Regularization and Optimization

Aziz Temirkhanov

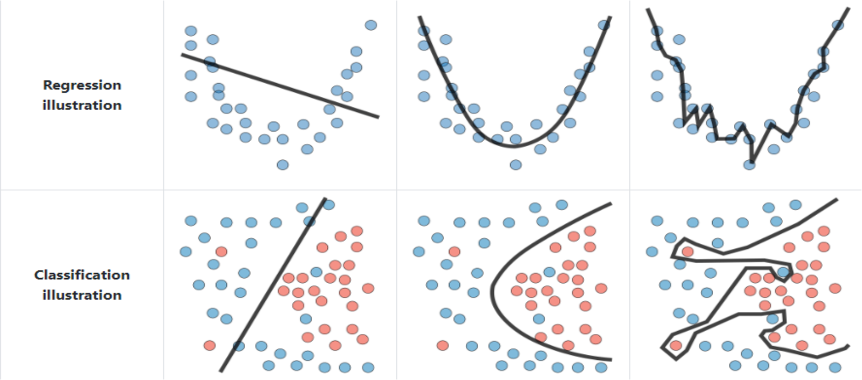
LAMBDA lab
Faculty of Computer Science
Higher School of Economics

March 5, 2024

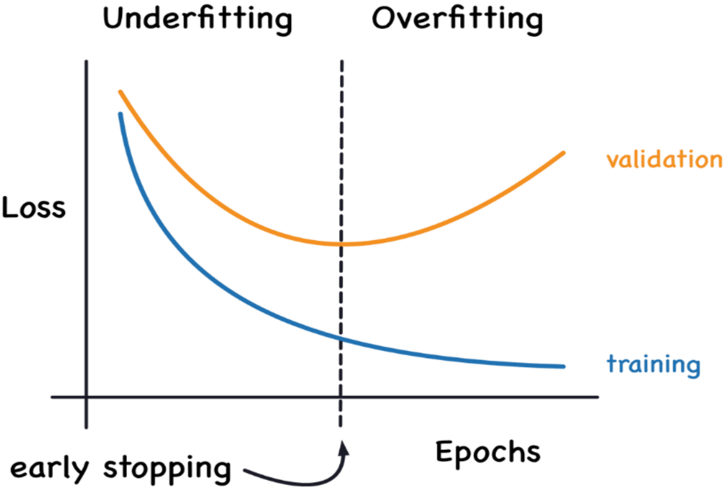
Outline

Overfitting

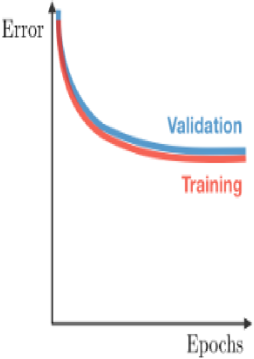
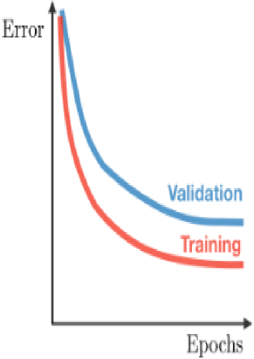
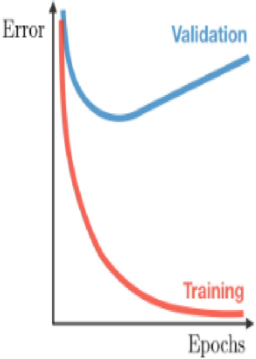
Overfitting



Overfitting



Overfitting

		
• Complexify model • Add more features • Train longer		• Perform regularization • Get more data

Overfitting

Possible remedies:

- Add regularizing term to the loss function, e.g. penalize for complex parameters
- Introduce random noise to the input data
- Introduce random noise to the labels
- Acquire more data samples
- Change the network topology
- ...

Dropout

Dropout

Let $z \in \mathbb{R}^{B \times N}$, B – batch size, N – hidden size be a batch of latent representations, i.e. logit of some intermediate layer.

