



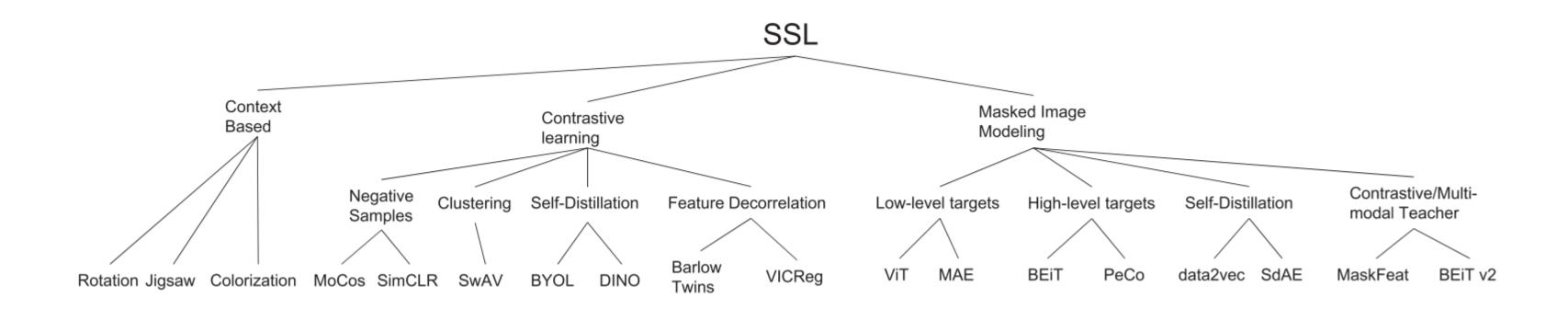
Sesión 5.0 Self-supervised learning l

Contrastive learning





Self-Supervised Learning

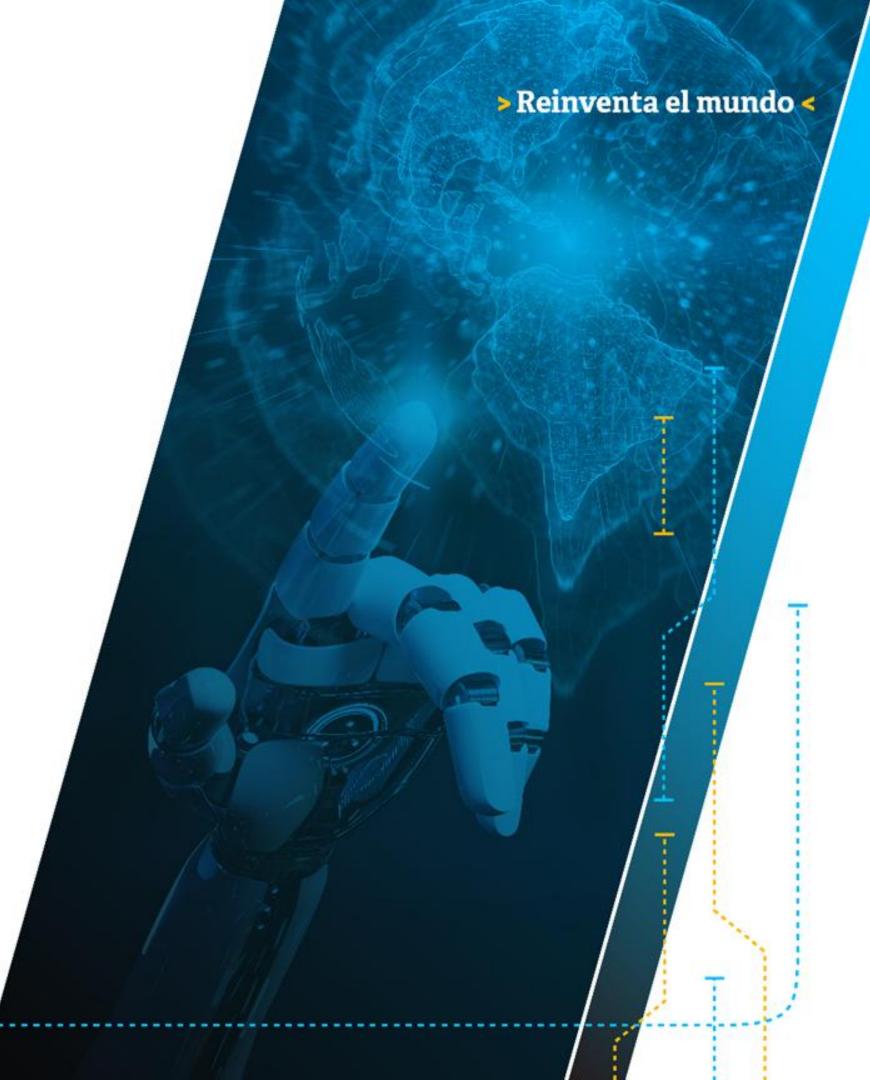




1.



