CSE546: Point Estimation
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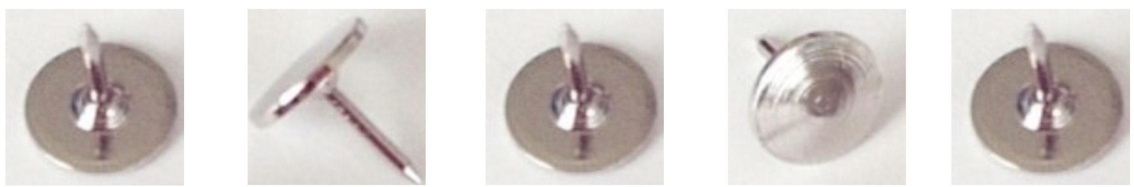
Slides adapted from Carlos Guestrin and Dan Klein

Your first consulting job

- A billionaire from the suburbs of Seattle asks you a question:
  - He says: I have thumbtack, if I flip it, what's the probability it will fall with the nail up?
  - You say: Please flip it a few times:



  - You say: The probability is:
    - P(H) = 3/5
  - **He says: Why???**
  - You say: Because…

Random Variables

- A random variable is some aspect of the world about which we (may) have uncertainty
  - R = Is it raining?
  - D = How long will it take to drive to work?
  - L = Where am I?

- We denote random variables with capital letters

- Random variables have domains
  - R in {true, false}   (sometimes write as {+r, ¬r})
  - D in $[0, \infty)$
  - L in possible locations, maybe {(0,0), (0,1), …}

Probability Distributions

- Discrete random variables have distributions

$P(T)$

T	P
warm	0.5
cold	0.5

$P(W)$

W	P
sun	0.6
rain	0.1
fog	0.3
meteor	0.0

- A discrete distribution is a TABLE of probabilities of values
- A probability (lower case value) is a single number

$$P(W = rain) = 0.1 \qquad P(rain) = 0.1$$

- Must have:

$$\forall x\, P(x) \geq 0 \qquad \sum_x P(x) = 1$$

Joint Distributions

- A *joint distribution* over a set of random variables: $X_1, X_2, \ldots X_n$ specifies a real number for each assignment (or *outcome*):

$$P(X_1 = x_1, X_2 = x_2, \ldots X_n = x_n)$$

$$P(x_1, x_2, \ldots x_n)$$

  – Size of distribution if n variables with domain sizes d?

  – Must obey:

$$P(x_1, x_2, \ldots x_n) \geq 0$$

$$\sum_{(x_1, x_2, \ldots x_n)} P(x_1, x_2, \ldots x_n) = 1$$

$$P(T, W)$$

T	W	P
hot	sun	0.4
hot	rain	0.1
cold	sun	0.2
cold	rain	0.3

- For all but the smallest distributions, impractical to write out

Marginal Distributions

- Marginal distributions are sub-tables which eliminate variables
- Marginalization (summing out): Combine collapsed rows by adding

$P(T,W)$

T	W	P
hot	sun	0.4
hot	rain	0.1
cold	sun	0.2
cold	rain	0.3

$$P(t) = \sum_s P(t,s)$$

$$P(s) = \sum_t P(t,s)$$

$P(T)$

T	P
hot	0.5
cold	0.5

$P(W)$

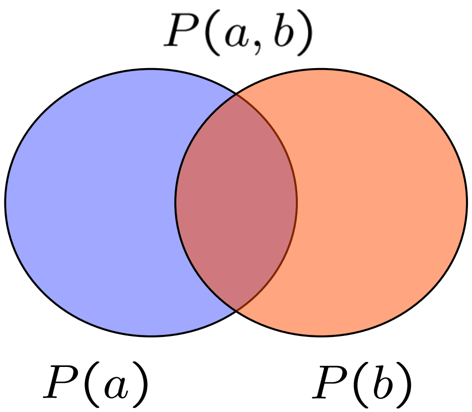
W	P
sun	0.6
rain	0.4

$$P(X_1 = x_1) = \sum_{x_2} P(X_1 = x_1, X_2 = x_2)$$

Conditional Probabilities

- A simple relation between joint and conditional probabilities
  - In fact, this is taken as the *definition* of a conditional probability

