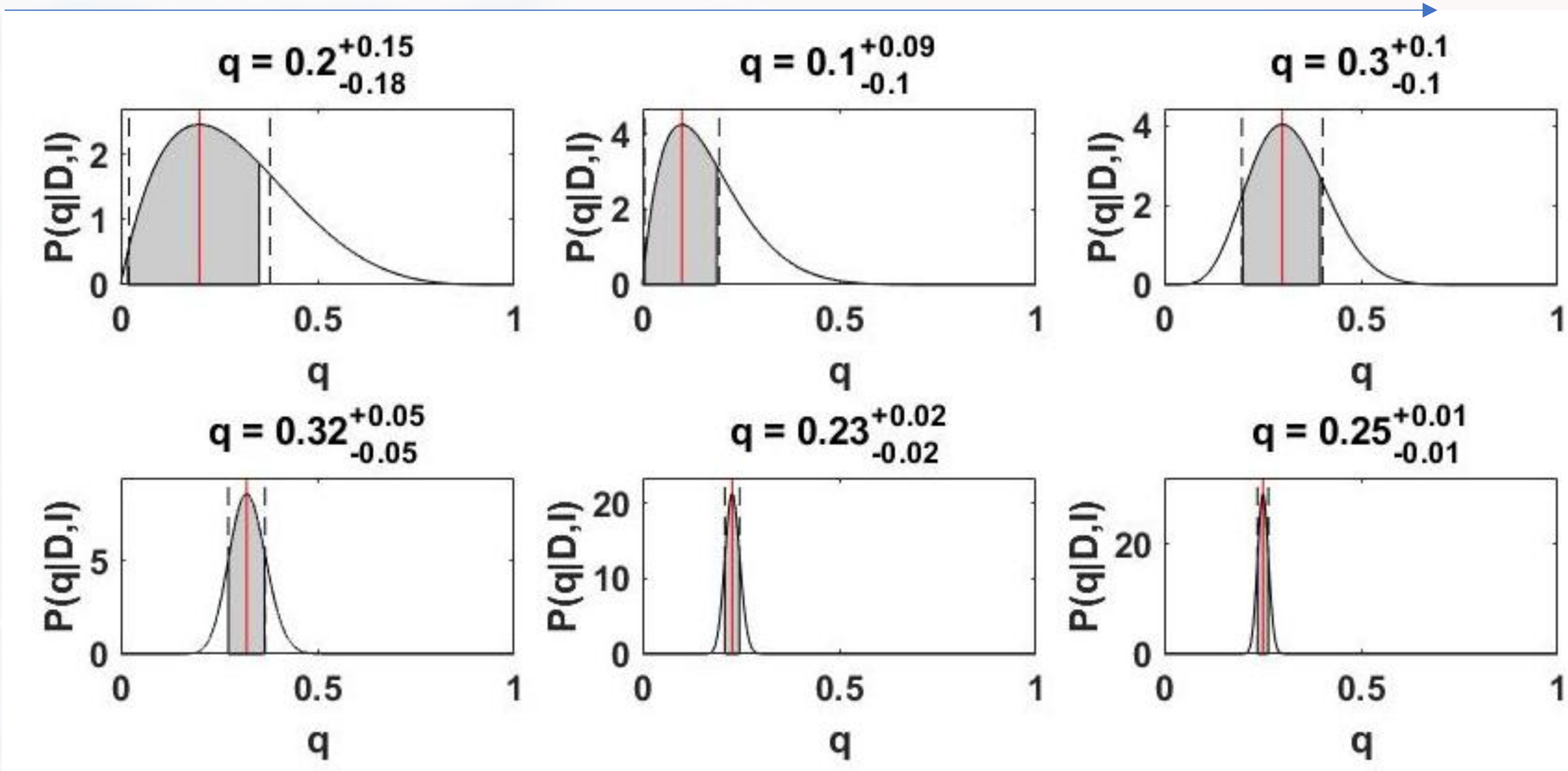
$$P(q|data\ set) = \frac{q^k(1-q)^{n-k}}{\int_0^1 q^k(1-q)^{n-k}\ dq}$$

```
[q1, b, _] = bayesian_bino(n1, k1)
```



