Probabilistic Machine learning

Introduction to probabilistic programming languages (PPLs)

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[Material partly made by Antonio Salmeron and Helge Langseth]

Plan

- **Day 1: Probabilistic Modeling**
  - Introduction to probabilistic modeling and inference
  - Introduction to probabilistic programming
  - Probabilistic programming in Pyro
- **Day 2 : Variational Inference for Probabilistic Machine Learning**
  - Introduction to Variational inference
  - Variational inference in Pyro
  - Variational AutoEncoders

What is NOT Covered in This PhD Course

To set clear expectations, the following topics are **not** included in this introductory course on Probabilistic AI:

- **Advanced Bayesian Nonparametrics:** Dirichlet Process, Chinese Restaurant Process, Hierarchical Bayesian models
- **Causal Inference:** Structural causal models, counterfactual reasoning, etc
- **Advanced Deep Probabilistic Models:** Normalizing Flows, Energy-based models, GANs
- **Diffussion Models**: Image generation, protein structures generation, etc.
- **Probabilistic Robotics and Control:** SLAM, Kalman filters in control, Probabilistic model predictive control, Reinforment Learning, etc.

For further learning, consider attending the Nordic Probabilistic AI School.

Deliverable

To get credits for the course, you need to hand in a deliverable/assignment with the following contents:

- Describe a problem/dataset for which a probabilistic model can be used for analysis. Examples include:
  - Based on your own PhD research (preferred!)
  - Taken from a public repository such as `www.kaggle.com` or `https://archive.ics.uci.edu`
- Design a probabilistic model for solving the problem.
- Implement your model in *Pyro*.
- Use the implementation to perform an analysis, for example:
  - Learn and apply a classifier
  - Perform Bayesian inference to compute distributions over quantities of interest (e.g., parameters, latent variables, etc.)
- Document your approach and findings in a short report (3-5 pages).

Deadline: 30th April 2025

A majestic oil painting of a raccoon Queen wearing red French royal gown. The painting is hanging on an ornate wall decorated with wallpaper.

Imagen

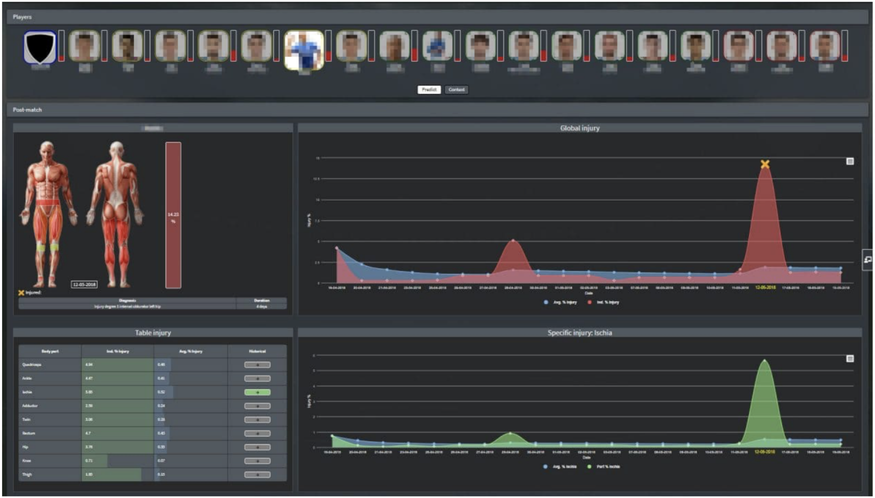
unprecedented photorealism × deep level of language understanding

Google Research, Brain Team

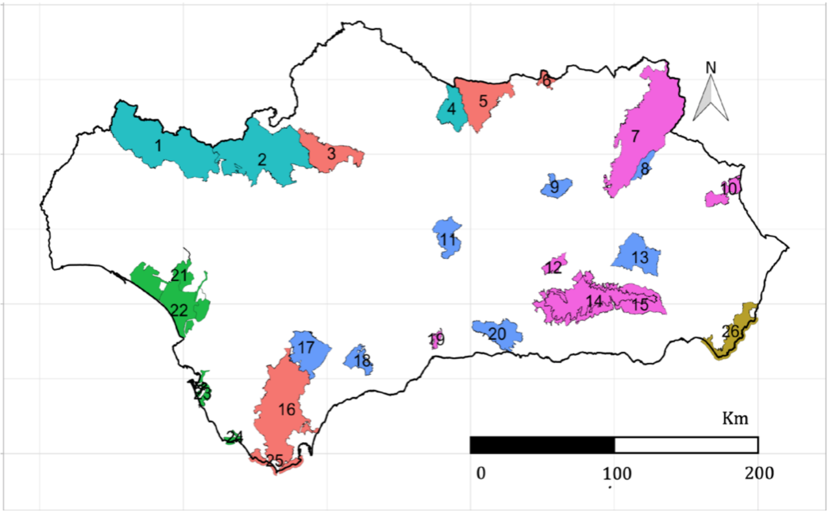
Generating images from written descriptions

