Optimization Techniques for Big Data Analysis

Chapter 4. First-Order Methods Applied to Neural Networks

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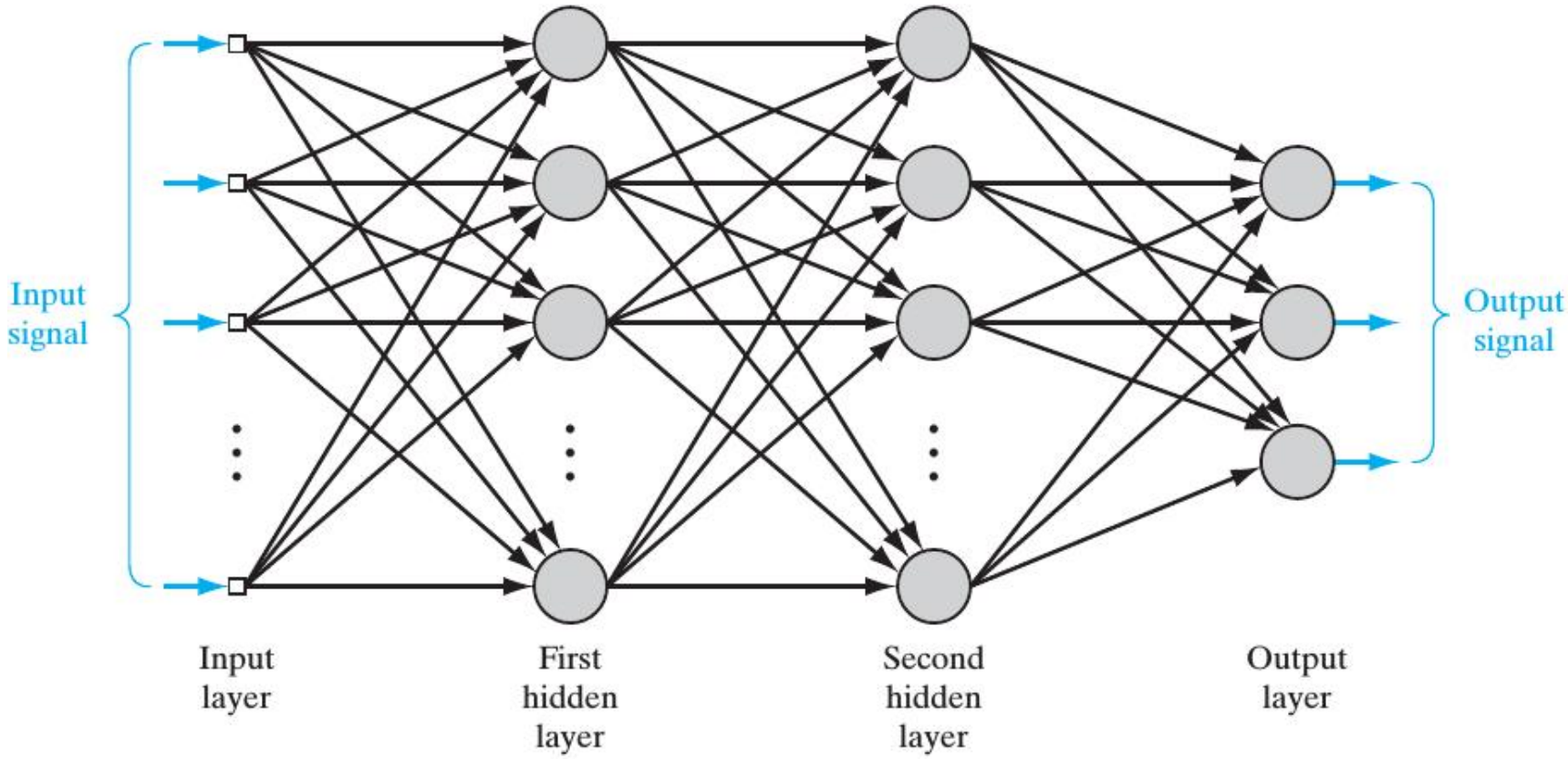
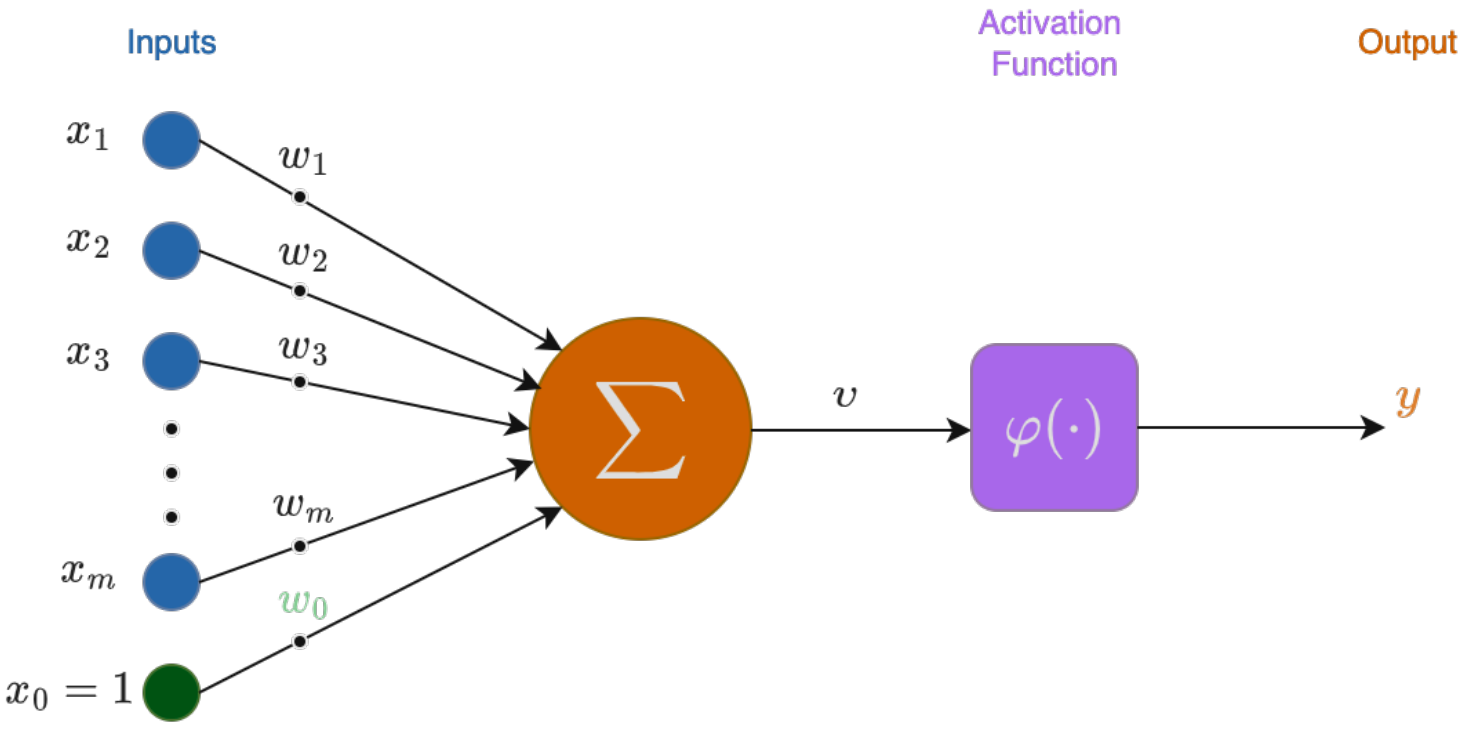
2024

