Master 2 Statistique & Data Science, Ingénierie Mathématique

Réseaux de neurones profonds pour l'apprentissage Deep neural networks for machine learning

Course V – Introduction to Artificial Neural Networks: Generative Models

Bruno Galerne 2024-2025



Credits

Most of the slides from **Charles Deledalle's** course "UCSD ECE285 Machine learning for image processing" (30 \times 50 minutes course)

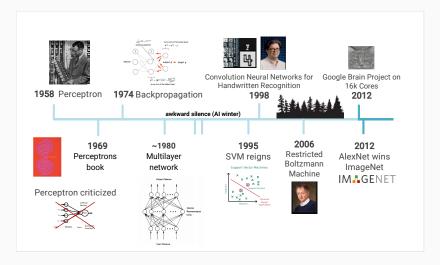


www.charles-deledalle.fr/
https://www.charles-deledalle.fr/pages/teaching.php#learning

2

Machine learning – Timeline

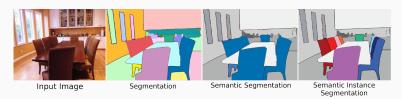
Timeline of (deep) learning



Segmentation

Segmentation

Segmentation – Terminology

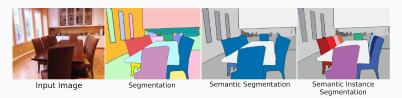


• Segmentation:

- Partition of an image into several "coherent" parts/segments,
- Without any attempt at understanding what these parts represent,
- Typically based on color, textures, smoothness of boundaries,
- Also referred to as super-pixel segmentation.

Segmentation

Segmentation – Terminology



- Semantic segmentation:
 - Each segment corresponds to a class label (objects + background),
 - Also referred to as scene parsing or scene labeling.
- Instance segmentation:
 - Find object boundaries between objects, including delineations between instances of the same object.
- **Semantic instance segmentation:** find object boundaries + labels.

U-net for image segmentation



(source: From [Ronneberger et al., 2015])

- First proposed in [Ronneberger et al., 2015].
- Idea: Classify each pixel
- Condense spatial information as for image classification.
- Re-affine spatially the classification step by step with mirror upsampling steps (transpose of conv2D with padding) and concatenation.

U-net for image segmentation

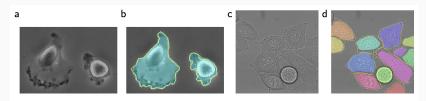
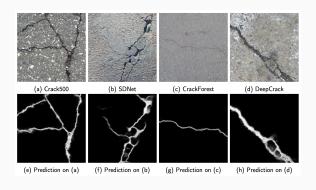


Fig. 4. Result on the ISBI cell tracking challenge. (a) part of an input image of the "PhC-U373" data set. (b) Segmentation result (cyan mask) with manual ground truth (yellow border) (c) input image of the "DIC-HeLa" data set. (d) Segmentation result (random colored masks) with manual ground truth (yellow border).

(source: From [Ronneberger et al., 2015])

- Improved state-of-the-art in cell-tracking.
- Can be extended to very different contexts provided enough labeled data.

U-net for image segmentation



(source: From [Drouyer, 2020])

- Example usage: Crack detection
- The network outputs the probability that each pixel belongs to a crack.

U-net for inverse problems

More generally a U-net can be trained to produce an image aligned with the input image.

