

DATA221 Intro Machine Learning

04 Gaussians

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THE UNIVERSITY OF
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Plan

- Least Squares Adjustment (demo)
- Definitions
- Anatomy of the Gaussian distribution
- Fitting one-dimensional Gaussian mixture distribution

Problems 1 and 2 on homework present different types of attacks on inference:

- Q2: Direct

You have a **likelihood for the data** given the parameters

$$P(x | \lambda)$$

$$P(\text{childHeight} | \mu, \sigma)$$

Likelihood sum is over the data points; one term for each observation

- Q1: Indirect

You have a likelihood for a **statistic based on the data** given the parameters (for instance a histogram or a moment)

$$P(z | \lambda) =$$

$$\text{Poisson}(\int_{Z_i}^{Z_{i+1}} \text{Exp}'l(x; \lambda) dx * N_{total})$$

Likelihood sum is over the histogram bins. One point for each bin.

What are you summing over? Is it data points or bins?

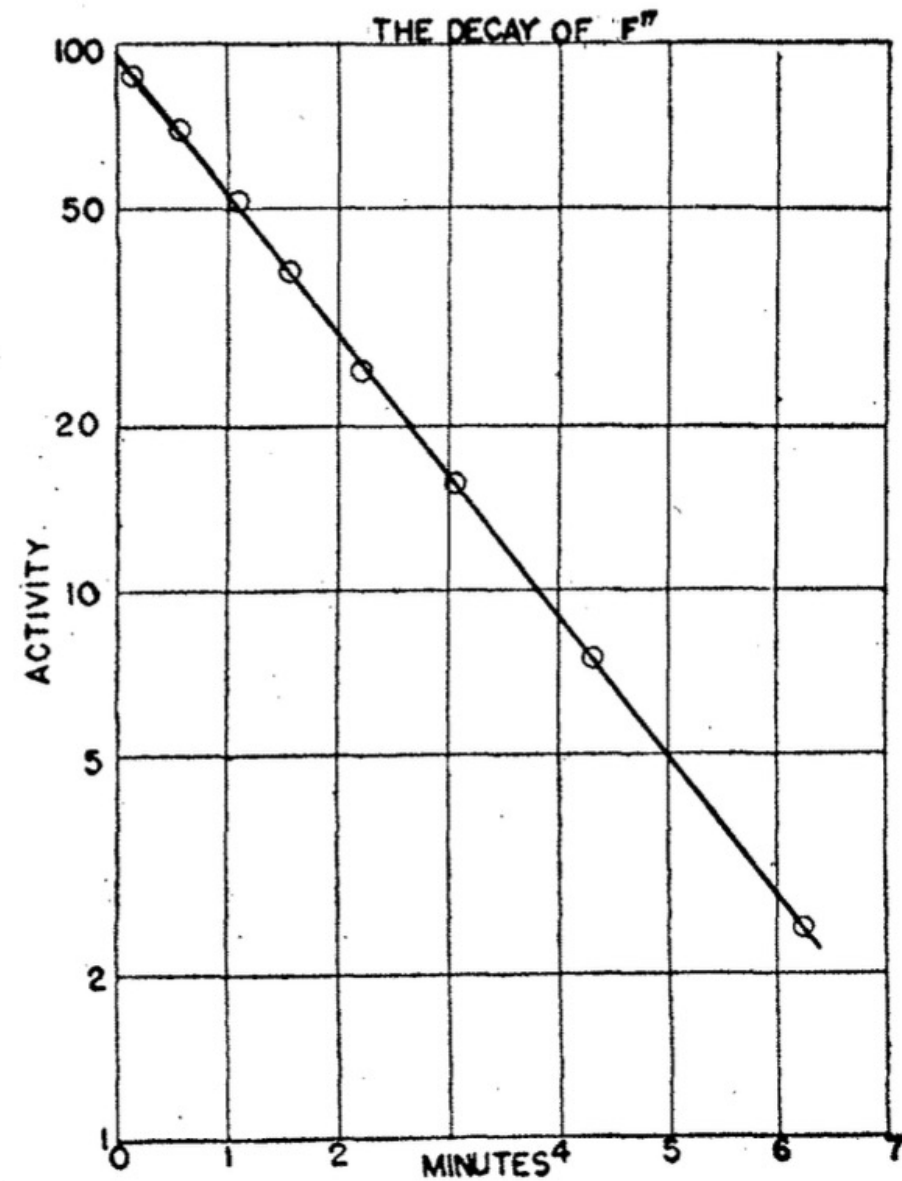
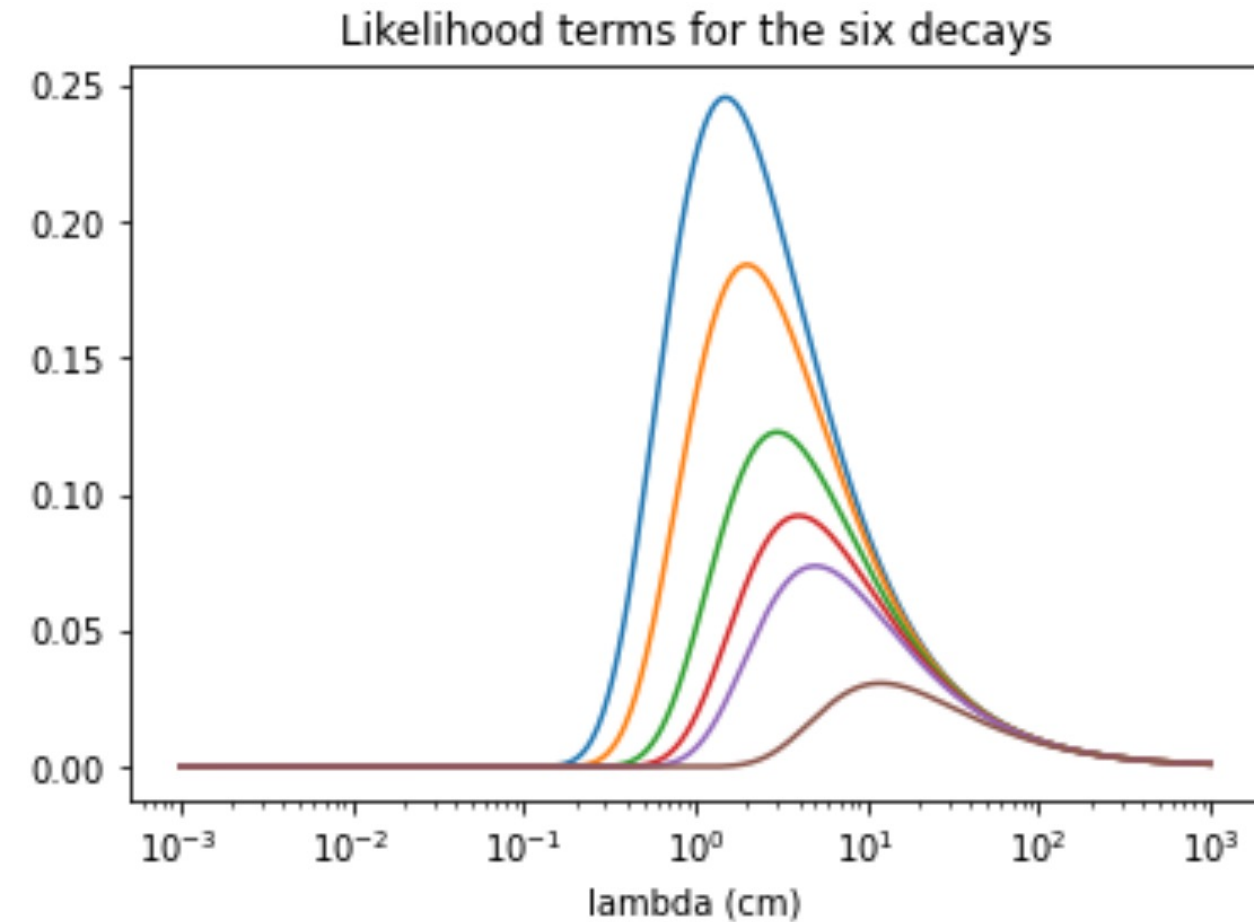


FIG. 1. A logarithmic plot of the decay of F^{17} ; the half-life of this substance is found to be 1.16 minutes.

