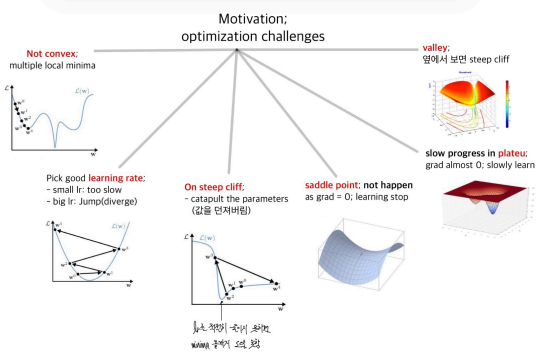
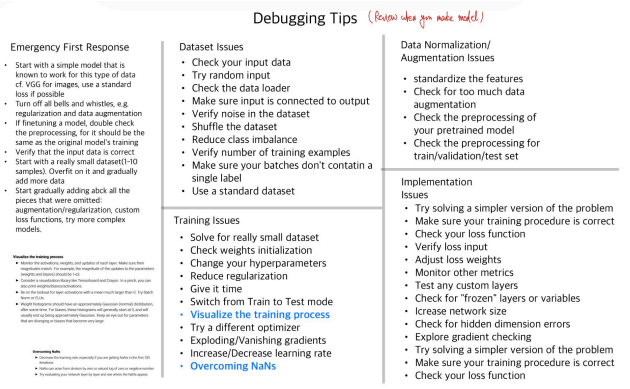
Lec5. optimization