$$P(a|b) = \frac{P(a,b)}{P(b)}$$



$$P(T,W)$$

T	W	P
hot	sun	0.4
hot	rain	0.1
cold	sun	0.2
cold	rain	0.3

$$P(W = r|T = c) = ???$$

Conditional Distributions

- Conditional distributions are probability distributions over some variables given fixed values of others

Conditional Distributions

$P(W|T)$

$$P(W|T = hot)$$

W	P
sun	0.8
rain	0.2

$$P(W|T = cold)$$

W	P
sun	0.4
rain	0.6

Joint Distribution

$$P(T, W)$$

T	W	P
hot	sun	0.4
hot	rain	0.1
cold	sun	0.2
cold	rain	0.3

The Product Rule

- Sometimes have conditional distributions but want the joint

$$P(x|y) = \frac{P(x,y)}{P(y)} \quad \Leftrightarrow \quad P(x,y) = P(x|y)P(y)$$

- Example:

$P(W)$

R	P
sun	0.8
rain	0.2

$P(D|W)$

D	W	P
wet	sun	0.1
dry	sun	0.9
wet	rain	0.7
dry	rain	0.3

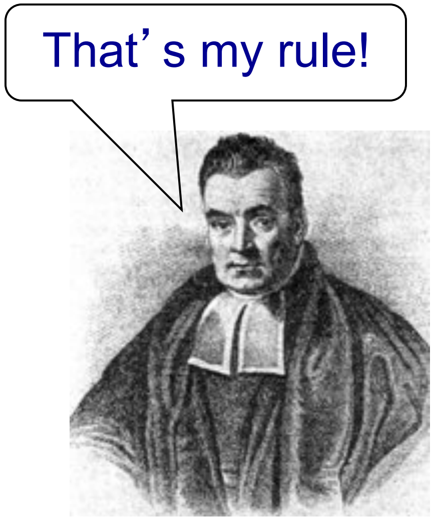
$P(D,W)$

D	W	P
wet	sun	0.08
dry	sun	0.72
wet	rain	0.14
dry	rain	0.06

Bayes’ Rule

- Two ways to factor a joint distribution over two variables:

$$P(x,y) = P(x|y)P(y) = P(y|x)P(x)$$



- Dividing, we get:

$$P(x|y) = \frac{P(y|x)}{P(y)}P(x)$$

- Why is this at all helpful?
  - Lets us build one conditional from its reverse
  - Often one conditional is tricky but the other one is simple
  - Foundation of many practical systems (e.g. ASR, MT)

- In the running for most important ML equation!

Thumbtack – Binomial Distribution

- P(Heads) = θ, P(Tails) = 1-θ

- Flips are *i.i.d.*: $D=\{x_i \mid i=1\ldots n\},\ P(D \mid \theta) = \Pi_i P(x_i \mid \theta)$
  - Independent events
  - Identically distributed according to Binomial distribution
- Sequence *D* of α_H Heads and α_T Tails

$$P(\mathcal{D} \mid \theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$$

Maximum Likelihood Estimation

- **Data:** Observed set D of α_H Heads and α_T Tails
- **Hypothesis:** Binomial distribution
- **Learning:** finding θ is an optimization problem
  - What's the objective function?

$$P(\mathcal{D} \mid \theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$$

- **MLE:** Choose θ to maximize probability of *D*

$$\begin{aligned} \widehat{\theta} &= \arg\max_{\theta} \; P(\mathcal{D} \mid \theta) \\ &= \arg\max_{\theta} \; \ln P(\mathcal{D} \mid \theta) \end{aligned}$$

