Special topics: Convolutional Neural Networks

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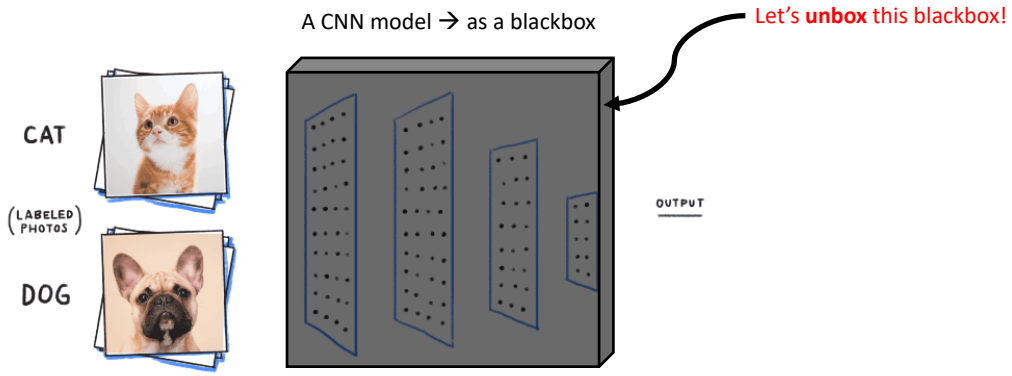
Slide & Code: https://github.com/chupibk/INT3414_22

Schedule

Week	Content	Class hour	Self-study hour
1	Introduction CNNs in Computer Vision	2	1
2	~~Foundations of CNNs~~ ~~Case study: Image classification problem~~ Basics of Neural networks Training with backpropagation Implementation with PyTorch	2	2-6
3	~~Training and tuning parameters~~ ~~Data augmentation - Data generator~~ Foundations of CNNs Transfer learning	2	2-6
4	Object detection	2	2-6
5	Segmentation	2	2-6
6, 7	Mid-term presentations	2	2-6
8, 9	Advanced topics using CNNs	2	2-6
10, 11, 12	Final project presentations	1	2-6
13	Class summarization	1-3	open

Recall week 1



The most important: design the problem to a solvable task using the blackbox

Image credit: https://becominghuman.ai/building-an-image-classifier-using-deep-learning-in-python-totally-from-a-beginners-perspective-be8dbaf22dd8

Week 2

Basics of Neural Networks and Deep Learning

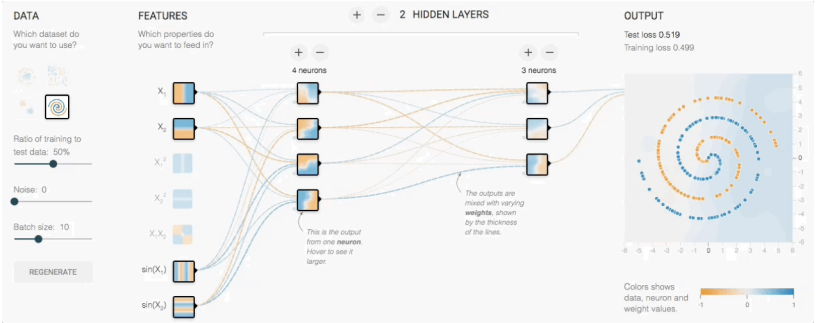
Implementation with PyTorch

Code

- Google Colab notebook
  - https://colab.research.google.com/drive/1hLRa43CbzXeE0-DY7UlTrbDUeITsS7Pe

Build a neural network

https://playground.tensorflow.org/



m observed data, 4 features

Input $X \in \mathbb{R}^{4\times m}$ — Hidden 1 $H^{(1)} \in \mathbb{R}^{4\times m}$ — Hidden 2 $H^{(2)} \in \mathbb{R}^{3\times m}$ — Output $y \in \mathbb{R}^{1\times m}$

