# Modelos Generativos 2

<u>Material auxiliar</u>

*Máster en Inteligencia Artificial aplicada a Mercados Financieros*

Jorge del Val

# Índice

1. Recap
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# Recap

# Recordando…

Para nosotros, cada dato $x_i$ es una *realización* de una variable aleatoria subyacente $\mathbf{x}$, con una distribución de probabilidad $p(x)$ desconocida

$$\mathbf{x} \sim p(x)$$

- El *aprendizaje no supervisado* es el campo que intenta inferir propiedades de $\mathbf{x}$ sólo con las muestras (datos).
- Los *modelos generativos* son un subconjunto del aprendizaje no supervisado que pretende *aproximar* $\mathbf{x}$ como una combinación de variables aleatorias "simples" que se puedan muestrear:

$$\mathbf{x} \approx G_\theta(\mathbf{z_1}, \mathbf{z_2}, \dots, \mathbf{z_k}) \triangleq \hat{\mathbf{x}}$$

# Entrenamiento

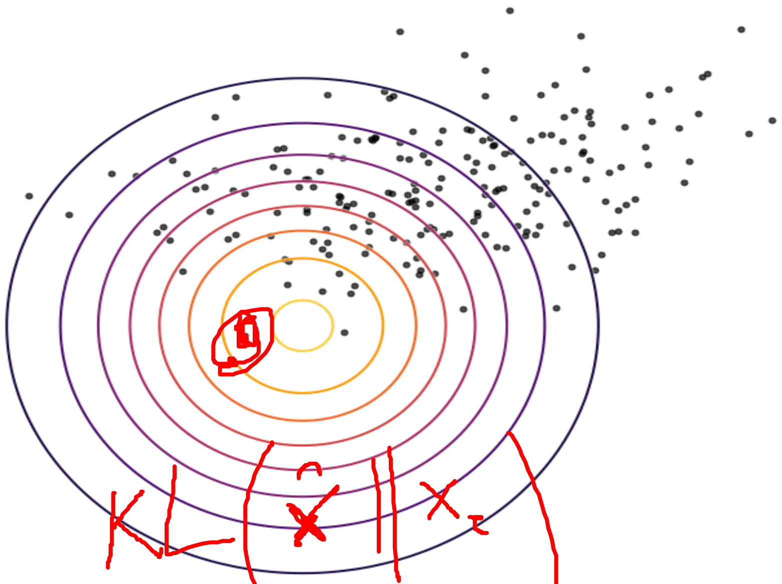
Queremos aproximar $\mathbf{x}$ como $\hat{\mathbf{x}} = G_\theta(\mathbf{z})$. ¿Cómo encontramos los parámetros θ óptimos?

**Maximiza la verosimilitud (likelihood) de tu modelo!!**

*Probabilidad de que tu modelo generara $x_i$*

$$\max_\theta \mathcal{L}(\theta | x_{train}) = \max_\theta \prod_{i=1}^{N} p_\theta(x_i)$$

$$\max_\theta \log \mathcal{L}(\theta | x_{train}) = \max_\theta \sum_{i=1}^{N} \log p_\theta(x_i)$$

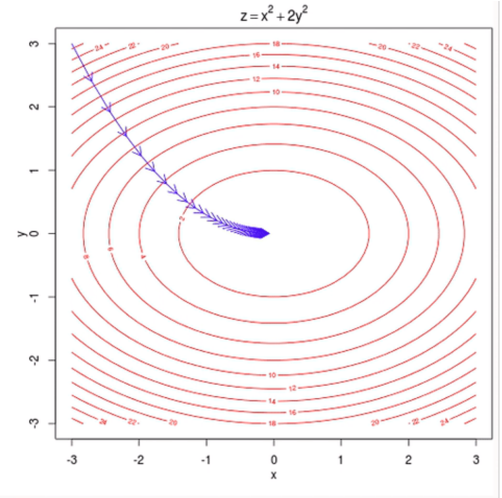


$KL(\hat{x} \| x_i)$

*Image credit: Colin Raffel*

Necesitamos $p_\theta(x)$ explícitamente!

# Optimización




## Optimizamos una función de coste (error)!

*Stochastic Gradient Descent*

$$\min_{\theta} L(\theta; \text{data}) \rightarrow \boxed{\theta_{t+1} = \theta_t - \alpha \nabla_\theta L}$$

```python
model = MyNetwork()
theta = model.parameters()
optimizer = torch.optim.Adam(theta, lr=0.001)

for x, y in dataloader:
    y_pred = model(x)
    loss = myloss(y, y_pred)
    loss.backwards()
    optimizer.step()
```

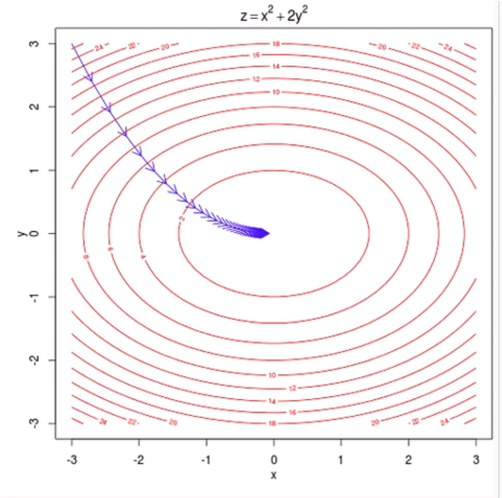
PyTorch

```python
model = MyNetwork()
theta = model.trainable_variables
optimizer = tf.train.AdamOptimizer(lr = 0.001)

for x, y in dataset:
    with tf.GradientTape() as g
        y_pred = model(x)
        loss = myloss(y, y_pred)
    grads = g.gradient(loss, theta)
    optimizer.apply_gradients(zip(grads, model.trainable_variables))
```

TensorFlow

# Optimización

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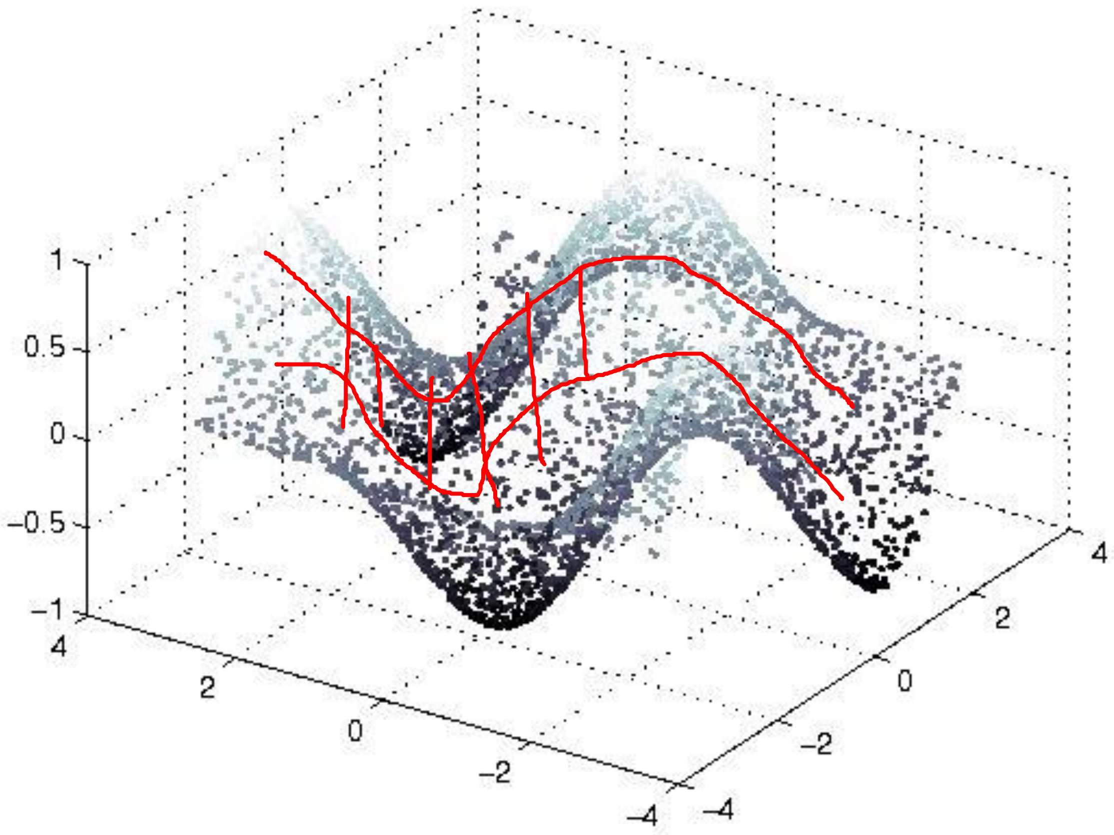
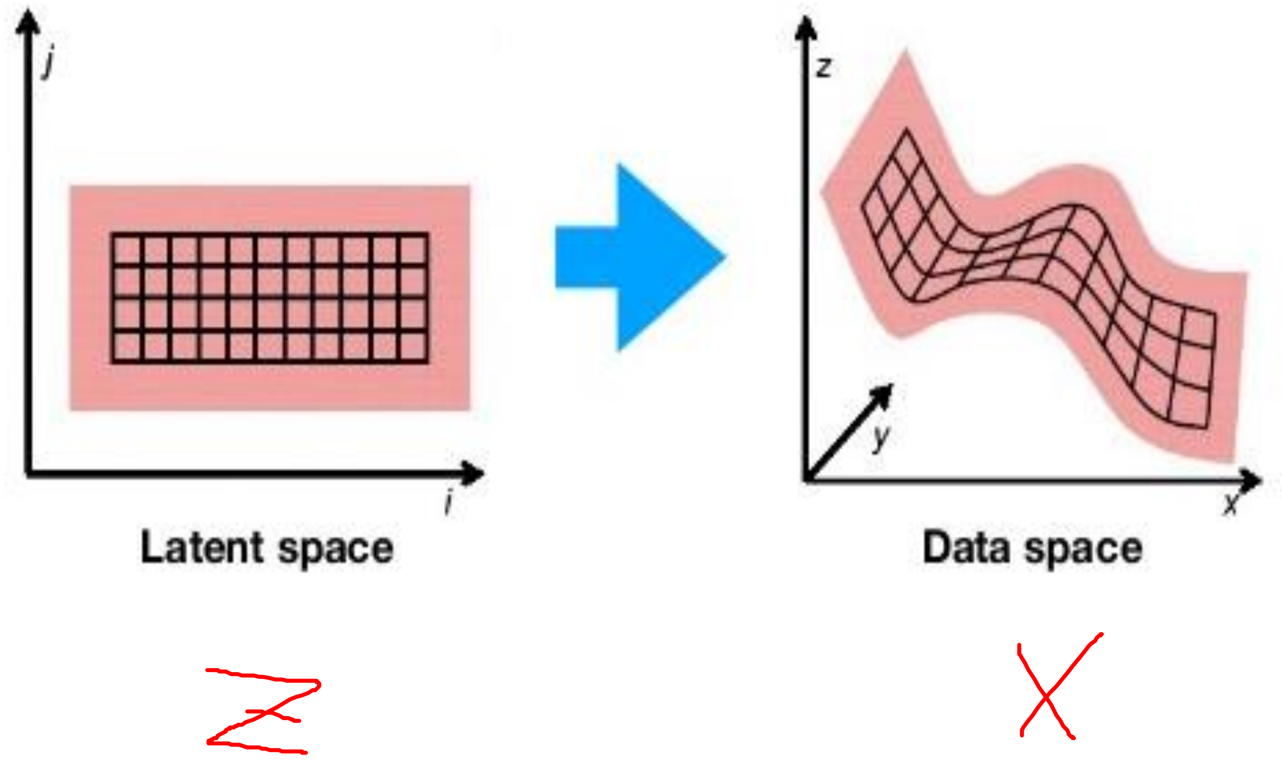
TensorFlow

