UTEC
UNIVERSIDAD DE INGENIERÍA Y TECNOLOGÍA

> Reinventa el mundo <

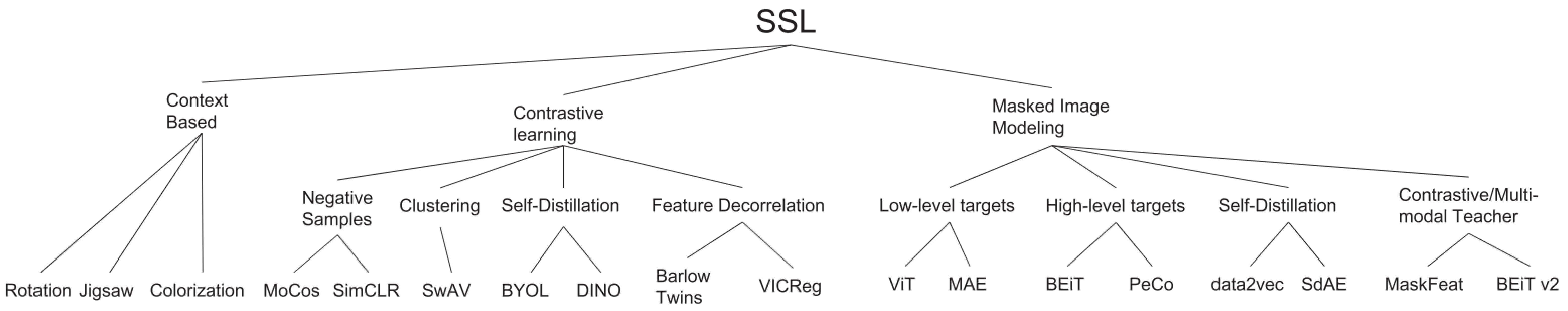
Sesión 5.0

Self-supervised learning I

Contrastive learning

TRANSFORMATEC

Self-Supervised *Learning*



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1.

Context-Based *Methods*

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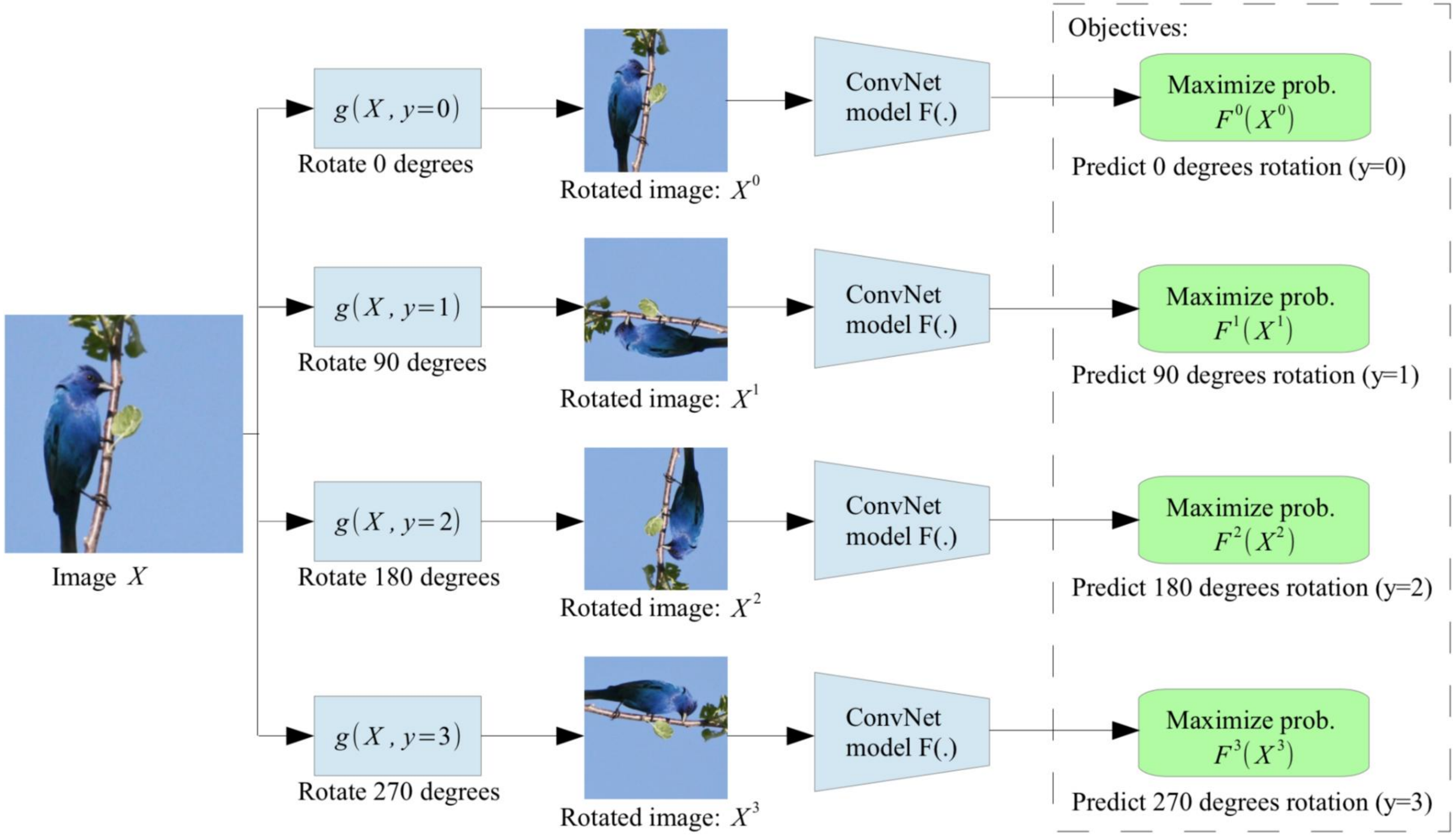
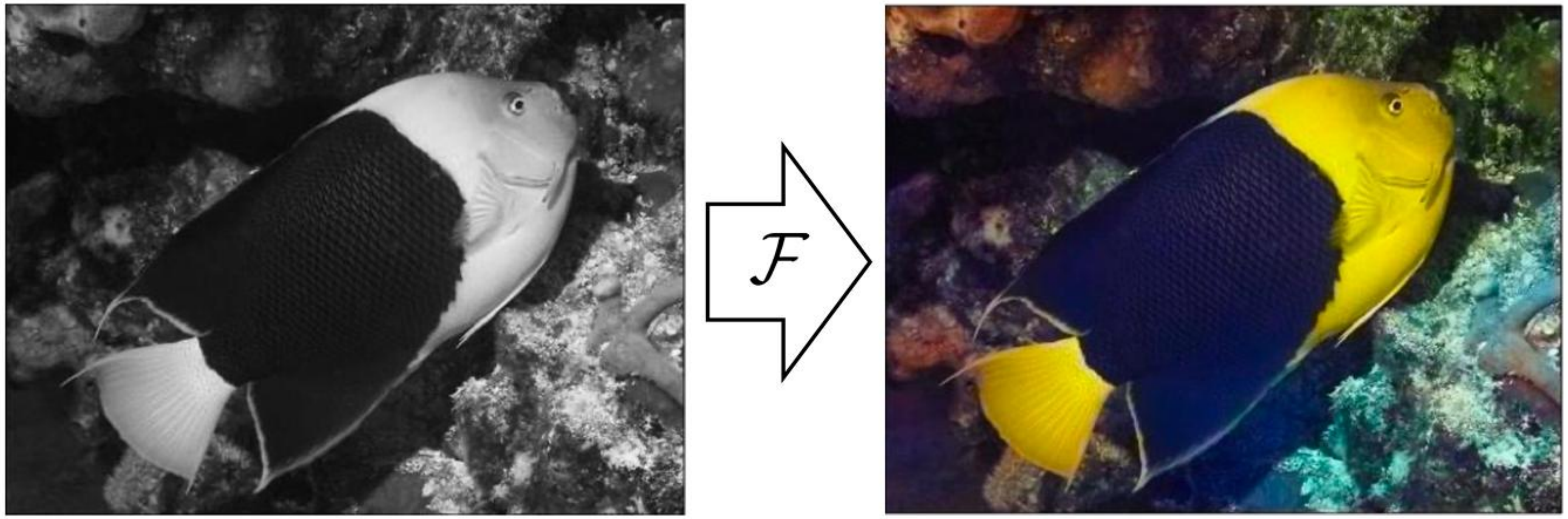
Rotation



Spyros Gidaris et al. (2018) “Unsupervised Representation Learning by Predicting Image Rotations”. arXiv preprint arXiv:1803.07728.

Image *Colorization*



Grayscale image: *L* channel

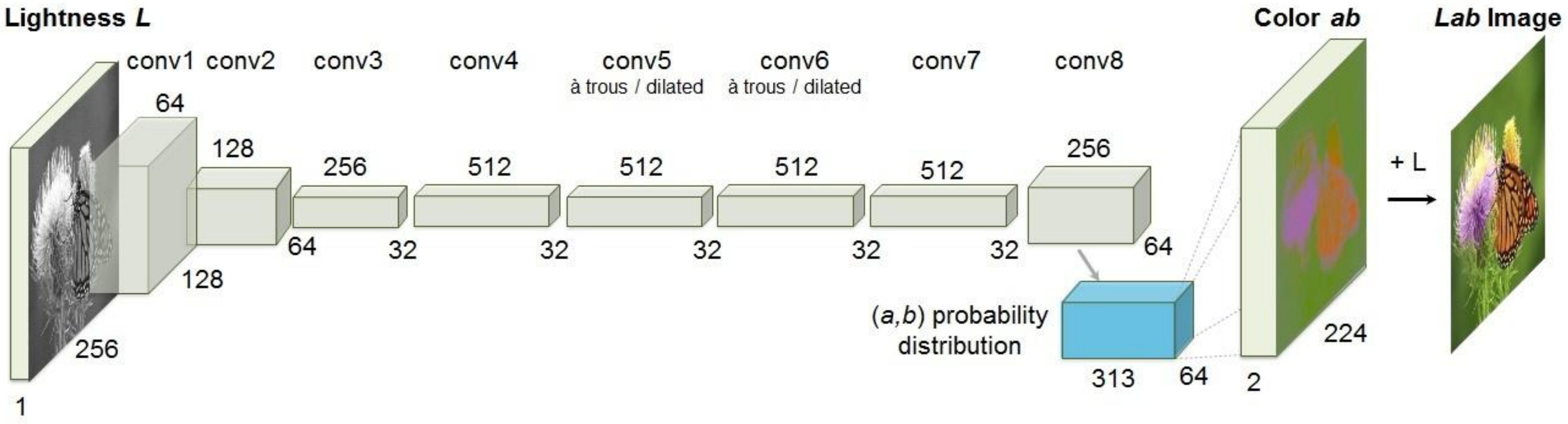
$\mathbf{X} \in \mathbb{R}^{H \times W \times 1}$

Concatenate (L,ab)

$(\mathbf{X}, \widehat{\mathbf{Y}})$

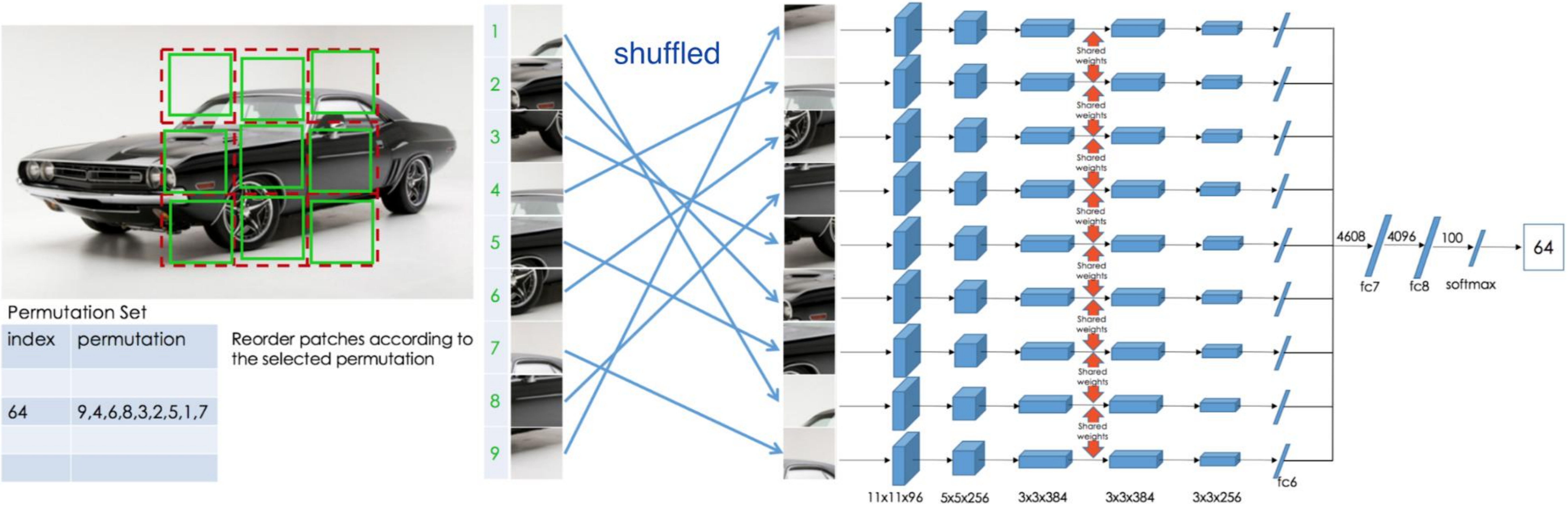
Richard Zhang et al. (2016) "Colorful Image Colorization". Computer Vision–ECCV 2016: 14th European Conference, Amsterdam, The Netherlands, October 11-14, 2016, Proceedings, Part III 14 (pp. 649-666). Springer International Publishing.

Image *Colorization*



Richard Zhang et al. (2016) “Colorful Image Colorization”.
Computer Vision–ECCV 2016: 14th European Conference, Amsterdam, The Netherlands, October 11-14, 2016, Proceedings, Part III 14 (pp. 649-666). Springer International Publishing.