Learning weights and biases

$W^{(1)}X + B^{(1)} = H^{(1)}$, $W^{(1)} \in \mathbb{R}^{4\times 4}$

$W^{(2)}H^{(1)} + B^{(2)} = H^{(2)}$, $W^{(2)} \in \mathbb{R}^{3\times 4}$

$W^{(3)}H^{(2)} + B^{(3)} = y$, $W^{(3)} \in \mathbb{R}^{1\times 3}$

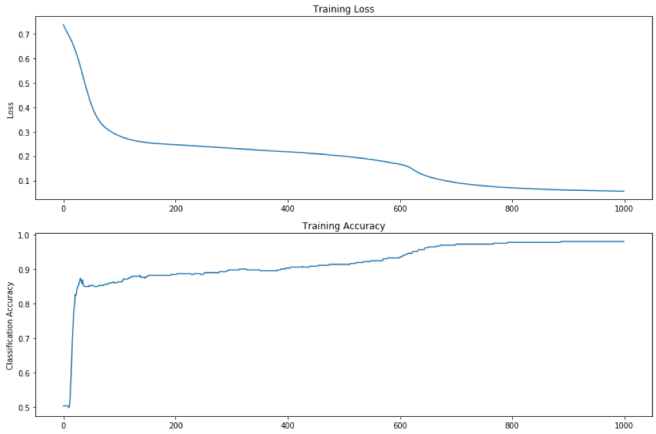
Implementation with PyTorch

```
model = nn.Sequential(
    nn.Linear(D_in, H),
    nn.ReLU(),
    nn.Linear(H, D_out),
    nn.Sigmoid()
)
```

```
loss_fn = nn.BCELoss()
lr = 0.01 #learning rate
optimizer = torch.optim.Adam(
      model.parameters(),
      lr=lr
)
```

```
for t in range(num_epochs):
    # Forward pass
    y_pred = model(x_train_t)

    # Compute loss
    loss = loss_fn(y_pred, y_train_t)

    # Clear the buffers
    optimizer.zero_grad()

    # Backward pass: compute gradients
    loss.backward()

    # update the parameters
    optimizer.step()
```

Visualize the training loss



Steps in training a CNN – Keras

- Prepare data: x_train, y_train, x_val, y_val, x_test, y_test
  - x: (b, h, w, c)
  - y: (b, n)
- Define a CNN model
  - Conv + dense layers
- Compile the model
  - Define a loss function: cross entropy loss
  - Set an optimizer & its parameters
  - Define evaluation metrics

model.compile(...)

- Train the model
  - Feed the actual data and do weight updating
    - Feed several times (# of epochs)
    - Feed a small amount at a time (batch_size)

model.fit(...)

```
model.compile(loss=keras.losses.categorical_crossentropy,
              optimizer=keras.optimizers.Adadelta(),
              metrics=['accuracy'])
```

Loss function: Cross entropy

p(x): true distribution
q(x): estimated distribution
x: discrete variable

$$H(p,q) = -\sum_{\forall x} p(x)\log(q(x))$$

Other form:

y: ground truth vector
$\hat{y}$: estimated vector
$(\cdot)$: vector dot product

$$L = -\mathbf{y}\cdot\log(\hat{\mathbf{y}})$$

Loss function example

```
def cross_entropy(y_true, y_pred, eps=1e-12):
    '''
    Log loss is undefined for p=0 or p=1,
        so probabilities are
        clipped to (eps, 1 - eps).
    '''
    y_true = np.clip(y_true, eps, 1. - eps)
    y_pred = np.clip(y_pred, eps, 1. - eps)
    log_likelihood = -np.log(y_pred)
    loss = -(y_true * np.log(y_pred)).sum()
    return loss
```

```
cross_entropy([1, 0, 0, 0], [0.9, 0, 0, 0.1])
```

```
0.10536051571528555
```

```
cross_entropy([1, 0, 0, 0], [0.1, 0.8, 0.1, 0])
```

```
2.3025850930218996
```