Sample a binary mask $m \in \{0, 1\}^{B \times N}$ $m_{ij} \sim Bernoulli(1 - p)$, where p - dropout rate, typically $0.1 \leq p \leq 0.5$

Dropout

Train mode:

1. Sample new mask m
2. $y = m \odot z \times \frac{1}{1-p}$.

- Normalization by $\frac{1}{1-p}$ is required to preserve the expectation of neurons:

$$\mathbb{E}[y] = \mathbb{E}[m \odot z \cdot \frac{1}{1-p}] = \frac{1}{1-p} \cdot z \odot \mathbb{E}[m] = \frac{1}{1-p} \cdot z \cdot (1-p) = z \quad (1)$$

- The mask needs to be stored for backward pass

Dropout

Eval mode:

- As we normalized the output during training, it is an identical transform during testing:

$$y = z$$

- Dropout makes training slower but improves test quality

Batch Normalization

Batch Normalization

Main idea:

stabilize training by forcing zero mean and unit variance of features

Let:

$$X \in \mathbb{R}^{B \times N} = (x_1^{(N)}, x_2^{(N)}, \dots, x_B^{(N)})^T$$

Train mode:

1. Compute batch statistics:

$$\mu = \frac{1}{B}\sum_{i=1}^{B} x_i, \qquad \sigma^2 = \frac{1}{B}\sum_{i=1}^{B}(x_i - \mu)^2 \tag{2}$$

$$\mu, \sigma^2 \in \mathbb{R}^N$$

2. Normalize x, recall that every operation is element-wise:

$$\hat{x}_i = \frac{x_i - \mu}{\sqrt{\sigma^2 + \epsilon}} \tag{3}$$

Batch Normalization

All operations are differentiable, so we need to compute

$$\frac{d\ell}{d\hat{x}_i}, \frac{d\ell}{d\mu}, \frac{d\ell}{d\sigma^2}, \frac{d\ell}{dx_i}$$

during backward pass

Then, apply trainable element-wise affine transform:

$$y_i = \hat{x}_i \odot w + b; \quad w, b \in \mathbb{R}^N \tag{4}$$

We give the model freedom to set the desired mean and variance for x_i

Batch Normalization

We do not have access to a batch of data during the test.
Thus, we will accumulate statistics from the training batches:

$$\begin{aligned} running\_mean &= running\_mean \cdot (1 - m) + \mu \cdot m \\ running\_var &= running\_var \cdot (1 - m) + \sigma^2 \cdot m \cdot \frac{B}{B - 1} \end{aligned} \tag{5}$$

Here, m – is a momentum parameter (usually $m = 0.1$ to ensure slow updates).
In the beginning, *running_mean* is initialized with a zero-valued vector and *running_var* as ones. These vectors are not considered trainable.

Batch Normalization

1. Normalizing using accumulated statistics:

$$\hat{x}_i = \frac{x_i - running\_mean}{\sqrt{running\_var + \epsilon}} \tag{6}$$

2. Apply affine transform:

$$y_i = \hat{x}_i \odot w + b \tag{7}$$

Optimization

SGD

- $\{x_i, y_i\}_{i=1}^{\ell}$ – training set
- B – batch size
- $\mathcal{L}(\cdot, \cdot)$ – loss function
- W – all trainable parameters of the model
- $f_W(\cdot)$ – neural network

At the step t we have:

$$\mathcal{L}^t(w) = \frac{1}{B} \sum_{i=1}^{B} \mathbf{L}(f_W(x_i), y_i), \quad t_i \sim \mathcal{U}(\{1, ..., \ell\}) \tag{8}$$

SGD

SGD algorithm:

1. $g_t = \nabla_w \mathcal{L}^t(w_{t-1})$ – compute the gradient.
2. $m_t = \mu m_{t-1} + g_t$ – compute the momentum. This concept came from physics. Momentum accelerates the decrease in loss due to bigger steps in the right direction. It also helps with local minima, jumping over not deep local points.
3. $w_t = w_{t-1} - \eta_t m_t$ – now update the parameters with momentum, multiplying by a factor of learning rate. Learning rate η_t is arbitrary and can vary at each step (epoch) of training or be a constant.