Easy to gradient descent any function with current frameworks!! ☺

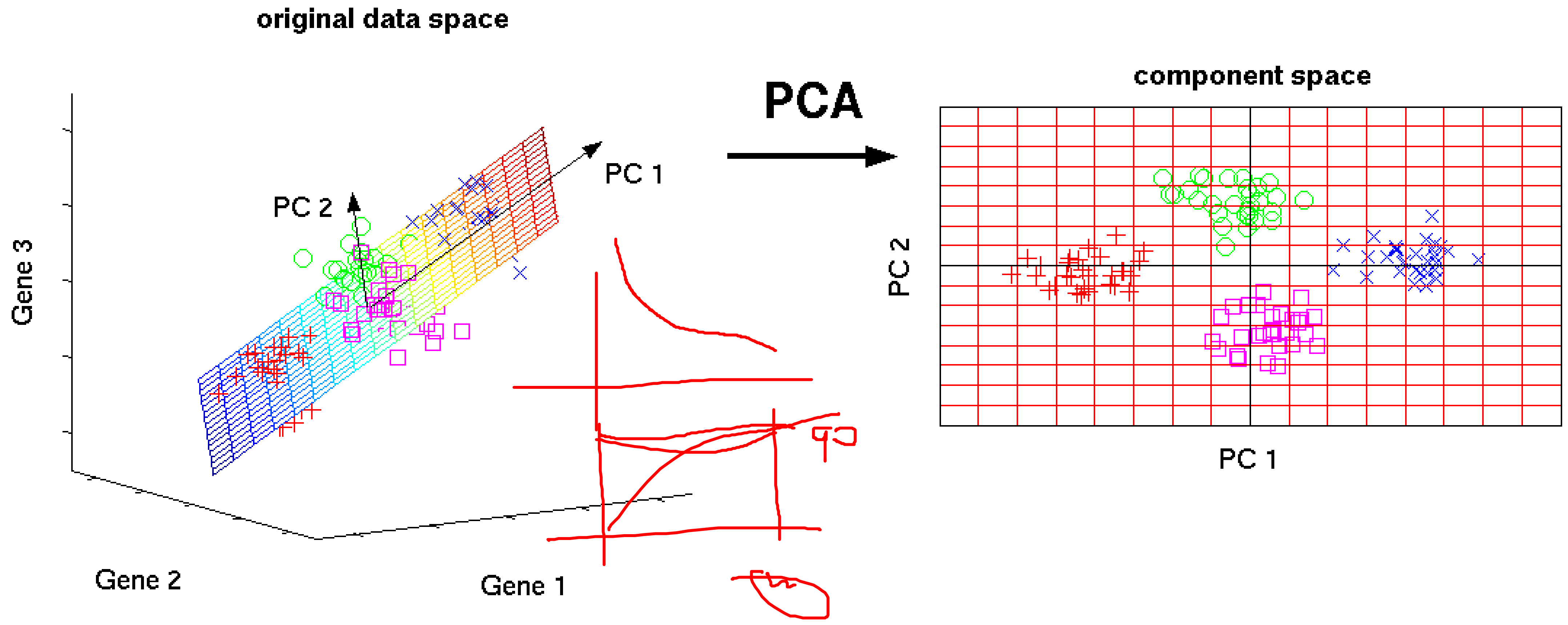

1
0.5
0
-0.5
-1
4
2
0
-2
-4
4
2
0
-2
-4

# Dimensiones latentes de los datos



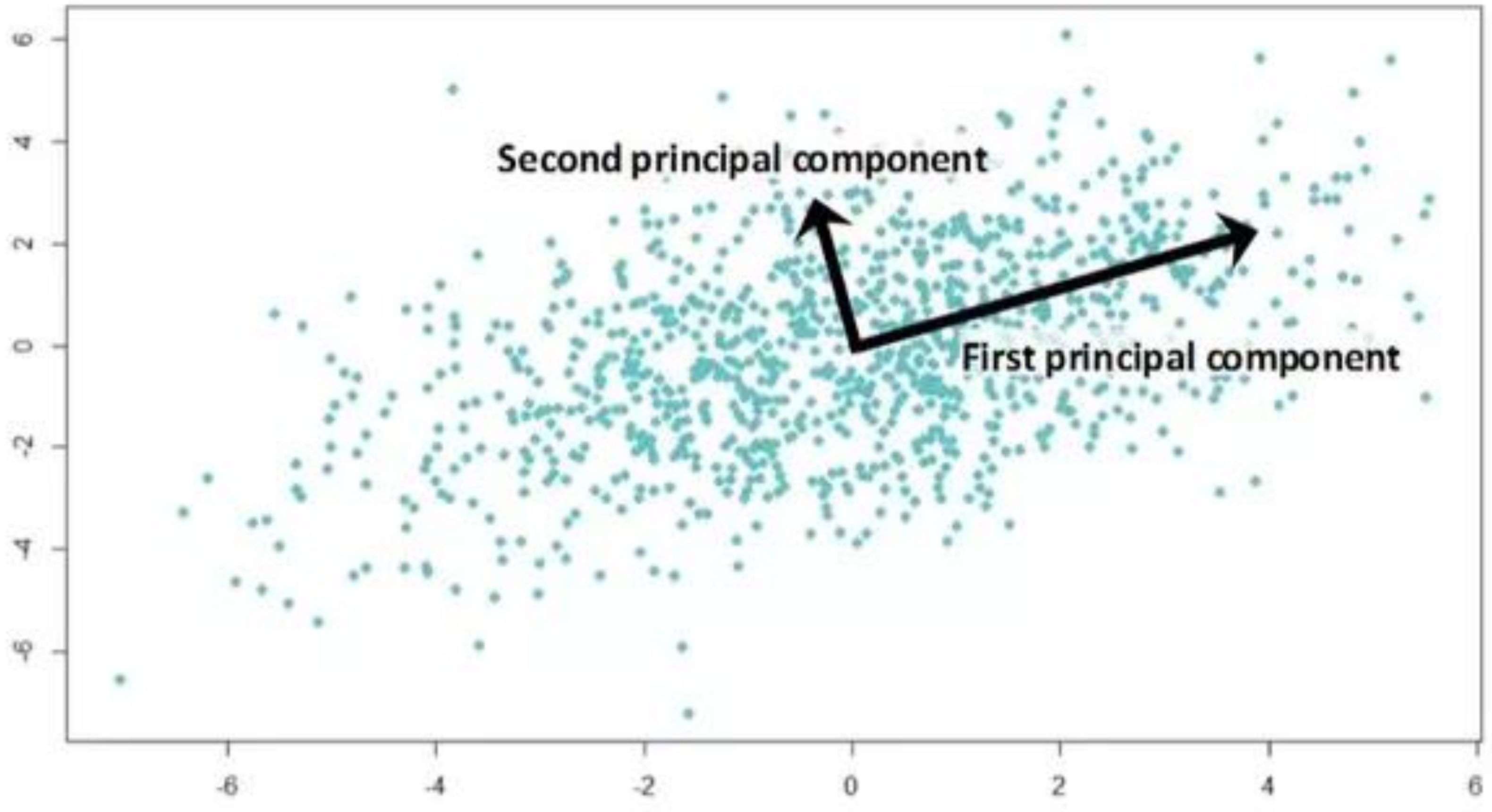

*Images credit Ward A.D. et al 2007*

# Principal Component Analysis

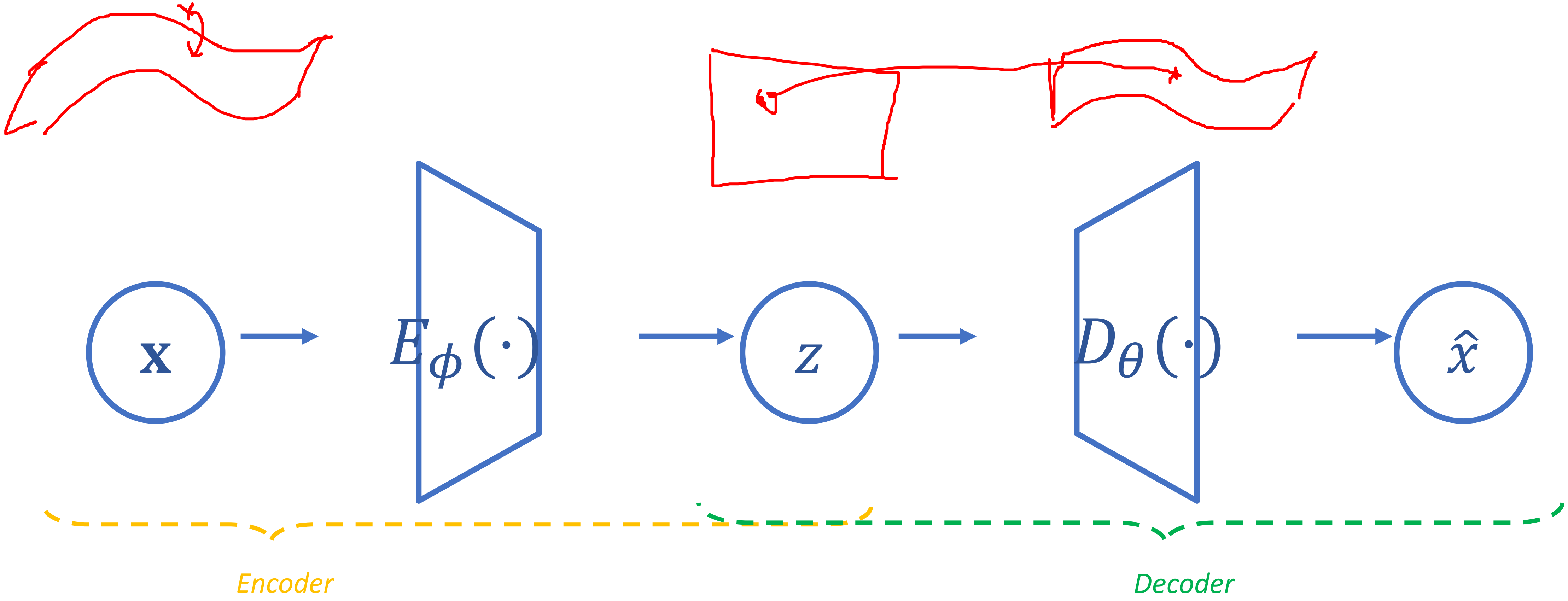


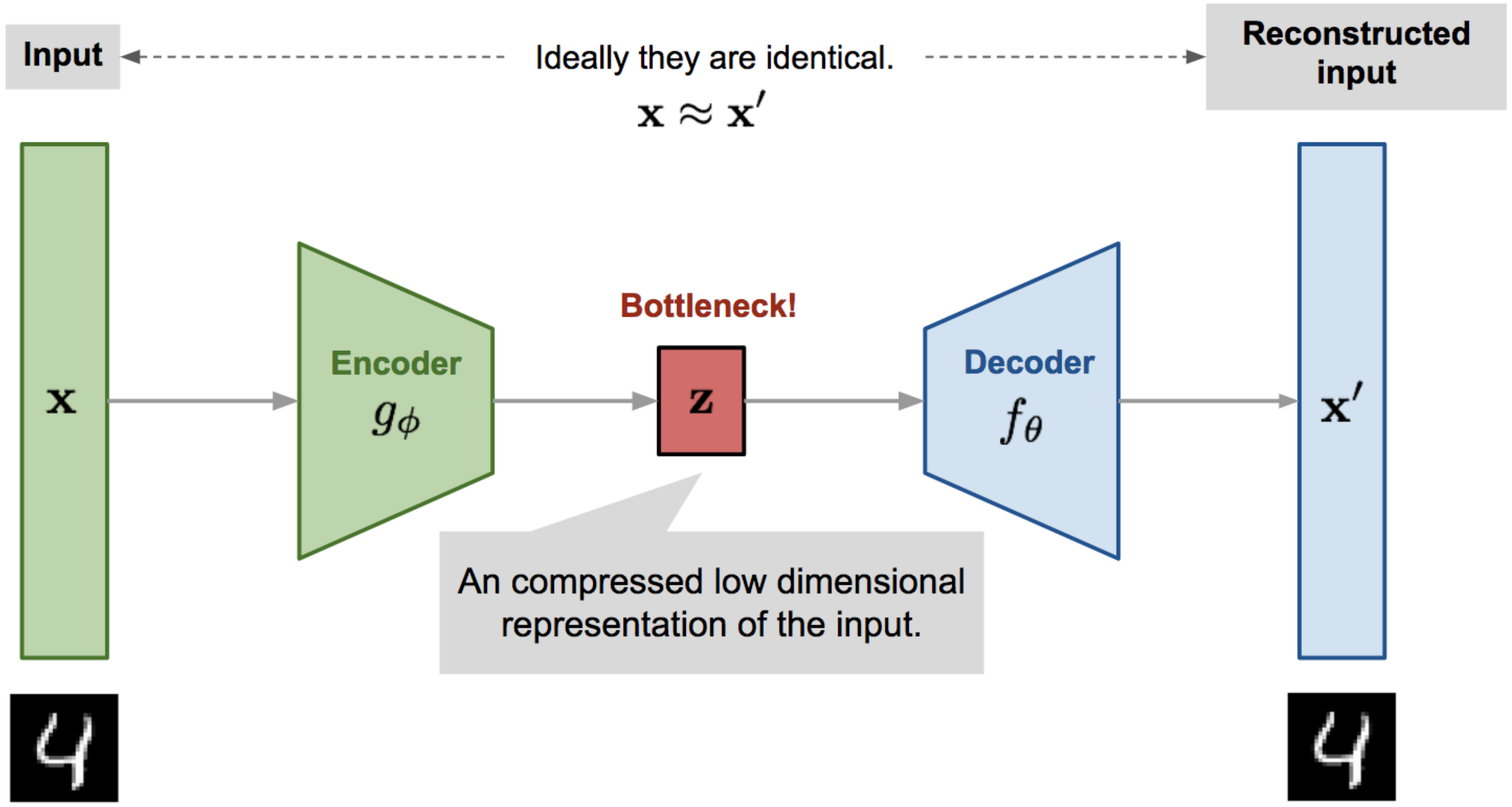

PCA asume que el manifold es lineal!