The simplest case of parameterization ambiguity: distribution of a single parameter

MacKay Ch3:

$$P(x | \lambda) = \begin{cases} \frac{1}{\lambda} e^{-x/\lambda} / Z(\lambda) & 1 < x < 20 \\ 0 & \text{otherwise} \end{cases}$$

Wikipedia “Exponential distribution”

$$\lambda e^{-\lambda x}$$

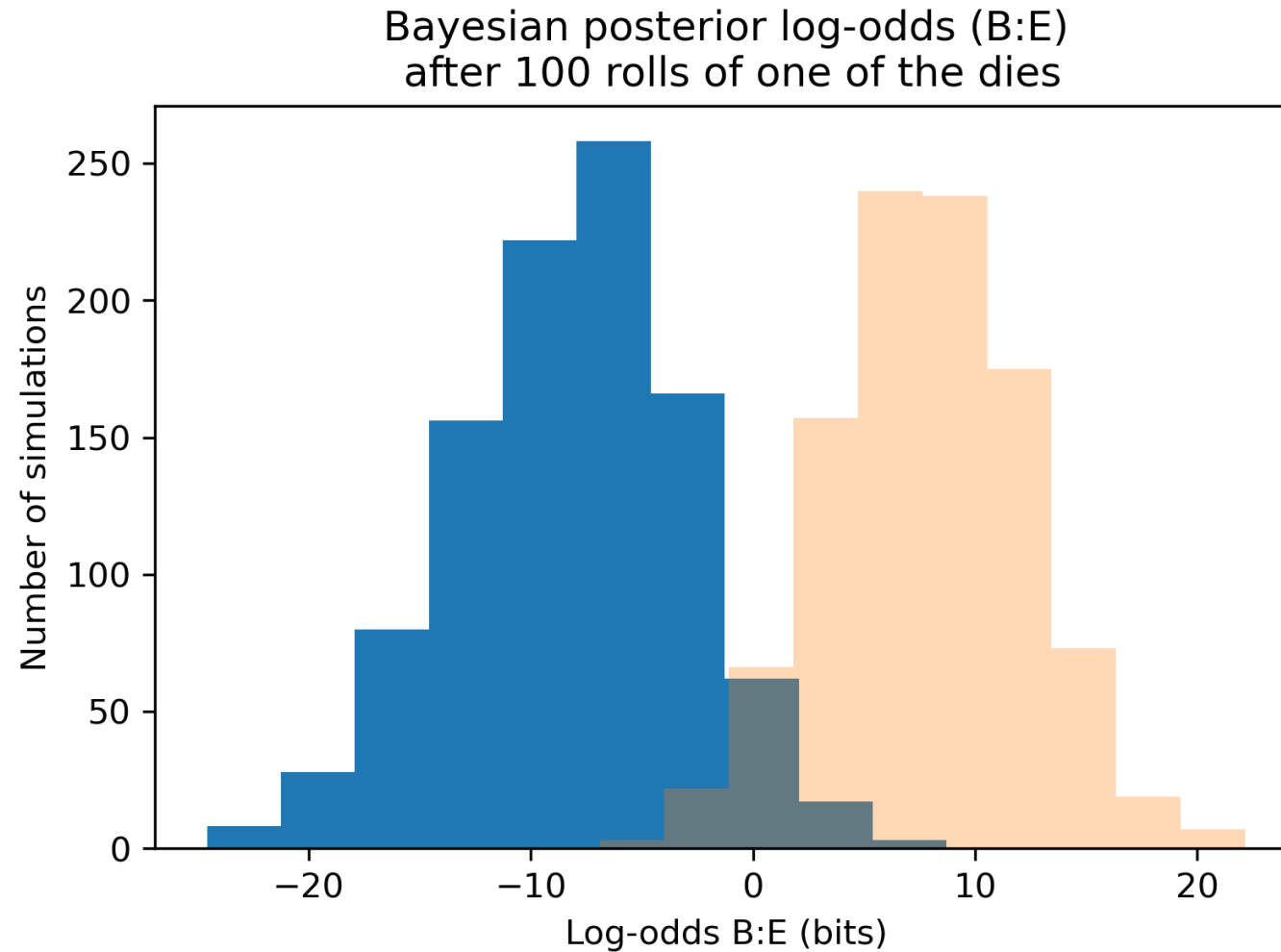
decay rate

Wikipedia “Alternate parameterization”