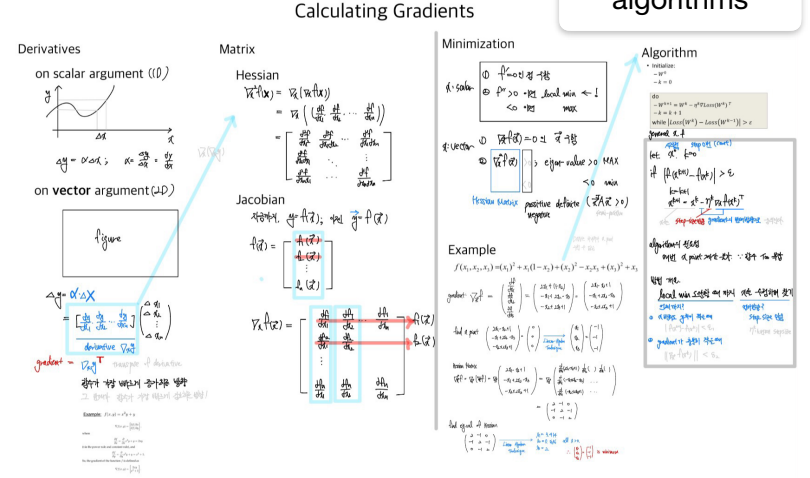
Motivation



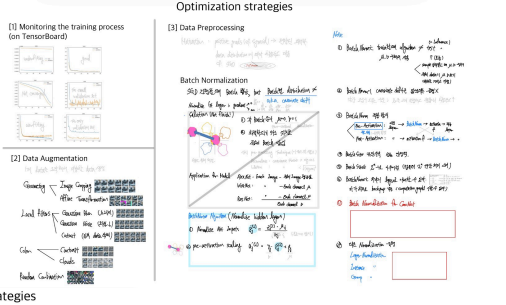
Debugging Tips

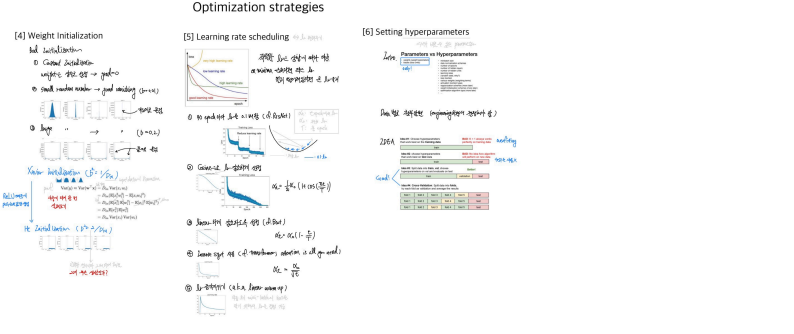


Optimization algorithms



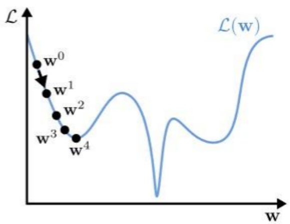
Optimization strategies



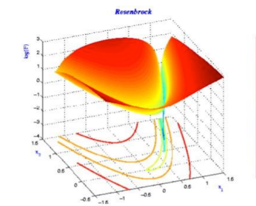


Motivation;
optimization challenges

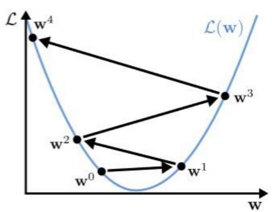
Not convex;
multiple local minima



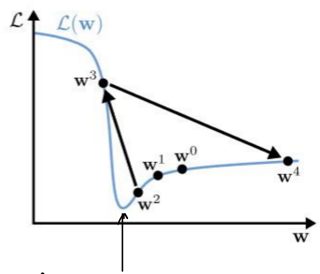
valley;
옆에서 보면 steep cliff



Pick good **learning rate**;
- small lr: too slow
- big lr: Jump(diverge)

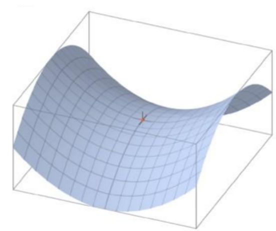


On steep cliff;
- catapult the parameters
  (값을 던져버림)

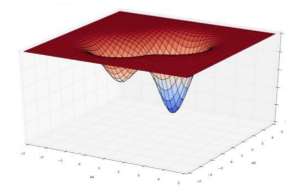


lr을 적절히 줄이지 못하면
minima 끝까지 도달 못함

saddle point; **not happen**
as grad = 0; learning stop



slow progress in plateu;
grad almost 0; slowly learn



Optimization algorithms

TMI:

다양한 형태로 Momentum식 구현 가능 (다른 뜻!)

$v_{t+1} = \rho v_t - \alpha \nabla f(x_t)$ ≠ $v_{t+1} = \rho v_t + \nabla f(x_t)$

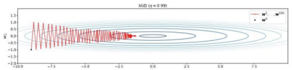
$x_{t+1} = x_t + v_{t+1}$ $\quad$ $x_{t+1} = x_t - \alpha v_{t+1}$

$= x_t + (\rho v_t - \alpha \nabla f(x_t))$ $\quad$ $= x_t - (\alpha \rho v_t + \alpha \nabla f(x_t))$

Gradient Descent

↓ pick mini-batch ($B = 2^n$ 개 data) 매번 다 계산 불가

SGD



Algorithm

① initialize w^0 η B

② Draw random mini batch $\{(x_1, y_1), \cdots (x_B, y_B)\}$

③ for 각 element (x_1, y_1)

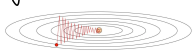
forward: $x_b \longrightarrow \hat{y}_b$

backward: $\nabla_w L_b(w^t) = \nabla_w L_b(\hat{y}_b, y_b, w)$

④ Update gradient $w^{t+1} = w^t - \eta \frac{1}{B} \sum \nabla_w L_b(w^t)$ Loss

problem of SGD : how to find good lr?

① Jittering in shallow dimension



② Stuck in local minima & saddle point

③ noisy gradient

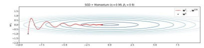
∵ 전체가 아닌, minibatch의 gradient

TMI proof: SGD works with mathematics later!

Solution of SGD

Momentum

SGD + Momentum



Jittering하면 dampen(약화). 스러면 가속

$m^{t+1} = \beta_1 m^t + (1-\beta_1) \nabla_w L_B(w^t)$

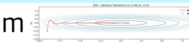
(m^{t+1}: velocity, β_1: momentum)

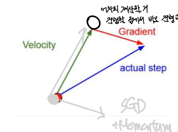
$w^{t+1} = w^t + \eta m^{t+1}$

(η: learning rate)

여러 방법들 中 weighted sum(β_1, $1-\beta_1$)으로 표현된 방법은 고른 것. learning rate는 마지막에 1번 적용하는 데 주의 (중복X)

SGD + Nestrov Momentum





목적: 계산 효율적.