# Principal Component Analysis



# Autoencoders





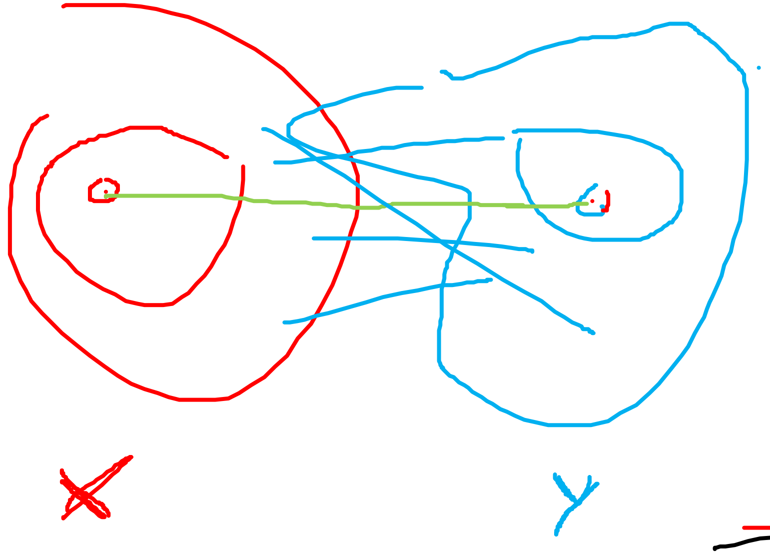

**… pero no podemos usar la variable *z* para muestrear; ninguna relación con la distribución de probabilidad ☹**

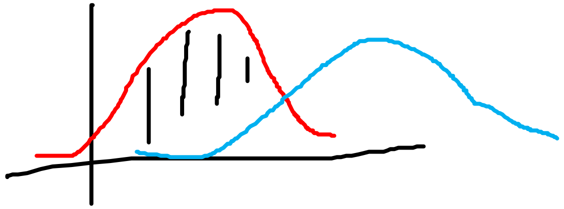
$E[\quad]$

# Let's go mathy!: Divergencia de Kullback-Leibler (KL)

$\int |p(x) - p(y)|\, dx$

$d(x, y)$

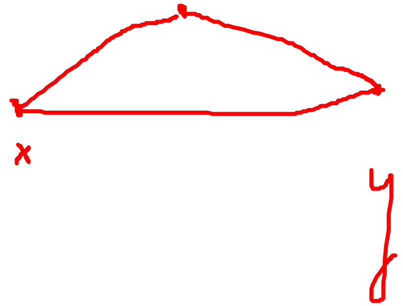


# Cómo medimos la “distancia” entre dos distribuciones?

$x \sim$

$\mathbb{E}[x -$

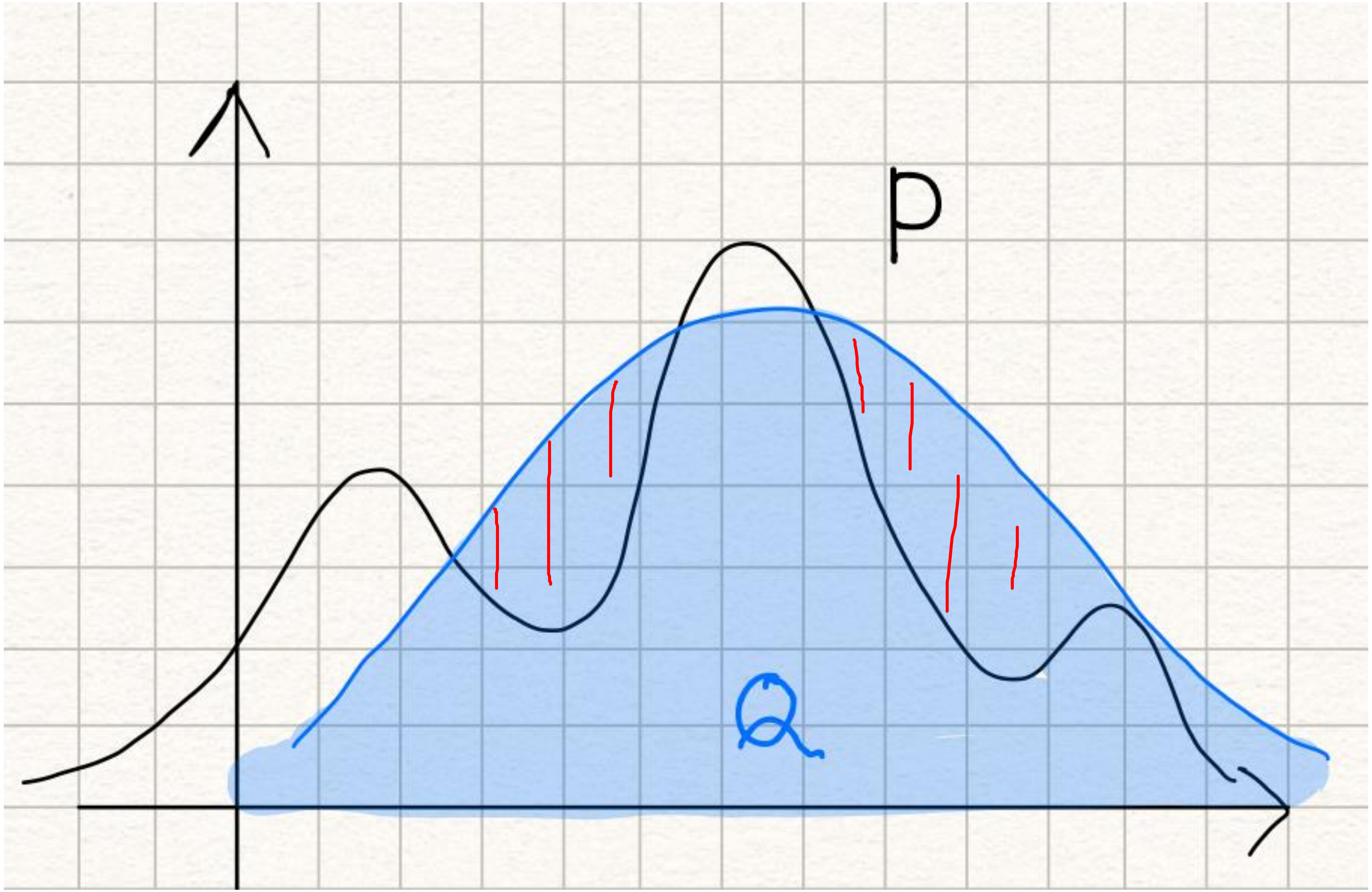



$$KL(p||q) = \mathbb{E}_{x\sim p(x)}\left[\log\frac{p(x)}{q(x)}\right] = \int_x p(x)\log\frac{p(x)}{q(x)}\,dx$$

