Notes

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Some notes about Machine Learning concepts.

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1 TODOs

- Transposed Convolution
- Batch-Normalization

2 Maximum Likelihood Estimation (MLE)[4] [5]

Maximum likelihood estimation is a method that determines values for the parameters of a model. The parameter values are found such that they maximise the likelihood that the process described by the model produced the data that were actually observed.

We first have to decide which model we think best describes the process of generating the data.

Then what we want to calculate is the total probability of observing all of the data, i.e. the joint probability distribution of all observed data points. To do this we would need to calculate some conditional probabilities, which can get very difficult. So it is here that we will make our first assumption. *The assumption is that each data point is generated independently of the others.* This assumption makes the maths much easier. If the events (i.e. the process that generates the data) are independent, then the total probability of observing all of data is the product of observing each data point individually (i.e. the product of the marginal probabilities).

$$f(x_1, \ldots, x_n; \theta) = \prod_{i=1}^{n} f(x_i; \theta)$$

$$L(\theta) = \prod_{i=1}^{n} f_\theta(x_i)$$

We now search for the parameters θ that maximize the Likelihood-function L, i.e. $\theta_{ML} = \arg\max_{\theta \in \Theta} L(\theta)$. We can do this by differentiation. All we have to do is find the derivative of the function.

The above expression for the total probability is actually quite a pain to differentiate, so it is almost always simplified by taking the natural logarithm of the expression. This is absolutely fine because the natural logarithm is a monotonically increasing function. This means that if the value on the x-axis increases, the value on the y-axis also increases. This is important because it ensures that the maximum value of the log of the probability occurs at the same point as the original probability function.

$$log(L(\theta)) = log(\prod_{i=1}^{n} f_\theta(x_i)) = \sum_{i=1}^{n} log(f_\theta(x_i))$$

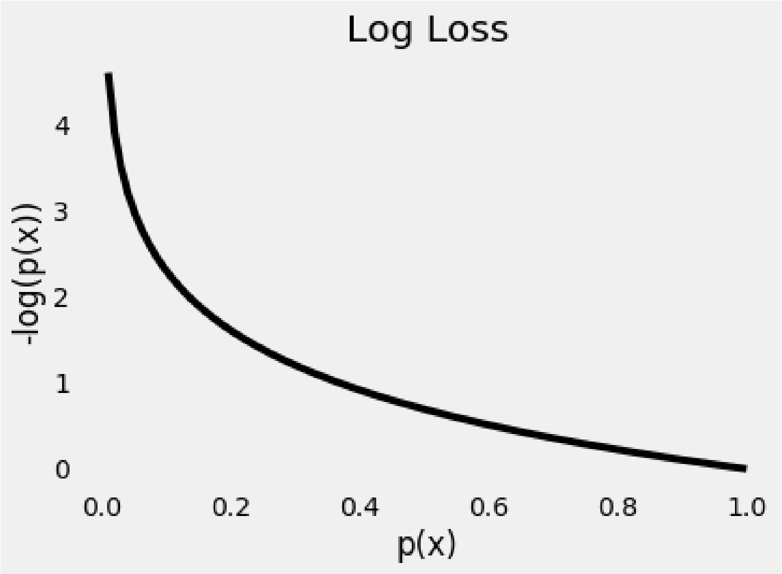


Figure 1: Negative log loss

3 Binary cross entropy [7]

$$H_p(q) = -\frac{1}{N}\sum_{i=1}^{N} y_i \cdot log(p(y_i)) + (1 - y_i) \cdot (1 - p(y_i))$$

where y_i is the true class label and $p(y_i)$ is the predicted probability of x_i coming from the positive class $y = 1$. Basically: **sum of negative logs of predicted true class probabilities** (weighted by number of samples). Look at figure 1 for negative log loss.