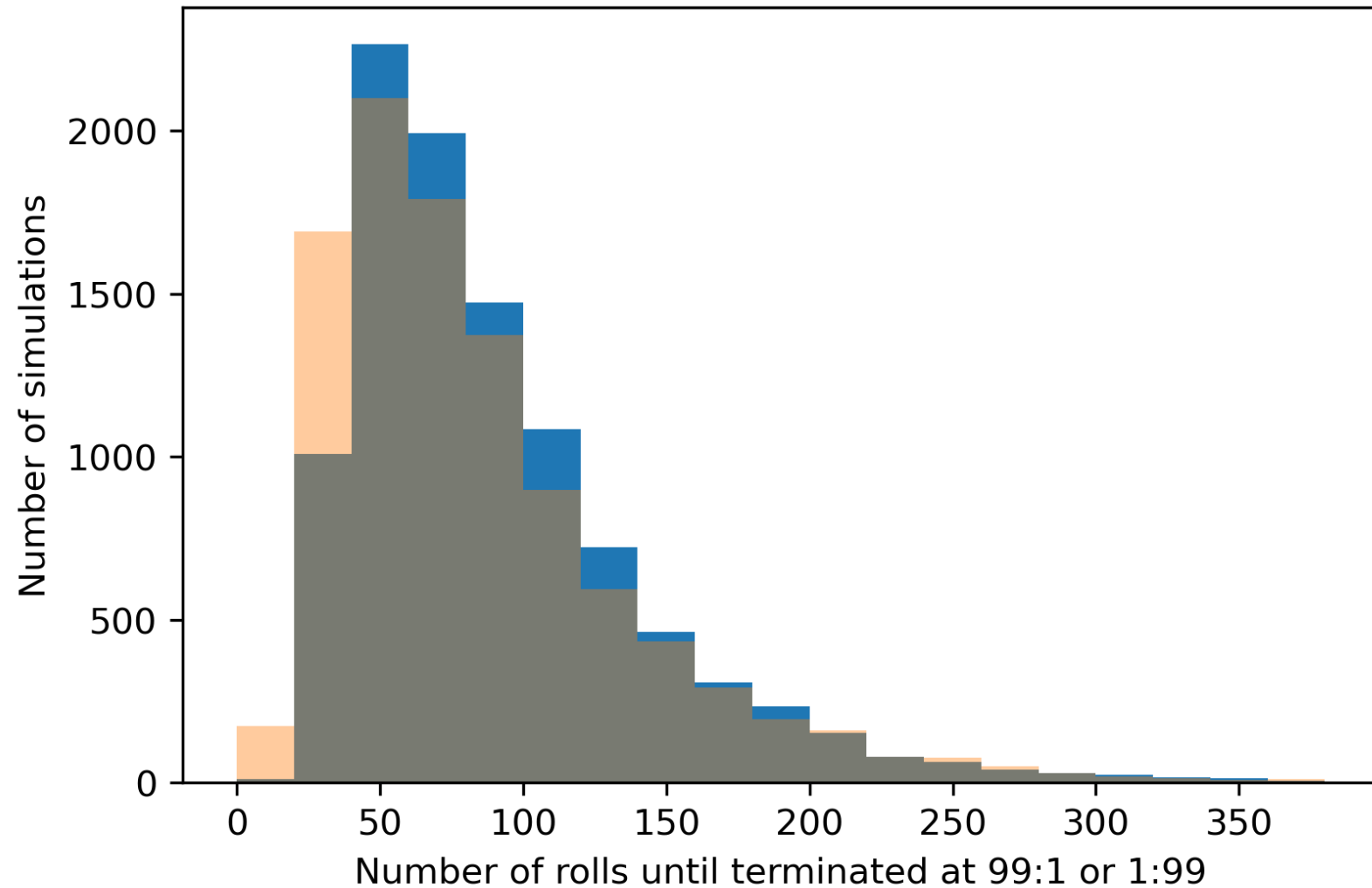
$$\frac{1}{\beta} e^{-x/\beta}$$

decay length /
decay time

Dice problem



Dice problem



Inferring parameters

θ : value of model parameter

Y : training data

$$P(\theta | Y) = P(Y | \theta) P(\theta) / P(Y)$$

↑
Distribution
to help me
find the
parameter
value

posterior

↑
This is the
likelihood

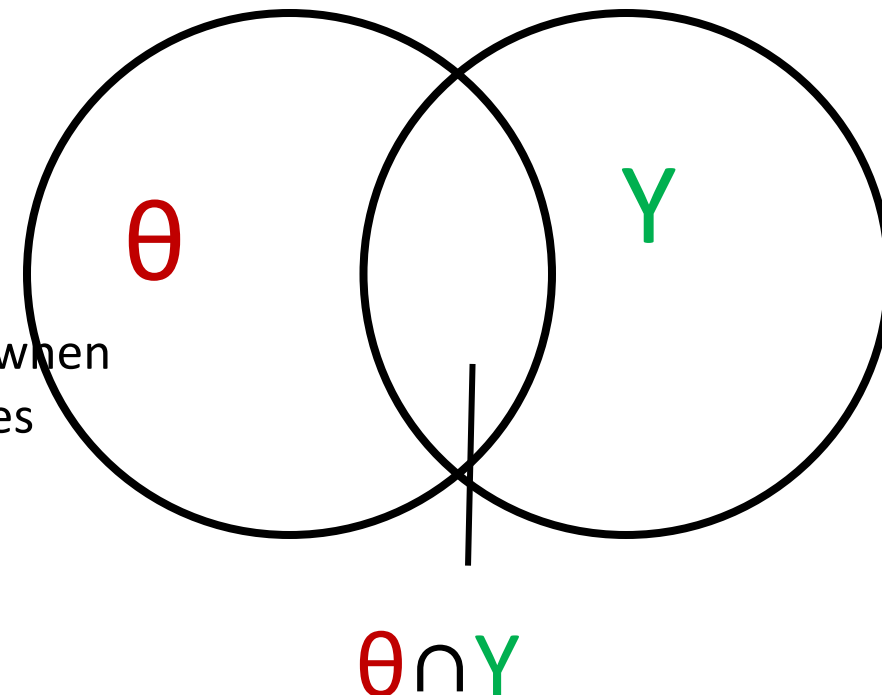
likelihood

↑
Prior
distribution
for
parameter

prior

↑
Equivalent to
“normalization
constant” worry when
multiple outcomes

evidence



Inferring parameters

θ : value of model parameter

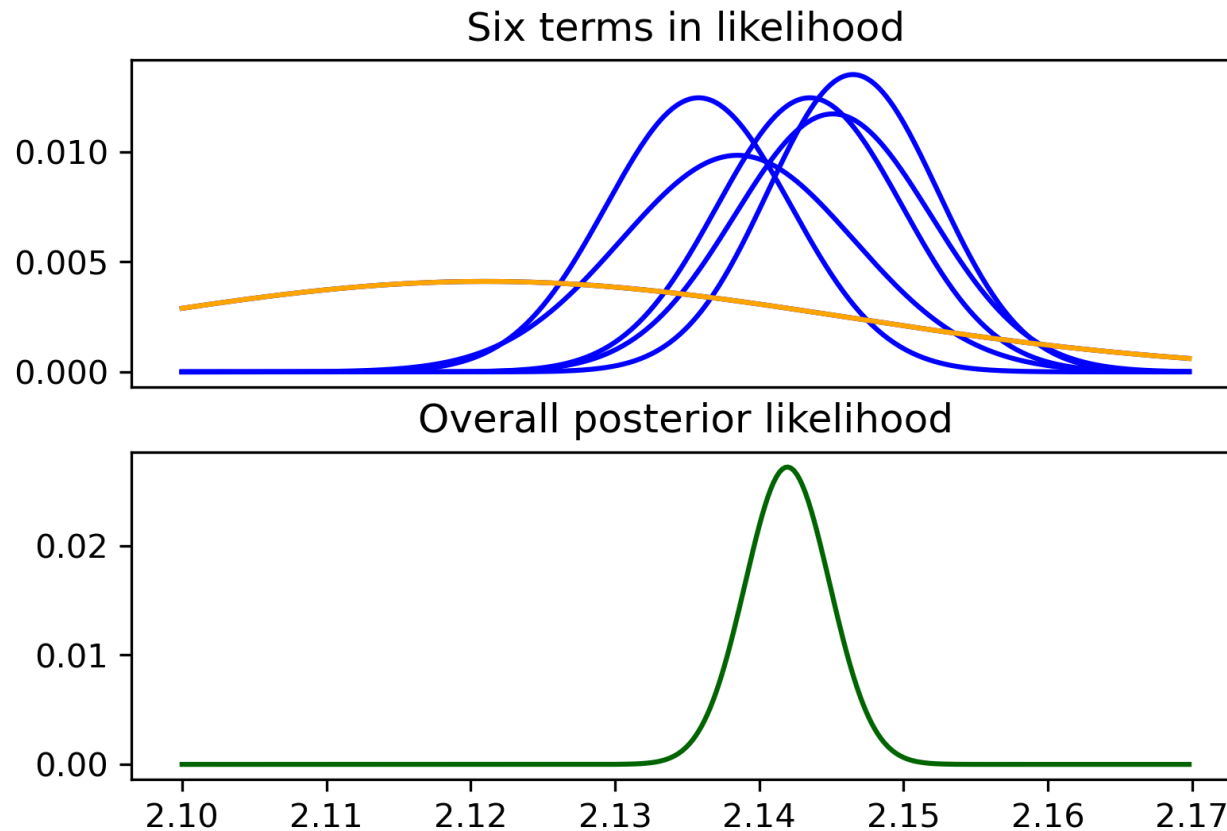
Y : training data

$$P(\text{parameter } \theta \mid \text{data } Y) = P(Y \mid \theta) P(\theta) / P(Y)$$

$$P(\text{diagnosis } \theta \mid \text{test result } Y) = P(Y \mid \theta) P(\theta) / P(Y)$$

For problem 1, all of these are functions of θ (λ)

Least-squares adjustment with normal posteriors



This is the simplest Bayesian inference problem I can think of with a one-dimensional, continuous variable; the probability density at every stage is a well-behaved normal distribution.

The log-likelihoods are parabolas.

Caution: this weighted-average approach takes the standard deviations as known with certainty.

$$\text{Posterior}(x) = P_1(x) P_2(x) P_3(x) P_4(x) P_5(x) \text{Prior}(x)$$

LEASTSQADJUST.ipynb

Least-squares adjustment

$$\begin{aligned}\text{Prior}(x) &= N(m_0, s_0) = \frac{1}{\sqrt{2\pi s_0^2}} e^{-\frac{(x-m_0)^2}{2s_0^2}} \\ \text{Likelihood}_1(x) &= N(m_1, s_1) = \frac{1}{\sqrt{2\pi s_1^2}} e^{-\frac{(x-m_1)^2}{2s_1^2}}\end{aligned}$$

In one dimension, imagine I have a variable x .

I want the best number I can get for $P(x | \text{DATA})$ (the posterior)
but all I have are a basket full of $p(\text{DATA}_i | x)$. (the likelihoods)

Bayes' rule to the rescue!

$$P(x | \text{DATA}) = P(x) P(\text{DATA} | x) / p(\text{DATA})$$

Least-squares adjustment

$$\text{Prior}(x) = N(m_0, s_0) = \frac{1}{\sqrt{2\pi s_0^2}} e^{-\frac{(x-m_0)^2}{2s_0^2}}$$

$$\text{Likelihood}_1(x) = N(m_1, s_1) = \frac{1}{\sqrt{2\pi s_1^2}} e^{-\frac{(x-m_1)^2}{2s_1^2}}$$

$$\text{Likelihood}_2(x) = N(m_2, s_2) = \frac{1}{\sqrt{2\pi s_2^2}} e^{-\frac{(x-m_2)^2}{2s_2^2}}$$

$$\text{Likelihood}_3(x) = N(m_3, s_3) = \frac{1}{\sqrt{2\pi s_3^2}} e^{-\frac{(x-m_3)^2}{2s_3^2}}$$

...

$$\text{Posterior} = \text{Prior} * L1 * L2 * L3 \dots$$

Take prior to be constant for now; take logs of all the likelihoods:

Prior(x) = constant

$$\text{Likelihood}_1(x) = N(m_1, s_1) = \frac{1}{\sqrt{2\pi s_1^2}} e^{-\frac{(x-m_1)^2}{2s_1^2}}$$

$$\text{Likelihood}_2(x) = N(m_2, s_2) = \frac{1}{\sqrt{2\pi s_2^2}} e^{-\frac{(x-m_2)^2}{2s_2^2}}$$

$$\text{Likelihood}_3(x) = N(m_3, s_3) = \frac{1}{\sqrt{2\pi s_3^2}} e^{-\frac{(x-m_3)^2}{2s_3^2}}$$

...

Posterior = Prior * L1 * L2 * L3 ...

Least-squares adjustment

$$\log \text{Prior}(x) = \log C = C$$

$$\text{LLikelihood_1}(x) = \log N(m_1, s_1) = -\frac{1}{2} \log(2\pi s_1^2) - \frac{(x-m_1)^2}{2s_1^2}$$

$$\text{LLikelihood_2}(x) = \log N(m_2, s_2) = -\frac{1}{2} \log(2\pi s_2^2) - \frac{(x-m_2)^2}{2s_2^2}$$

$$\text{LLikelihood_3}(x) = \log N(m_3, s_3) = -\frac{1}{2} \log(2\pi s_3^2) - \frac{(x-m_3)^2}{2s_3^2}$$

...

$$\log \text{Posterior} = \log \text{Prior} + \text{LL1} + \text{LL2} + \text{LL3} \dots$$

Least-squares adjustment

$$\log \text{Prior}(x) = \log C = C$$

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...

While these are straightforward functions of the s_i , these are just parabolas as a function of x . Sum of parabolas is a ...