Loss function for a dataset of size N

$$J = -\frac{1}{N}\left(\sum_{i=1}^{N} \mathbf{y_i} \cdot \log(\hat{\mathbf{y}}_\mathbf{i})\right)$$

Evaluation metrics

total N=150	Predicted YES	Predicted NO
Actual: YES	True positive TP = 80	False Negative FN = 25
Actual: NO	False Positive FP = 10	True negative TN = 35

$$accuracy = \frac{number\ of\ correct\ predictions}{total\ number\ of\ predictions\ made}$$

$$= \frac{TP + TN}{N} = \frac{80 + 35}{150} = 0.7$$

$$recall = \frac{number\ of\ correct\ positive\ predictions}{number\ of\ all\ positive\ samples}$$

$$= \frac{TP}{TP + FN} = \frac{80}{80 + 25} = 0.76$$

$$precision = \frac{number\ of\ correct\ positive\ predictions}{number\ of\ positive\ predictions\ made}$$

$$= \frac{TP}{TP + FP} = \frac{80}{80 + 10} = 0.89$$

$$F1 = 2 * \frac{1}{\frac{1}{precision} + \frac{1}{recall}}$$

Harmonic mean between precision and recall

Evaluation metrics for multi-class classification

	Predicted YES	Predicted NO
Actual: YES	True positive	False Negative
Actual: NO	False Positive	True negative

Recall = TP/Total actual positive

Precision = TP/Total predicted positive

	GoldLabel_A	GoldLabel_B	GoldLabel_C	
Predicted_A	**30**	20	10	TotalPredicted_A=60
Predicted_B	50	**60**	10	TotalPredicted_B=120
Predicted_C	20	20	**80**	TotalPredicted_C=120
	TotalGoldLabel_A=100	TotalGoldLabel_B=100	TotalGoldLabel_C=100	

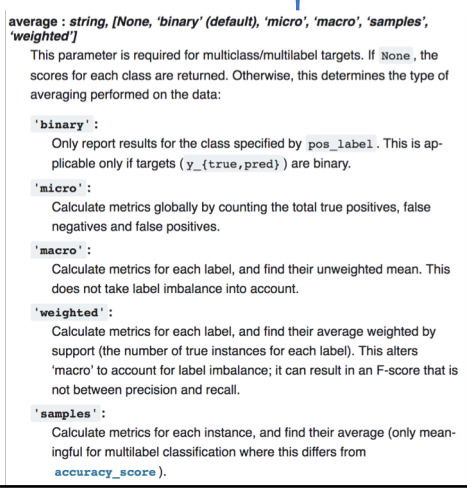
Recall label X = TP_X / Total actual X

Precision label X = TP_X / Total predicted_X

Ref: http://text-analytics101.rxnlp.com/2014/10/computing-precision-and-recall-for.html

sklearn.metrics

sklearn.metrics.precision_score(*y_true*, *y_pred*, *labels=None*, *pos_label=1*, *average='binary'*, *sample_weight=None*)



average : *string, [None, 'binary' (default), 'micro', 'macro', 'samples', 'weighted']*

This parameter is required for multiclass/multilabel targets. If `None`, the scores for each class are returned. Otherwise, this determines the type of averaging performed on the data:

`'binary'`:
Only report results for the class specified by `pos_label`. This is applicable only if targets (`y_{true,pred}`) are binary.

`'micro'`:
Calculate metrics globally by counting the total true positives, false negatives and false positives.

`'macro'`:
Calculate metrics for each label, and find their unweighted mean. This does not take label imbalance into account.

`'weighted'`:
Calculate metrics for each label, and find their average weighted by support (the number of true instances for each label). This alters 'macro' to account for label imbalance; it can result in an F-score that is not between precision and recall.

`'samples'`:
Calculate metrics for each instance, and find their average (only meaningful for multilabel classification where this differs from `accuracy_score`).