3.1 Diving deeper

Entropy is a measure of uncertainty associated with a given distribution $q(y)$.

$$H(q) = -\sum_{c=1}^{C} q(y_c) \cdot log(q(y_c))$$

Example with two classes (and log base 2):

- All points from one class: $H(q) = -1 \cdot log(1) = 0 \Rightarrow$ no uncertainty
- 50:50 distribution: $H(q) = -log(0.5) = 1 \Rightarrow$ maximum uncertainty

So if we know the true distribution of a random variable, we can compute its entropy. But what if we don't know the true distribution? We can try to approximate the true distribution with some other distribution, namely $p(y)$.

Cross-Entropy. Let's assume our points follow this other distribution $p(y)$. But we know they are actually coming from the true distribution $q(y)$. If we compute entropy like this, we are actually computing the cross-entropy between both distributions:

$$H_p(q) = -\sum_{c=1}^{C} q(y_c) \cdot log(p(y_c))$$

If we, somewhat miraculously match $p(y)$ to $p(y)$ perfectly, the computed values for both cross-entropy and entropy will match as well. Since this is likely never happening, cross-entropy will have a BIGGER value than the entropy computed on the true distribution.

$$H_p(q) - H(q) \geq 0$$

The difference between cross-entropy and entropy is called **Kullback-Leibler Divergence** (KL Divergence), it is a measure of dissimilarity between two distributions:

$$D_{KL}(q||p) = H_p(q) - H(q) = \sum_{c=1}^{C} q(y_c) \cdot [log(q(y_c)) - log(p(y_c))]$$

This means that, the closer $p(y)$ gets to $q(y)$, the lower the divergence and, consequently, the cross-entropy, will be. So, we need to find a good $p(y)$ to use... but, this is what our classifier should do, isn't it? And indeed it does! It looks for the best possible $p(y)$, which is the one that minimizes the cross-entropy.

For our log loss we use $q(y_c) = 1/N_c$, so the number of samples we have for class c.

4 Generative Adversarial Networks (GANs) [8]

4.1 How do generative models work? How do GANs compare to others?

To simplify the discussion somewhat, we will focus on generative models that work via the principle of maximum likelihood. Not every generative model uses maximum likelihood. Some generative models do not use maximum likelihood by default, but can be made to do so (GANs fall into this category). (Reminder MLE: $\theta^* = \arg\max_\theta \prod_{i=1}^{m} p_{model}(x^{(i)}; \theta)$).

We can think of maximum likelihood estimation as minimizing the KL divergence between the data generating distribution and the model:

$$\theta^* = \arg\min_\theta D_{KL}(p_{data}(x)||p_{model}(x; \theta)).$$

If we were able to do this preciely, then if p_{data} lies within the family of distributions $p_{model}(x; \theta)$, the model would recover p_{data} exactly. In practice, we do not have access to p_{data} itself, but only to a training set consiting of m samples from p_{data}. We use these to define $\hat{p}_{data}$, an **empirical distribution** that places mass only on exactly those m points, approximating p_{data}. Minimizing the KL divergence between $\hat{p}_{data}$ and p_{model} is exactly equivalent to maximizing the log-likelihood of the training set.

4.2 How do GANs work?

The basic idea of GANs: set up game between two players. One of them is called **generator** and creates samples that are intended to come from the same distribution as the training data. The other player is the **discriminator** who examines samples to determine whether they are real or fake.

Formally, GANs are a structured probabilistic model containing latent variables z and observed variables x.

The two players in the game are represented by two functions, each of which is differentiable both with respect to its inputs and with respect to its parameters.

- Discriminator: D takes x as input and uses $\theta^{(D)}$ as parameters
- Generator: G takes z as input and uses $\theta^{(G)}$ as parameters

Both players have cost functions that are defined in terms of both players' parameters.