Context-Based Methods





Rotation

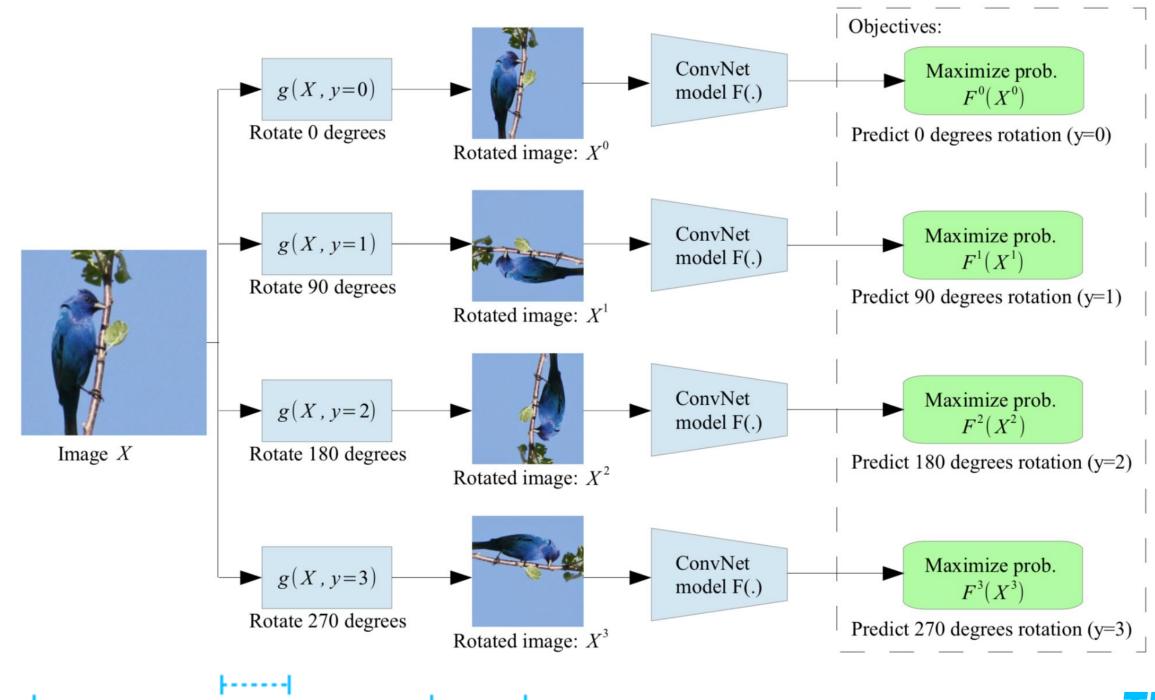




Image Colorization

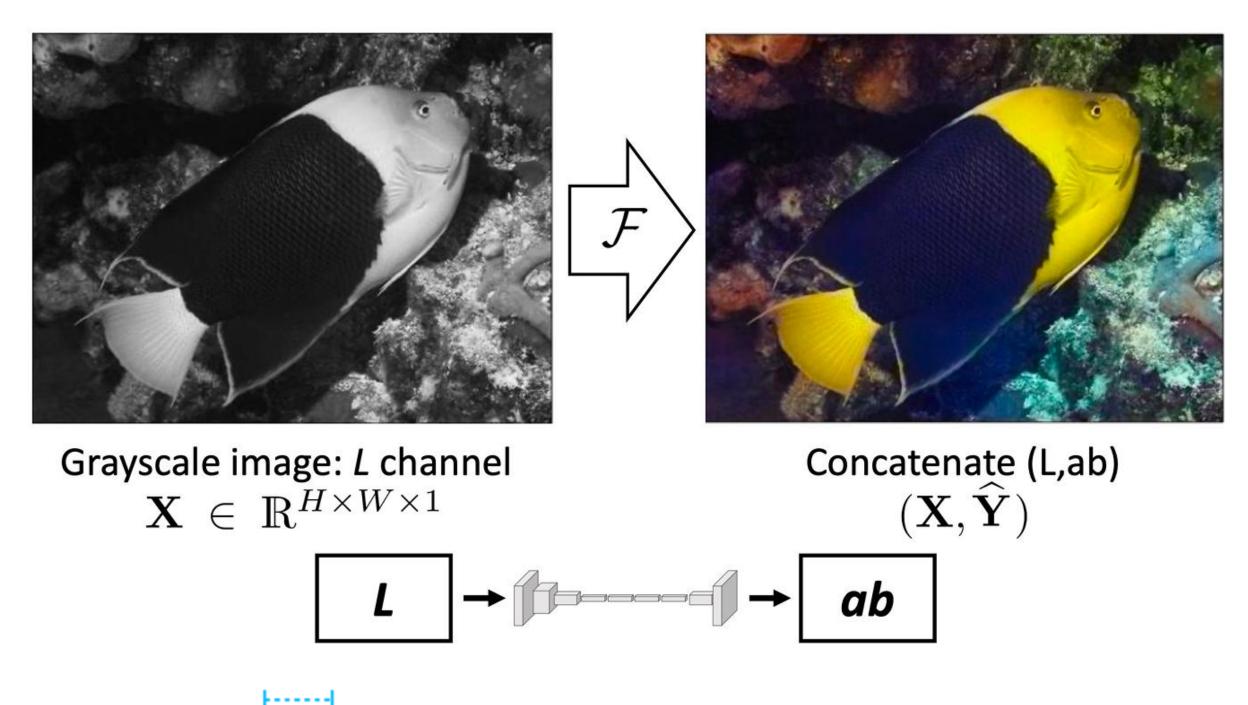
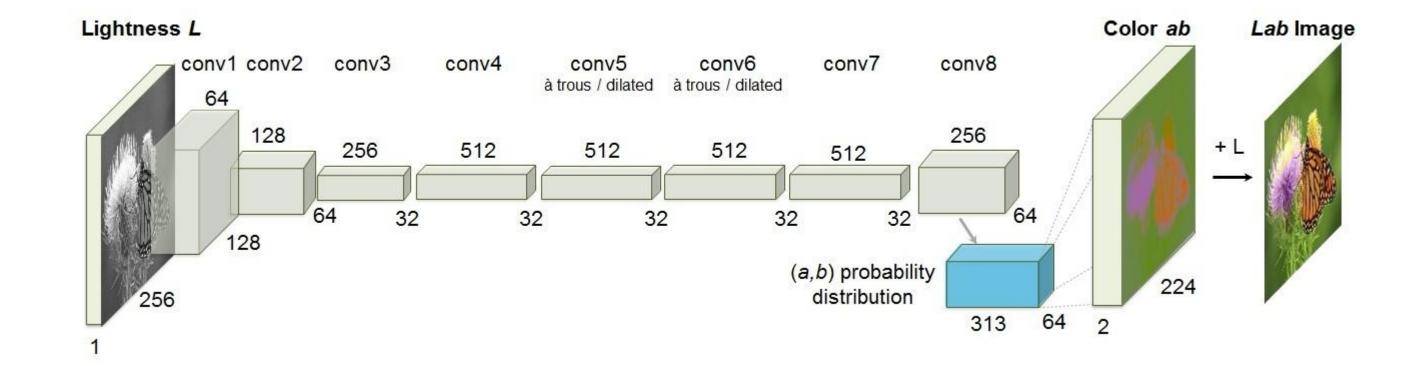


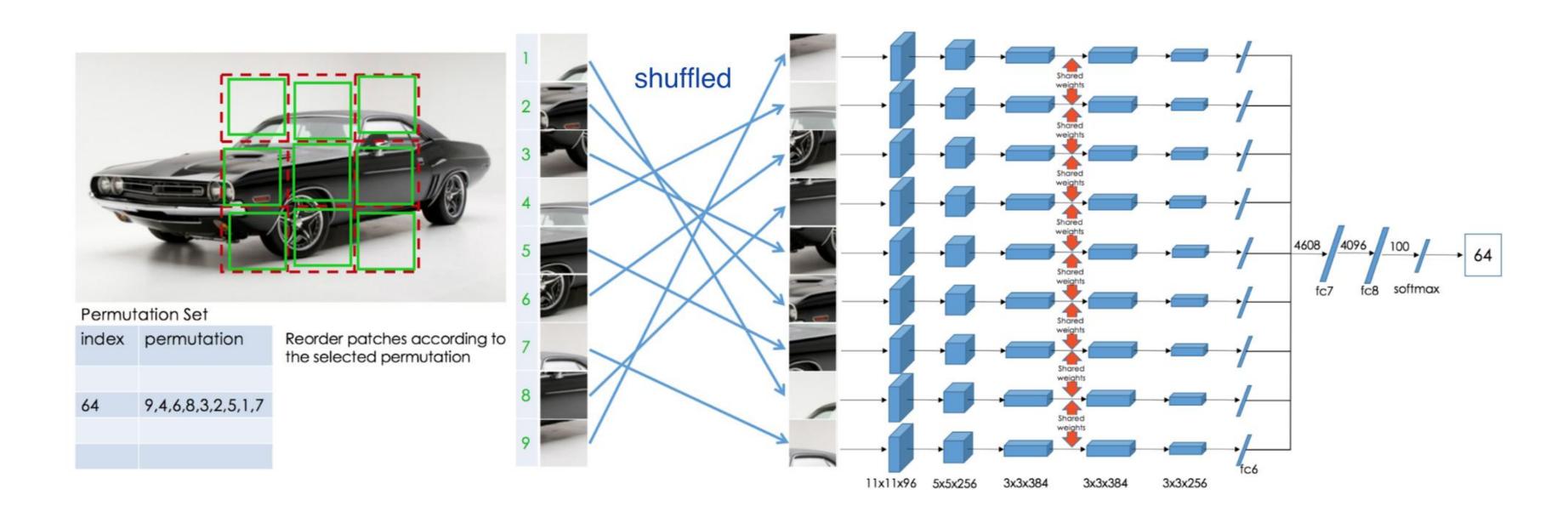


Image Colorization





Jigsaw Puzzles



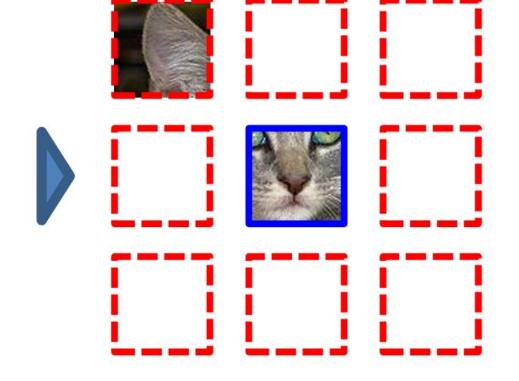


Context Prediction

Example:



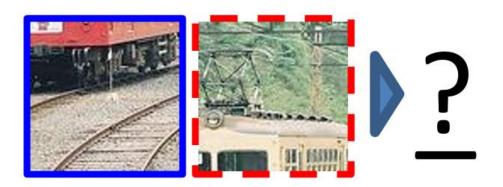




Question 1:

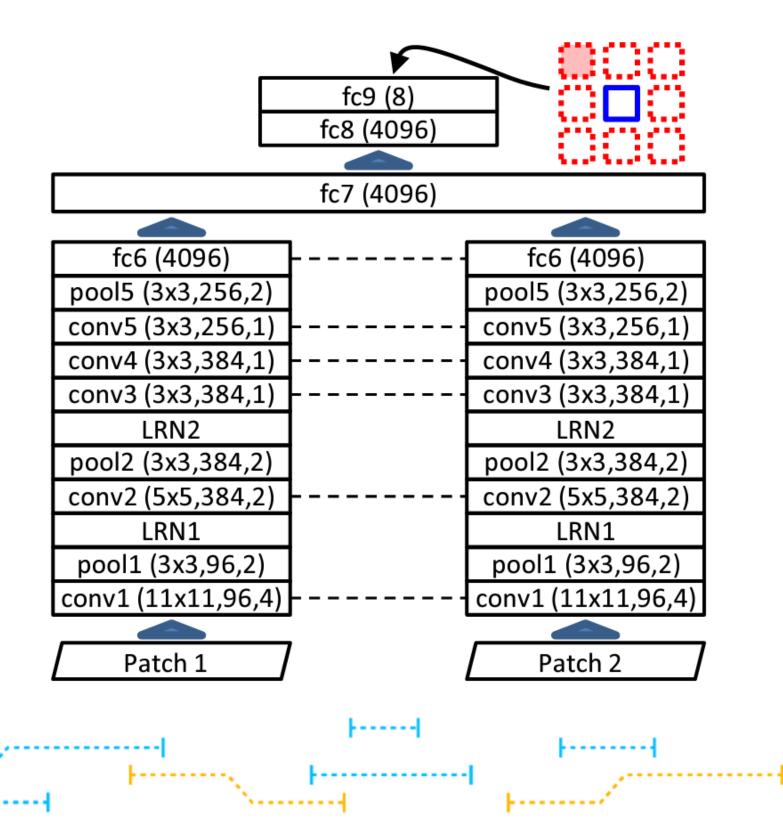


Question 2:





Context Prediction



Question 1:



Question 2:

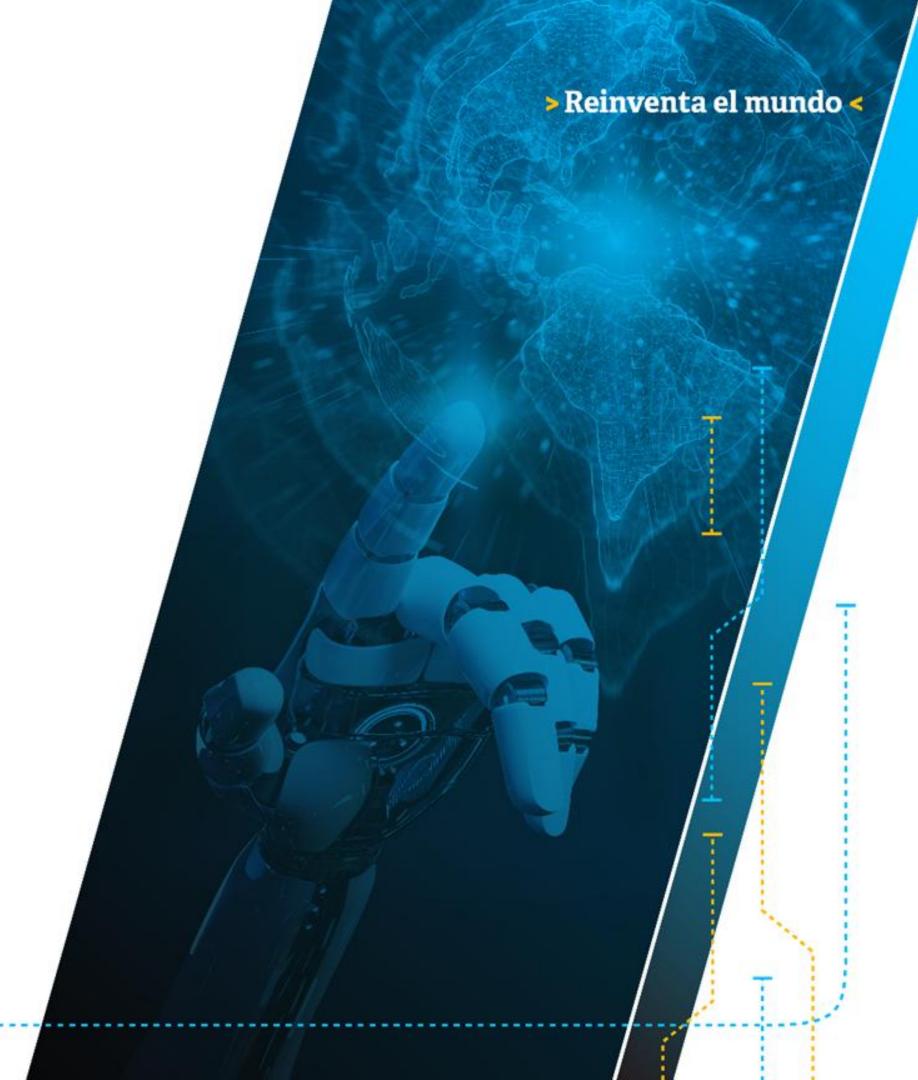




2.

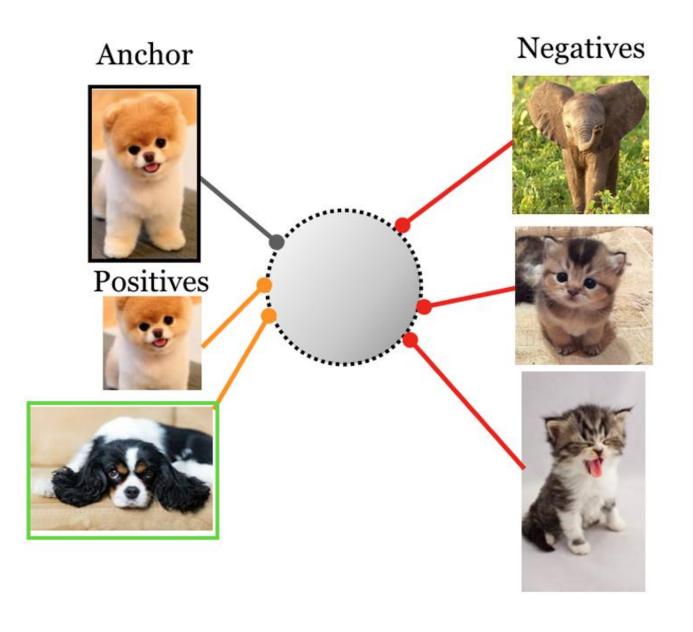


Contrastive Learning





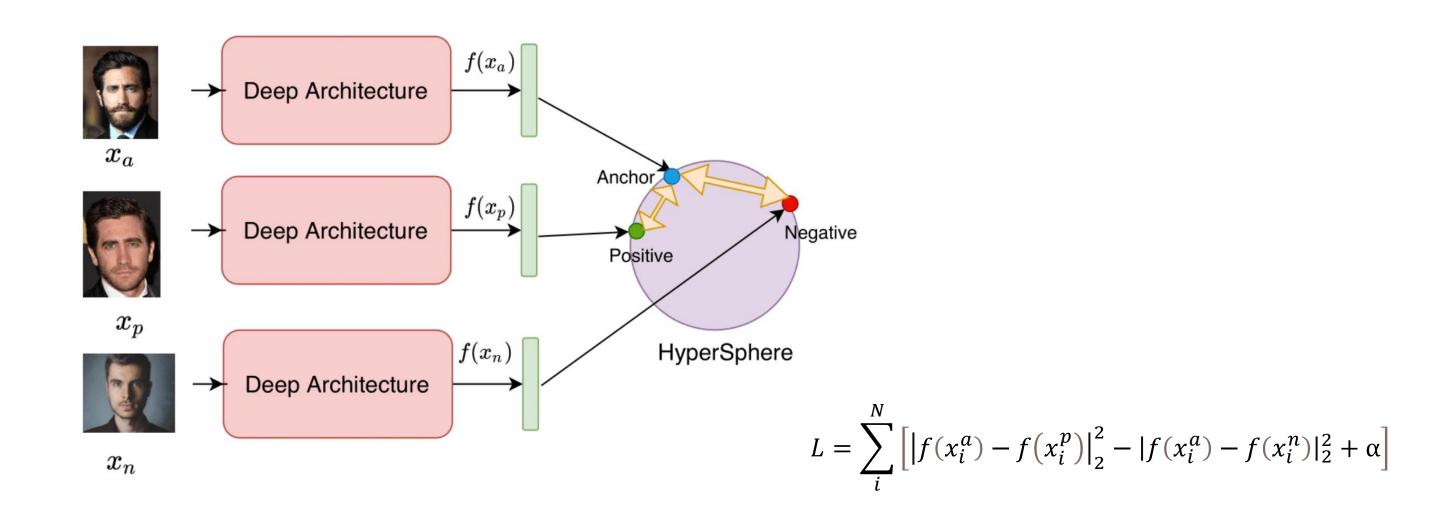
Self-Supervised Learning





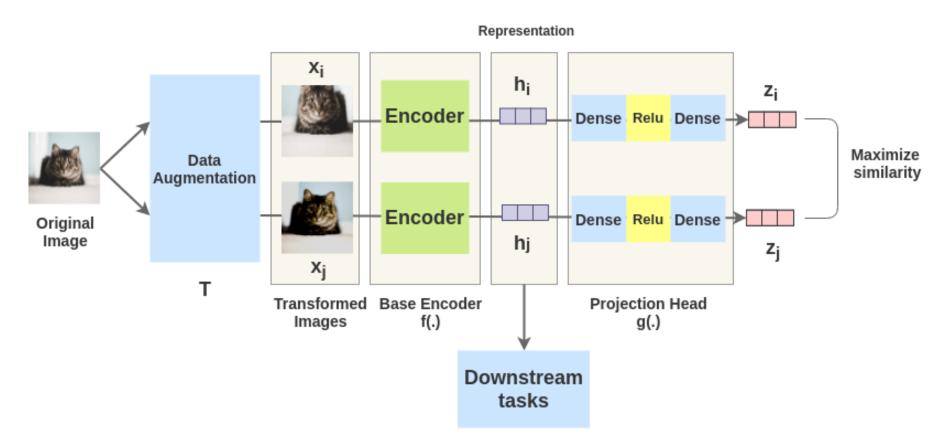
Triplet Loss

Es una técnica de aprendizaje supervisado, el cual es predecesor de propuestas en self-supervised.





SimCLR



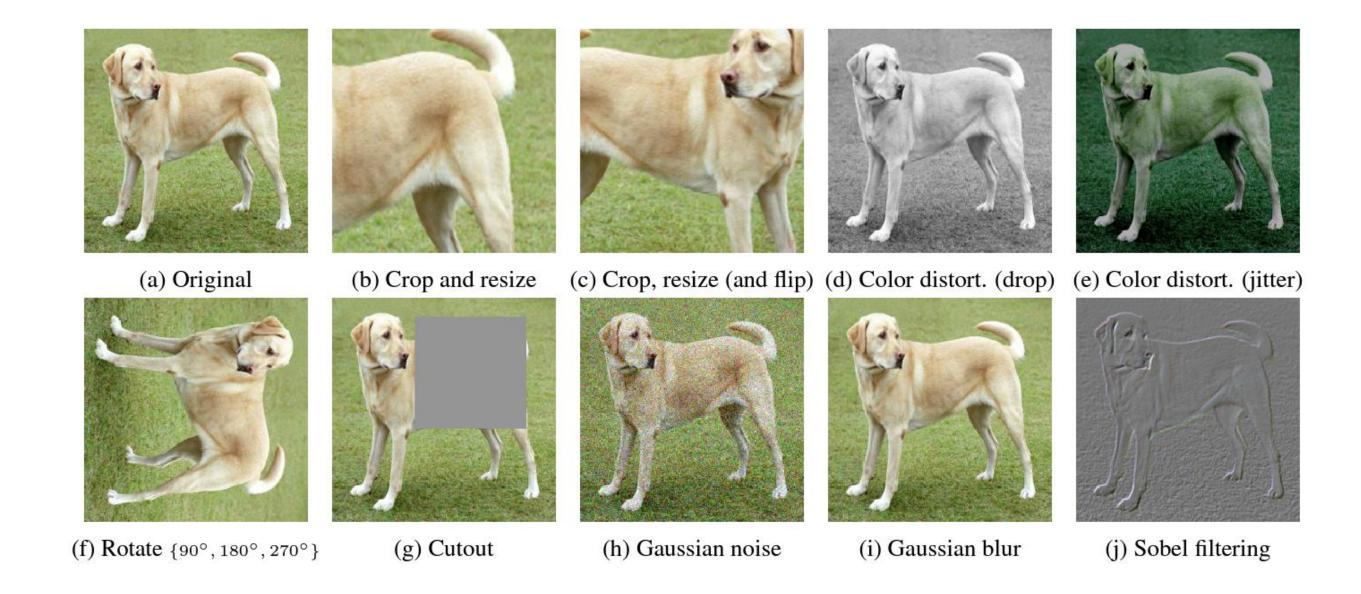
Normalized Temperature-scaled Cross-Entropy (NT-Xent):

