DeepLearning

AIC 和 BIC 准则

Notes

模型选择问题在 **模型复杂度** 与 **模型对数据集描述能力** 之间寻求最佳平衡；

AIC 准则

赤池信息准则（Akaike Information Criterion，AIC），AIC 定义为：

$$AIC = 2k - 2ln(L)$$

其中 k 为参数个数，L 为似然函数。从一组可供选择的模型中选择最佳模型时，**通常选择 AIC 最小的模型**：

- 当两个模型之间存在较大差异时，差异主要体现在似然函数项，当似然函数差异不显著时，上式第一项，即模型复杂度则起作用，从而**参数个数少**的模型是较好的选择；
- 一般而言，当模型复杂度提高（k 增大）时，似然函数 L 也会增大，从而使 AIC 变小，但是 k 过大时，似然函数增速减缓，导致 AIC 增大，模型过于复杂容易造成过拟合现象；
- 目标是选取AIC最小的模型，AIC不仅要提高模型拟合度（极大似然），而且引入了惩罚项，使模型参数尽可能少，有助于降低过拟合的可能性；

BIC 准则

贝叶斯信息准则（Bayesian Information Criterion，BIC），BIC 定义为：

$$BIC = kln(n) - 2ln(L)$$

其中，k 为模型参数个数，n 为样本数量，L 为似然函数。从一组可供选择的模型中选择最佳模型时，**通常选择 BIC 最小的模型**；

比较

AIC 和BIC 的公式中后半部分是一样的；当 $n \geq 10^2$ 时，$kln(n) \geq 2k$，所以，BIC 相比AIC 在**大数据量时对模型参数惩罚得更多**，导致 BIC 更倾向于选择参数少的简单模型。所以还是**考虑使用 BIC 准则**；

Links

- 参考链接：AIC和BIC准则详解

交叉熵、相对熵、JS 散度

熵

熵（信息熵）指的是信息量的期望；

$$H(X) = -\sum_{i=1}^{n} p(x_i)\log(p(x_i))$$

相对熵（KL 散度）

相对熵（KL 散度）用来衡量两个分布的差异；

$$D_{KL}(p||q) = \sum_{i=1}^{n} p(x_i)\ log\left(\frac{p(x_i)}{q(x_i)}\right)$$

相对熵是非对称的，使用时 $p(x)$ 用来表示样本的真实分布，而 $q(x)$ 用来表示模型所预测的分布；

交叉熵

交叉熵可以通过相对熵变化而来，在机器学习中通常直接用交叉熵作为损失函数；

$$H(p,q)=-\sum_{i=1}^{n}p(x_i)\log(q(x_i))$$

JS 散度

JS 散度用来衡量两个分布的相似度，是基于相对熵的变体，解决了相对熵的非对称问题；

$$JS(P_1||P_2)=\frac{1}{2}KL(P_1||\frac{P_1+P_2}{2})+\frac{1}{2}KL(P_2||\frac{P_1+P_2}{2})$$

Wasserstein 距离

Wasserstein 距离用来度量两个概率分布之间的距离，解决了当两个分布 P, Q 相差很远时，KL 散度和 JS 散度梯度消失的问题；

$$W(P_1,P_2)=\inf_{\gamma\sim\Pi(P_1,P_2)}\mathbb{E}_{(x,y)\sim\gamma}[||x-y||]$$

Optimizer in Deep Learning

梯度下降法（Gradient Descent）

梯度下降法的计算过程就是沿梯度下降的方向求解极小值，也可以沿梯度上升方向求解最大值。使用梯度下降法更新参数：

$$\theta_{t+1}=\theta_t-\alpha\cdot\nabla_\theta J(\theta)$$

批量梯度下降法（BGD）

在整个训练集上计算梯度，对参数进行更新：

$$\theta_{t+1}=\theta_t-\alpha\cdot\frac{1}{n}\cdot\sum_{i=1}^{n}\nabla_\theta J_i(\theta,x^i,y^i)$$

