Variational Auto-Encoders
Part One

CS109B Data Science 2

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Outline

- Motivation for Variational Autoencoders (VAE)
- Inference in Neural Networks
  - Bayesian Linear Regression
  - Bayesian Neural Networks
  - Introduction to variational methods
  - Variational Autoencoder as an inference model
- Variational Autoencoders as generative model
  - Separability of VAE
  - Tips & tricks
  - Other generative models

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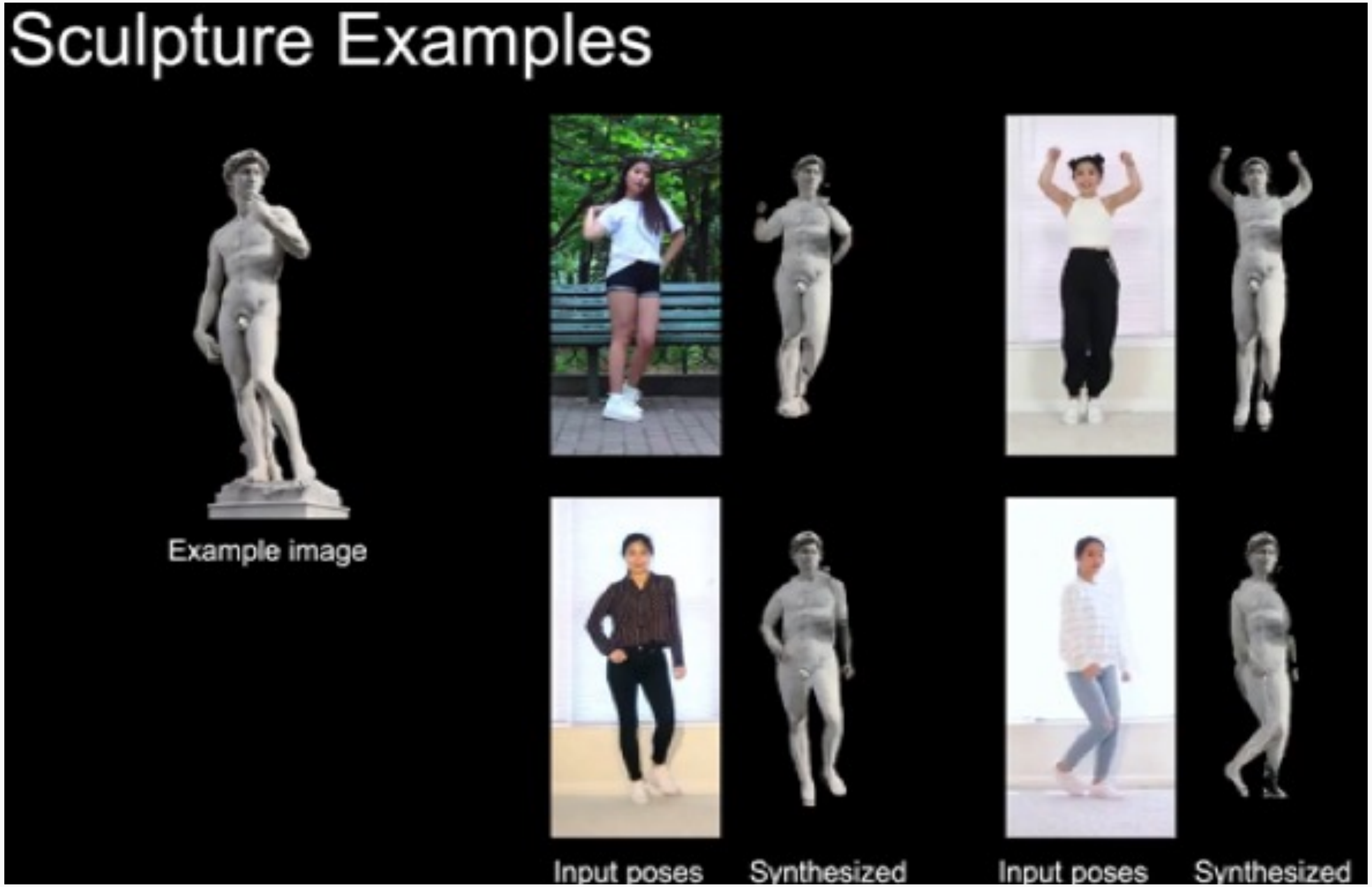
State of the Art in AI – sans NLP



https://nvlabs.github.io/few-shot-vid2vid/

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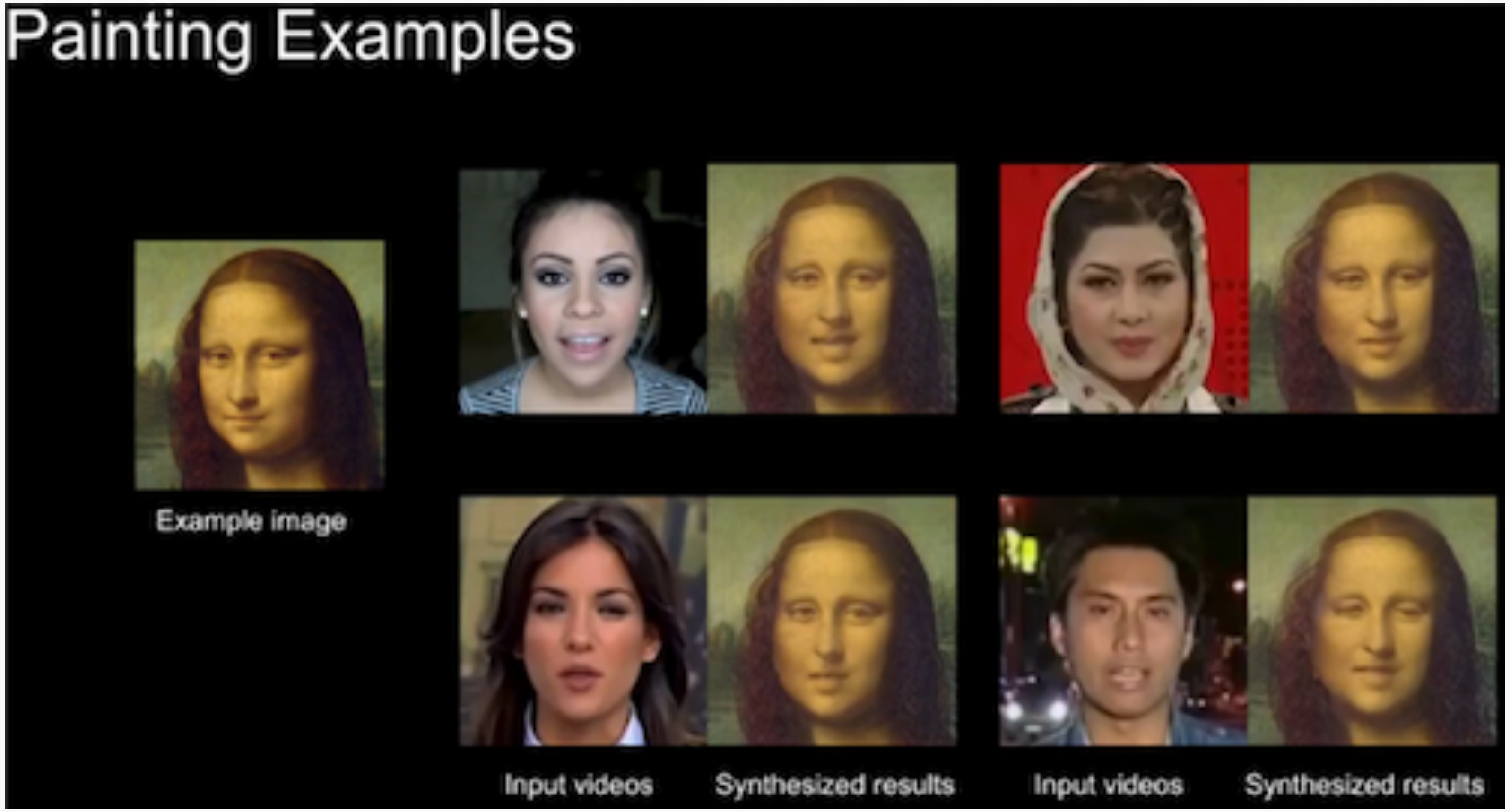

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Generative Modeling

https://github.com/tkarras/progressive_growing_of_gans

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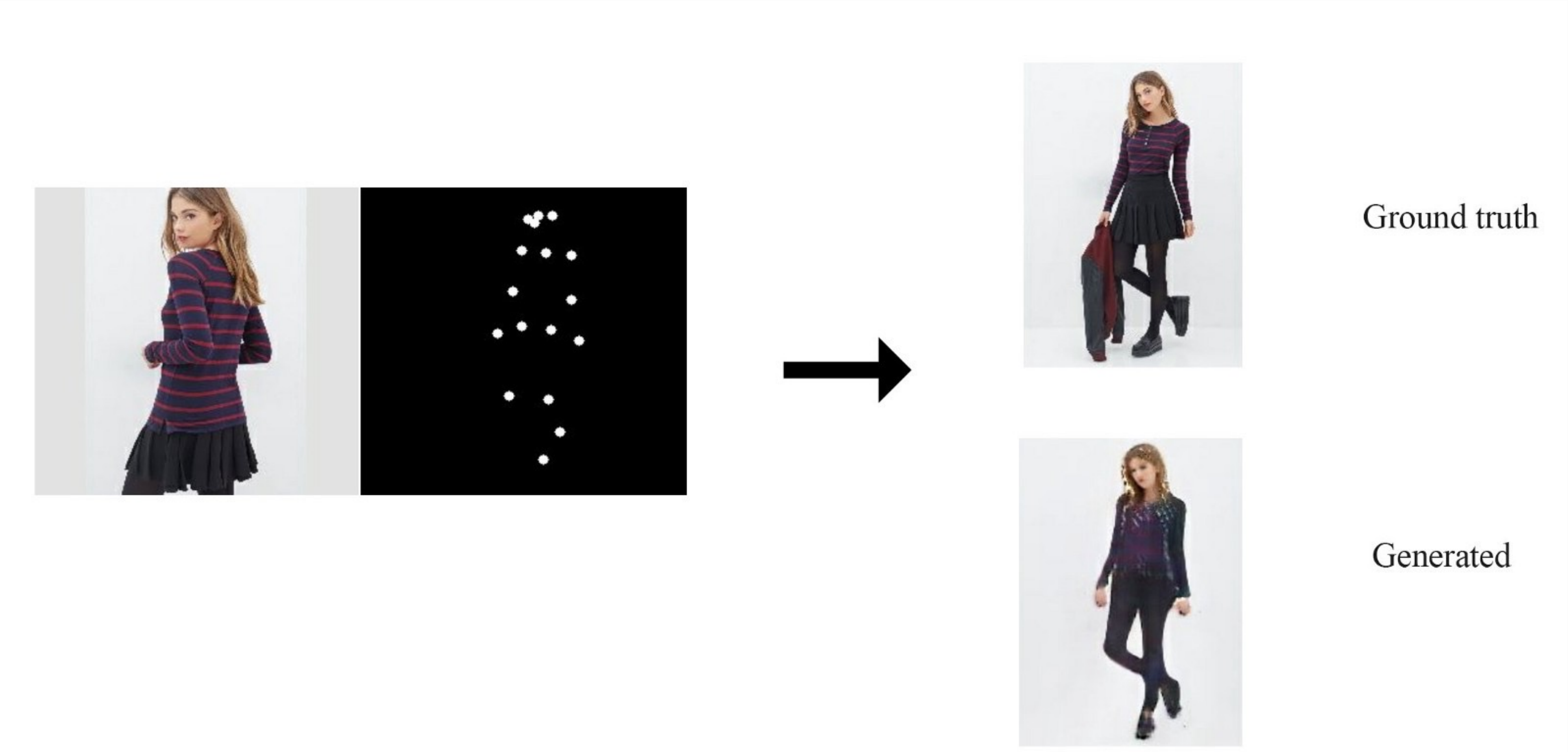
Generative Modeling