check out `bayesian_bino.py`

increasing n

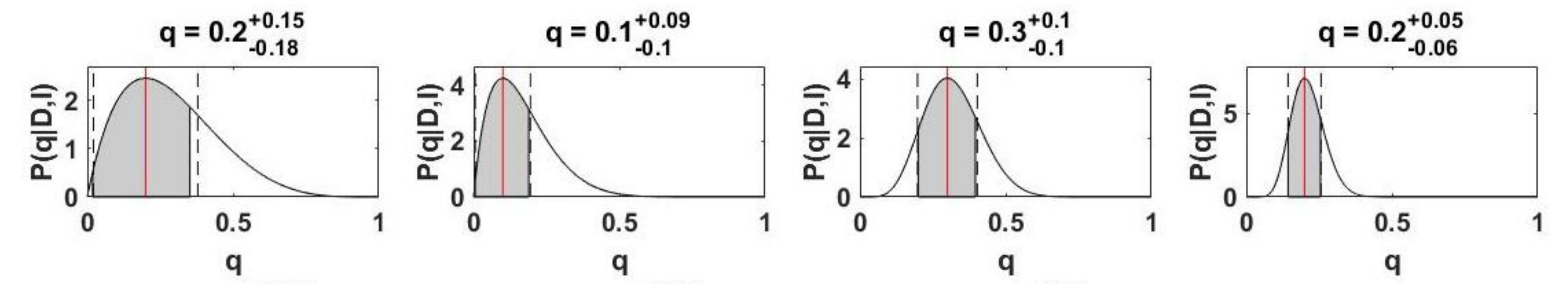


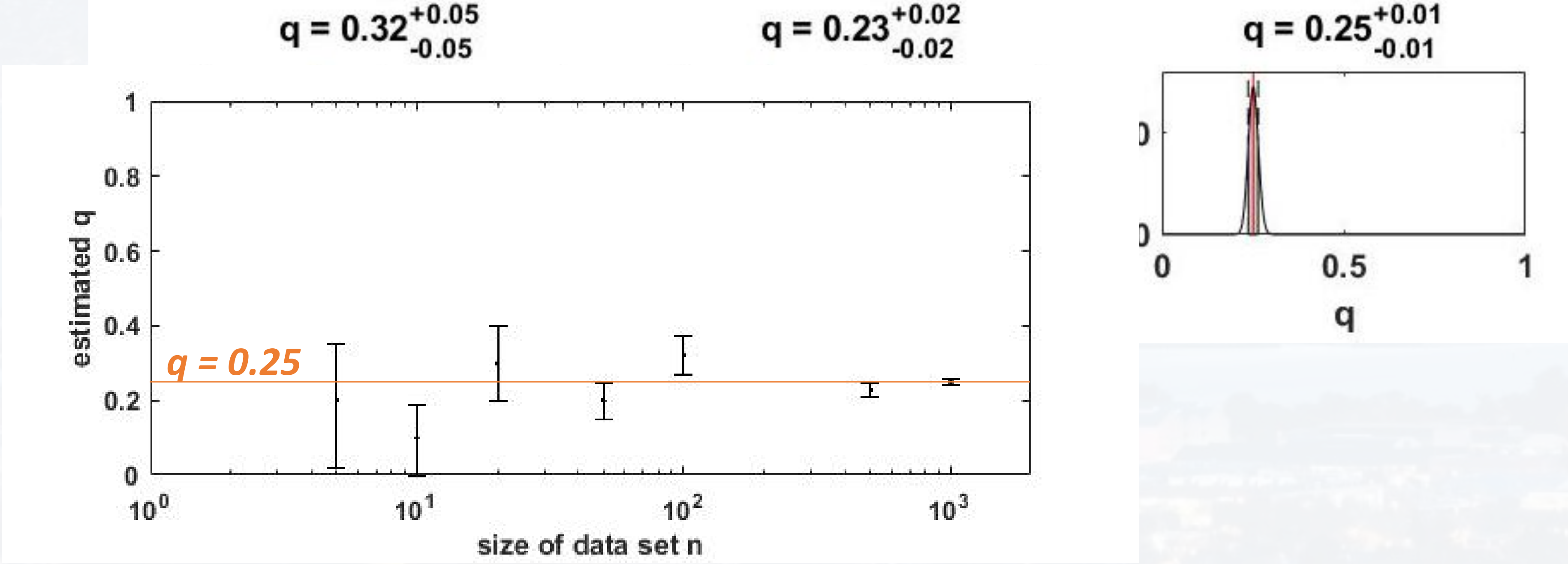
n	estimated q
5	$0.2^{+0.15}_{-0.18}$
10	$0.1^{+0.09}_{-0.1}$
20	$0.3^{+0.1}_{-0.1}$
50	$0.2^{+0.05}_{-0.06}$
100	$0.32^{+0.05}_{-0.05}$
500	$0.23^{+0.02}_{-0.02}$
1,000	$0.25^{+0.01}_{-0.01}$
infinity	0.25