Understanding the backpropagation

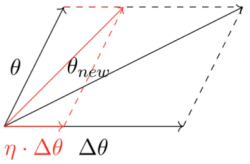
Updating parameters (1/2)

- Loss function w.r.t to θ = **[w,b]** where w and b are weights and biases

$$L = -\mathbf{y} \cdot \log(\hat{\mathbf{y}})$$

We want to find best θ that minimizes L → How?

- For a given θ, let's change it a small amount Δθ =u
  i.e., θ = θ + Δθ
  Even better, using a controllable parameter (learning rate)
  θ = θ + η.Δθ



- What will happen to L?

Using Taylor series:

∇L(θ) = [∂L(θ)/∂w , ∂L(θ)/∂b]

gradient

$$\mathscr{L}(\theta + \eta u) = \mathscr{L}(\theta) + \eta * u^T \nabla_\theta \mathscr{L}(\theta) + \frac{\eta^2}{2!} * u^T \nabla^2 \mathscr{L}(\theta) u + \frac{\eta^3}{3!} * \ldots + \frac{\eta^4}{4!} * \ldots$$

Updating parameters (2/2)

$$\mathscr{L}(\theta + \eta u) = \mathscr{L}(\theta) + \eta * u^T \nabla_\theta \mathscr{L}(\theta) + \frac{\eta^2}{2!} * u^T \nabla^2 \mathscr{L}(\theta) u + \frac{\eta^3}{3!} * \ldots + \frac{\eta^4}{4!} * \ldots$$

η <<1 → can ignore these values

When updating θ, we want the loss decreases
→ This means

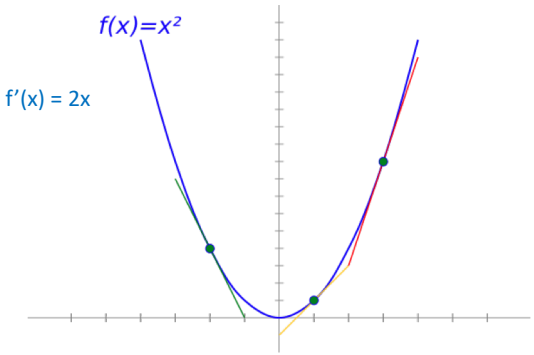
$$u^T \nabla_\theta \mathscr{L}(\theta) < 0$$

The angle between two vectors

$$-1 \leq cos(\beta) = \frac{u^T \nabla_\theta \mathscr{L}(\theta)}{||u|| * ||\nabla_\theta \mathscr{L}(\theta)||} \leq 1$$

u.∇L(θ) is minimum when vector u and gradient is opposite
i.e., cos(β) = -1 or β = 180° with respect to the gradient

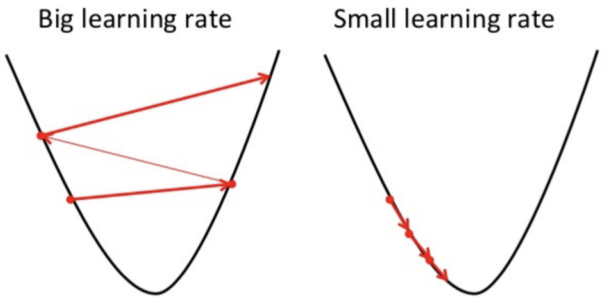
An intuitive example of gradient descent



x<0 → f'<0 → the function is decreasing
Update x so that in the opposite of current x
→ x - e, e has same sign with f' (<0)
→ x goes to 0

x>0 → f'>0 → the function is increasing
Update x so that in the opposite of current x
→ x - e, e has same sign with f' (>0)
→ x goes to 0