$\log p - \log q$

$KL(p||q) \neq KL(q||p)$

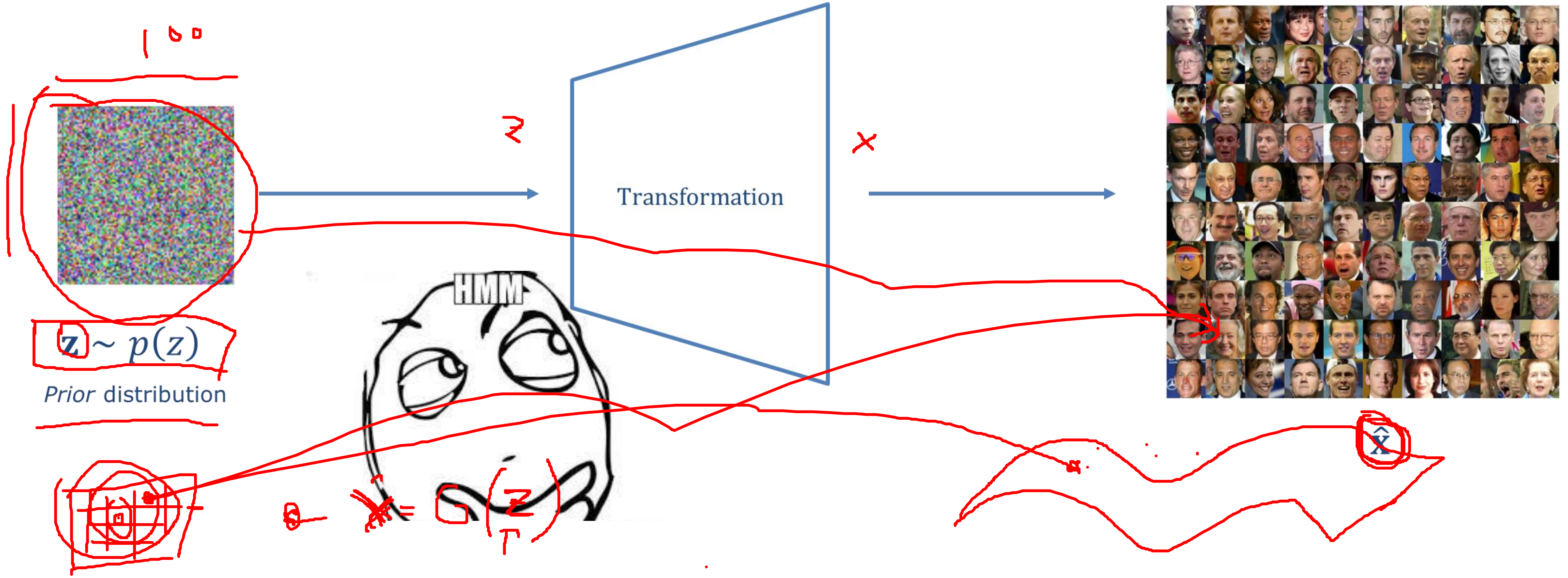
$KL \geq 0$


P
Q

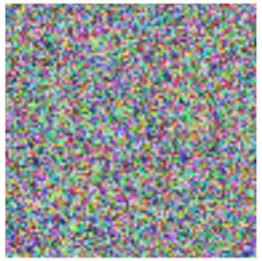
# Variational Autoencoders

# Lo que queremos!

$z \sim N( \quad )$

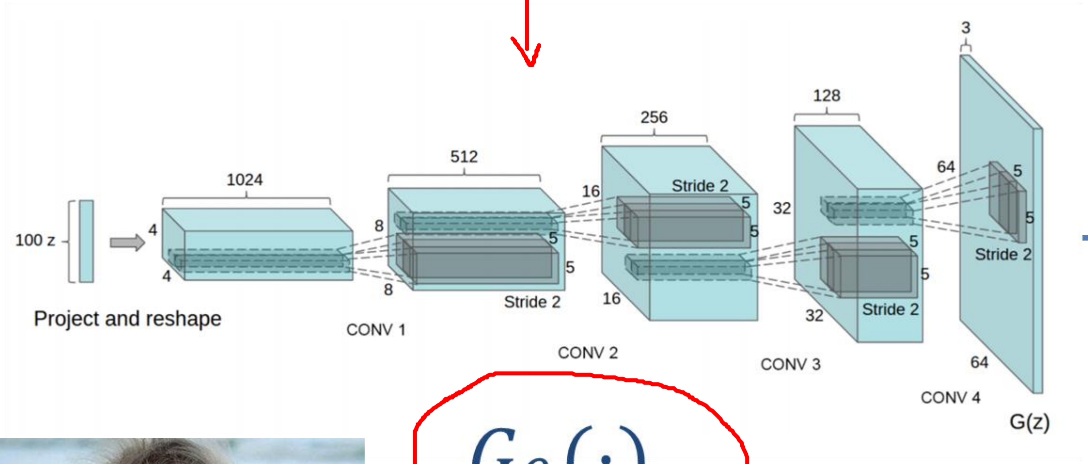


# Deep Latent Variable Models



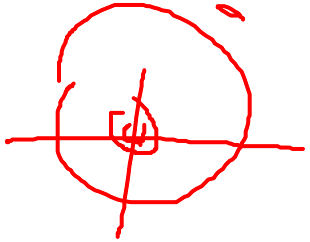
$\mathbf{z} \sim p(z)$

*Prior* distribution

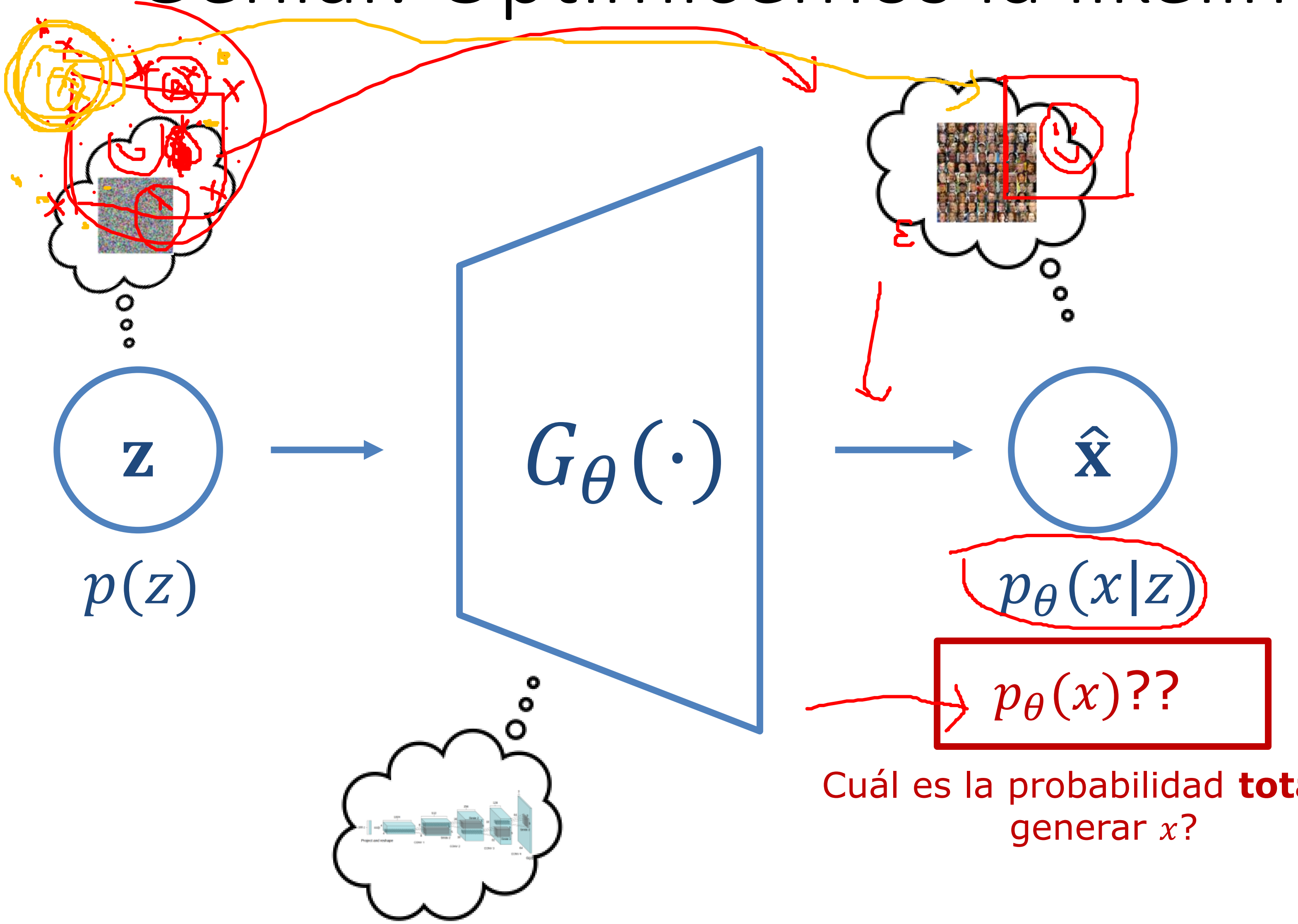



$G_\theta(\cdot)$


$\hat{\mathbf{x}} = G_\theta(\mathbf{z})$

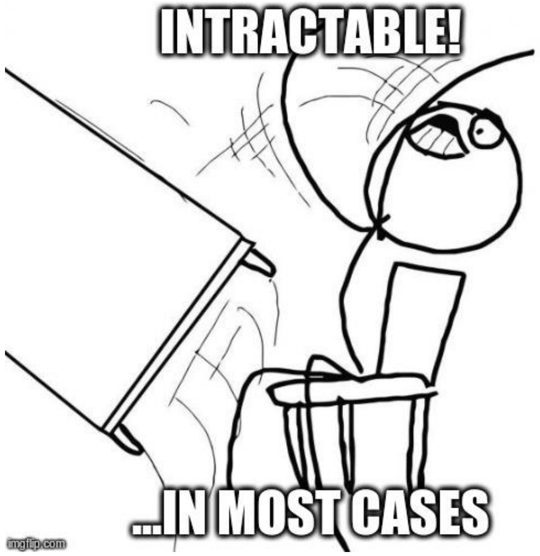