Least-squares adjustment

$$\log \text{Prior}(x) = \log C = C$$

$$\text{Likelihood}_1(x) = \log N(m_1, s_1) = -\frac{1}{2} \log(2\pi s_1^2) - \frac{(x-m_1)^2}{2s_1^2}$$

reorganize terms in powers of x

$$\log \text{Posterior} = -\frac{1}{2} \sum \frac{1}{s_i^2} x^2 + \frac{2}{2} \sum \frac{m_i}{s_i^2} x - \frac{1}{2} \sum \frac{m_i^2}{s_i^2}$$

$$\frac{d \log(\text{posterior})}{dx} = -\sum \frac{1}{s_i^2} x + \sum \frac{m_i}{s_i^2} = 0$$

$$x_{\max} = \frac{\sum \frac{m_i}{s_i^2}}{\sum \frac{1}{s_i^2}} \quad S_{\text{tot}} = \frac{1}{\sqrt{\sum \frac{1}{s_i^2}}}$$

Ta-da! (Undergrad-level combination of measurements)

$$x_{\max} = \frac{\sum \frac{m_i}{s_i^2}}{\sum \frac{1}{s_i^2}} \quad s_{\text{tot}} = \frac{1}{\sqrt{\sum \frac{1}{s_i^2}}}$$

When you have a collection of normally-distributed likelihoods with known means and standard deviations

(These represent measurements and someone's judgement of the uncertainty attached to each measurement.)

We have a procedure that turns likelihood functions into algebra

And the product of N normal distributions is a normal distribution that is much tighter.

Ta-da! (Undergrad-level combination of measurements)

$$x_{\max} = \frac{\sum \frac{m_i}{s_i^2}}{\sum \frac{1}{s_i^2}} \quad s_{\text{tot}} = \frac{1}{\sqrt{\sum \frac{1}{s_i^2}}} \quad \text{Posterior (x)} = N(x_{\max}, s_{\text{tot}})$$

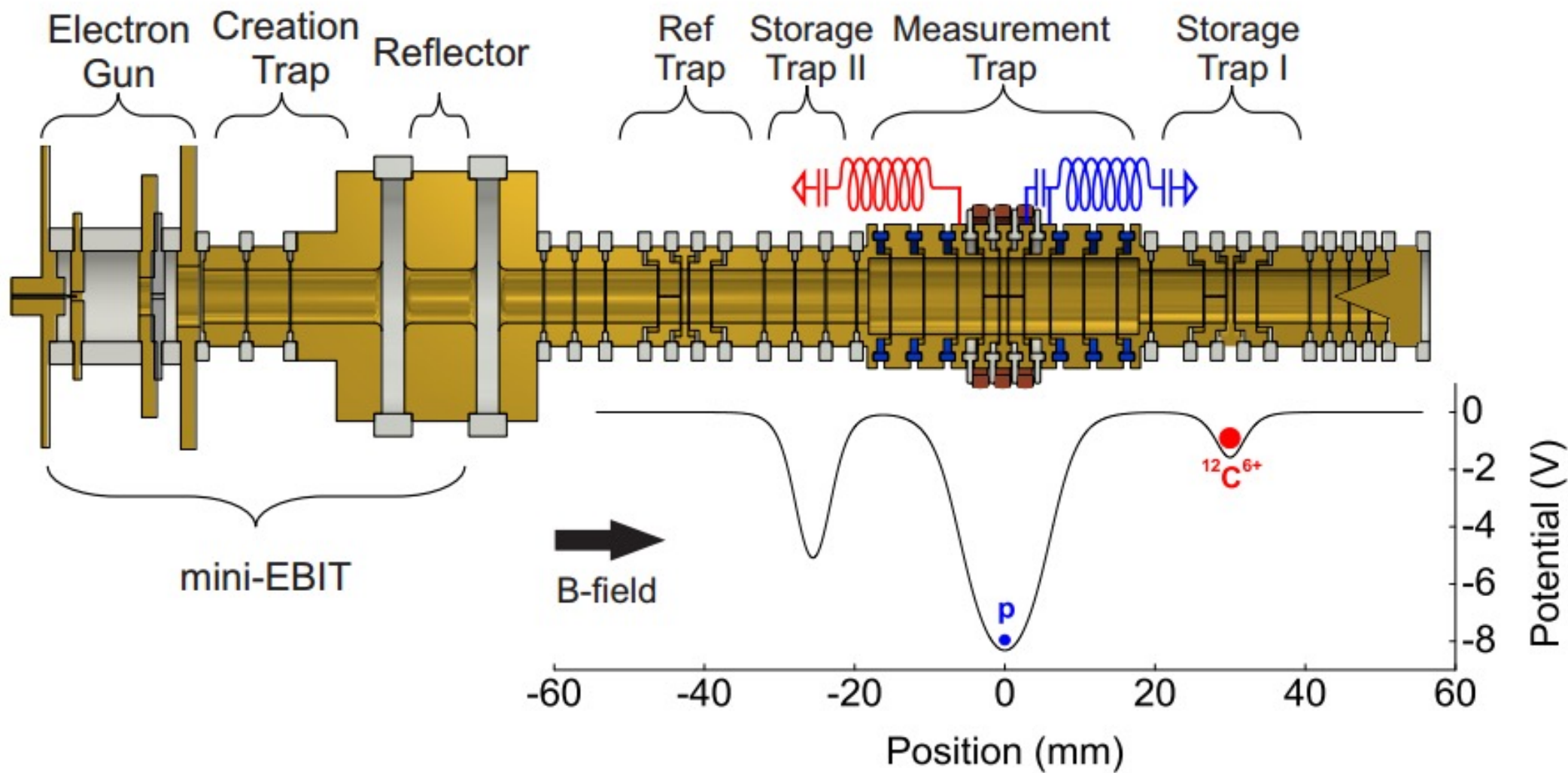
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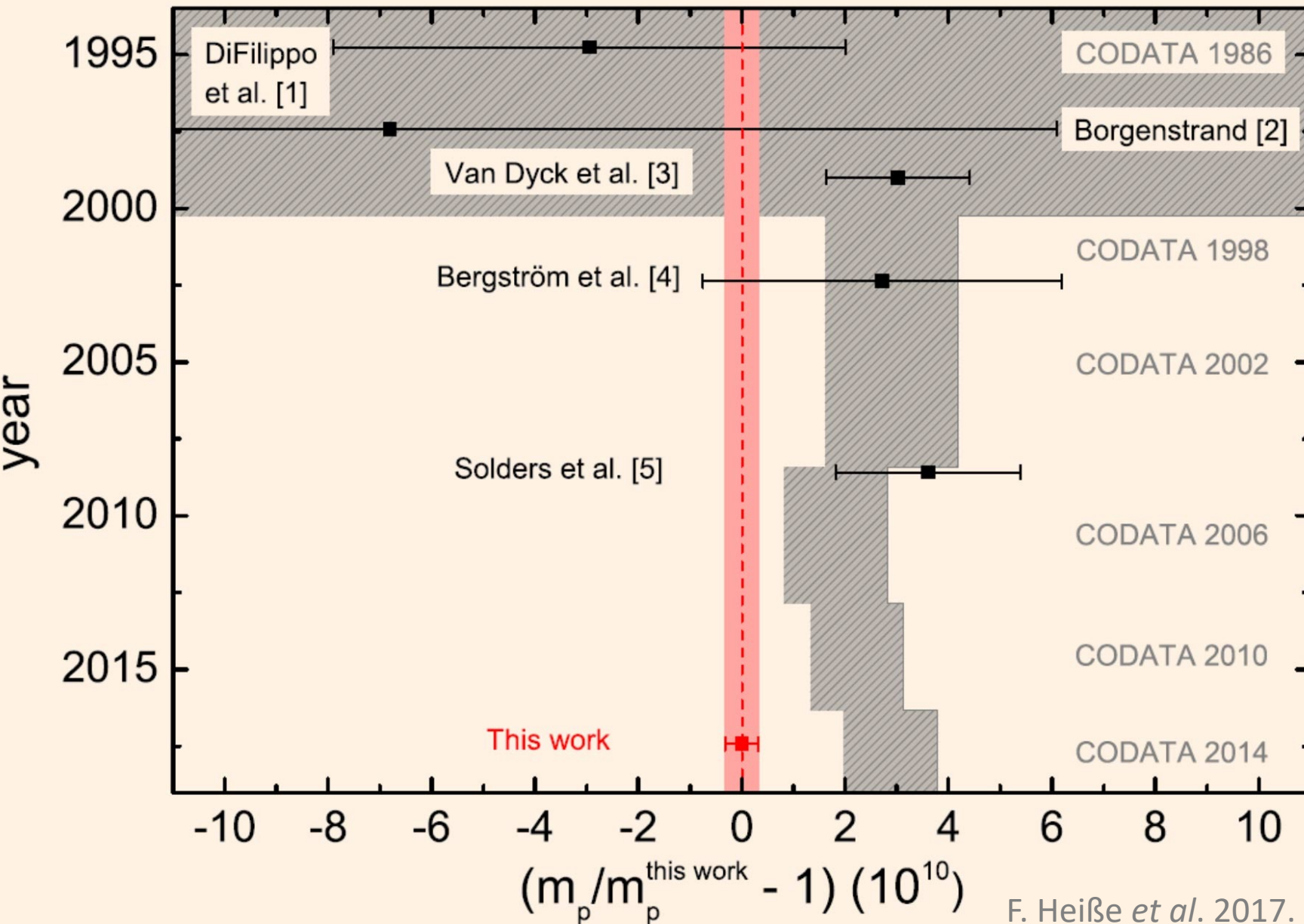
And the product of N normal distributions is a normal distribution that is much tighter.