Learning rate



Gradient descent

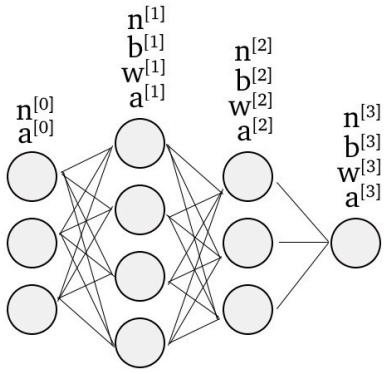
The simplest updating rule using gradient

$$w_{t+1} = w_t - \eta \nabla w_t$$
$$b_{t+1} = b_t - \eta \nabla b_t$$
$$where, \nabla w_t = \frac{\partial \mathscr{L}(w,b)}{\partial w}_{at\ w=w_t, b=b_t}, \nabla b = \frac{\partial \mathscr{L}(w,b)}{\partial b}_{at\ w=w_t, b=b_t}$$

In order to update the parameters, we need to compute all the partial derivatives with respect to the components of θ
(i.e., weights w and biases b)

HOW?

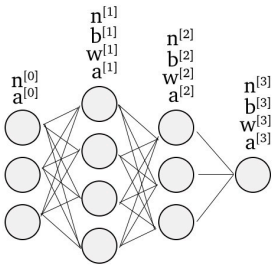
Calculating derivation



- $n^{[l]}$ - The number of neurons in the layer *l*.
- $W^{[l]}$ - The weight matrix associated with the layers *l* and *l*-1, of the size ($n^{[l]} \times n^{[l-1]}$). $w_{jk}^{[l]}$ refers to the weight associated with the neuron *j* in the layer *l* and the neuron *k* in the layer *l*-1.
- $b^{[l]}$ - The vector of biases associated with the layer *l*, of the size ($n^{[l]} \times 1$).
- $a^{[l]}$ - The vector of activations of the neurons in the layer *l*, of the size ($n^{[l]} \times 1$).
- $z^{[l]}$ - The vector of the weighted output of the neurons in the layer *l*, of the size ($n^{[l]} \times 1$).
- $g^{[l]}$ - The activation function applied to the output of the neurons in the layer *l*, $a^{[l]} = g^{[l]}(z^{[l]})$.

Source: https://medium.com/binaryandmore/beginners-guide-to-deriving-and-implementing-backpropagation-e3c1a5a1e536

Calculating derivation



Forward propagation

$$z^{[l]} = w^{[l]}.a^{[l-1]} + b^{[l]}$$

$$\mathrm{a}^{[l]} = g^{[l]}(z^{[l]})$$

Loss (Cost) function

$$\mathrm{C} = \text{-}(\mathrm{y}\log\hat{y} + (1-y)\log(1-\hat{y}))$$

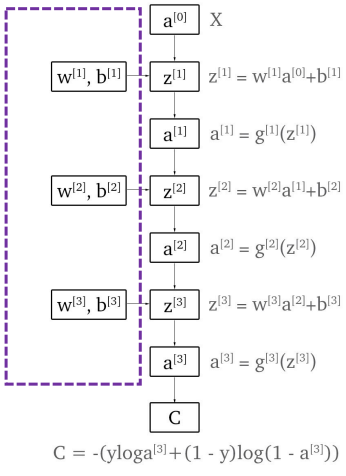
Update rules

$$w^{[l]} = w^{[l]} - \alpha\frac{\partial C}{\partial w^{[l]}}$$

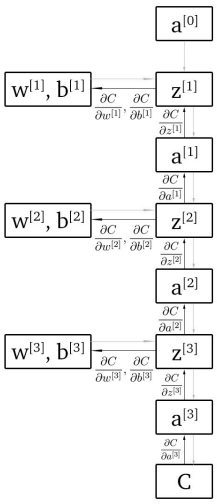
$$b^{[l]} = b^{[l]} - \alpha\frac{\partial C}{\partial b^{[l]}}$$