$$\mathcal{L}_{i,j} = -\log \frac{\exp(\operatorname{sim}(z_i, z_j)/\tau)}{\sum_{k=1}^{2N} 1[k \neq i] \exp(\operatorname{sim}(z_i, z_k)/\tau)}$$

donde
$$sim(z_i, z_j) = \frac{z_i \cdot z_j}{|z_i||z_j|}$$



SimCLR

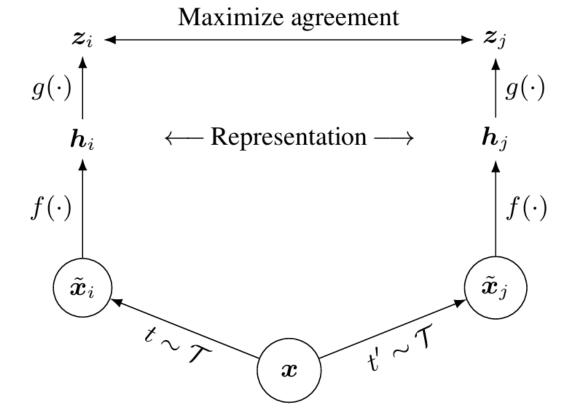




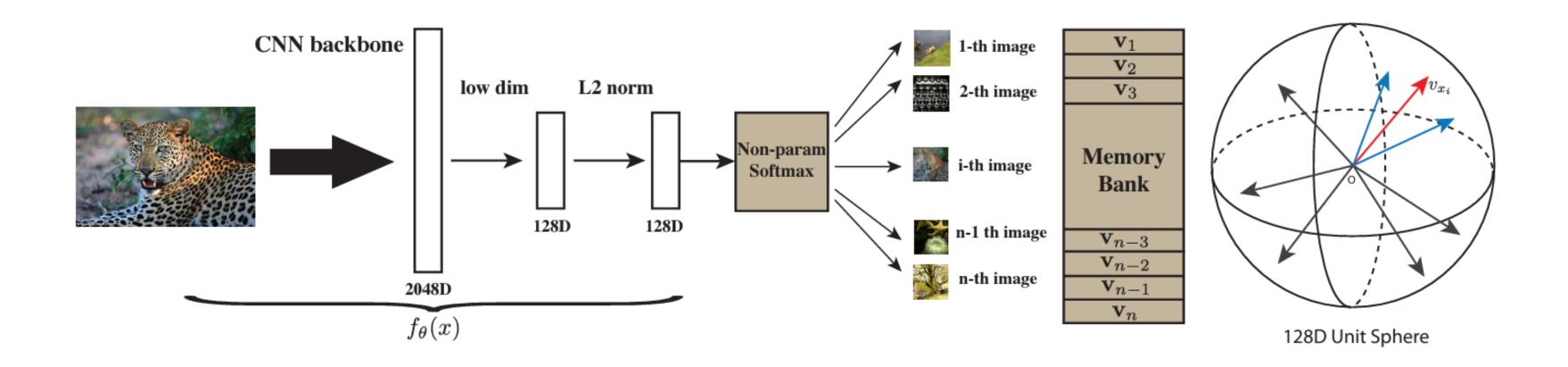
SimCLR

Algorithm 1 SimCLR's main learning algorithm.

```
input: batch size N, constant \tau, structure of f, g, \mathcal{T}.
for sampled minibatch \{oldsymbol{x}_k\}_{k=1}^N do
   for all k \in \{1, \dots, N\} do
        draw two augmentation functions t \sim T, t' \sim T
        # the first augmentation
        \tilde{\boldsymbol{x}}_{2k-1} = t(\boldsymbol{x}_k)
       \boldsymbol{h}_{2k-1} = f(\tilde{\boldsymbol{x}}_{2k-1})
                                                                 # representation
        \boldsymbol{z}_{2k-1} = g(\boldsymbol{h}_{2k-1})
                                                                        # projection
        # the second augmentation
        \tilde{\boldsymbol{x}}_{2k} = t'(\boldsymbol{x}_k)
       \boldsymbol{h}_{2k} = f(\tilde{\boldsymbol{x}}_{2k})
                                                                 # representation
        \boldsymbol{z}_{2k} = g(\boldsymbol{h}_{2k})
                                                                        # projection
   end for
   for all i \in \{1, \dots, 2N\} and j \in \{1, \dots, 2N\} do
        s_{i,j} = oldsymbol{z}_i^{	op} oldsymbol{z}_j / (\|oldsymbol{z}_i\| \|oldsymbol{z}_j\|) # pairwise similarity
   end for
   define \ell(i,j) as \ell(i,j) = -\log \frac{\exp(s_{i,j}/\tau)}{\sum_{k=1}^{2N} \mathbb{1}_{[k \neq i]} \exp(s_{i,k}/\tau)}
   \mathcal{L} = \frac{1}{2N} \sum_{k=1}^{N} \left[ \ell(2k-1, 2k) + \ell(2k, 2k-1) \right]
   update networks f and g to minimize \mathcal{L}
end for
return encoder network f(\cdot), and throw away g(\cdot)
```

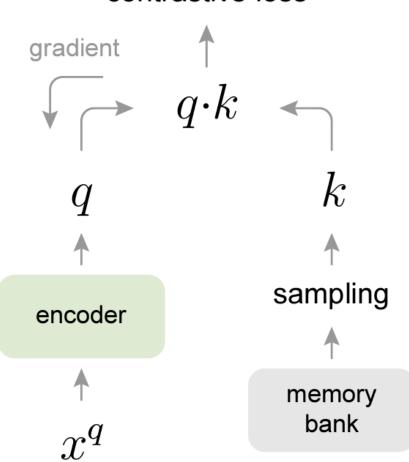








contrastive loss



La probabilidad de que una imagen v pertenezca a una instancia i está dada por:

$$p(i|v) = \frac{\exp(v_i^T v/\tau)}{\sum_{j=1}^n \exp(v_j^T v/\tau)}$$

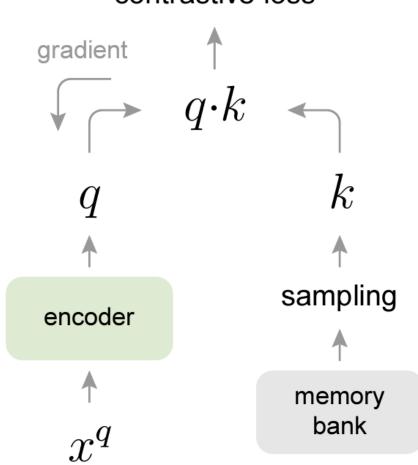
Loss function:

$$J(\theta) = -\sum_{i=1}^{n} \log p(i|f_{\theta}(x_i))$$





contrastive loss



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Problemas:

- Muchas clases (una por muestra en la memoria).
- Es difícil calcular p(i|v)



contrastive loss gradient sampling encoder memory bank

Cambiamos a un problema de clasificación binaria:

Definimos un evento binario *D*, donde:

- D = 1 significa que la muestra es real.
- D = 0 significa que la muestra es ruido.



contrastive loss gradient sampling encoder memory bank x^q

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Definimos un evento binario *D*, donde:

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Calculamos la probabilidad posteriori:

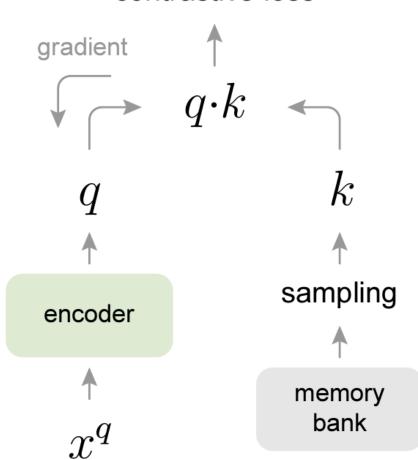
$$P(D = 1|i, v) = \frac{P(i|v)P(D = 1)}{P(i|v)P(D = 1) + P_n(i)P(D = 0)}$$

donde:

- P(D=1) es la probabilidad de que una muestra provenga del conjunto real de datos.
- P(D=0) es la probabilidad de que una muestra provenga del ruido.
- $P_n(i)$ es la probabilidad de la muestra bajo la distribución de ruido (se asume distribución uniforme).



contrastive loss



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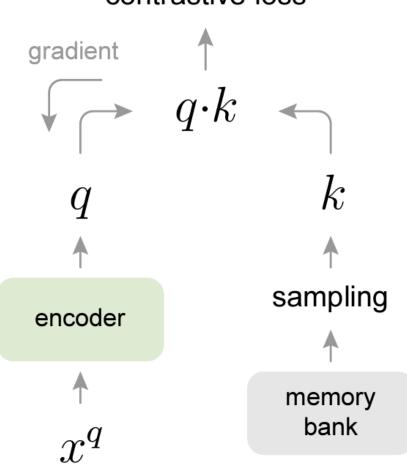
Hacemos:

- Los datos reales ocurren con probabilidad $\frac{1}{1+m}$.
- El ruido ocurre con probabilidad $\frac{m}{1+m}$.





contrastive loss



Cambiamos a un problema de clasificación binaria:

Definimos un evento binario D, donde:

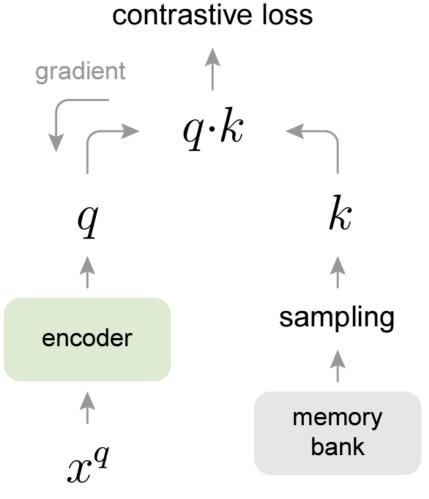
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Calculamos la probabilidad posteriori:

$$P(D = 1|i, v) = \frac{P(i|v) \cdot \frac{1}{1+m}}{P(i|v) \cdot \frac{1}{1+m} + P_n(i) \cdot \frac{m}{1+m}} = \frac{P(i|v)}{P(i|v) + mP_n(i)}$$



and the Contract



Cambiamos a un problema de clasificación binaria:

Definimos un evento binario *D*, donde:

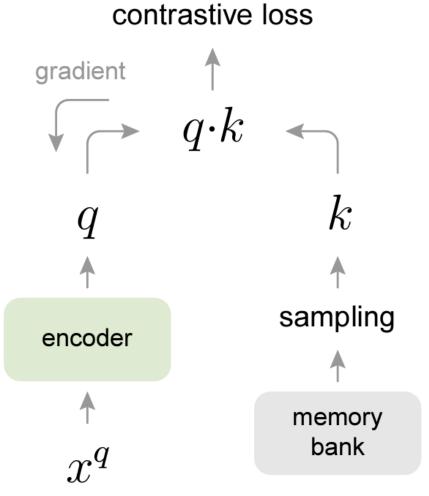
- D = 1 significa que la muestra es real.
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Calculamos la probabilidad posteriori:

$$h(i,v) = \frac{P(i|v)}{P(i|v) + mP_n(i)}$$

Asumimos distribución uniforme para $P_n(i)$, entonces: $P_n(i) = 1/n$





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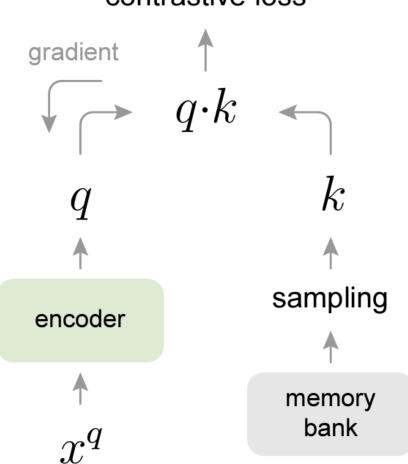
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Aun tenemos a P(i|v)



contrastive loss



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$$h(i,v) = \frac{P(i|v)}{P(i|v) + mP_n(i)}$$

Nos interesa: $P(i|v) = \frac{\exp(v^T v_i/\tau)}{7}$ donde Z es el término de normalización:

$$Z = \sum_{j=1}^{n} \exp(v^T v_j / \tau)$$

Aproximamos con muestreo Monte Carlo usando m muestras negativas:

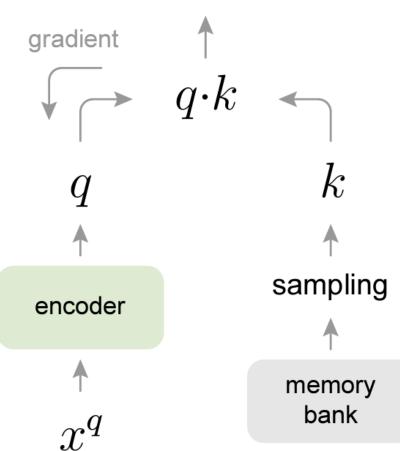
$$Z \approx n \cdot \frac{1}{m} \sum_{k=1}^{m} \exp(v^{T} v_{j_{k}} / \tau)$$







contrastive loss



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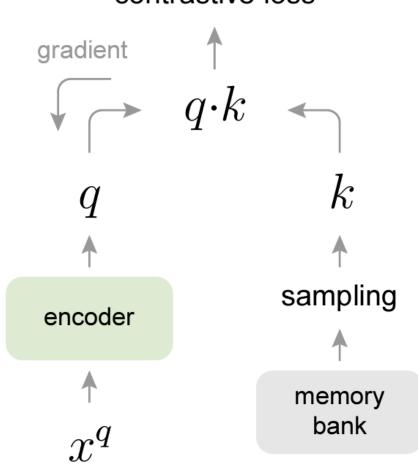
Aproximamos con muestreo Monte Carlo usando m muestras negativas:

$$Z \approx n \cdot \mathbb{E}_j \left[\exp(v^T v_j / \tau) \right] \approx n \cdot \frac{1}{m} \sum_{k=1}^m \exp(v^T v_{j_k} / \tau)$$





contrastive loss



Cambiamos a un problema de clasificación binaria:

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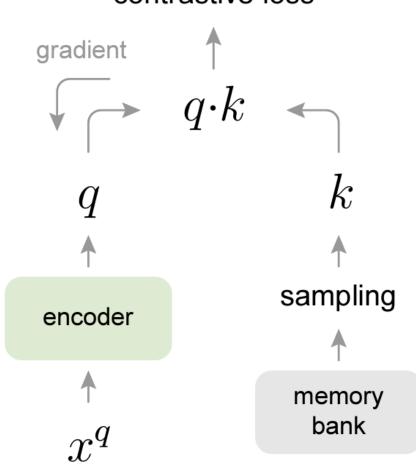
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Calculamos la probabilidad posteriori:

$$h(i,v) = \frac{P(i|v)}{P(i|v) + mP_n(i)} = \frac{\frac{\exp(v^T v_i/\tau)}{\frac{n}{m} \sum_{k=1}^{m} \exp(v^T v_{j_k}/\tau)}}{\frac{\exp(v^T v_i/\tau)}{\frac{n}{m} \sum_{k=1}^{m} \exp(v^T v_{j_k}/\tau)} + m \cdot \frac{1}{n}}$$



contrastive loss



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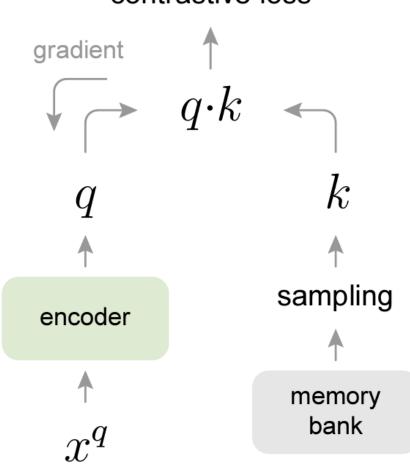
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contrastive loss



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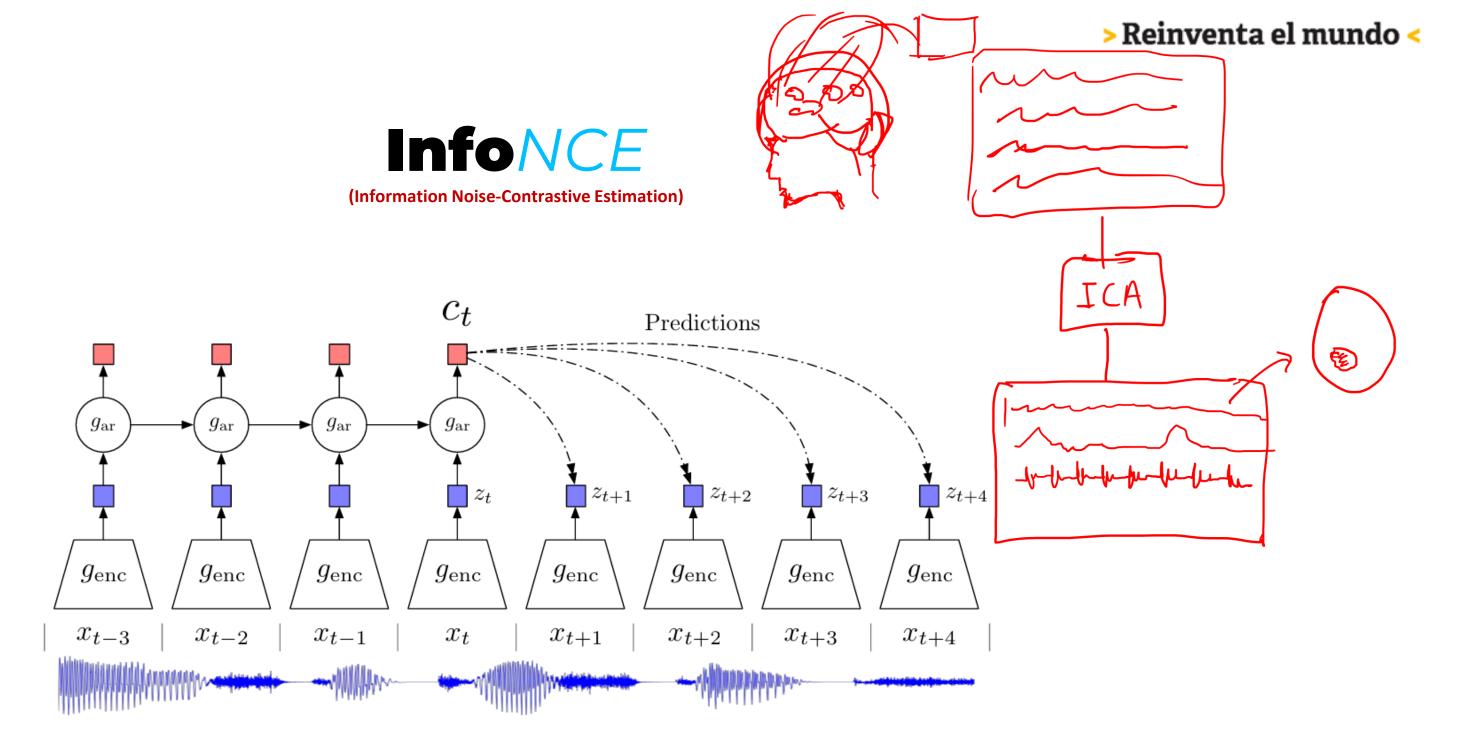
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Loss function:

$$J_{NCE}(\theta) = -\mathbb{E}_{P_d}[\log h(i, v)] - m \cdot \mathbb{E}_{P_n}[\log(1 - h(i, v'))]$$





$$I(x;c) = \sum_{x,c} p(x,c) \log \frac{p(x|c)}{p(x)}$$



b(xn) = brobla)

Mutual Information

La información mutua es una medida de dependencia entre dos variables aleatorias X y Y.