因为要计算整个数据集，收敛速度慢，但其优点在于更趋近于全局最优解；

随机梯度下降法（SGD）

每次只随机选择一个样本计算梯度，对参数进行更新：

$$\theta_{t+1}=\theta_t-\alpha\cdot\nabla_\theta J_i(\theta,x^i,y^i)$$

训练速度快，但是容易陷入局部最优点，导致梯度下降的波动非常大；

小批量梯度下降法（Mini-batch Gradient Descent）

每次随机选择 n 个样本计算梯度，对参数进行更新：

$$\theta_{t+1}=\theta_t-\alpha\cdot\frac{1}{m}\cdot\sum_{i=x}^{i=x+m-1}\cdot\nabla_\theta J_i(\theta,x^i,y^i)$$

这种方法是 BGD 和 SGD 的折衷；

动量优化法

Momentum

参数更新时在一定程度上保留之前更新的方向，同时又利用当前 batch 的梯度微调最终的更新方向。在 SGD 的基础上增加动量，则参数更新公式如下：

$$
\begin{aligned}
m_{t+1} &= \mu \cdot m_t + \alpha \cdot \nabla_\theta J(\theta) \\
\theta_{t+1} &= \theta_t - m_{t+1}
\end{aligned}
$$

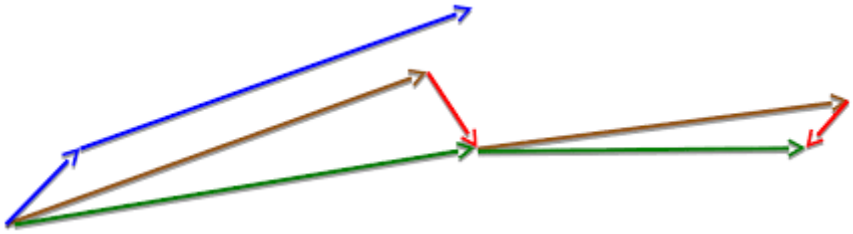
在梯度方向发生改变时，Momentum 能够降低参数更新速度，从而减少震荡；在梯度方向相同时，Momentum 可以加速参数更新，从而加速收敛。

NAG（Nesterov Accelerated Gradient）

与 Momentum 不同的是，NAG 是在更新梯度是做一个矫正，即提前往前探一步，并对梯度作修改。参数更新公式如下：

$$
\begin{aligned}
m_{t+1} &= \mu \cdot m_t + \alpha \cdot \nabla_\theta J(\theta - \mu \cdot m_t) \\
\theta_{t+1} &= \theta_t - m_{t+1}
\end{aligned}
$$

两者的对比：蓝色为 Momentum， 剩下的是 NAG；



自适应学习率

AdaGrad

AdaGrad 算法期望在模型训练时有一个较大的学习率，而随着训练的不断增多，学习率也跟着下降。参数更新公式如下：

$$
\begin{aligned}
g &\leftarrow \nabla_\theta J(\theta) \\
r &\leftarrow r + g^2 \\
\Delta\theta &\leftarrow \frac{\delta}{\sqrt{r+\epsilon}} \cdot g \\
\theta &\leftarrow \theta - \Delta\theta
\end{aligned}
$$

学习率随着 **梯度的平方和**（r）的增加而减少. 缺点：

- 需要手动设置学习率 δ ，如果 δ 过大，会使得正则化项 $\frac{\delta}{\sqrt{r+\epsilon}}$ 对梯度的调节过大；
- 中后期，参数的更新量会趋近于 0，使得模型无法学习；

Adadelta

Adadelta 算法将 梯度的平方和 改为 **梯度平方的加权平均值**。参数更新公式如下：

$$
\begin{aligned}
g_t &\leftarrow \nabla_\theta J(\theta) \\
E[g^2]_t &\leftarrow \gamma \cdot E[g^2]_{t-1} + (1-\gamma) \cdot g_t^2 \\
\Delta\theta_t &\leftarrow -\frac{\eta}{\sqrt{E[g^2]_t + \epsilon}} \cdot g_t \\
\theta_{t+1} &\leftarrow \theta_t + \Delta\theta_t
\end{aligned}
$$

上式中仍存在一个需要自己设置的全局学习率 η，可以通过下式**消除全局学习率的影响**：

$$
\begin{aligned}
E[\Delta\theta^2]_t &\leftarrow \gamma \cdot E[\Delta\theta^2]_{t-1} + (1-\gamma) \cdot \Delta\theta_t^2 \\
\Delta\theta_t &\leftarrow -\frac{\sqrt{E[\Delta\theta^2]_{t-1} + \epsilon}}{\sqrt{E[g^2]_t + \epsilon}} \cdot g_t \\
\theta_{t+1} &\leftarrow \theta_t + \Delta\theta_t
\end{aligned}
$$