Scheme of a DNN



Basic unit: the neuron



The basic operation of a single neuron corresponds to:

$$y = \varphi\left(\sum_{j=1}^{m} x_j w_j + w_0\right) = \varphi\left(\mathbf{w}^T \mathbf{x}\right)$$

DNN output function

For a neural network of with one hidden layer, the p-th output for one input $\mathbf{x}_i = [x_{1,i}, x_{2,i}, \cdots, x_{j,i}, \cdots, x_{d,i}]^T$ is given by,

$$o_p(\mathbf{x}_i) = \varphi^{(2)} \left(\sum_{l=1}^{m_1} w_{pl}^{(2)} \varphi^{(1)} \left(\sum_{j=1}^{d} w_{lj}^{(1)} x_{j,i} + w_{l0}^{(1)} \right) + w_{p0}^{(2)} \right)$$

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To estimate it, the forward pass does the following:

$$\text{Layer 1} \rightarrow v_{l,i}^{(1)} = \sum_{j=0}^{d} w_{lj}^{(1)} x_{j,i} \quad z_{l,i}^{(1)} = \varphi^{(1)} \left(v_{l,i}^{(1)} \right)$$

$$\text{Layer 2} \rightarrow v_{p,i}^{(2)} = \sum_{l=0}^{m_1} w_{pl}^{(2)} z_{l,i}^{(1)} \quad z_{p,i}^{(2)} = \varphi^{(2)} \left(v_{p,i}^{(2)} \right)$$

Cost function

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Note that the DNN could have multiple outputs, in that case be $\mathbf{y}_i = [y_{1,i}, \cdots, y_{p,i}, \cdots, y_{q,i}]$, the q-dimensional vector with the labels for the i-th sample.

$$\mathcal{L}(\mathbf{W}) = \frac{1}{n}\sum_{i=1}^{n}\sum_{p=1}^{q} e_{p,i}^2 = \frac{1}{n}\sum_{i=1}^{n}\sum_{p=1}^{q} (o_{p,i} - y_{p,i})^2$$

Weights update rule

During one iteration of the learning algorithm:

$$w^{(t)}[k+1] = w^{(t)}[k] - \eta \frac{\partial \mathcal{L}}{\partial w^{(t)}}$$

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Considering the former example, if $t = 2$ the updating rule looks like:

$$w_{pl}^{(2)}[k+1] = w_{pl}^{(2)}[k] - \frac{\eta}{n} \sum_{i=1}^{n} \left(\frac{\partial \ell_{p,i}}{\partial e_{p,i}} \frac{\partial e_{p,i}}{\partial \varphi_{p,i}^{(2)}} \frac{\partial \varphi_{p,i}^{(2)}}{\partial v_{p,i}^{(2)}} \frac{\partial v_{p,i}^{(2)}}{w_{pl}^{(2)}[k]} \right)$$