Naive Bayes, Bayesian Parameter Estimation, MAP:

check out `bayesian_bino.py`

increasing n





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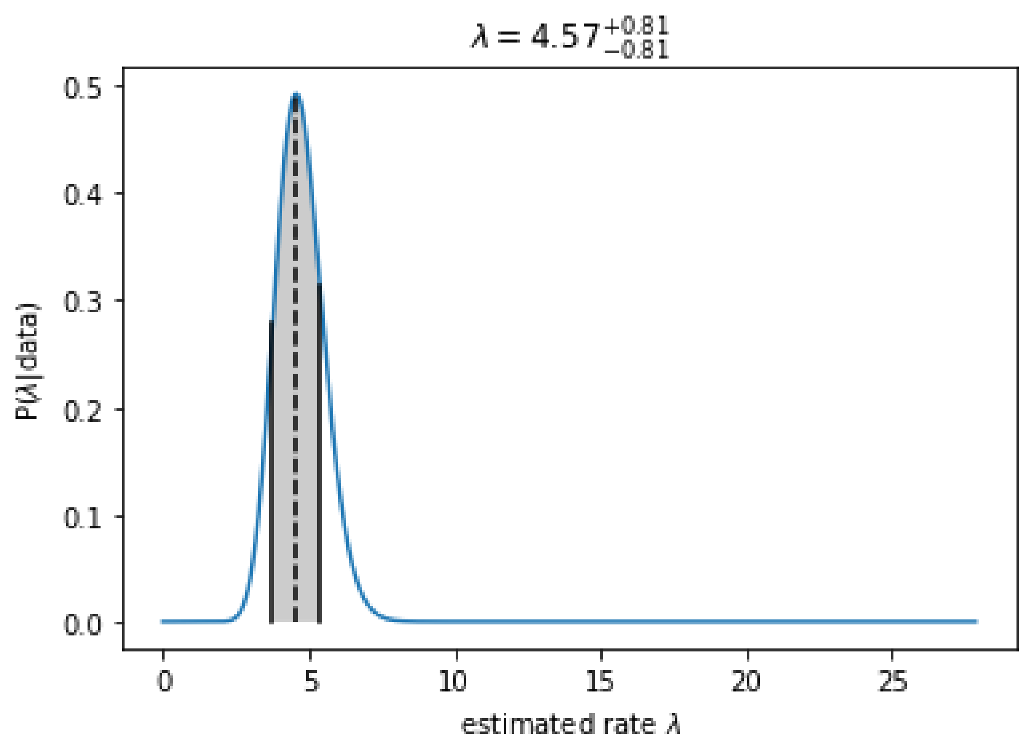
infinity	0.25

Bayesian Parameter Estimation works with **any other pdf**

What is the average number of WhatsUp messages I get every day?