$v_{t+1} = \rho v_t - \alpha \nabla f(x_t + \rho v_t)$

$x_{t+1} = x_t + v_{t+1}$

$m_{t+1} = \rho m_t - \alpha \nabla f(\tilde{w}_t)$

$\tilde{w}_t = w_t + \rho m_t$

$\tilde{w}_{t+1} = \tilde{w}_t + m_{t+1}$

$= \tilde{w}_t + \rho m_t - \alpha \nabla f(\tilde{w}_t)$

- Jittering ↓
- RNN에 효과적임

Scaling

AdaGrad

Adaptive Gradient Estimation

```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared += dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

grad_squared += dx * dx: 계속 누적

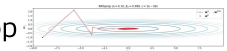
np.sqrt(grad_squared) → ∞

scaling: dimension (parameter) 별로 다른 gradient 적용되도록

lr: adaptive lr로 표현

→ step_size → 0 방지하기 위해

RMSProp



```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared = decay_rate * grad_squared + (1 - decay_rate) * dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

decay_rate 추가, weighted sum 형태

lr을 크게 선정해도, learning OK (잘 adaptive하게 조정됨)

Adam(good)

Momentum + RMSprop

Understanding with Math later!

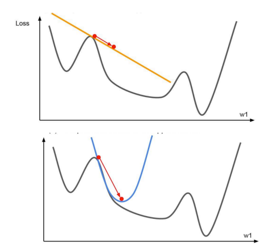
```
first_moment = 0
second_moment = 0
for t in range(1, num_iterations):
  dx = compute_gradient(x)
  first_moment = beta1 * first_moment  + (1 - beta1) * dx
  second_moment = beta2 * second_moment + (1 - beta2) * dx * dx
  first_unbias = first_moment / (1 - beta1 ** t)
  second_unbias = second_moment / (1 - beta2 ** t)
  x -= learning_rate * first_unbias / (np.sqrt(second_unbias) + 1e-7))
```

Momentum

Bias correction

AdaGrad / RMSProp

TMI: Second-order optimization

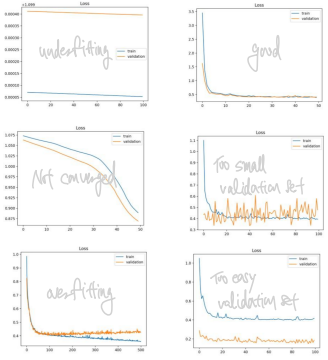


RNN은 사용X. 계산량 너무 많음.

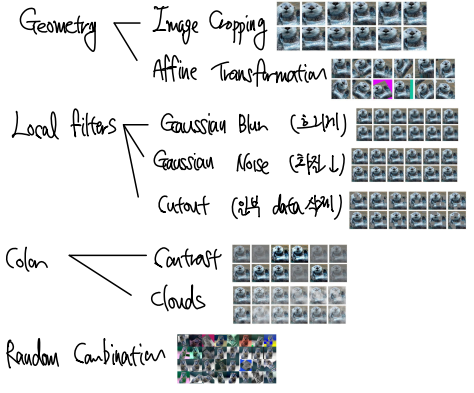
사용한다면, 훨씬 빠르게 최적화 가능.

Optimization strategies

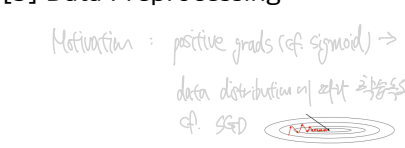
[1] Monitoring the training process (on TensorBoard)