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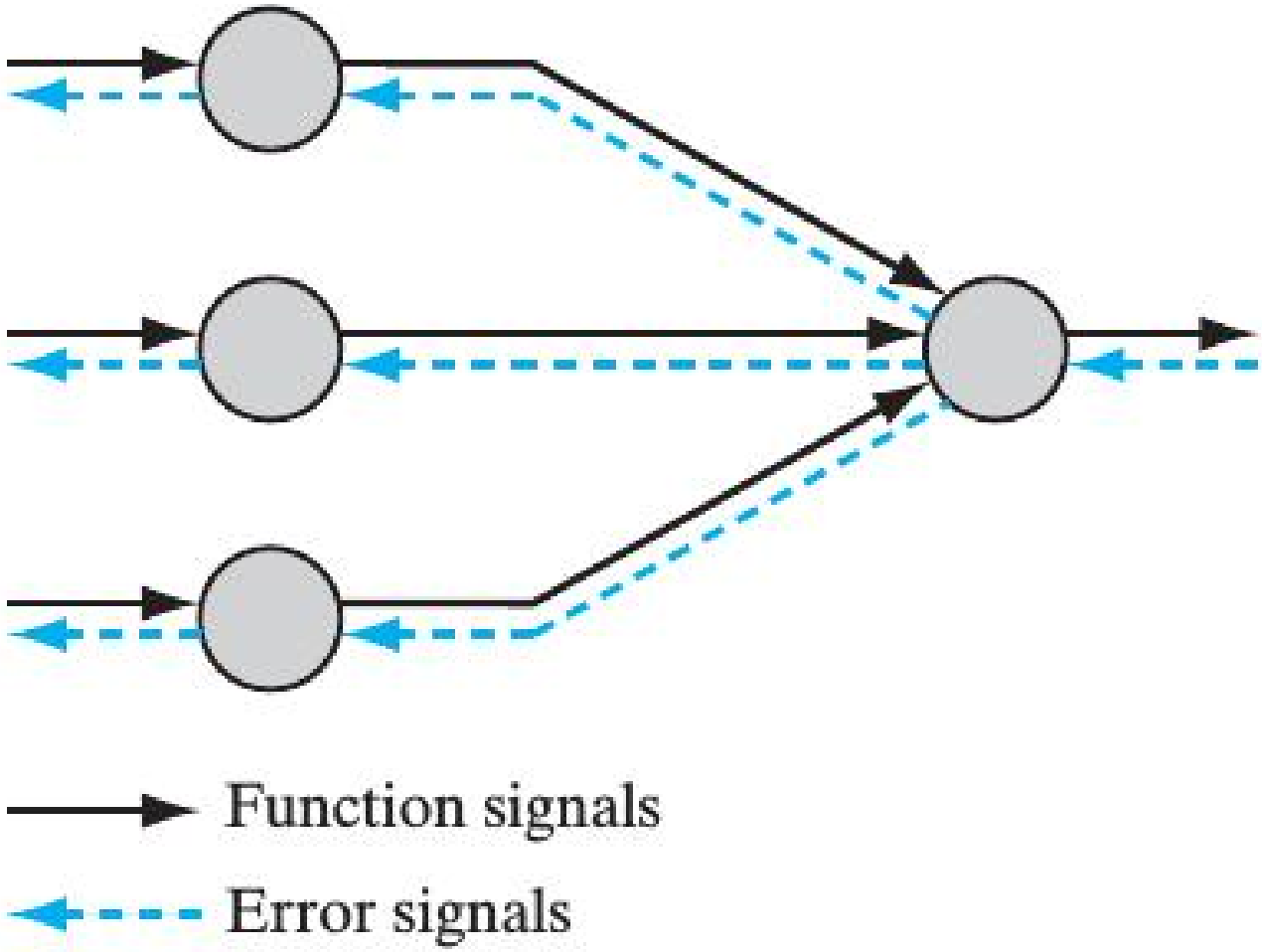
The updating rule for $t = 1$ (backward pass) looks like this:

$$w_{lj}^{(1)}[k+1] = w_{lj}^{(1)}[k+1] - \frac{\eta}{n} \sum_{i=1}^{n} \sum_{p=1}^{q} \left(\delta_{p,i} \frac{\partial \upsilon_{p,i}^{(2)}}{z_{l,i}^{(1)}} \frac{\partial z_{l,i}^{(1)}}{\partial \varphi_{l,i}^{(1)}} \frac{\partial \varphi_{l,i}^{(1)}}{\partial \upsilon_{l,i}^{(1)}} \frac{\partial \upsilon_{l,i}^{(1)}}{\partial w_{lj}^{(1)}[k]} \right)$$

Signal flows



Gradient calculation

All factors in the updating rules can be calculated easily:

$$\frac{\partial \ell_{p,i}}{\partial e_{p,i}} \rightarrow 2(o_{p,i} - y_{p,i})$$

$$\frac{\partial e_{p,i}}{\partial \varphi_{p,i}^{(2)}} \rightarrow 1$$

$$\frac{\partial \varphi_{p,i}^{(2)}}{\partial \upsilon_{p,i}^{(2)}} \rightarrow \varphi^{'(2)}\left(\upsilon_{p,i}^{(2)}\right)$$

$$\frac{\partial \upsilon_{p,i}^{(2)}}{\partial w_{pl}^{(2)}} \rightarrow z_{l,i}^{(1)}$$

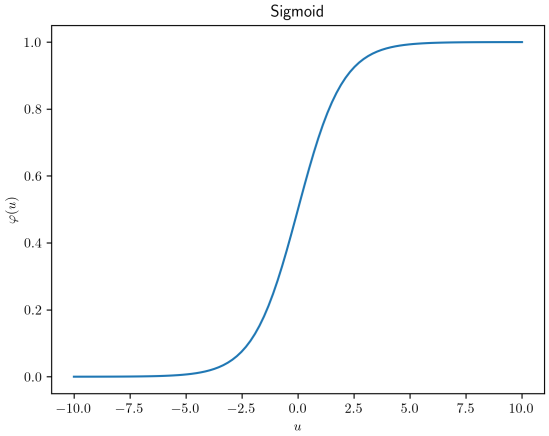
$$\frac{\partial \upsilon_{p,i}^{(2)}}{\partial z_{l,i}^{(1)}} \rightarrow w_{p,l}^{(2)}$$

$$\frac{\partial z_{l,i}^{(1)}}{\partial \varphi_{l,i}^{(1)}} \rightarrow 1$$

$$\frac{\partial \varphi_{l,i}^{(1)}}{\partial \upsilon_{l,i}^{(1)}} \rightarrow \varphi^{'(1)}(\upsilon_{l,i}^{(1)})$$

$$\frac{\partial \upsilon_{l,i}^{(1)}}{\partial w_{lj}^{(1)}} \rightarrow x_{j,i}$$