Jigsaw *Puzzles*



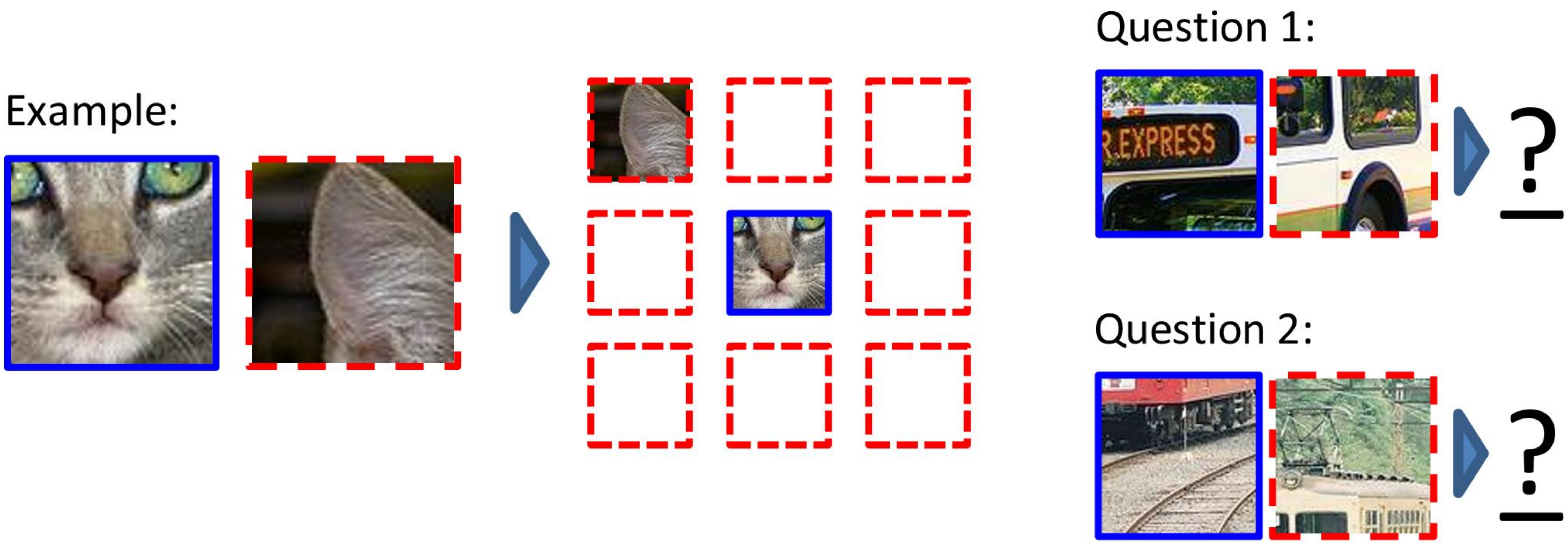
Permutation Set

index	permutation
64	9,4,6,8,3,2,5,1,7

Reorder patches according to the selected permutation

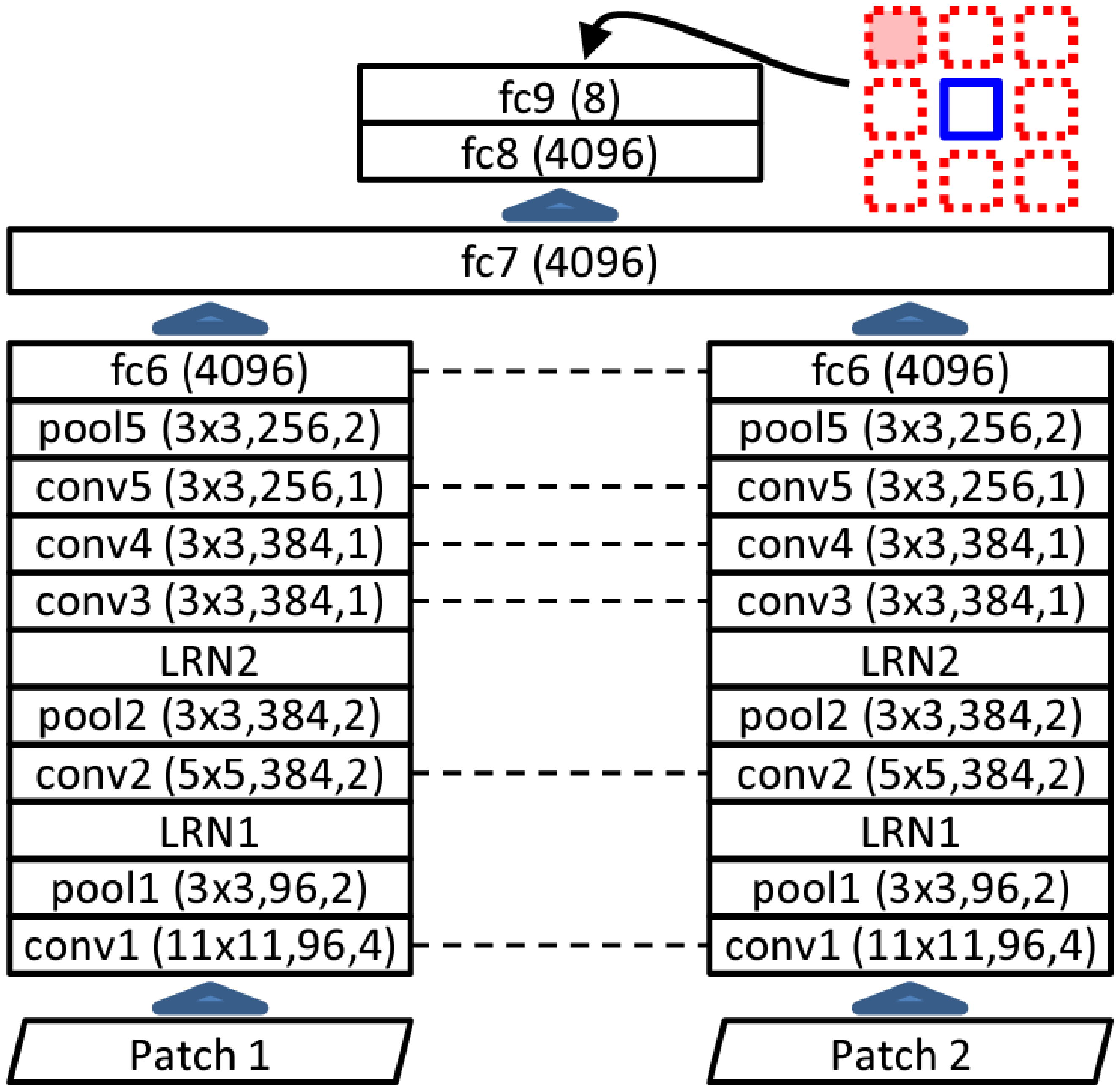
Mehdi Noroozi and Paolo Favaro (2016) "Unsupervised Learning of Visual Representations by Solving Jigsaw Puzzles". European conference on computer vision (pp. 69-84). Cham: Springer International Publishing.

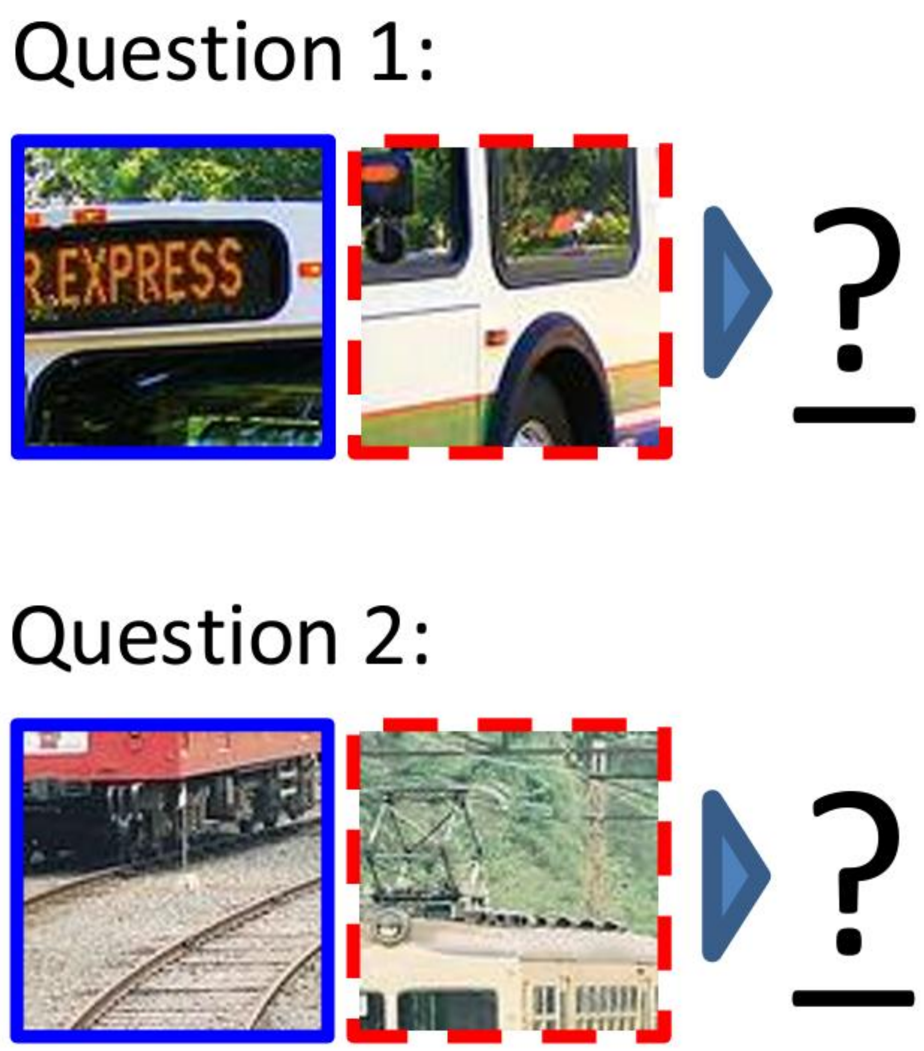
Context *Prediction*



Carl Doersch et al. (2015) "Unsupervised Visual Representation Learning by Context Prediction". Proceedings of the IEEE international conference on computer vision (pp. 1422-1430).

Context *Prediction*





Carl Doersch et al. (2015) "Unsupervised Visual Representation Learning by Context Prediction". Proceedings of the IEEE international conference on computer vision (pp. 1422-1430).

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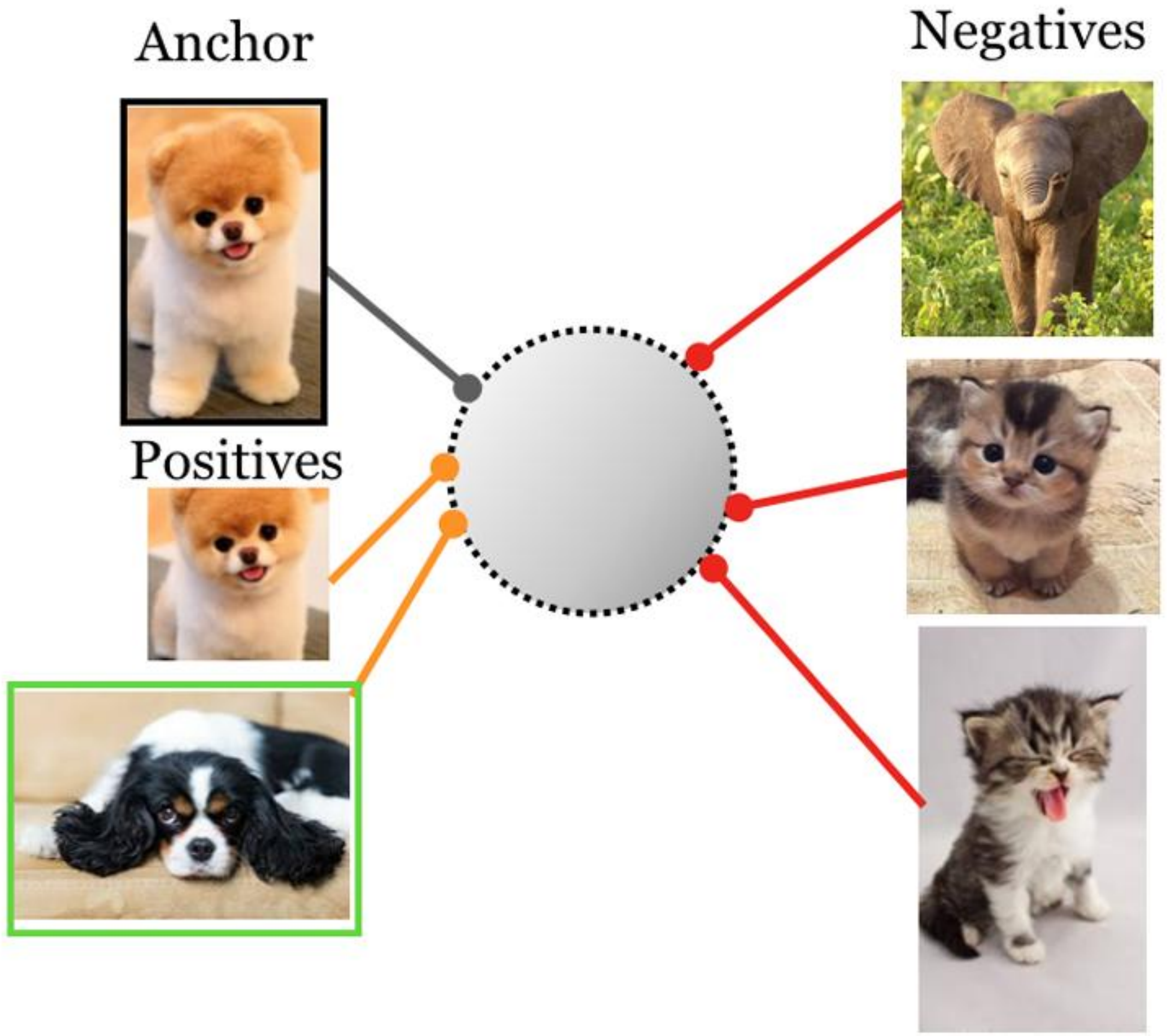
2.

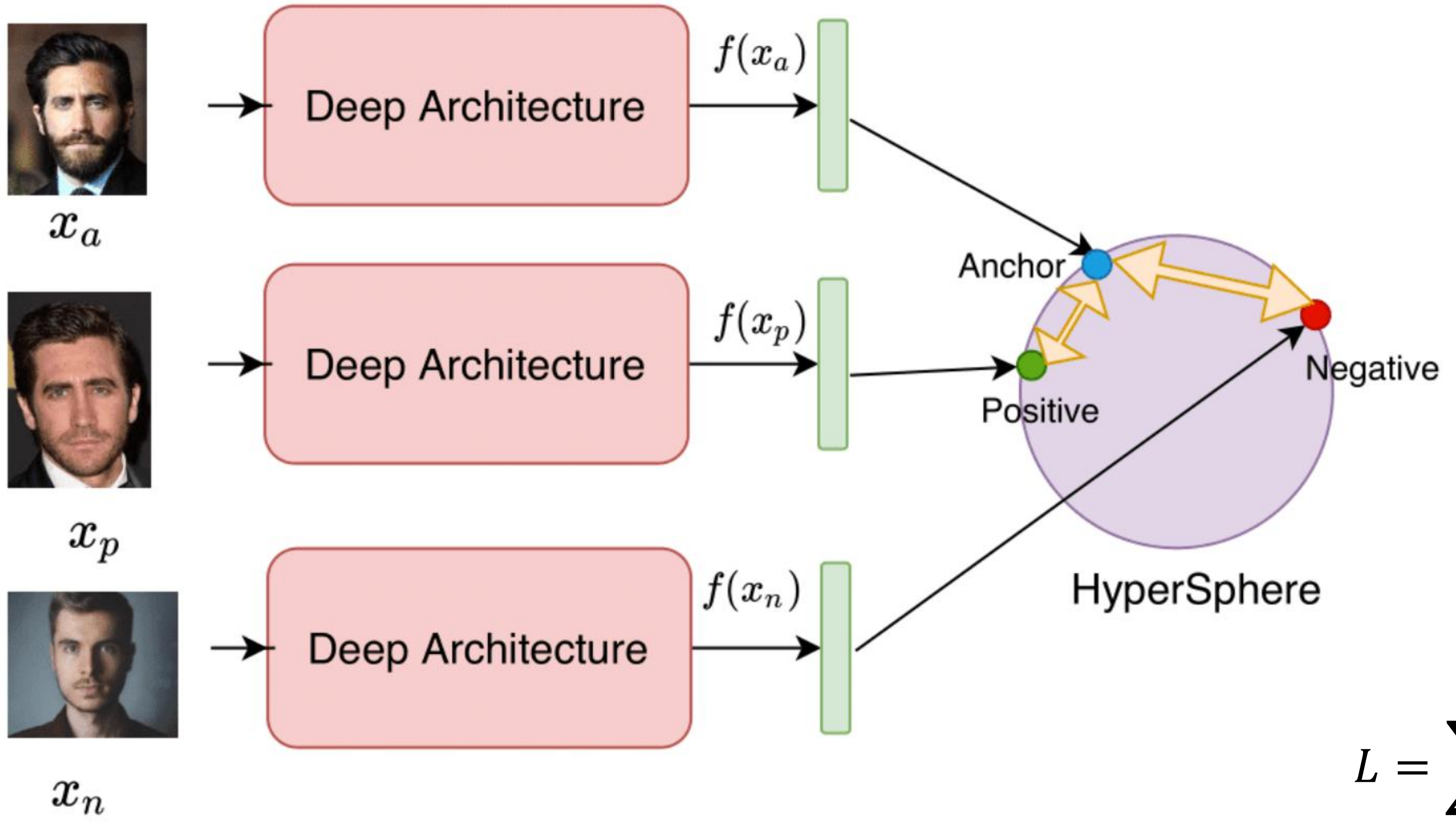
Contrastive *Learning*

Self-Supervised *Learning*



Triplet *Loss*

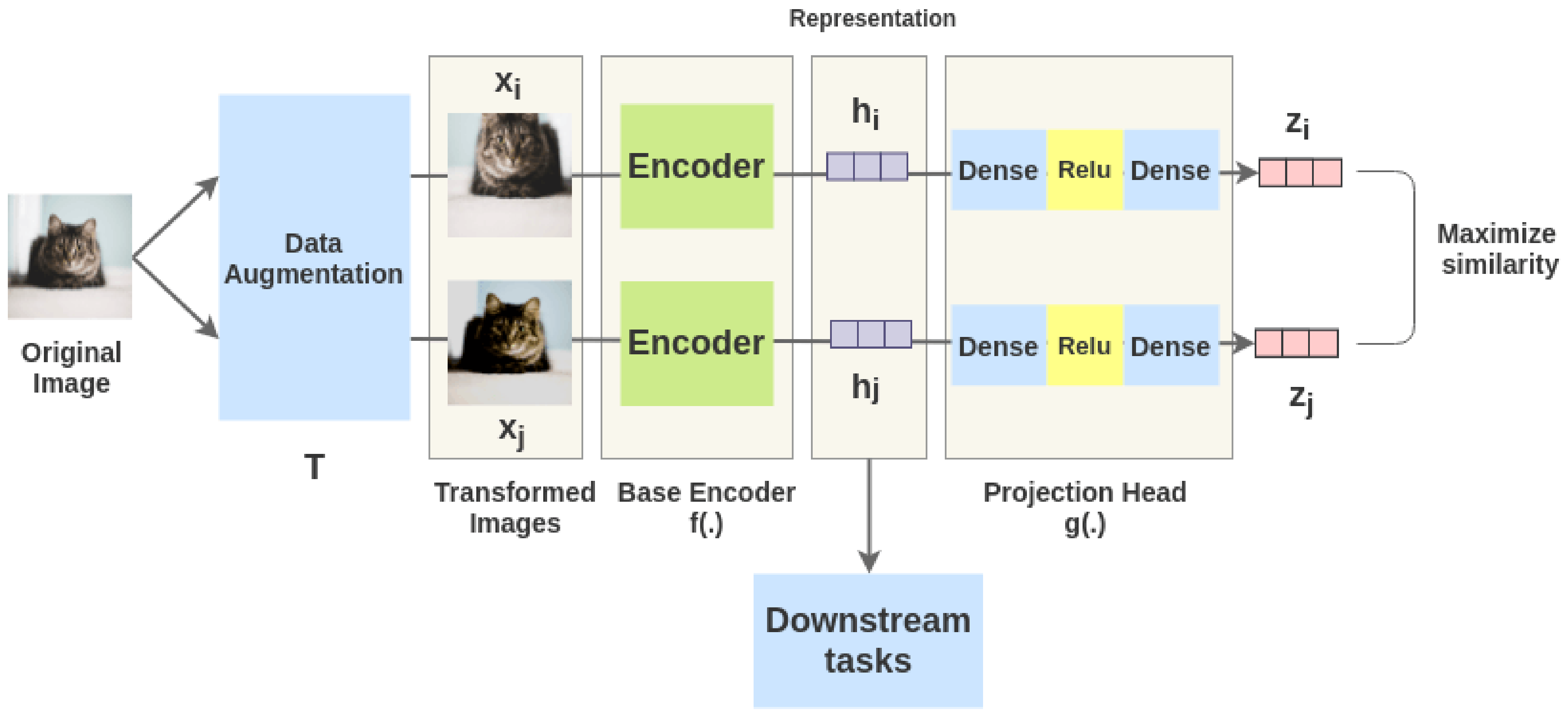
Es una técnica de aprendizaje supervisado, el cual es predecesor de propuestas en self-supervised.



$$L = \sum_{i}^{N} \left[\left| f(x_i^a) - f(x_i^p) \right|_2^2 - \left| f(x_i^a) - f(x_i^n) \right|_2^2 + \alpha \right]$$

Florian Schroff et al. (2015) "FaceNet: A Unified Embedding for Face Recognition and Clustering". Proceedings of the IEEE conference on computer vision and pattern recognition. 2015. p. 815-823.