RMSProp

RMSProp 算法是 AdaGrad 算法的改进，修改 梯度平方和 为 **梯度平方的指数加权移动平均**，解决了学习率急剧下降的问题。参数更新公式如下：

$$
\begin{aligned}
g_t &\leftarrow \nabla_\theta J(\theta) \\
E[g^2]_t &\leftarrow \rho \cdot E[g^2]_{t-1} + (1-\rho) \cdot g_t^2 \\
\Delta\theta &\leftarrow \frac{\delta}{\sqrt{E[g^2]_t + \epsilon}} \cdot g \\
\theta &\leftarrow \theta - \Delta\theta
\end{aligned}
$$

Adam（Adaptive Moment Estimation）

Adam 算法在动量的基础上，结合了偏置修正。参数更新公式如下：

$$
\begin{aligned}
g_t &\leftarrow \Delta_\theta J(\theta) \\
m_t &\leftarrow \beta_1 \cdot m_{t-1} + (1-\beta_1) \cdot g_t \\
v_t &\leftarrow \beta_2 \cdot v_{t-1} + (1-\beta_2) \cdot g_t^2 \\
\hat{m}_t &\leftarrow \frac{m_t}{1-(\beta_1)^t} \\
\hat{v}_t &\leftarrow \frac{v_t}{1-(\beta_2)^t} \\
\theta_{t+1} &= \theta_t - \frac{\delta}{\sqrt{\hat{v}_t} + \epsilon} \cdot \hat{m}_t
\end{aligned}
$$

论文伪代码：

Algorithm 1: *Adam*, our proposed algorithm for stochastic optimization. See section 2 for details, and for a slightly more efficient (but less clear) order of computation. g_t^2 indicates the elementwise square $g_t \odot g_t$. Good default settings for the tested machine learning problems are $\alpha = 0.001$, $\beta_1 = 0.9$, $\beta_2 = 0.999$ and $\epsilon = 10^{-8}$. All operations on vectors are element-wise. With β_1^t and β_2^t we denote β_1 and β_2 to the power t.

Require: α: Stepsize
Require: $\beta_1, \beta_2 \in [0, 1)$: Exponential decay rates for the moment estimates
Require: $f(\theta)$: Stochastic objective function with parameters θ
Require: θ_0: Initial parameter vector
$m_0 \leftarrow 0$ (Initialize 1st moment vector)
$v_0 \leftarrow 0$ (Initialize 2nd moment vector)
$t \leftarrow 0$ (Initialize timestep)
while θ_t not converged **do**
$t \leftarrow t + 1$
$g_t \leftarrow \nabla_\theta f_t(\theta_{t-1})$ (Get gradients w.r.t. stochastic objective at timestep t)
$m_t \leftarrow \beta_1 \cdot m_{t-1} + (1 - \beta_1) \cdot g_t$ (Update biased first moment estimate)
$v_t \leftarrow \beta_2 \cdot v_{t-1} + (1 - \beta_2) \cdot g_t^2$ (Update biased second raw moment estimate)
$\widehat{m}_t \leftarrow m_t / (1 - \beta_1^t)$ (Compute bias-corrected first moment estimate)
$\widehat{v}_t \leftarrow v_t / (1 - \beta_2^t)$ (Compute bias-corrected second raw moment estimate)
$\theta_t \leftarrow \theta_{t-1} - \alpha \cdot \widehat{m}_t / (\sqrt{\widehat{v}_t} + \epsilon)$ (Update parameters)
end while
return θ_t (Resulting parameters)

Links

- 参考链接：优化算法 Optimizer 比较和总结
- Adam 论文链接：Kingma D P, Ba J. Adam: A method for stochastic optimization[J]. arXiv preprint arXiv:1412.6980, 2014.