Your first parameter learning algorithm

$$\hat{\theta} = \arg\max_{\theta} \ln P(\mathcal{D} \mid \theta)$$
$$= \arg\max_{\theta} \ln \theta^{\alpha_H}(1-\theta)^{\alpha_T}$$

- Set derivative to zero, and solve!

$$\frac{d}{d\theta} \ln P(\mathcal{D} \mid \theta) = \frac{d}{d\theta}\left[\ln \theta^{\alpha_H}(1-\theta)^{\alpha_T}\right]$$
$$= \frac{d}{d\theta}\left[\alpha_H \ln \theta + \alpha_T \ln(1-\theta)\right]$$
$$= \alpha_H \frac{d}{d\theta} \ln \theta + \alpha_T \frac{d}{d\theta} \ln(1-\theta)$$
$$= \frac{\alpha_H}{\theta} - \frac{\alpha_T}{1-\theta} = 0$$

$$\hat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$$

But, how many flips do I need?

$$\widehat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$$

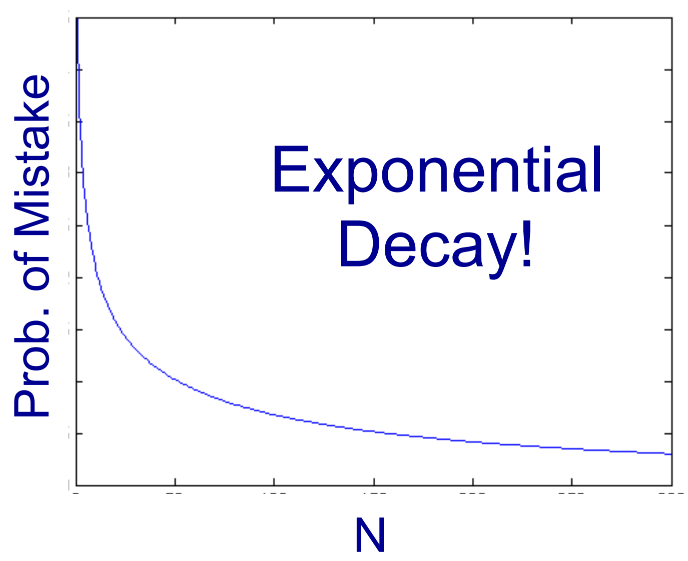
- Billionaire says: I flipped 3 heads and 2 tails.
- You say: θ = 3/5, I can prove it!
- He says: What if I flipped 30 heads and 20 tails?
- You say: Same answer, I can prove it!
- **He says: What's better?**
- You say: Umm… The more the merrier???
- He says: Is this why I am paying you the big bucks???

A bound (from Hoeffding's inequality)

- For $N = \alpha_H + \alpha_T$, and $\widehat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$

- Let θ^* be the true parameter, for any $\varepsilon > 0$:

$$P(|\,\widehat{\theta} - \theta^*\,| \geq \epsilon) \;\leq\; 2e^{-2N\epsilon^2}$$



PAC Learning

- PAC: Probably Approximate Correct
- Billionaire says: I want to know the thumbtack θ, within ε = 0.1, with probability at least 1-δ = 0.95.
- How many flips? Or, how big do I set N?

$$P(|\,\widehat{\theta} - \theta^* \,| \geq \epsilon) \;\leq\; 2e^{-2N\epsilon^2}$$