SimCLR



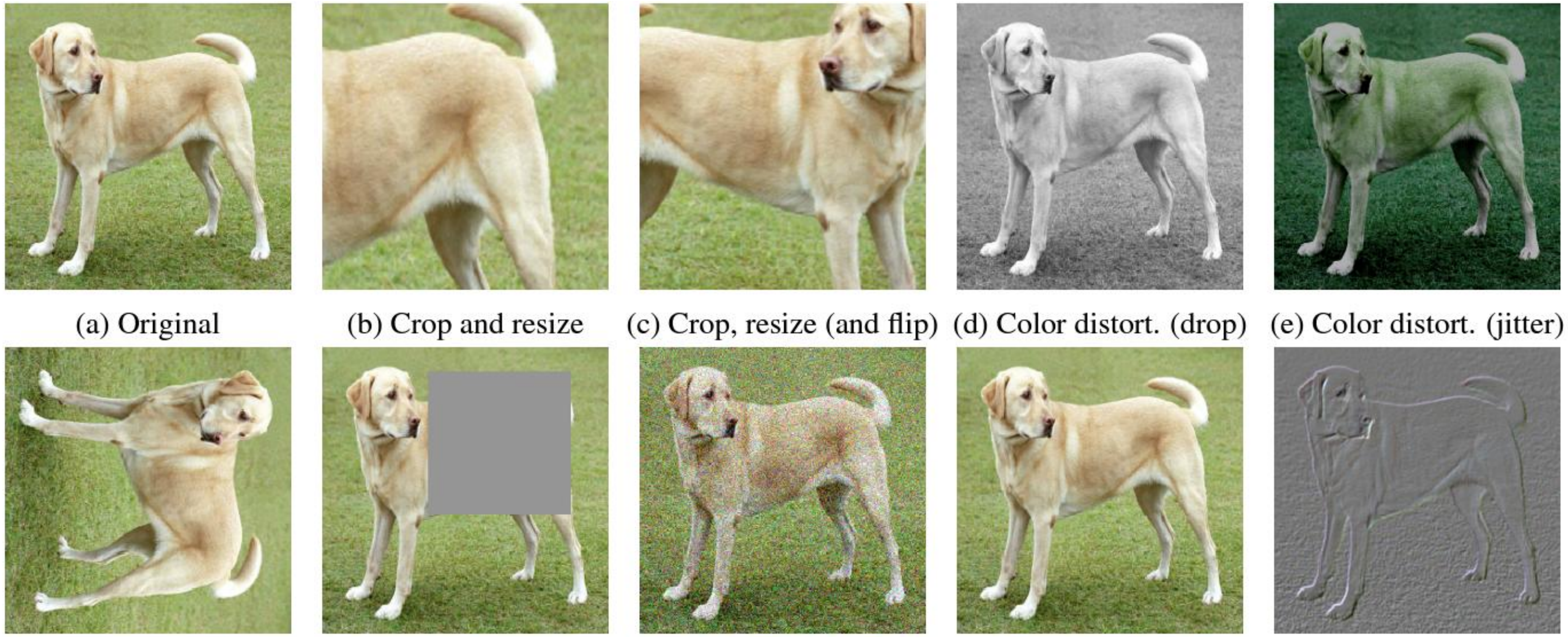
Normalized Temperature-scaled Cross-Entropy (NT-Xent):

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

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

Ting Chen et al. (2020) "A Simple Framework for Contrastive Learning of Visual Representations". International conference on machine learning. PMLR, 2020. p. 1597-1607.

SimCLR



(a) Original (b) Crop and resize (c) Crop, resize (and flip) (d) Color distort. (drop) (e) Color distort. (jitter)

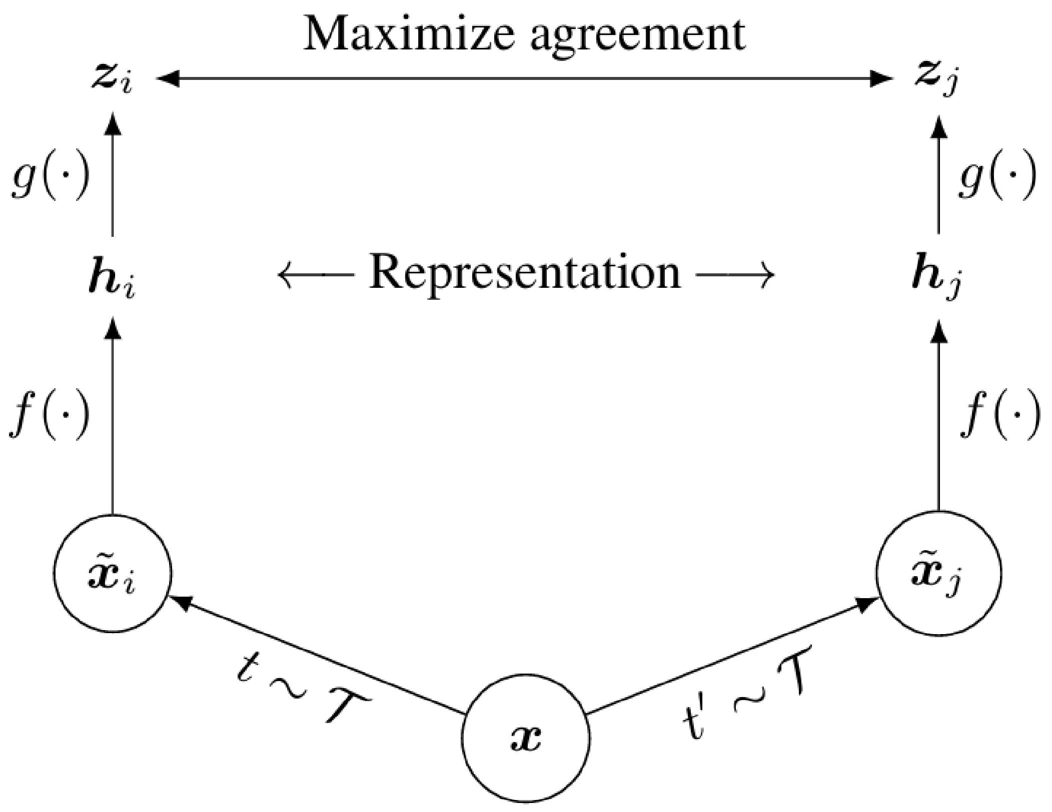
(f) Rotate {90°, 180°, 270°} (g) Cutout (h) Gaussian noise (i) Gaussian blur (j) Sobel filtering

Ting Chen et al. (2020) "A Simple Framework for Contrastive Learning of Visual Representations".
International conference on machine learning. PMLR, 2020. p. 1597-1607.

SimCLR

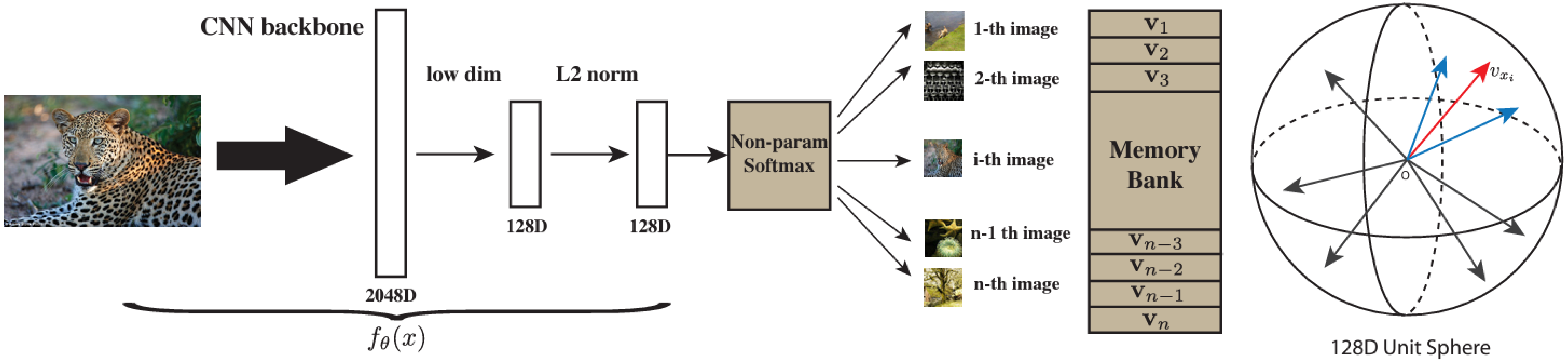
Algorithm 1 SimCLR's main learning algorithm.

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



Ting Chen et al. (2020) "A Simple Framework for Contrastive Learning of Visual Representations".
International conference on machine learning. PMLR, 2020. p. 1597-1607.

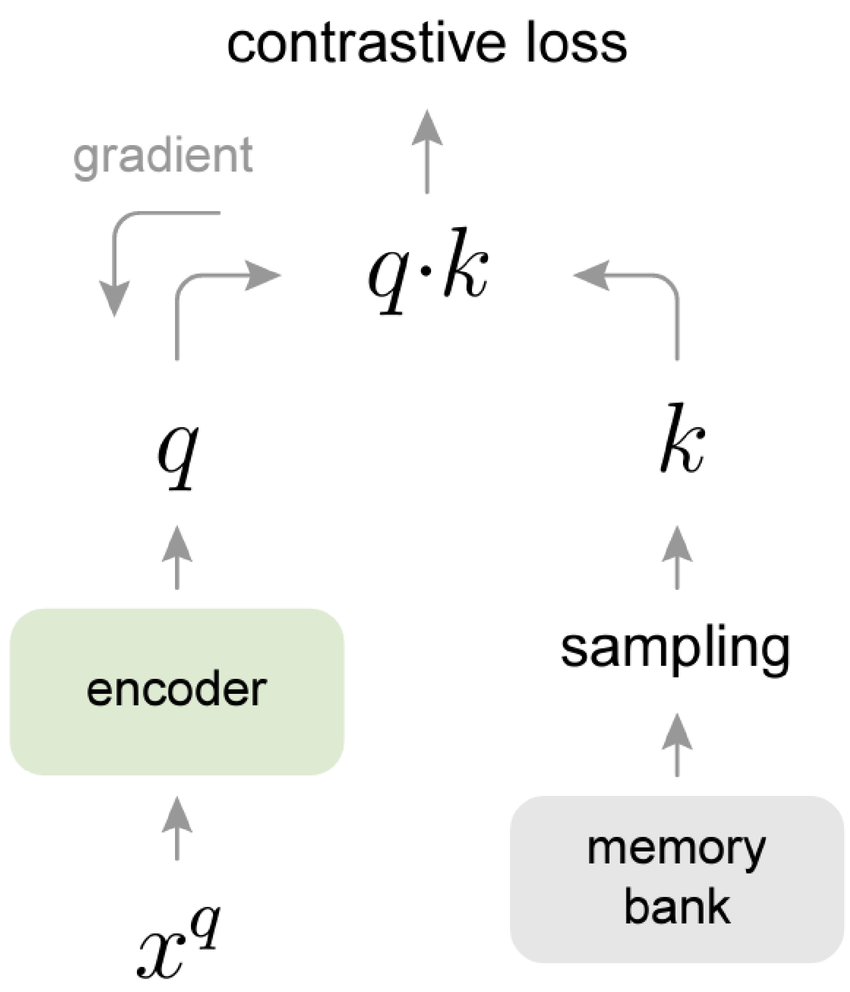
Noise-Contrastive *Estimation (NCE)*



Zhirong Wu et al. (2018) "Unsupervised Feature Learning via Non-Parametric Instance Discrimination". Proceedings of the IEEE conference on computer vision and pattern recognition (pp. 3733-3742).

Noise-Contrastive *Estimation (NCE)*

E



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

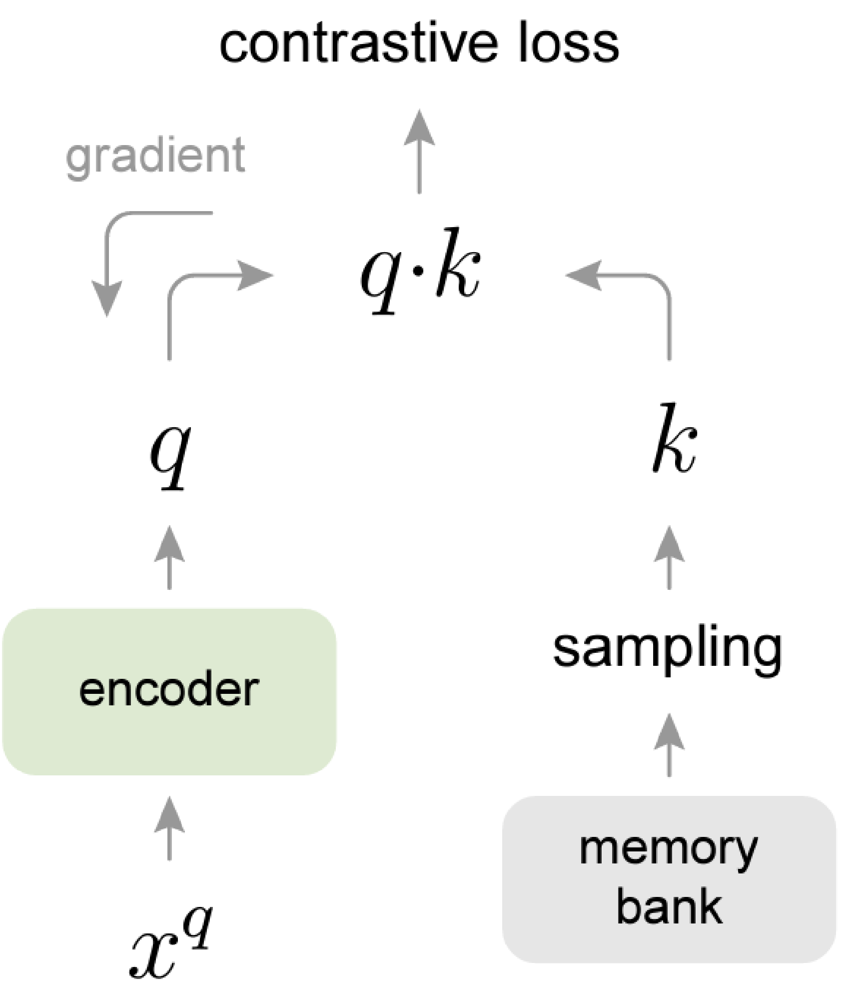
$$p(i|v) = \frac{\exp(v_i^T v/\tau)}{\sum_{j=1}^{n} \exp(v_j^T v/\tau)}$$

Loss function:

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

Zhirong Wu et al. (2018) "Unsupervised Feature Learning via Non-Parametric Instance Discrimination".
Proceedings of the IEEE conference on computer vision and pattern recognition (pp. 3733-3742).

Noise-Contrastive *Estimation (NCE)*



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Loss function:

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

Problemas:

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

Zhirong Wu et al. (2018) "Unsupervised Feature Learning via Non-Parametric Instance Discrimination". Proceedings of the IEEE conference on computer vision and pattern recognition (pp. 3733-3742).

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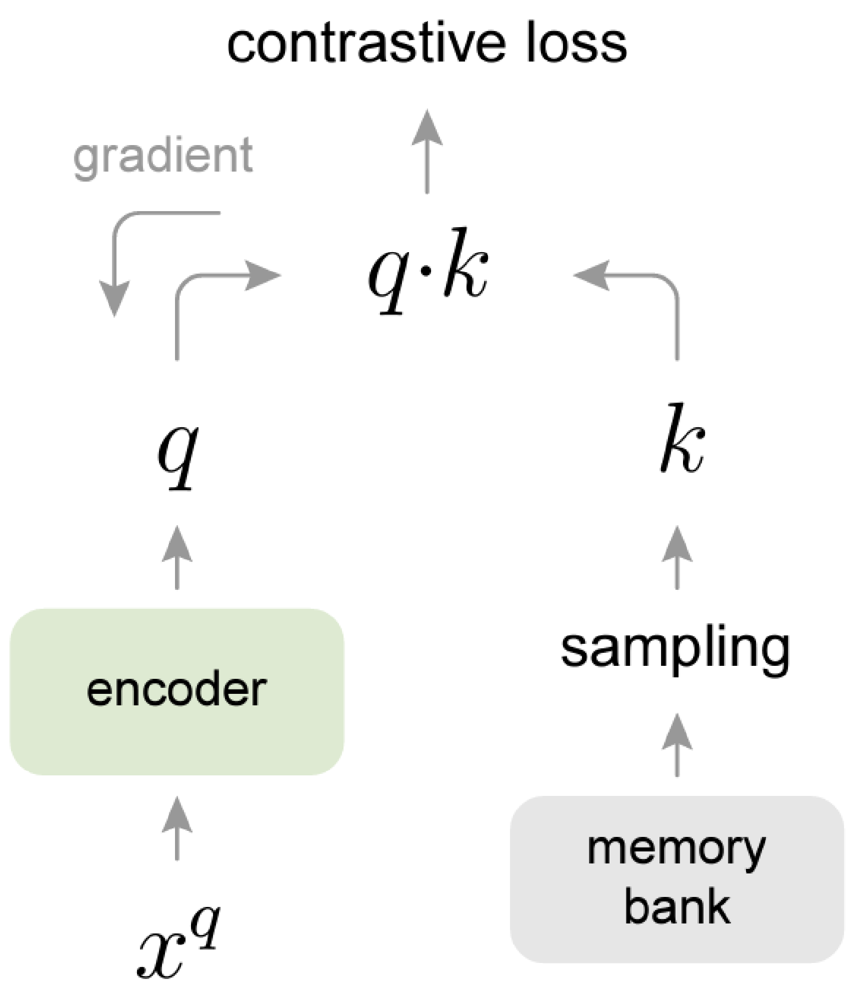

Cambiamos a un problema de clasificación binaria:

Definimos un evento binario D, donde:

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

Zhirong Wu et al. (2018) "Unsupervised Feature Learning via Non-Parametric Instance Discrimination". Proceedings of the IEEE conference on computer vision and pattern recognition (pp. 3733-3742).

