Deep Neural Networks (3)
Computational Graphs, Learning Algorithms, Initialisation

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Machine Learning Practical — MLP Lecture 5
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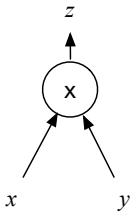
Computational Graphs

Computational graphs

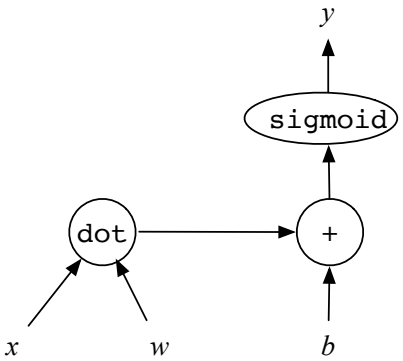
- Each node is an operation
- Data flows between nodes (scalars, vectors, matrices, tensors)
- More complex operations can be formed by composing simpler operations

Computational graph example 1



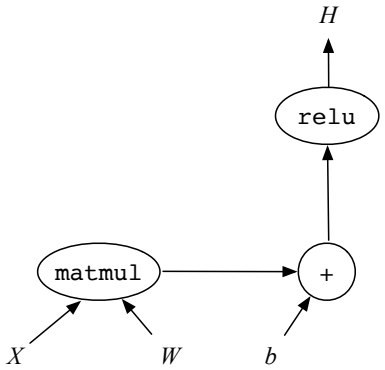
Graph for $\times$ to compute $z = xy$

Computational graph example 2



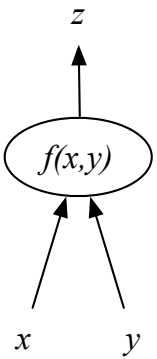
Graph for logistic regression:
$y = \text{sigmoid}(\boldsymbol{w}^\top \boldsymbol{x} + b)$

Computational graph example 3

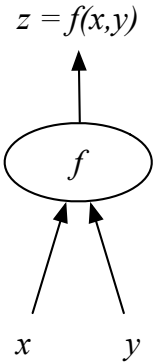


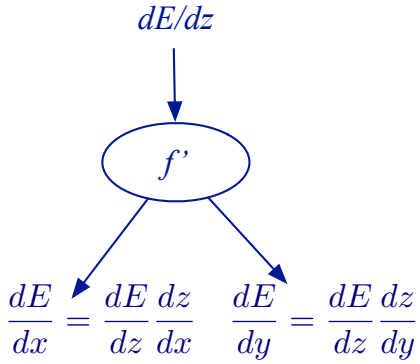
Graph for ReLU layer:
$\boldsymbol{H} = \text{relu}(\boldsymbol{W}\boldsymbol{X} + \boldsymbol{b})$

Computational graphs and back-propagation



Computational graphs and back-propagation





Chain rule of differentiation as the backward pass through the computational graph

Computational graphs

- Each node is an operation
- Data flows between nodes (scalars, vectors, matrices, tensors)
- More complex operations can be formed by composing simpler operations
- Implement chain rule of differentiation as a backward pass through the graph
- Back-propagation: Multiply the local gradient of an operation with an incoming gradient (or sum of gradients)
- See http://colah.github.io/posts/2015-08-Backprop/

How to set the learning rate?

Weight Updates

- Let $d_i(t) = \partial E / \partial w_i(t)$ be the gradient of the error function E with respect to a weight w_i at update time t
- "Vanilla" gradient descent updates the weight along the negative gradient direction:

$$\Delta w_i(t) = -\eta d_i(t)$$
$$w_i(t+1) = w_i(t) + \Delta w_i(t)$$

  Hyperparameter η - *learning rate*
- Initialise η, and update as the training progresses (learning rate schedule)

Learning Rate Schedules

- Proofs of convergence for stochastic optimisation rely on a learning rate that reduces through time (as $1/t$) - Robbins and Munro (1951)
- Learning rate schedule – typically initial larger steps followed by smaller steps for fine tuning: Results in *faster convergence* and *better solutions*

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- Learning rate schedule – typically initial larger steps followed by smaller steps for fine tuning: Results in *faster convergence* and *better solutions*
- **Time-dependent** schedules

$$\Delta w_i(t) = -\eta(t) d_i(t)$$

  - **Piecewise constant**: pre-determined η for each epoch
  - **Exponential**: $\eta(t) = \eta(0) \exp(-t/r)$ ($r \sim$ training set size)
  - **Reciprocal**: $\eta(t) = \eta(0)(1 + t/r)^{-c}$ ($c \sim 1$)