- Segmentation [Ronneberger et al., 2015]
- Denoising (see e.g. DRUNet [Zhang et al., 2022])
- Image to image translation (Pix2pix [Isola et al., 2017])
- Inverse problems: trained to remove artefacts from a crude solution:

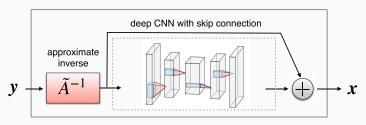
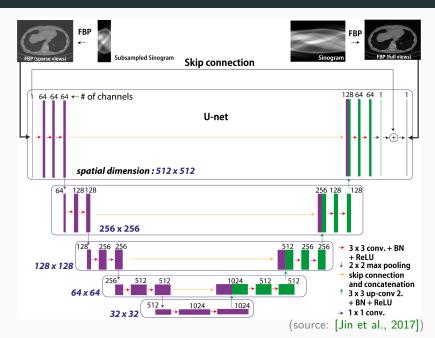


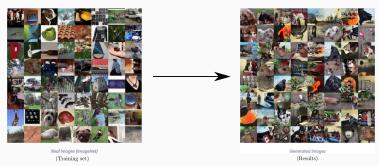
Fig. 7. When an approximate inverse \tilde{A}^{-1} of the forward model is known, a common approach in the supervised setting is to train a deep CNN to remove noise and artifacts from an initial reconstruction obtained by applying \tilde{A}^{-1} to the measurements. (source: [Ongie et al., 2020])

U-net for inverse problems



Motivations – Image generation

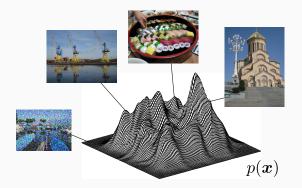
• **Goal:** Generate images that look like the ones of your training set.



- What? Unsupervised learning.
- Why? Different reasons and applications:
 - Can be used for simulation, e.g., to generate labeled datasets,
 - Must capture all subtle patterns → provide good features,
 - Can be used for other tasks: super-resolution, style transfer, ...

Image generation - Explicit density

lacktriangle Learn the distribution of images p(x) on a training set.



 ${\bf 2}$ Generate samples from this distribution.

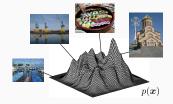
Image generation - Gaussian model

• Consider a Gaussian model for the distribution of images x with n pixels:

$$oldsymbol{x} \sim \mathcal{N}(oldsymbol{\mu}, oldsymbol{\Sigma})$$

$$p(\boldsymbol{x}) = \frac{1}{\sqrt{2\pi^n} |\boldsymbol{\Sigma}|^{1/2}} \exp\left[(\boldsymbol{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} - \boldsymbol{\mu}) \right]$$

- μ : mean image,
- Σ : covariance matrix of images.







Gaussian prior $x \sim \mathcal{N}(\mu, \Sigma)$

Image generation – Gaussian model

ullet Take a training dataset ${\mathcal T}$ of images:

$$\mathcal{T} = \{oldsymbol{x}_1, \dots, oldsymbol{x}_N \}$$

$$= \left\{ \begin{array}{c} \dots \\ \dots \end{array} \right.$$

Estimate the mean

$$\hat{m{\mu}} = rac{1}{N} \sum_i m{x}_i =$$

• Estimate the covariance matrix: $\hat{m{\Sigma}} = \frac{1}{N} \sum_i (m{x}_i - \hat{m{\mu}}) (m{x}_i - \hat{m{\mu}})^T = \hat{m{E}} \hat{m{\Lambda}} \hat{m{E}}^T$

Image generation – Gaussian model

You now have learned a generative model:

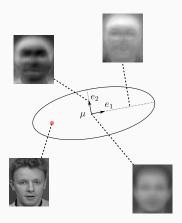


Image generation - Gaussian model

How to generate samples from $\mathcal{N}(\hat{\mu}, \hat{\Sigma})$?

$$\left\{egin{array}{ll} m{z} & \sim \mathcal{N}(0, \mathrm{Id}_n) & \leftarrow \mathsf{Generate} \ m{x} & = \hat{m{\mu}} + \hat{m{E}}\hat{m{\Lambda}}^{1/2}m{z} \end{array}
ight.$$



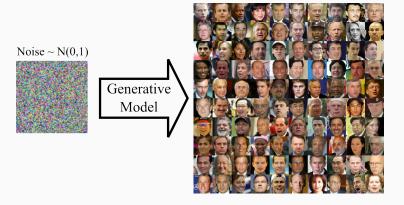
The model does not generate realistic faces.