Computation graph

Need to compute the partial derivative of C wrt learnable parameters



Chain rules



$$\frac{\partial C}{\partial w^{[1]}} = \frac{\partial C}{\partial a^{[3]}}.\frac{\partial a^{[3]}}{\partial z^{[3]}}.\frac{\partial z^{[3]}}{\partial a^{[2]}}.\frac{\partial a^{[2]}}{\partial z^{[2]}}.\frac{\partial z^{[2]}}{\partial a^{[1]}}.\frac{\partial a^{[1]}}{\partial z^{[1]}}.\frac{\partial z^{[1]}}{\partial w^{[1]}}$$

$$\frac{\partial C}{\partial b^{[1]}} = \frac{\partial C}{\partial a^{[3]}}.\frac{\partial a^{[3]}}{\partial z^{[3]}}.\frac{\partial z^{[3]}}{\partial a^{[2]}}.\frac{\partial a^{[2]}}{\partial z^{[2]}}.\frac{\partial z^{[2]}}{\partial a^{[1]}}.\frac{\partial a^{[1]}}{\partial z^{[1]}}.\frac{\partial z^{[1]}}{\partial b^{[1]}}$$

$$\frac{\partial C}{\partial w^{[2]}} = \frac{\partial C}{\partial a^{[3]}}.\frac{\partial a^{[3]}}{\partial z^{[3]}}.\frac{\partial z^{[3]}}{\partial a^{[2]}}.\frac{\partial a^{[2]}}{\partial z^{[2]}}.\frac{\partial z^{[2]}}{\partial w^{[2]}}$$

$$\frac{\partial C}{\partial b^{[2]}} = \frac{\partial C}{\partial a^{[3]}}.\frac{\partial a^{[3]}}{\partial z^{[3]}}.\frac{\partial z^{[3]}}{\partial a^{[2]}}.\frac{\partial a^{[2]}}{\partial z^{[2]}}.\frac{\partial z^{[2]}}{\partial b^{[2]}}$$

$$\frac{\partial C}{\partial w^{[3]}} = \frac{\partial C}{\partial a^{[3]}}.\frac{\partial a^{[3]}}{\partial z^{[3]}}.\frac{\partial z^{[3]}}{\partial w^{[3]}}$$

$$\frac{\partial C}{\partial b^{[3]}} = \frac{\partial C}{\partial a^{[3]}}.\frac{\partial a^{[3]}}{\partial z^{[3]}}.\frac{\partial z^{[3]}}{\partial b^{[3]}}$$

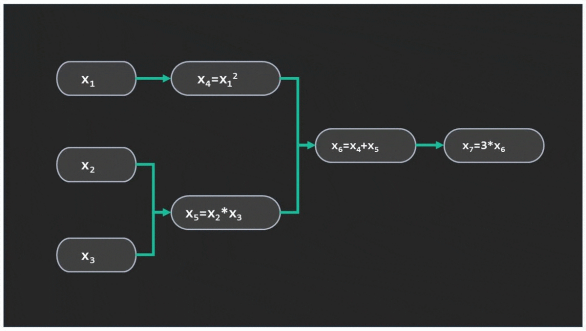
Automatic differentiation: Autograd

Autograd is a PyTorch package for the differentiation for all operations on Tensors.
It performs the backpropagation starting from a variable (i.e., the tensor of the loss function).

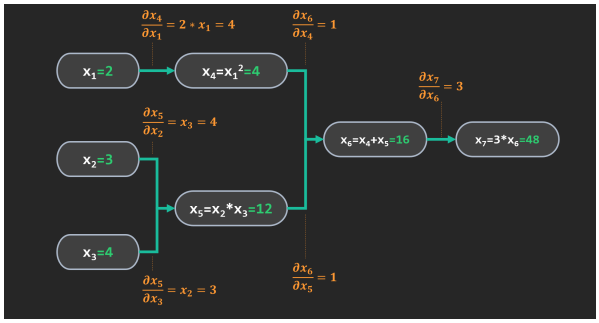
`loss.backward()` This executes the backward pass and computes all the backpropagation gradients automatically.

`w.grad` We access individual gradient through the attributes grad of a variable.

How autodiff works?