- Discriminator: wishes to minimize $J^{(D)}(\theta^{(D)}, \theta^{(G)})$ while controlling only $\theta^{(D)}$
- Generator: wishes to minimize $J^{(G)}(\theta^{(D)}, \theta^{(G)})$ while controlling only $\theta^{(G)}$

Because each player's cost depends on the other player's parameters, but each player cannot control the other player's parameters, this scenario is most straightforward to describe as a game rather than as an optimization problem. The solution to an optimization problem is a (local) minimum, a point in parameter space where all neighboring points have greater or equal cost. The solution to a game is a Nash equilibrium. Here, we use the terminology of local differential Nash equilibria (Ratliff et al., 2013). In this context, a Nash equilibrium is a tuple $(\theta^{(D)}, \theta^{(G)})$ that is a local minimum of $J^{(D)}$ w.r.t $\theta^{(D)}$ and a local minimum of $J^{(G)}$ w.r.t $\theta^{(G)}$.

The training process. The training process consists of simultaneous SGD. On each step, two minibatches are sampled: a minibatch of x values from the dataset and a minibatch of z values drawn from the model's prior over latent variables. Then two gradient steps are made simultaneously: one updating $\theta^{(D)}$ to reduce $J^{(D)}$ and one updating $\theta^{(G)}$ to reduce $J^{(G)}$. In both cases, it is possible to use the gradient-based optimization algorithm of your choice. Adam (Kingma and Ba, 2014) is usually a good choice.

4.3 Cost functions

Several different cost functions may be used within the GANs framework.

4.3.1 The discriminators cost, $J^{(D)}$

The cost used for the discriminator is:

$$J^{(D)}(\theta^{(D)}, \theta^{(G)}) = -\frac{1}{2}\mathbb{E}_{x\sim p_{data}} logD(x) - \frac{1}{2}\mathbb{E}_z log(1 - D(G(z))).$$

This is just the standard cross-entropy cost that is minimized when training a standard binary classifier with a sigmoid output. The only difference is that the classifier is trained on two minibatches of data; one coming from the dataset, where the label is 1 for all examples, and one coming from the generator, where the label is 0 for all examples. ($Reminder:\ Entropy = H(q) = -\sum_{c=1}^{C} q(y_c) \cdot log(q(y_c)) = \mathbb{E}_{q\sim P} log(P(q))$ [1].

All versions of the GAN game encourage the discriminator to minimize this equation. In all cases, the discriminator has the same optimal strategy.

We see that by training the discriminator, we are able to obtain an estimate of the ratio $\frac{p_{data}(x)}{p_{model}(x)}$. Estimating this ratio enables us to compute a wide variety of divergences and their gradients. This is the key approximation technique that sets GANs apart from VACs and Boltzmann machines.

4.3.2 Minimax

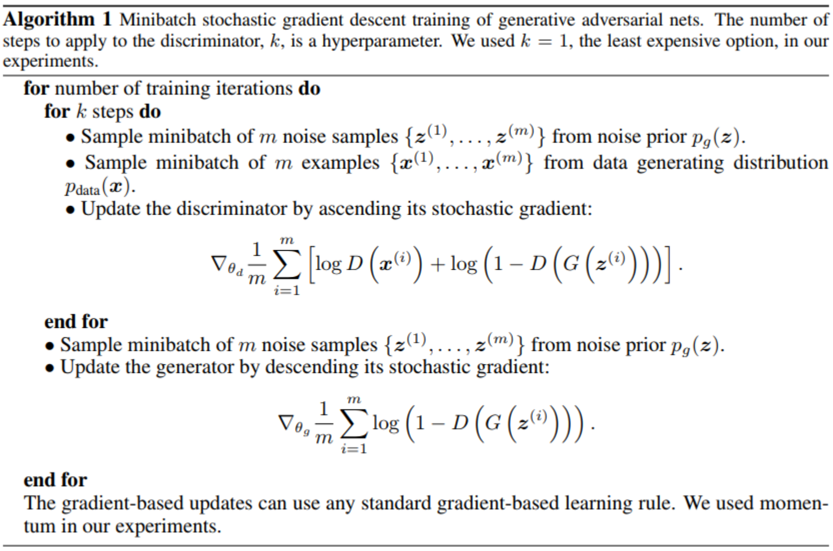
A complete specification of the game requires that we specify a cost function also for the generator. From a game theoretic perspective D and G play the following two-player minimax game with value function $V(G, D)$:

$$min_G max_D V(D, G) = E_{x\sim p_{data}}(x)[logD(x)] + E_{z\sim p_z(z)}[log(1 - D(G(z)))].$$

The discriminator tries to maximize the objective function, therefore we can perform gradient ascent on the objective function. The generator tries to minimize the objective function, therefore we can perform gradient descent on the objective function. Look at figure 2 for the algorithm.