# Genial! Optimicemos la likelihood!




Cuál es la probabilidad **total** de generar $x$?

$$p_\theta(x) = \int p_\theta(x|z)\, p(z)\, dz$$



# Diferentes modelos – diferentes métodos

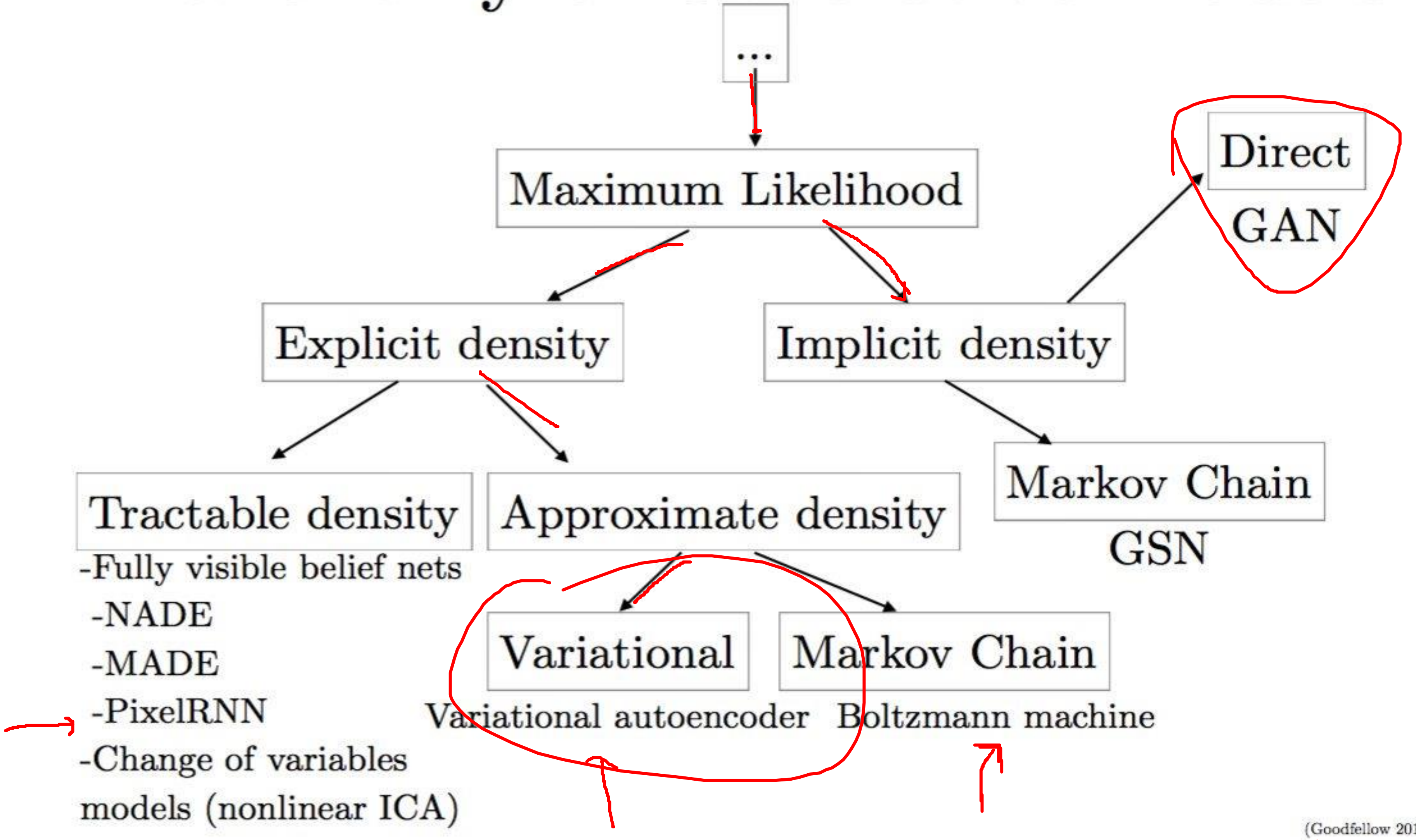
GMM

1. Tenemos $p_\theta(\hat{x})$ explícitamente: **maximizamos likelihood**.

2. $p_\theta(\hat{x})$ es intratable: lo podemos aproximar
   - Markov Chain Monte Carlo (MCMC) methods
   - Variational methods (e.g. Variational Autoencoders)

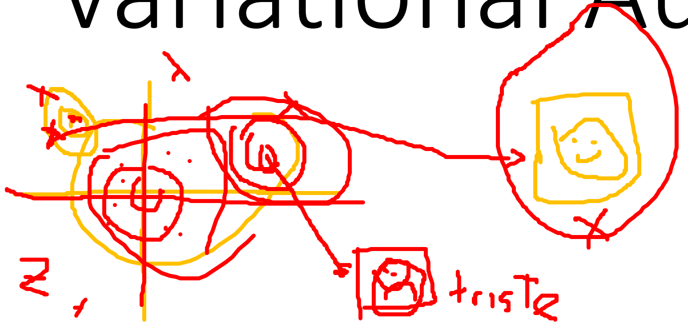
3. No necesitamos $p_\theta(\hat{x})$; está implícito!
   - Adversarial methods (e.g. GANs)