神经网络中的 Normalization 的发展历程

> 参考链接：[笔记] 神经网络中 Normalization 的发展历程

Local Response Normalization

(1) 重要思想：借鉴“侧抑制”（Lateral Inhibitio）的思想实现**局部神经元抑制**，即使得局部的神经元产生竞争机制，使其中响应值大的变得更大，响应值小的变得更小（这一点我从数值上并没有看不出来）；在运用 Local Response Normalization 过程中，我觉得需要注意的是它是对 **FeatureMap** 的一个正则化操作

(2) 公式：

$$b_{x,y}^i = a_{x,y}^i \Big/ \left(k + \alpha \sum_{j=\max(0,i-n/2)}^{\min(N-1,i+n/2)} (a_{x,y}^j)^2 \right)^\beta$$

其中，i, j 表示 FeatureMap 的索引，$a_{(x,y)}^j$ 表示第 j 个 FeatureMap 中位于 (x, y) 处的响应值；常用的值为：$k = 2, n = 5, \alpha = 10^{-4}, \beta = 0.75$ 。

(3) 2015 年的 VGG 中发现 Local Response Normalization 的方法并没有什么作用，故后来很少再被采用；

(4) 参考链接：

- 深度学习饱受争议的局部响应归一化(LRN)详解

Batch Normalization

(1) 主要思想：使用 Batch Normalization 层能够**使网络的训练更加稳定**，**加速神经网络的收敛速度**（当网络训练的收敛速度慢时可以考虑使用 BN 层），使得神经网络**对于初始化的敏感度下降**，并且**具有一定的正则化效果**；知乎大佬说 BN 层的优势是可以**防止"梯度弥散"**（我感觉不出来）；

(2) 公式：

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

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

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

其中，γ 和 β 两个仿射参数，是为了经过 BN 层处理后的数据仍**可以**恢复到之前的分布，从而**提升了网络结构的 Capacity**，即在做出一定改变的同时，仍保留之前的能力。注意，**上面用的是 "可以" 这个词汇，具体"是不是"**，还是要看模型训练的结果，训练的过程即**正常的求导梯度下降法**，公式如下：

$$\frac{\partial \ell}{\partial \widehat{x}_i} = \frac{\partial \ell}{\partial y_i} \cdot \gamma$$

$$\frac{\partial \ell}{\partial \sigma_{\mathcal{B}}^2} = \sum_{i=1}^{m} \frac{\partial \ell}{\partial \widehat{x}_i} \cdot (x_i - \mu_{\mathcal{B}}) \cdot \frac{-1}{2}(\sigma_{\mathcal{B}}^2 + \epsilon)^{-3/2}$$

$$\frac{\partial \ell}{\partial \mu_{\mathcal{B}}} = \sum_{i=1}^{m} \frac{\partial \ell}{\partial \widehat{x}_i} \cdot \frac{-1}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}}$$

$$\frac{\partial \ell}{\partial x_i} = \frac{\partial \ell}{\partial \widehat{x}_i} \cdot \frac{1}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} + \frac{\partial \ell}{\partial \sigma_{\mathcal{B}}^2} \cdot \frac{2(x_i - \mu_{\mathcal{B}})}{m} + \frac{\partial \ell}{\partial \mu_{\mathcal{B}}} \cdot \frac{1}{m}$$

$$\frac{\partial \ell}{\partial \gamma} = \sum_{i=1}^{m} \frac{\partial \ell}{\partial y_i} \cdot \widehat{x}_i$$

$$\frac{\partial \ell}{\partial \beta} = \sum_{i=1}^{m} \frac{\partial \ell}{\partial y_i}$$

(3) 代码实现：

- 使用注意点：
    - `batch_size` 应该尽可能设置得大一些；
    - 建议将bn层放在卷积层和激活层（例如 `Relu`）之间，且卷积层不要使用偏置 bias；
- PyTorch：

BATCHNORM2D

CLASS `torch.nn.BatchNorm2d(num_features, eps=1e-05, momentum=0.1, affine=True, track_running_stats=True)` [SOURCE]

Applies Batch Normalization over a 4D input (a mini-batch of 2D inputs with additional channel dimension) as described in the paper Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift .

$$y = \frac{x - \mathrm{E}[x]}{\sqrt{\mathrm{Var}[x] + \epsilon}} * \gamma + \beta$$

The mean and standard-deviation are calculated per-dimension over the mini-batches and γ and β are learnable parameter vectors of size C (where C is the input size). By default, the elements of γ are set to 1 and the elements of β are set to 0. The standard-deviation is calculated via the biased estimator, equivalent to *torch.var(input, unbiased=False)*.