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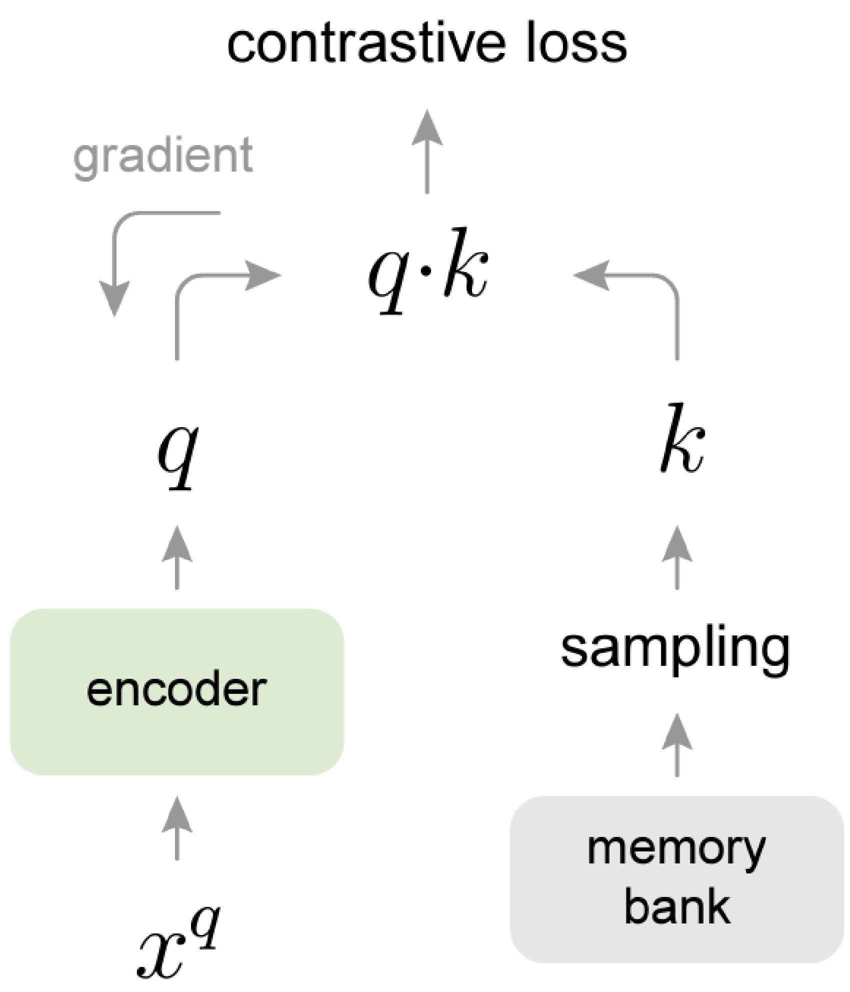

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Calculamos la probabilidad posteriori:

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

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).

Zhirong Wu et al. (2018) "Unsupervised Feature Learning via Non-Parametric Instance Discrimination". Proceedings of the IEEE conference on computer vision and pattern recognition (pp. 3733-3742).

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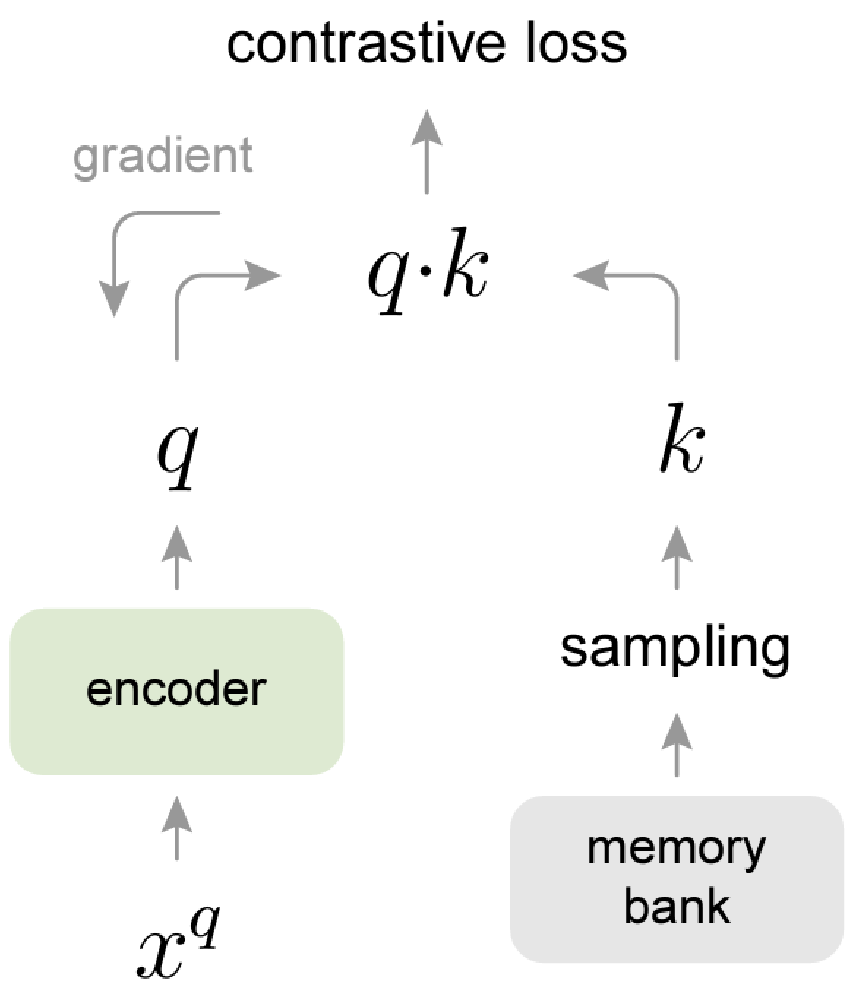

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Hacemos:

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

Zhirong Wu et al. (2018) "Unsupervised Feature Learning via Non-Parametric Instance Discrimination". Proceedings of the IEEE conference on computer vision and pattern recognition (pp. 3733-3742).

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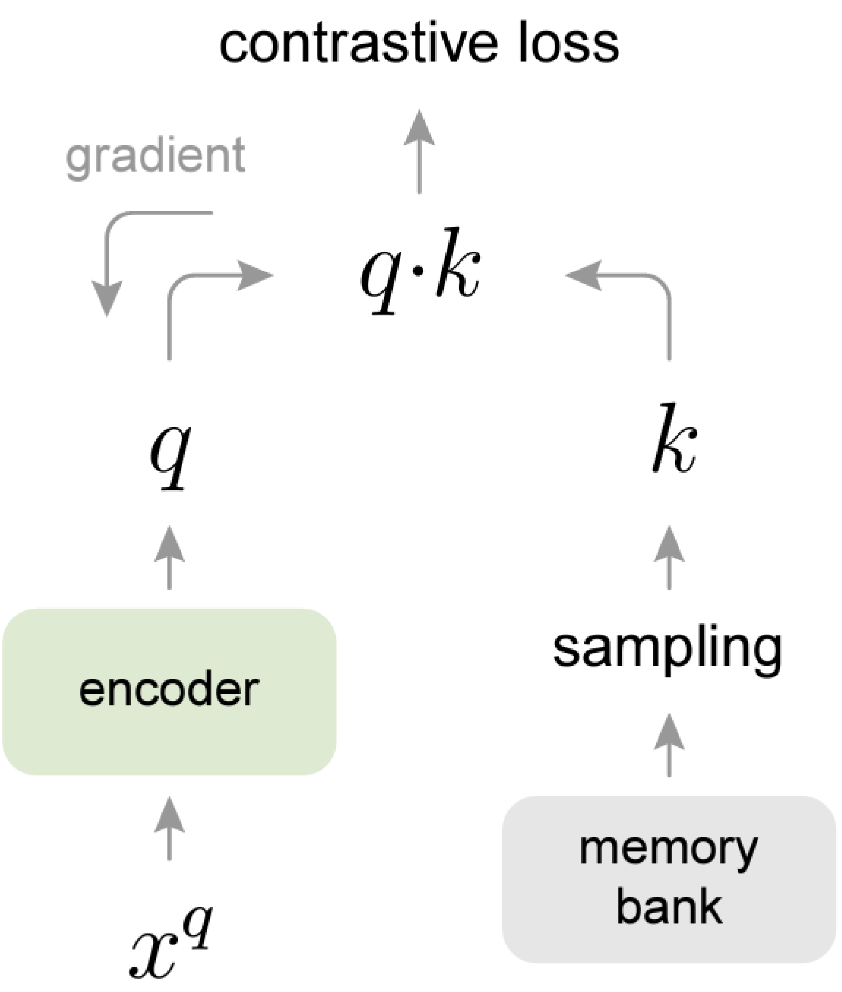

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Zhirong Wu et al. (2018) "Unsupervised Feature Learning via Non-Parametric Instance Discrimination". Proceedings of the IEEE conference on computer vision and pattern recognition (pp. 3733-3742).

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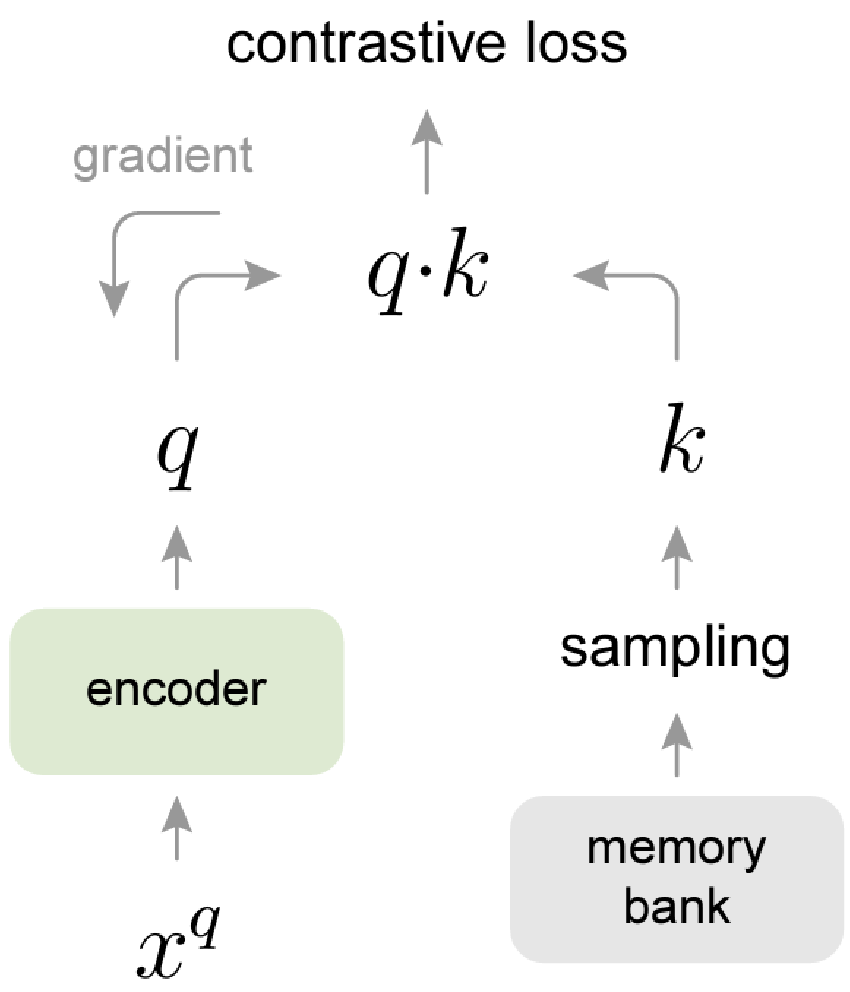

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$$h(i, v) = \frac{P(i|v)}{P(i|v) + mP_n(i)}$$

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

Zhirong Wu et al. (2018) "Unsupervised Feature Learning via Non-Parametric Instance Discrimination".
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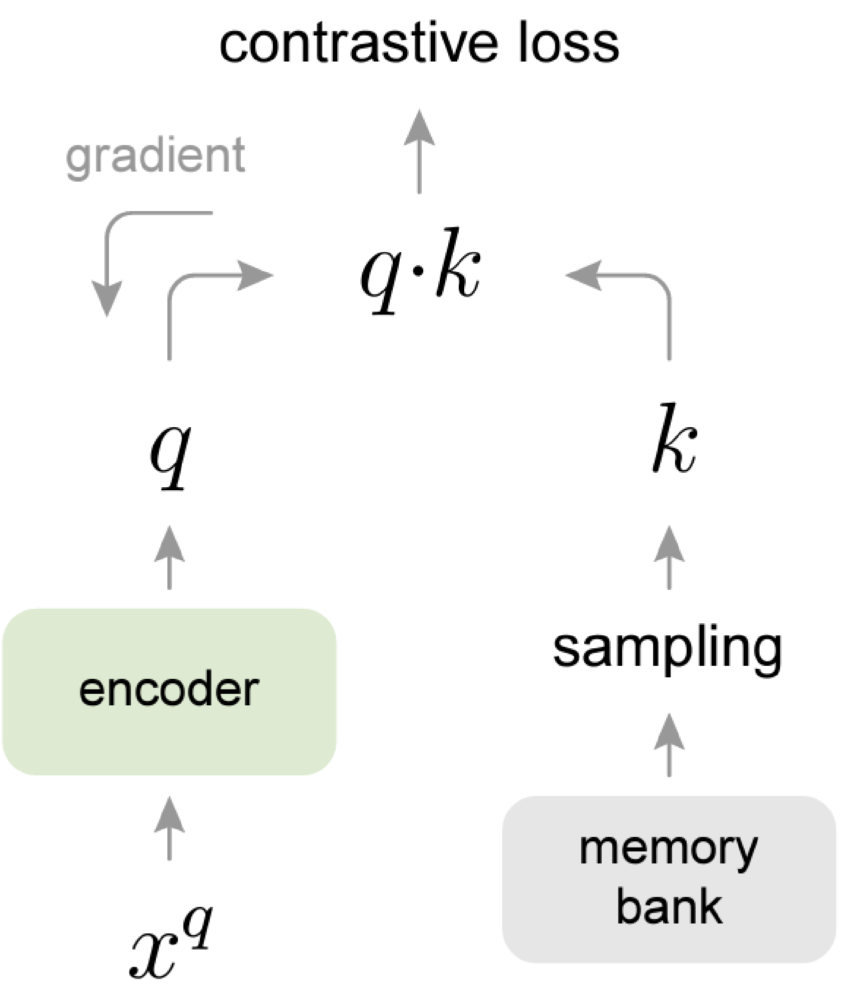

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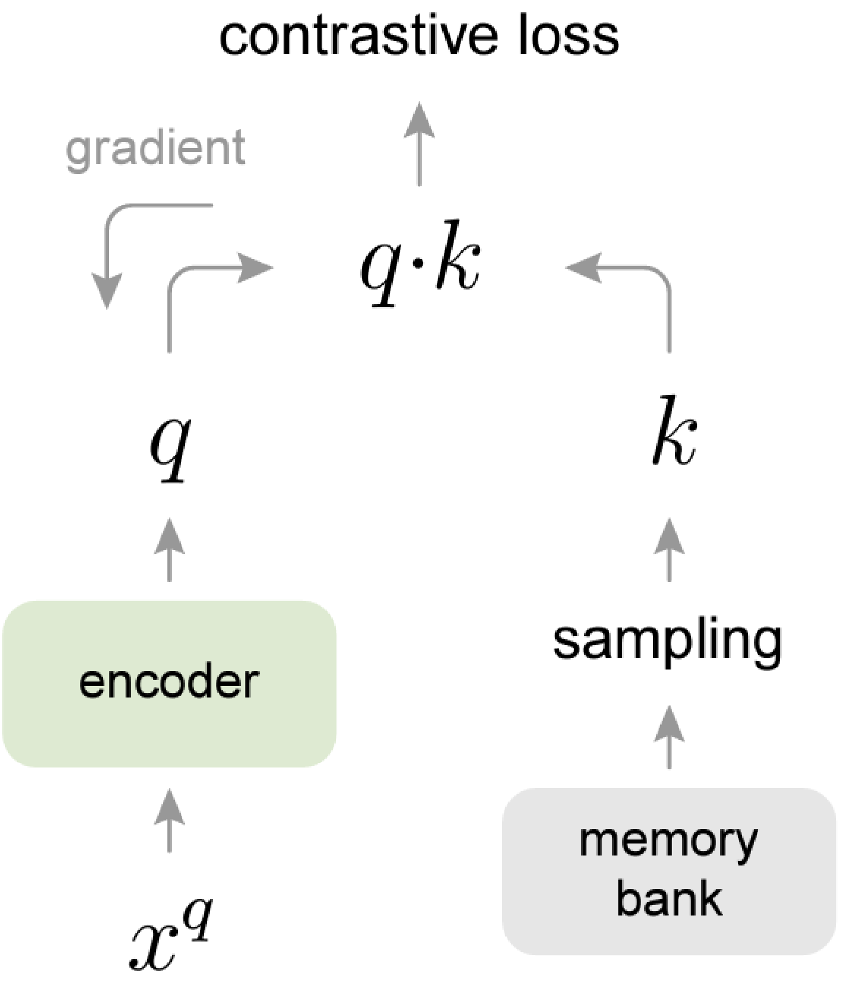
Aun tenemos a $P(i|v)$

Zhirong Wu et al. (2018) "Unsupervised Feature Learning via Non-Parametric Instance Discrimination". Proceedings of the IEEE conference on computer vision and pattern recognition (pp. 3733-3742).