The Gaussian distribution assumption is too simplistic.

Each generated image is just a linear random combination of the eigenvectors.

The generator corresponds to a linear neural network (without non-linearities).

Image generation – Beyond Gaussian models



But the concept is interesting: can we find a transformation such that each random code can be mapped to a photo-realistic image?

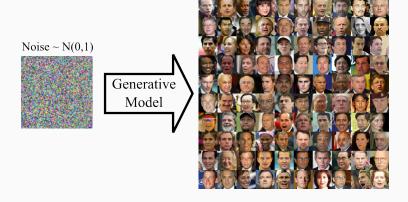
We need to find a way to assess if an image is photo-realistic.

Main references:

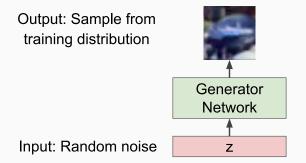
• Original paper: [Goodfellow et al., 2014]

NIPS 2016 tutorial: [Goodfellow, 2017]

Image generation - Beyond Gaussian models

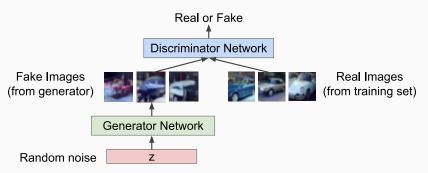


- Goal: design a complex model with high capacity able to map latent random noise vectors $z \in \mathbb{R}^k$ to a realistic image $x \in \mathbb{R}^d$.
- Idea: Take a deep neural network



What about the loss? Measure if the generated image is photo-realistic.

Define a loss measuring how much you can fool a classifier that has learned to distinguish between real and fake images.



- Discriminator network: Try to distinguish between real and fake images.
- **Generator network:** Fool the discriminator by generating realistic images.

Recap on binary classification

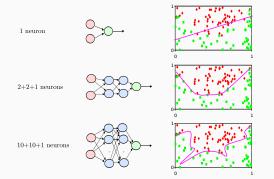
• Given a labeled dataset

$$\mathcal{D} = \{ (\boldsymbol{x}^{(i)}, y^{(i)}), \ i = 1, \dots, N \} \subset \mathbb{R}^d \times \{0, 1\}$$

with binary labels $y^{(i)} \in \{0,1\}$ that corresponds to two classes C_0 and C_1 .

• A parametric classifier $f_{\boldsymbol{\theta}}: \mathbb{R}^d \to [0,1]$ outputs a probability such that

$$p = f_{\theta}(x) = \mathbb{P}(x \in C_1)$$
 and $1 - p = 1 - f_{\theta}(x) = \mathbb{P}(x \in C_0)$



Estimated decision regions: $\hat{C} = \{ m \in \mathbb{R}^d \mid f_*(m) > 1 \}$

$$\hat{C}_1 = \{ m{x} \in \mathbb{R}^d, \ f_{m{ heta}}(m{x}) \geqslant rac{1}{2} \}$$
 and $\hat{C}_0 = \mathbb{R}^d \setminus \hat{C}_1.$

Complexity/capacity of the network

$$\Rightarrow$$

Trade-off between generalization and overfitting.

Recap on binary classification

 Training: Logistic regression for binary classification: Maximum likelihood of the dataset (opposite of binary crosss-entropy: BCELoss in PyTorch):

$$\max_{\theta} \sum_{i=1}^{N} \left[y^{(i)} \log f_{\theta}(\boldsymbol{x}^{(i)}) + (1 - y^{(i)}) \log \left(1 - f_{\theta}(\boldsymbol{x}^{(i)}) \right) \right]$$