Examples: ML for Self-driving cars

Can I predict an event in advance so that I can avoid it?



What should I do to prevent players from being injured?



Monitoring protected areas

"I always wondered how it would be if a
Superior species landed on Earth and showed us
How they played chess. Now I know it."

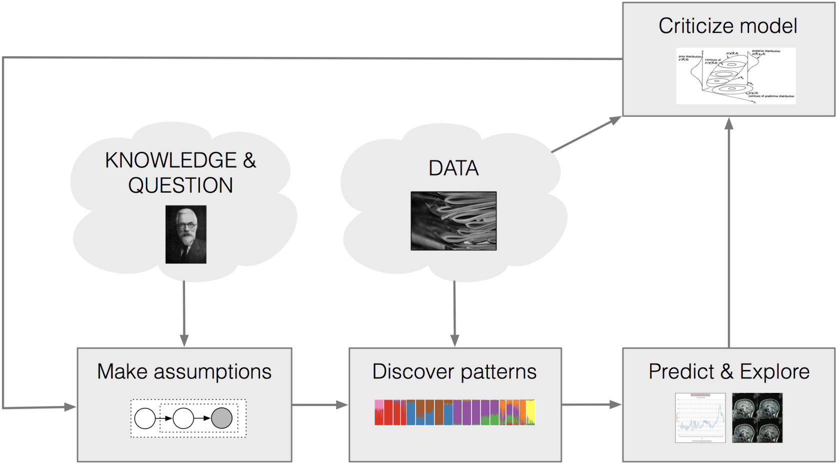
Peter Heine Nielsen.
Chess Grand Master and Magnus Carlsen's coach

Definition:

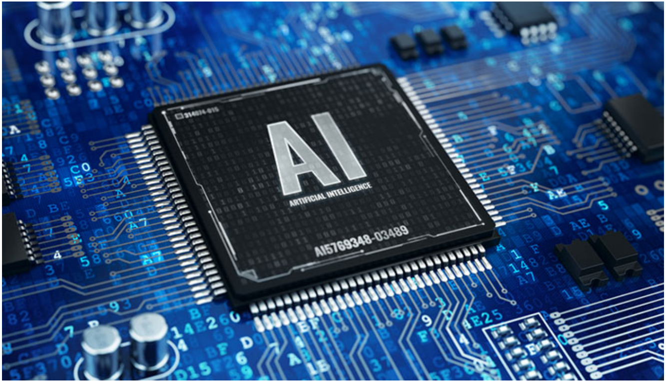
- **Probabilistic Machine Learning** integrates probability theory with machine learning to model uncertainty about predictions, parameters, and data-generating processes.
- By treating unknown quantities as **random variables**, it quantifies confidence in inferences and predictions - an important aspect for real-world decision-making.

Motivating Example: Medical Diagnosis

- Instead of making a **binary decision** (e.g., "the patient has the disease" or "the patient does not"), a **probabilistic approach** provides a distribution over possible diagnoses.
- For example, a **probabilistic model** determines that a patient has a 70% chance of having a particular disease based on symptoms and test results, helping in making **informed medical decisions**.

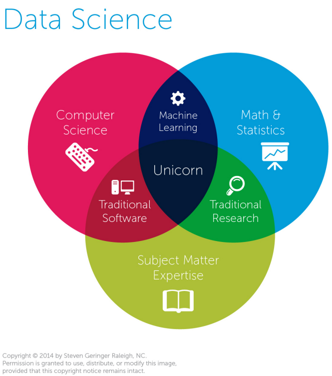


[Box, 1980; Rubin, 1984; Gelman+ 1996; Blei, 2014]



The development of machine learning systems requires enormous efforts.