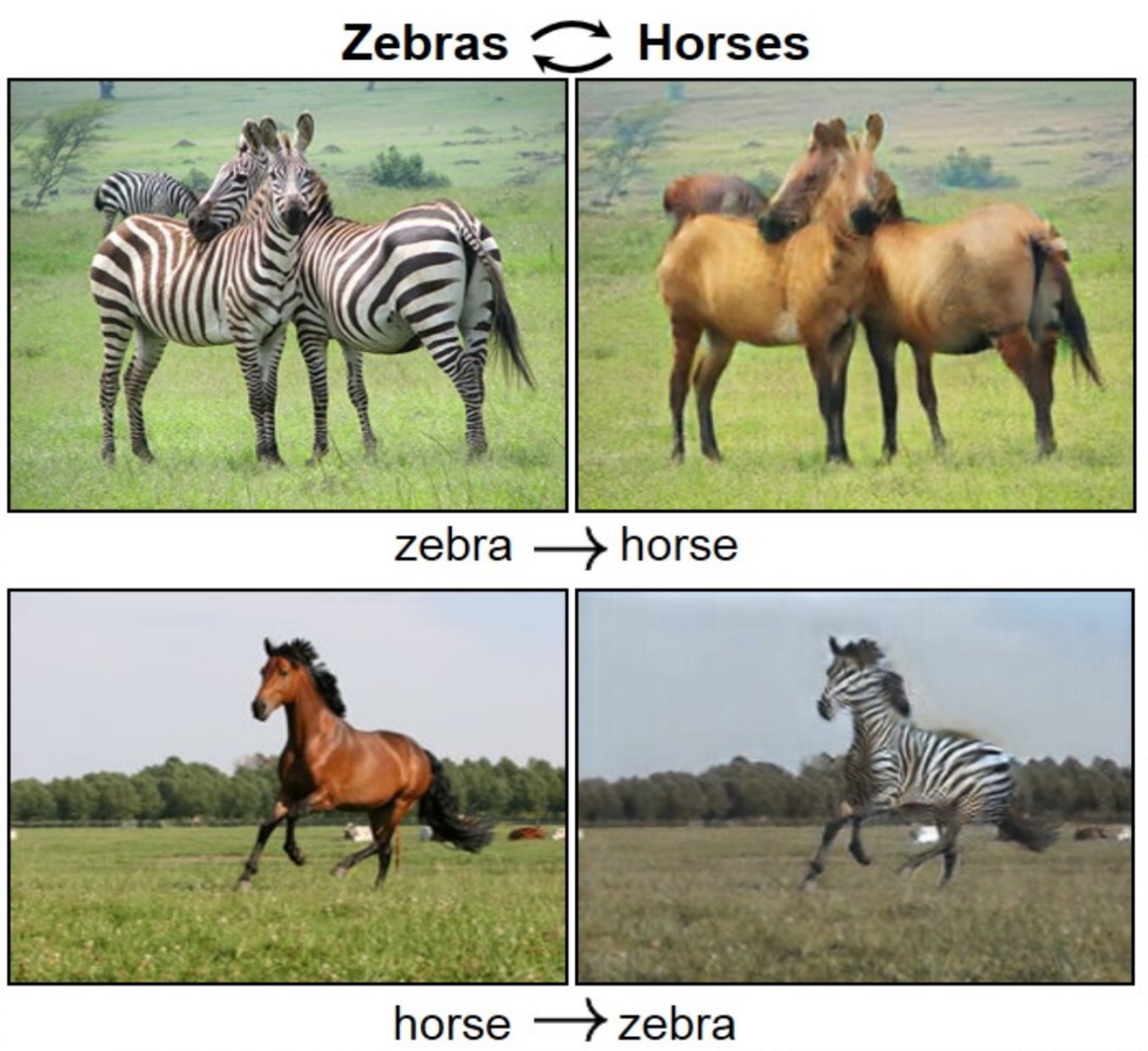
Figure 7: Generated samples

https://arxiv.org/pdf/1708.05509.pdf

Generative Modeling



Generative Modeling



(a) MidiNet model 1

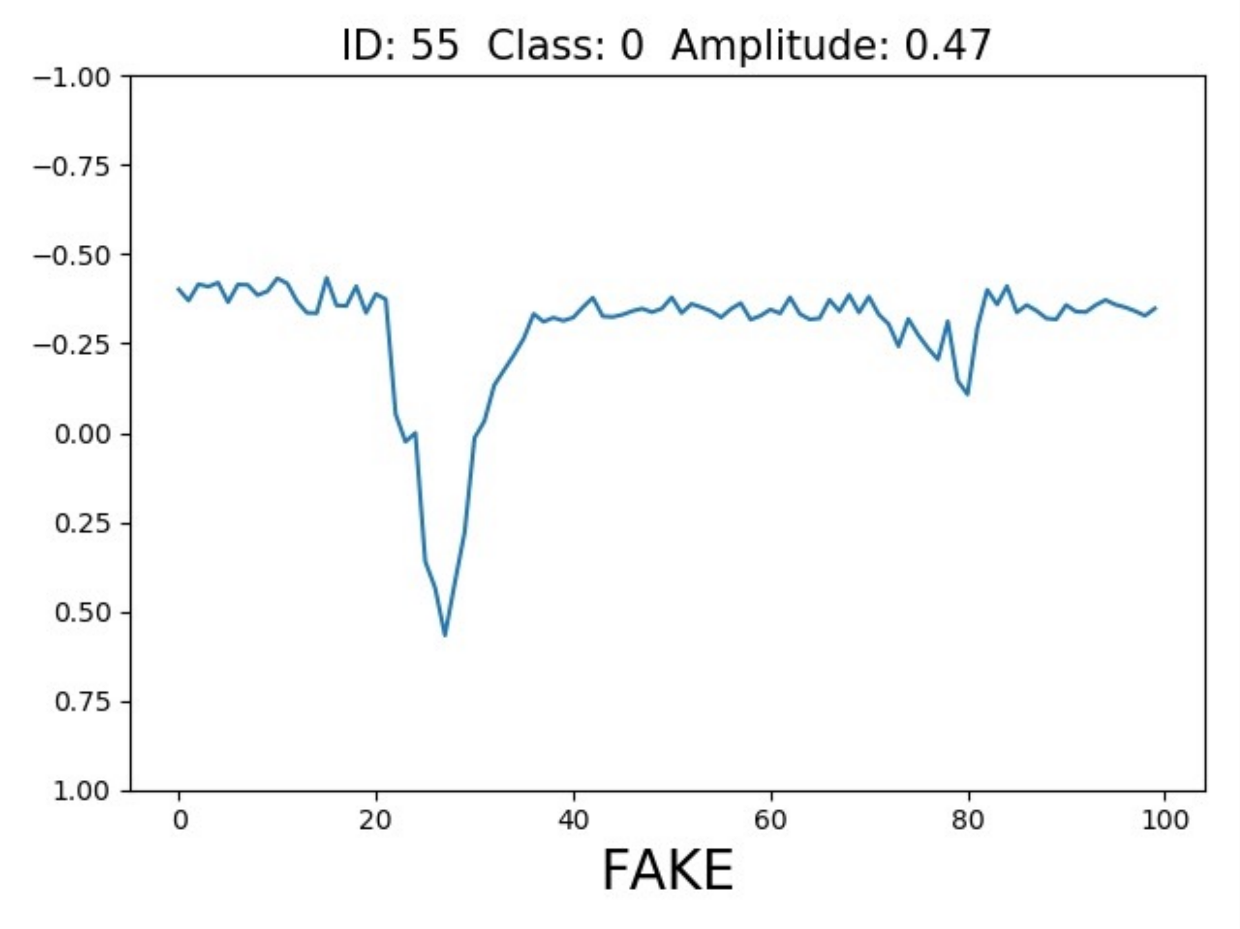
(b) MidiNet model 2

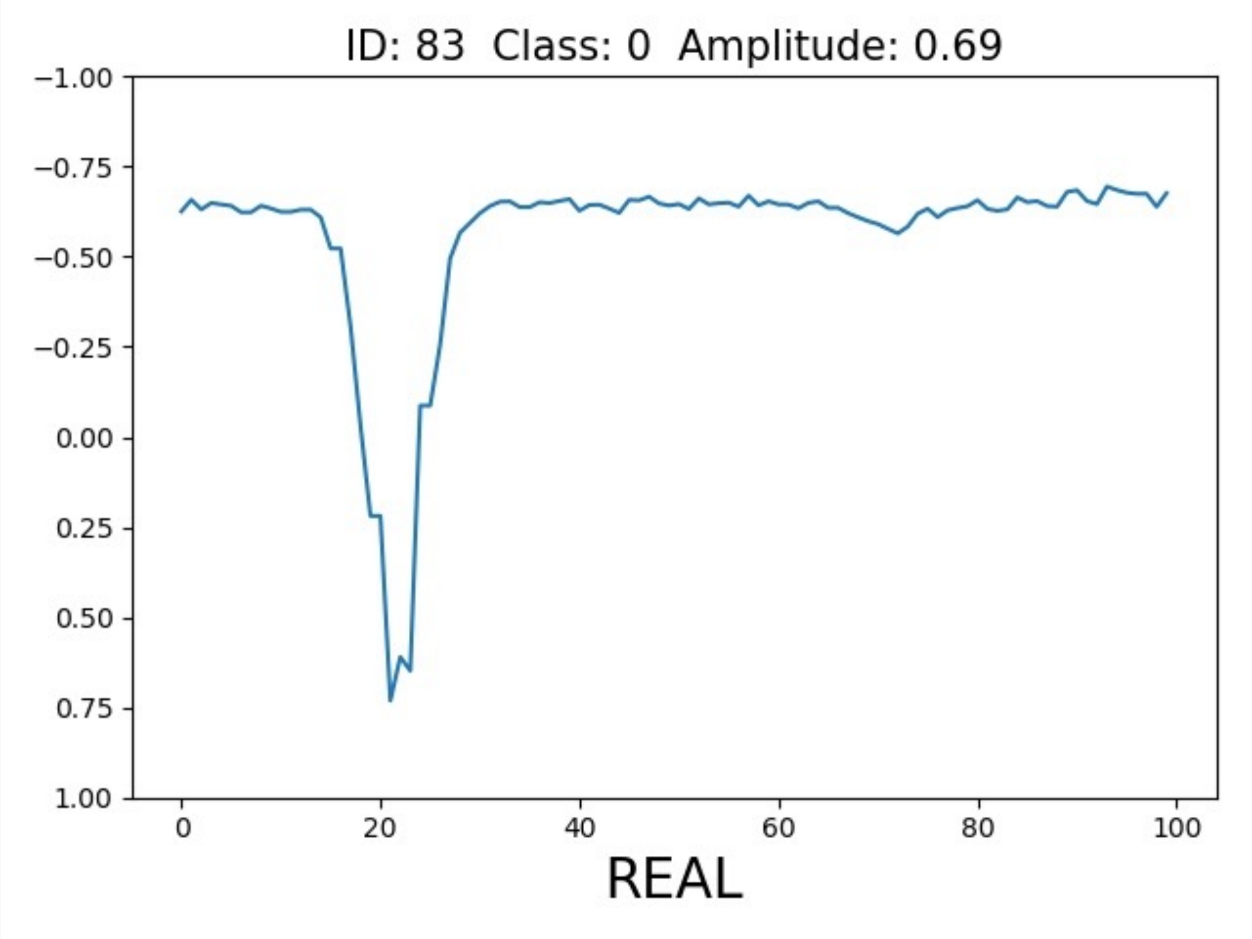
(c) MidiNet model 3

Figure 3. Example result of the melodies (of 8 bars) generated by different implementations of MidiNet.

Another use of generating new data is to give us ideas and options. Suppose we're planning a house. We can give the computer the space we have available, and its location. From this, the computer can can give us some ideas.

Big networks require big data, and getting high-quality, labeled data is difficult. If we're generating that data our selves, we can make as much of it as we like.



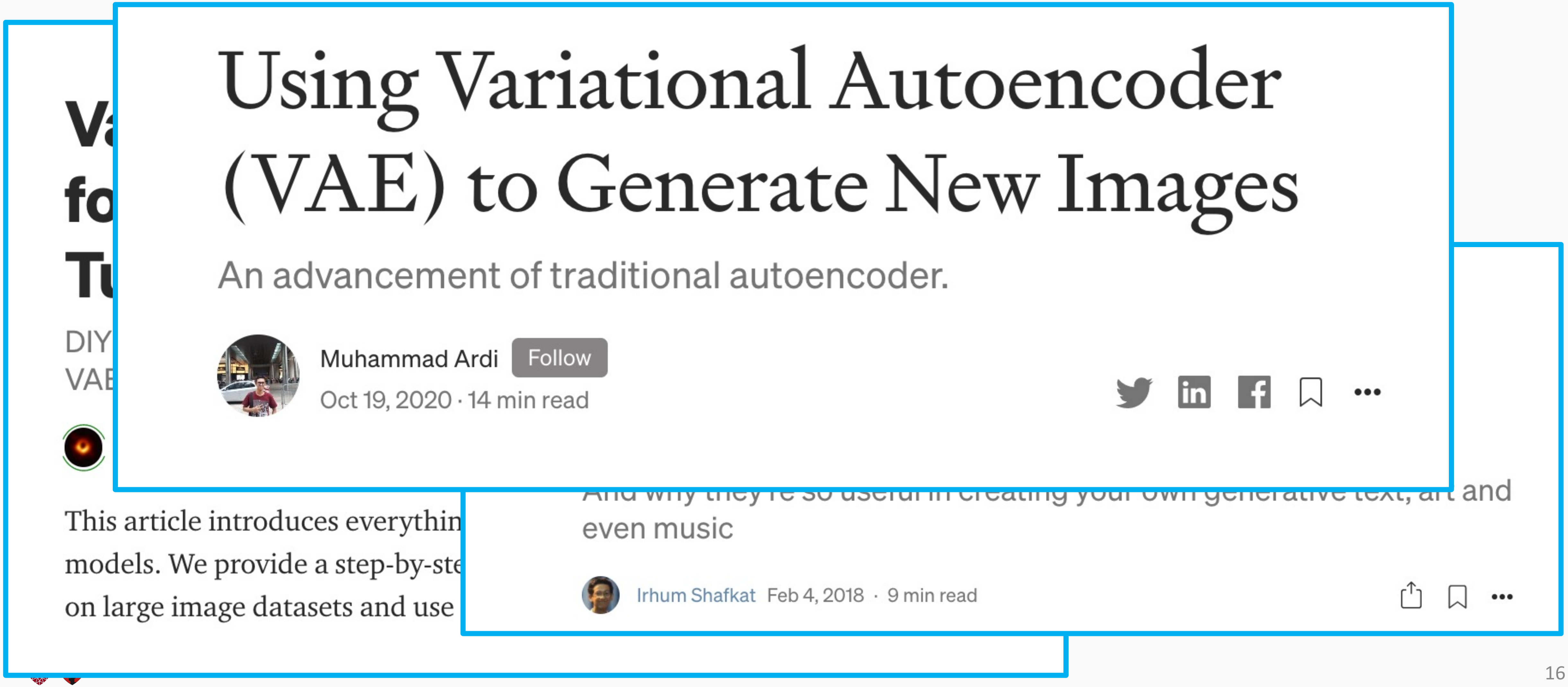


To summarize:

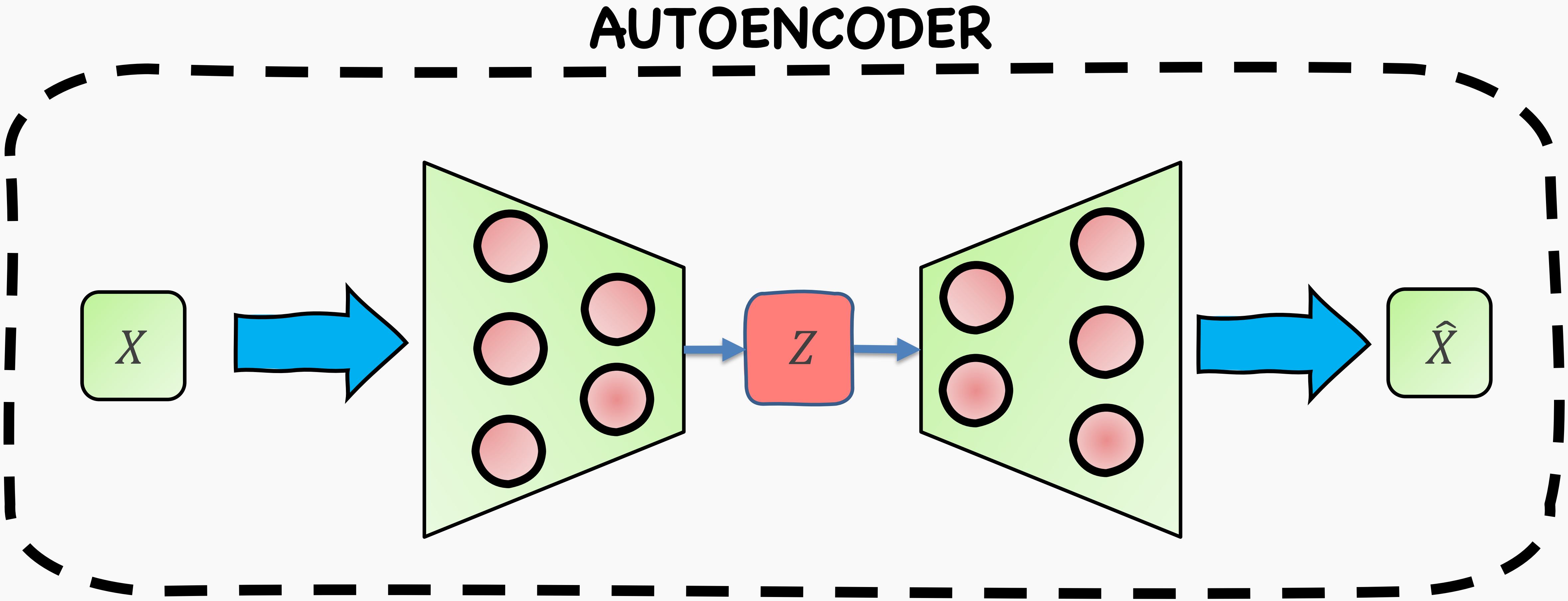
VAEs are a form of generative models

Variational AutoEncoder

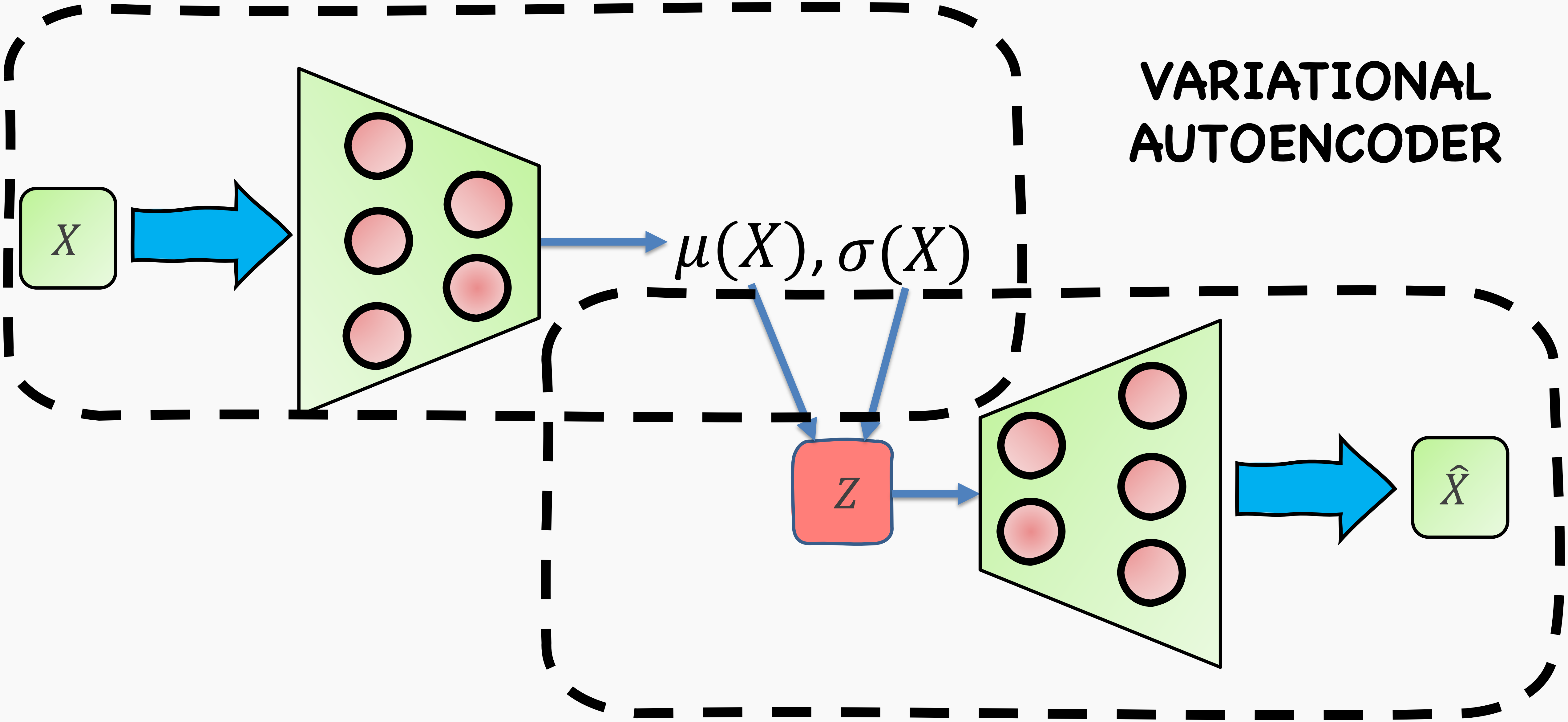
Popular explanations of VAE as generative models



RECAP: Vanilla AutoEncoder



Variational AutoEncoder



Variational Autoencoders

Typical explanations include:

- We want a continuous latent space representation
- We use a *simple* Reparameterization "trick"
- We add an Estimated Lower Bound **(ELBO)** error to reconstruction term

Why are Variational Autoencoders built this way?

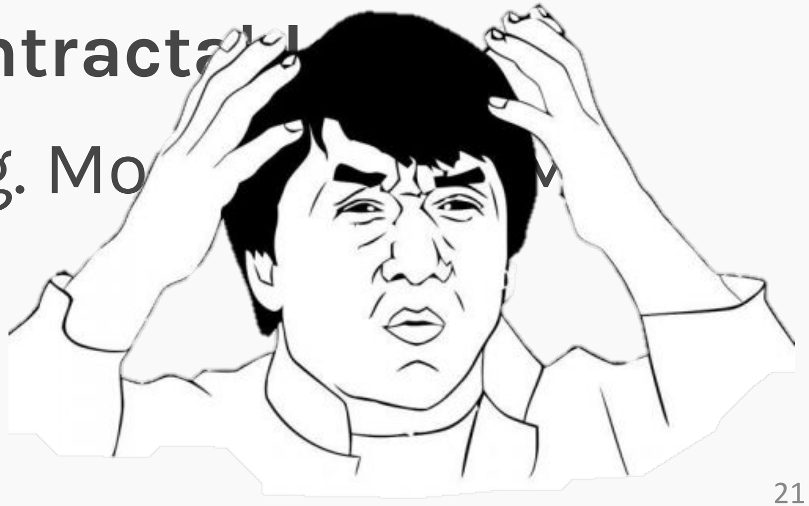
Variational AutoEncoder: Original Paper

Let us consider some dataset $X = \{x^{(i)}\}_{i=1}^{N}$ consisting of N i.i.d. samples of some continuous or discrete variable x. We assume that the data are generated by some random process, involving an unobserved continuous random variable z.