When applied, it is observed that optimizing the generator objective function does not work so well, this is because when the sample is generated it is likely to be classified as fake, the model would like to learn from the gradients but the gradients turn out to be relatively flat. This makes it difficult for the model to learn. Therefore, the generator objective function is changed to: $max_G \mathbb{E}_{z\sim p(z)} log(D(G(z)))$

Instead of minimizing the likelihood of the discriminator being correct, we maximize the likelihood of the discriminator being wrong. Therefore, we perform gradient ascent on the generator according to this objective function [2].



Algorithm 1 Minibatch stochastic gradient descent training of generative adversarial nets. The number of steps to apply to the discriminator, k, is a hyperparameter. We used $k = 1$, the least expensive option, in our experiments.

```
for number of training iterations do
  for $k$ steps do
    • Sample minibatch of $m$ noise samples $\{z^{(1)}, \dots, z^{(m)}\}$ from noise prior $p_g(z)$.
    • Sample minibatch of $m$ examples $\{x^{(1)}, \dots, x^{(m)}\}$ from data generating distribution $p_{\text{data}}(x)$.
    • Update the discriminator by ascending its stochastic gradient:
        $\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^{m} \left[ \log D\left(x^{(i)}\right) + \log\left(1 - D\left(G\left(z^{(i)}\right)\right)\right) \right].$
  end for
  • Sample minibatch of $m$ noise samples $\{z^{(1)}, \dots, z^{(m)}\}$ from noise prior $p_g(z)$.
  • Update the generator by descending its stochastic gradient:
      $\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log\left(1 - D\left(G\left(z^{(i)}\right)\right)\right).$
end for
The gradient-based updates can use any standard gradient-based learning rule. We used momentum in our experiments.
```

Figure 2: Minimax algorithm for GANs [9]

5 Deep Convolutional Generative Adversarial Networks (DCGAN)

DCGANs are a family of architectures that resulted in stable training across a range of datasets and allowed for training higher resolution and deeper generative models.

Architecture guidelines for stable Deep Convolutional GANs:

- Replace any pooling layers with strided convolutions (discriminator) and fractional-strided convolutions (generator).
- Use batchnorm in both the generator and the discriminator. No batchnorm at generator output and discriminator input layer.
- Remove fully connected hidden layers for deeper architectures.
- Use ReLU activation in generator for all layers except for the output, which uses Tanh.
- Use LeakyReLU activation in the discriminator for all layers.
- Use Sigmoid at discriminator output, Tanh at generator.

More details:

- Mini-batch SGD with mini-batch size of 128
- Weight-initialization from zero-centered normal distribution with standard deviation of 0.02