- It can be a **highly technical** task.



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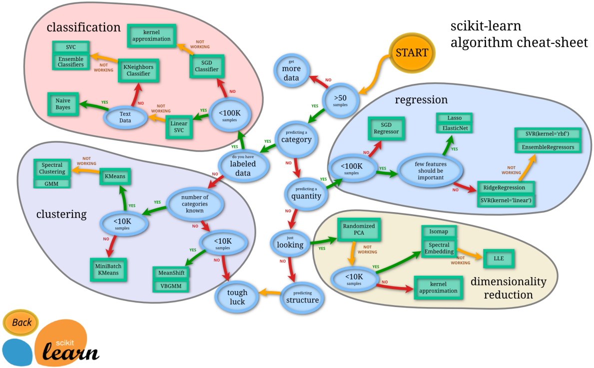

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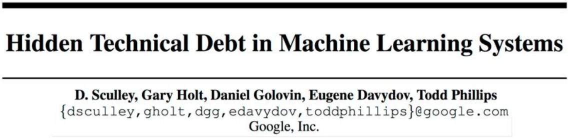
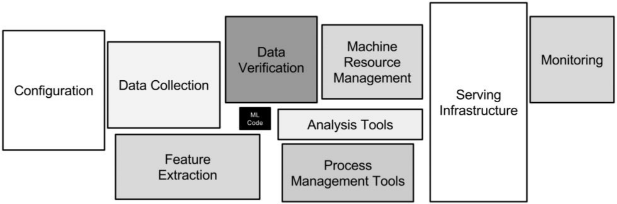


Hidden Technical Debt in Machine Learning Systems

D. Sculley, Gary Holt, Daniel Golovin, Eugene Davydov, Todd Phillips
{dsculley,gholt,dgg,edavydov,toddphillips}@google.com
Google, Inc.



The development of **machine learning systems** requires enormous efforts.

- It can be a **highly technical** task.
- It requires of **highly qualified experts.**
- It is difficult to find the **ML model most suitable** for an application.
- Programming a ML model is a **complex task**; many problems are intermingled.

Machine Learning Libraries

Claire D. Costa. Best Python Libraries for Machine Learning and Deep Learning.
https://towardsdatascience.com/best-python-libraries-for-machine-learning-and-deep-learning-b0bd40c7e8c

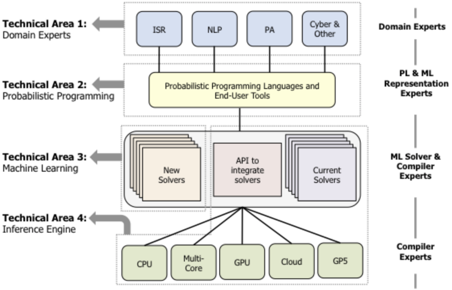
Machine Learning Libraries:

- **High-quality**, well-maintained, and open-source libraries
- Provide **high-level abstractions**.
- Hide **low level details** under the hood.
- Increase the **adoption** of the technologies.

What about in Probabilistic AI?

Which are the "high-level libraries" in Probabilistic AI?

Programming languages (PPLs)

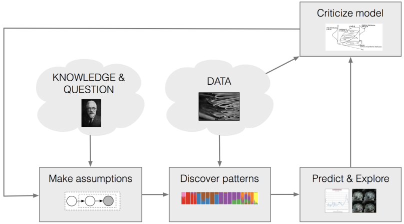


PPLs as high-level programming languages for **probabilistic ML systems**:

- Stacked architecture.
- Different Domain Experts can code their models using the same language.
- ML experts can focus on the development of ML methods/algorithms (ML solvers).
- Compiler experts can focus on running these ML solvers on specialized hardware.

Why probabilistic programming languages (PPLs)?

Box's Loop



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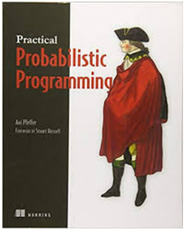
Benefits of PPLs for developing probabilistic machine learning systems:

- Simplify probabilistic machine learning model code.
- Reduce development time and cost to encourage experimentation.
- Reduce the necessary level of expertise.
- "Democratization" of the development of probabilistic ML systems.