…

We are interested in a general algorithm that works in case of:

1. *Intractability:* $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$ is **intracta**
2. *Large Dataset:* Sampling based solutions eg. Mo
   would be too slow



[Auto-Encoding Variational Bayes (Diederik P. Kingma et al)]

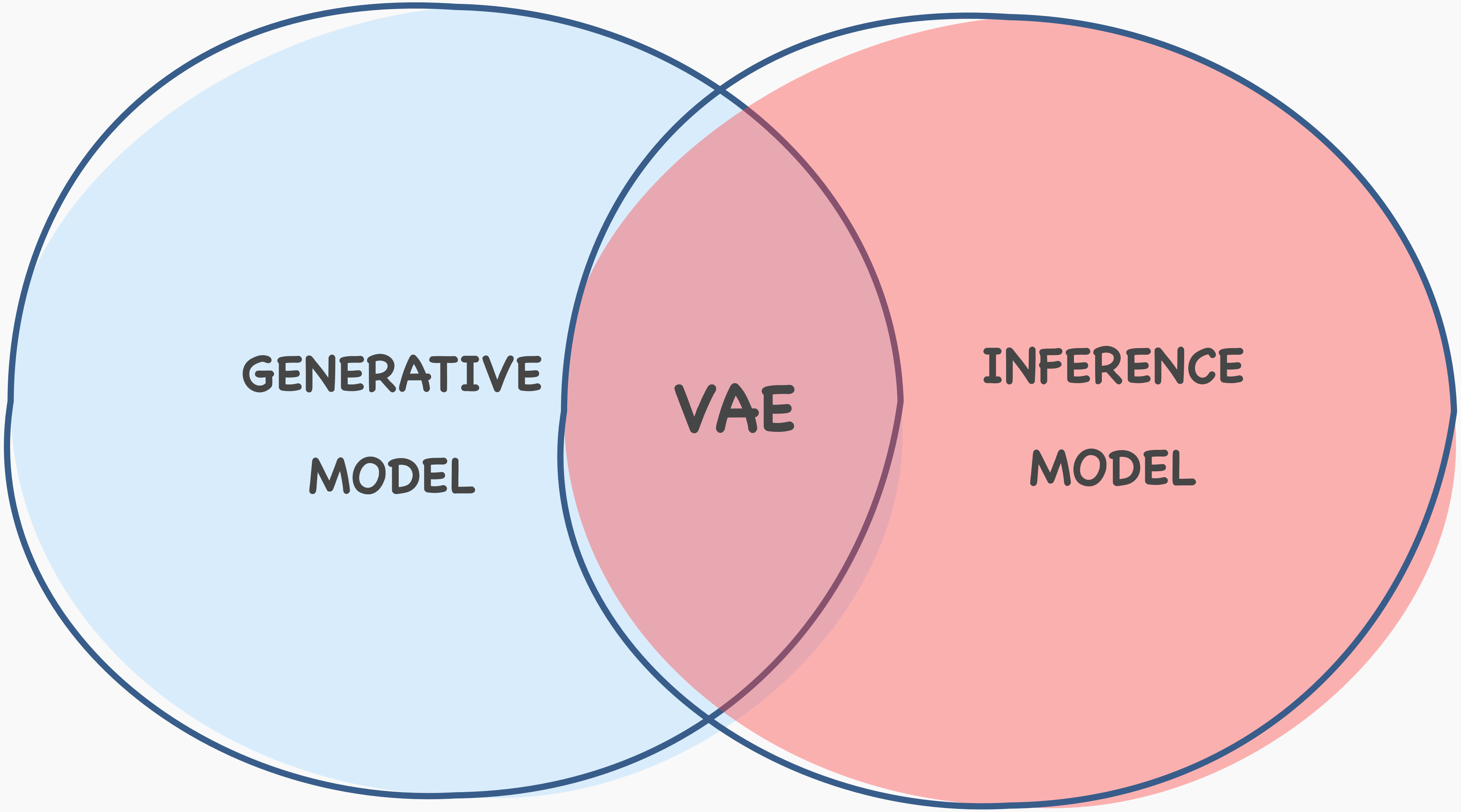
Variational Autoencoders as Inference models

The story of Variational Auto-encoders is like Coca-Cola

- Originally invented by John Pemberton to counter his own morphine addiction.
- Eventually found commercial success as a sugary drink and now is synonymous with soft beverages.

Source : https://en.wikipedia.org/wiki/Coca-Cola

Variational AutoEncoders




Are you ready?
BAYESIAN
LINEAR REGRESSION
BAYESIAN
NEURAL NETWORKS
VARIATIONAL
METHODS
VARIATIONAL
AUTO-ENCODERS
N
W
E
S

Bayesian Linear Regression

Inference Review

Bootstrap combined with Maximum Likelihood can give us the distribution of the coefficients.

Such a method is:

- Easy to understand
- Easy to implement
- Statistically equivalent to analytical solution

Inference Review

Let us begin by considering the case of linear regression:

$$y = f(x) + \epsilon \qquad \text{where} \qquad f(x) = \beta_0 + \beta_1 x$$

We interpret the ε term to be noise introduced by random variations in nature, or imprecisions of our scientific instruments and everything else.

If we knew the exact form of $f(x)$, for example, $f(x) = \beta_0 + \beta_1 x$, and there was no noise in the data , then estimating the $\hat{\beta}'s$ would have been exact.

Sometimes $\boldsymbol{\varepsilon}$ is considered as "catch-it-all" term

Confidence intervals for the predictors estimates (cont)

However, two things happen, which result in mistrust of the values of $\hat{\beta}'s$:

- observational error is always there – this is called ***aleatoric*** error, or ***irreducible*** error.
- we do not know the exact form of $f(x)$ - this is called ***misspecification*** error and it is part of the *epistemic* error.

We will put everything into the catch-it-all term ε.

Because of ε, every time we measure the response y for a fix value of x, we will obtain a different observation, and hence a different estimate of $\hat{\beta}'s$.

Confidence intervals for the predictors estimates (cont)

So, if we just have one set of measurements of $\{X, Y\}$, our estimates of $\hat{\beta}_0$ and $\hat{\beta}_1$ are just for this particular realization.

Question: If this is just one realization of the reality how do we know the truth? How do we deal with this conundrum?

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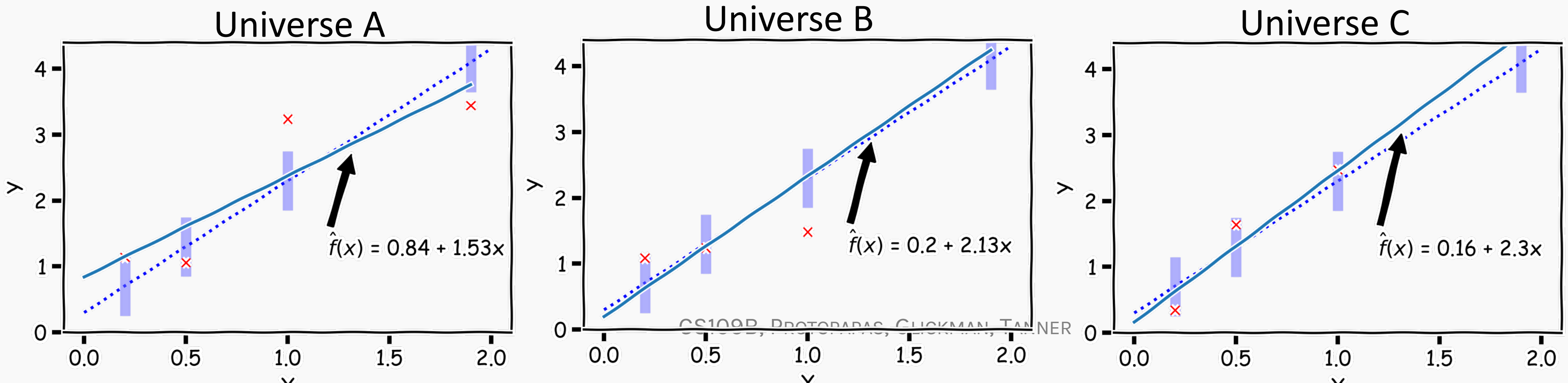
Imagine (magic realism) we have parallel universes, and we repeat this experiment on each of the other universes.



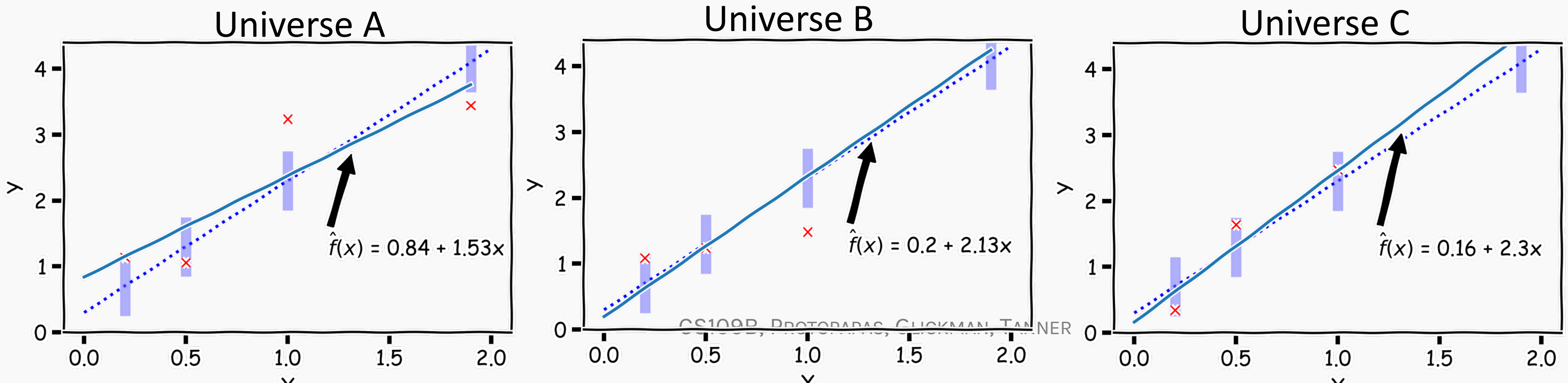
Confidence intervals for the predictors estimates (cont)

So, if we just have one set of measurements of $\{X, Y\}$, our estimates of $\hat{\beta}_0$ and $\hat{\beta}_1$ are just for this particular realization.

We use bootstrap to create different dataset.
Bootstrap is sampling with replacement.
Bootstrapping was covered **extensively** in CS109A.

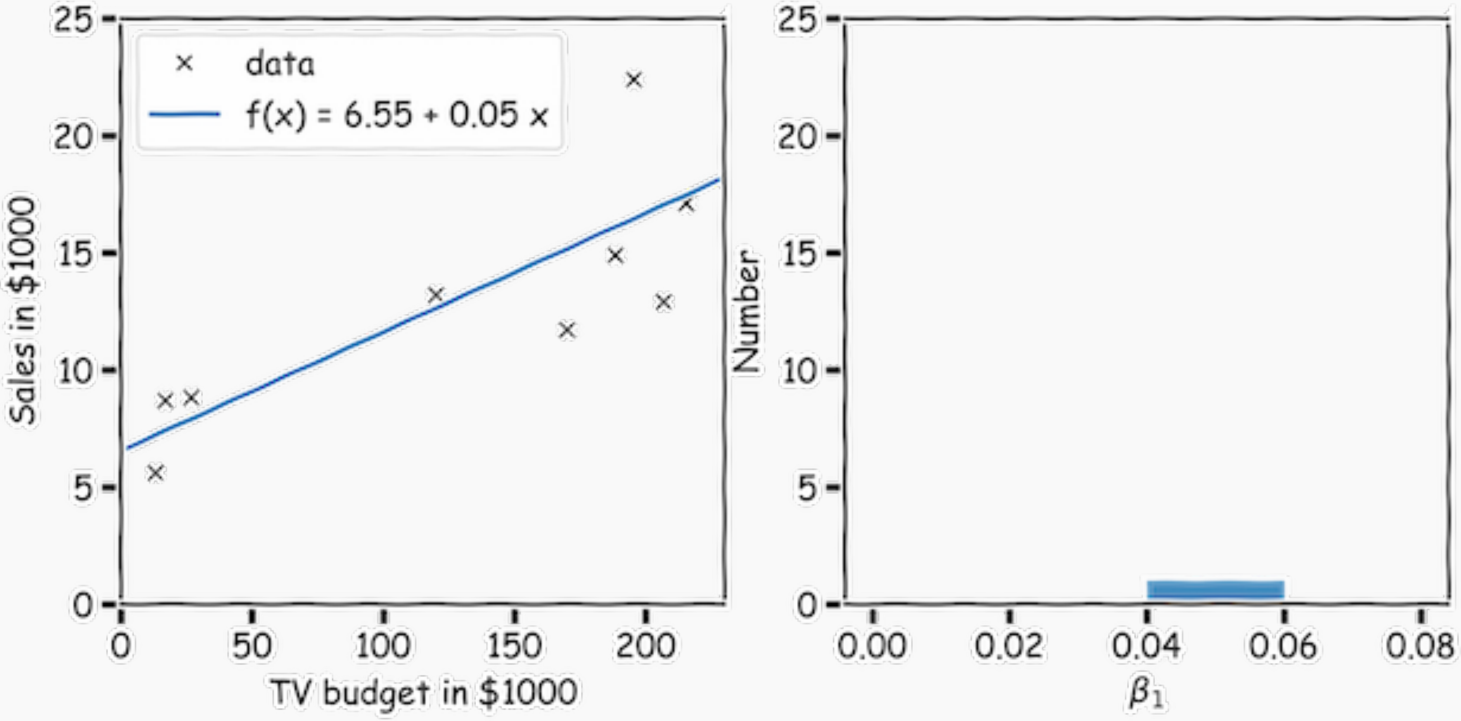
Question: If this is just one realizati
truth? How do we deal with this c

Imagine (magic realism) we have parallel universes, and we repeat this experiment on each of the other universes.



Confidence intervals for the predictors estimates (cont)

In our magical realisms, we can now sample multiple times. One universe, one sample, one set of estimates for $\hat{\beta}_0, \hat{\beta}_1$

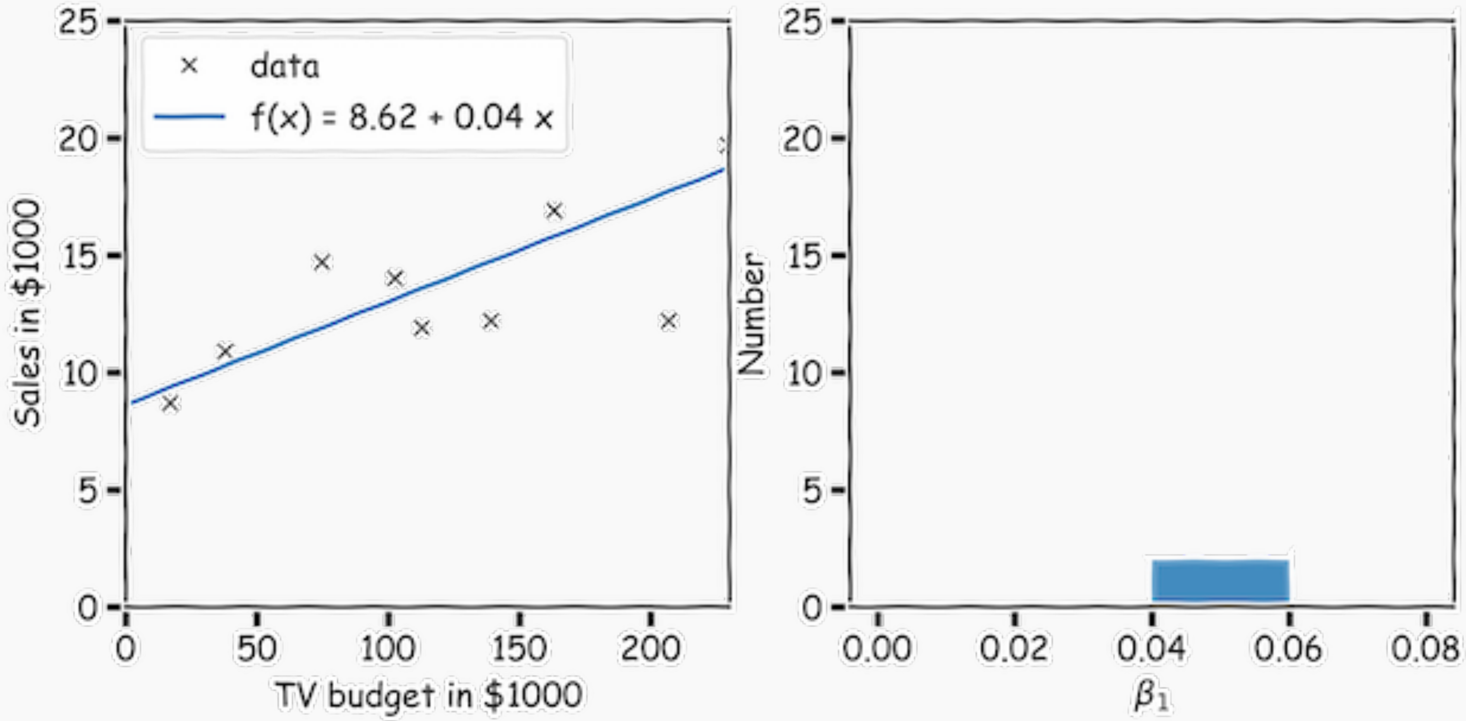


There will be an equivalent plot for $\hat{\beta}_0$ which we don't show here for simplicity