- For neural networks, the probability f_{θ} is obtained using the **sigmoid** function $\sigma(t) = \frac{e^t}{1+e^t} = \frac{1}{1+e^{-t}}$ as the activation function of the last layer.
- Beware that $y^{(i)} = 0$ or 1 so only one term is non-zero.
- One could instead regroup the terms of the sum according to the label values:

$$\max_{\boldsymbol{\theta}} \sum_{\substack{(\boldsymbol{x}^{(i)}, y^{(i)}) \in \mathcal{D} \\ \text{s.t. } y^{(i)} = 1}}^{N} \log f_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) + \sum_{\substack{(\boldsymbol{x}^{(i)}, y^{(i)}) \in \mathcal{D} \\ \text{s.t. } y^{(i)} = 0}}^{N} \log \left(1 - f_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)})\right)$$

- Discriminator network: Consider two sets
 - $\mathcal{D}_{\text{real}}$: a dataset of n real images (real = labeled with $y^{(i)} = 1$),
 - $\mathcal{D}_{\text{fake}}$: a dataset of m fake images $\pmb{x}=G_{\theta_g}(\pmb{z})$ (fake = labeled with $y^{(i)}=0$).
- Goal: Find the parameters θ_d of a binary classification network $x\mapsto D_{\theta_d}(x)$ meant to classify real and fake images. Minimize the binary cross-entropy, or maximize its negation

$$\max_{\theta_d} \underbrace{\sum_{\boldsymbol{x}_{\mathsf{real}} \in \mathcal{D}_{\mathsf{real}}} \log D_{\theta_d}(\boldsymbol{x}_{\mathsf{real}})}_{\text{force predicted labels to be 1}} + \underbrace{\sum_{\boldsymbol{x}_{\mathsf{fake}} \in \mathcal{D}_{\mathsf{fake}}} \log (1 - D_{\theta_d}(\boldsymbol{x}_{\mathsf{fake}}))}_{\text{force predicted labels to be 0}}$$

• How: Use gradient ascent (Adam).

- Generator network: Consider a given discriminative model $x \mapsto D_{\theta_d}(x)$ and consider $\mathcal{D}_{\mathsf{rand}}$ a set of m random latent vectors.
- Goal: Find the parameters θ_g of a network $z \mapsto G_{\theta_g}(z)$ generating images from random vectors z such that it fools the discriminator

$$\min_{\theta_g} \sum_{\boldsymbol{z} \in \mathcal{D}_{\mathsf{rand}}} \log(1 - D_{\theta_d}(G_{\theta_g}(\boldsymbol{z}))) \tag{1}$$

our generated fake images are not fake (away from 0)

or alternatively (works better in practice)

$$\max_{\theta_g} \sum_{\substack{\boldsymbol{z} \in \mathcal{D}_{\mathsf{rand}} \\ \mathsf{force the discriminator to think that} \\ \mathsf{our generated fake images are real (close to 1)}}}$$

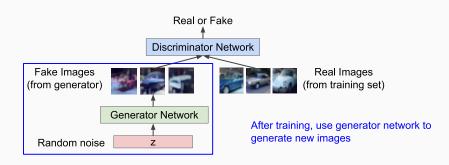
How: Gradient descent for (1) or gradient ascent for (2) (Adam)

- Train both networks jointly.
- Minimax loss in a two player game (each player is a network):

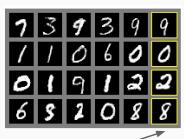
$$\min_{\boldsymbol{\theta}_g} \max_{\boldsymbol{\theta}_d} \ \sum_{\boldsymbol{x} \in \mathcal{D}_{\mathsf{real}}} \log D_{\boldsymbol{\theta}_d}(\boldsymbol{x}) + \sum_{\boldsymbol{z} \in \mathcal{D}_{\mathsf{rand}}} \log (1 - D_{\boldsymbol{\theta}_d}(\underbrace{G_{\boldsymbol{\theta}_g}(\boldsymbol{z})}_{\mathsf{fake}})$$

- Training algorithm: Repeat until convergence
 - **1** Fix θ_q , update θ_d with one step of gradient ascent,
 - **2** Fix θ_d , update θ_g with one step of gradient descent for (1),

(or one step of gradient ascent for (2).)