Activation Functions



Sigmoid

$$\varphi(u) = \frac{\exp(u)}{1+\exp(u)} = \frac{1}{1+\exp(-u)}$$

$$\varphi^{'}(u) = \varphi(u)(1-\varphi(u))\partial u$$

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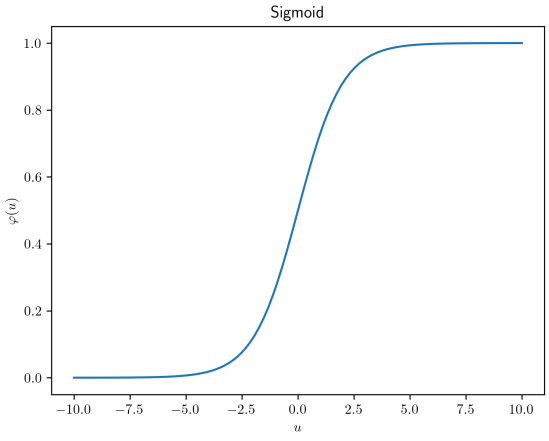

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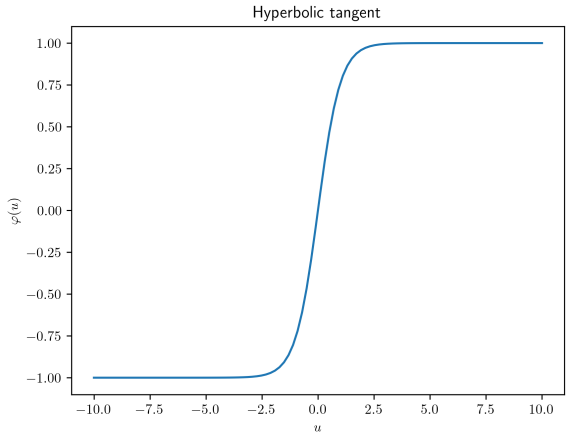

Hyperbolic tangent

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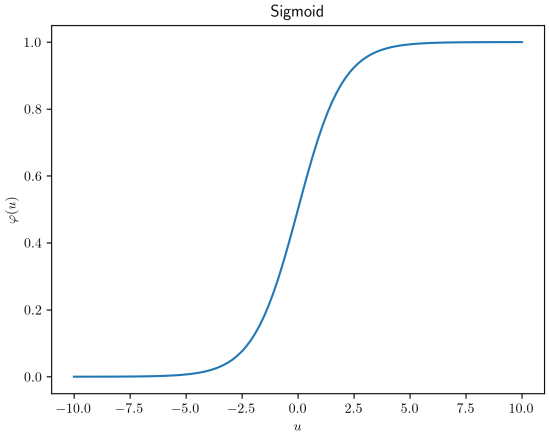

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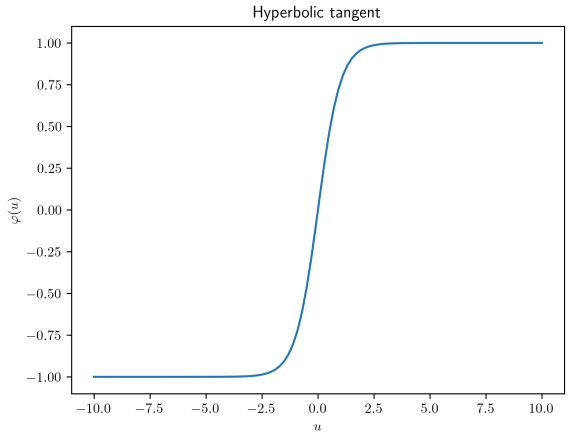

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Softmax

$$\varphi(u_p) = \frac{\exp(u_p)}{\sum_{l=1}^{C}\exp(u_l)}, \quad \frac{\partial\varphi(u_p)}{\partial u_l} = \varphi(u_p)(\iota_{pl}-\varphi(u_l)), \quad \iota_{pl} = \begin{cases} 1 & \text{if} \quad p = l \\ 0 & \text{if} \quad p \neq l \end{cases}$$

Remarks

It is worth highlighting the following:

- The objective function is non-convex.
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Think about what the algorithm needs to keep in memory for a whole epoch (forward and backward passes)

Stochastic Gradient Methods

$$f(\mathbf{w}) = \mathbb{E}[\ell_{\mathbf{w}}(\mathbf{x})] + r(\mathbf{w})$$

For the standard gradient descent, during iteration k, we need access to the actual gradient vector $\nabla_{\mathbf{w}} f(\mathbf{w}_k)$.

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In this case, the expectation $f(\mathbf{w})$ must be replaced by an instantaneous approximation of it, $f_s(\mathbf{w}) = \ell_{\mathbf{w}}(\mathbf{x}) + r(\mathbf{w})$. This is what we label it as the stochastic approach:

$$\mathbf{w}_{k+1} = \mathbf{w}_k - \eta \nabla_{\mathbf{w}} f_s(\mathbf{w}_k)$$

Stochastic Gradient Methods

Working with gradient estimates instead of the gradient itself implies certain impairments that we have to take into account.

$$s_k\left(\mathbf{w}_k\right) = \nabla_{\mathbf{w}} f_s\left(\mathbf{w}_k\right) - \nabla_{\mathbf{w}} f\left(\mathbf{w}_k\right)$$

This noise perturbation is known as *Gradient Noise Process*

1. Prevents the stochastic iterate from converging to the optimum $\mathbf{w}^*$ when constant step sizes are used (less convergence level).
2. Some deterioration in performance occurs since the iterate $\mathbf{w}_k$ will instead fluctuate close to $\mathbf{w}^*$ in the steady state regime.