BOOTSTRAP

Confidence intervals for the predictors estimates (cont)

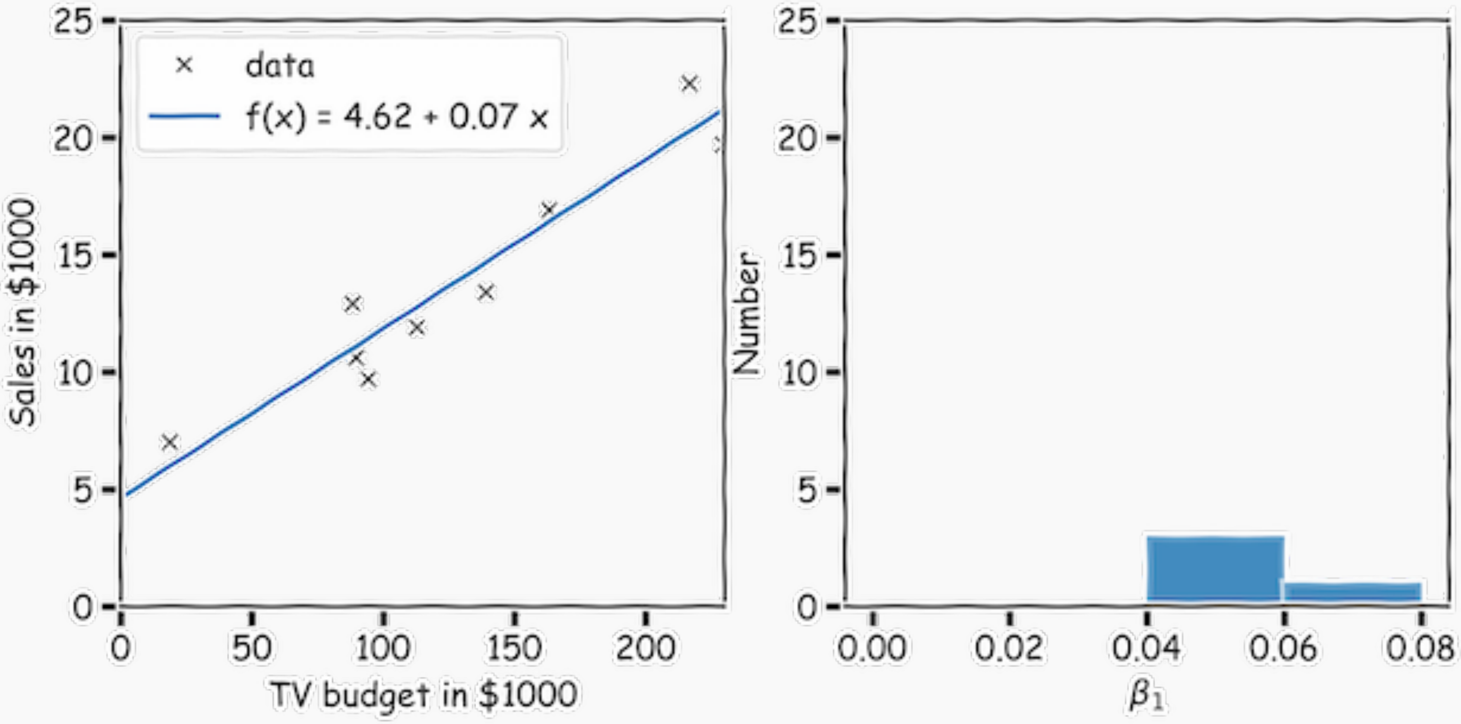
Another sample, another estimate of $\hat{\beta}_0, \hat{\beta}_1$



BOOTSTRAP

Confidence intervals for the predictors estimates (cont)

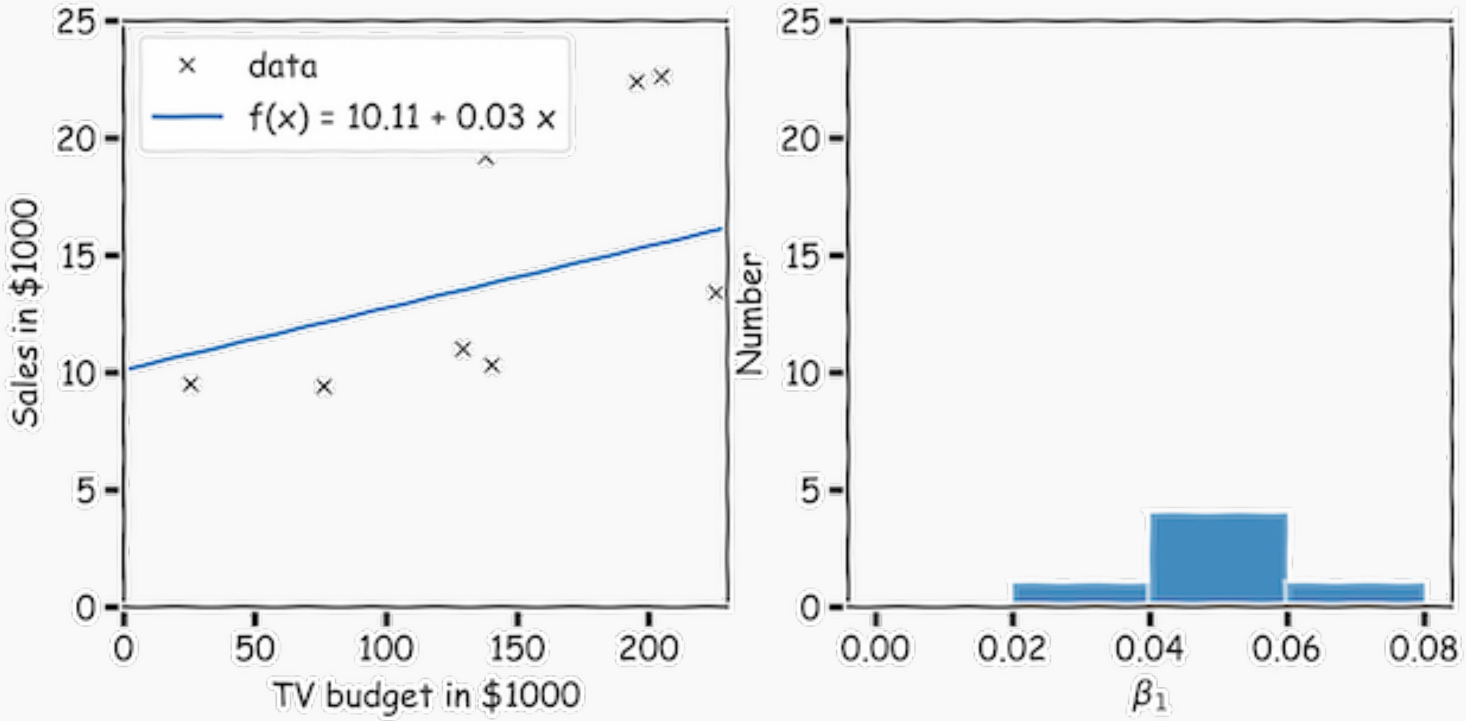
again



BOOTSTRAP

Confidence intervals for the predictors estimates (cont)

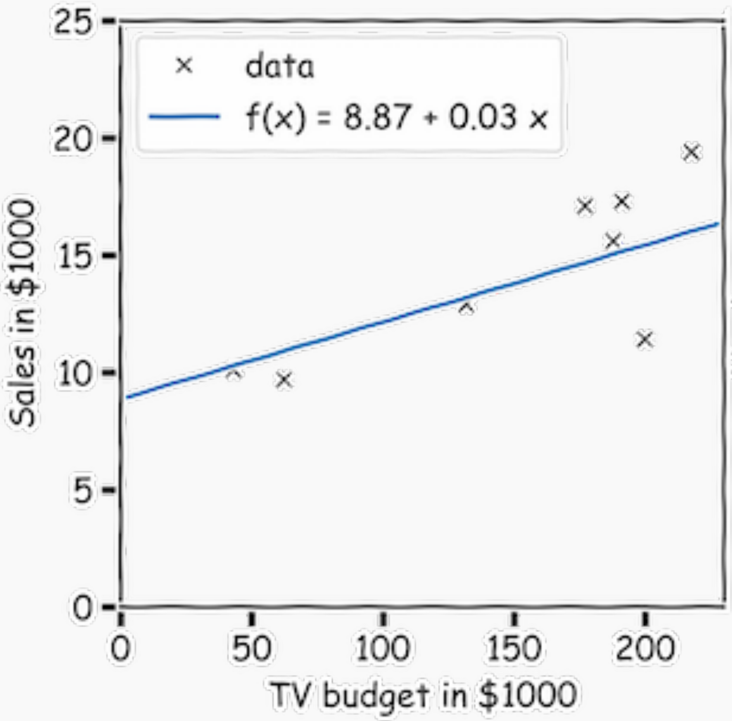
and again

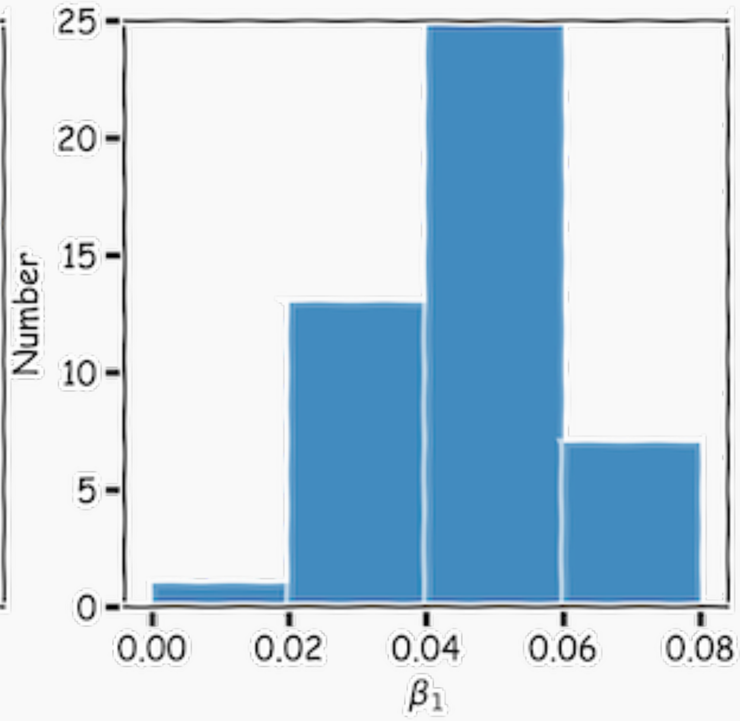


BOOTSTRAP

Confidence intervals for the predictors estimates (cont)

repeat this for 100 times, until we have enough samples of $\hat{\beta}_0, \hat{\beta}_1$.



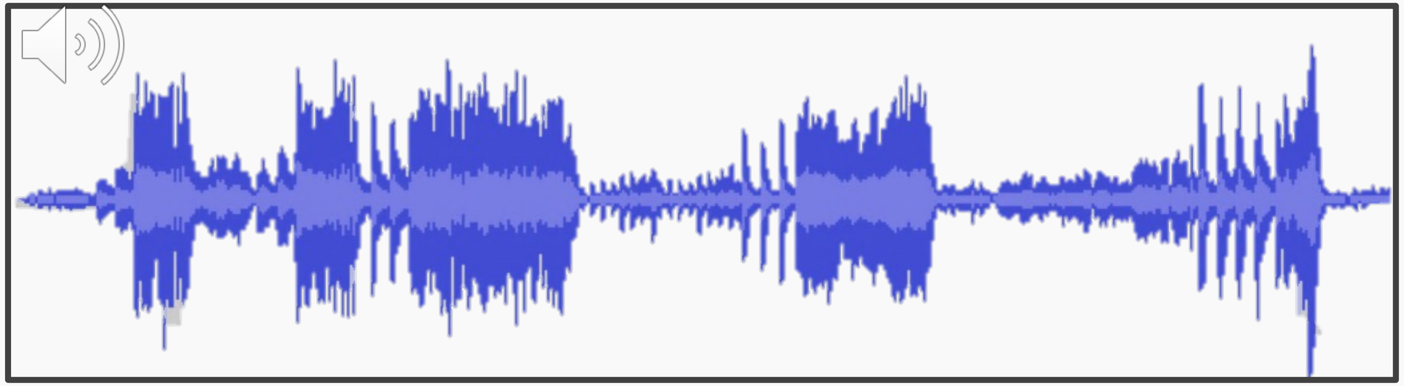


BOOTSTRAP

BOOTSTRAP ISSUES?

- Although easy to implement, it is computationally expensive.
- The output distribution is sensitive to input data.
- As it uses maximum likelihood point estimates, it is not a natural candidate for inference.

The marriage of Figaro

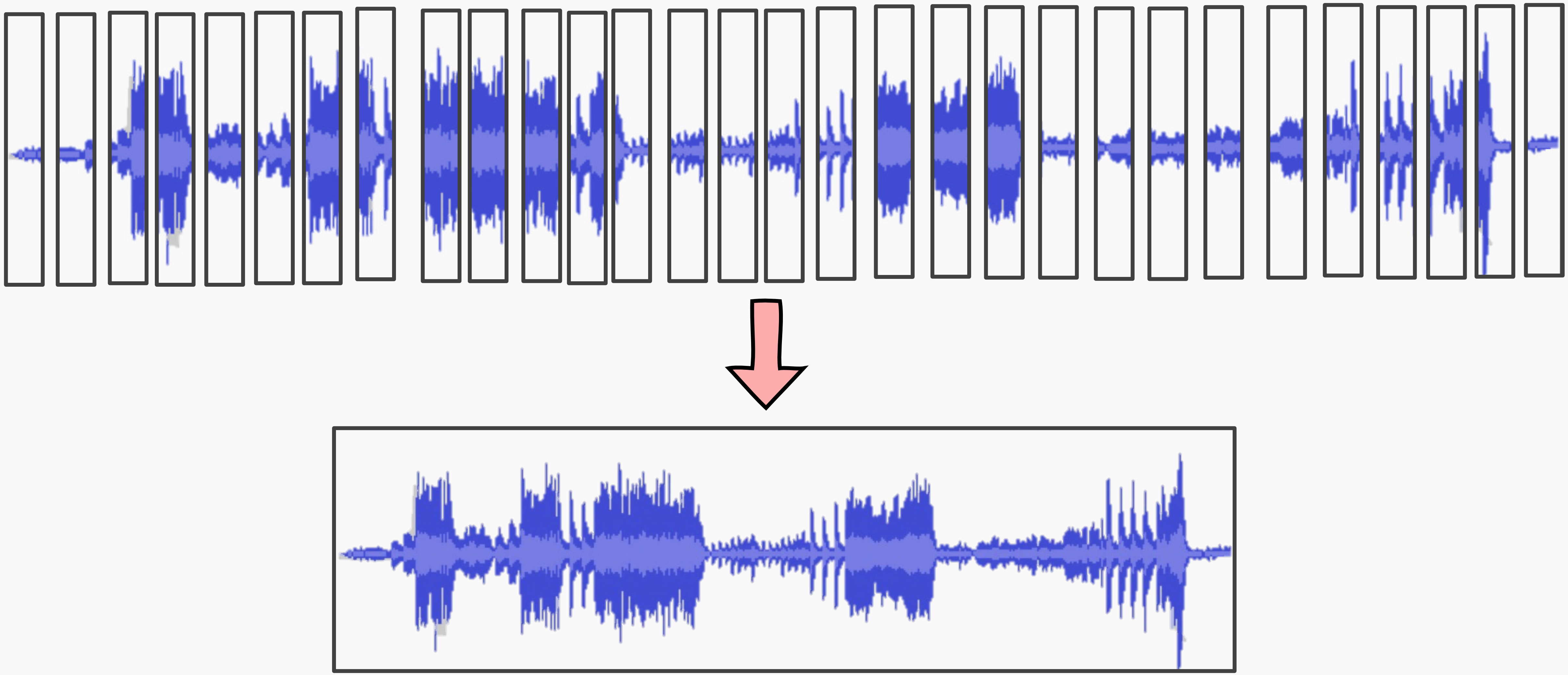


The composition is a "collection" of notes, as seen by the waveform above

The Marriage of Figaro – Bootstrap edition

MysteryGuitarMan – [The marriage of Figaro]()

The Marriage of Figaro – Bootstrap edition



What we want

INFERENCE WISHLIST?

- We want the full probability distribution of the parameters given the data, i.e., let β=[β_0, β_1], then we are looking for $P(\beta\ |data)$.
- We want the posterior predictive distribution of the output given the data. i.e., $P(Y|X)$.