Generated samples





Nearest neighbor from training set

Generated samples (CIFAR-10)



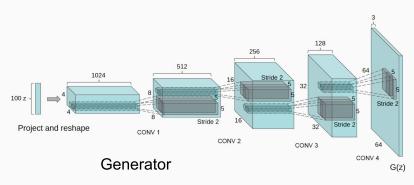


Nearest neighbor from training set

Convolutional GAN

[Radford et al., 2016]

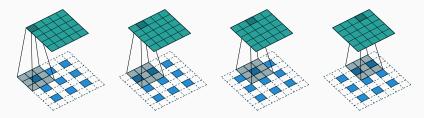
- Generator: upsampling network with fractionally strided convolutions
 (i.e. the transpose operator of convolution+subsampling, called
 ConvTranspose2d in PyTorch),
- Discriminator: convolutional network with strided convolutions.



Transposed convolution arithmetic

Fractionally strided convolutions:

- This is the transpose operator of convolution+subsampling (convolution with stride).
- Called ConvTranspose2d in PyTorch



The transpose of convolving a 3×3 kernel over a 5×5 input padded with a 1×1 border of zeros using 2×2 strides (i.e., $i=5,\ k=3,\ s=2$ and p=1). It is equivalent to convolving a 3×3 kernel over a 3×3 input (with 1 zero inserted between inputs) padded with a 1×1 border of zeros using unit strides (i.e., $i'=3,\ \tilde{i}'=5,\ k'=k,\ s'=1$ and p'=1).

(source: From [Dumoulin and Visin, 2016])

Convolutional GAN

[Radford et al., 2016]



Generations of realistic bedrooms pictures, from randomly generated latent variables.

Convolutional GAN

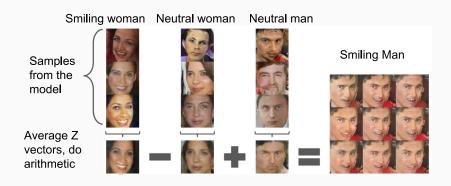
[Radford et al., 2016]



Interpolation in between points in latent space.

Convolutional GAN - Arithmetic

[Radford et al., 2016]



Generative Adversarial Networks (GAN)

Convolutional GAN – Arithmetic

[Radford et al., 2016]



Generative Adversarial Networks (GAN)

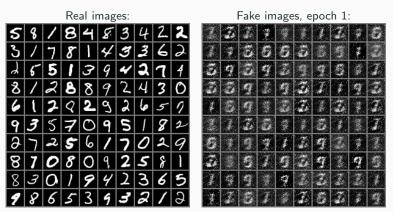
Generative Aversarial Networks: Style GAN [Karras et al., 2019]



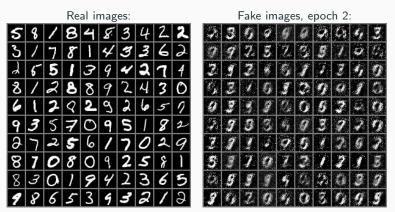
Image size: 1024× 1024 px

(source: Karras et al.)

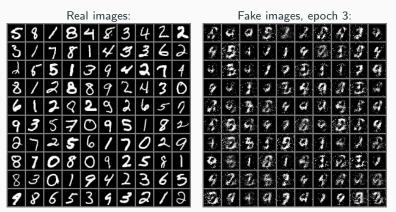
- Adam optimizer
- Learning rate 0.0002 for both the discriminator and the generator



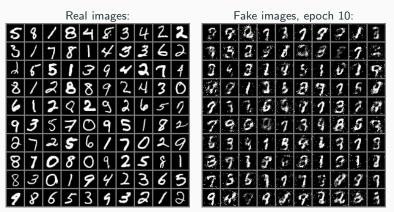
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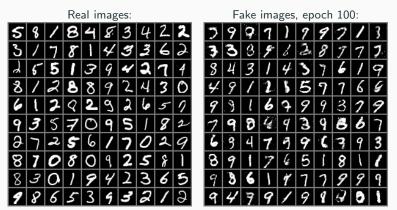
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Training GANs is quite unstable!