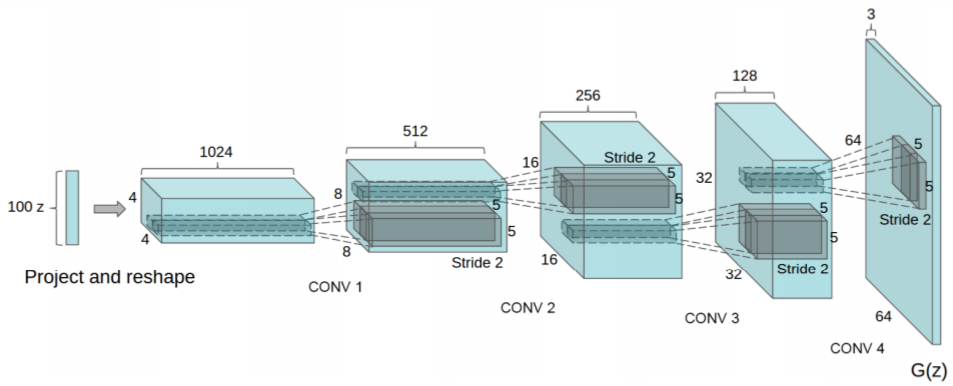


Figure 1: DCGAN generator used for LSUN scene modeling. A 100 dimensional uniform distribution Z is projected to a small spatial extent convolutional representation with many feature maps. A series of four fractionally-strided convolutions (in some recent papers, these are wrongly called deconvolutions) then convert this high level representation into a 64×64 pixel image. Notably, no fully connected or pooling layers are used.

- Leaky-ReLU slope of 0.2
- Adam optimizer, learning rate of 0.0002, leaving momentum of 0.5

6 Important formulas

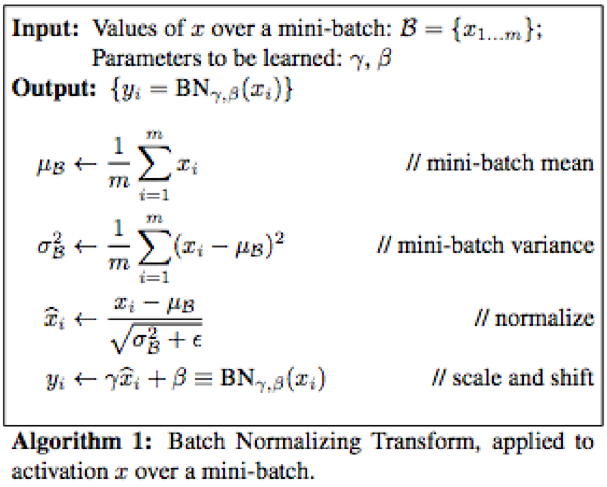
6.1 Convolution

O : output size, W : input size, F : filter kernel size, P : padding, S : stride

- Convolution: $O = \frac{W-F+2P}{S} + 1$
- Transposed Convolution: $O = S(W-1) + F - 2P$

7 Batch Normalization

The idea of batch normalization is to normalize the outputs of each layer, as you normally do it with the input to the neural network (i.e. normalize image pixel values to [0..1]). In a first step the mean and variance of the mini-batch get calculated and the values get normalized to have zero mean and standard deviation one (in most cases this happens before they get passed on to the activation function). Because such a normalization isn't always desired (imagine you have a sigmoid activation function, nearly all activations wouldn't even reach 0 or 1) two learnable parameters γ and β get introduced that modify the mean and variance.



```
Input: Values of $x$ over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$;
       Parameters to be learned: $\gamma$, $\beta$
Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

  $\mu_\mathcal{B} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i$                                  // mini-batch mean
  $\sigma_\mathcal{B}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_\mathcal{B})^2$             // mini-batch variance
  $\widehat{x}_i \leftarrow \frac{x_i - \mu_\mathcal{B}}{\sqrt{\sigma_\mathcal{B}^2 + \epsilon}}$                        // normalize
  $y_i \leftarrow \gamma\widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i)$                  // scale and shift
```

Algorithm 1: Batch Normalizing Transform, applied to activation x over a mini-batch.

Figure 3:

7.1 Why does batch normalization work?

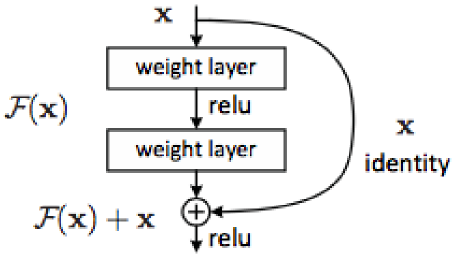
In the case that the input distribution of a learning system, such as a neural network, changes, one speaks of a so-called covariate shift. If this change happens on the input of internal nodes of (deep) neural networks, it is called an internal covariate shift.