Mon:	5	event	- has no duration
Tue:	7		- is rare
Wed:	1		
Thu:	3		→ Poissonian
Fri:	9		
Sat:	2		
Sun:	5		



likelihood function $P(k|\lambda) = \frac{\lambda^k}{k!} e^{-\lambda}$

$$P(q|D) = \frac{\boxed{P(D|q)}P(q)}{P(D)}$$

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Naive Bayes, Bayesian Parameter Estimation, MAP:

Idea
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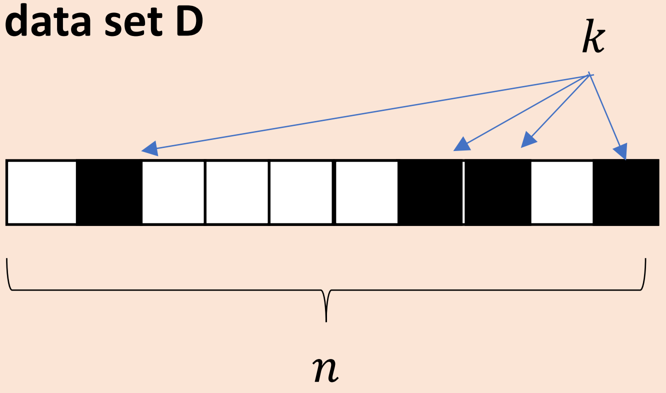
Laplace Approximation and MAP

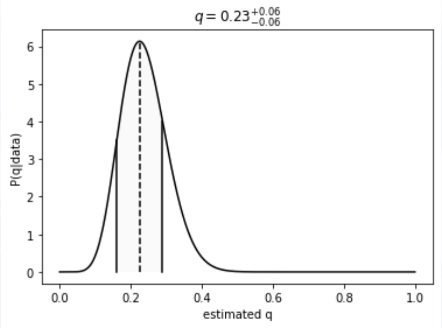
What if there is new data?

data set D

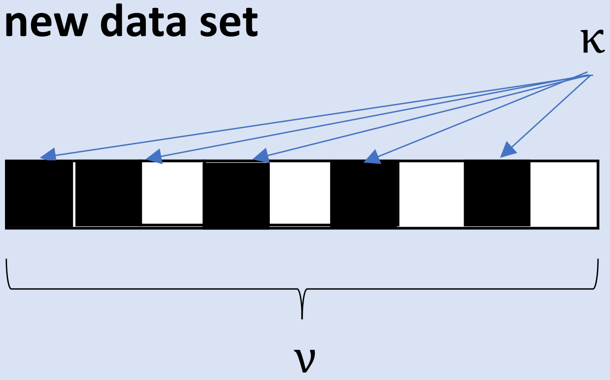


$\cancel{q = ?}$

$$\boxed{P(q|D) = \frac{q^k(1-q)^{n-k}}{\int_0^1 q^k(1-q)^{n-k}\, dq}}$$



new data set



if there **is** prior information ***I*** about q:

$$P(q|new\ data\ set, I) = \frac{P(new\ data\ set|q, I)\ \boldsymbol{P(q, I)}}{P(new\ data\ set)}$$

What if there is new data?

$$P(q|new\ data\ set, I) = \frac{P(new\ data\ set|q, I)\ \boldsymbol{P(q, I)}}{P(new\ data\ set)}$$

$$P(q|D) = \frac{q^k(1-q)^{n-k}}{\int_0^1 q^k(1-q)^{n-k}\ dq}$$

$$= \frac{q^{\kappa}(1-q)^{\nu-\kappa}\ q^k(1-q)^{n-k}}{\int_0^1 q^{\kappa}(1-q)^{\nu-\kappa}\ q^k(1-q)^{n-k}\ dq}$$

$$= \frac{q^{k+\kappa}(1-q)^{\nu-\kappa+n-k}}{\int_0^1 q^{k+\kappa}(1-q)^{\nu-\kappa+n-k}\ dq}$$

often: $\kappa = \alpha - 1$
$\beta = \nu - \kappa - 1$

$$= \frac{q^{k+\alpha-1}(1-q)^{n-k+\beta-1}}{\boxed{\int_0^1 q^{k+\alpha-1}(1-q)^{n-k+\beta-1}\ dq}}$$

Beta function **(conjugate prior of the binomial distribution)**

Naive Bayes, Bayesian Parameter Estimation, MAP:

What if there is new data?