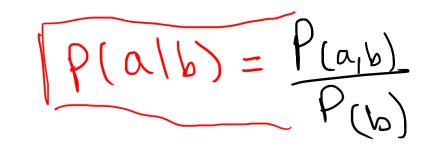
$$I(X;Y) = D_{KL}(p(x,y)||p(x) \otimes p(y))$$

donde:

- p(x, y) es la distribución conjunta de X y Y.
- p(x) y p(y) son las distribuciones marginales de X y Y, respectivamente.







> Reinventa el mundo <

Mutual Information

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$$I(X;Y) = D_{KL}(p(x,y)||p(x) \otimes p(y)) = \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x,y) \log \frac{p(x,y)}{p(x)p(y)} dond$$

$$\sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x,y) \log \frac{p(y|x)}{p(x)} dond$$

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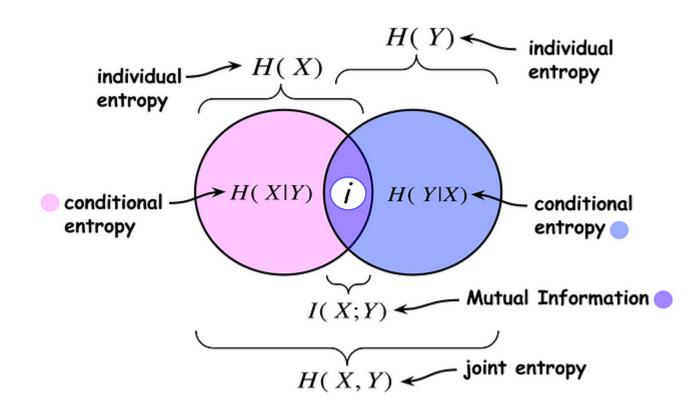
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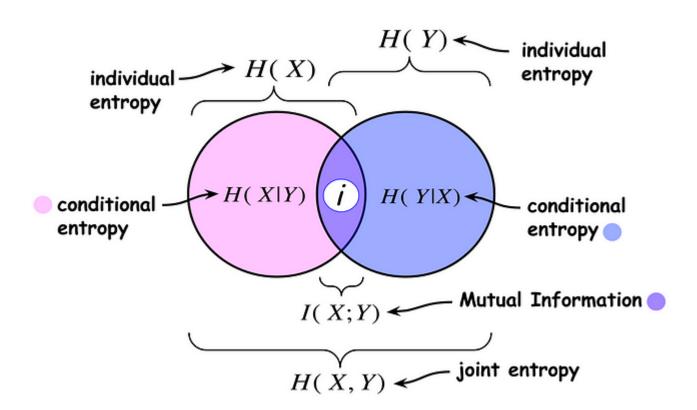
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- donde: p(x, y) es la distribución conjunta de X y Y.

 p(x) y p(y) son las distribuciones marginales de *X* y *Y*, respectivamente.



Interpretación:

- I(X;Y) mide cuánta información sobre X se obtiene conociendo Y (y viceversa).
- Si X e Y son independientes, entonces p(x, y) = p(x)p(y), lo que implica I(X;Y) = 0, es decir, no comparten información.
- Si X e Y son completamente dependientes, la información mutua es máxima y coincide con la entropía de cualquiera de las dos variables si son idénticas.







InfoNCE

(Information Noise-Contrastive Estimation)

Partimos de NCE loss:
$$p(d=i|X,c_t) = \frac{p(x_i|c_t) \prod_{l \neq i} p(x_l)}{\sum_{j=1}^{N} p(x_j|c_t) \prod_{l \neq j} p(x_l)} = \frac{\frac{p(x_i|c_t)}{p(x_i)}}{\sum_{j=1}^{N} \frac{p(x_j|c_t)}{p(x_j)}}$$





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Definimos InfoNCE loss:
$$\mathcal{L}_{\mathrm{N}} = -\mathbb{E}\left[\log \frac{f_k(x_{t+k}, c_t)}{\sum_{x_j \in X} f_k(x_j, c_t)}\right]$$
 donde: $f_k(x_{t+k}, c_t) \propto \frac{p(x_{t+k}|c_t)}{p(x_{t+k})}$



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Lo interesante es que garantiza:
$$I(x_{t+k}, c_t) \geq \log(N) - \mathcal{L}_N$$





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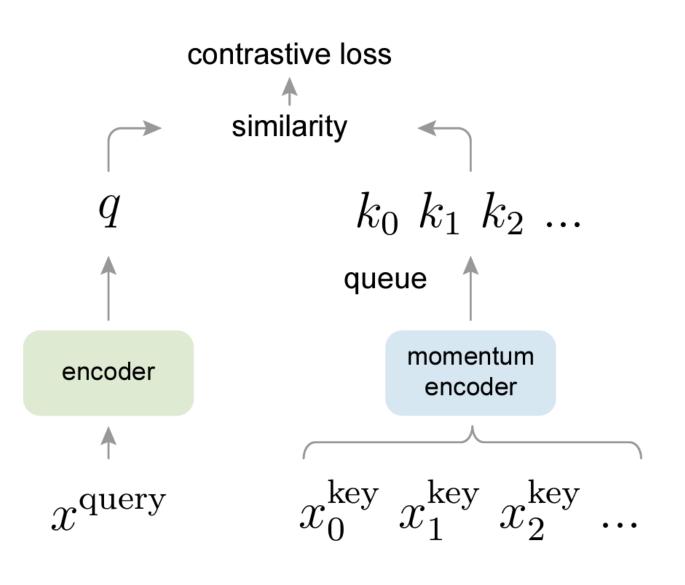
Definimos InfoNCE loss:
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 donde: $f_{k}(x_{t+k}, c_{t}) \propto \frac{p(x_{t+k}|c_{t})}{p(x_{t+k})}$

Lo interesante es que garantiza:
$$I(x_{t+k}, c_t) \geq \log(N) - \mathcal{L}_N$$

$$\begin{aligned} \textbf{Demostración:} \quad & \mathcal{L}_{\mathrm{N}}^{\mathrm{opt}} = -\mathop{\mathbb{E}}_{X} \log \left[\frac{\frac{p(x_{t+k}|c_{t})}{p(x_{t+k})}}{\frac{p(x_{t+k}|c_{t})}{p(x_{t+k})} + \sum_{x_{j} \in X_{\mathrm{neg}}} \frac{p(x_{j}|c_{t})}{p(x_{j})}} \right] = \mathop{\mathbb{E}}_{X} \log \left[1 + \frac{p(x_{t+k})}{p(x_{t+k}|c_{t})} \sum_{x_{j} \in X_{\mathrm{neg}}} \frac{p(x_{j}|c_{t})}{p(x_{j})} \right] \\ & \approx \mathop{\mathbb{E}}_{X} \log \left[1 + \frac{p(x_{t+k})}{p(x_{t+k}|c_{t})} (N-1) \mathop{\mathbb{E}}_{x_{j}} \frac{p(x_{j}|c_{t})}{p(x_{j})} \right] = \mathop{\mathbb{E}}_{X} \log \left[1 + \frac{p(x_{t+k})}{p(x_{t+k}|c_{t})} (N-1) \right] \\ & \geq \mathop{\mathbb{E}}_{X} \log \left[\frac{p(x_{t+k})}{p(x_{t+k}|c_{t})} N \right] = -I(x_{t+k}, c_{t}) + \log(N) \end{aligned}$$







Dado un query q y un conjunto de keys $\{k_0,k_1,\dots\}$, se minimiza el InfoNCE loss:

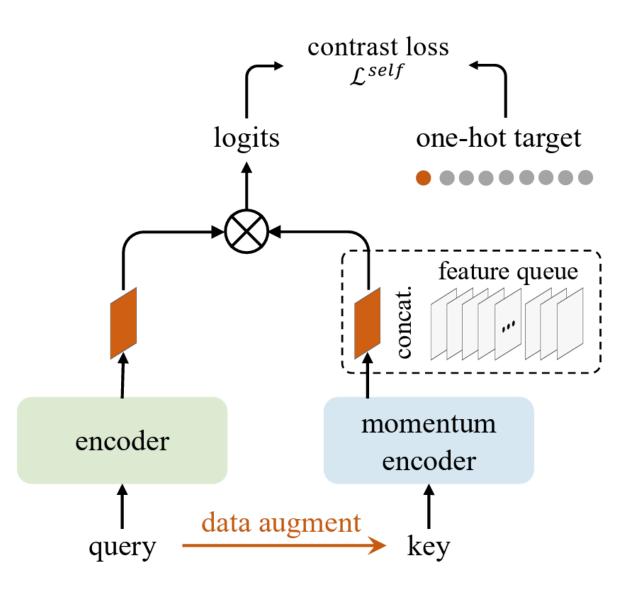
$$\mathcal{L}_{q} = -\log \frac{\exp(q \cdot k^{+}/\tau)}{\sum_{i=0}^{K} \exp(q \cdot k_{i}/\tau)}$$

donde:

- k^+ es la clave positiva (matching key).
- k_i son claves negativas.
- τ es un hiperparámetro de temperatura.