We could use Bayes Theorem

$$\boxed{P(\beta\ |data) = \frac{P(data\ |\beta) * P(\beta)}{P(data)}}$$

RECAP: Bayes Theorem

Likelihood

Prior distribution over β

$$P(\beta\,|data) = \frac{P(data\,|\beta) * P(\beta)}{P(data)}$$

Posterior distribution over β

Evidence

Evidence

$$P(data) = \int P(data|\beta)P(\beta)d\beta$$

ISSUES WITH ANALYTICAL FORM

- Unless for very simple distributions, the **evidence**, $P(data)$ is hard to compute.
- It is difficult to express the posterior as a closed form, which we will need to perform inference.

This product may not have a closed form solution

$$P(\beta|data) = \frac{P(data\,|\beta) * P(\beta)}{\int P(data|\beta)P(\beta)d\beta}$$

This integral is very hard to compute

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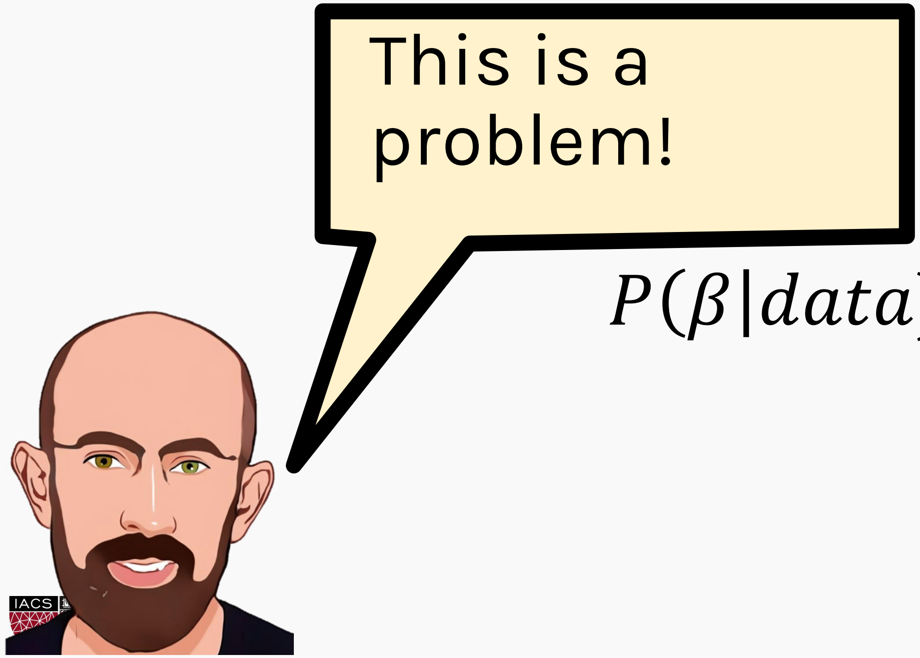

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Maybe you should look at my notes

This product may not have a closed form solution

$$P(\beta|data) = \frac{P(data\,|\beta) * P(\beta)}{\int P(data|\beta)P(\beta)d\beta}$$

This integral is very hard to compute

RECAP: Bayes Theorem

$$P(\beta|data) = \frac{P(data\,|\beta) * P(\beta)}{\int P(data|\beta)P(\beta)d\beta}$$

$$P(\beta|data) \propto P(data|\beta) * P(\beta)$$

For any **given** value of $\beta_0\,,\beta_1$ we can find the posterior probability ***up to a proportionality constant***:

$$P(\beta|data) = C * P(data|\beta) * P(\beta)$$

RECAP: Bayes Theorem

For any **given** value of β_0 , β_1 we can find the posterior probability ***up to a proportionality constant***:

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LINEAR REGRESSION EXAMPLE

let: $y = f(x) + \epsilon$

where: $f(x) = \beta_0 + \beta_1 x$

Assume β_0 & β_1 have normally distributed priors ~ $\mathcal{N}(0, \sigma_{0,1})$ where $\sigma_{0,1}$ are arbitrarily large enough variance.

RECAP: Bayes Linear Regression

We assume that the likelihood $P(data|\beta)$ is also normal, $\mathcal{N}(\beta_0 + \beta_1 x, \sigma_D)$

Hence, for given values of parameters, β_0, β_1, and for each $(x_i, y_i) \in data$

$$P((x_n, y_n)|\boldsymbol{\beta}) = \frac{1}{\sqrt{2\pi\sigma_D^2}} e^{-\left(\frac{(y_n - (\beta_o + \beta_1 x_n))^2}{2\sigma_D^2}\right)}$$

$$P(data|\boldsymbol{\beta}) = \prod_n^N \frac{1}{\sqrt{2\pi\sigma_D^2}} e^{-\left(\frac{(y_n - (\beta_o + \beta_1 x_n))^2}{2\sigma_D^2}\right)}$$

RECAP: Bayes Linear Regression

Calculating the prior distribution is much easier for the chosen values of β_o & β_1

$$P(\beta) = \frac{1}{\sqrt{2\pi\sigma_0^2}} e^{-\frac{\beta_0^2}{2\sigma_0^2}} * \frac{1}{\sqrt{2\pi\sigma_1^2}} e^{-\frac{\beta_1^2}{2\sigma_1^2}}$$

TECHNICAL DETAIL

Here we assume that the parameters β_0 & β_1 are independent random variables, hence the joint distribution (β_0, β_1) is the product of the individual distributions

Putting it all together

$$P(\beta|data) = C * P(data|\beta^i) * P(\beta^i)$$

$$P(\beta|data) \;\ldots\; \prod^{N} \frac{1}{\ldots} \;\ldots\; \frac{(y_n-(\beta_o+\beta_1 x_n))^2}{2\sigma_D^2} * \frac{1}{\sqrt{2\pi\sigma_0^2}} e^{-\frac{\beta_0^2}{2\sigma_0^2}} * \frac{1}{\sqrt{2\pi\sigma_1^2}} e^{-\frac{\beta_1^2}{2\sigma_1^2}}$$

Now we can crunch some numbers

Proportionality constant

Likelihood

Prior over β

INFERENCE WISHLIST?

Even if we cannot get the analytical solution for the parameters, we can compare how *likely* a given value of $\beta^{(i)}$ is to another value $\beta^{(j)}$ using the equations from before

$$\frac{P\left(\beta^{(i)}\middle|data\right)}{P\left(\beta^{(j)}\middle|data\right)} = \frac{P\left(data\middle|\beta^{(i)}\right) * P\left(\beta^{(i)}\right)}{P\left(data\middle|\beta^{(j)}\right) * P\left(\beta^{(j)}\right)}$$

This way, we are still using Bayesian inference, and we can work with equations that are computable.

A (very) brief recap of sampling

$$\frac{P\left(\beta^{(i)}\middle|data\right)}{P\left(\beta^{(j)}\middle|data\right)} = \frac{P\left(data\middle|\beta^{(i)}\right) * P\left(\beta^{(i)}\right)}{P\left(data\middle|\beta^{(j)}\right) * P\left(\beta^{(j)}\right)}$$

- Sampling methods using Bayesian inference with relative comparison between candidate points are popular methods to calculate para... distributions.
- Popular sampling methods include **Monte Carlo sampling** and **Markov Chain Monte Carlo** (MCMC) sampling methods.
- We will consider a much popular variant of MCMC, **Metropolis ak... ndom walk** for our discussion, but other variants can also be used to d... posterior distributions.

But how can we find the parameter distributions by such a comparison?

MCMC Sampling

MCMC - Metropolis Hastings

Metropolis-Hastings is very powerful and a widely-used sampler.

If we are looking for the distribution for some parameter, $\boldsymbol{\theta}$, it reduces the problem of sampling from a difficult distribution $p(\theta|data)$ to:

- making proposals: $q\left(\theta^{(j)}|\theta^{(j-1)}\right)$
- evaluating ratios: $\dfrac{p(\theta^*|data)/q(\theta^*|\theta^{(j-1)})}{p(\theta^{(j-1)}|data)/q(\theta^{(j-1)})|\theta^*)}$

The proposals can be trivial, for e.g., random walk (choose $\theta^{(j)}$ from a normal distribution centered at $\theta^{(j-1)}$).

Note: Only efficiency, not correctness is affected by the proposal.

Metropolis Hastings

TECHNICAL DETAILS

The Metropolis-Hastings algorithm is outlined below:

1. Select an initial value θ_0
2. For $i = 1, \ldots, m$ repeat:
   a) Draw a candidate $\theta^* \sim q\left(\theta^* \middle| \theta^{(j-1)}\right)$
   b) $\alpha = \dfrac{p(\theta^*|data)/q(\theta^*|\theta^{(j-1)})}{p(\theta^{(j-1)}|data)/q(\theta^{(j-1)})|\theta^*)} = \dfrac{p(\theta^*|data)q(\theta^{(j-1)})|\theta^*)}{p(\theta^{(j-1)}|data)q(\theta^*|\theta^{(j-1)})}$
   c) If $\alpha \geq 1$, accept θ^* & set $\theta^{(j)} \leftarrow \theta^*$

      Else if $0 < \alpha < 1$ accept θ^* & set $\theta^{(j)} \leftarrow \theta^*$ with probability η

      reject θ^* & set $\theta^{(j)} \leftarrow \theta^*$ with probability $1 - \eta$

Metropolis Hastings

TECHNICAL DETAILS

The Metropolis-Hastings algorithm is outlined below:

q(.) is the proposal. For example,
$\theta^* \sim \mathrm{N}(\theta^{(j-1)}, \sigma)$

1. Select an initial value θ_0

2. For $i = 1, \ldots, m$ repeat:

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   c) If $\alpha \geq 1$, accept θ^* & set $\theta^{(j)} \leftarrow \theta^*$

   Else if $0 < \alpha < 1$ accept θ^* & set $\theta^{(j)} \leftarrow \theta^*$ with probability α

   reject θ^* with probability $1 - \alpha$

How? Draw a random number, ρ. If $\rho > (1 - \alpha)$ accept.

Metropolis Hastings – Random Walk

A special case of the Metropolis-Hastings algorithm is the ***Metropolis*** where the distribution q is symmetric i.e.,

$$\boxed{q\left(\theta^*\middle|\theta^{(j-1)}\right) = q(\theta^{(j-1)}|\theta^*)}$$

This makes the algorithm much simpler, as

$$\boxed{\alpha = \frac{p(\theta^*|data)q(\theta^{(j-1)})|\theta^*)}{p(\theta^{(j-1)}|data)q(\theta^*|\theta^{(j-1)})}}$$

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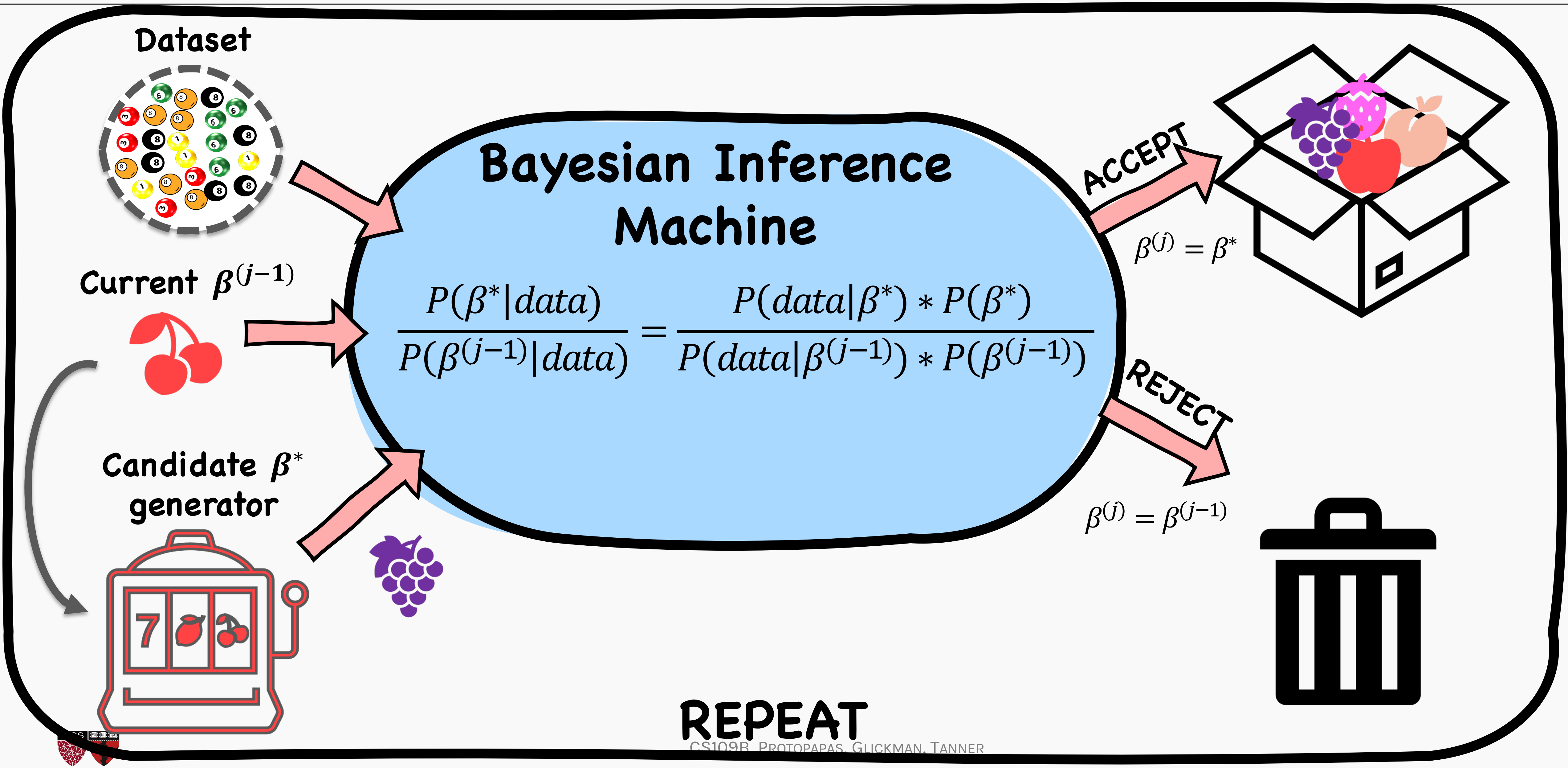
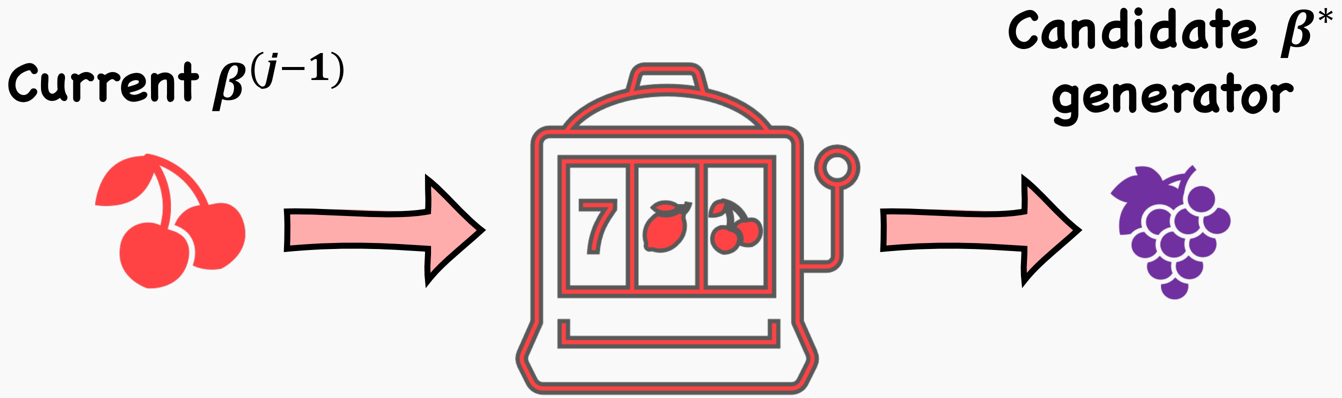
We can show using Bayes theorem:

$$\boxed{\alpha = \frac{p(data|\theta^*)}{p(data|\theta^{(j-1)})}\frac{p(\theta^*)}{p(\theta^{(j-1)})}}$$

MCMC Factory



MCMC Factory - What is a generator

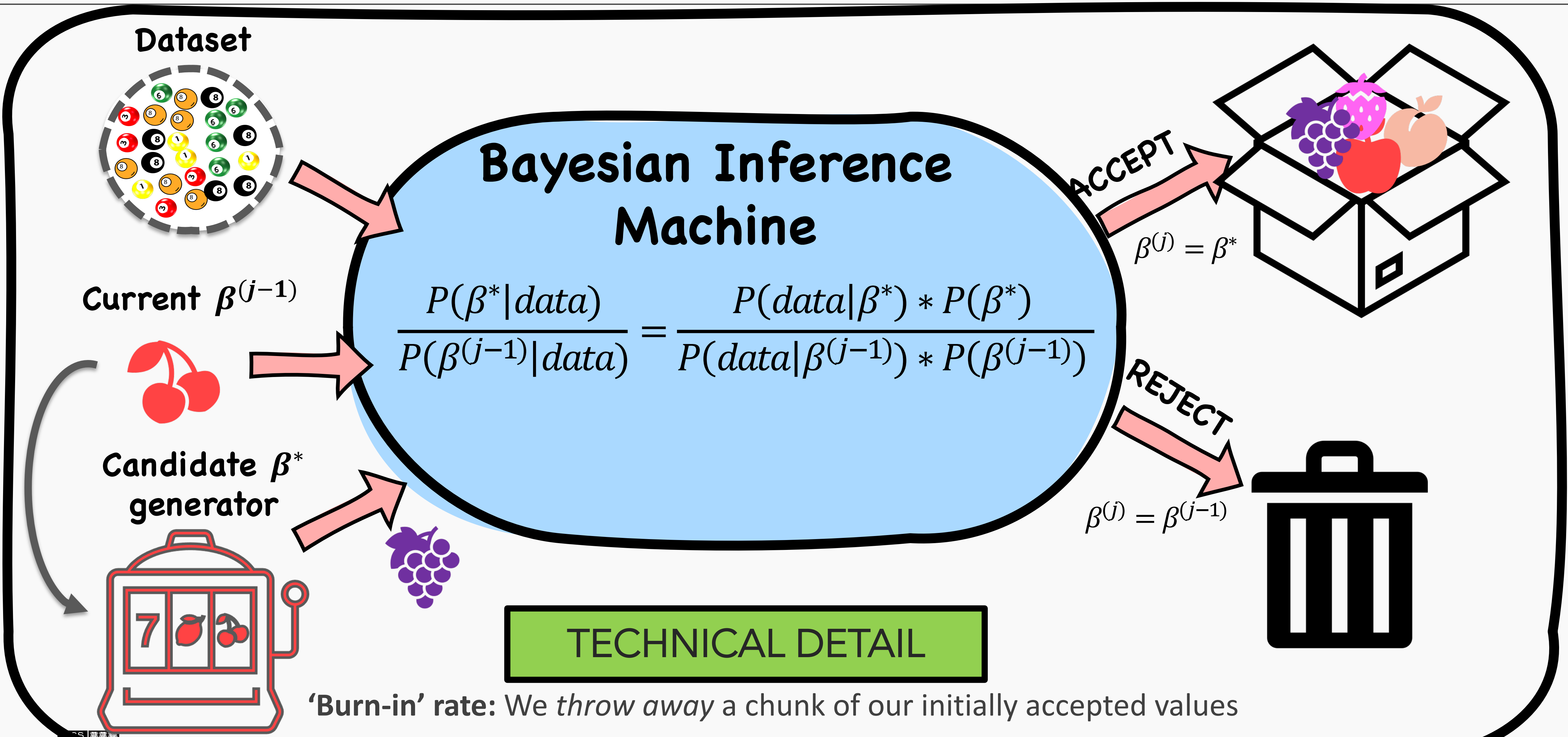


- The candidate $\boldsymbol{\beta}^{*}$ generator takes the currently accepted $\beta^{(j-1)}$ value and draws a value from a distribution, for example:

$$\beta^{*} \sim \mathcal{N}\left(\beta^{(j-1)}, \sigma\right)$$

- This ensures that we don't get wildly crazy candidates, but ones quite similar to the current $\boldsymbol{\beta}$.