Also by default, during training this layer keeps running estimates of its computed mean and variance, which are then used for normalization during evaluation. The running estimates are kept with a default `momentum` of 0.1.

If `track_running_stats` is set to `False`, this layer then does not keep running estimates, and batch statistics are instead used during evaluation time as well.

NOTE

This `momentum` argument is different from one used in optimizer classes and the conventional notion of momentum. Mathematically, the update rule for running statistics here is $\hat{x}_{\text{new}} = (1 - \text{momentum}) \times \hat{x} + \text{momentum} \times x_t$, where $\hat{x}$ is the estimated statistic and x_t is the new observed value.

    - 可以设置 `affine=False`，则不再设置后面的仿射参数；
    - 当设置（默认值） `track_running_state=True` 时，模型会使用动量法更新**两个全局的动态统计量** `running_mean` 和 `running_var` 来归一定输入的 `mini_batch`；如何设置 `track_running_state=False` 时，则模型直接使用 `mini_batch` 作为统计量；（所以在测试的时候，最好就是将这个设置为 `False`）
    - 在模型预测阶段，我们需要设置 BN 层 `training=False`，即直接使用 `model.eval()`；
- Tensorflow：（这里以 Tensorflow 2 为主，具体分析的话，可以发现它和 Tensorflow 1 的很多形为存在不同之处）

tf.keras.layers.BatchNormalization

See Stable | See Nightly

TensorFlow 1 version | View source on GitHub

Layer that normalizes its inputs.

Inherits From: `Layer`, `Module`

```
tf.keras.layers.BatchNormalization(
    axis=-1, momentum=0.99, epsilon=0.001, center=True, scale=True,
    beta_initializer='zeros', gamma_initializer='ones',
    moving_mean_initializer='zeros',
    moving_variance_initializer='ones', beta_regularizer=None,
    gamma_regularizer=None, beta_constraint=None, gamma_constraint=None,
    renorm=False, renorm_clipping=None, renorm_momentum=0.99, fused=None,
    trainable=True, virtual_batch_size=None, adjustment=None, name=None, **kwargs
)
```

Batch normalization applies a transformation that maintains the mean output close to 0 and the output standard deviation close to 1.

Importantly, batch normalization works differently during training and during inference.

During training (i.e. when using `fit()` or when calling the layer/model with the argument `training=True`), the layer normalizes its output using the mean and standard deviation of the current batch of inputs. That is to say, for each channel being normalized, the layer returns `(batch - mean(batch)) / (var(batch) + epsilon) * gamma + beta`, where:

- `epsilon` is small constant (configurable as part of the constructor arguments)
- `gamma` is a learned scaling factor (initialized as 1), which can be disabled by passing `scale=False` to the constructor.
- `beta` is a learned offset factor (initialized as 0), which can be disabled by passing `center=False` to the constructor.

During inference (i.e. when using `evaluate()` or `predict()` or when calling the layer/model with the argument `training=False` (which is the default), the layer normalizes its output using a moving average of the mean and standard deviation of the batches it has seen during training. That is to say, it returns `(batch - self.moving_mean) / (self.moving_var + epsilon) * gamma + beta`.

`self.moving_mean` and `self.moving_var` are non-trainable variables that are updated each time the layer in called in training mode, as such:

- `moving_mean = moving_mean * momentum + mean(batch) * (1 - momentum)`
- `moving_var = moving_var * momentum + var(batch) * (1 - momentum)`

  - 可以看到，Tensorflow 在设计上和 pytorch 有所不同，tensorflow 直接将 BN 层设计成了 `traning` 模式 和 `inference` 模式；在 `traning` 模式下，模型会不断更新 `moving_mean` 和 `moving_var` 这两个变量，`mini_batch` 的统计量直接由输入得到；而在 `inference` 模式下，模型则固定 `moving_mean` 和 `moving_var` 两个变量作为 `mini_batch` 的统计量（这可能就是基于了同分布的假设）；至于这个模式的变换，通过在调用 BN 层时设置一个 `trainig` 参数实现，下面具体看一下他的文档

Call arguments:

- `inputs`: Input tensor (of any rank).
- `training`: Python boolean indicating whether the layer should behave in training mode or in inference mode.
  - `training=True`: The layer will normalize its inputs using the mean and variance of the current batch of inputs.
  - `training=False`: The layer will normalize its inputs using the mean and variance of its moving statistics, learned during training.