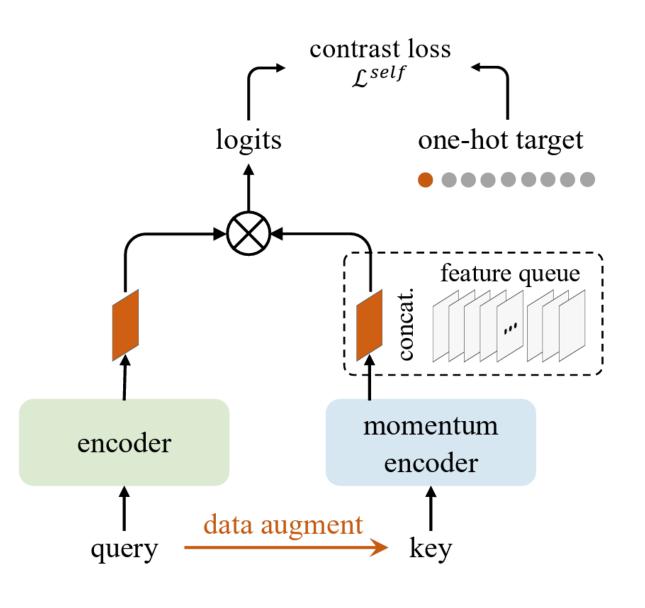


Dictionary queue

Es una cola FIFO (First In, First Out) que almacena representaciones de imágenes (*keys*) de los mini-batches previos en el entrenamiento. Su propósito principal es proporcionar un conjunto grande de ejemplos negativos para el aprendizaje contrastivo, desacoplando el tamaño del mini-batch del tamaño del diccionario.







Momentum updates

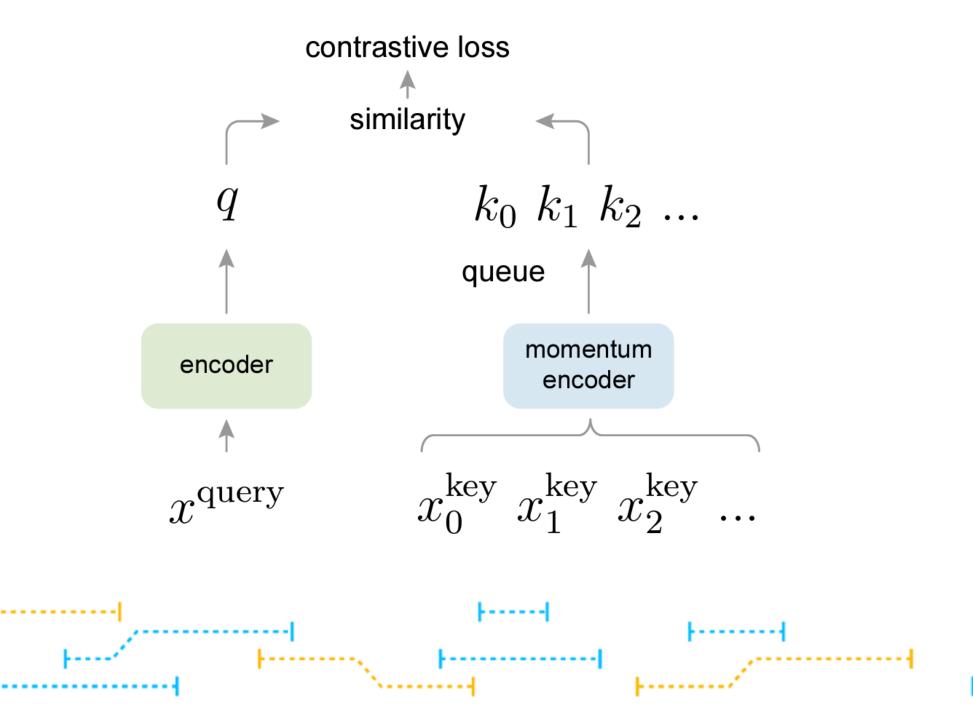
En lugar de copiar el codificador del query al key en cada paso (lo cual introduce inestabilidad), se usa una actualización por momentum:

$$\theta_k \leftarrow m\theta_k + (1-m)\theta_q$$

esto mantiene la consistencia de las representaciones a lo largo del entrenamiento.



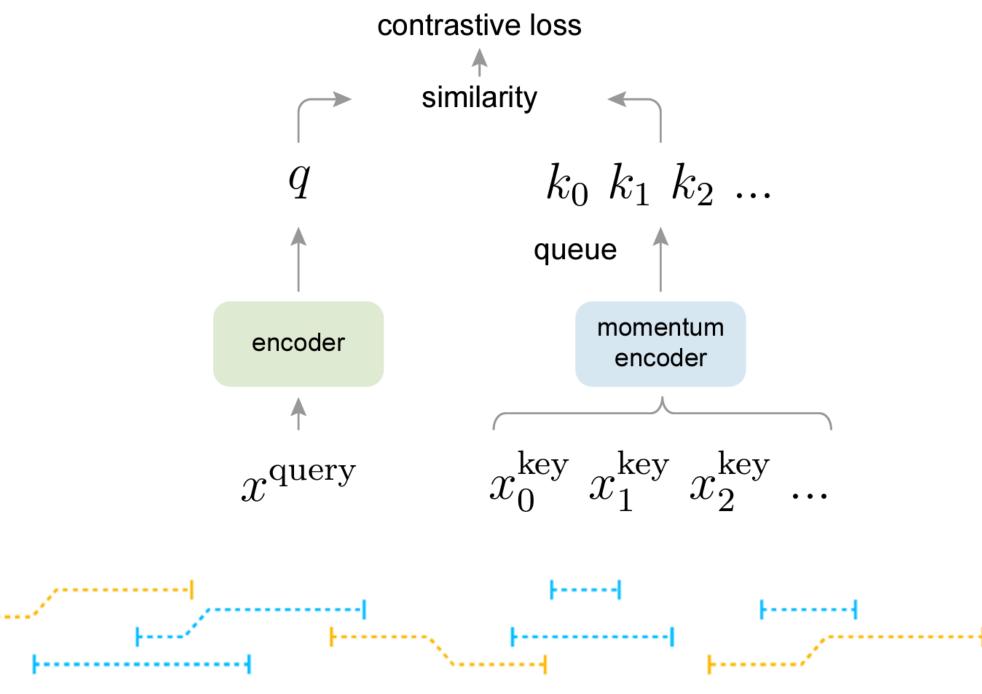




CODE?







Algorithm 1 Pseudocode of MoCo in a PyTorch-like style.

```
# f_q, f_k: encoder networks for query and key
# queue: dictionary as a queue of K keys (CxK)
# m: momentum
# t: temperature
f_k.params = f_q.params # initialize
for x in loader: # load a minibatch x with N samples
  x_q = aug(x) # a randomly augmented version
  x_k = aug(x) # another randomly augmented version
   q = f_q.forward(x_q) # queries: NxC
   k = f_k.forward(x_k) # keys: NxC
   k = k.detach() # no gradient to keys
   # positive logits: Nx1
   l_pos = bmm(q.view(N, 1, C), k.view(N, C, 1))
   # negative logits: NxK
   l_neg = mm(q.view(N,C), queue.view(C,K))
   # logits: Nx(1+K)
   logits = cat([l_pos, l_neg], dim=1)
   # contrastive loss, Eqn.(1)
  labels = zeros(N) # positives are the 0-th
   loss = CrossEntropyLoss(logits/t, labels)
   # SGD update: query network
   loss.backward()
   update(f_q.params)
   # momentum update: key network
   f_k.params = m*f_k.params+(1-m)*f_q.params
   # update dictionary
  enqueue (queue, k) \# enqueue the current minibatch
   dequeue (queue) # dequeue the earliest minibatch
```

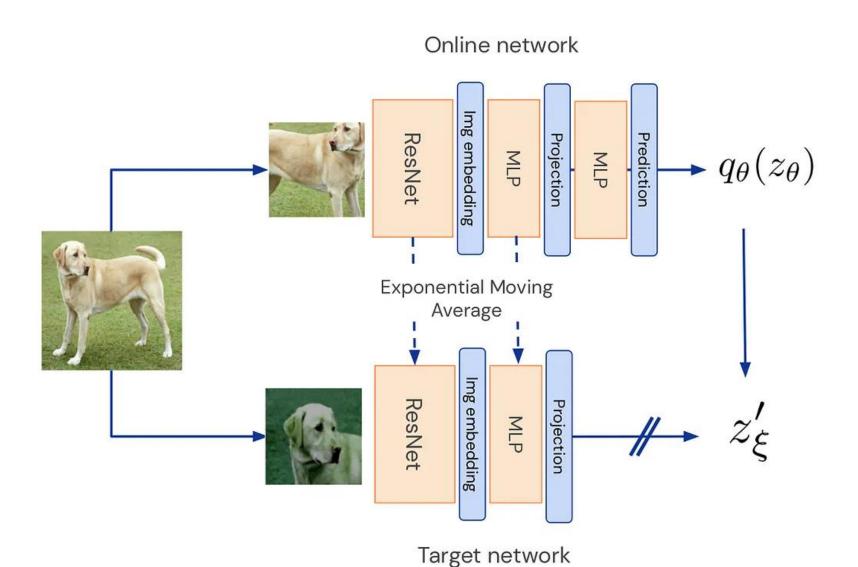
bmm: batch matrix multiplication; mm: matrix multiplication; cat: concatenation.

TRANSFORMATEC

Kaiming He et al. (2020) "Momentum Contrast for Unsupervised Visual Representation Learning". Proceedings of the IEEE/CVF conference on computer vision and pattern recognition. 2020. p. 9729-9738.



Bootstrap Your Own Latent (BYOL)



Online network:

Se entrena activamente en cada paso de optimización.