The generator can suffer *mode collapse*: It always produces the same image (one mode only).

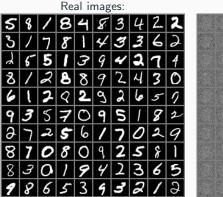
Same as before but with SGD instead of Adam.

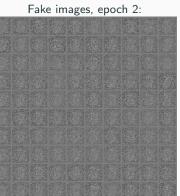


Fake images, epoch 1:

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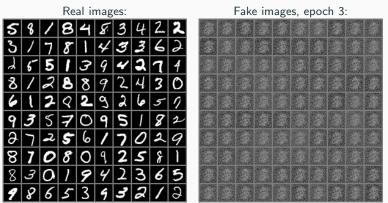
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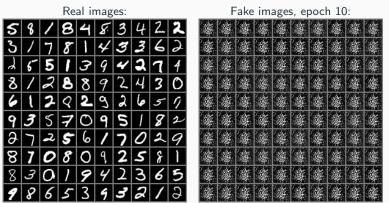
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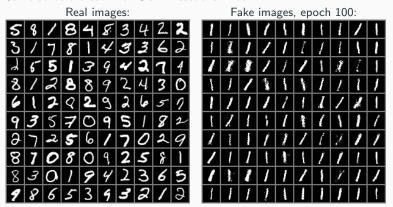
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Conditional GANs

 Conditional GANs: Train the generator and the discriminator by passing some information about the images.

Example: Class conditional generator and discriminator

• Generator: Generate a fake "3".

• Discriminator: Is it a real or a fake "3"?

Unconditional training:

$$\min_{\boldsymbol{\theta}_g} \max_{\boldsymbol{\theta}_d} \ \sum_{\boldsymbol{x} \in \mathcal{D}_{\mathsf{real}}} \log D_{\boldsymbol{\theta}_d}(\boldsymbol{x}) + \sum_{\boldsymbol{z} \in \mathcal{D}_{\mathsf{rand}}} \log (1 - D_{\boldsymbol{\theta}_d}(\underline{G_{\boldsymbol{\theta}_g}(\boldsymbol{z})})$$

Class conditional training:

$$\min_{\theta_g} \max_{\theta_d} \sum_{(\boldsymbol{x}, \boldsymbol{c}) \in \mathcal{D}_{\text{real}}} \log D_{\theta_d}(\boldsymbol{x}, \boldsymbol{c}) + \sum_{(\boldsymbol{z}, \boldsymbol{c}) \in \mathcal{D}_{\text{rand}}} \log (1 - D_{\theta_d}(\underbrace{G_{\theta_g}(\boldsymbol{z}, \boldsymbol{c})}_{\text{fake}}, \boldsymbol{c}))$$

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• Discussion: How to do this in practice?

Conditional GANs

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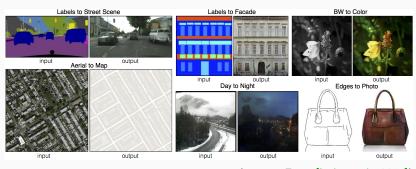
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• Discussion: How to do this in practice? Use torch.nn.Embedding.