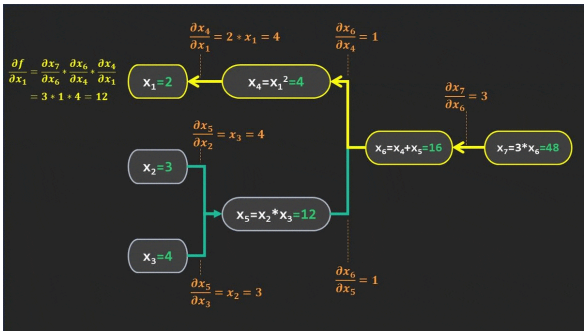


Forward pass



Partial derivatives of each node wrt its inputs

How autodiff works?



Ref: https://medium.com/@rhome/automatic-differentiation-26d5a993692b

Optimizers

What is an optimizer?

Prediction

$$\hat{y} = f(x; w, b) = f(x; \theta) \text{ where } \theta = [w, b]$$

w: weights
b: biases

Loss function

$$L(\theta) = -y \cdot log(\hat{y})$$

Optimizers are algorithms/methods that change the attributes of the model in order to reduce the objective function

Objective:

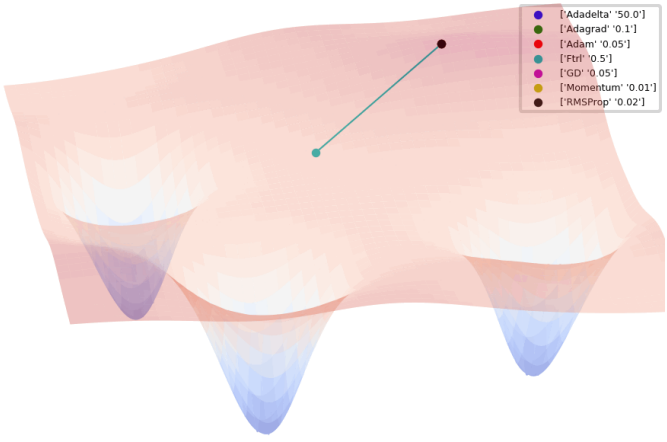
$$min_\theta L(\theta)$$

How?

Start from a random position of theta
Iteratively update it

$$\theta = \theta + \eta\Delta\theta$$

Iterative weight updating



Visualization credit: https://github.com/Jaewan-Yun/optimizer-visualization

Optimizers

- Gradient descent (GD)
- Stochastic gradient descent (SGD)
- Mini-batch gradient descent
- Momentum gradient descent
- Adaptive gradient descent (AdaGrad)
- Root mean square propagation gradient descent (RMSProp)
- Adaptive moment estimation (Adam)

Gradient descent update rule

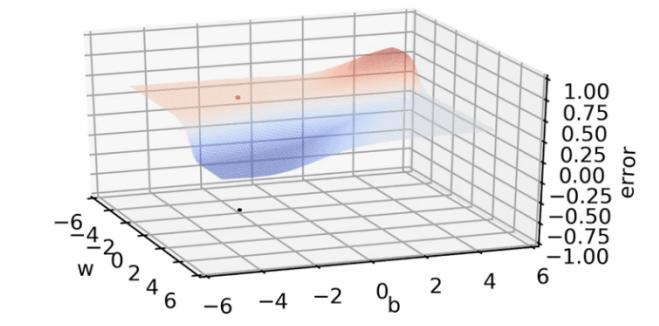
- Randomly initialize w,b
- Iterate over data
  - Compute y-hat
  - Compute loss L(w,b)
  - Update

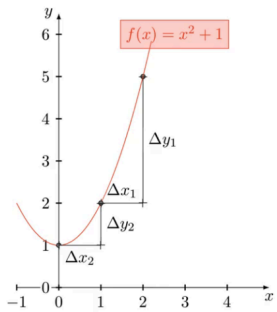
$$w_{t+1} = w_t - \eta \nabla w_t$$
$$b_{t+1} = b_t - \eta \nabla b_t$$
$$where, \nabla w_t = \frac{\partial \mathscr{L}(w,b)}{\partial w}_{at\ w=w_t, b=b_t}, \nabla b = \frac{\partial \mathscr{L}(w,b)}{\partial b}_{at\ w=w_t, b=b_t}$$