$$\delta \geq 2e^{-2N\epsilon^2} \geq P(\text{mistake})$$

$$\ln\delta \geq \ln 2 - 2N\epsilon^2$$

$$N \geq \frac{\ln(2/\delta)}{2\epsilon^2}$$

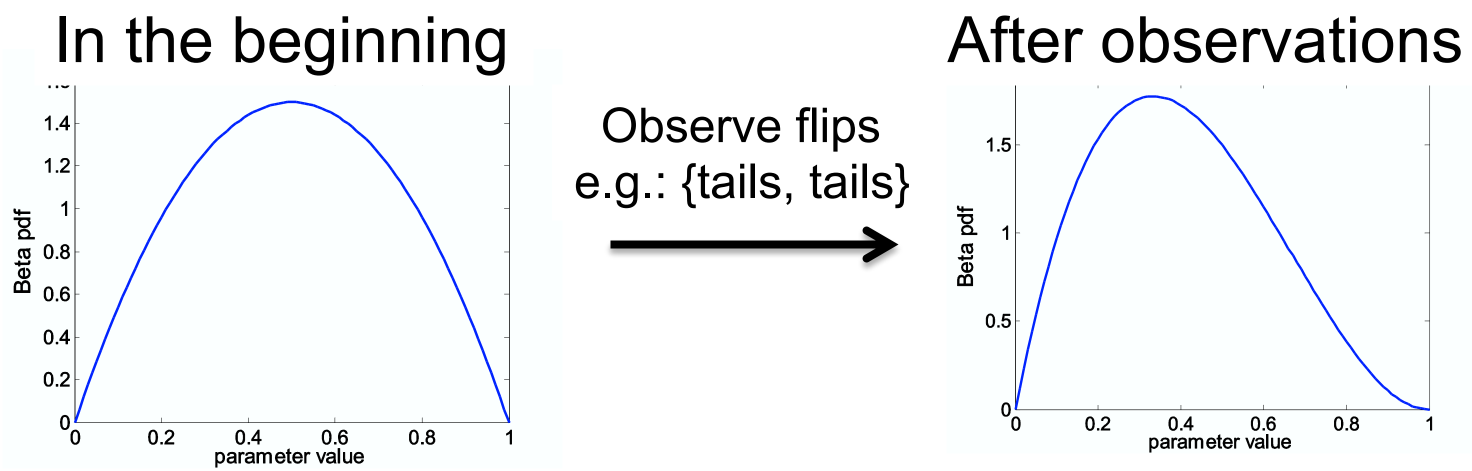
Interesting! Lets look at some numbers!

- ε = 0.1, δ=0.05

$$N \geq \frac{\ln(2/0.05)}{2 \times 0.1^2} \approx \frac{3.8}{0.02} = 190$$

What if I have prior beliefs?

- Billionaire says: Wait, I know that the thumbtack is "close" to 50-50. What can you do for me now?
- **You say: I can learn it the Bayesian way…**
- Rather than estimating a single θ, we obtain a distribution over possible values of θ

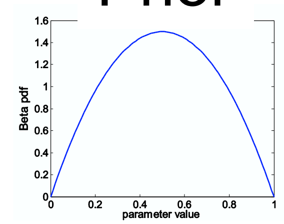


Bayesian Learning

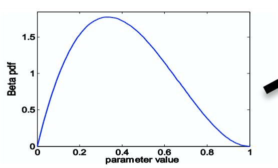
- Use Bayes rule:

Data Likelihood

Prior



Posterior



$$P(\theta \mid \mathcal{D}) = \frac{P(\mathcal{D} \mid \theta)P(\theta)}{P(\mathcal{D})}$$

Normalization

- Or equivalently: $P(\theta \mid \mathcal{D}) \propto P(\mathcal{D} \mid \theta)P(\theta)$
- Also, for uniform priors:
  → reduces to MLE objective

$$P(\theta) \propto 1 \qquad P(\theta \mid \mathcal{D}) \propto P(\mathcal{D} \mid \theta)$$