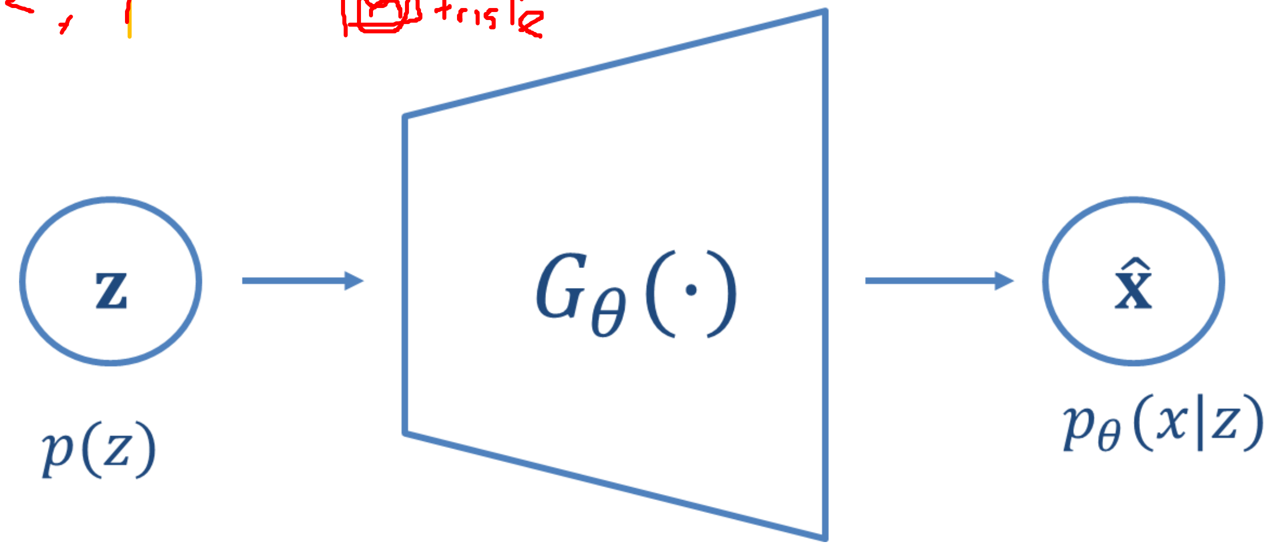
# Taxonomy of Generative Models



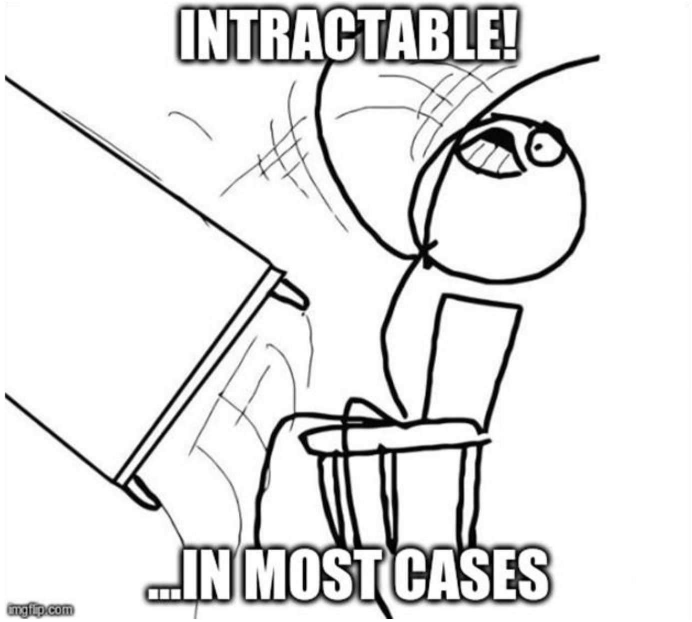

(Goodfellow 2016)