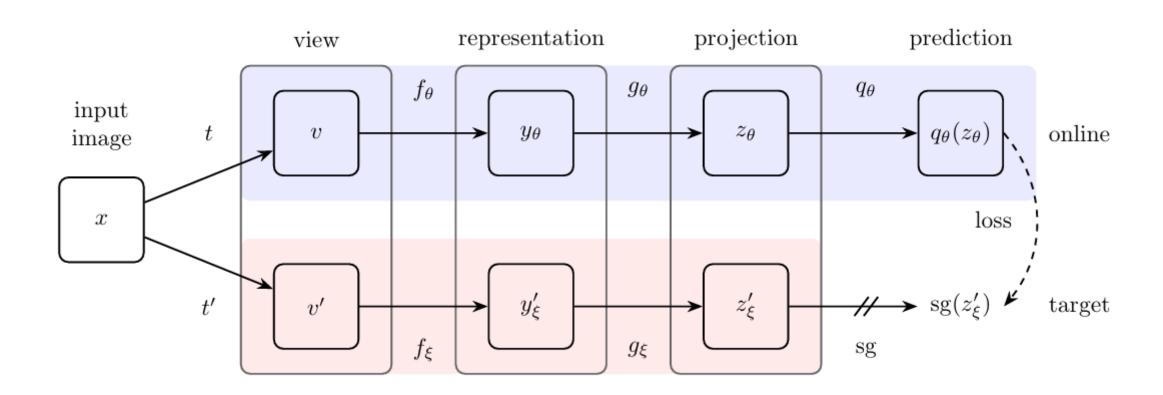
Target network:

No se entrena directamente, sino que es una versión suavizada de la red online, actualizada con **exponential moving average**:

$$\xi \leftarrow \tau \xi + (1 - \tau)\theta$$



Bootstrap Your Own Latent (BYOL)



$$\mathcal{L}_{\theta,\xi} \triangleq \left\| \overline{q_{\theta}}(z_{\theta}) - \overline{z}_{\xi}' \right\|_{2}^{2} = 2 - 2 \cdot \frac{\langle q_{\theta}(z_{\theta}), z_{\xi}' \rangle}{\left\| q_{\theta}(z_{\theta}) \right\|_{2} \cdot \left\| z_{\xi}' \right\|_{2}}$$

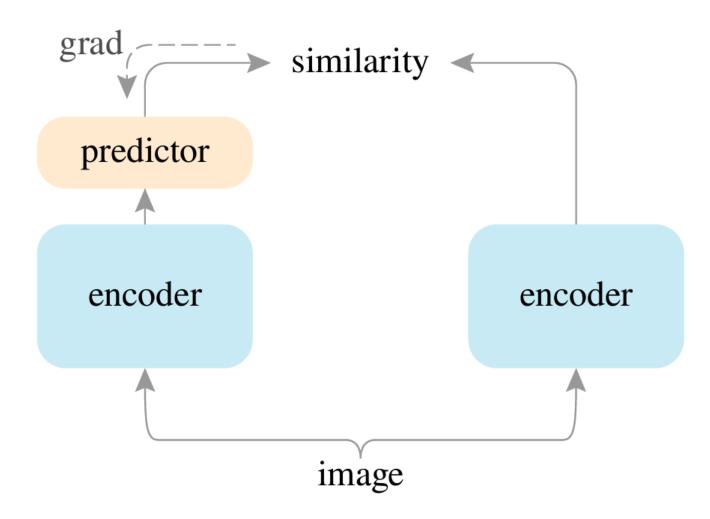












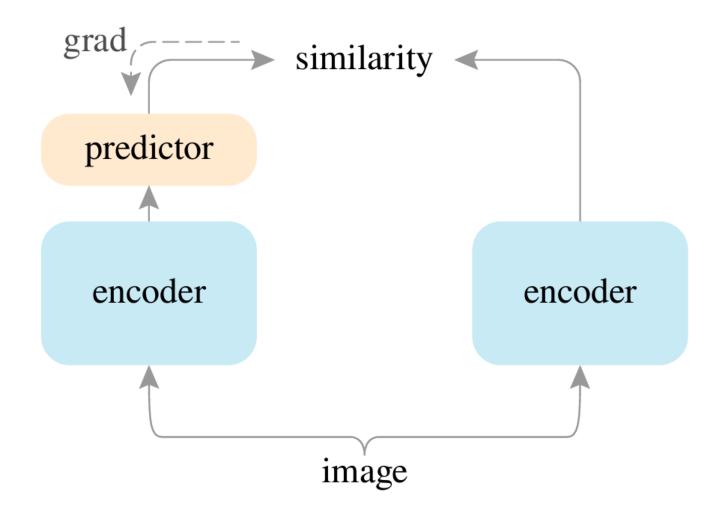
Negative cosine similarity

$$\mathcal{D}(p_1, z_2) = -\frac{p_1}{\|p_1\|_2} \cdot \frac{z_2}{\|z_2\|_2}$$

Symmetric loss

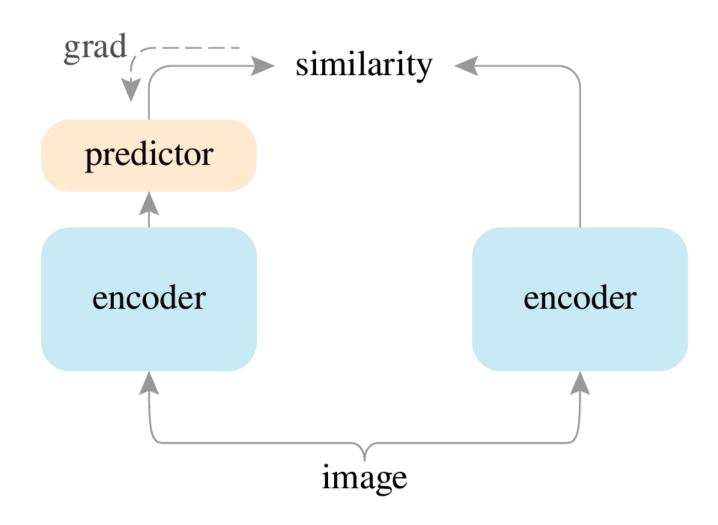
$$\mathcal{L} = \frac{1}{2}\mathcal{D}(p_1, z_2) + \frac{1}{2}\mathcal{D}(p_2, z_1).$$





CODE?





Algorithm 1 SimSiam Pseudocode, PyTorch-like

```
# f: backbone + projection mlp
# h: prediction mlp

for x in loader: # load a minibatch x with n samples
    x1, x2 = aug(x), aug(x) # random augmentation
    z1, z2 = f(x1), f(x2) # projections, n-by-d
    p1, p2 = h(z1), h(z2) # predictions, n-by-d

    L = D(p1, z2)/2 + D(p2, z1)/2 # loss

    L.backward() # back-propagate
    update(f, h) # SGD update

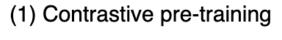
def D(p, z): # negative cosine similarity
    z = z.detach() # stop gradient

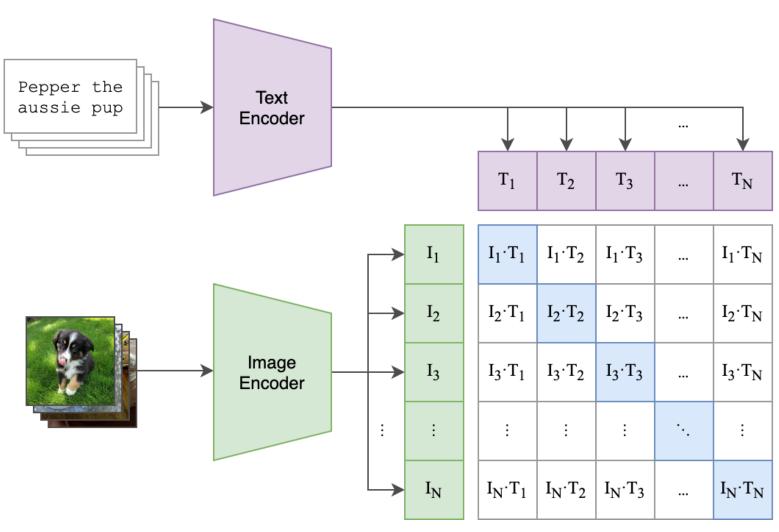
p = normalize(p, dim=1) # 12-normalize
    z = normalize(z, dim=1) # 12-normalize
    return -(p*z).sum(dim=1).mean()
```



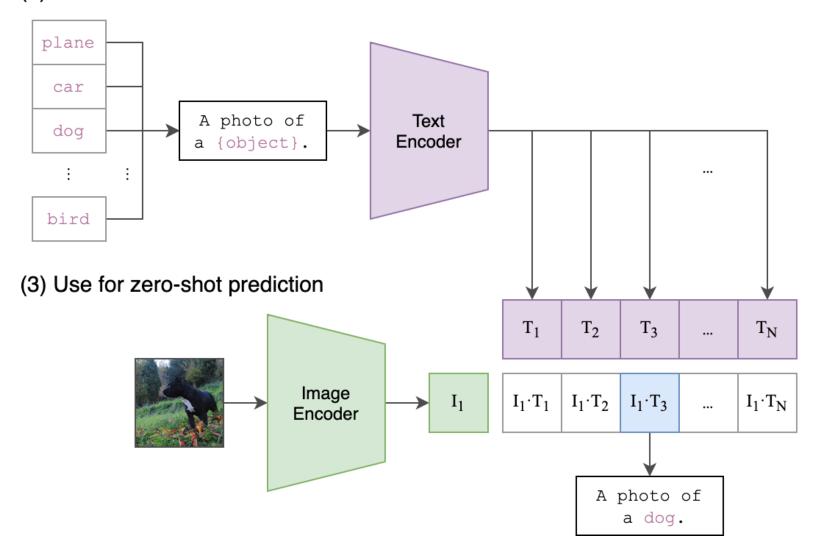


(Contrastive Language-Image Pre-training)





(2) Create dataset classifier from label text







> Reinventa el mundo <

GRACIAS

Victor Flores Benites