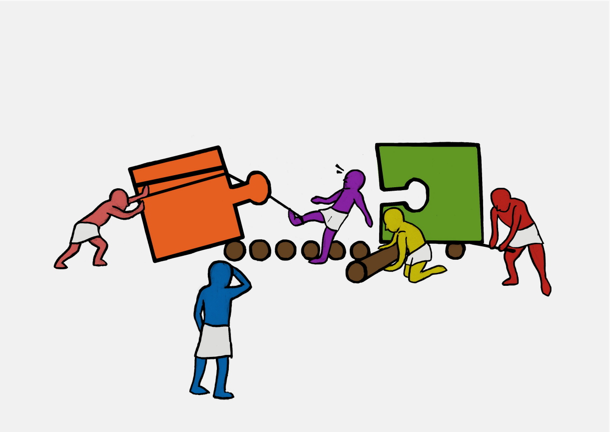
MCMC Factory



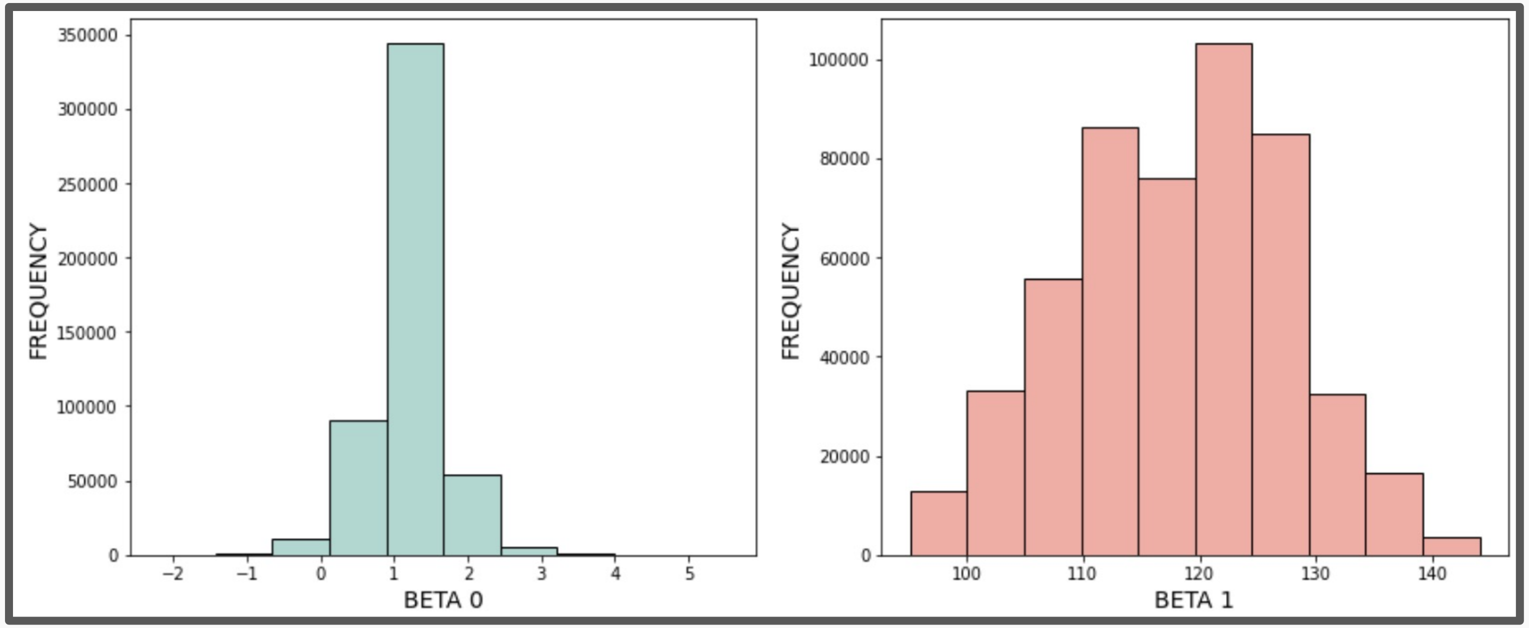
TECHNICAL DETAIL

‘Burn-in’ rate: We *throw away* a chunk of our initially accepted values

Exercise: Linear Regression MCMC from scratch



The aim of this exercise is to perform Monte Carlo Markov Chain (MCMC) from scratch for linear regression.
On completing the exercise you should be able to see the following distribution. One for each of the beta value:




Time to scale the hills of
Bayesian NNs!
BAYESIAN
LINEAR REGRESSION
BAYESIAN
NEURAL NETWORKS
N
W
E
S

Bayesian Neural Network

Bayesian Linear Regression

We assume that the likelihood $P(data|\beta)$ is also normal, $\mathcal{N}(\beta_0 + \beta_1 x, \sigma_D)$

Hence, for given values of parameters, β_0, β_1, and for each $(x_i, y_i) \in data$

$$P(\{x_n, y_n\}|\boldsymbol{\beta}) = \frac{1}{\sqrt{2\pi\sigma_D^2}} e^{-\left(\frac{(y_n - (\beta_o + \beta_1 x_n))^2}{2\sigma_D^2}\right)}$$

$$P(data|\boldsymbol{\beta}) = \prod_n^N \frac{1}{\sqrt{2\pi\sigma_D^2}} e^{-\left(\frac{(y_n - (\beta_o + \beta_1 x_n))^2}{2\sigma_D^2}\right)}$$

Bayesian Neural Network

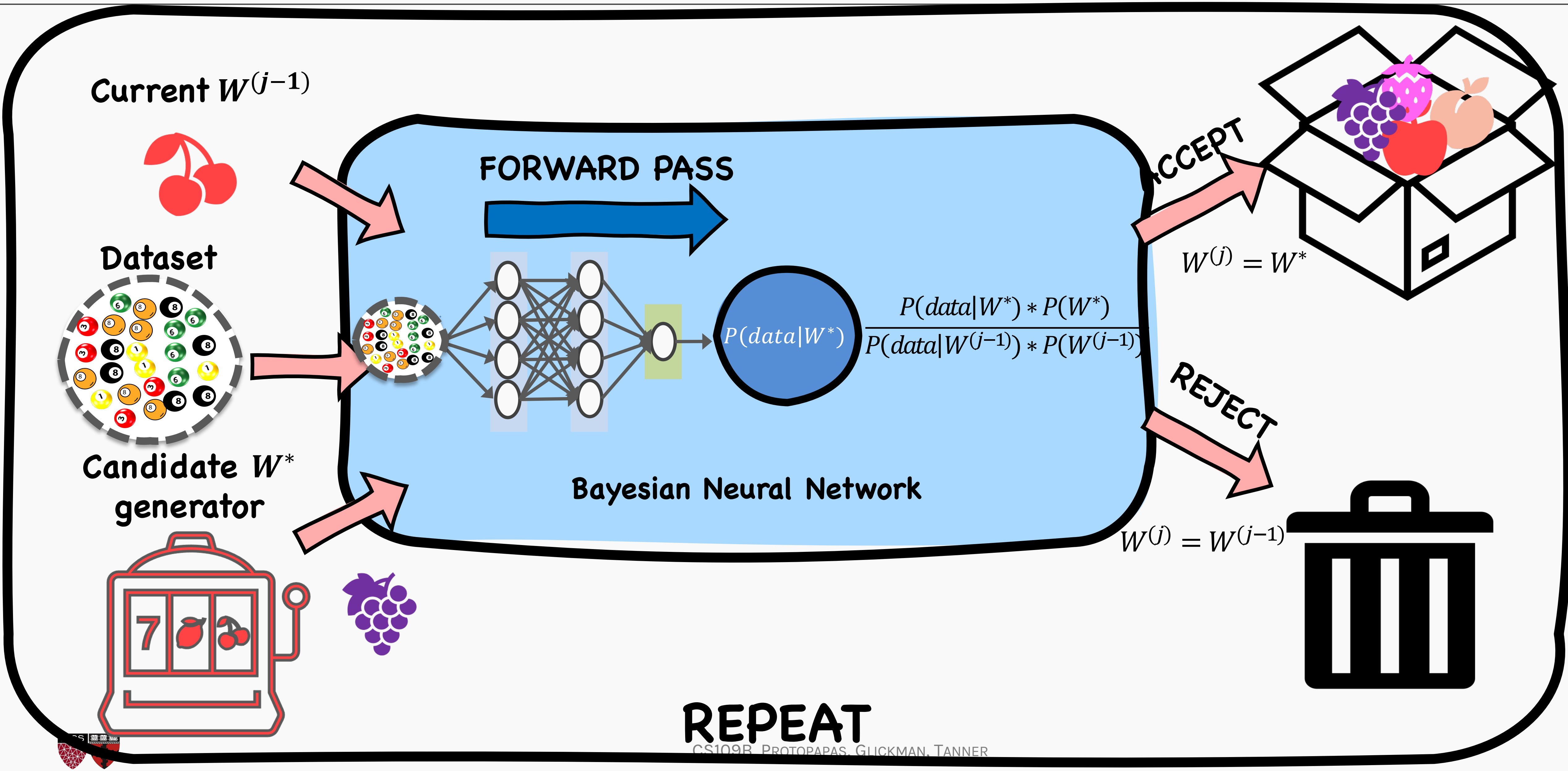
We assume that the likelihood $P(data|\beta)$ is also normal, $\mathcal{N}(NN_W(x), \sigma_D)$

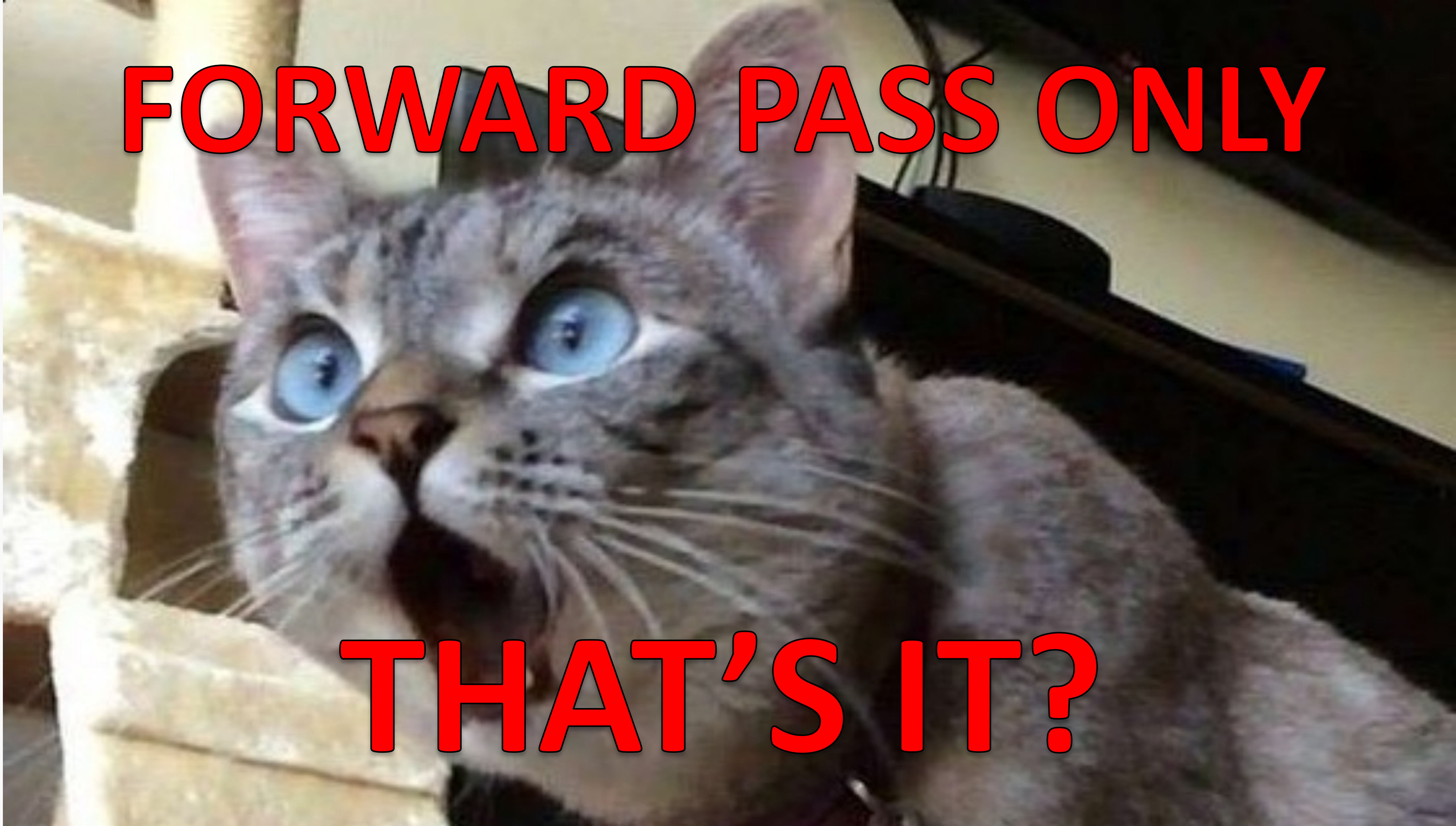
Hence, for given values of parameters, W, and for each $(x_i, y_i) \in data$

$$P(\{x_n, y_n\}|W) = \frac{1}{\sqrt{2\pi\sigma_D^2}} e^{-\left(\frac{(y_n - NN_W(x_n))^2}{2\sigma_D^2}\right)}$$