Input shape: Arbitrary. Use the keyword argument `input_shape` (tuple of integers, does not include the samples axis) when using this layer as the first layer in a model.

Output shape: Same shape as input.
About setting `layer.trainable = False` on a `BatchNormalization` layer:

The meaning of setting `layer.trainable = False` is to freeze the layer, i.e. its internal state will not change during training: its trainable weights will not be updated during `fit()` or `train_on_batch()`, and its state updates will not be run.

Usually, this does not necessarily mean that the layer is run in inference mode (which is normally controlled by the `training` argument that can be passed when calling a layer). "Frozen state" and "inference mode" are two separate concepts.

> Usually, this does not necessarily mean that the layer is run in inference mode (which is normally controlled by the `training` argument that can be passed when calling a layer). "Frozen state" and "inference mode" are two separate concepts.
>
> However, in the case of the `BatchNormalization` layer, **setting `trainable = False` on the layer means that the layer will be subsequently run in inference mode** (meaning that it will use the moving mean and the moving variance to normalize the current batch, rather than using the mean and variance of the current batch).
>
> This behavior has been introduced in TensorFlow 2.0, in order to enable `layer.trainable = False` to produce the most commonly expected behavior in the convnet fine-tuning use case.
>
> Note that:
>
> - This behavior only occurs as of TensorFlow 2.0. In 1.*, setting `layer.trainable = False` would freeze the layer but would not switch it to inference mode.
> - Setting `trainable` on an model containing other layers will recursively set the `trainable` value of all inner layers.
> - If the value of the `trainable` attribute is changed after calling `compile()` on a model, the new value doesn't take effect for this model until `compile()` is called again.

  - BN 层含有两个比较关键的参数，`trainable` 用来表示 BN 层是否可训练，控制的是上面的仿射参数的状态；`training` 参数则用来控制 `inference` 状态；另外，当设置 `trainable=False` 时，tensorflow 2 中的 BN 层将自动进入 `inference` 状态（这个和 tensorflow 1 不同）；
  - 在 `model.compile()` 之后修改 BN 层的 `trainable` 属性，需要重新调用 `model.compile()` 才会起作用；

(4) 参考链接：

- 深度学习中 Batch Normalization为什么效果好？
- Batch Normalization详解以及pytorch实验

Weight Normalization

(1) 主要思想：相比于 BN 层，WN 层并不是对输入的特征数据进行归一化操作，而是**对神经网络中指定的层的参数做归一化操作**；WN 层摆脱了对于 Batch 的依赖，这意味着 WN 层完全可以用在 RNN 网络中，以及对于噪声敏感的任务；WN 层的计算成本低，可以**减少模型的运行时间**；