PPLs



1st Generation of PPLs :

- Bugs, WinBugs, Jags, Figaro, etc.
- Turing-complete probabilistic programming languages. (i.e. they can represent any computable probability distribution).
- Inference engine based on Monte Carlo methods.
- Not able to scale to large data samples/high-dimensional models.

2nd Generation of PPLs :

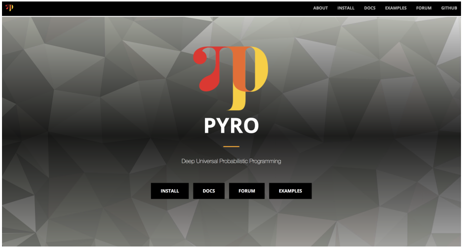
- Infer.net, Factorie, Amidst, etc.
- Inference engine based on message passage algorithms and/or variational inference methods.
- Scale to large data samples/high-dimensional models.
- Restricted probabilistic model families (i.e. factor graphs, conjuage exponential family, etc.)

PPLs

3rd Generation of PPLs :

- Pyro, Stan, PyMC, InferPy, etc.
- Black Box Variational Inference and Hamiltonian Monte-Carlo.
- Scale to large data samples/high-dimensional models.
- Turing-complete probabilistic programming languages.
  - Strong focus on probabilistic models with **deep neural networks**.
- Most rely on deep learning frameworks (Pytorch, JAX, TensorFlow, etc).
  - Specialized hardware like GPUs, TPUs, etc.
  - Automatic differentiation methods.

Pyro



Pyro's main features (`www.pyro.ai`) :

- Initially developed by UBER (the car riding company).
- Community of contributors and a dedicated team at Broad Institute (US).
- Rely on Pytorch (Deep Learning Framework).
- Enable GPU accelaration and distributed learning.

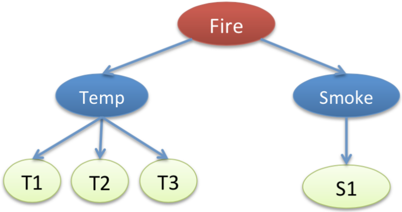
Probabilistic Graphical Models

A Bayesian Network is a **directed acyclic graph (DAG)** where:

- **Nodes represent random variables** (e.g., Fire, Temp., Smoke, and Sensors).
- **Edges represent probabilistic dependencies** between variables. If there is an edge from node A to node B, it means that A has a direct influence on B.

Example: The network structure captures **causal relationships** between events. In our case:

- **Fire** is the root cause, influencing both **Temperature** and **Smoke**.
- **Temperature** affects three independent temperature sensors (**T1, T2, T3**).
- **Smoke** affects a single smoke sensor (**S1**).



$$p(f, t, s, t_1, t_2, t_3, s_1) = p(t_1|t)p(t_2|t)p(t_3|t)p(s_1|s)p(t|f)p(s|f)p(f)$$

Bayesian networks: definition

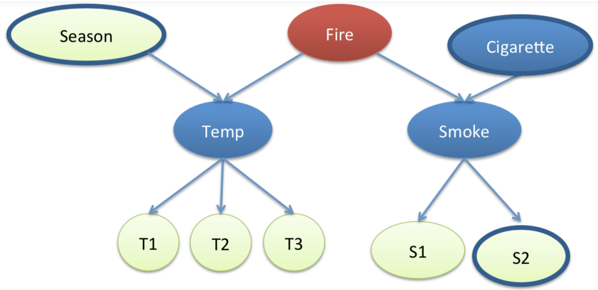
A Bayesian network over random variables $X_1, \dots, X_n$ consists of

- A DAG $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ with $\mathcal{V} = \{X_1, \dots, X_n\}$
- A set of local conditional distributions $\mathcal{P} = \{p(X_i|pa(X_i)), X_i \in \mathcal{V}\}$ where $pa(X_i)$ denotes the parents of X_i according to $\mathcal{E}$