Bayesian Learning for Thumbtacks

$$P(\theta \mid \mathcal{D}) \;\propto\; P(\mathcal{D} \mid \theta)P(\theta)$$

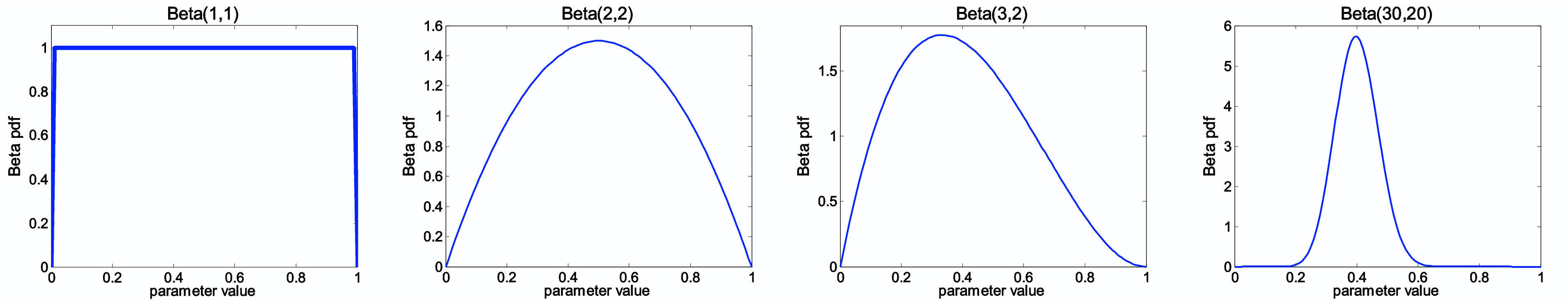
Likelihood function is Binomial:

$$P(\mathcal{D} \mid \theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$$

- What about prior?
  - Represent expert knowledge
  - Simple posterior form
- Conjugate priors:
  - Closed-form representation of posterior
  - **For Binomial, conjugate prior is Beta distribution**

Beta prior distribution – P(θ)

$$P(\theta) = \frac{\theta^{\beta_H - 1}(1-\theta)^{\beta_T - 1}}{B(\beta_H, \beta_T)} \sim Beta(\beta_H, \beta_T)$$



- Likelihood function: $P(\mathcal{D} \mid \theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$
- Posterior: $P(\theta \mid \mathcal{D}) \propto P(\mathcal{D} \mid \theta) P(\theta)$

$$P(\theta \mid \mathcal{D}) \propto \theta^{\alpha_H}(1-\theta)^{\alpha_T}\ \theta^{\beta_H - 1}(1-\theta)^{\beta_T - 1}$$

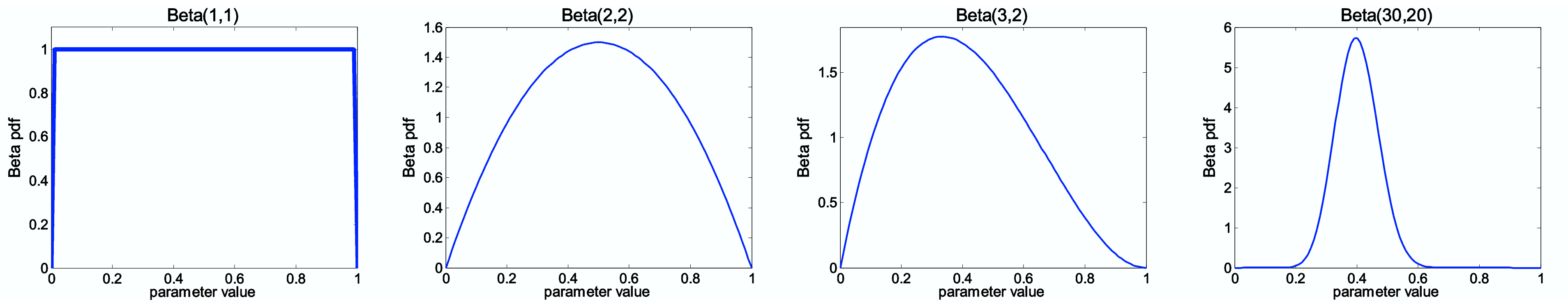
$$= \theta^{\alpha_H + \beta_H - 1}(1-\theta)^{\alpha_T + \beta_t + 1}$$