Stochastic Gradient Methods.Performance metrics

1. *Mean Square Deviation (MSD)* that refers to the fluctuations level of the sequence of the coefficients around the optimum value.
2. On the other hand the *Excess Risk (ER)* refers to the mean deviation at the end of convergence of the objective function along the sequence of coefficients with respect to the objective function particularized at the optimum value.

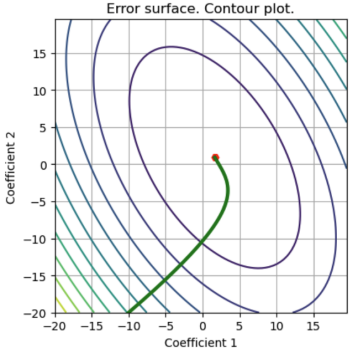
For fixed step size, we have (let us remind that for decaying step size $MSD = ER = 0$ but paying extra convergence time):

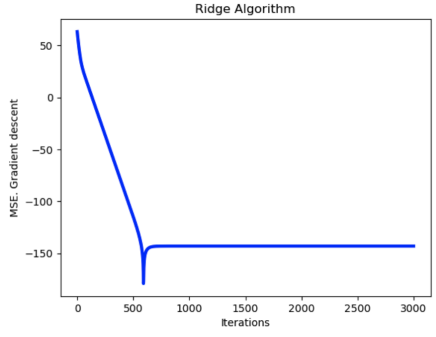
$$MSD \triangleq \lim_{k\to\infty} E\left\{\|\mathbf{w}_k - \mathbf{w}^*\|_2^2\right\}$$
$$ER = \lim_{k\to\infty} E\left\{f\left(\mathbf{w}_k\right) - f\left(\mathbf{w}^*\right)\right\}$$

Examples

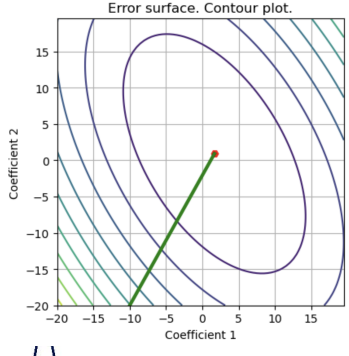
Have a look at the examples; in all of them, the addressed problem corresponds to ridge regression:

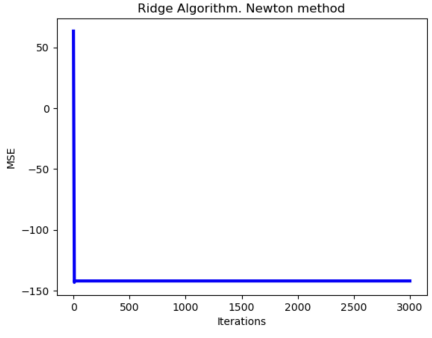
`Example_4_1`: Learning curve and error surface for FOM.



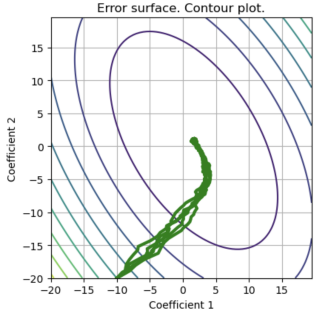


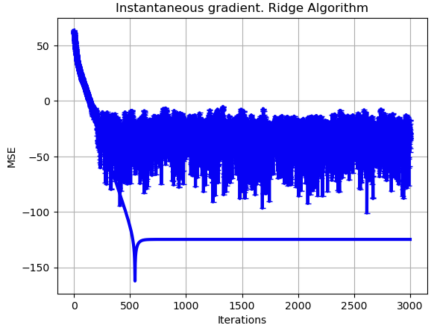
`Example_4_2`: Learning curve and error surface for SOM.