Pix2pix: Image-to-Image Translation with Conditional Adversarial Nets [Isola et al., 2017]



- ullet Training using a set of image pairs $(oldsymbol{x}_i,oldsymbol{y}_i)$
- GAN conditioned on input image x to produce y = G(x).
- Opens the way for new creative tools

Pix2pix: Image-to-Image Translation with Conditional Adversarial Nets [Isola et al., 2017]

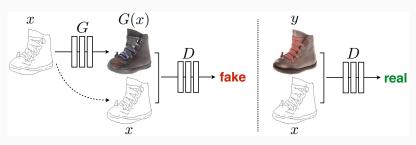
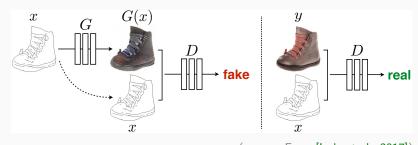
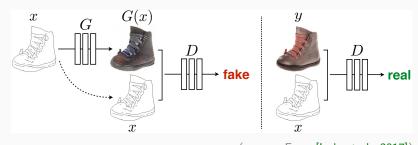


Figure 2: Training a conditional GAN to map edges \rightarrow photo. The discriminator, D, learns to classify between fake (synthesized by the generator) and real {edge, photo} tuples. The generator, G, learns to fool the discriminator. Unlike an unconditional GAN, both the generator and discriminator observe the input edge map.



Architecture details:

- Generator: **U-net architecture** (see recap later)
- Discriminator: Patch discriminator applied to each 70×70 patch, and the score is spatially average.
- Both are fully convolutional so larger images can be used at test time.

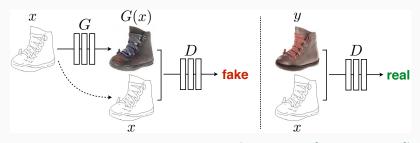


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(source: From [Isola et al., 2017])

- Generator: U-net architecture (see recap later)
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Question: What is missing here?

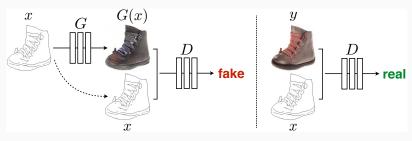


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(source: From [Isola et al., 2017])

- Generator: **U-net architecture** (see recap later)
- Discriminator: Patch discriminator applied to each 70×70 patch, and the score is spatially average.
- Both are fully convolutional so larger images can be used at test time.

Question: What is missing here? No latent code z in the generator, but randomness thanks to dropout in the network. Still stochasticity is limited given an input x.



(source: From [Isola et al., 2017])

Training loss:

• The training of generator combines a GAN loss and an ℓ_1 loss:

$$\min_{\boldsymbol{\theta}_g} \max_{\boldsymbol{\theta}_d} \sum_{(\boldsymbol{x}, \boldsymbol{y}) \in \mathcal{D}} \log D_{\boldsymbol{\theta}_d}(\boldsymbol{y}, \boldsymbol{x}) + \log(1 - D_{\boldsymbol{\theta}_d}(\underbrace{G_{\boldsymbol{\theta}_g}(\boldsymbol{x})}_{\text{fake}}, \boldsymbol{x}) + \|\underbrace{G_{\boldsymbol{\theta}_g}(\boldsymbol{x})}_{\text{fake}} - \boldsymbol{y}\|_1$$

- ullet The discriminator looks at generated patches while the ℓ_1 loss is global.
- This is a mixed loss between classical supervised training and unsupervised GAN training.



Figure 4: Different losses induce different quality of results. Each column shows results trained under a different loss. Please see https://phillipi.github.io/pix2pix/ for additional examples.

Adversarial loss for inverse problems

- With the pix2pix example we see that an adversarial loss is used to produce realistic images.
- Using only ℓ_1 or ℓ_2 loss leads to blurry results. This is known as "regression to the mean" issue.
- Adversarial losses helps to improve the visual aspect, but can also hallucinate details. Use with care in scientific context.
- Introducing generative capabilities to networks is especially important for tasks where content has to be inferred with few to no available information, such as super-resolution.