$$= Beta(\alpha_H + \beta_H, \alpha_T + \beta_T)$$

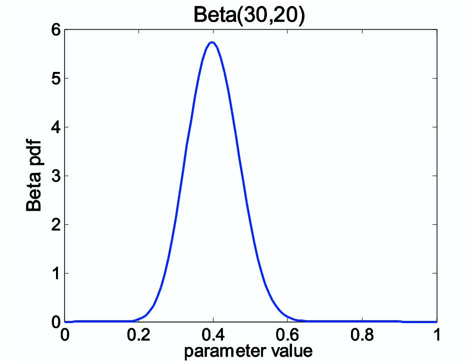
Posterior distribution

- Prior: $Beta(\beta_H, \beta_T)$
- Data: α_H heads and α_T tails
- Posterior distribution:

$$P(\theta \mid \mathcal{D}) \sim Beta(\beta_H + \alpha_H, \beta_T + \alpha_T)$$



Bayesian Posterior Inference



- Posterior distribution:

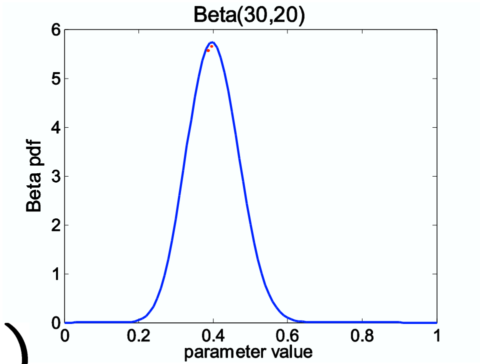
$$P(\theta \mid \mathcal{D}) \sim Beta(\beta_H + \alpha_H, \beta_T + \alpha_T)$$

- Bayesian inference:
  - No longer single parameter
  - For any specific f, the function of interest
  - Compute the expected value of f

$$E[f(\theta)] = \int_0^1 f(\theta) P(\theta \mid \mathcal{D}) d\theta$$

  - Integral is often hard to compute

MAP: Maximum a posteriori approximation



$$P(\theta \mid \mathcal{D}) \sim Beta(\beta_H + \alpha_H, \beta_T + \alpha_T)$$

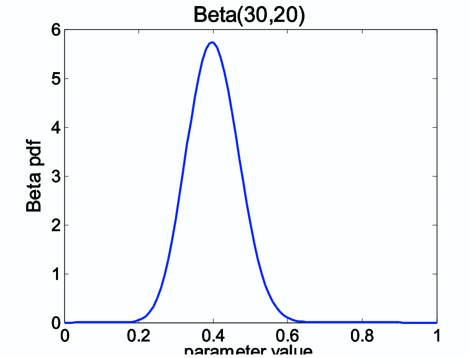
$$E[f(\theta)] = \int_0^1 f(\theta) P(\theta \mid \mathcal{D}) d\theta$$

- As more data is observed, Beta is more certain
- MAP: use most likely parameter to approximate the expectation

$$\widehat{\theta} = \arg\max_{\theta} P(\theta \mid \mathcal{D})$$

$$E[f(\theta)] \approx f(\widehat{\theta})$$

MAP for Beta distribution



$$P(\theta \mid \mathcal{D}) = \frac{\theta^{\beta_H+\alpha_H-1}(1-\theta)^{\beta_T+\alpha_T-1}}{B(\beta_H+\alpha_H,\beta_T+\alpha_T)} \sim Beta(\beta_H+\alpha_H,\beta_T+\alpha_T)$$