Noise-Contrastive *Estimation (NCE)*



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Calculamos la probabilidad posteriori:

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

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

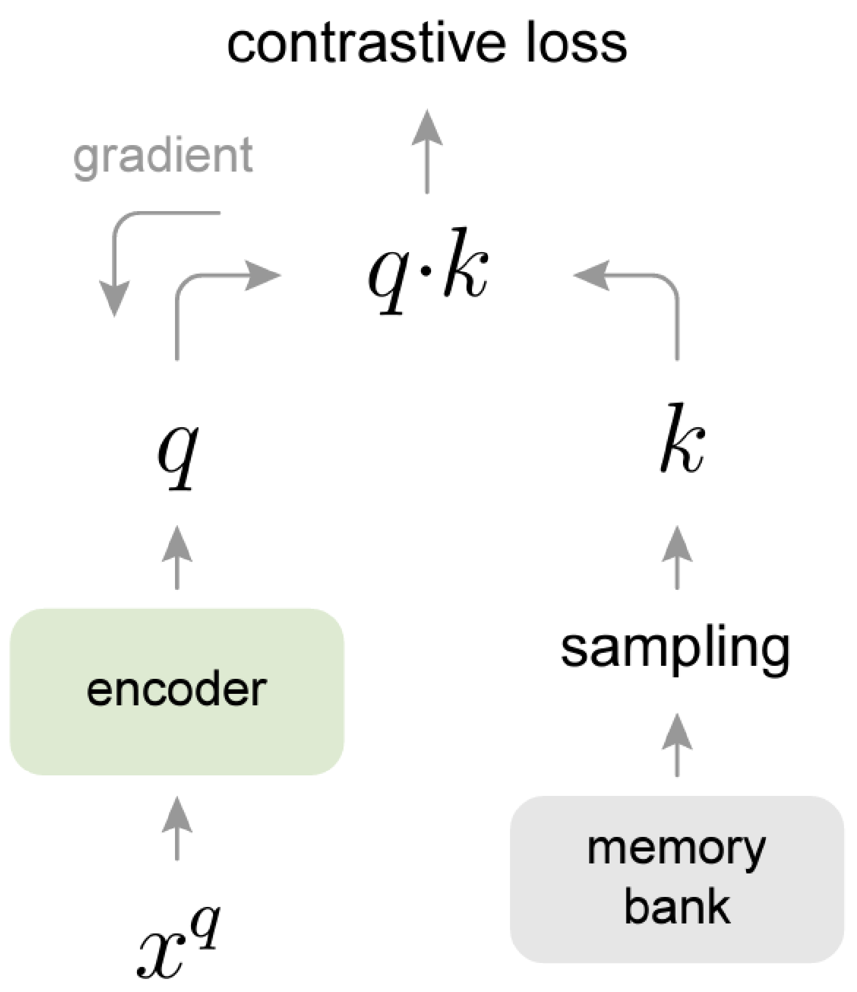
$$Z = \sum_{j=1}^{n} \exp(v^T v_j/\tau)$$

Aproximamos con muestreo Monte Carlo usando m muestras negativas:

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

Zhirong Wu et al. (2018) “Unsupervised Feature Learning via Non-Parametric Instance Discrimination”. Proceedings of the IEEE conference on computer vision and pattern recognition (pp. 3733-3742).

Noise-Contrastive *Estimation (NCE)*



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

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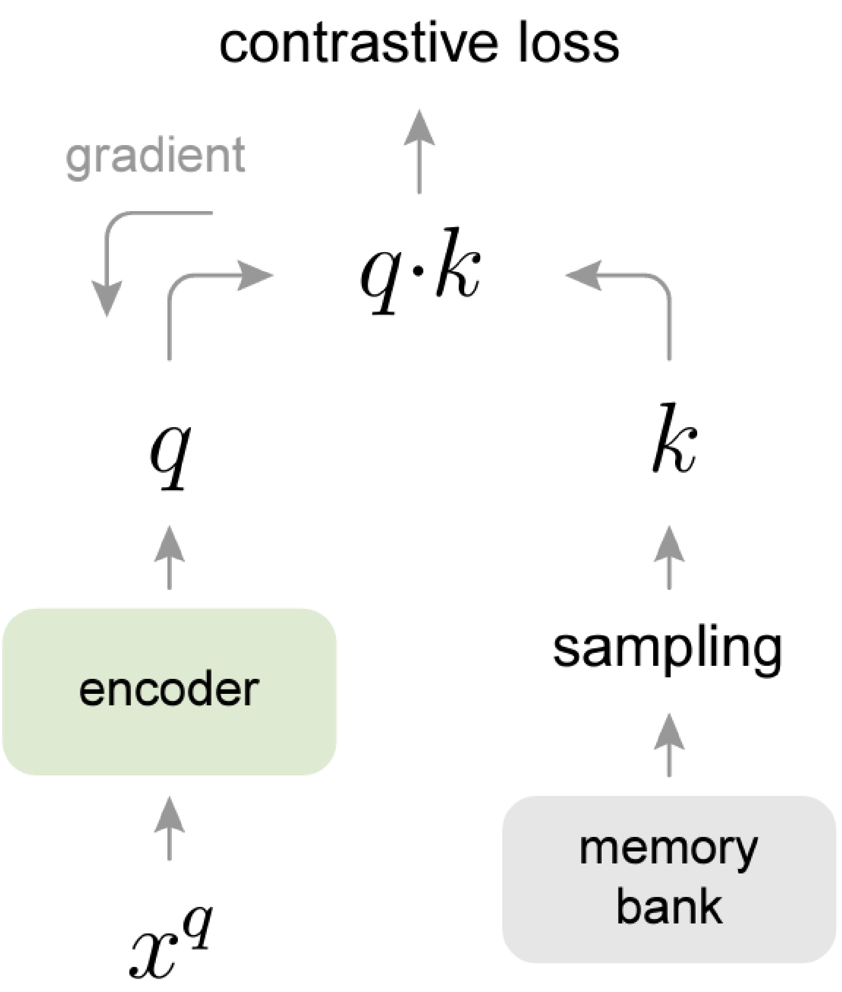
Zhirong Wu et al. (2018) "Unsupervised Feature Learning via Non-Parametric Instance Discrimination". Proceedings of the IEEE conference on computer vision and pattern recognition (pp. 3733-3742).

Noise-Contrastive *Estimation (NCE)*



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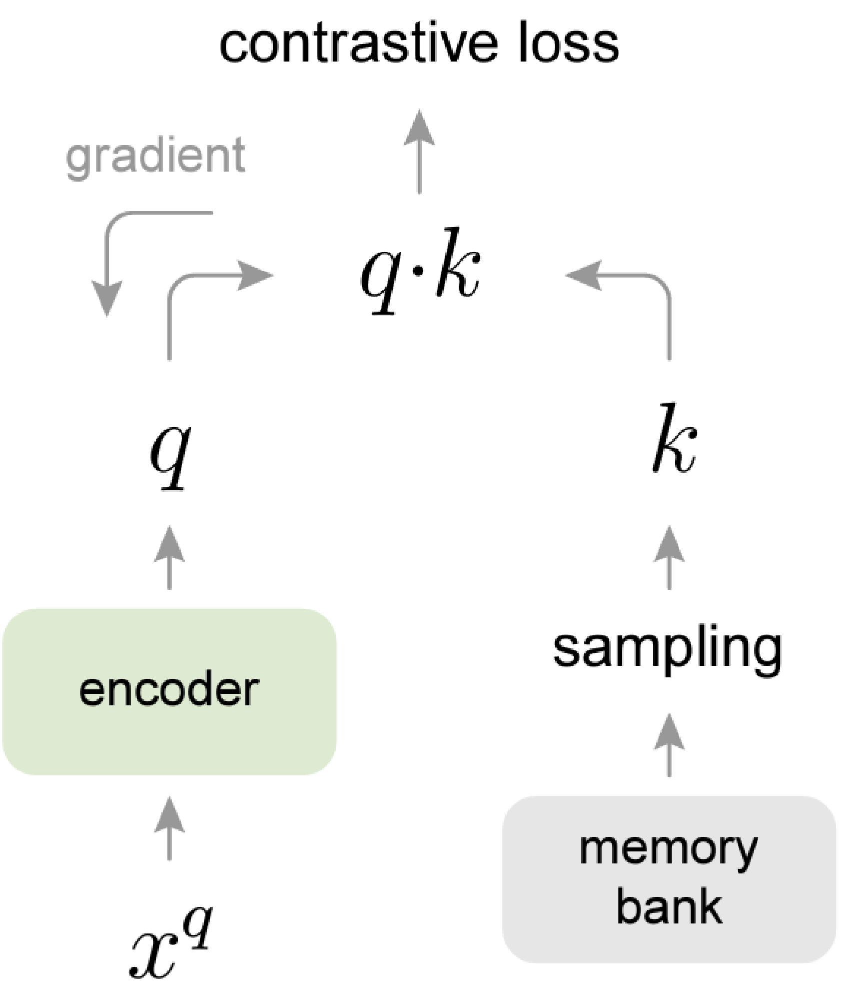
Zhirong Wu et al. (2018) "Unsupervised Feature Learning via Non-Parametric Instance Discrimination". Proceedings of the IEEE conference on computer vision and pattern recognition (pp. 3733-3742).

Noise-Contrastive *Estimation (NCE)*



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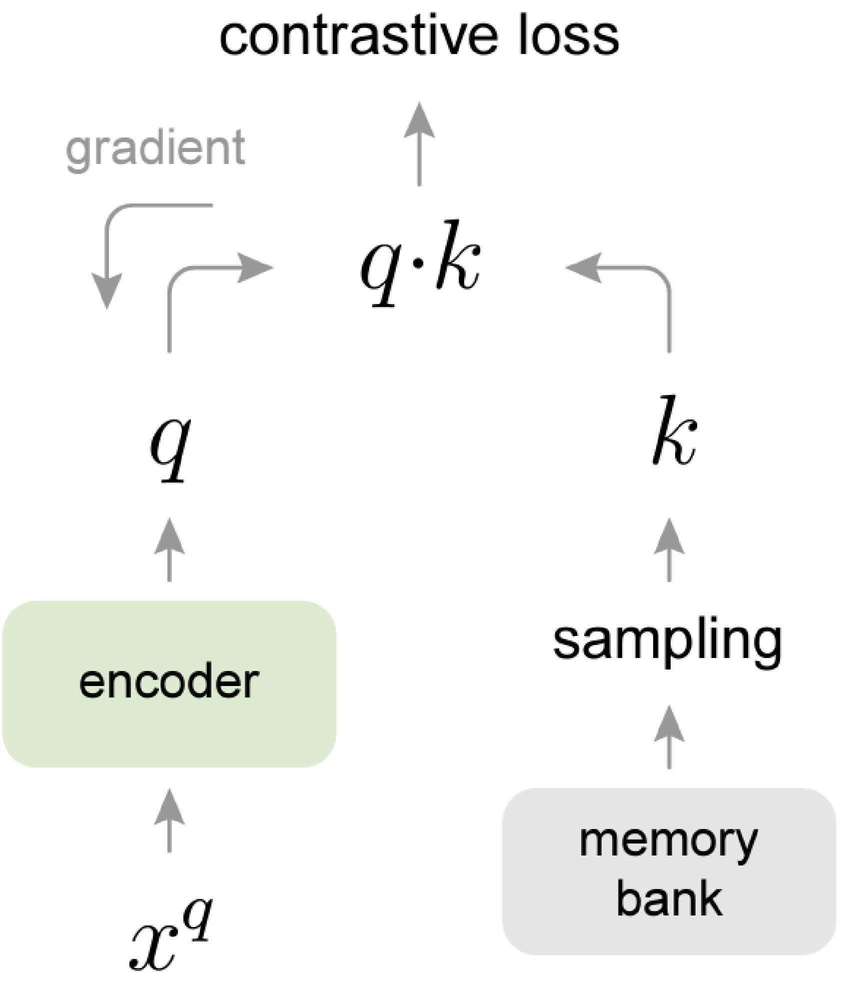
Calculamos la probabilidad posteriori:

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

Zhirong Wu et al. (2018) "Unsupervised Feature Learning via Non-Parametric Instance Discrimination". Proceedings of the IEEE conference on computer vision and pattern recognition (pp. 3733-3742).

Noise-Contrastive *Estimation (NCE)*



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

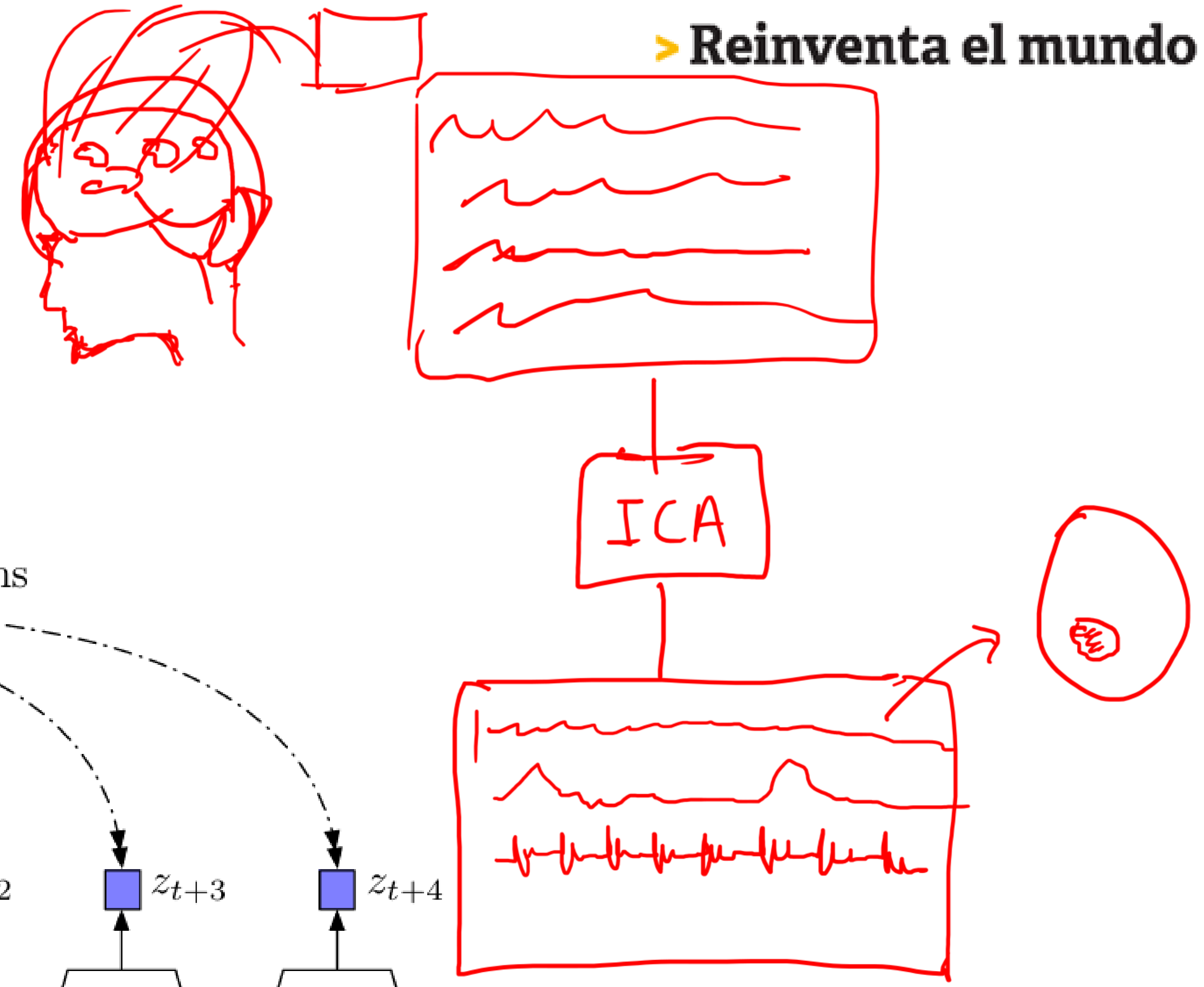
Loss function:

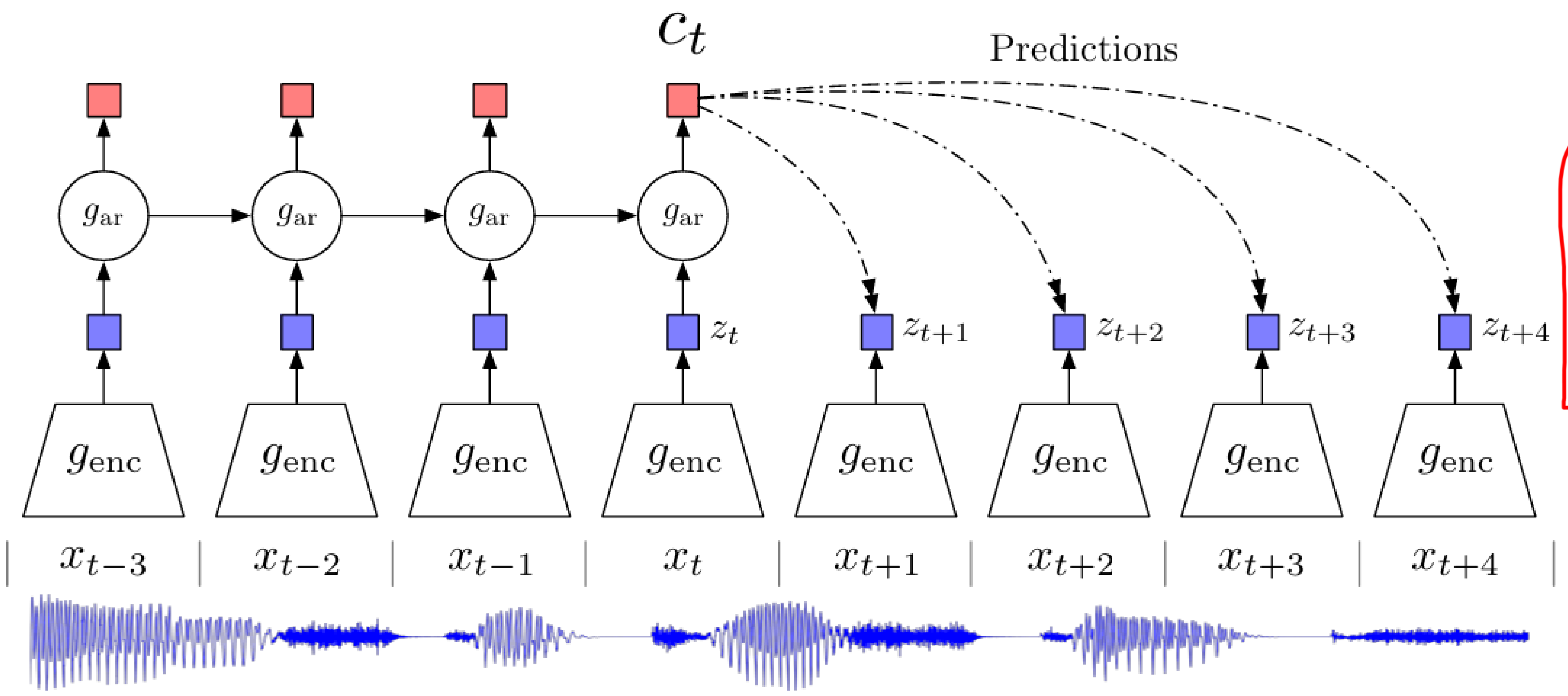
$$J_{NCE}(\theta) = -\mathbb{E}_{P_d}[\log h\,(i, v)] - m \cdot \mathbb{E}_{P_n}[\log(1 - h(i, v'))]$$

Zhirong Wu et al. (2018) "Unsupervised Feature Learning via Non-Parametric Instance Discrimination". Proceedings of the IEEE conference on computer vision and pattern recognition (pp. 3733-3742).

InfoNCE

(Information Noise-Contrastive Estimation)





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

Aaron van den Oord et al. (2019) "Representation Learning with Contrastive Predictive Coding". arXiv preprint arXiv:1807.03748.

$p(x,y) = p(x)p(y)$?

Mutual *Information*

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

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

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.

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

Mutual *Information*

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

$$I(X;Y) = \mathrm{D}_{KL}\big(p(x,y)||p(x) \otimes p(y)\big) = \sum_{x\in\mathcal{X}} \sum_{y\in\mathcal{Y}} p(x,y) \log \frac{p(x,y)}{p(x)p(y)}$$

$\rightarrow p(y|x)$

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$$\updownarrow$$

$$\sum_j \sum_i p(x,y) \log \frac{p(y|x)}{p(y)}$$

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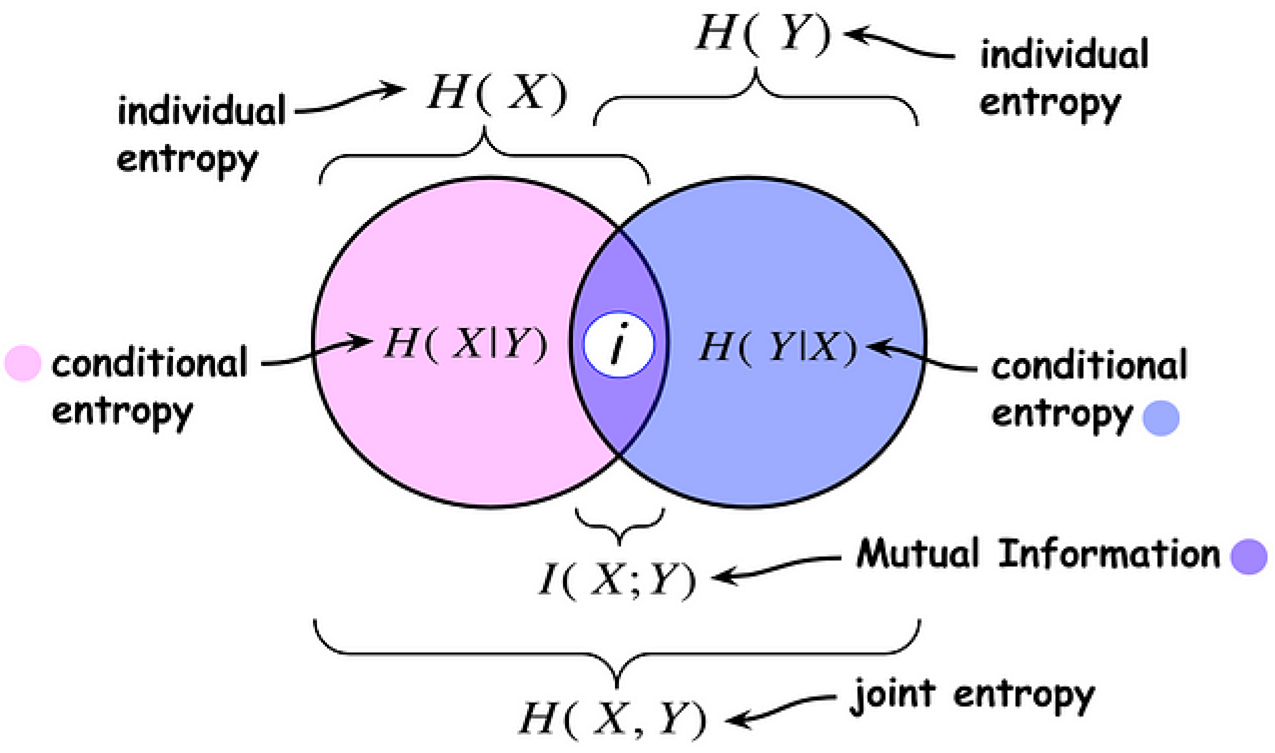

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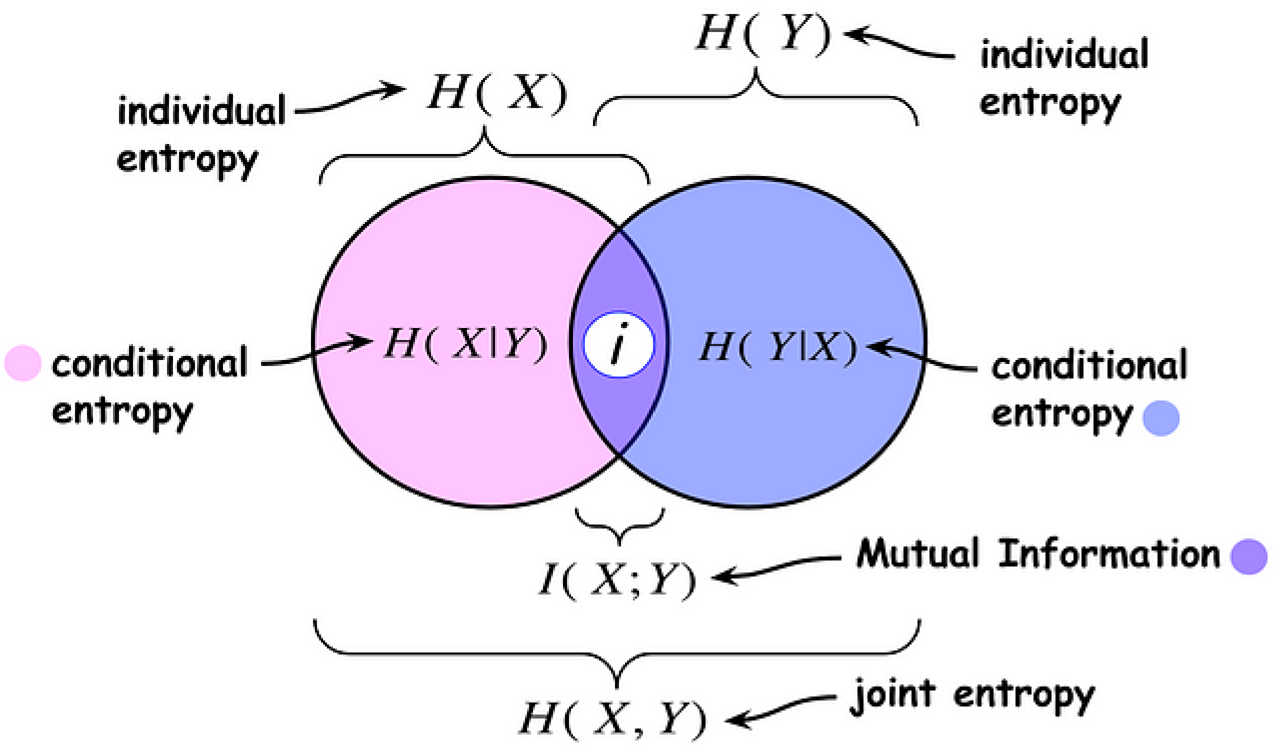

Interpretación:

- $I(X;Y)$ 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.

Info*NCE*

(Information Noise-Contrastive Estimation)

Partimos de **NCE loss**:

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

Aaron van den Oord et al. (2019) "Representation Learning with Contrastive Predictive Coding". arXiv preprint arXiv:1807.03748.

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

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Demostración:

$$\mathcal{L}_{\mathrm{N}}^{\mathrm{opt}} = -\mathop{\mathbb{E}}_{X}\log\left[\frac{\frac{p(x_{t+k}|c_t)}{p(x_{t+k})}}{\frac{p(x_{t+k}|c_t)}{p(x_{t+k})}+\sum_{x_j\in X_{\mathrm{neg}}}\frac{p(x_j|c_t)}{p(x_j)}}\right] = \mathop{\mathbb{E}}_{X}\log\left[1+\frac{p(x_{t+k})}{p(x_{t+k}|c_t)}\sum_{x_j\in X_{\mathrm{neg}}}\frac{p(x_j|c_t)}{p(x_j)}\right]$$

$$\approx \mathop{\mathbb{E}}_{X}\log\left[1+\frac{p(x_{t+k})}{p(x_{t+k}|c_t)}(N-1)\mathop{\mathbb{E}}_{x_j}\frac{p(x_j|c_t)}{p(x_j)}\right] = \mathop{\mathbb{E}}_{X}\log\left[1+\frac{p(x_{t+k})}{p(x_{t+k}|c_t)}(N-1)\right]$$

$$\geq \mathop{\mathbb{E}}_{X}\log\left[\frac{p(x_{t+k})}{p(x_{t+k}|c_t)}N\right] = -I(x_{t+k},c_t)+\log(N)$$

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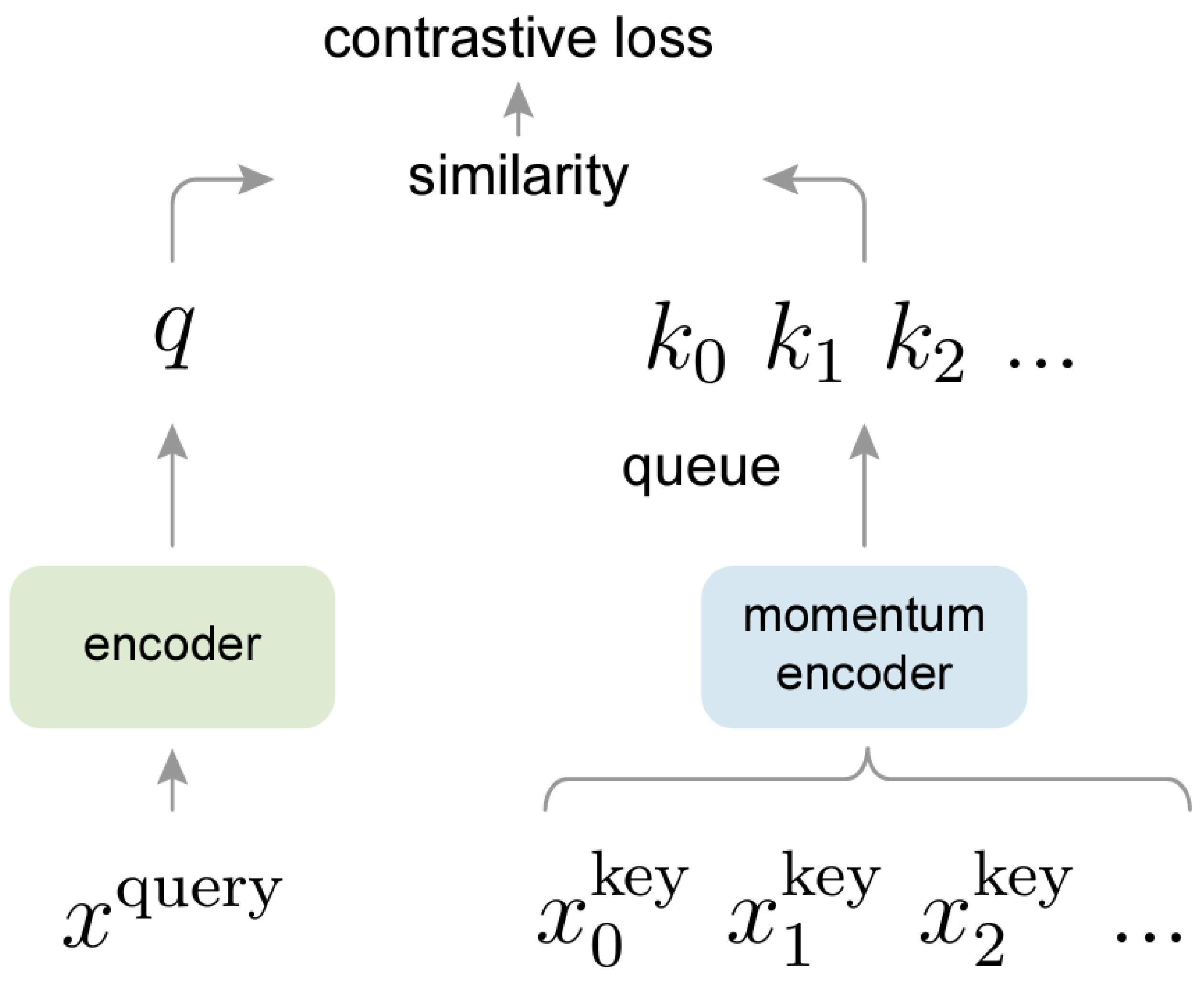
MoCo

(Momentum Contrast)

MoCo entrena un modelo para buscar representaciones similares dentro de un diccionario.



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.

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.

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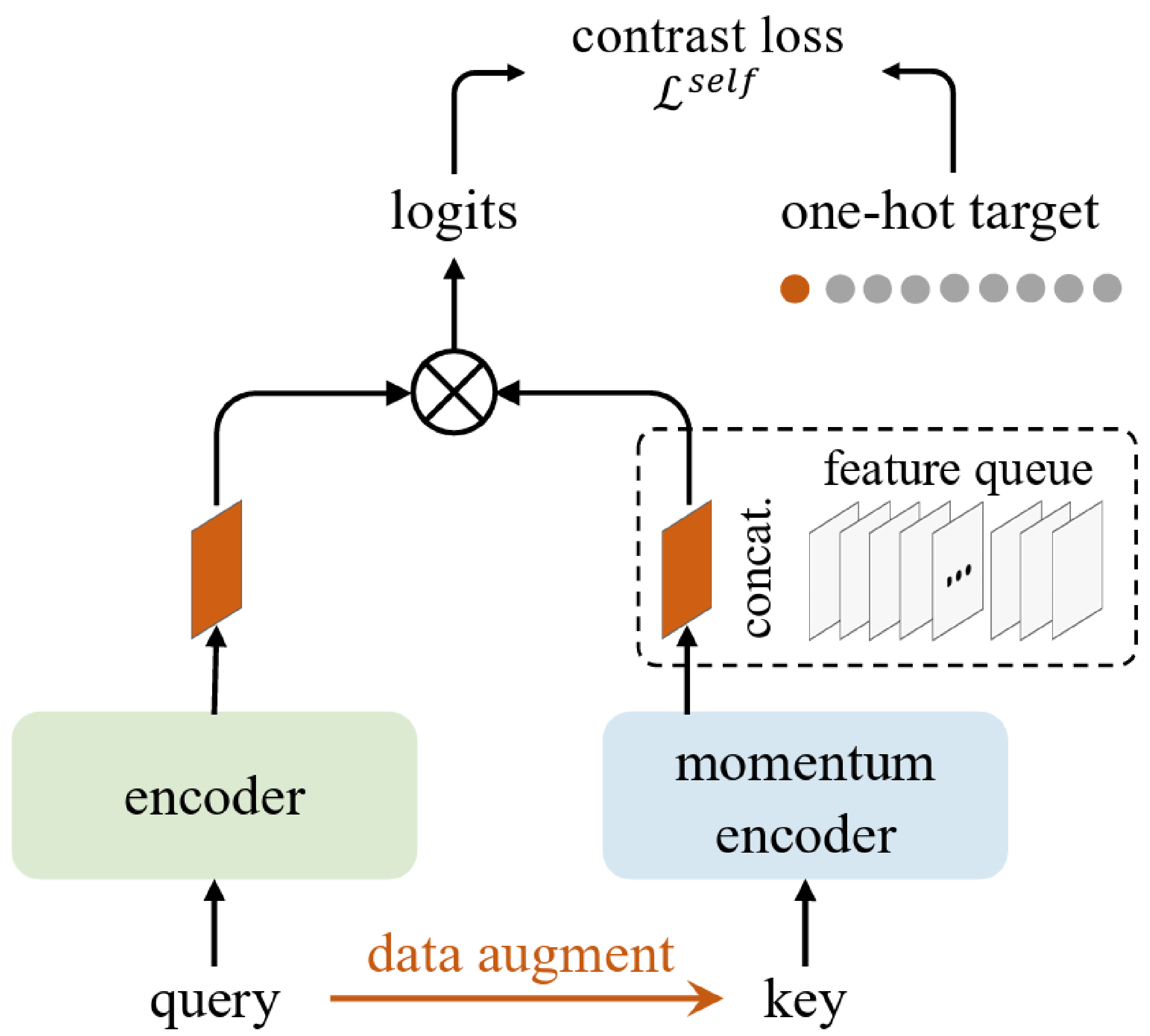

Dictionary queue

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.