Caution: this procedure does not know or care whether the measurements agree with each other.



This is a balance that compares the mass of the proton to the mass of $^{12}\text{C}^{6+}$

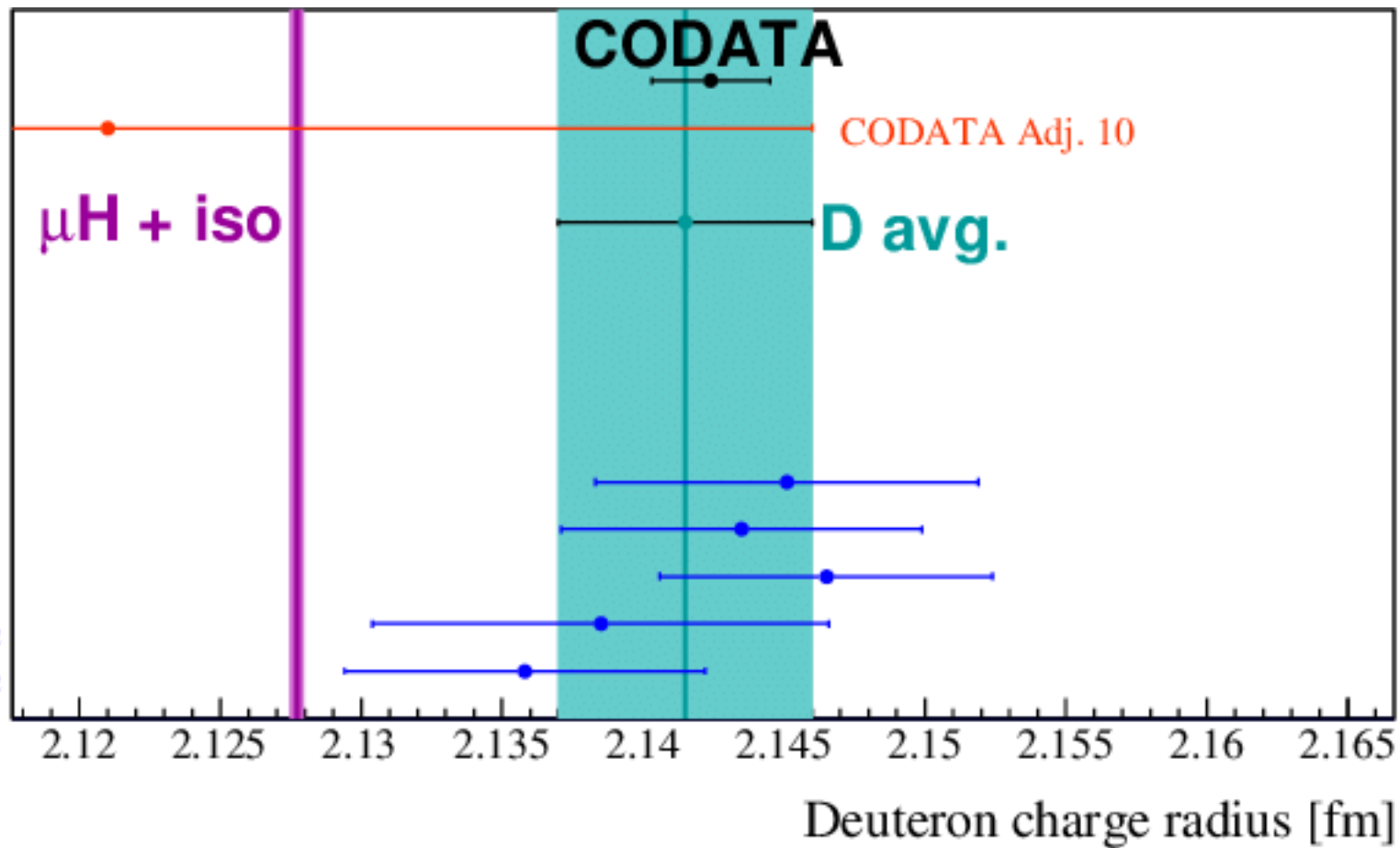
F. Heiße *et al.* 2017. High-Precision Measurement of the Proton's Atomic Mass. *Phys. Rev. Lett* 119 (3): 033001; doi: 10.1103/PhysRevLett.119.033001



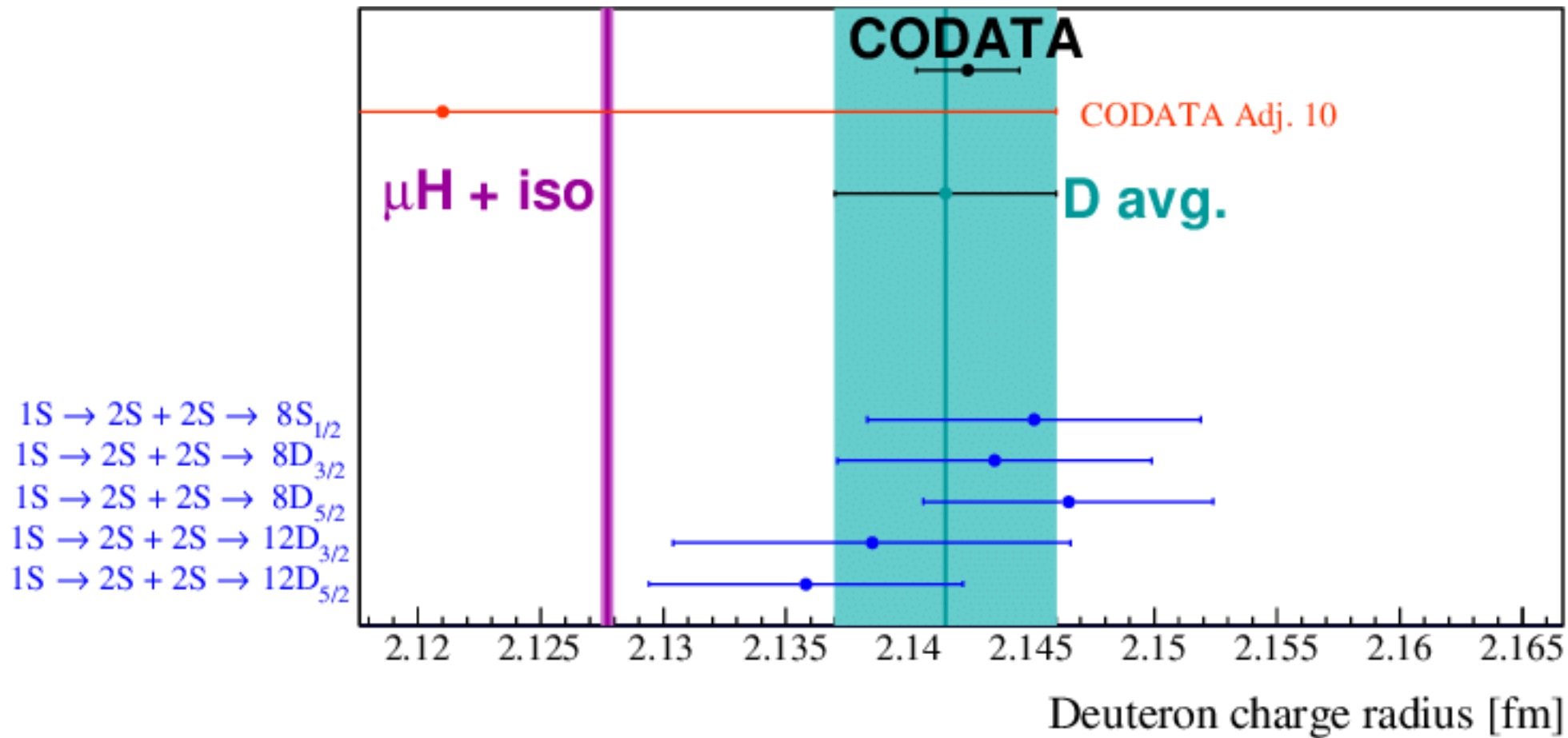
Multiple researchers, with advancing technology, have taken cracks at measuring the mass of the proton.