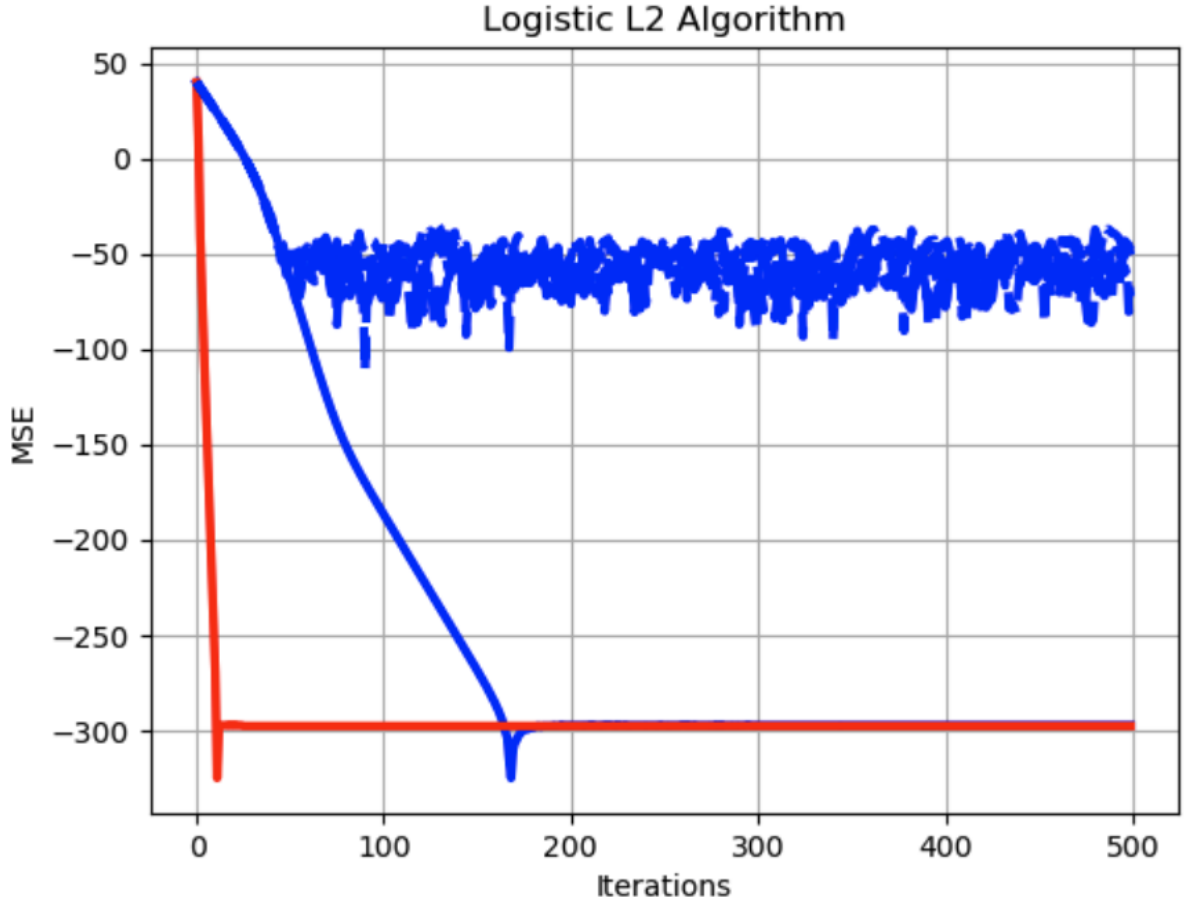
`Example_4_3`: Learning curve and error surface for SGD.



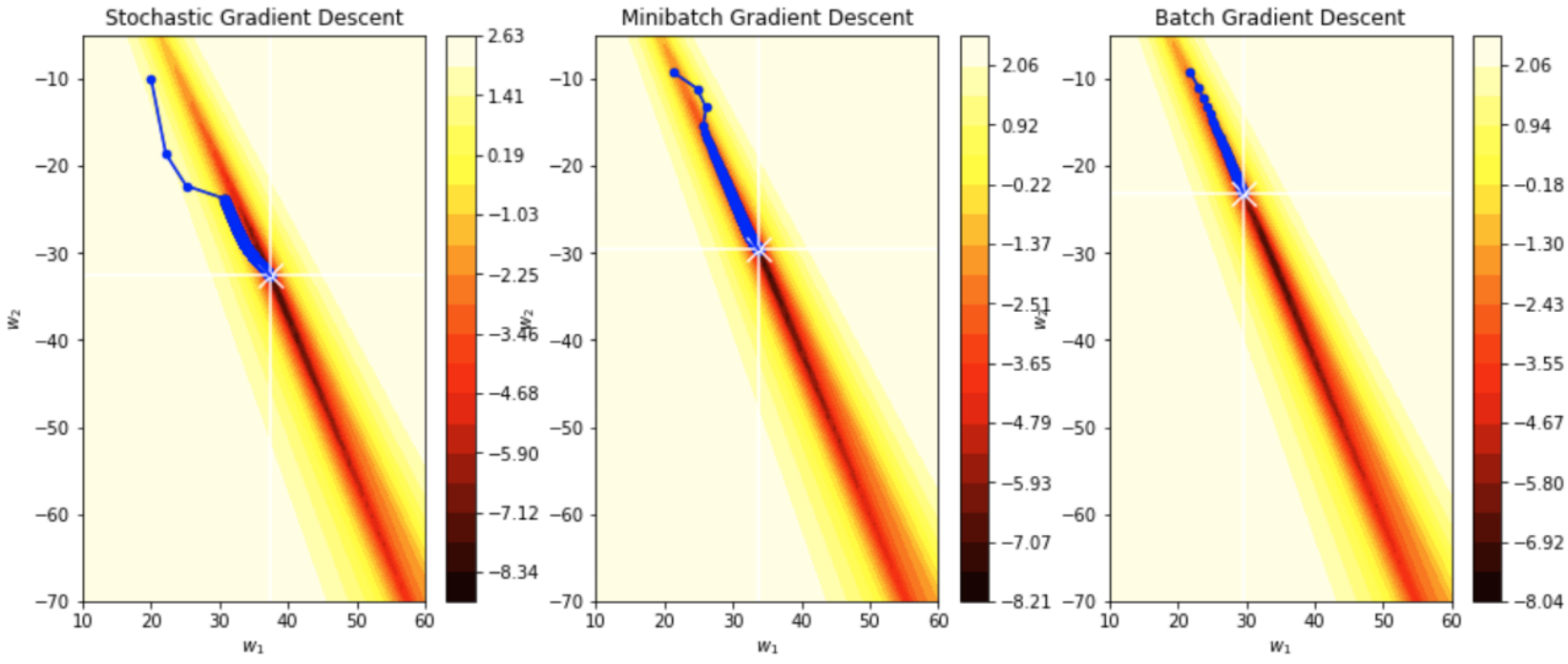


Case studies

- `Case_study_4_1`: This is just an overview of the previous examples putting all together.
- `Case_study_4_2`: This is a similar exercise but focuses on the logistic functions instead.