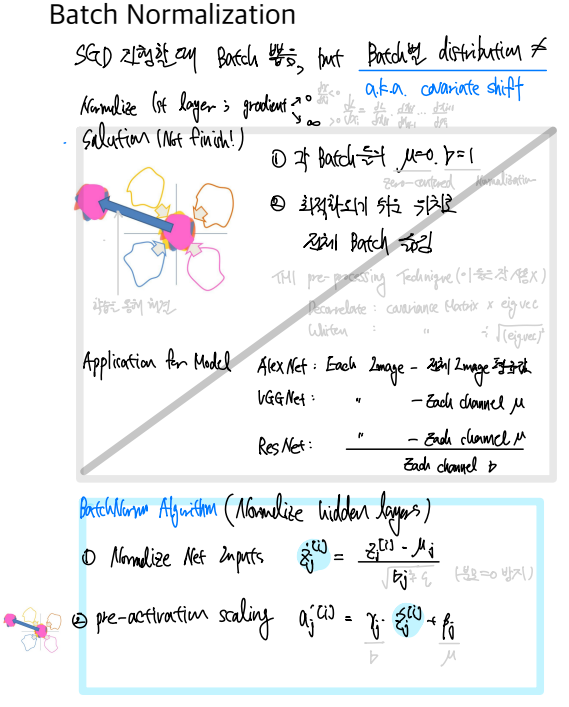
[2] Data Augmentation



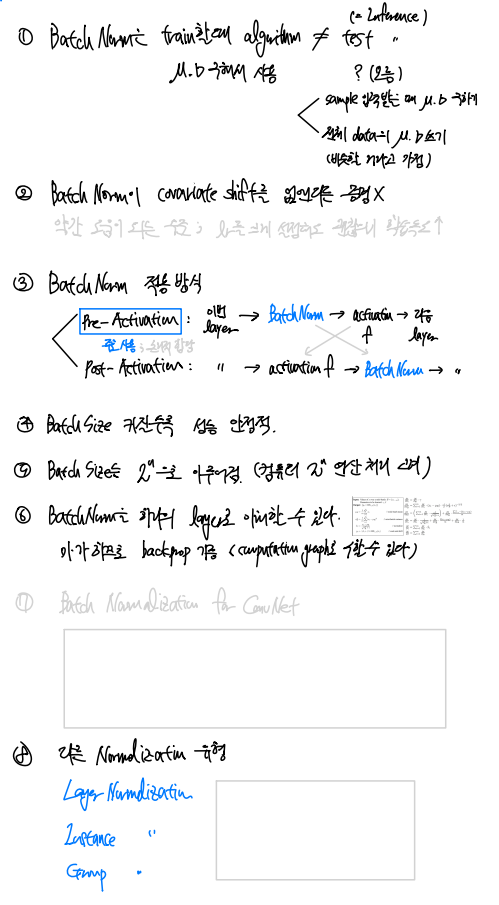
[3] Data Preprocessing



Batch Normalization



Note



Optimization strategies

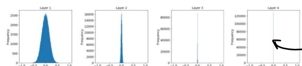
[4] Weight Initialization

Bad Initialization

① Constant Initialization

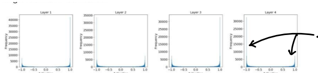
weight는 상수로 설정 → grad=0

② small random number → grad vanishing (b=0.01)



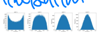
가운데로 몰림

③ large " → " (b=0.2)



끝으로 몰림

Xavier Initialization ($b^2 = 1/D_{in}$) input data의 Dimension



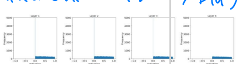
proof.

$$\begin{aligned} \mathrm{Var}(y) &\approx \mathrm{Var}(w^T x) = D_{in}\,\mathrm{Var}(x_i w_i) \\ &= D_{in}(\mathbb{E}[x_i^2 w_i^2] - \mathbb{E}[x_i w_i]^2) \\ &= D_{in}(\mathbb{E}[x_i^2]\,\mathbb{E}[w_i^2] - \mathbb{E}[x_i]^2\,\mathbb{E}[w_i]^2) \\ &= D_{in}\mathbb{E}[x_i^2]\,\mathbb{E}[w_i^2] \\ &= D_{in}\,\mathrm{Var}(x_i)\,\mathrm{Var}(w_i) \end{aligned}$$

iid 가정, iid

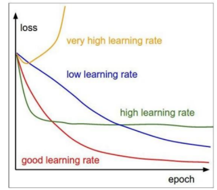
ReLU 때문에 positive값만 생성

He Initialization ($b^2 = 2/D_{in}$)



절반만 생기니까 2배하여 해결

[5] Learning rate scheduling ⇔ lr 바꿔주기

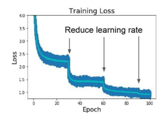


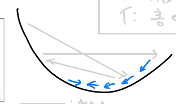
적절한 lr는 상황에 따라 다름

ex. minima 근처라면 작은 lr
멀리 떨어져있다면 큰 lr 유리

① 30 epoch 마다 lr을 0.1 배함 (cf. ResNet)

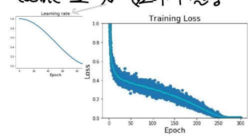
α_t: t epoch에서 lr
α_0: 처음 lr
T: 총 epoch





---- : 처음 lr   —— : 0.1·lr

② Cosine으로 lr 감소하게 설정

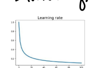


$$\alpha_t = \frac{1}{2}\alpha_0\left(1+\cos\left(\frac{\pi t}{T}\right)\right)$$