Likelihood $p(x_i\|\theta)$	Model parameters θ	Conjugate prior (and posterior) distribution $p(\theta\|\Theta), p(\theta\|\mathbf{x},\Theta) = p(\theta\|\Theta')$	Prior hyperparameters Θ
Bernoulli	*p* (probability)	Beta	$\alpha,\ \beta \in \mathbb{R}$
Binomial with known number of trials, *m*	*p* (probability)	Beta	$\alpha,\ \beta \in \mathbb{R}$
Negative binomial with known failure number, *r*	*p* (probability)	Beta	$\alpha,\ \beta \in \mathbb{R}$
Poisson	*λ* (rate)	Gamma	$k,\ \theta \in \mathbb{R}$ $\alpha,\ \beta$[note 4]
Categorical	***p*** (probability vector), *k* (number of categories; i.e., size of ***p***)	Dirichlet	$\boldsymbol{\alpha} \in \mathbb{R}^k$
Multinomial	***p*** (probability vector), *k* (number of categories; i.e., size of	Dirichlet	$\boldsymbol{\alpha} \in \mathbb{R}^k$

see example "Model Selection" about discrete signals

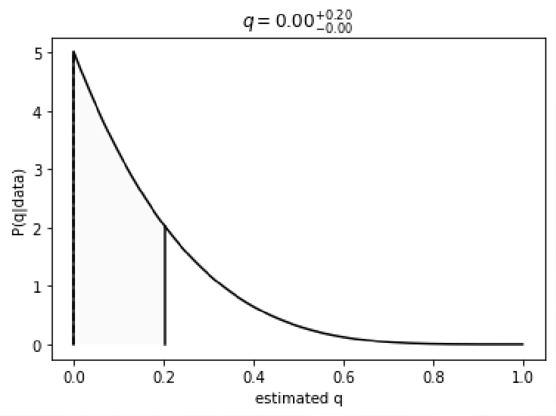
What if there is new data?

$$P(q|new\ data\ set, I) = \frac{q^{\kappa}(1-q)^{\nu-\kappa}\ q^{k}(1-q)^{n-k}}{\int_0^1 q^{\kappa}(1-q)^{\nu-\kappa}\ q^{k}(1-q)^{n-k}\ dq}$$

Idea
Sharing new Information
Laplace Approximation and MAP

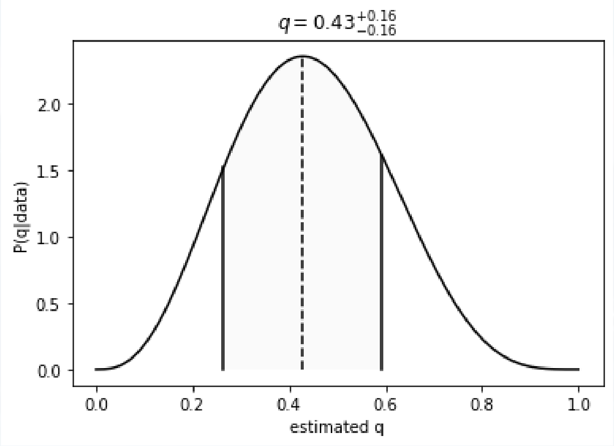
```
n1 = 4
k1 = np.random.binomial(n1, q = 0.2)
[_, _, Prior] = bayesian_bino(n1, k1)
```