# Variational Autoencoder

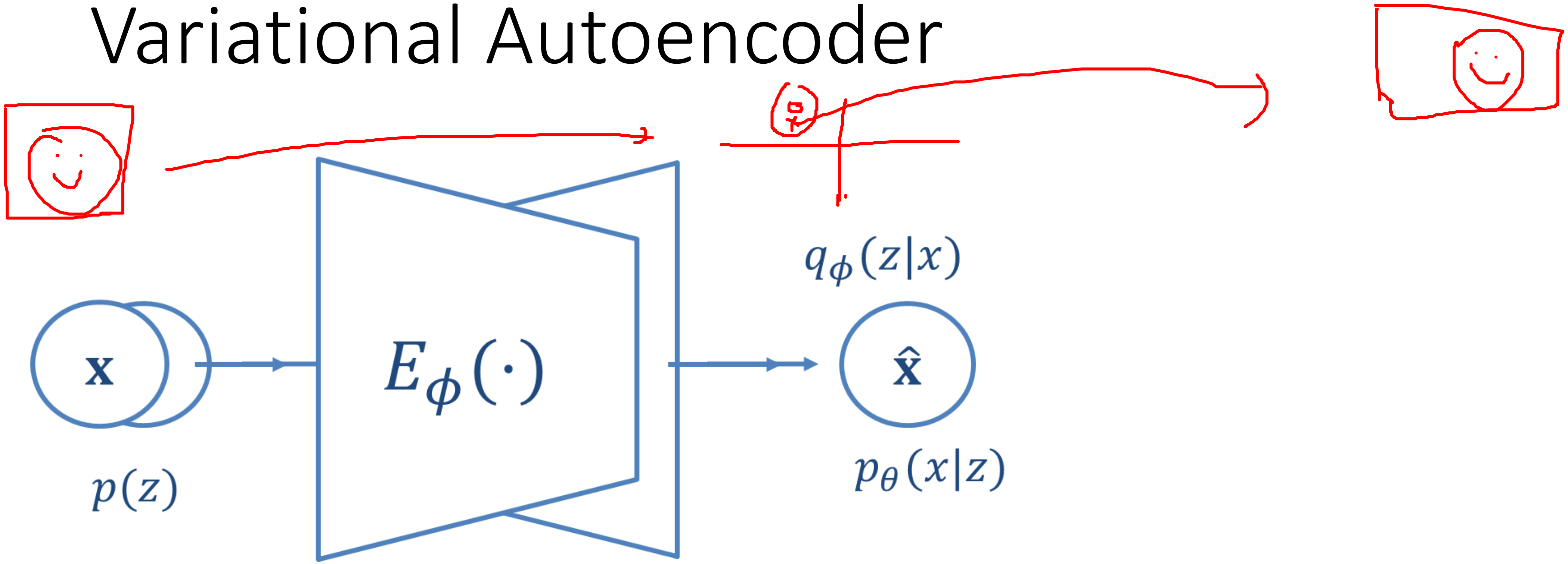


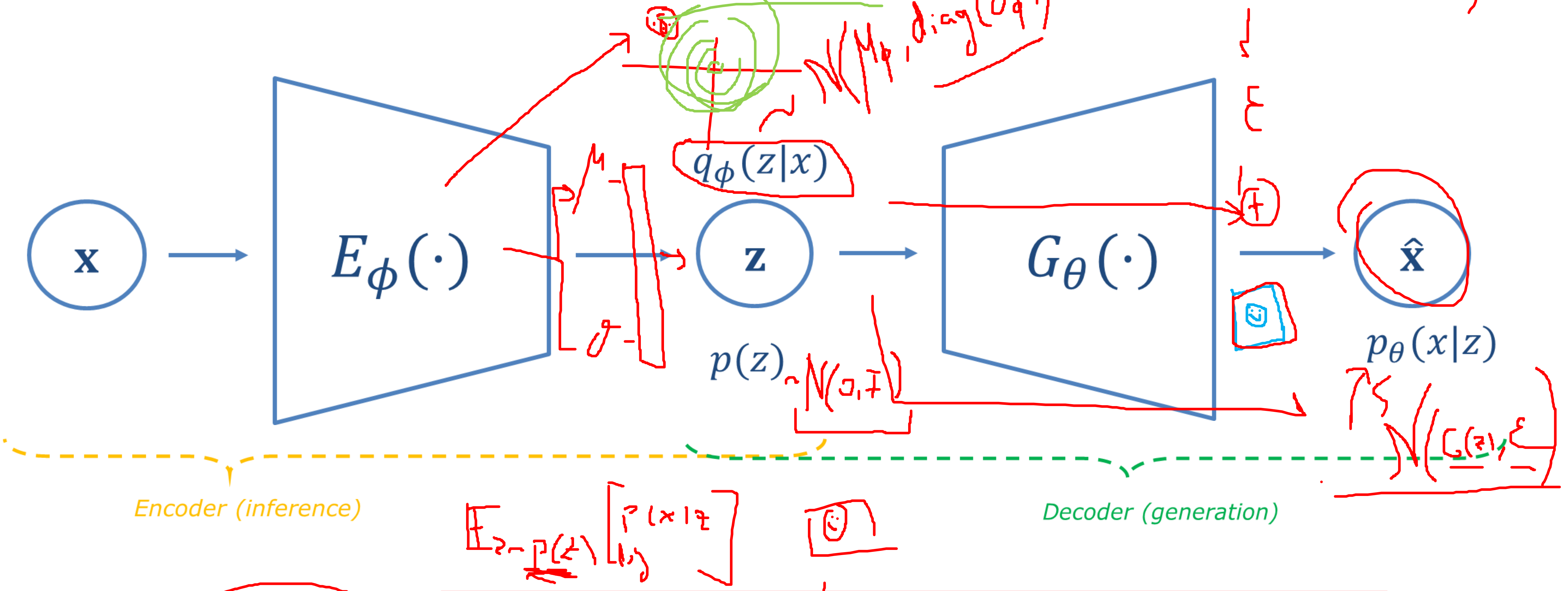

$$p_\theta(x) = \int_{Z} p_\theta(x|z)\,p(z)dz$$



# Variational Autoencoder



# Variational Autoencoder

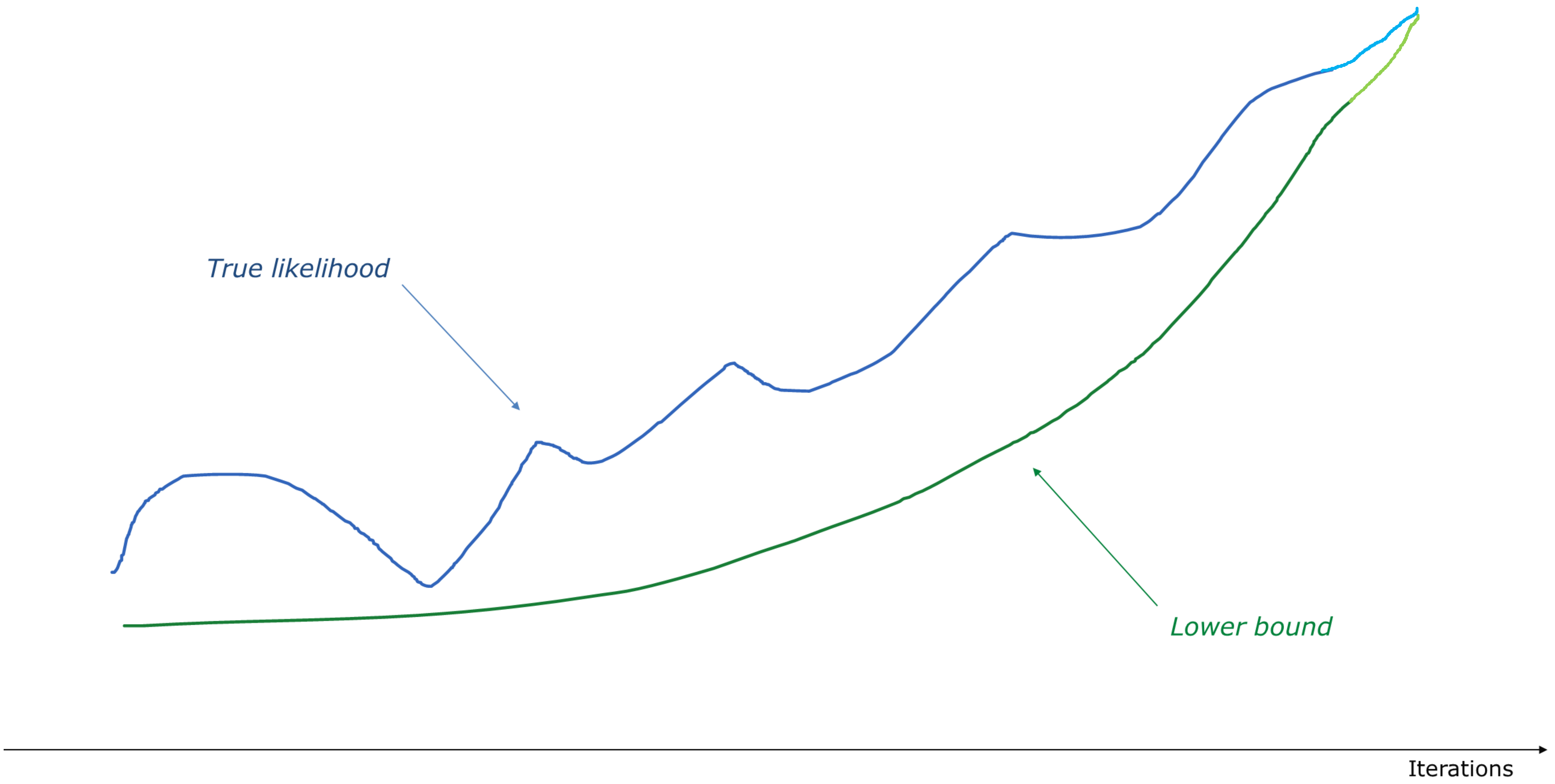



$$\log p_\theta(x) \geq \boxed{\mathbb{E}_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] - \mathrm{KL}[q_\phi(z|x) \,\|\, p(z)]}$$

$\|\hat{x} - x\|^2/\varepsilon$

ELBO

*Maximize this instead!*


True likelihood
Lower bound
Iterations

# ¿Por qué? *Nerd warning*

$$\log p_\theta(x) =$$

$$\log \int_z p_\theta(x|z)p(z)dz = \log \int_z p_\theta(x|z)p(z)\frac{q(z|x)}{q(z|x)}dz = \log \mathbb{E}_{z\sim q}\left[\frac{p_\theta(x|z)p(z)}{q(z|x)}\right] \leq$$

$$\mathbb{E}_{z\sim q}\left[\log\frac{p_\theta(x|z)p(z)}{q(z|x)}\right] = \mathbb{E}_{z\sim q}\left[\log p_\theta(x|z) - \log\frac{p(z)}{q(z|x)}\right] = \mathbb{E}_{z\sim q}[\log p_\theta(x|z)] +$$

$$\mathbb{E}_{z\sim q}\left[\log\frac{q(z|x)}{p(z)}\right] = \mathbb{E}_{z\sim q}[\log p_\theta(x|z)] - \mathrm{KL}(\mathrm{q(z|x)} || \mathrm{p(z)})$$

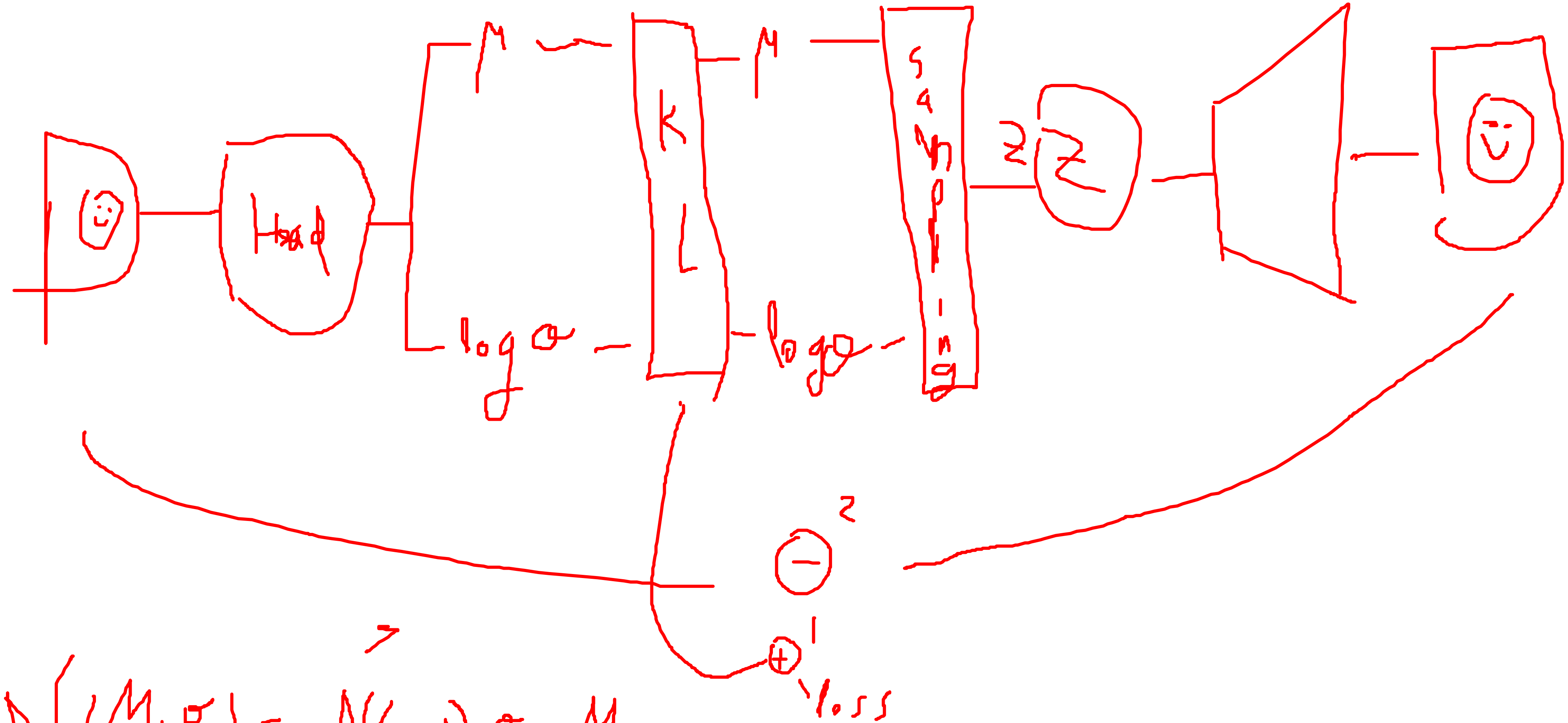
# Variational Autoencoders

**Pros:**

- Inferencia eficiente gratis!
  - o Buena herramienta para modelar la estructura interna de los datos
- Entrenamiento estable
- Buen fundamento teórico