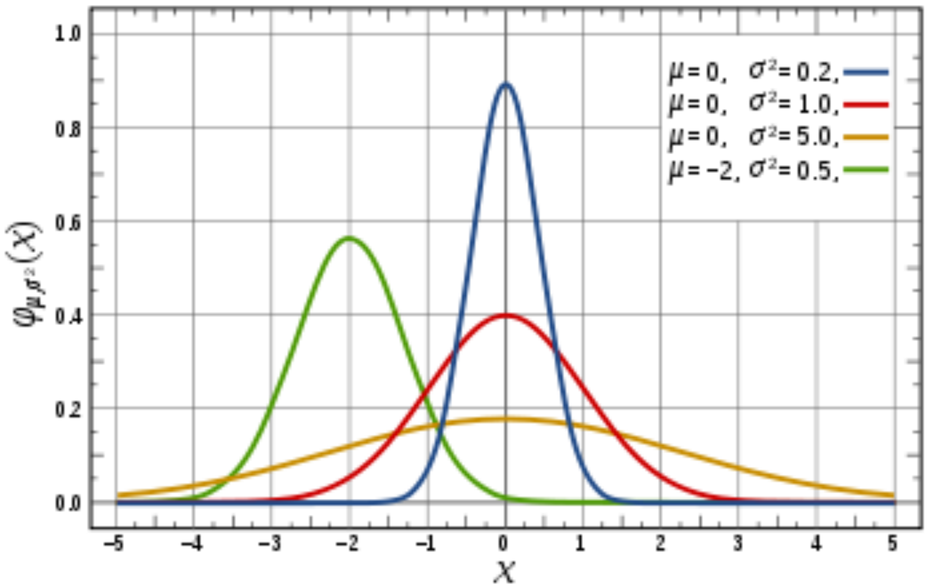
- MAP: use most likely parameter:

$$\widehat{\theta} = \arg\max_{\theta} P(\theta \mid \mathcal{D}) = \frac{\alpha_H+\beta_H-1}{\alpha_H+\beta_H+\alpha_T+\beta_T-2}$$

- Beta prior equivalent to extra thumbtack flips
- As $N \rightarrow 1$, prior is "forgotten"
- **But, for small sample size, prior is important!**

What about continuous variables?

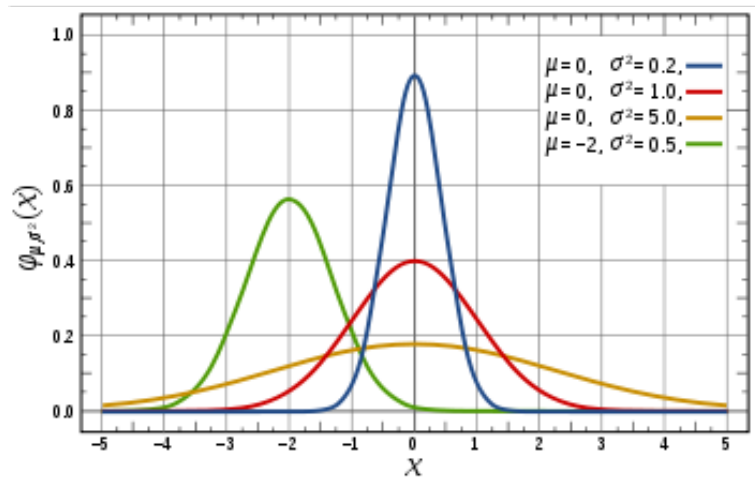
- Billionaire says: If I am measuring a continuous variable, what can you do for me?
- **You say: Let me tell you about Gaussians…**



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

Some properties of Gaussians

- Affine transformation (multiplying by scalar and adding a constant) are Gaussian
  - $X \sim N(\mu,\sigma^2)$
  - $Y = aX + b \rightarrow Y \sim N(a\mu+b,a^2\sigma^2)$



- Sum of Gaussians is Gaussian
  - $X \sim N(\mu_X,\sigma^2_X)$
  - $Y \sim N(\mu_Y,\sigma^2_Y)$
  - $Z = X+Y \rightarrow Z \sim N(\mu_X+\mu_Y, \sigma^2_X+\sigma^2_Y)$

- Easy to differentiate, as we will see soon!