Imagine a multilayer fully-connected neural network that is trying to learn. At each training step each layer tries to improve the networks performance by updating its weights based on the activations fed into that layer. The problem is that (especially for layers deep down in the network) weight changes in previous layers drastically change the data distribution this layer observes at each step (this is the aforementioned internal covariance shift). This slows down training and reduces the overall performance. Batch normalization reduces this effect to some extent by ensuring that the data distributions variance and mean remain stable.

Additionally the mean and variance are only computed on each mini-batch instead of the whole training set. This adds some noise to the layer activations and acts as a gentle regularization.

8 Residual Blocks [6]

The authors of ResNet observed, no matter how deep a network is, it should not be any worse than the shallower network. That's because if we argue that neural net could approximate any complicated function, then it could also learn identity function, i.e. input = output, effectively skipping the learning progress on some layers. But, in real world, this is not the case because of the vanishing gradient and curse of dimensionality problems.


x
weight layer
relu
$\mathcal{F}(\mathbf{x})$
weight layer
x
identity
$\mathcal{F}(\mathbf{x}) + \mathbf{x}$
relu

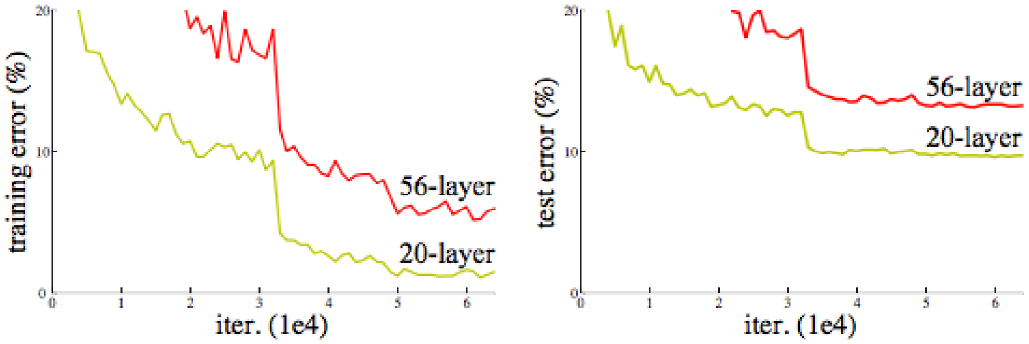


Figure 1. Training error (left) and test error (right) on CIFAR-10 with 20-layer and 56-layer "plain" networks. The deeper network has higher training error, and thus test error. Similar phenomena on ImageNet is presented in Fig. 4.

Hence, it might be useful to explicitly force the network to learn an identity mapping, by learning the residual of input and output of some layers (or subnetworks). Suppose the input of the subnetwork is x, and the true output is $H(x)$. The residual is the difference between them: $F(x) = H(x) - x$. As we are interested in finding the true, underlying output of the subnetwork, we then rearrange that equation into $H(x) = F(x) + x$

So that's the difference between ResNet and traditional neural nets. Where traditional neural nets will learn $H(x)$ directly, ResNet instead models the layers to learn the residual of input and output of subnetworks. This will give the network an option to just skip subnetworks by making $F(x) = 0$, so that $H(x) = x$. In other words, the output of a particular subnetwork is just the output of the last subnetwork.

During backpropagation, learning residual gives us nice property. Because of the formulation, the network could choose to ignore the gradient of some subnetworks, and just forward the gradient from higher layers to lower layers without any modification. As an extreme example, this means that ResNet could just forward gradient from the last layer, e.g. layer 151, directly to the first layer. This gives ResNet additional nice to have option which might be useful, rather than just strictly doing computation in all layers.

Reflection Padding [3]

Padded pixels are computed by reflecting the input image pixels about the border:

SR	QRSTUVWX	WV
KJ	IJKLMNOP	ON
CB	ABCDEFGH	GF
KJ	IJKLMNOP	ON
SR	QRSTUVWX	WV
aZ	YZabcdef	ed
ih	ghijklmn	ml
qp	opqrstuv	ut
ih	ghijklmn	ml
aZ	YZabcdef	ed

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