(2) 公式：将参数 w 拆分成方向和长度两个部分

$$y = \Phi(w * x + b) \Rightarrow y = \Phi(g * \frac{v}{||v||} * x + b)$$

我们把公式转换一下，就可以发现 **BN 层其实等同于使用参数的统计值对数据进行归一化**，

$$\Rightarrow y = \Phi(gv * \frac{v}{||v||} + b)$$

参数的学习，直接通过梯度下降的方法即可

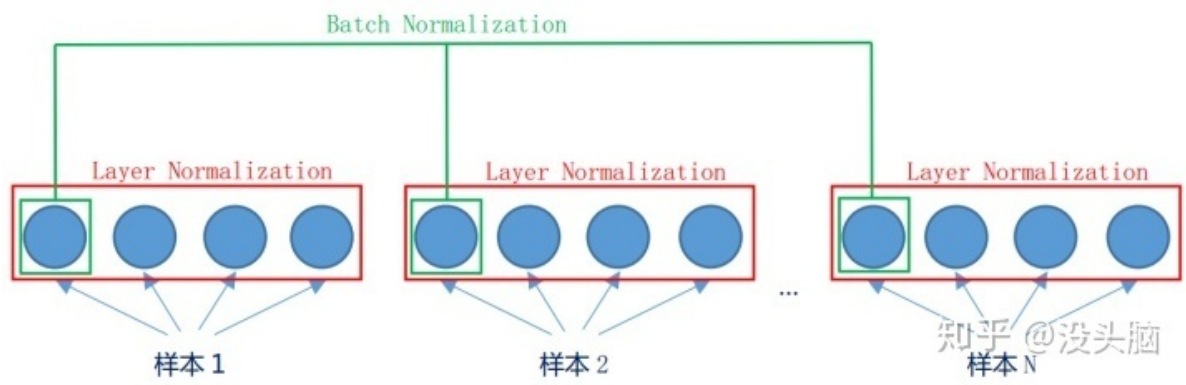
$$\nabla_g L = \frac{\nabla_{\mathbf{w}} L \cdot \mathbf{v}}{||\mathbf{v}||} \qquad \nabla_{\mathbf{v}} L = \frac{g}{||\mathbf{v}||} \nabla_{\mathbf{w}} L - \frac{g \nabla_g L}{||\mathbf{v}||^2} \mathbf{v}$$

(3) 参考链接：

- 模型优化之Weight Normalization
- 详解深度学习中的Normalization，BN/LN/WN

Layer Normalization

(1) 主要思想：LN 层和 BN 层非常相似，不同之处在于，BN 层是对一个 Batch 中的**所有样本的不同维度**做 Normalization，而 LN 是对**单个样本的所有维度**做 Normalization；LN 层是为了解决 BN 层**对 `batch` 数据和内存的依赖**，并**减少 normalization 的时间**；



(2) 公式：（注意，**这里的统计量是一个标量**）

$$\mu^l = \frac{1}{H}\sum_{i=1}^{H} a_i^l, \quad \sigma^l = \sqrt{\frac{1}{H}\sum_{i=1}^{H}(a_i^l - \mu^l)^2}$$

在 RNN 中，我们对每个时间片的输入都使用 LN 层来进行归一化，t 时刻循环网络层的输入可以表示为：

$$\mathbf{a}^t = W_{hh}h^{t-1} + W_{xh}\mathbf{x}^t$$

则可以在 a^t 上应用 LN 层：

$$\mathbf{h}^t = f(\frac{\mathbf{g}}{\sqrt{(\sigma^t)^2+\epsilon}} \odot (\mathbf{a}^t - \mu^t) + \mathbf{b}) \qquad \mu^t = \frac{1}{H}\sum_{i=1}^{H} a_i^t \qquad \sigma^t = \sqrt{\frac{1}{H}\sum_{i=1}^{H}(a_i^t - \mu^t)^2}$$

(3) 参考链接：

- 模型优化之Layer Normalization

Instance Normalization

(1) 主要思想：IN 层和 LN 层相似，仅**对单个样本进行归一化，但是 IN 层并不进行仿射变换**；

(2) 公式：

$$\mu_{nc}(x) = \frac{1}{HW}\sum_{h=1}^{H}\sum_{w=1}^{W} x_{nchw}$$

$$\sigma_{nc}(x) = \sqrt{\frac{1}{HW}\sum_{h=1}^{H}\sum_{w=1}^{W}(x_{nchw} - \mu_{nc}(x))^2 + \epsilon}$$

这边需要注意，IN 层和 LN 层还有一点不同是，**IN 层是作用在 FeatureMap 的单个 Channel 上的**，所以它计算出来的统计量是一个向量；

(3) 代码：

- PyTorch：

INSTANCENORM2D

CLASS `torch.nn.InstanceNorm2d(num_features, eps=1e-05, momentum=0.1, affine=False, track_running_stats=False)` [SOURCE]

Applies Instance Normalization over a 4D input (a mini-batch of 2D inputs with additional channel dimension) as described in the paper Instance Normalization: The Missing Ingredient for Fast Stylization.

$$y = \frac{x - \mathrm{E}[x]}{\sqrt{\mathrm{Var}[x] + \epsilon}} * \gamma + \beta$$

The mean and standard-deviation are calculated per-dimension separately for each object in a mini-batch. γ and β are learnable parameter vectors of size C (where C is the input size) if `affine` is `True`. The standard-deviation is calculated via the biased estimator, equivalent to *torch.var(input, unbiased=False)*.

By default, this layer uses instance statistics computed from input data in both training and evaluation modes.