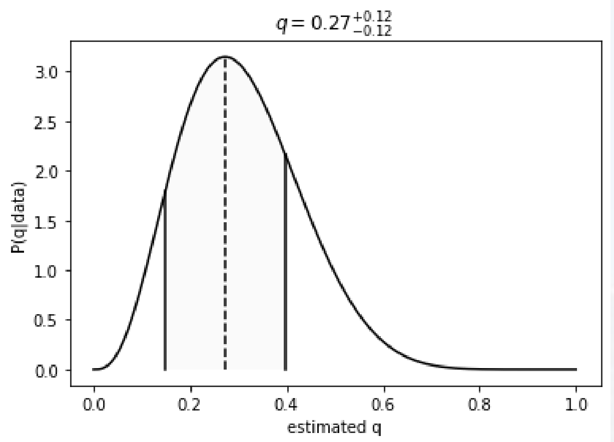
```
n2 = 7
k2 = np.random.binomial(n2, q = 0.2)
[_, _, _] = bayesian_bino(n2, k2)
```



$$P(q, I) = \frac{q^{k}(1-q)^{n-k}}{\int_0^1 q^{k}(1-q)^{n-k}\ dq}$$

```
[_ , _, _] = bayesian_bino(n2, k2, Prior = Prior)
```



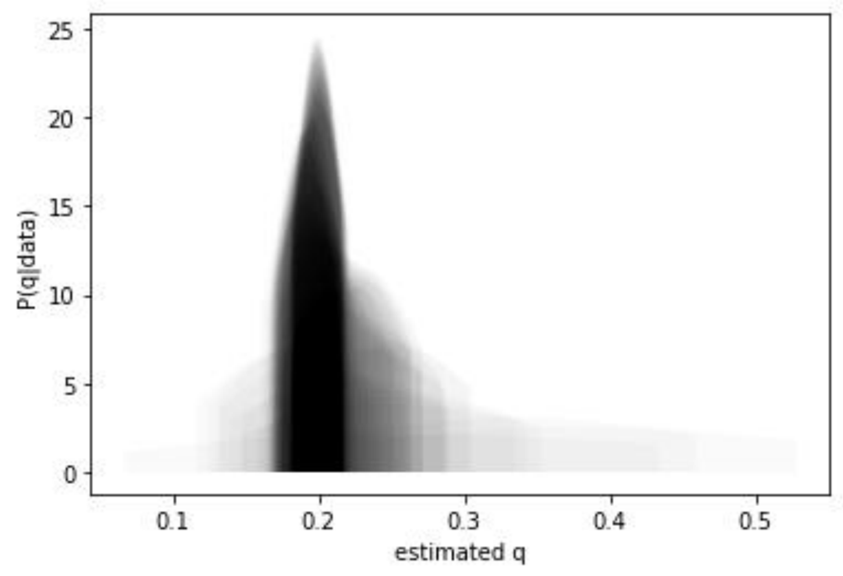


Naive Bayes, Bayesian Parameter Estimation, MAP:

What if there is new data?

$$P(q|new\ data\ set, I) = \frac{q^{\kappa}(1-q)^{\nu-\kappa}\ \ q^{k}(1-q)^{n-k}}{\int_0^1 q^{\kappa}(1-q)^{\nu-\kappa}\ \ q^{k}(1-q)^{n-k}\ \ dq}$$

The **posterior** from the **previous** experiment is the **prior** of the **next** experiment



→ we become more certain about the model parameters
→ learning!

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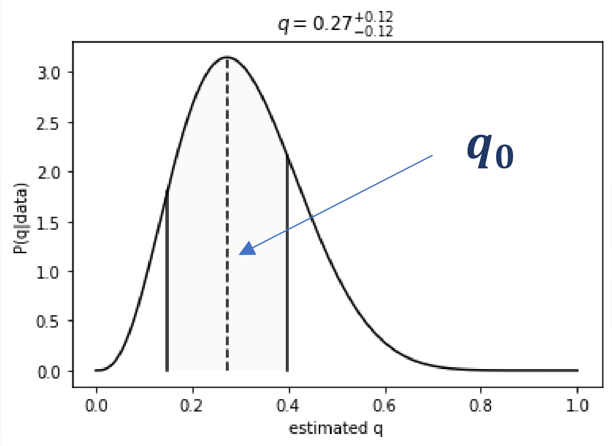
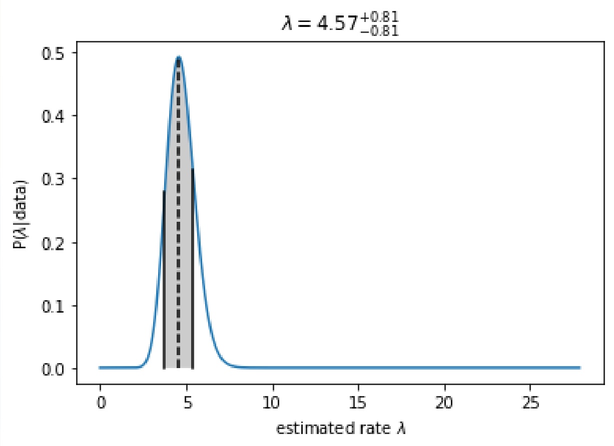