F. Heiße *et al.* 2017. High-Precision Measurement of the Proton's Atomic Mass. *Phys. Rev. Lett* 119 (3): 033001; doi: 10.1103/PhysRevLett.119.033001

$1S \rightarrow 2S + 2S \rightarrow 8S_{1/2}$
 $1S \rightarrow 2S + 2S \rightarrow 8D_{3/2}$
 $1S \rightarrow 2S + 2S \rightarrow 8D_{5/2}$
 $1S \rightarrow 2S + 2S \rightarrow 12D_{3/2}$
 $1S \rightarrow 2S + 2S \rightarrow 12D_{5/2}$



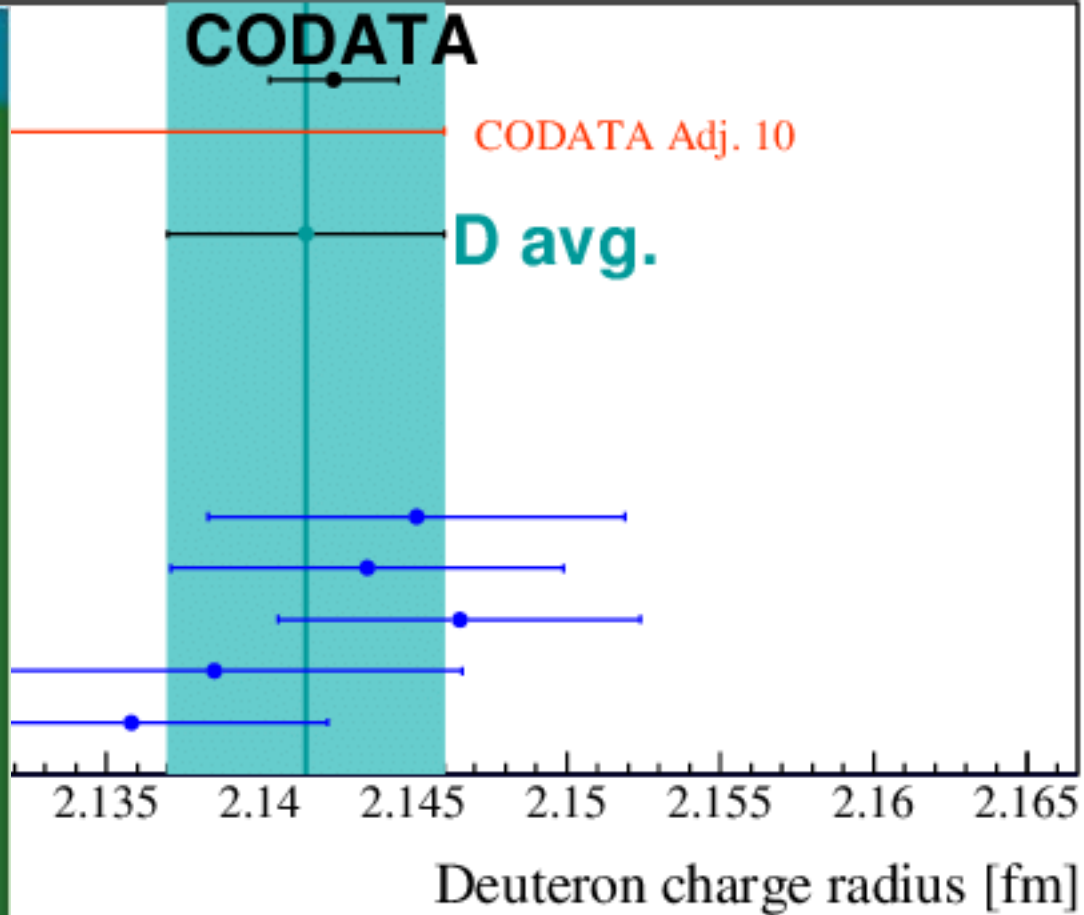
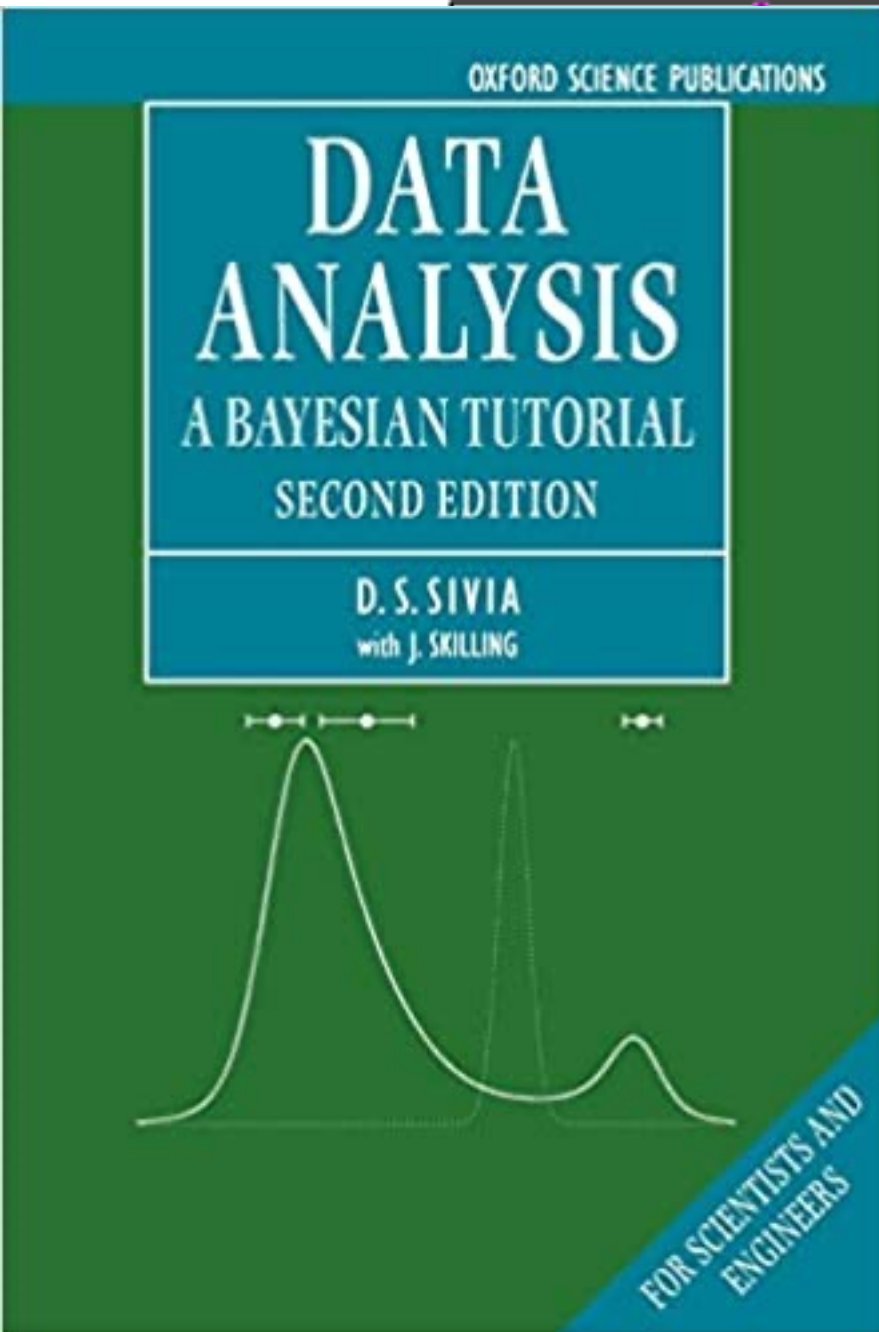
In a different measurement campaign, there are multiple (technically different) measurement approaches to the deuteron charge radius.



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In a measurement-evaluation doctrine called “Least Squares Adjustment,” information about the physical constant (deuteron charge radius) is combined from multiple experiments using a very lightweight version of Bayesian inference.

Goes by the term “metaanalysis” in other fields.



In a different measurement campaign, there are multiple (technically different) measurement approaches to the deuteron charge radius.

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nt version of Bayesian inference.

other fields.

Least squares without weights is usually a mistake!

- Unweighted least squares implicitly solves the problem where the additive errors on each point are normal and identically distributed. This is not usually the case!
- For count data (Poisson distribution) variance is proportional to N , standard deviation proportional to \sqrt{N} . (HW1 Q1)
- For proportion data (Binomial distribution / N) variance is proportional to $1/N$; standard deviation proportional to $1/\sqrt{N}$. Since we usually know the proportion, standard deviation is

$$\text{Standard Error of the Mean (binomial)} = \sqrt{p(1-p) / N}$$

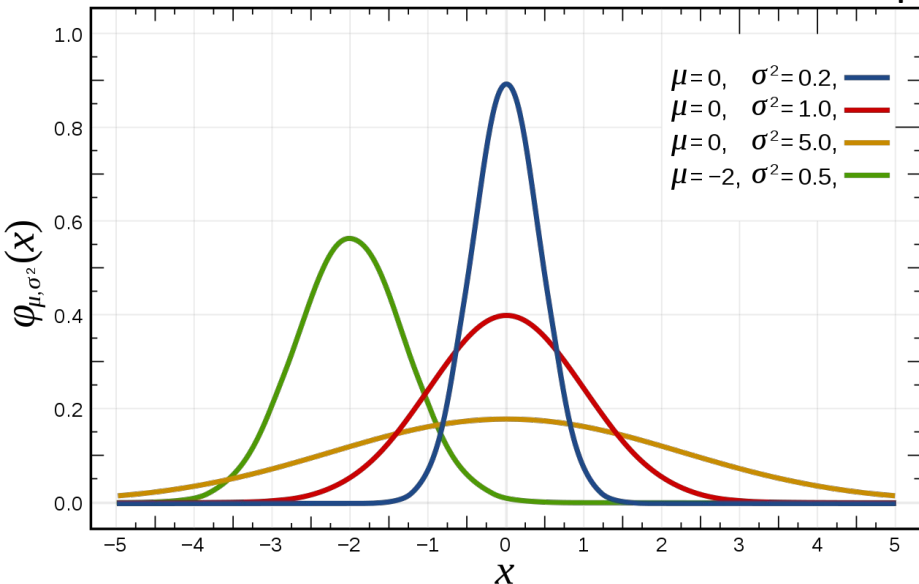
Anatomy of the normal distribution

$$\mathcal{N}(x|\mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp -\frac{(x-\mu)^2}{2\sigma^2}$$