If `track_running_stats` is set to `True`, during training this layer keeps running estimates of its computed mean and variance, which are then used for normalization during evaluation. The running estimates are kept with a default `momentum` of 0.1.

NOTE

This `momentum` argument is different from one used in optimizer classes and the conventional notion of momentum. Mathematically, the update rule for running statistics here is $\hat{x}_{\text{new}} = (1 - \text{momentum}) \times \hat{x} + \text{momentum} \times x_t$, where $\hat{x}$ is the estimated statistic and x_t is the new observed value.

NOTE

`InstanceNorm2d` and `LayerNorm` are very similar, but have some subtle differences. `InstanceNorm2d` is applied on each channel of channeled data like RGB images, but `LayerNorm` is usually applied on entire sample and often in NLP tasks. Additionally, `LayerNorm` applies elementwise affine transform, while `InstanceNorm2d` usually don't apply affine transform.

可以看到，代码中也有一个 `track_running_stats` 参数；并且，可以设置 `affine=True` 来额外添加仿射参数；

- Tensorflow：

  ### tfa.layers.InstanceNormalization

  View source on GitHub

  Instance normalization layer.

  Inherits From: `GroupNormalization`

  ```
  tfa.layers.InstanceNormalization(
      **kwargs
  )
  ```

  Tensorflow 2 中，IN 层则在 `tensorflow_addons` 包中；

(4) 有两个场景建议不要使用 IN 层：

- **MLP 或者 RNN 中**：因为在 MLP 或者 RNN 中，每个通道上只有一个数据，这时会自然不能使用 IN；
- **FeatureMap 比较小时**：因为此时 IN 的采样数据非常少，得到的归一化统计量将不再具有代表性；

(5) 参考链接：

- 模型优化之Instance Normalization

Consine Normalization

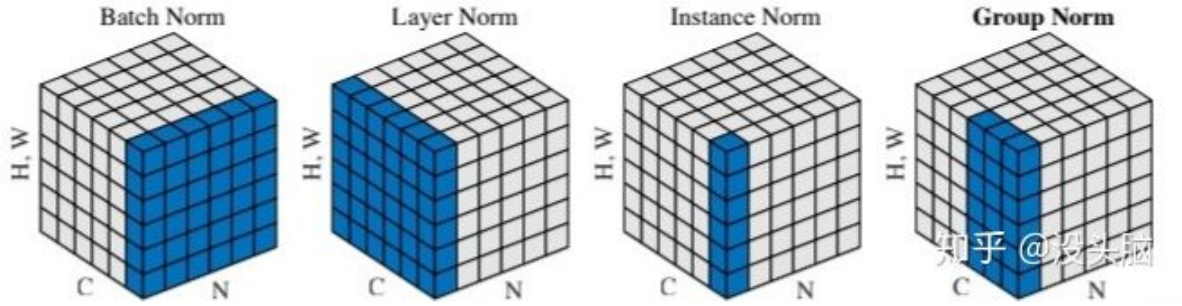
(1) 主要思想：CN 层和前面的思想都不太一样，其不对输入数据做归一化，也不对参数做归一化，而是对输入数据和参数之间的点乘做出改动，改为**计算两者的余弦相似度** $\cos(\theta)$；**CN 层将模型的输出进行归一化，使得输出有界，但是也因此丢弃了原本输出中所含的 Scale 信息，所以其作用有待探讨**；

(2) 公式：

$$w * x \Rightarrow \frac{w * x}{|w| * |x|}$$

Group Normalization

(1) 主要思想：**GN 层更像是 LN 层和 IN 层的一般化形式，通过参数 G 进行控制**；当 $G = 1$，GN 层即等价于 IN 层；当 $G = C$ 时，GN 层即等价于 LN 层；



(2) 公式：

$$\mu_{ng}(x) = \frac{1}{(C/G)HW} \sum_{c=gC/G}^{(g+1)C/G} \sum_{h=1}^{H} \sum_{w=1}^{W} x_{nchw}$$

$$\sigma_{ng}(x) = \sqrt{\frac{1}{(C/G)HW} \sum_{c=gC/G}^{(g+1)C/G} \sum_{h=1}^{H} \sum_{w=1}^{W} (x_{nchw} - \mu_{ng}(x))^2 + \epsilon}$$