Introduction to Deep Learning

Mnacho Echenim

Grenoble INP-Ensimag

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Notes

Feature preprocessing

- The range of input parameters can be very diverse
  - One way of improving a neural network is to have a uniform representation of inputs
  - Force inputs to have comparable ranges
- Two main techniques
  - Data normalization, or min-max normalization
    - Preprocess training data to collect min and max values along each dimension, obtain the vectors m and M of minima and maxima, respectively
  - **Data standardization**
    - Impose the distribution of training data to have a mean of 0 and standard deviation of 1
    - Compute the mean μ and standard deviation σ of the training data

Notes

An input standardizing layer

- Constructor parameters:
  - Mean of the training input
  - StdDev of the training input
  - Underlying layer
- Forward propagation
  - Standardize the input
  - Invoke forward propagation on the underlying layer with the standardized input
- Backpropagation
  - Deferred to the underlying layer
- Parameter update
  - Deferred to the underlying layer

Notes

Faster training with input standardization

- Compute mean μ and stddev σ of training data S
- Construct preprocessed training data $S' = \left\{ \frac{x-\mu}{\sigma} \,\middle|\, x \in S \right\}$
- Construct input standardizing layer with two modes:
  - Training mode: input is fed to underlying layer with no modification $\rightarrow$ less costly
  - Testing mode: input is standardized before being fed to underlying layer
- Train network with S'
- Set mode to Testing to evaluate network performance

Notes

Batch normalization: Presentation

- *"One of the most exciting recent innovations in optimizing deep neural networks"* (Deep Learning book)
- Original design: optimization of the training phase of a neural network
  - Especially for very deep neural networks
- Impressive results:
  - With the at the time best-performing ImageNet classification network
  - Matched its performance with 14 times less training steps

Notes

Features

- Larger learning rates can be applied
- More activation functions can be used
- The initialization of parameters is less of a problem
- Batch normalization also improves generalization
  - Regularization techniques such as Dropout are less necessary
- **But** more computations are required
  - Not trivial to implement efficiently

Notes

On Internal Covariate Shift

- Neural networks rely on the assumption that the distribution of data is the same during the training and testing phase
  - Optimal parameters for the training phase should work well on the testing phase

Question

How does this distribution of data evolve within hidden layers?

- Example: a neural network with 2 hidden layers
  - The output is $\alpha^2 = f_2(f_1(\alpha^0;\theta^1);\theta^2)$
  - α^0 has distribution $\mathcal{D}_0$, α^1 has distribution $\mathcal{D}_1(\mathcal{D}_0,\theta^1)$
- Gradient descent:
  - $\theta^1 \leftarrow \theta^1 - \eta\nabla_{\theta^1}\mathcal{C}$: optimization w.r.t. distribution $\mathcal{D}_0$
  - $\theta^2 \leftarrow \theta^2 - \eta\nabla_{\theta^2}\mathcal{C}$: optimization w.r.t. distribution $\mathcal{D}_1$
- But after the update of θ^1, the distribution for α^1 is $\mathcal{D}'_1 \neq \mathcal{D}_1$; the optimization of θ^2 may not be efficient

Notes

Principle of Batch Normalization

- Goal: reduce internal covariate shift
- How: by applying a technique similar to input standardization to hidden layers
  - The parameter updates of preceding layers then have less efect on a given layer

Params: γ, β

Input : $(\alpha_{(1)},\ldots,\alpha_{(M)})$, an input mini-batch

$\mu \leftarrow \frac{1}{M}\sum_{m=1}^{M}\alpha_{(m)}$;

$\sigma \leftarrow \sqrt{\frac{1}{M}\sum_{m=1}^{M}(\alpha_{(m)}-\mu)^2}$;

for $m \leftarrow 1$ **to** M **do**

  $\widehat{\alpha_{(m)}} \leftarrow \frac{\alpha_{(m)}-\mu}{\sigma}$;

  $\chi_{(m)} \leftarrow \gamma\widehat{\alpha_{(m)}} + \beta$;

end

return $(\chi_{(1)},\ldots,\chi_{(M)})$

Algorithm 1: Batch normalization algorithm

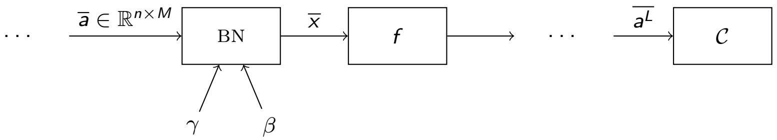
Notes

Remarks on batch normalization computations

- A batch normalization layer has a weights matrix $\Omega = \mathbf{Id}$ and an activation function $\Phi : \mathbb{R}^{n\times M} \to \mathbb{R}^{n\times M}$, for which each column depends on the entire batch
- At Line 4 of the algorithm, it is standard to replace σ by $\sqrt{\sigma^2+\epsilon}$, with $\epsilon \approx 10^{-3}$
- All operations on vectors are applied componentwise
- γ and β are not hyperparameters, they are parameters to be learned
- Because $\Omega = \mathbf{Id}$, computations for backpropagation and gradient descent can be carried out componentwise