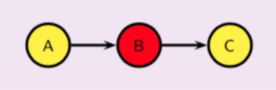
Every Bayesian network encodes a joint distribution factorized as

$$p(X_1, \dots, X_n) = \prod_{i=1}^{n} p(X_i|pa(X_i))$$

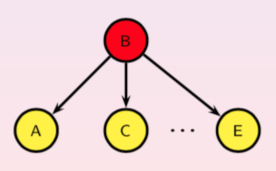
Bayesian networks: modular structure



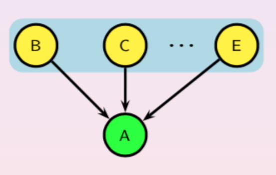
- Serial connection



- Diverging connection



- Converging connection



Inference

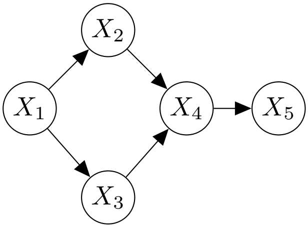
Inference in Bayesian networks

Assume a Bayesian network over variables $\mathbf{X} = \{X_1, \dots, X_n\}$

$$\left.\begin{array}{c}\text{Bayesian network}\\[1em] +\\[1em] \text{Evidence } (\mathbf{X}_E)\end{array}\right\} \Rightarrow P(\mathbf{X}_I|\mathbf{X}_E)?$$

Inference methods

- Exact
  - Brute force: compute $P(\mathbf{X}, \mathbf{X}_E)$ and marginalize out $\mathbf{X} \setminus \mathbf{X}_I$
  - Take advantage of the network structure
- Approximate
  - Sampling
  - Deterministic



- We are interested in X_5
- All variables are discrete
- $E = \emptyset$

$$
\begin{aligned}
p(x_5) &= \sum_{x_1 \ldots x_4} p(x_1, x_2, x_3, x_4, x_5) \\
&= \sum_{x_1 \ldots x_4} p(x_1)p(x_2|x_1)p(x_3|x_1)p(x_4|x_2, x_3)p(x_5|x_4) \\
&= \sum_{x_2 \ldots x_4} \sum_{x_1} p(x_1)p(x_2|x_1)p(x_3|x_1)p(x_4|x_2, x_3)p(x_5|x_4) \\
&= \sum_{x_2 \ldots x_4} p(x_4|x_2, x_3)p(x_5|x_4) \boxed{\sum_{x_1} p(x_1)p(x_2|x_1)p(x_3|x_1)} \\
&= \sum_{x_2 \ldots x_4} p(x_4|x_2, x_3)p(x_5|x_4)h(x_2, x_3)
\end{aligned}
$$

We have reached a similar problem as initially, but with one variable less.

Variable elimination algorithm

Input

$\mathcal{P}$: Conditional distributions in the network
$\mathbf{X}$: Variables in the network
X_I: Target variable
$\mathbf{X}_E$: Observed variables
$\mathbf{Y}$: All variables in $\mathbf{X}$ except X_I ($\mathbf{Y} = \mathbf{X} \setminus \{X_I\}$).

1. Restrict all the distributions in $\mathcal{P}$ to the evidence $\mathbf{X}_E = \mathbf{x}_E$
2. For each $Y \in \mathbf{Y}$,
    1. Let $\mathcal{P}_Y$ be the set of distributions in $\mathcal{P}$ that contain Y.
    2. $q := \prod_{p \in \mathcal{P}_Y} p$.
    3. $r := \sum_y q$.
    4. $\mathcal{P} := \mathcal{P} \setminus \mathcal{P}_Y \cup \{r\}$.
3. $p(x_I) = \prod_{p \in \mathcal{P}} p$.
4. Normalize p

Variable elimination algorithm

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Considerations about exact inference

- Product of functions raises complexity
  - Exponentially in the case of discrete variables
- Complexity also depends on the elimination order
- Representation of densities turns out to be relevant
  - Closed-form solutions to product and marginalization are preferable

Monte Carlo inference algorithms

- A Bayesian network is a representation of a joint probability distribution over $\mathbf{X} \Rightarrow$ it describes some population consisting of all the possible configurations of $\mathbf{X}$
- If the entire population was available, the inference problem could be solved exactly, basically by counting cases
- **Problem:** Population size can be huge or even infinite.
- Monte Carlo methods operate by drawing an artificial **sample** from it using some random mechanism
- The sample (much smaller than the population), is used to estimate the distribution of each variable of interest.