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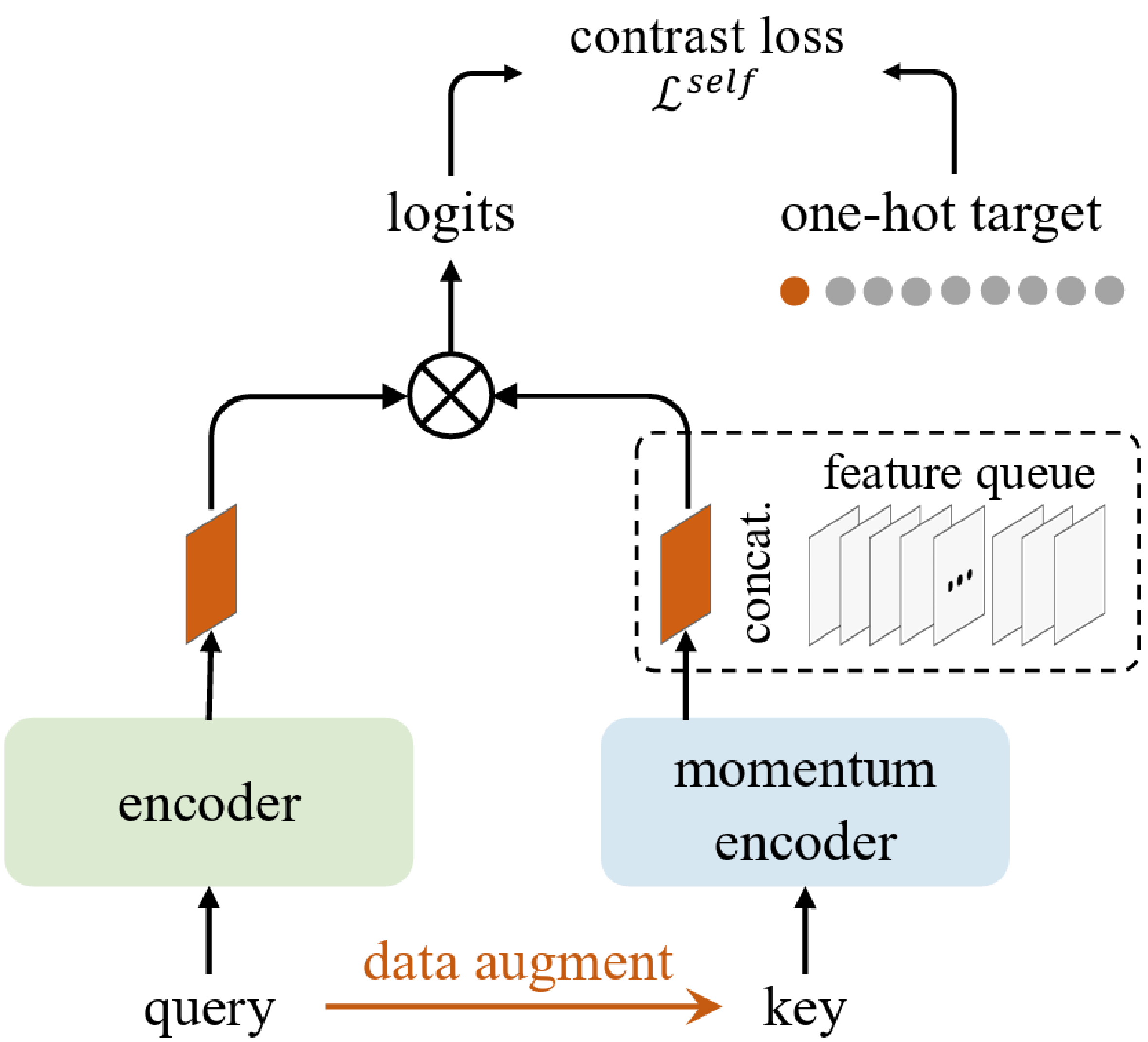

Momentum updates

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.

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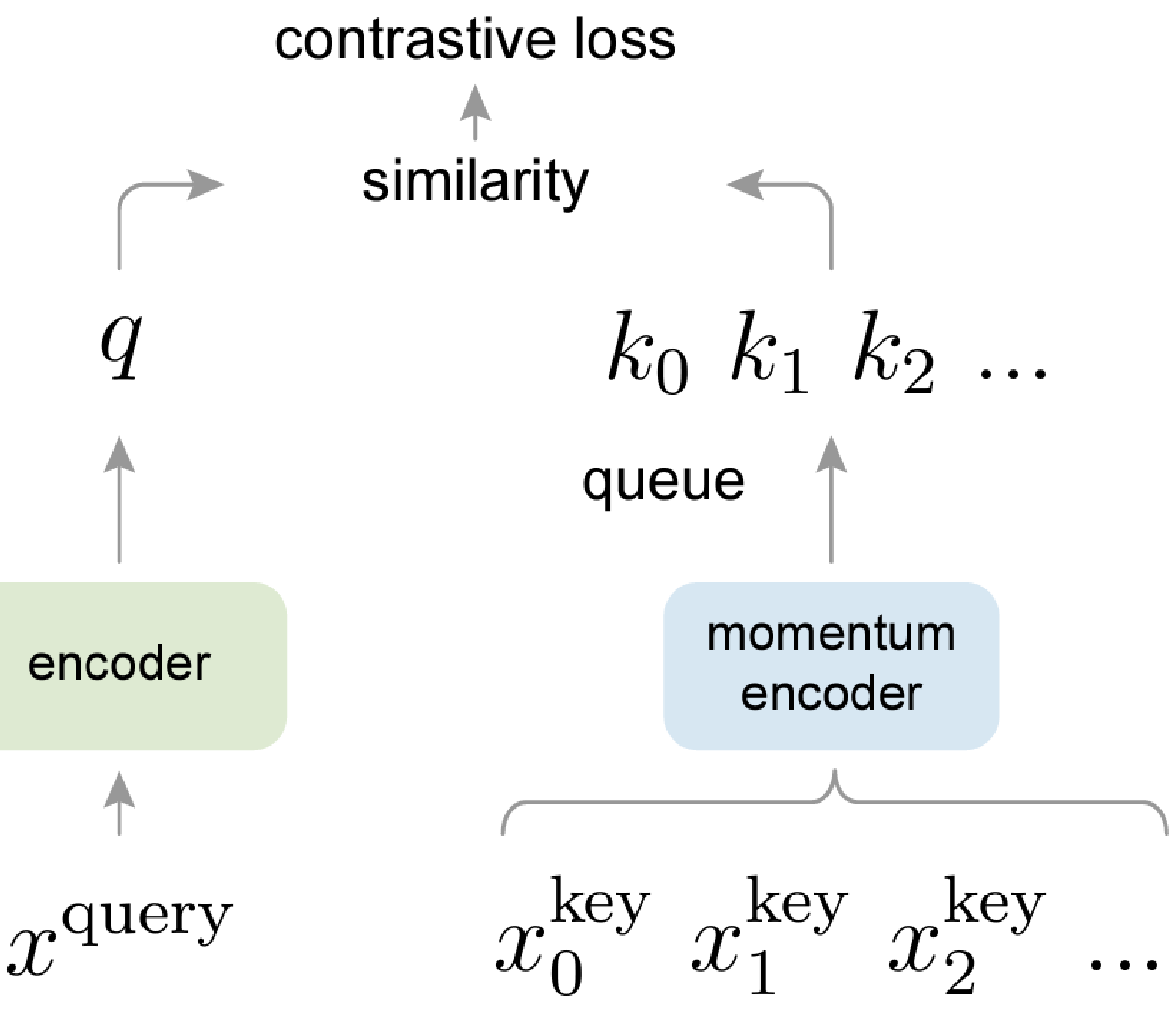

CODE?

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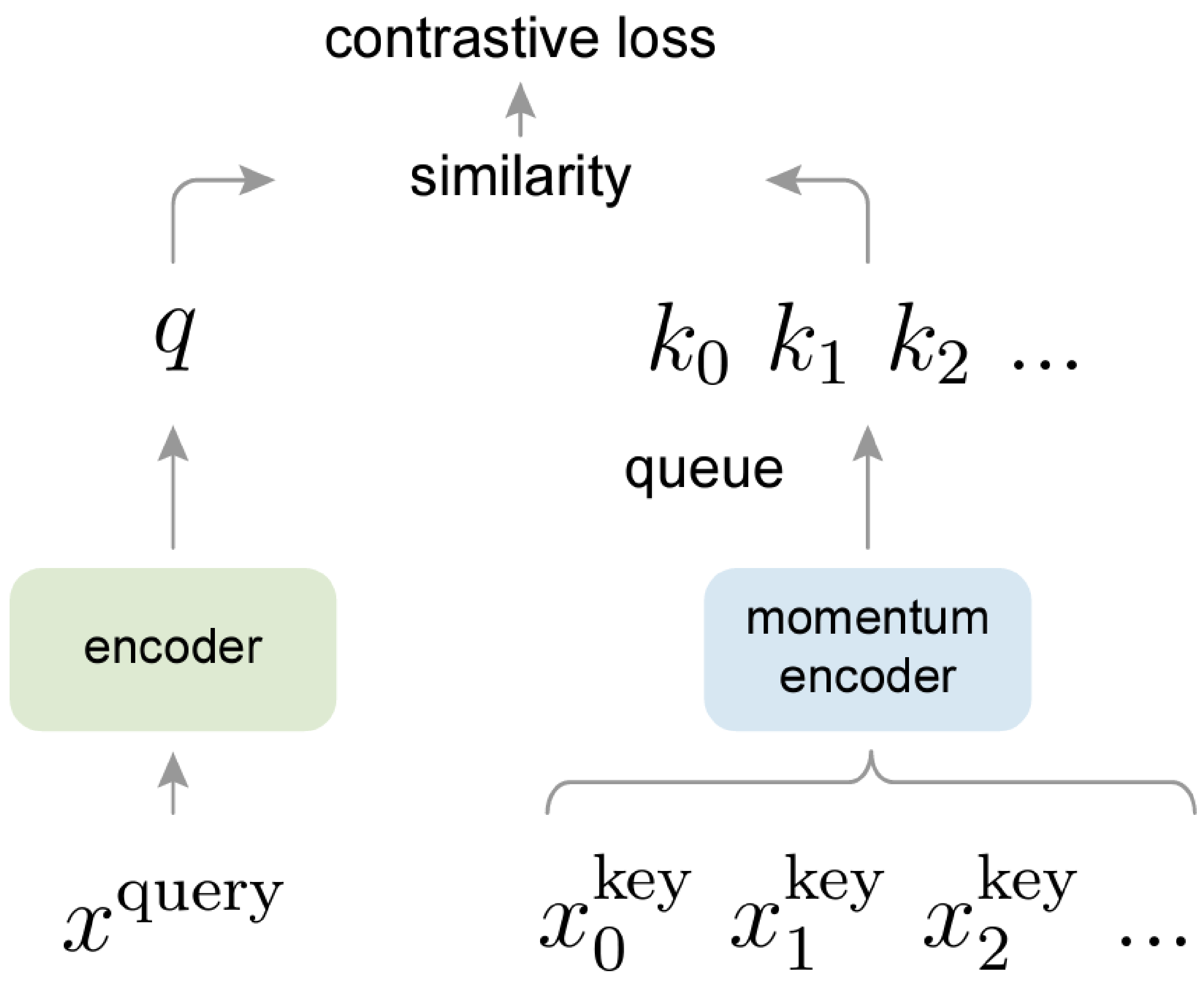