D:	**data set**
q:	**parameter**
q_0:	**q for which *P(q|D)* reaches max**

for large *D*, the posterior seems to approach a Gaussian

Laplace approximation: 2nd order Taylor approximation of $ln[P(q|D)]$

$$L = ln[P(q|D)] \approx ln[P(q_0|D)] + \underbrace{\frac{d}{dq} ln[P(q|D)]|_{q=q_0}(q - q_0)}_{\textbf{= 0 (evaluated at maximum)}} + \frac{1}{2}\frac{d^2}{dq^2} ln[P(q|D)]|_{q=q_0}(q - q_0)^2$$

$$P(q|D) \approx P(q_0|D) \exp\left\{\frac{1}{2}\frac{d^2}{dq^2} ln[P(q|D)]|_{q=q_0}(q - q_0)^2\right\}$$

Naive Bayes, Bayesian Parameter Estimation, MAP:

$$P(q|D) \approx P(q_0|D)\exp\left\{\frac{1}{2}\frac{d^2}{dq^2} ln[P(q|D)]|_{q=q_0}(q - q_0)^2\right\}$$

$$\mu = q_0$$

$$\sigma^2 = \frac{1}{\frac{d^2}{dq^2} ln[P(q|D)]|_{q=q_0}}$$

D:	**data set**
q:	**parameter**
q_0:	**q for which *P(q/D)* reaches max**

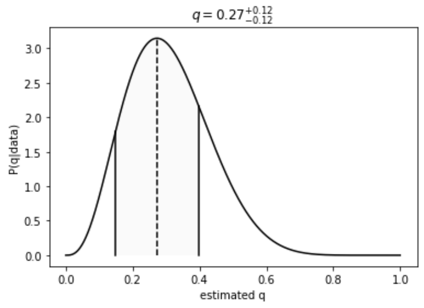
for **example**, if $P(D|q)$ is a **binomial** distribution:

$$P(q|D) \sim q^k(1-q)^{n-k}$$

$$\left.\begin{array}{l} q_0 = \frac{k}{n} \\ \sigma = \sqrt{\frac{q_0(1-q_0)}{n}} \end{array}\right\} \quad q = \frac{k}{n} \pm \sqrt{\frac{q_0(1-q_0)}{n}}$$

for large n:
approaches frequentist results
(like maximum likelihood estimation, MLE)

$$P(q|D) \approx P(q_0|D)\exp\left\{\frac{1}{2}\frac{d^2}{dq^2}ln[P(q|D)]|_{q=q_0}(q-q_0)^2\right\}$$



D:	**data set**
q:	**parameter**
q_0:	**q for which $P(q/D)$ reaches max**

note:

- using Bayesian Parameter Estimation, we find the **pdf** $P(q|D)$ of the desired parameter q
- the $P(q|D)$ is flat for small D, but becomes more defined for large D → **reflects the exact amount of information with have about *q***
- **integration** around the maximum of $P(q|D)$ provides **confidence intervals** about q
- for large D, we can apply the **Laplace approximation**, which is equal to the frequentist result
- finding $q_0 = \underset{q}{argmax}\{P(q|D)\}$, is called **maximum a posteriori (MAP)** estimate
- maximum likelihood estimation, MLE (see later): $q_0 = \underset{q}{argmax}\{P(D|q)\}$,

Thank you very much for your attention!