$m_0 = 0$, $0 \leq \mu \leq 1$, usually $\mu = 0.9$

SGD with Regularization

We can add L^2 **regularization**:

$$\mathcal{L}^t(w) \mapsto \mathcal{L}^t_\lambda(w) := \mathcal{L}^t(w) + \frac{\lambda}{2}\|w\|_2^2 \tag{9}$$

$$\nabla_w \|w\|_2^2 = 2w$$

1. $g_t = \nabla_w \mathcal{L}^t(w_{t-1}) + \lambda w_{t-1}$
2. $m_t = \mu m_{t-1} + g_t$
3. $w_t = w_{t-1} - \eta_t m_t$

It is essentially a weight decaying by a factor of less than 1:

$$w_t = w_{t-1}(1 - \eta_t \lambda) - \eta_t(\mu m_{t-1} + \nabla_w \mathcal{L}^t(w_{t-1}))$$

Adam

Adam:

- Has adaptive learning rate (like in AdaGrad, RMSProp)
- Has Momentum

1. $g_t = \nabla_w \mathcal{L}^t(w_{t-1}) + \lambda w_{t-1}$ – calculate gradient with penalty factor (weight decay)
2. $m_t = \beta_1 m_{t-1} + (1 - \beta_1) g_t$ – calculate the first moment
3. $v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$ – calculate the second moment. Here gradients are squared element-wise.
4. $\hat{m}_t = \frac{m_t}{1-\beta_1^t}, \quad \hat{v}_t = \frac{v_t}{1-\beta_2^t}$ – bias correction for first and second moment estimations
5. $w_t = w_{t-1} - \eta_t \frac{\hat{m}_t}{\hat{v}_t + \epsilon}$ - update weights

Adam

Initially,

$$m_0 = 0, v_0 = 0$$

And

$$\lambda, \beta_1, \beta_2, \epsilon \text{ -- hyperparams}$$

$$\beta_1 = 0.9, \beta_2 = 0.999, \epsilon = 10^{-8}$$

Whereas λ – is an optional one.
Adam accelerates on the slopes and lows down at the narrow points to achieve stable convergence. See this paper or the original one for the reference.

AdamW

The difference between **Adam** and **AdamW** is the approach for tackling weight decay. The decay factor is being used in gradient calculation in the **Adam** algorithm, whether in **AdamW** weight decay applied at the weights updating phase, similarly to **SGD**:

1. $g_t = \nabla_w \mathcal{L}^t(w_{t-1})$ – calculate gradient
2. $m_t = \beta_1 m_{t-1} + (1 - \beta_1) g_t$
3. $v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$ – element-wise square
4. $\hat{m}_t = \frac{m_t}{1-\beta_1^t}, \quad \hat{v}_t = \frac{v_t}{1-\beta_2^t}$
5. $w_t = w_{t-1}(1 - \eta_t \lambda) - \eta_t \frac{\hat{m}_t}{\hat{v}_t + \epsilon}$

LR Schedulers

It is often a non-trivial task to choose a learning rate η_t
You can update it once per training epoch

- Constant. $\eta_t = \eta_0$. Often gives suboptimal quality
- StepRL. $\forall t \in \{t_0, ... t_n\} : \eta_{cur} = \eta_t, \eta_0 > \eta_1 > ...$
- ExponentialLR. $\eta_t = \gamma \eta_{t-1}, \gamma < 1$
- CosineLR. $\eta_t = \eta_0 \cdot \frac{1}{2}(1 + \cos(\frac{\pi t}{T}))$, T – maximum number of epochs
- Linear warmup LR. Linearly increase lr first n-batches $\eta_0^{(0)} \mapsto \eta_0^{(n)}$. Then apply any scheduler.
- Reduce LR on a plateau. Reduce LR when validation loss stagnates, thus requiring a validation set


Thank
you