“The normalizing constant”

x- dependence
shape and position
of distribution

peak density proportional to $1/\sigma$



Anatomy of the normal distribution

$$\log \mathcal{N}(x|\mu, \sigma) = -\frac{1}{2} \log(2\pi) - \log \sigma - \frac{(x-\mu)^2}{2\sigma^2}$$

Constant term,
not going to give
us trouble

Term depends
only on σ

Term depends on
 σ and μ

Anatomy of the normal distribution

$$\log \mathcal{N}(x|\mu, \sigma) = -\frac{1}{2} \log(2\pi) - \log \sigma - \frac{(x-\mu)^2}{2\sigma^2}$$

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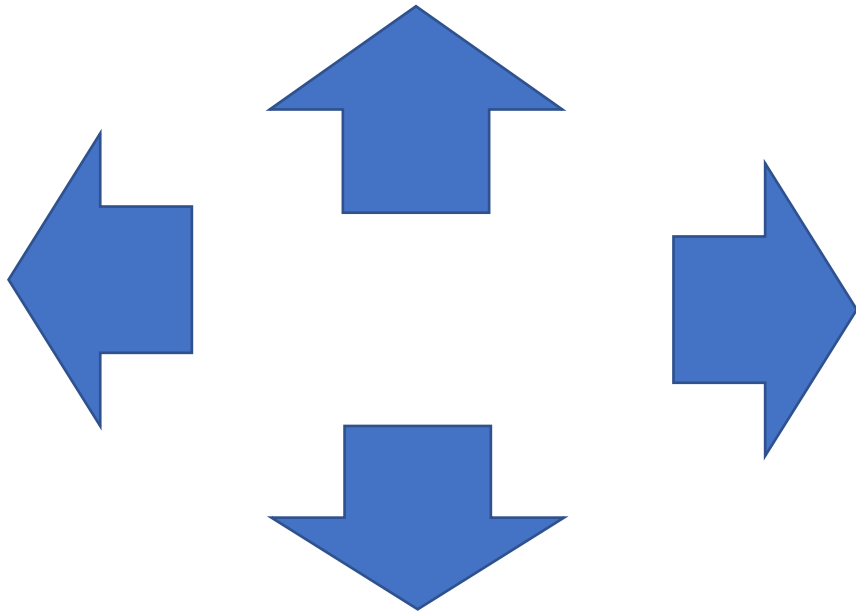
Term depends on
 σ and μ

Penalizes
distributions that
are too spread
out

Tells us where
the center is

Anatomy of the normal distribution

$$\log \mathcal{N}(x|\mu, \sigma) = -\frac{1}{2} \log(2\pi) - \log \sigma - \frac{(x-\mu)^2}{2\sigma^2}$$



When σ is too large, this term makes likelihood small

When σ is too small, this term penalizes the likelihood because the distribution will miss the data.

Normal(x_1) x Normal (x_2) ??

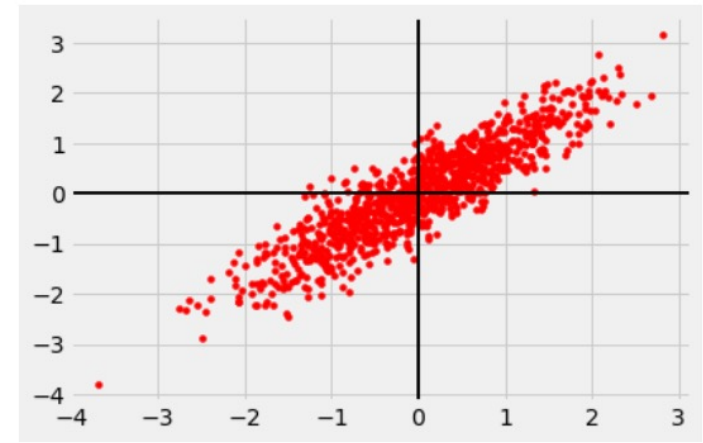
$$\mathcal{N}(x_1, x_2 | \mu_1, \mu_2, \sigma_{11}, \sigma_{22}) = \frac{1}{(2\pi)} \frac{1}{\sigma_{11}\sigma_{22}} \exp -\frac{1}{2} \left(\frac{(x_1 - \mu_1)^2}{\sigma_{11}} + \frac{(x_2 - \mu_2)^2}{\sigma_{22}} \right)$$

If I take the product of two 1-D normal distributions, I get a perfectly good probability distribution, but it isn't quite flexible enough for my data-modeling needs.

This factorizes into the product of a term that depends only on x_1 and σ_1 and a term only in x_2 and σ_2 .

This expression doesn't permit me to make distributions where the probability density of x_1 depends on the value of x_2

Multivariate normal



$$\Sigma = \begin{bmatrix} \sigma_{11}^2 & \sigma_{12}^2 \\ \sigma_{12}^2 & \sigma_{22}^2 \end{bmatrix}$$

$$\mathcal{N}(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{(\sigma_{11}^2 \sigma_{22}^2 - \sigma_{12}^2)} \exp -\frac{1}{2} \left(\begin{bmatrix} x_0 - \mu_0 & x_1 - \mu_1 \end{bmatrix} \begin{bmatrix} \sigma_{11}^2 & \sigma_{12}^2 \\ \sigma_{12}^2 & \sigma_{22}^2 \end{bmatrix}^{-1} \begin{bmatrix} x_0 - \mu_0 \\ x_1 - \mu_1 \end{bmatrix} \right)$$

Constant term,
not going to give
us trouble

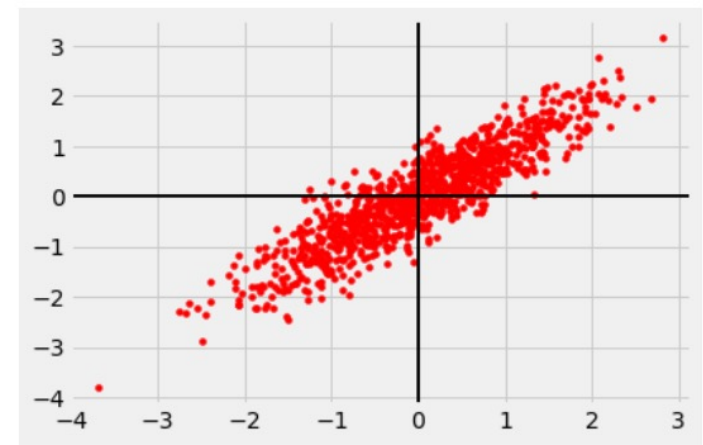
Term depends
only on Σ

Two powers of $\mathbf{x}-\boldsymbol{\mu}$

Multivariate normal

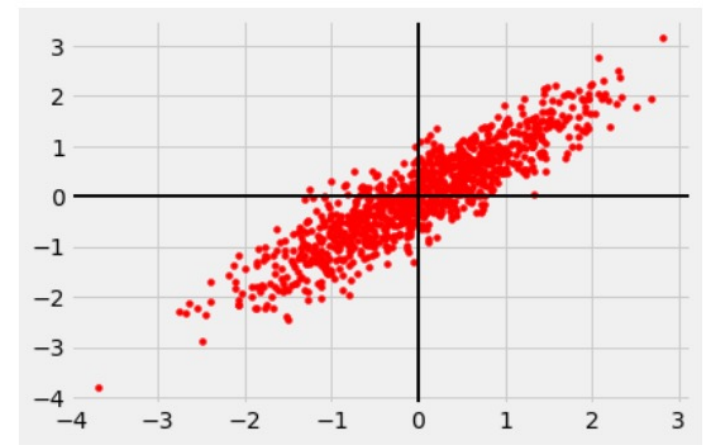
$$\Sigma = \begin{bmatrix} \sigma_{11}^2 & \cdots & \sigma_{1D}^2 \\ \vdots & \ddots & \vdots \\ \sigma_{D1}^2 & \cdots & \sigma_{DD}^2 \end{bmatrix}$$

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{D/2}} \exp -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu})$$



Multivariate normal

$$\Sigma = \begin{bmatrix} \sigma_{11}^2 & \cdots & \sigma_{1D}^2 \\ \vdots & \ddots & \vdots \\ \sigma_{D1}^2 & \cdots & \sigma_{DD}^2 \end{bmatrix}$$

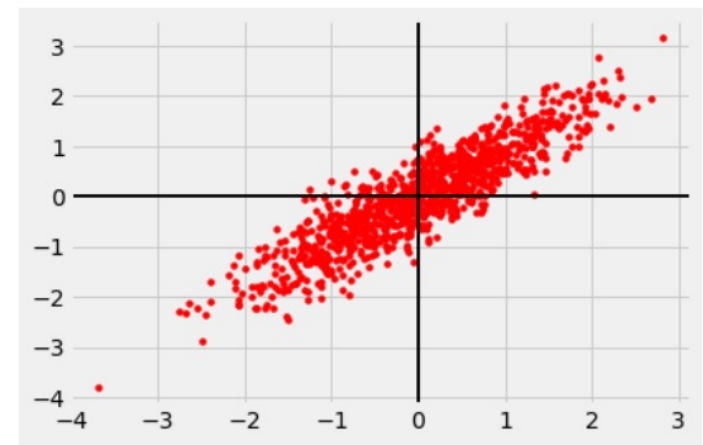


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How many parameters do I need for a D-dimensional multivariate Gaussian ?