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Key issues in a Monte Carlo inference algorithm:

1. The sampling mechanism
2. The functions (estimators) which compute the probabilities from the sample

Importance sampling. General setting

- Assume we have a random variable X with density $p(x)$
- Importance sampling is a technique designed for estimating the expected value of a function $f(X)$. It is based on the following transformation:

$$\mathbb{E}_p[f(x)] = \int f(x)p(x)dx = \int \frac{p(x)}{p^*(x)} f(x)p^*(x)dx = \mathbb{E}_{p^*}\left[\frac{p(x)}{p^*(x)} f(x)\right],$$

where p^* is a density function called the sampling or proposal distribution, s.t. $p^*(x) > 0$ whenever $p(x) > 0$.

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  where p^* is a density function called the sampling or proposal distribution, s.t. $p^*(x) > 0$ whenever $p(x) > 0$.
- Therefore, $\mathbb{E}_p[f(x)]$ can be estimated by drawing a sample $x^{(1)}, \ldots, x^{(m)}$ from p^* and computing

$$\hat{\mathbb{E}}_p[f(x)] = \frac{1}{m}\sum_{j=1}^{m} \frac{p(x^{(j)})}{p^*(x^{(j)})} f(x^{(j)}),$$

  which is specially convenient if p^* is easier to handle than p

Markov Chain Monte Carlo (MCMC)

- We start with an initial configuration of the variables in the network
- A new item in the sample is generated conditional on the previous configuration
- The elements of the sample are no longer independent, instead they form a **Markov chain**

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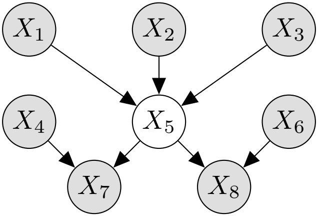
Gibbs sampling

A new item in the sample is generated by simulating each variable at a time conditional on the value of the other variables sampled so far:

- Assume $\mathbf{X} = \{X_1, \ldots, X_n\}$
- Let $\mathbf{x}^{(i)} = (x_1^{(i)}, \ldots, x_n^{(i)})$ be the current configuration
- A new configuration, $\mathbf{x}^{(i+1)}$ is generated by sampling each variable X_k, $k = 1, \ldots, n$ with

$$p(x_j^{(i+1)} | x_1^{(i+1)}, \ldots, x_{j-1}^{(i+1)}, x_{j+1}^{(i)}, \ldots, x_n^{(i)})$$



$$p^*(X_5) \propto p(X_5|X_1, X_2, X_3)p(X_7|X_4, X_5)p(X_8|X_5, X_6)$$

Problems

- Generating an initial configuration with positive probability can be hard
- The dependence between elements of the sample can make it converge slowly

Learning From Data

Thumbtack example

We have tossed a thumb tack 100 times. It has landed pin up 80 times, and we now look for the probability θ of pin up ($\rightsquigarrow$ model that best fits the observations/data):

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We can measure how well a model fits the data using the likelihood:

$$\begin{aligned} p(\text{data}|\theta) &= p(\text{pin up}, \text{pin up}, \text{pin down}, \ldots, \text{pin up}|\theta) \\ &= p(\text{pin up}|\theta) \cdot p(\text{pin up}|\theta) \cdot p(\text{pin down}|\theta) \cdot \ldots \cdot p(\text{pin up}|\theta) \end{aligned}$$

Thumbtack example

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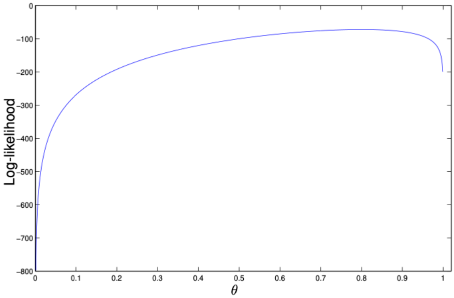
We select the parameter $\hat{\theta}$ that maximizes:

$$\hat{\theta} = \arg\max_{\theta} p(\text{data}|\theta) \left(\text{or } \log p(\text{data}|\theta) \right)$$
$$= \arg\max_{\theta} \prod_{i=1}^{100} p(x_i|\theta)$$
$$= \arg\max_{\theta} \theta^{80}(1-\theta)^{20}.$$