Minibatch


Stochastic Gradient Descent
Minibatch Gradient Descent
Batch Gradient Descent
w_1
w_2
−10
−20
−30
−40
−50
−60
−70
10
20
30
40
50
60
2.63
1.41
0.19
−1.03
−2.25
−3.46
−4.68
−5.90
−7.12
−8.34
2.06
0.92
−0.22
−1.37
−2.51
−3.65
−4.79
−5.93
−7.07
−8.21
2.06
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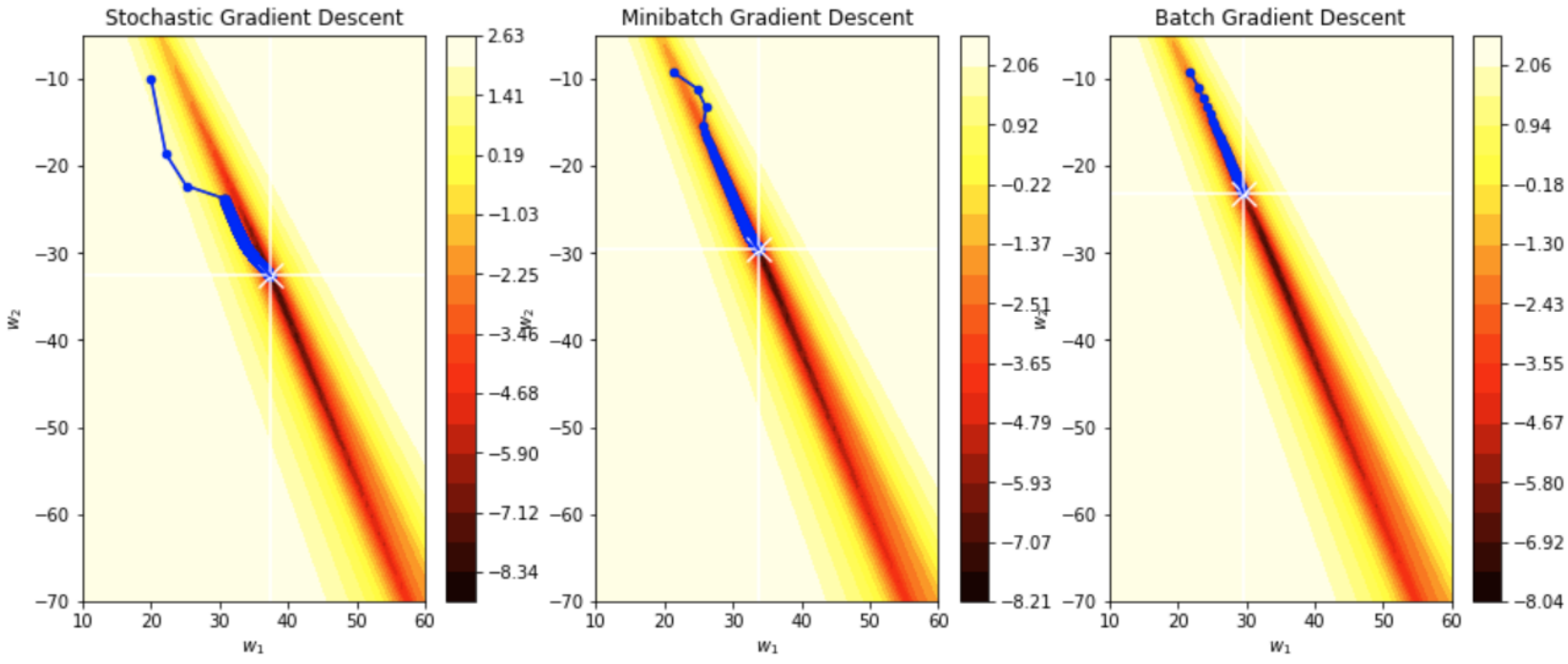
−8.04

Minibatch



Stochastic behaviour has positive effects regarding saddle points!

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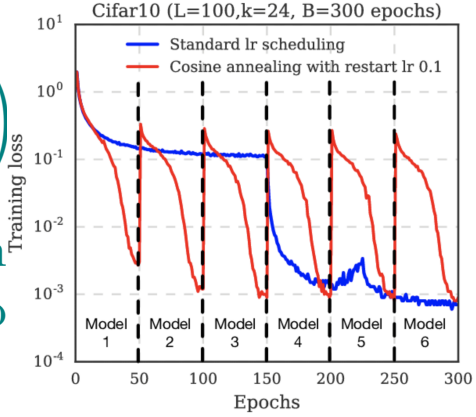
- Learning rate schedulers:
  - Cosine annealing (warm restart) [1]:

$$\eta_k = \eta_{min} + \frac{1}{2}(\eta_{max} - \eta_{min}) \left(1 + \cos\left(\frac{T_{cur}}{T}\right)\right)$$

T_{cur} accounts for how many epochs have been performed since the last restart. You can also increase T by a T_{mul} factor every restart.



Adaptive Gradient Algorithm (Adagrad)

Decay the learning rate for parameters in proportion to their update history (more updates means more decay).

The update rule used is:

$$\mathbf{g}_{k+1} = \mathbf{g}_k + (\nabla f(\mathbf{w}_k))^2$$
$$\mathbf{w}_{k+1} = \mathbf{w}_k - \frac{\eta}{\sqrt{\mathbf{g}_{k+1}} + \varepsilon} \odot \nabla f(\mathbf{w}_k)$$

with $\mathbf{g}_0 = \mathbf{0}$. The step size is adjusted automatically: parameters with large accumulated gradient have a smaller step, and parameters with small accumulated gradient have a larger update.