Multivariate normal

$$\Sigma = \begin{bmatrix} \sigma_{11}^2 & \cdots & \sigma_{1D}^2 \\ \vdots & \ddots & \vdots \\ \sigma_{D1}^2 & \cdots & \sigma_{DD}^2 \end{bmatrix}$$

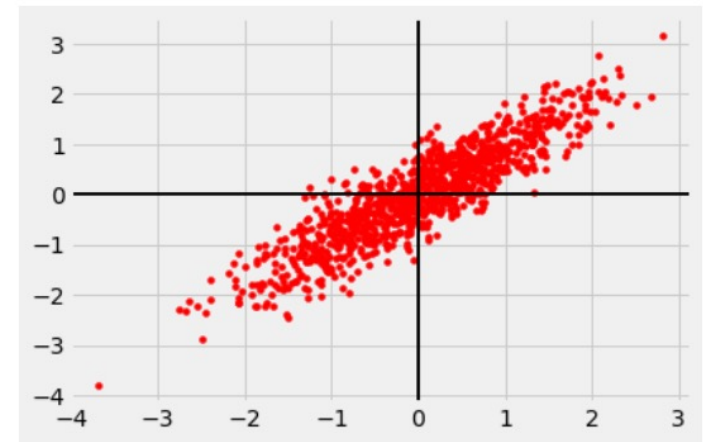


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How many parameters do I need for a D-dimensional multivariate Gaussian ?

$$\boldsymbol{\mu} : D \quad \boldsymbol{\Sigma} : (D^2 + D)/2$$

Multivariate normal



$$\mathcal{N}(\mathbf{x}|\mathbf{x}_0, \mathbf{\Sigma}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\mathbf{\Sigma}|^{D/2}} \exp -\frac{1}{2}(\mathbf{x} - \mathbf{x}_0)^T \mathbf{\Sigma}^{-1}(\mathbf{x} - \mathbf{x}_0)$$

Constant term,
not going to give
us trouble

Term depends
only on Σ

Two powers of $\mathbf{x}-\mathbf{x}_0$

Σ covariance matrix

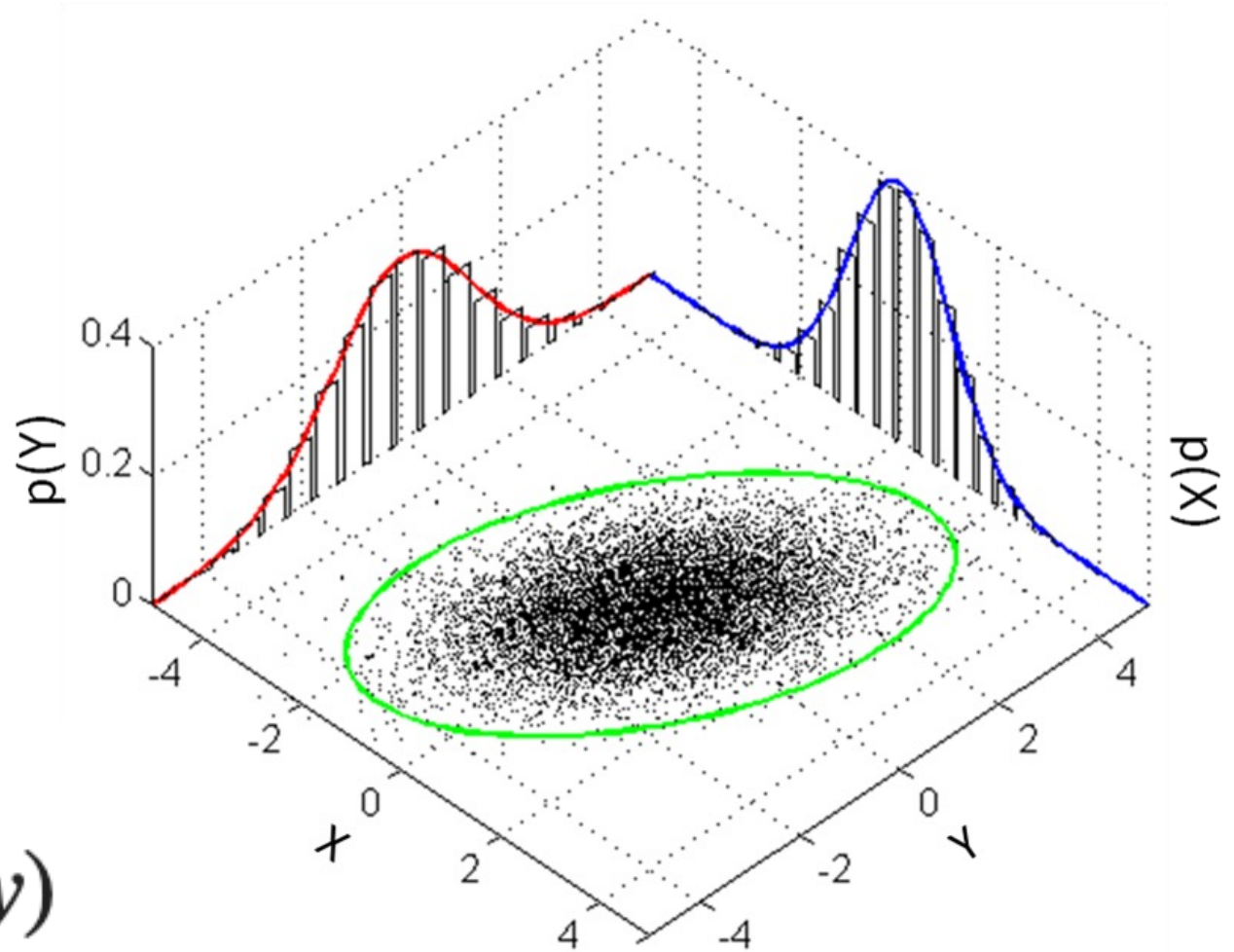
Σ^{-1} “precision” matrix

Jargon: Marginalization

To “marginalize” is to take a distribution of many variables and turn it into a distribution of fewer variables by integrating the product of the density and the prior probability of each of the unwanted variables.

When we are able to do this, this gives us the one-dimensional probability distribution (for the parameter of interest) that we seek, in essence averaging over all likely values of the variables not of interest.

$$P(x) = \int dy P(x|y)P(y)$$



Unsupervised learning

I don't have labels, just data $\{\mathbf{x}_i\}_{i=1}^N$

My model is a function that does something useful with new data.

Tasks may include

detecting outliers (points where the density is low; **density estimation**)

dimensionality reduction (produce coordinates in a low-dimensional space; compress the data while retaining its essence)

clustering (output is a cluster id)

Supervised learning

Supervised learning: the **dataset** is a collection of **labeled examples** $\{ \mathbf{x}_i, y_i \}_{i=1}^N$

N examples

\mathbf{x} is called a **feature vector** and

y is the set of **labels**

\mathbf{x} , y can be in \mathbb{R}^n or can be discrete, categorical labels, or some more complex kind of input and output

Goal of supervised learning is to produce a model that turns a feature vector into an approximation of the label.

Jargon

parameter = numbers that determine “the model.”

hyperparameter = number that controls the behavior of the learning algorithm

regression = prediction of a real-valued label

fitting = determining the parameters of the model

classification = prediction of a label from a finite set of labels

shallow learning algorithm – fits the parameters of the model from the features of the training data.

deep learning algorithm fits the parameters of the model from the output of layers that are fed by the training features.

Generative vs. discriminative

If I fit a probability distribution to my data, I can evaluate

$P(\text{newdata} \mid \text{model})$ and

$P(\text{label} \mid \text{model}, \text{newdata})$

but I also can draw samples from the distribution. Models of this sort are called “generative” models because they permit me to “generate” new data consistent with the model parameters.

Models that just find the function of x that gives the right answer y (say, by fitting weights directly rather than finding weights from fitted distribution parameters) are called “discriminative” models.