Notes

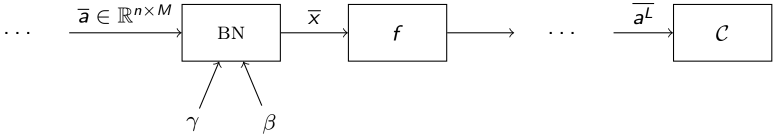
Backpropagation in batch normalization



- During backpropagation, the batch norm layer receives $\left[\nabla_{x_{(m)}}\mathcal{C}\right]_i$ as an input, where $m \in [\![1, M]\!]$ and $i \in [\![1, n]\!]$
- The quantities to compute are:
  - $\nabla_\gamma \mathcal{C}$, for the update of γ
  - $\nabla_\beta \mathcal{C}$, for the update of β
  - $\nabla_{a_{(j)}} \mathcal{C}$, where $j \in [\![1, M]\!]$, for the backpropagation to the previous layer

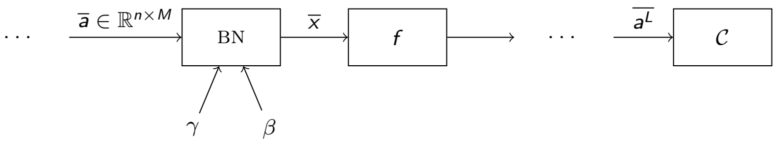
Notes

Backpropagation in batch normalization (2)



Notes

Backpropagation in batch normalization (3)



Notes

Where should batch normalization be applied?

- There are two possibilities:
  - After the activation

$$\left[\overline{\alpha^j}\right]' = \mathrm{BN}\left(\overline{\alpha^j}\right)$$

  - Between the net input and the activation

$$\left[\overline{\alpha^j}\right]' = \Phi\left(\mathrm{BN}\left(\overline{\zeta^j}\right)\right)$$

- Original paper by Ioffe and Zsegedy: apply between the net input and the activation
  - But still some debate
  - May depend on activation function
  - It may be worthwhile to test both solutions

Notes

Mini-batch size

- Trade-off between gradient stability and efficient computation
- Until recently sizes could be very large, up to a few thousand
- Masters, Luschi: *Revisiting Small Batch Training for Deep Neural Networks*, 2018
  - Better to choose sizes between 2 and 32

Notes

Adjusting hyperparameters

- Some of them have recommended values it is better to start with
  - Example: exponential decay rates in Adam: recommended values are $\rho_1 = 0.9$ and $\rho_2 = 0.999$
- Some common techniques
  - Manual search: can be more of an art than a science
  - Grid search: systematic search of different combinations of hyperparameters; select the combination that works best
  - Random search: randomly sample combinations of hyperparameters

Notes

Dropout recommendation

Dropout should be tuned at the same time as the size of hidden layers

- Turn dropout off ($p = 1$)
- Adjust layer sizes until the network fits the training data
- Keep the same layer sizes and retrain the network with dropout turned back on

Notes

Training, validation and test sets

Data is generally partitioned into 3 sets:

- Training set: used to optimize the parameters of the neural network
- Validation set: used to tune the hyperparameters
  - Learning rate
  - Decay rate
  - Momentum parameter
  - Architecture of the network
- Test set: used to forecast how well the network will perform on unknown data

Standard partitioning rule

Partition the data as follows:

- 70% for the training set
- 15% for the validation set
- 15% for the test set

Notes

On cross-validation

- Generally recommended when there is not much data available train and test a model
  - Principle: iteratively use every sample in the dataset at some point in the test phase
- Basic algorithm:

  Input: A network N, number of folds k and dataset $\mathcal{S}$

  create a partition $(\Pi_1, \ldots, \Pi_k)$ of $\mathcal{S}$;
  for $i \leftarrow 1$ **to** k **do**
      train N on $\mathcal{S} \setminus \Pi_i$;
      $\mathcal{E}_i \leftarrow$ validate(N, Π_i);
  end
  return $\frac{\sum_{i=1}^{k} \mathcal{E}_i}{k}$

- Features:
  - Advantage: can reduce overfitting
  - Drawback: training can take much more time
  - Many existing variations (leave-one-out, nested, ...)

Notes

Open questions

- Why does gradient descent work so well on neural networks?
  - The error function is not convex
  - It is very unlikely that gradient descent will reach the global minimum
  - Yet, for an appropriate neural network architecture, the local minimum yields values that are quite close to the global one
- Why can complicated functions even be approximated?
  - Why are so many impressive results obtained on quantum mechanics simulations, image processing, speech recognition or games?
  - The same global algorithm permits to obtain these results; what similarities are there between these functions?
  - Why are there intuitively simple functions that are difficult to approximate?
    - MLPs are not good at learning equality: `https://arxiv.org/pdf/1812.01662.pdf`

Notes

Resources on deep learning techniques in finance

- B. Huge, A. Savine. *Differential Machine Learning*
  - `https://arxiv.org/pdf/2005.02347.pdf`
  - **Principle:** supervised learning or values and differentials
  - TensorFlow implementation available
- B. Lapeyre, J. Lelong. *Neural network regression for Bermudan option pricing*
  - `https://arxiv.org/pdf/1907.06474.pdf`
  - **Principle:** use a neural network to approximate the conditional expectations used to price Bermudan options
- S. Becker, P. Cheridito, A. Jentzen. *Deep optimal stopping*
  - `https://arxiv.org/pdf/1804.05394.pdf`
  - **Principle:** use Reinforcement Learning to compute optimal stopping times (used to price Bermudan options)

Notes

Other resources

- Practical advice for building and debugging a neural network:
  - `https://pcc.cs.byu.edu/2017/10/02/practical-advice-for-building-deep-neural-networks/`
  - `http://cs231n.github.io/neural-networks-3/`
- Seminar by Pierre Courtiol at Collège de France: `https://www.college-de-france.fr/site/stephane-mallat/seminar-2018-02-21-11h15.htm`

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