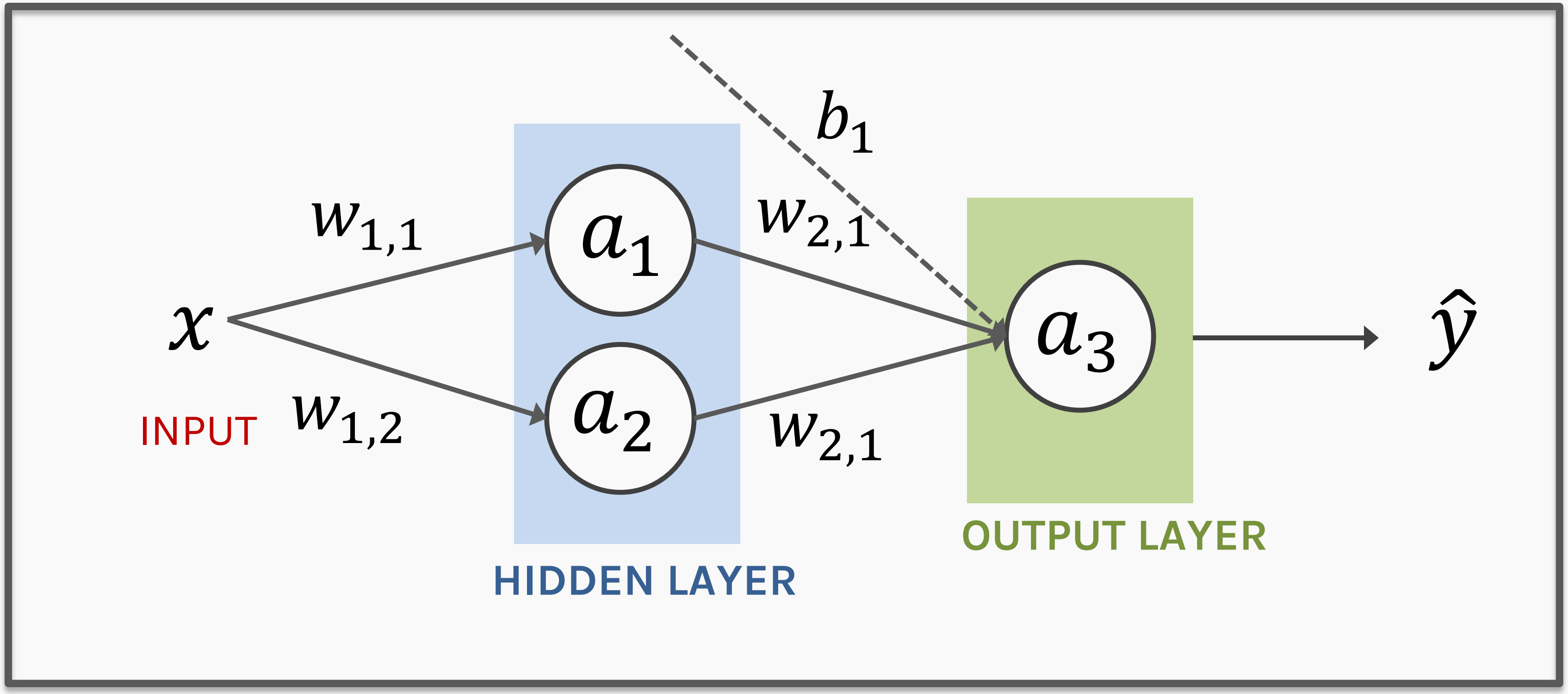
$$P(data|W) = \prod_n^N \frac{1}{\sqrt{2\pi\sigma_D^2}} e^{-\left(\frac{(y_n - NN_W(x_n))^2}{2\sigma_D^2}\right)}$$

Bayesian Neural Network

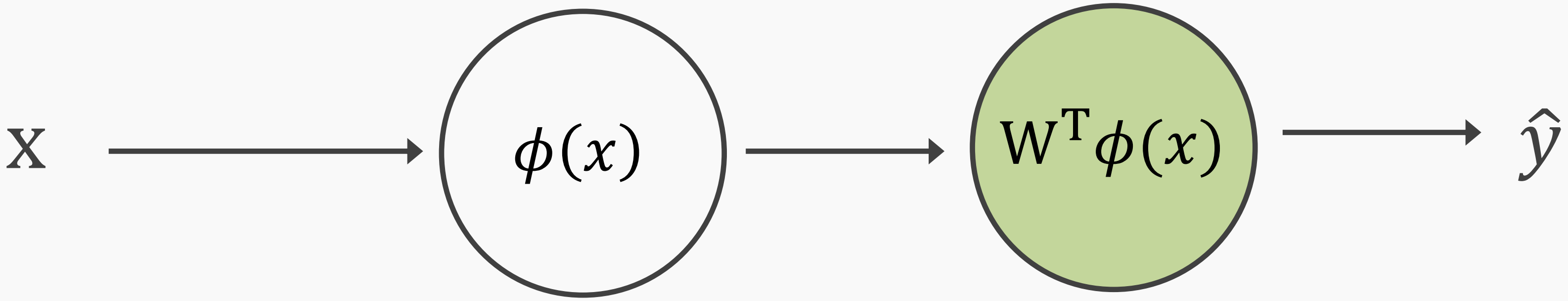



FORWARD PASS ONLY
THAT’S IT?

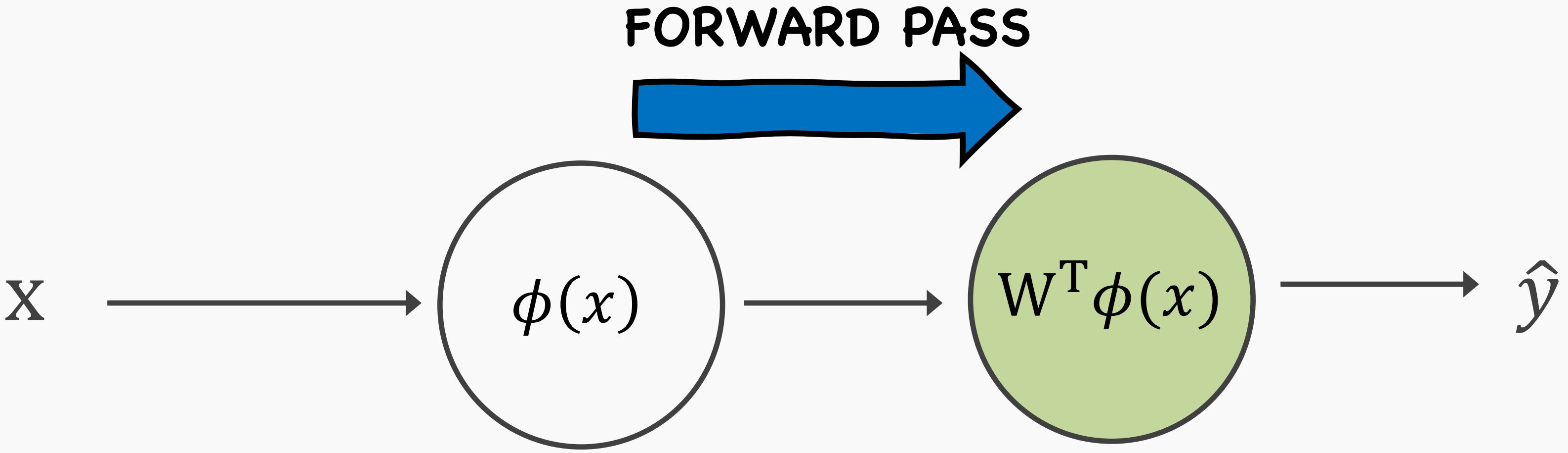
Example: A simple Bayesian Neural Network (BNN)



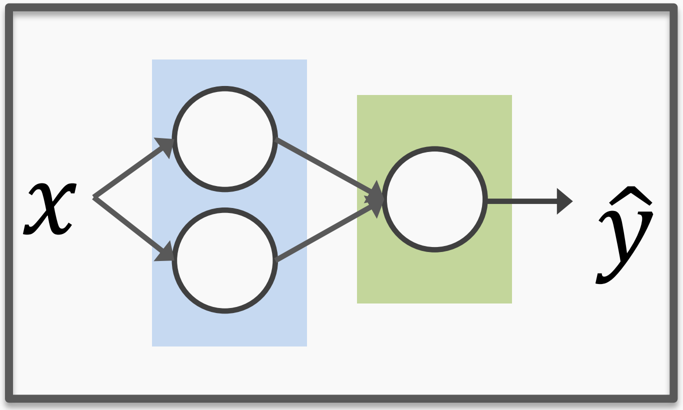
Neural Network Architecture



Bayesian Neural Network (BNN)

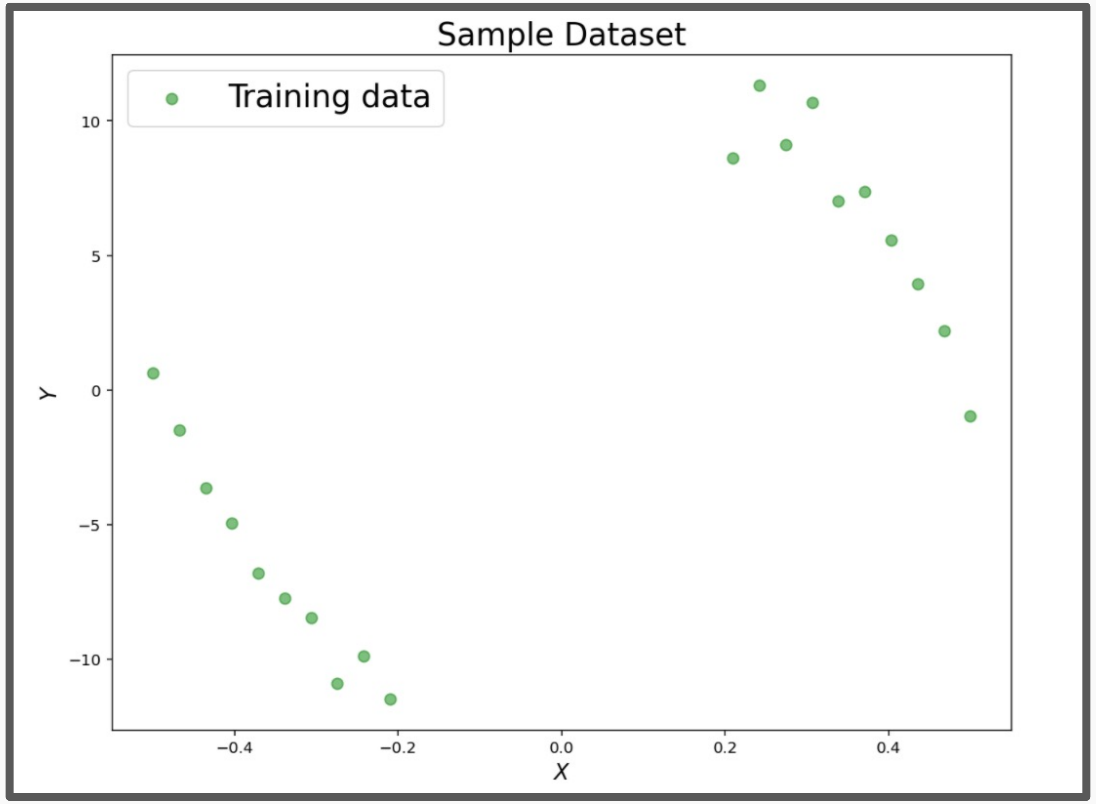


1. Select an initial value $W^{(0)}$ (this represent all weights in the network)
2. For $i = 1, \ldots, m$ repeat:
   a) Draw a candidate $W^* \sim q\left(W^* \middle| W^{(j-1)}\right)$
   b) $\alpha = \dfrac{p(data|W^*)}{p(data|W^{(j-1)})} \dfrac{p(W^*)}{p(W^{(j-1)})}$
   c) If $\alpha \geq 1$, accept W^* & set $W^{(j)} \leftarrow W^*$
      else if $0 < \alpha < 1$ accept W^* & set $W^{(j)} \leftarrow W^*$ with probability α
      reject θ^* probability $1 - \alpha$

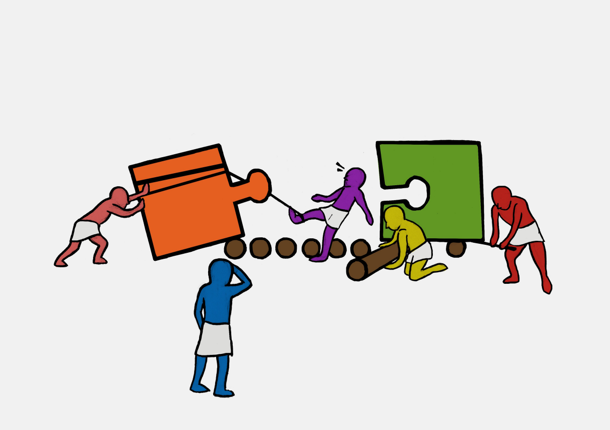


Bayesian **Neural Network**

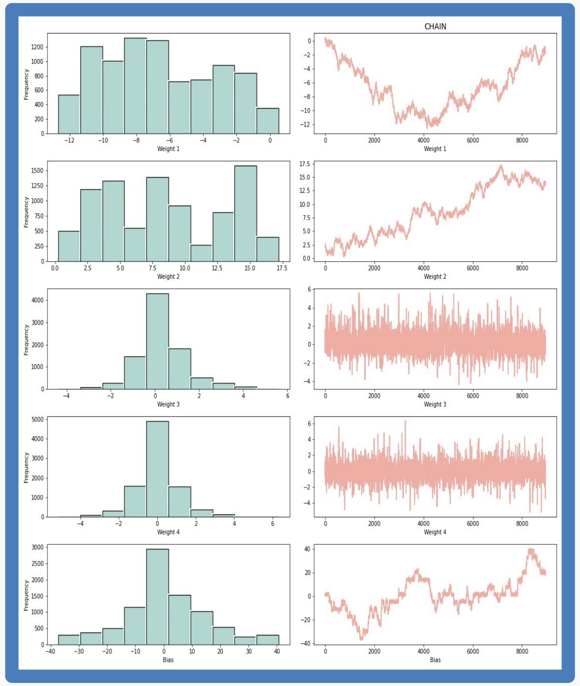
Let us consider the dataset below for regression



Exercise: MCMC from Scratch for Neural Networks

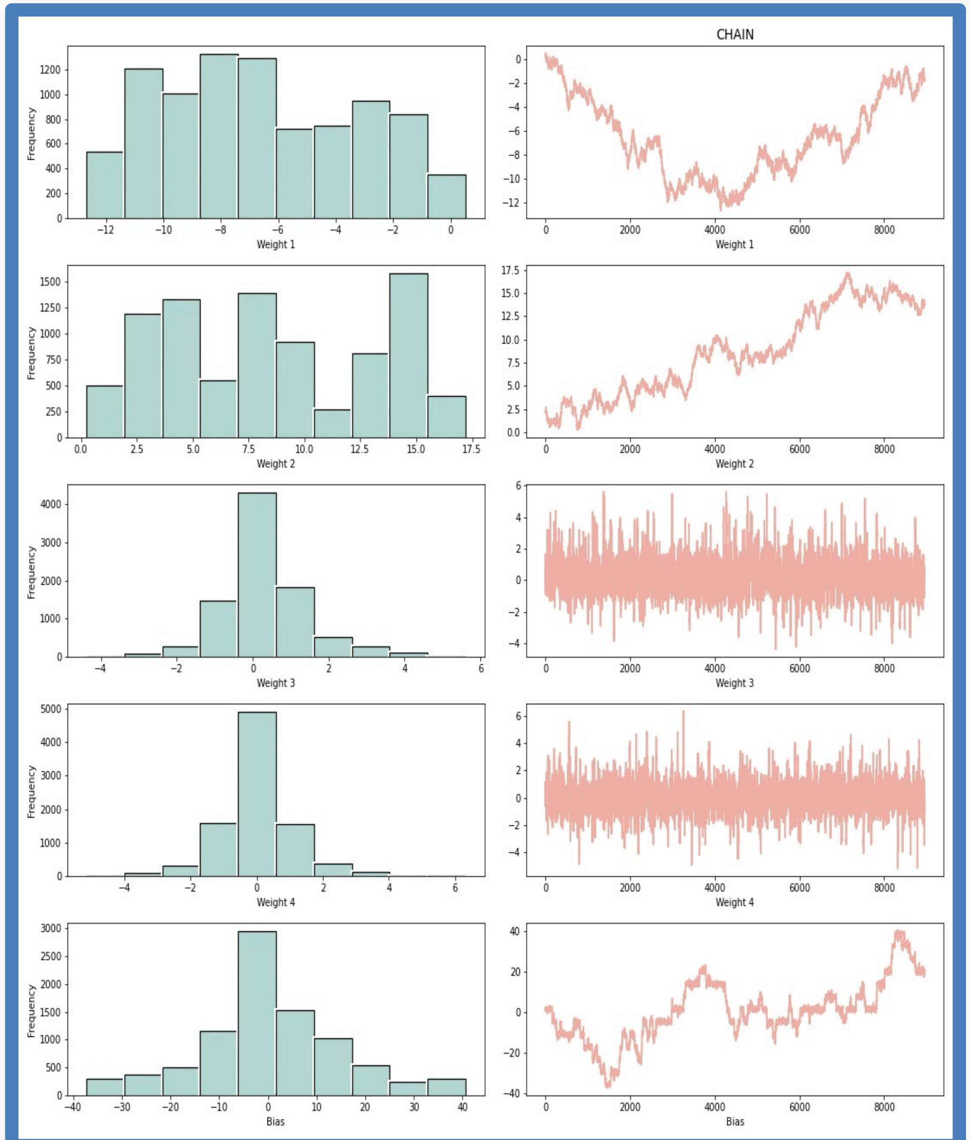


The aim of this exercise is to perform Metropolis Monte Carlo Markov Chain (MCMC) from scratch (as in exercise 1) for a simple neural network.
On completing the exercise, you should be able to see the following distribution. One for each of the beta value:



Warning: This is not going to converge unless we start very near the mode of the distribution!

FULL MCMC ISSUES



MCMC we will not work for NN's with more than a few dozens of parameters.