SRGAN [Ledig et al., 2017]

Adversarial loss: Same as GAN but replace the latent code by the LR image

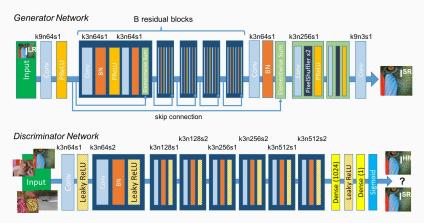
$$\begin{split} \min_{\theta_{\text{SR}}} \max_{\theta_{\text{D}}} \sum \log D_{\theta_D}(\boldsymbol{x}^{\text{HR}}) + \log(1 - D_{\theta_D}(\boldsymbol{x}^{\text{SR}})) + \lambda L_{\text{content}}(\boldsymbol{x}^{\text{SR}}, \boldsymbol{x}^{\text{HR}}) \\ \text{where} \quad \boldsymbol{x}^{\text{SR}} = G_{\theta_{\text{SR}}}(\boldsymbol{x}^{\text{LR}}) \quad \text{and} \quad \boldsymbol{x}^{\text{LR}} = \boldsymbol{H}(\boldsymbol{x}^{\text{HR}}) \end{split}$$

Content loss: Euclidean distance between the $L^{\rm th}$ feature tensors obtained with VGG for the SR and HR images, respectively:

$$L_{\mathsf{content}}(oldsymbol{x}^{\mathsf{SR}},oldsymbol{x}^{\mathsf{HR}}) = \|oldsymbol{h}^{\mathsf{SR}} - oldsymbol{h}^{\mathsf{HR}}\|_2^2 \quad \mathsf{with} \quad egin{dcases} oldsymbol{h}^{\mathsf{RR}} = \mathsf{VGG}^L(oldsymbol{x}^{\mathsf{SR}}) \ oldsymbol{h}^{\mathsf{HR}} = \mathsf{VGG}^L(oldsymbol{x}^{\mathsf{HR}}) \ oldsymbol{x}^{\mathsf{SR}} = \mathsf{G}_{ heta_{\mathsf{SR}}}(oldsymbol{x}^{\mathsf{LR}}) \end{cases}$$

- Force images to have similar high level feature tensors.
- Supposed to be closer to perceptual similarity [Johnson et al., 2016].

SRGAN [Ledig et al., 2017]

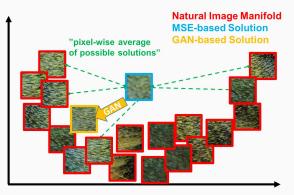


Architecture of Generator and Discriminator Network with corresponding kernel size (k), number of feature maps (n) and stride (s) indicated for each convolutional layer.

(source: From [Ledig et al., 2017])

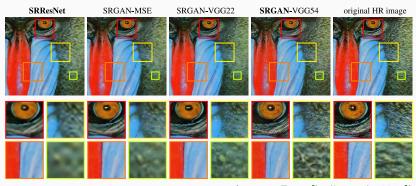
Both networks are trained by alternating their gradient based updates.

SRGAN [Ledig et al., 2017]



(source: From [Ledig et al., 2017])

- ullet The SR problem is ill-posed o infinite number of solutions,
- ullet MSE promotes a pixel-wise average of them o over-smooth,
- GAN drives reconstruction towards the "natural image manifold".



(source: From [Ledig et al., 2017])

imes4 upsampling (16imes more pixels)

• SRResNet: ResNet SR generator trained with MSE,

SRGAN-MSE: generator and discriminator with MSE content loss,

SRGAN-VGG22: generator and discriminator with VGG22 content loss,

SRGAN-VGG54: generator and discriminator with VGG54 content loss.





SRResNet





(source: From [Ledig et al., 2017])

\times 4 upsampling (16 \times more pixels)

- Even though some details are lost, they are replaced by "fake" but photo-realistic objects (instead of blurry ones).
- Remark that SRResNet is blurrier but achieves better PSNR.

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Questions?

(Most) Slides from Charles Deledalle

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