Number of updates in one epoch

- Batch gradient descent → 1
- Stochastic gradient descent → N (N = number of data samples)
- Mini-batch gradient descent → N/B (B = batch size)

Gradient descent in flat vs steep area





Visualization credit: Niranjan Kumar

Momentum

Go faster if the same direction is repeated

$$v_t = \gamma * v_{t-1} + \eta \nabla w_t$$
$$w_{t+1} = w_t - v_t$$

AdaGrad (adaptive learning rate)

- Perform larger updates for infrequent parameters and smaller updates for frequent parameters
  - Parameter that is not zero most of the times -> small learning rate
  - Parameter that is zero most of the times, when it is on → higher learning rate to boost the gradient update

$$v_t = v_{t-1} + (\nabla w_t)^2$$
$$w_{t+1} = w_t - \frac{\eta}{\sqrt{(v_t)} + \epsilon} \nabla w_t$$

Non-sparse parameters will have large history value due to frequent updates
→ Small learning rate

Root Mean Square Propagation (RMSProp)

Decaying the history to prevent the rapid growth of the denominator in AdaGrad

$$v_t = \beta * v_{t-1} + (1-\beta)(\nabla w_t)^2$$

$$w_{t+1} = w_t - \frac{\eta}{\sqrt{(v_t)} + \epsilon} \nabla w_t$$

Adaptive moment estimation (Adam)

- Combine Momentum & RMSProp

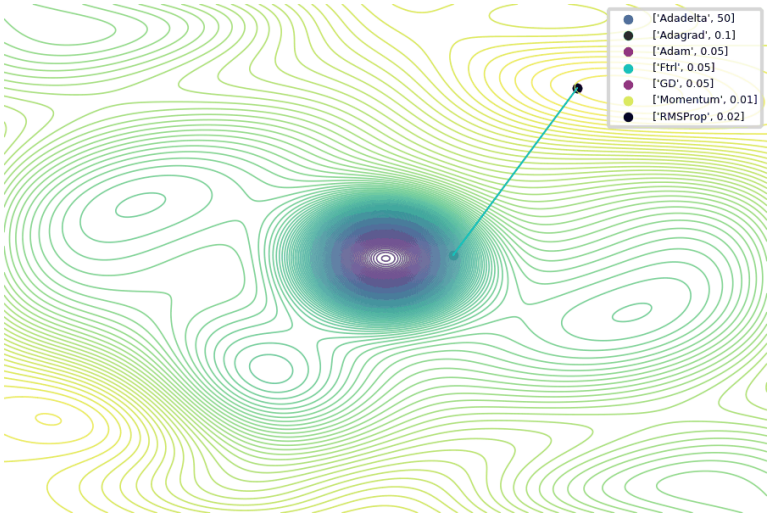
$$m_t = \beta_1 * v_{t-1} + (1-\beta_1)(\nabla w_t)$$

→ use history to compute update

$$v_t = \beta_2 * v_{t-1} + (1-\beta_2)(\nabla w_t)^2$$

→ use history to adjust learning rate (shrink or boost)

$$w_{t+1} = w_t - \frac{\eta}{\sqrt{(v_t)} + \epsilon} m_t$$



Visualization credit: https://github.com/Jaewan-Yun/optimizer-visualization

Learning hyperparameters

- Learning rate
- Momentum
- Decay
- Epsilon (fuzz factor)
- Beta_1, beta_2 -> Adam

References

- Intuition of gradient descent
  - https://hackernoon.com/the-reason-behind-moving-in-the-direction-opposite-to-the-gradient-f9566b95370b
- Backpropagation
  - https://medium.com/binaryandmore/beginners-guide-to-deriving-and-implementing-backpropagation-e3c1a5a1e536
- Optimizers:
  - https://hackernoon.com/demystifying-different-variants-of-gradient-descent-optimization-algorithm-19ae9ba2e9bc