③ linear 하게 감소하도록 설정 (cf. Bert)

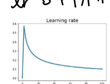
$$\alpha_t = \alpha_0\left(1-\frac{t}{T}\right)$$

④ Inverse sqrt 사용 (cf. transformer; attention is all you need)



$$\alpha_t = \frac{\alpha_0}{\sqrt{t}}$$

⑤ lr 증가시키기 (a.k.a. linear warm up)



학습 초기 mini-batch의 bias를 막기 위해서. lr는 점점 가중

[6] Setting hyperparameters

<우리가 바꿀수 있는 parameter

Intro.

Parameters vs Hyperparameters

- weights (weight parameters)
- biases (bias units)

only!

- minibatch size
- data normalization schemes
- number of epochs
- number of hidden layers
- number of hidden units
- learning rates
- (random seed, why?)
- loss function
- various weights (weighting terms)
- activation function types
- regularization schemes (more later)
- weight initialization schemes (more later)
- optimization algorithm type (more later)
- ...

Data 별로 천차만별 (engineering하면서 결정해야 함)

IDEA

Idea #1: Choose hyperparameters that work best on the **training data** — **BAD**: K = 1 always works perfectly on training data — overfitting

train

Idea #2: choose hyperparameters that work best on **test** data — **BAD**: No idea how algorithm will perform on new data — test는 사용X

train	test

Good!

Idea #3: Split data into **train**, **val**; choose hyperparameters on val and evaluate on test — **Better!**

train	validation	test

Idea #4: **Cross-Validation**: Split data into **folds**, try each fold as validation and average the results

fold 1	fold 2	fold 3	fold 4	fold 5	test
fold 1	fold 2	fold 3	fold 4	fold 5	test
fold 1	fold 2	fold 3	fold 4	fold 5	test

Debugging Tips

Emergency First Response

- Start with a simple model that is known to work for this type of data cf. VGG for images, use a standard loss if possible
- Turn off all bells and whistles, e.g. regularization and data augmentation
- If finetuning a model, double check the preprocessing, for it should be the same as the original model's training
- Verify that the input data is correct
- Start with a really small dataset(1-10 samples). Overfit on it and gradually add more data
- Start gradually adding abck all the pieces that were omitted: augmentation/regularization, custom loss functions, try more complex models.

Visualize the training process

- Monitor the activations, weights, and updates of each layer. Make sure their magnitudes match. For example, the magnitude of the updates to the parameters (weights and biases) should be 1-e3.
- Consider a visualization library like Tensorboard and Crayon. In a pinch, you can also print weights/biases/activations.
- Be on the lookout for layer activations with a mean much larger than 0. Try Batch Norm or ELUs.
- Weight histograms should have an approximately Gaussian (normal) distribution, after some time. For biases, these histograms will generally start at 0, and will usually end up being approximately Gaussian. Keep an eye out for parameters that are diverging or biases that become very large.

Overcoming NaNs

- Decrease the learning rate, especially if you are getting NaNs in the first 100 iterations.
- NaNs can arise from division by zero or natural log of zero or negative number.
- Try evaluating your network layer by layer and see where the NaNs appear.

Dataset Issues

- Check your input data
- Try random input
- Check the data loader
- Make sure input is connected to output
- Verify noise in the dataset
- Shuffle the dataset
- Reduce class imbalance
- Verify number of training examples
- Make sure your batches don't contatin a single label
- Use a standard dataset

Training Issues

- Solve for really small dataset
- Check weights initialization
- Change your hyperparameters
- Reduce regularization
- Give it time
- Switch from Train to Test mode
- **Visualize the training process**
- Try a different optimizer
- Exploding/Vanishing gradients
- Increase/Decrease learning rate
- **Overcoming NaNs**

Data Normalization/ Augmentation Issues

- standardize the features
- Check for too much data augmentation
- Check the preprocessing of your pretrained model
- Check the preprocessing for train/validation/test set

Implementation Issues

- Try solving a simpler version of the problem
- Make sure your training procedure is correct
- Check your loss function
- Verify loss input
- Adjust loss weights
- Monitor other metrics
- Test any custom layers
- Check for "frozen" layers or variables
- Icrease network size
- Check for hidden dimension errors
- Explore gradient checking
- Try solving a simpler version of the problem
- Make sure your training procedure is correct
- Check your loss function