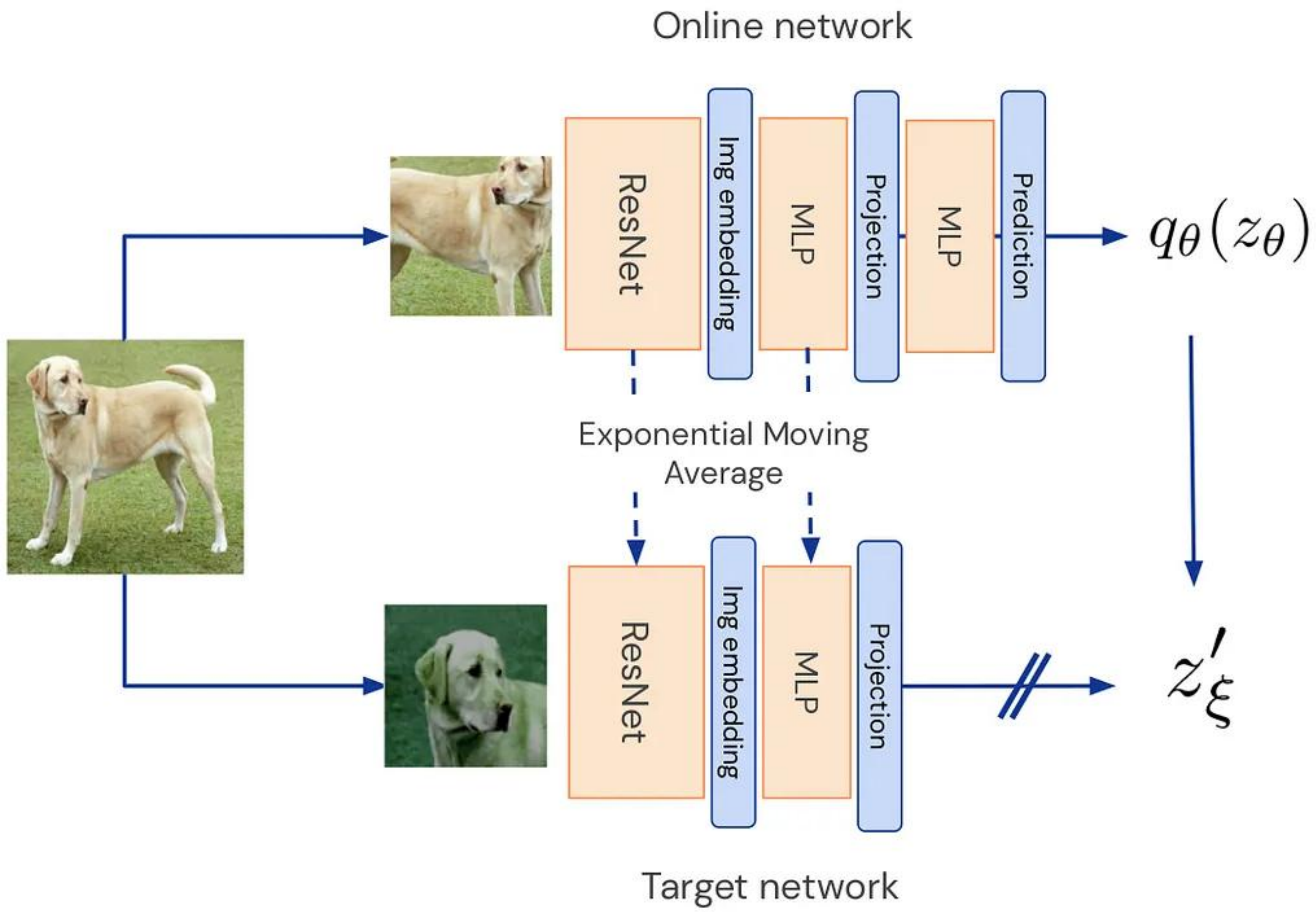
Algorithm 1 Pseudocode of MoCo in a PyTorch-like style.

```
# 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.

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**:

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

Jean-Bastien Grill et al. (2020) "Bootstrap your own latent-a new approach to self-supervised learning". Advances in neural information processing systems, 33, 21271-21284.

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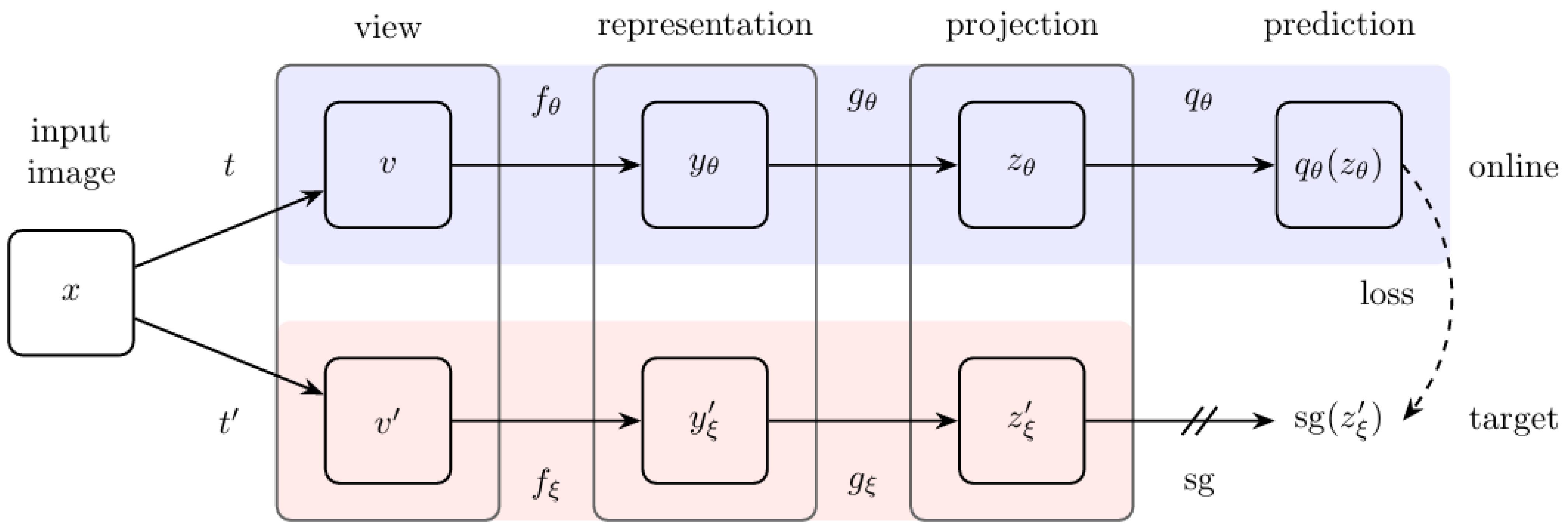

$$\mathcal{L}_{\theta,\xi} \triangleq \left\| \overline{q_\theta}(z_\theta) - \overline{z}'_\xi \right\|_2^2 = 2 - 2 \cdot \frac{\langle q_\theta(z_\theta), z'_\xi \rangle}{\left\| q_\theta(z_\theta) \right\|_2 \cdot \left\| z'_\xi \right\|_2}$$

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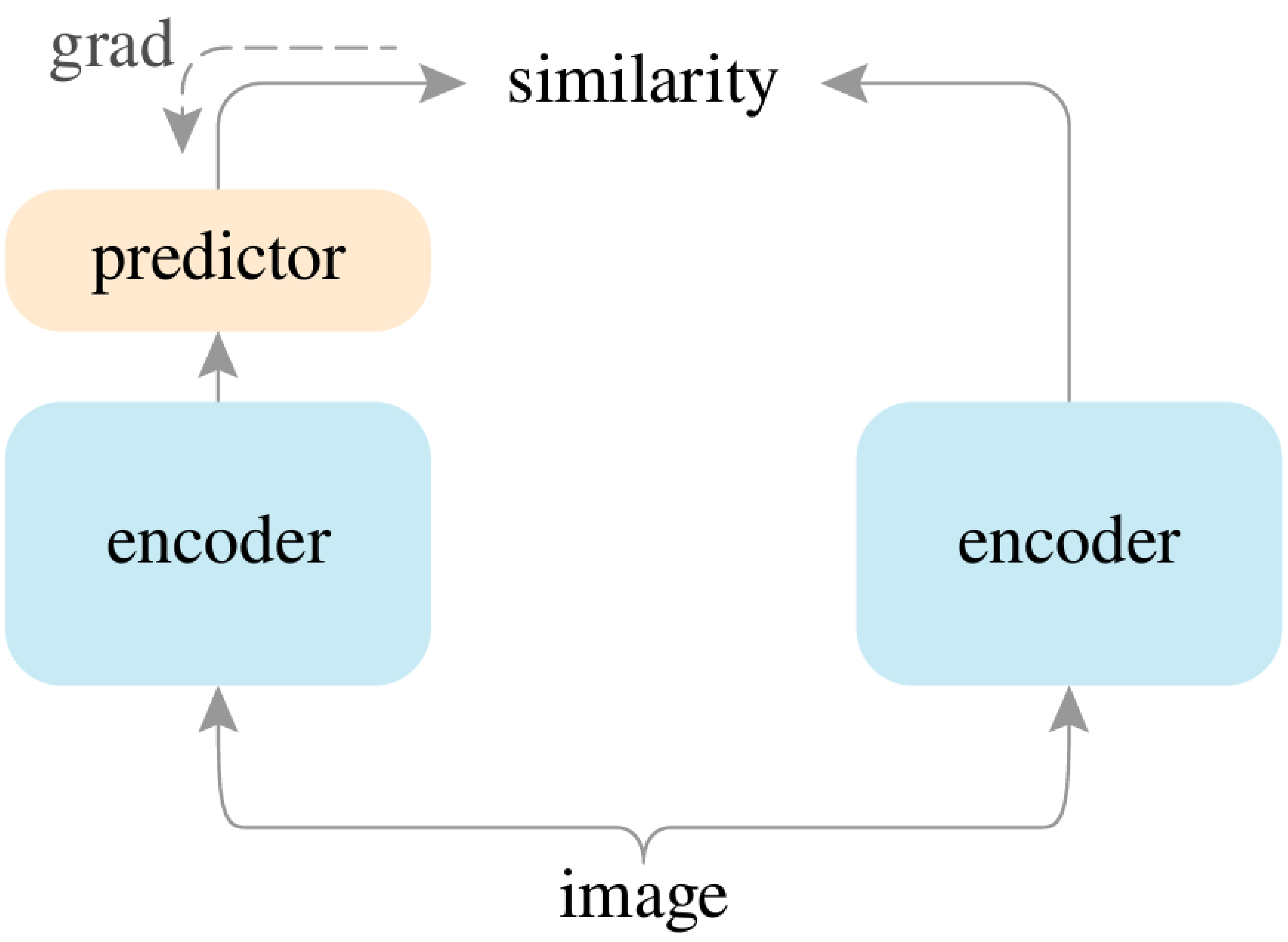
SimSiam

N samples

Xinlei Chen and Kaiming He (2021) "Exploring Simple Siamese Representation Learning".
Proceedings of the IEEE/CVF conference on computer vision and pattern recognition (pp. 15750-15758).

SimSiam



Negative cosine similarity

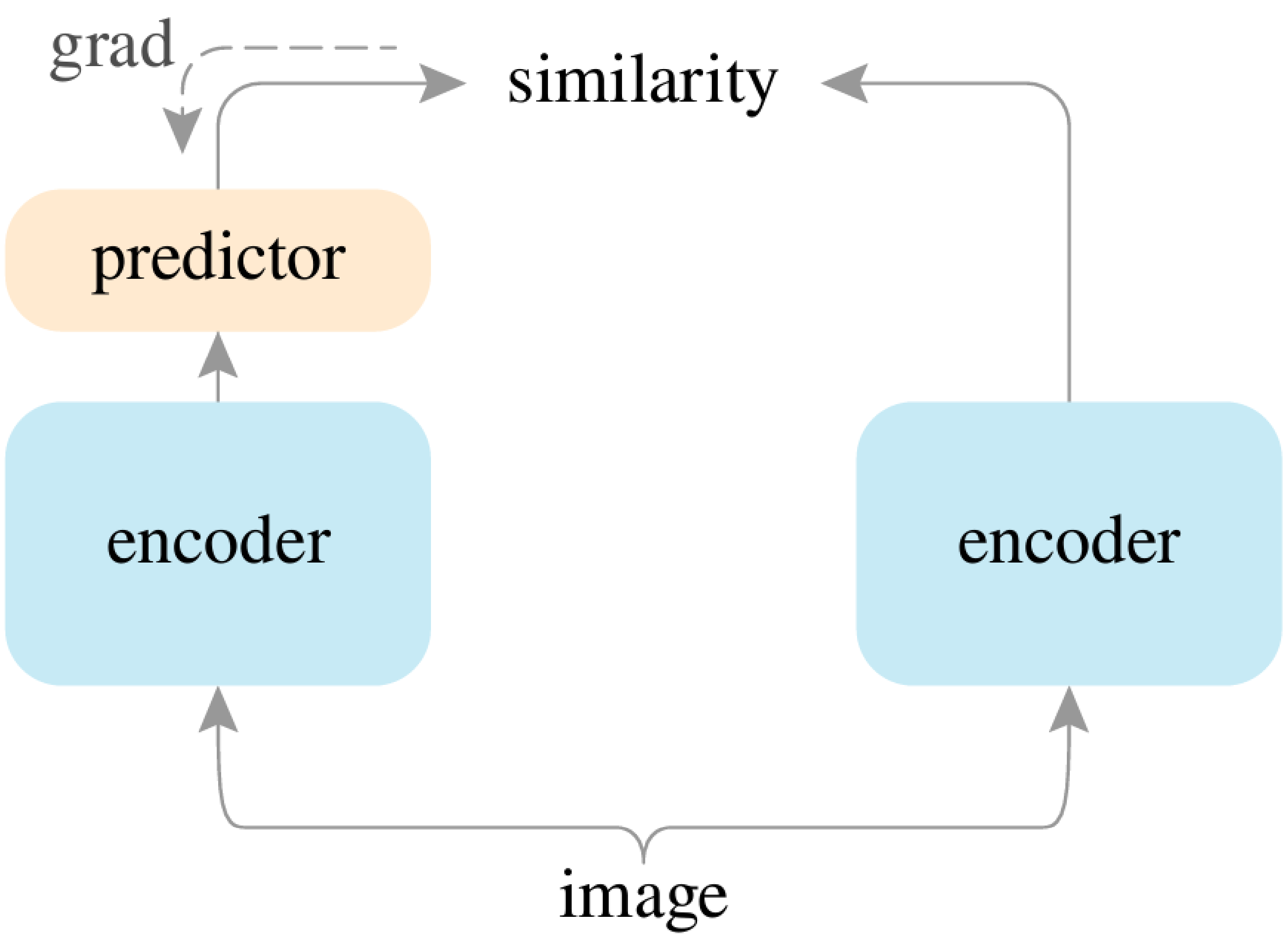
$$\mathcal{D}(p_1, z_2) = -\frac{p_1}{\|p_1\|_2} \cdot \frac{z_2}{\|z_2\|_2}$$

Symmetric loss

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

Xinlei Chen and Kaiming He (2021) "Exploring Simple Siamese Representation Learning". Proceedings of the IEEE/CVF conference on computer vision and pattern recognition (pp. 15750-15758).

SimSiam



CODE?

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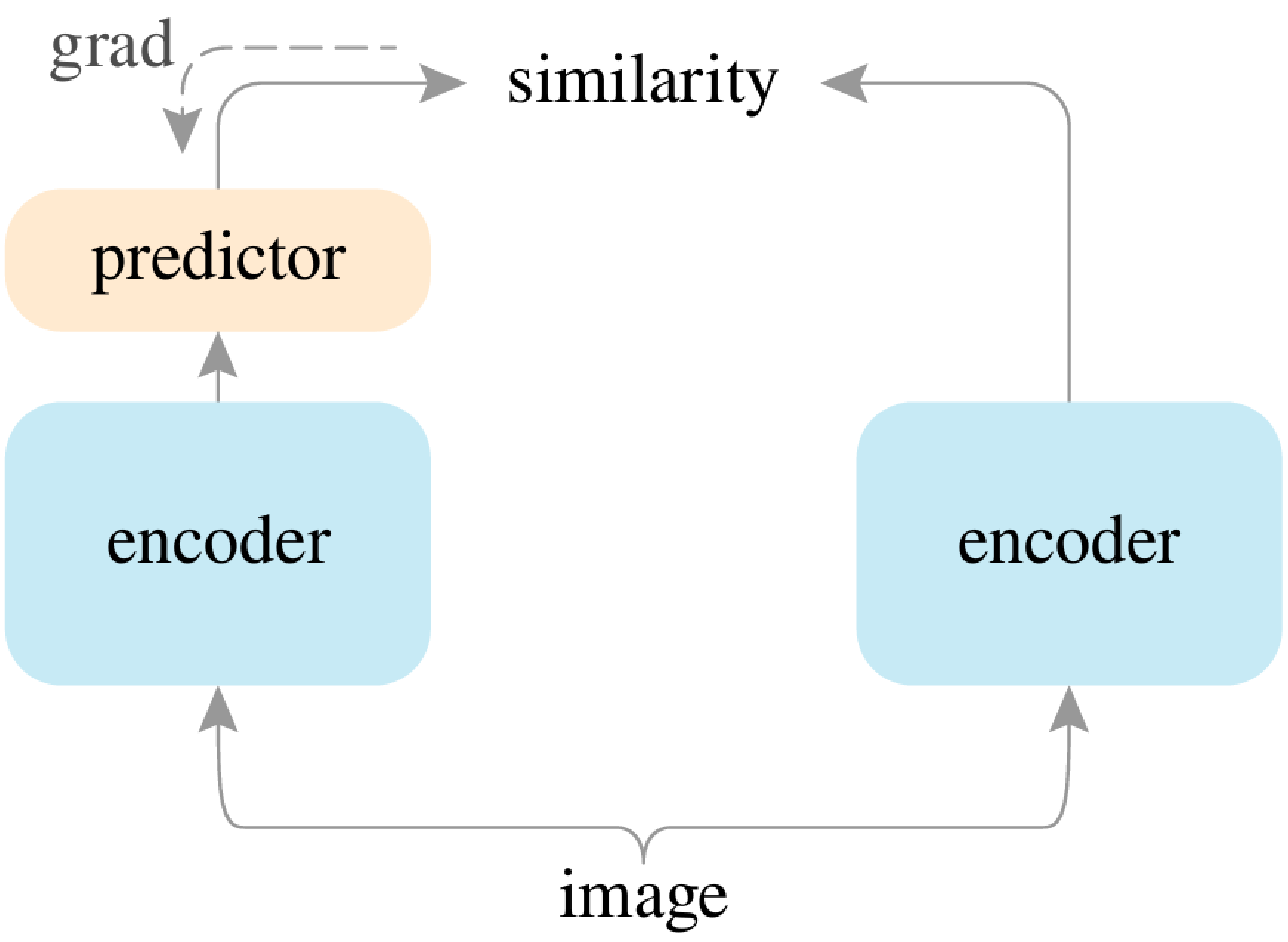


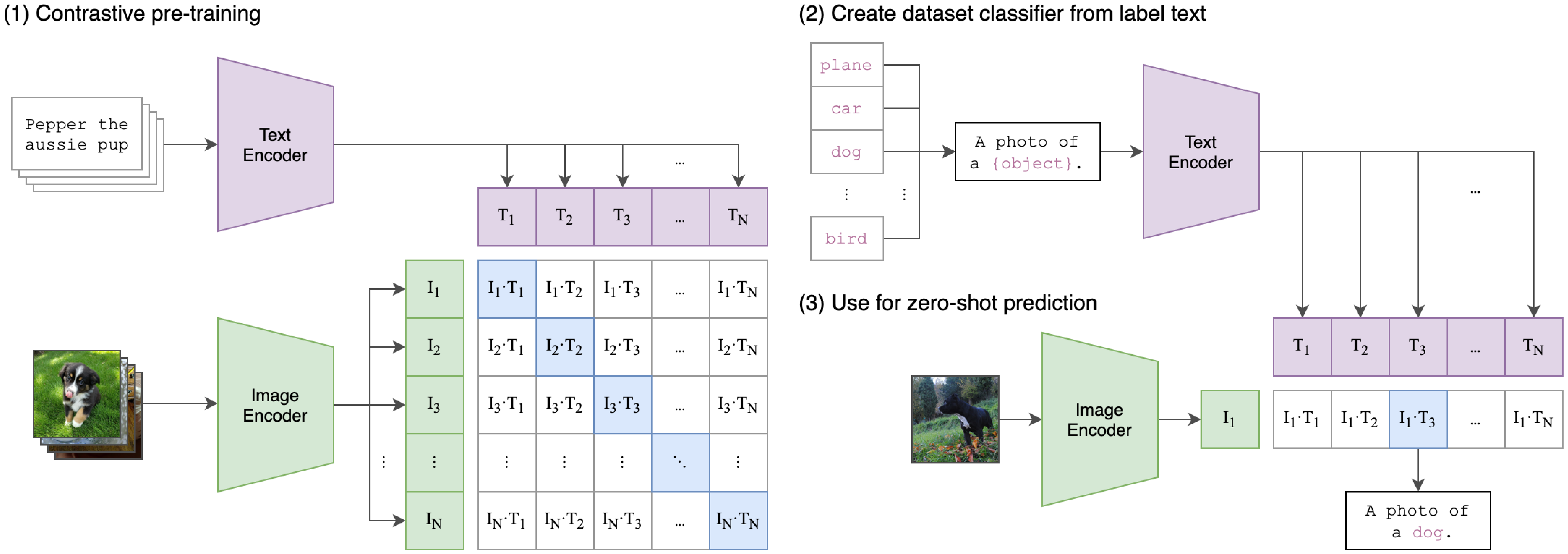
Algorithm 1 SimSiam Pseudocode, PyTorch-like

```
# 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) # l2-normalize
   z = normalize(z, dim=1) # l2-normalize
   return -(p*z).sum(dim=1).mean()
```


Xinlei Chen and Kaiming He (2021) "Exploring Simple Siamese Representation Learning". Proceedings of the IEEE/CVF conference on computer vision and pattern recognition (pp. 15750-15758).

CLIP

(Contrastive Language-Image Pre-training)



Alec Radford et al. (2021) "Learning Transferable Visual Models From Natural Language Supervision". International conference on machine learning (pp. 8748-8763). PMLR.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