This feature of Adagrad makes it also useful for dealing with sparse data.

RMSProp / Adadelta.

In Adagrad, the sum of the gradients is always increasing; thus the algorithm stops learning eventually.

Unlike Adagrad, in **RMSProp** instead of allowing this sum to increase continuously over the training period, we allow the sum to decrease.

$$\mathbf{g}_{k+1} = \beta \mathbf{g}_k + (1-\beta)\left(\nabla f(\mathbf{w}_k)\right)^2$$
$$\mathbf{w}_{k+1} = \mathbf{w}_k - \frac{\eta}{\sqrt{\mathbf{g}_{k+1}} + \varepsilon} \odot \nabla f(\mathbf{w}_k)$$

with $\mathbf{g}_0 = \mathbf{0}$, $\beta \simeq 0.9$. RMSProp exhibits the same property of speeding up the updating of the weights along one dimension and slowing down the motion along the other.

A similar algorithm to RMSProp, developed independently, is **Adadelta** [3].

Adaptive moment estimator (Adam)

Adam intuitively consists in adding momentum to RMSProp to improve its convergence speed.

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$$\mathbf{v}_{k+1} = \beta_1 \mathbf{v}_k - (1 - \beta_1) \nabla f(\mathbf{w}_k)$$

$$\mathbf{g}_{k+1} = \beta_2 \mathbf{g}_k + (1 - \beta_2) \left(\nabla f(\mathbf{w}_k)\right)^2$$

$$\mathbf{w}_{k+1} = \mathbf{w}_k - \frac{\eta}{\sqrt{\mathbf{g}_{k+1}} + \varepsilon} \odot \mathbf{v}_{k+1}$$

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To address the giant update steps happening at the beginning of training, Adam applies a bias correction: $\hat{\mathbf{v}}_{k+1} = \frac{\mathbf{v}_{k+1}}{1-\beta_1^k}$ and $\hat{\mathbf{g}}_{k+1} = \frac{\mathbf{g}_{k+1}}{1-\beta_2^k}$. Usually $\beta_1 = 0.9$ and $\beta_2 = 0.999$.

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Case_studies and examples

Go to the repository and take a look to following notebooks:

- `Example_4_4`: Ridge regression using Adam optimizer.
- `Case_study_4_3`: Vanilla NN for a regression problem using SGD.
- `Case_study_4_4`: Same network than before but using Adam optimizer.
- `Case_study_4_5`: Vanilla NN for solving the XOR problem.
- `Case_study_4_6`: Vanilla NN for a nonlinear classification problem.

Parallel and distributed gradient

Gradient methods are also amenable to parallel and distributed implementations:

- Parallel refers to using multiple processors in the same computer.
- Distributed is a more general concept, in which the computations are distributed among many different computers. It has to deal with:
  - Latency problems
  - Synchronicity problems

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Let us recall the gradient update rule for the least squares problem:

$$\mathbf{w}_{k+1} = \mathbf{w}_k - \mu_k \left[\frac{2}{n} \sum_{i=1}^{n} \left(\mathbf{w}_k^T \mathbf{x}_i - y_i \right) \mathbf{x}_i \right]$$

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If we have a computer with $M = 1$ processor, for each iteration k, the processor must:

- Obtain the n vector operations of the sum
- Perform the sum
- Perform the update

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The most time-consuming part is obtaining the n sum terms, which you may notice are independent.

So, if we have hardware with $M > 1$, we can split the computations of the sum terms across them.

Map - Reduce

Map - Reduce is a programming paradigm developed for processing data in distributed file systems (Hadoop). Its logic is based on two operations: 1) Map and 2) Reduce.

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Applied to GD it would work like this:

- Map step: split the n-sized training dataset into M subsets (partitions) with L training samples each, and let each processor obtain $\mathbf{p}_{m,k}, m \in 1, 2, ..., M$:

$$\mathbf{p}_{m,k} = \sum_{j=(m-1)L}^{mL-1} \left(\mathbf{w}_k^T \mathbf{x}_j - y_j\right) \mathbf{x}_j$$

Map - Reduce

- Reduce step: update the gradient:

$$\mathbf{w}_{k+1} = \mathbf{w}_k - 2\frac{\mu_k}{n}\sum_{m=1}^{M}\mathbf{p}_{m,k}$$

This step collects the computations done in the Map step to obtain an update.

Map - Reduce

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This step collects the computations done in the Map step to obtain an update.

If Reduce computation time is negligible compared to the Map computation time, the parallel version may speed up the computation by a factor up to M.

This, however, is hard to reach in real life due to other possible bottlenecks, such as memory access.

Distributed gradient

- The Map-Reduce scheme can also be used in a distributed setting, but we must consider communication-related problems (latency), especially in **synchronous** schemes, as we need all computers to wait for the others to make an update.
- It is possible to develop more advanced, **asynchronous** approaches, such as HOGWILD! [2], that only requires nodes (processors) access to shared memory with the possibility of overwriting each other work.
- If the optimization problem is sparse (most gradient updates only modify small parts of the decision variable), HOGWILD! achieves an early optimal rate of convergence.

Acknowledgments

I would like to acknowledge several sources I have used to create slides

- Akshay L Chandra, "Learning Parameters, Part 5: AdaGrad, RMSProp, and Adam". `https://towardsdatascience.com/learning-param...`
- Artem Oppermann, "Optimization in Deep Learning: AdaGrad, RMSProp, ADAM". `https://artemoppermann.com/optimization-in-deep...`

Questions?

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Thank You

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