**Cons:**

- No genera muy buenas muestras

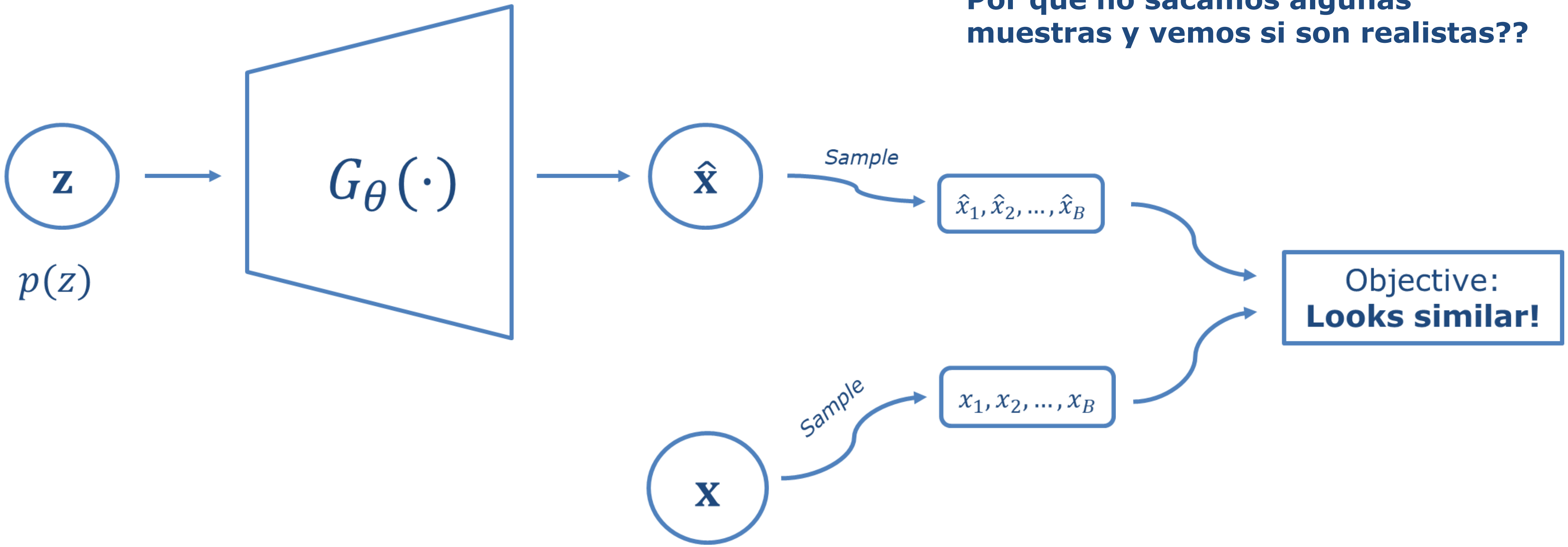



$$X \sim N(\mu, \sigma) = N(0,1)\cdot\sigma + \mu$$

# Generative Adversarial Networks

# Generative Adversarial Networks

**Por qué no sacamos algunas muestras y vemos si son realistas??**



*Pero… ¿Cómo medimos similitud entre grupos de muestras?*

# Similitud entre muestras

Una solución: **entrenar un <u>clasificador</u>** $D_\phi(x)$ **para discriminar!**

- Si el clasificador no puede decir si una muestra es real o no, ambas distribuciones están cerca.
- Entrenamos con la *cross-entropy loss* estandar:

$$\max_\phi L_d(\phi) = \max_\phi \left( \mathbb{E}_{x_r \sim p_{real}} \log\left(D_\phi(x_r)\right) + \mathbb{E}_{x_f \sim p_{fake}} \log\left(1 - D_\phi(x_f)\right)\right)$$

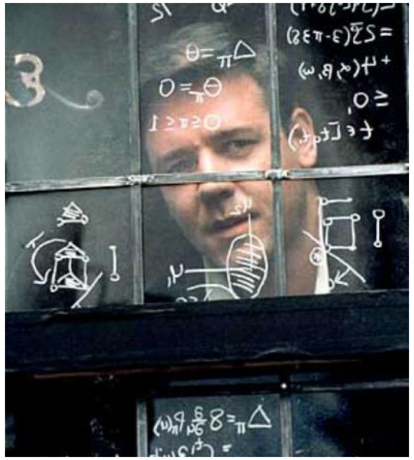
Se puede probar que el coste de un clasificador *óptimo* $L_d(\phi^*)$ está relacionado con la *cercanía* entre ambas distribuciones (Jensen-Shannon divergence).

# The GAN game

Queremos minimizar la “cercanía” entre las muestras generadas y las reales medida por el coste del discriminador:

$$\min_{\theta} \text{"closeness"}$$

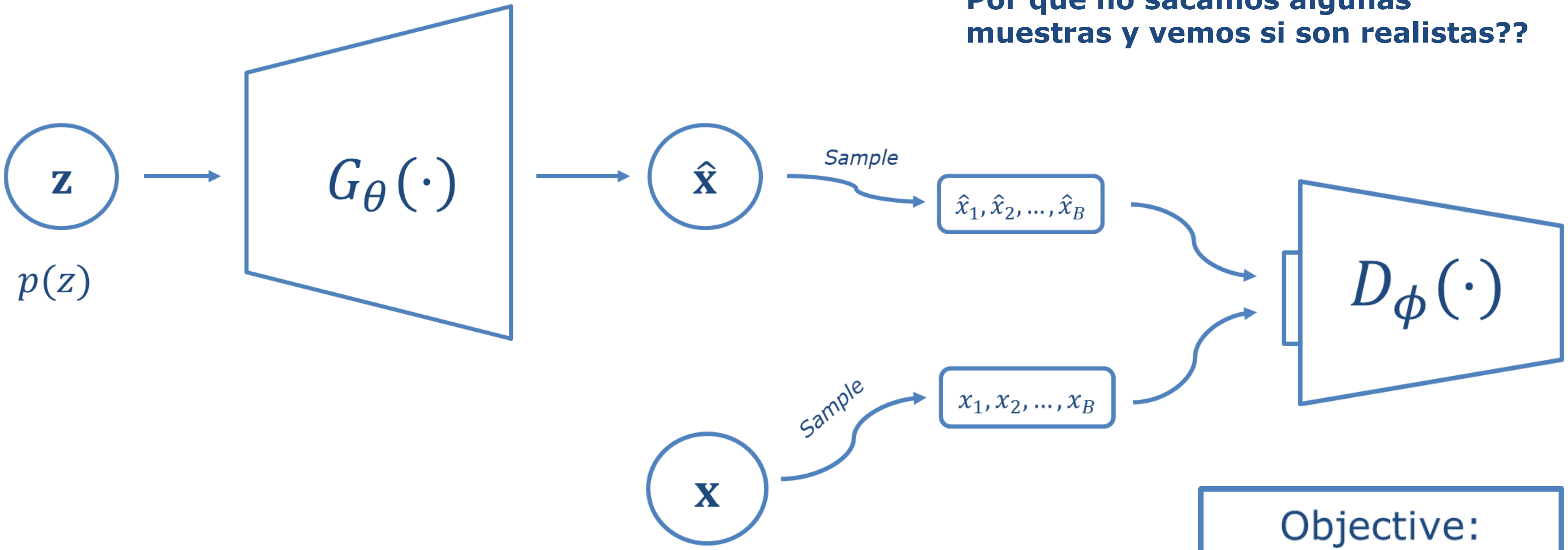
$$= \min_{\theta}\left(\max_{\phi}\left(\mathbb{E}_{x_r \sim p_{real}} \log\left(D_{\phi}(x_r)\right) + \mathbb{E}_{x_f \sim p_{fake}} \log\left(1 - D_{\phi}(x_f)\right)\right)\right)$$



<u>Es formalmente un juego minimax de dos jugadores!</u>

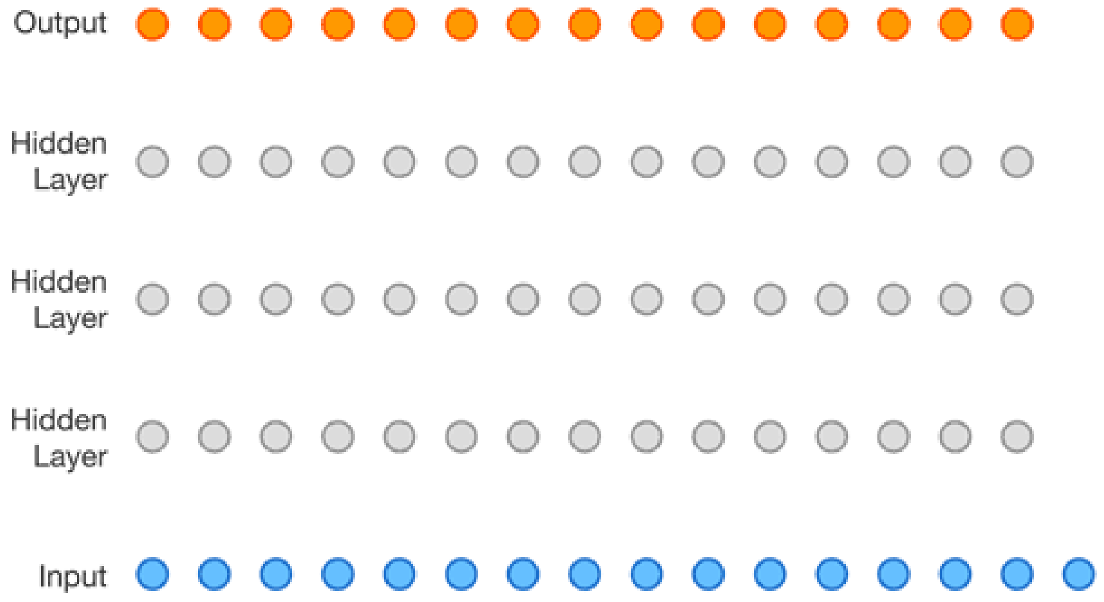
# Generative Adversarial Networks

**Por qué no sacamos algunas muestras y vemos si son realistas??**




Objective:
**Fool** $D_\phi$**!**

# Bonus: autoregressive models




$$p_\theta(x) = \prod_{t=1}^{T} p_\theta(x_t | x_1, \dots, x_{t-1})$$

*Divide et impera!*