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  - **Reciprocal**: $\eta(t) = \eta(0)(1 + t/r)^{-c}$ ($c \sim 1$)
- **Performance-dependent** η – e.g. "NewBOB": fixed η until validation set stops improving, then halve η each epoch (i.e. constant, then exponential)

Training with Momentum

$$\Delta w_i(t) = -\eta d_i(t) + \alpha \Delta w_i(t-1)$$

- $\alpha \sim 0.9$ is the *momentum* hyperparameter
- Weight changes start by following the gradient
- After a few updates they start to have *velocity* – no longer pure gradient descent
- Momentum term encourages the weight change to go in the previous direction
- Damps the random directions of the gradients, to encourage weight changes in a consistent direction

Adaptive Learning Rates

- Tuning learning rate (and momentum) parameters can be expensive (hyperparameter grid search) – it works, but we can do better
- Adaptive learning rates and per-weight learning rates
  - AdaGrad – normalise the update for each weight
  - RMSProp – AdaGrad forces the learning rate to always decrease, this constraint is relaxed with RMSProp
  - Adam – "RMSProp with momentum"

Well-explained by Andrej Karpathy at
http://cs231n.github.io/neural-networks-3/

AdaGrad

- Separate, normalised update for each weight
- Normalised by the sum squared gradient S

$$
\begin{aligned}
S_i(0) &= 0 \\
S_i(t) &= S_i(t-1) + d_i(t)^2 \\
\Delta w_i(t) &= \frac{-\eta}{\sqrt{S_i(t)} + \epsilon} d_i(t)
\end{aligned}
$$

$\epsilon \sim 10^{-8}$ is a small constant to prevent division by 0 errors

AdaGrad

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$$S_i(t) = S_i(t-1) + d_i(t)^2$$
$$\Delta w_i(t) = \boxed{\frac{-\eta}{\sqrt{S_i(t)} + \epsilon}} d_i(t)$$

  $\epsilon \sim 10^{-8}$ is a small constant to prevent division by 0 errors
- The update step for a parameter w_i is normalised by the (square root of) the sum squared gradients for that parameter
  - Weights with larger gradient magnitudes will have smaller effective learning rates
  - S_i cannot get smaller, so the effective learning rates monotonically decrease
- AdaGrad can decrease the effective learning rate too aggressively in deep networks

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Duchi et al, http://jmlr.org/papers/v12/duchi11a.html

RMSProp

- RProp (Riedmiller & Braun, http://dx.doi.org/10.1109/ICNN.1993.298623) is a method for batch gradient descent with an adaptive learning rate for each parameter, and uses only the sign of the gradient (which is equivalent to normalising by the gradient)
- RMSProp can be viewed as a stochastic gradient descent version of RProp normalised by a moving average of the squared gradient (Hinton, http://www.cs.toronto.edu/~tijmen/csc321/slides/lecture_slides_lec6.pdf) – similar to AdaGrad, but replacing the sum by a moving average for S:

$$S_i(t) = \beta S_i(t-1) + (1-\beta)\, d_i(t)^2$$

$$\Delta w_i(t) = \frac{-\eta}{\sqrt{S_i(t)} + \epsilon}\, d_i(t)$$

$\beta \sim 0.9$ is the decay rate

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  $\beta \sim 0.9$ is the decay rate
- Effective learning rates no longer guaranteed to decrease

Adam

- Hinton commented about RMSProp: "Momentum does not help as much as it normally does"

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- Adam (Kingma & Ba, https://arxiv.org/abs/1412.6980) can be viewed as addressing this – it is a variant of RMSProp with momentum:

$$M_i(t) = \alpha M_i(t-1) + (1-\alpha) d_i(t)$$
$$S_i(t) = \beta S_i(t-1) + (1-\beta) d_i(t)^2$$
$$\Delta w_i(t) = \frac{-\eta}{\sqrt{S_i(t)} + \epsilon} M_i(t)$$

Here a momentum-smoothed gradient is used for the update in place of the gradient. Kingma and Ba recommend $\alpha \sim 0.9$, $\beta \sim 0.999$

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Many hyperparameters:
batch-size, learning-rate, momentum,
learning-decay-rate, num-layers, num-units, ...