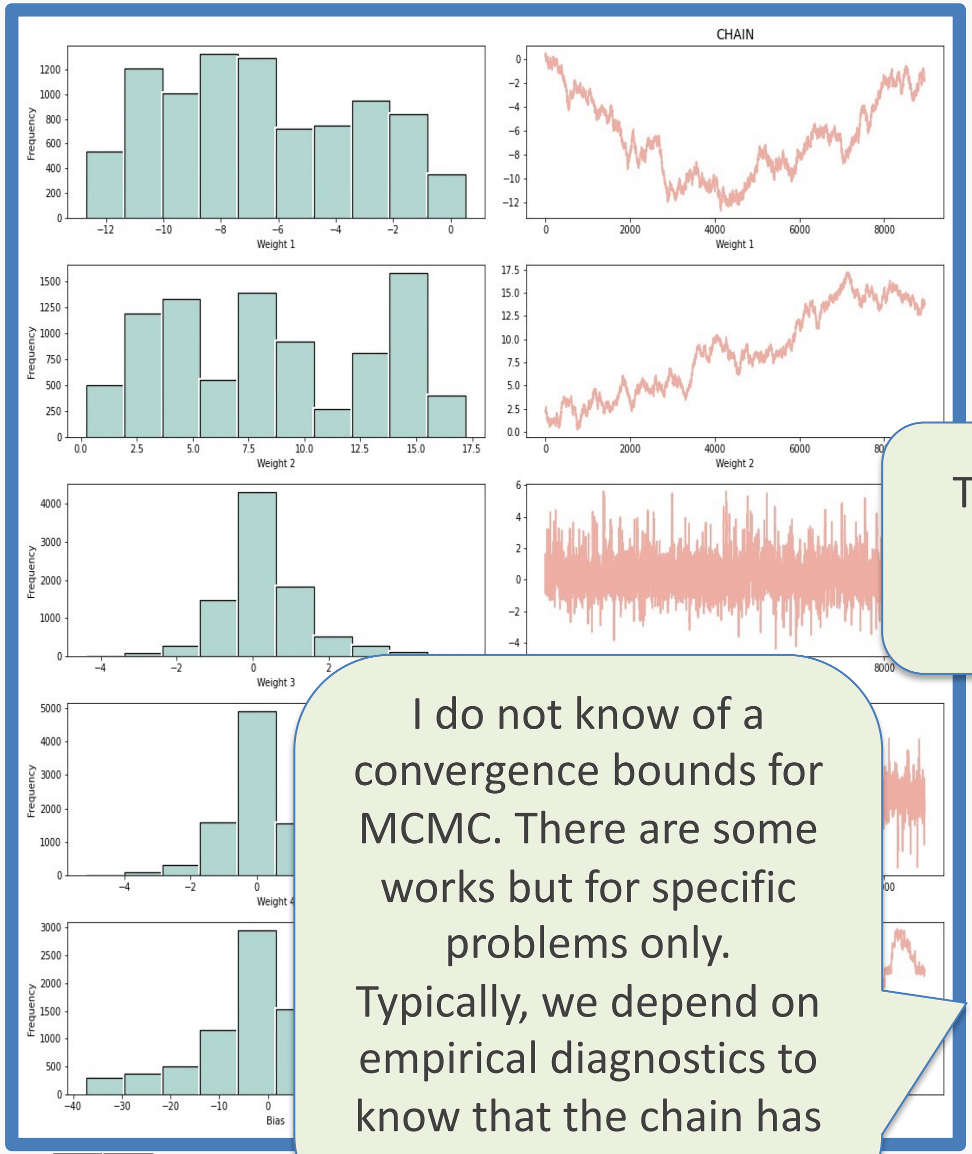
Why?

For each parameter (weight) we sample and calculate the likelihood $5 * n$ times, where n being the length of the chain.

We also throw away a significant number of samples.

Sufficient n also grows with the number of parameters and complexity of the posterior.

FULL MCMC ISSUES



MCMC we will not work for NN's with more than a few dozens of parameters.

Why?

For each parameter (we... t) we sample and ...elihood $5 * n$ times, where n being ... chain.

We also throw away a significant number of samples.

Sufficient n also grows with the number of parameters and complexity of the posterior.

Five times because we usually have acceptance rate of $\sim 20\%$.

Typically, we throw the first 10-20% of the samples for burn in.

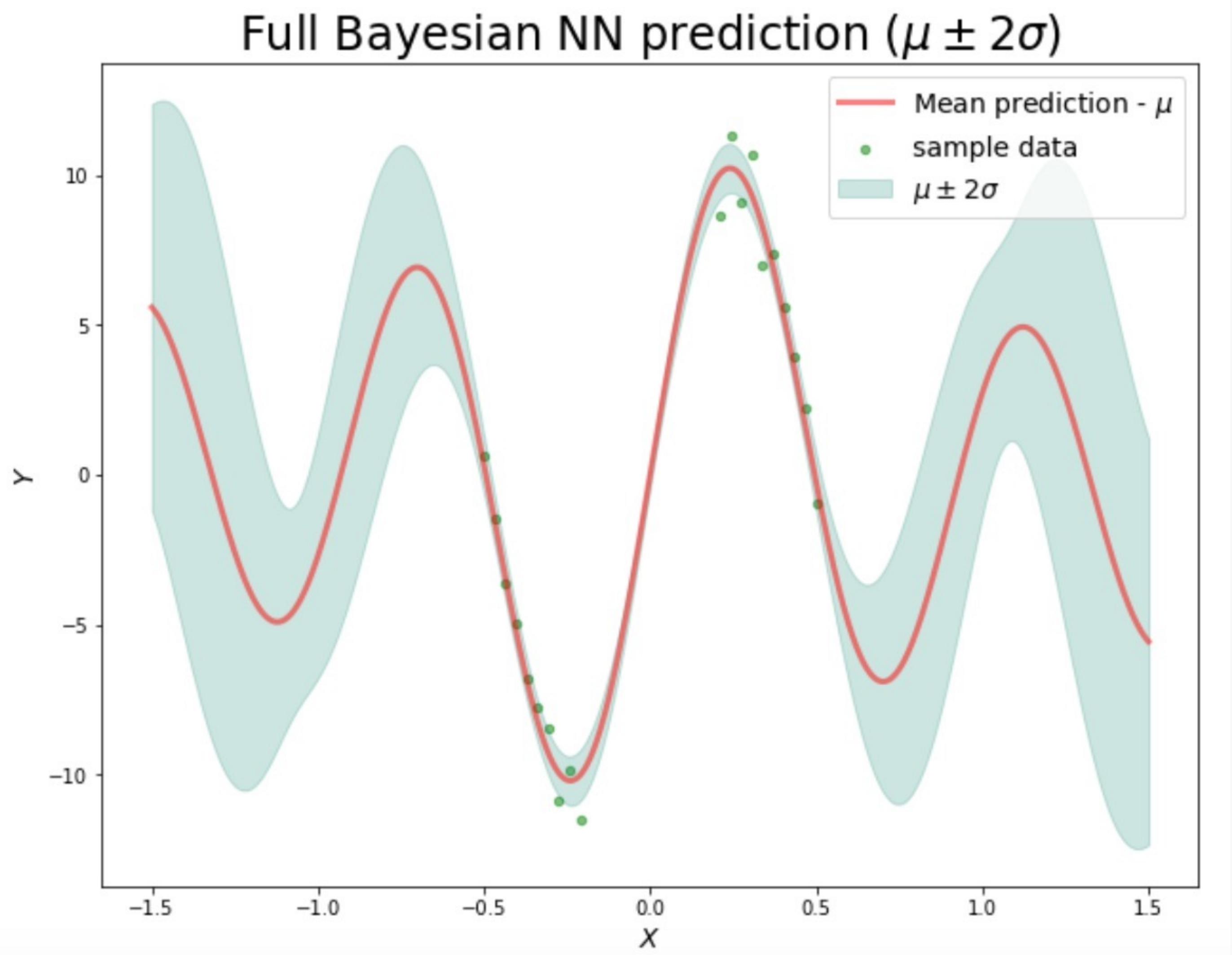
I do not know of a convergence bounds for MCMC. There are some works but for specific problems only.
Typically, we depend on empirical diagnostics to know that the chain has converged

Bayesian Neural Network: **Full MCMC with HMC**

Instead of the simple Metropolis MCMC, we could use a more sophisticated sampler HMC, as we did in HW3 and lab.

Here with Tensorflow Probability

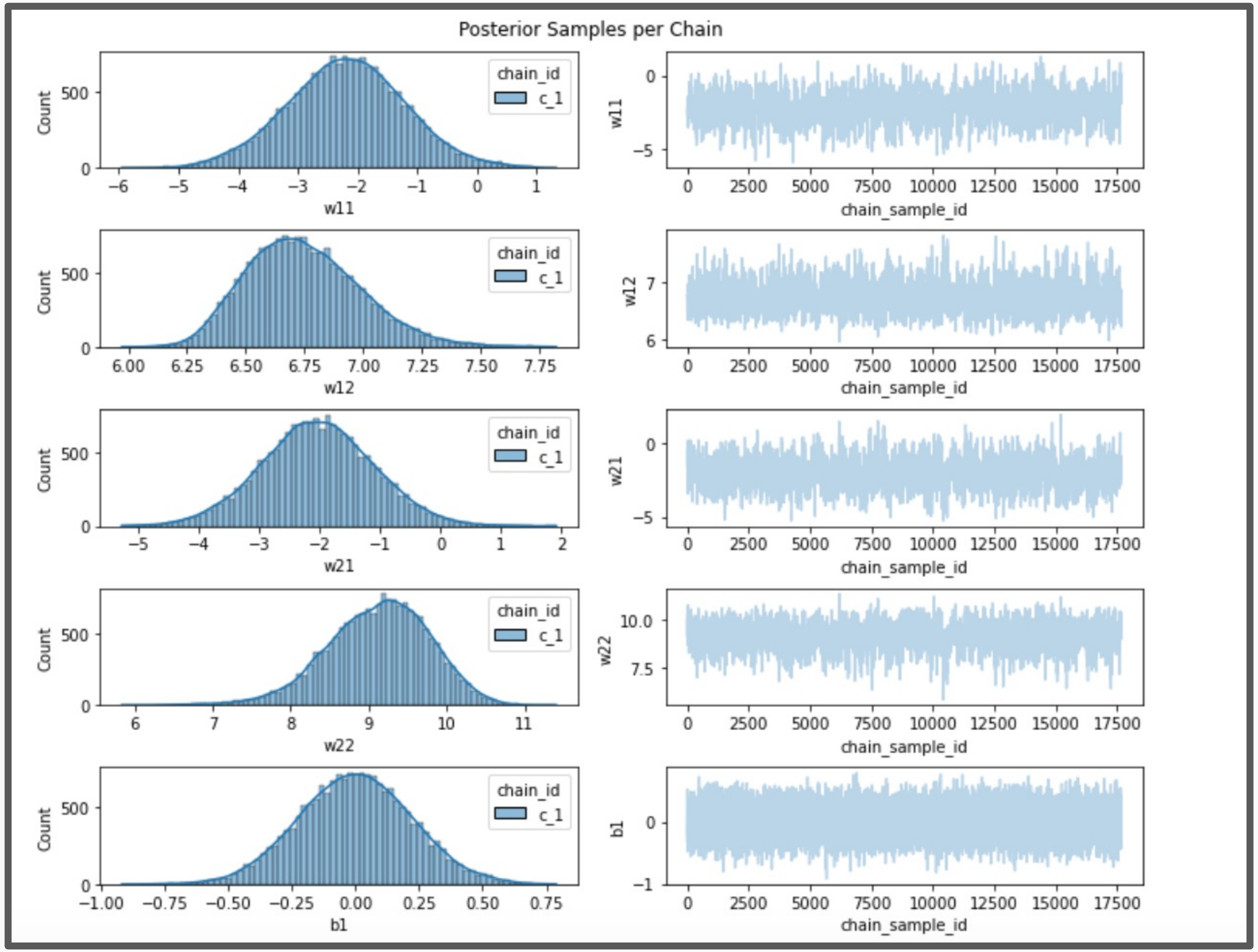
POSTERIOR DISTRIBUTION y



Bayesian Neural Network: **Full MCMC with HMC**

- The first set of plots on the right represents the distribution of the individual weights.
- The second set of plots on the right show the individual values of the weights considered while running the sampling algorithm.

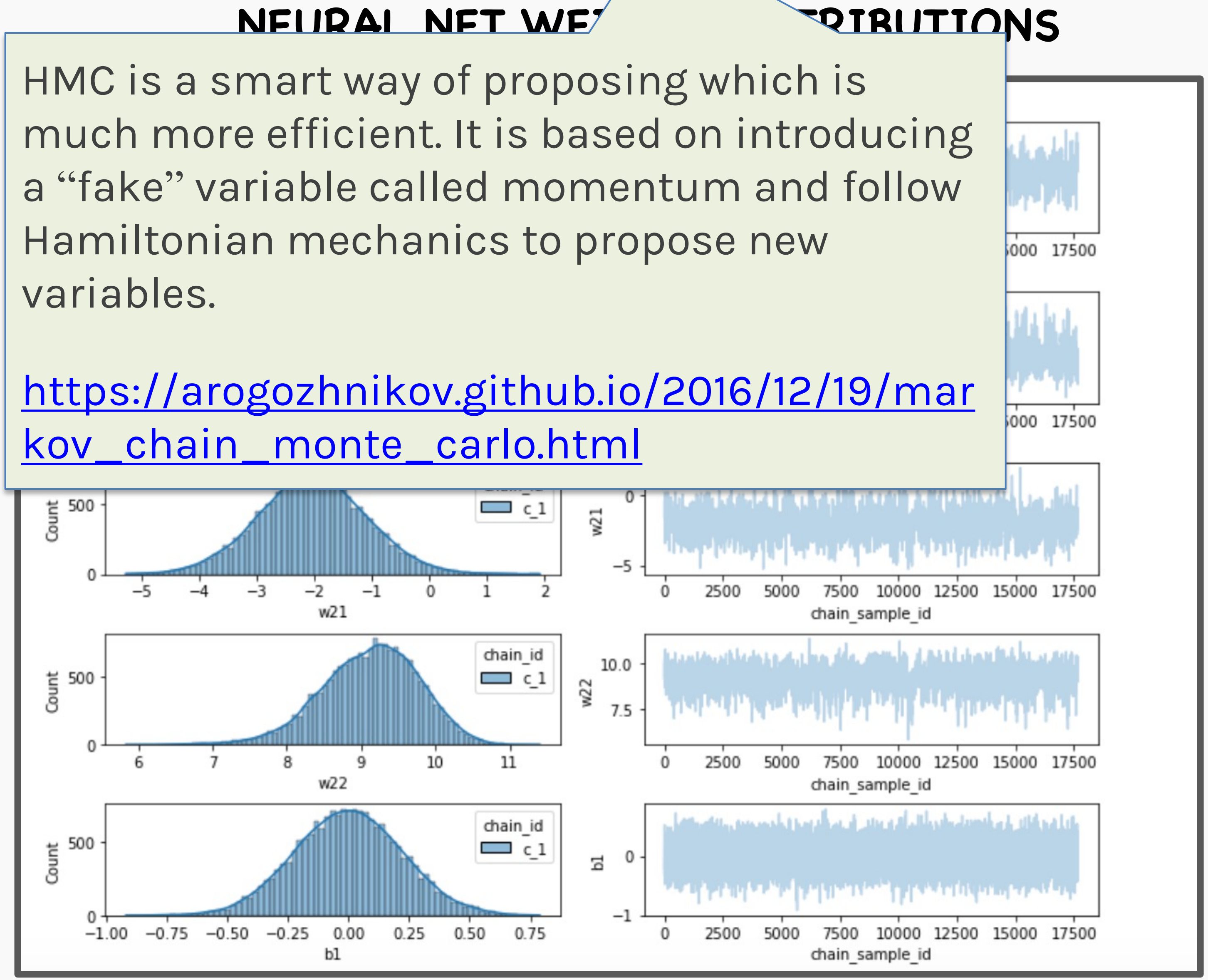
NEURAL NET WEIGHT DISTRIBUTIONS



Bayesian Neural Network: **Full MCMC with HMC**

- The first set of plots on the right represents the distribution of the individual weights.
- The second set of plots on the right show the individual values of the weights considered while running the sampling algorithm.

Activation: `sin()`
Burn rate: 30%



HMC is a smart way of proposing which is much more efficient. It is based on introducing a “fake” variable called momentum and follow Hamiltonian mechanics to propose new variables.

https://arogozhnikov.github.io/2016/12/19/markov_chain_monte_carlo.html

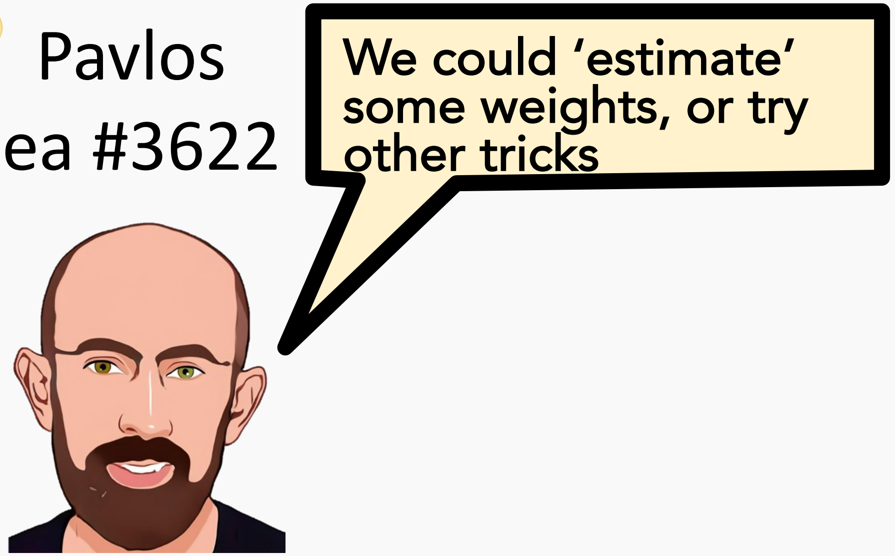
Bayesian Neural Network – Roadblocks MCMC doesn't work for higher dimension

BAYESIAN
INFERENCE
Guess we'll need
an alternate route!
VARIATIONAL
AUTO-ENCODERS
N
W
E
S

End of Part 1

Bayesian Neural Network: Hacks

Pavlos Idea #3622



W_{11} & W_{12} ML estimate