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By setting:

$$\frac{d}{d\theta}\theta^{80}(1-\theta)^{20} = 0 \qquad \left(\text{or } \frac{d}{d\theta}\log(\theta^{80}(1-\theta)^{20}) = 0\right)$$

we get the *maximum likelihood estimate*:

$$\hat{\theta} = 0.8.$$

- A random variable X
- A probability density/mass function p associated with X
- A parameter θ, whose value is fixed but unknown
- We assume p is known except for parameter θ, and denote this fact as $p(x|\theta)$
- For a sample $X_1, \ldots, X_n$ drawn from $f(x|\theta)$, the likelihood of the data is

$$p(x_1, \ldots, x_n|\theta) = \prod_{i=1}^{n} p(x_i|\theta)$$

  i.e. the joint density/mass of the sample regarded as a function of the parameter
- Learning problem is to find the parameter that maximize the log-likelihood of the data:

$$\max_{\theta} \ln p(x_1, \ldots, x_n|\theta)$$

Bayesian parameter learning

Basis

- Parameters are modeled as random variables and information about them can be included prior to observing data
- By Bayes' rule, the prior information is combined with the likelihood, yielding a posterior distribution that is used for making inferences about the parameter

More formally Parameter learning amounts to calculating the posterior distribution over the parameters given the data $\mathcal{D} = (\mathbf{x}_1, \ldots, \mathbf{x}_N)$:

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

$$p(\mathcal{D} \,|\, \boldsymbol{\theta}) = \prod_{i=1}^{N} p(\mathbf{x}_i \,|\, \boldsymbol{\theta}) \qquad \text{[Assuming independently sampled data]}$$

Posterior predictive distribution

For making predictions about future cases we use

$$p(\mathbf{X} \,|\, \mathcal{D}) = \int_{\boldsymbol{\theta}} p(\mathbf{X} \,|\, \boldsymbol{\theta}) p(\boldsymbol{\theta} \,|\, \mathcal{D}) d\boldsymbol{\theta}$$

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Posterior predictive distribution

For making predictions about future cases we use

$$p(\mathbf{X} \mid \mathcal{D}) = \int_{\boldsymbol{\theta}} p(\mathbf{X} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta} \mid \mathcal{D}) d\boldsymbol{\theta}$$

Model and data

Consider the variables $X_1, X_2, \ldots, X_N$ with $P(X_i|\theta) = \theta$:

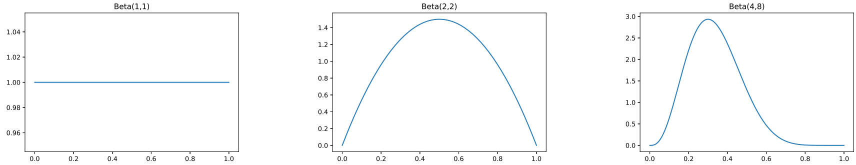
- $X_i = 1$ represents pin up and $X_i = 0$ represents pin down
- $\theta \in [0, 1]$ is the probability of pin up

Prior

The beta distribution Beta$(\theta \mid a, b)$ over θ:

$$p(\theta) \propto \theta^{a-1}(1 - \theta^{b-1}),$$

where a and b are hyper parameters.



Model and data

Suppose that $X_1, X_2, \ldots, X_N \sim \text{Ber}(\theta)$

- N_1 are the number of pin up
- N_0 are the number of pin down $(N = N_0 + N_1)$

Model and data

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Posterior

$$p(\theta \mid \mathcal{D}) = \text{Beta}(\theta \mid a + N_1, b + N_0)$$

Model and data

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Posterior

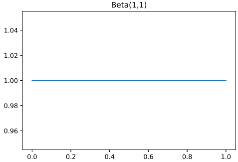
$$p(\theta \mid \mathcal{D}) = \text{Beta}(\theta \mid a + N_1, b + N_0)$$

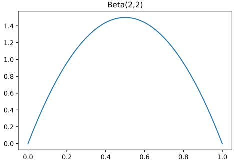
Posterior predictive distribution

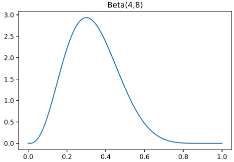
$$\begin{aligned} p(X_{N+1} = 1 \mid \mathcal{D}) &= \int_0^1 p(X_{N+1} = 1 \mid \theta) p(\theta \mid \mathcal{D}) d\theta \\ &= \int_0^1 \theta \text{Beta}(\theta \mid a + N_1, b + N_0) d\theta = \frac{a + N_1}{a + b + N} \end{aligned}$$

Assume that $N_0 = 5$ and $N_1 = 9$.

Prior







Posterior