How to set them?

$$\sqrt{S_i(t)} + \epsilon$$

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Coursework 1

http://www.inf.ed.ac.uk/teaching/courses/mlp/coursework-2018.html

- Build a baseline using the EMNIST dataset
- Compare RMSProp and Adam with SGD
- Cosine annealing learning rate scheduler
- L2 regularization / weight decay with Adam and cosine annealing
- Inspired by Loshchilov and Hutter, Fixing Weight Decay Regularization in Adam

Main aims of the coursework

- Read and understand a recent paper in the area
- Take the ideas from a paper, implement them in Python, carry out experiments to address research questions
- Write a clear, concise, correct report that includes
  - **What** you did
  - **Why** you did it
  - and provides an **interpretation** of your results, and some **conclusions**

How should we initialise deep networks?

Random weight initialisation

- Initialise weights to small random numbers r, sampling weights independently from a Gaussian or from a uniform distribution
  - control the initialisation by setting the mean (typically to 0) and variance of the weight distribution
- Biases may be initialised to 0
  - output (softmax) biases can be normalised to $\log(p(c))$, log of prior probability of the corresponding class c

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  - output (softmax) biases can be normalised to $\log(p(c))$, log of prior probability of the corresponding class c
- Calibration – variance of the input to a unit independent of the number of incoming connections ("fan-in", n_{in})
- Heuristic: $w_i \sim U(-\sqrt{1/n_{in}}, \sqrt{1/n_{in}})$ [U is uniform distribution]
  - Corresponds to a variance $\mathrm{Var}(w_i) = 1/(3n_{in})$
  - (Since, if $x \sim U(a, b)$, then $\mathrm{Var}(x) = (b-a)^2/12$ so if $x \sim U(-n, n)$, then $\mathrm{Var}(x) = n^2/3$)

Why $\mathrm{Var}(w) \sim 1/n$?

Consider a linear unit:

$$y = \sum_{i=1}^{n_{in}} w_i x_i$$

if w and x are zero-mean, then

$$\mathrm{Var}(y) = \mathrm{Var}(\sum_{i=1}^{n_{in}} w_i x_i) = n_{in}\,\mathrm{Var}(x)\,\mathrm{Var}(w)$$

if w and x are iid (independent and identically distributed)

So, if we want variance of inputs x and outputs y to be the same, set

$$\mathrm{Var}(w_i) = \frac{1}{n_{in}}$$

Nicely explained at http://andyljones.tumblr.com/post/110998971763/an-explanation-of-xavier-initialization

"GlorotInit" ("Xavier initialisation")

- We would like to constrain the variance of each layer to be $1/n_{in}$, thus

$$w_i \sim U(-\sqrt{3/n_{in}}, \sqrt{3/n_{in}})$$

- However we need to take the backprop into account, hence we would also like $\mathrm{Var}(w_i) = 1/n_{out}$
- As compromise set the variance to be $\mathrm{Var}(w_i) = 2/(n_{in} + n_{out})$
- This corresponds to Glorot and Bengio's normalised initialisation

$$w_i \sim U\left(-\sqrt{6/(n_{in} + n_{out})}, \sqrt{6/(n_{in} + n_{out})}\right)$$

Glorot and Bengio, "Understanding the difficulty of training deep feedforward networks", *AISTATS*, 2010.

http://www.jmlr.org/proceedings/papers/v9/glorot10a.html

Summary

- Computational graphs
- Learning rate schedules and gradient descent algorithms
- Initialising the weights
- **Reading**
  - Goodfellow et al, sections 6.5, 8.3, 8.5
  - Olah, "Calculus on Computational Graphs: Backpropagation", http://colah.github.io/posts/2015-08-Backprop/
  - Andrej Karpathy, CS231n notes (Stanford) http://cs231n.github.io/neural-networks-3/
- **Additional Reading**
  - Kingma and Ba, "Adam: A Method for Stochastic Optimization", ICLR-2015 https://arxiv.org/abs/1412.6980
  - Glorot and Bengio, "Understanding the difficulty of training deep feedforward networks", AISTATS-2010. http://www.jmlr.org/proceedings/papers/v9/glorot10a.html