Learning a Gaussian

- Collect a bunch of data
  - Hopefully, i.i.d. samples
  - e.g., exam scores
- Learn parameters
  - Mean: μ
  - Variance: σ

x_i $i =$	Exam Score
0	85
1	95
2	100
3	12
…	…
99	89

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

MLE for Gaussian: $P(x \mid \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$

- Prob. of i.i.d. samples $D=\{x_1,\ldots,x_N\}$:

$$P(\mathcal{D} \mid \mu, \sigma) = \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^N \prod_{i=1}^{N} e^{\frac{-(x_i-\mu)^2}{2\sigma^2}}$$

$$\mu_{MLE}, \sigma_{MLE} = \arg\max_{\mu,\sigma} P(\mathcal{D} \mid \mu, \sigma)$$

- Log-likelihood of data:

$$\begin{aligned} \ln P(\mathcal{D} \mid \mu, \sigma) &= \ln\left[\left(\frac{1}{\sigma\sqrt{2\pi}}\right)^N \prod_{i=1}^{N} e^{\frac{-(x_i-\mu)^2}{2\sigma^2}}\right] \\ &= -N \ln \sigma\sqrt{2\pi} - \sum_{i=1}^{N} \frac{(x_i-\mu)^2}{2\sigma^2} \end{aligned}$$

Your second learning algorithm: MLE for mean of a Gaussian

- What's MLE for mean?

$$
\begin{aligned}
\frac{d}{d\mu}\ln P(\mathcal{D} \mid \mu, \sigma) &= \frac{d}{d\mu}\left[-N \ln \sigma\sqrt{2\pi} - \sum_{i=1}^{N}\frac{(x_i-\mu)^2}{2\sigma^2}\right] \\
&= \frac{d}{d\mu}\left[-N \ln \sigma\sqrt{2\pi}\right] - \sum_{i=1}^{N}\frac{d}{d\mu}\left[\frac{(x_i-\mu)^2}{2\sigma^2}\right] \\
&= -\sum_{i=1}^{N}\frac{(x_i-\mu)}{\sigma^2} = 0 \\
&= -\sum_{i=1}^{N} x_i + N\mu = 0
\end{aligned}
$$

$$
\widehat{\mu}_{MLE} = \frac{1}{N}\sum_{i=1}^{N} x_i
$$

MLE for variance

- Again, set derivative to zero:

$$\frac{d}{d\sigma} \ln P(\mathcal{D} \mid \mu, \sigma) = \frac{d}{d\sigma}\left[-N \ln \sigma\sqrt{2\pi} - \sum_{i=1}^{N} \frac{(x_i-\mu)^2}{2\sigma^2}\right]$$

$$= \frac{d}{d\sigma}\left[-N \ln \sigma\sqrt{2\pi}\right] - \sum_{i=1}^{N} \frac{d}{d\sigma}\left[\frac{(x_i-\mu)^2}{2\sigma^2}\right]$$

$$= -\frac{N}{\sigma} + \sum_{i=1}^{N} \frac{(x_i-\mu)^2}{\sigma^3} = 0$$

$$\widehat{\sigma}^2_{MLE} = \frac{1}{N}\sum_{i=1}^{N}(x_i - \widehat{\mu})^2$$

Learning Gaussian parameters

- MLE:

$$\widehat{\mu}_{MLE} = \frac{1}{N}\sum_{i=1}^{N} x_i$$

$$\widehat{\sigma}^2_{MLE} = \frac{1}{N}\sum_{i=1}^{N} (x_i - \widehat{\mu})^2$$

- BTW. MLE for the variance of a Gaussian is **biased**
  - Expected result of estimation is **not** true parameter!
  - Unbiased variance estimator:

$$\widehat{\sigma}^2_{unbiased} = \frac{1}{N-1}\sum_{i=1}^{N} (x_i - \widehat{\mu})^2$$

Bayesian learning of Gaussian parameters

- Conjugate priors
  - Mean: Gaussian prior
  - Variance: Wishart Distribution

- Prior for mean:

$$P(\mu \mid \eta, \lambda) = \frac{1}{\lambda\sqrt{2\pi}} e^{\frac{-(\mu-\eta)^2}{2\lambda^2}}$$