Gradient Descent

Johanni Brea

Einführung Machine Learning

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- There is a course at EPFL on Optimization for machine learning
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- A simple optimizer that works usually well for parametric models is

  gradient descent.

Table of Contents

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1. Input: loss function L, initial guess $\beta^{(0)} = \left(\beta_0^{(0)}, \ldots, \beta_p^{(0)}\right)$ learning rate η, maximal number of steps T.
2. For $t = 1, \ldots, T$
   - $\delta_i = \eta \dfrac{\partial L}{\partial \beta_i}\left(\beta^{(t-1)}\right)$
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Automatic Differentiation software uses the chain rule and symbolic derivatives for primitive functions, to compute the derivative of almost any code we write.

Practical Considerations

- Choosing a good learning rate can be tricky.
- Scaling the loss function has an impact on gradient descent.
  It is e.g. advisable to have L independent of the size of the data set, e.g. replace $L = \sum_{i=1}^{n}(y_i - \beta x_i)^2$ by $L = \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta x_i)^2$.
- Additive constants in the loss function L that do not depend on the parameters have no impact on gradient descent; they are often removed from the loss function.
- Preprocessing the input and output may have a strong effect on gradient descent. There are domain-specific “best preprocessing practices” (e.g. for images or audio). Standardizing inputs (and outputs in the case of regression) is an option.

Table of Contents

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The solution of gradient descent depends on the initial condition.

Table of Contents

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Computing the loss over all samples $1, \ldots, n$ can be computationally costly.
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1. Input: loss function L, initial guess $\beta^{(0)} = \left(\beta_0^{(0)}, \dots, \beta_p^{(0)}\right)$ learning rate η, maximal number of steps T, batch size B.
2. For $t = 1, \dots, T$
   - Determine batch of training indices $\mathcal{I}$
   - $\delta_i = \eta \dfrac{\partial L}{\partial \beta_i}\left(\beta^{(t-1)}; \mathcal{I}\right)$
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where $L(\beta; \mathcal{I})$ is the loss function evaluated on the training samples with indices in $\mathcal{I}$, e.g.

$$L\left(\beta; \mathcal{I}\right) = \frac{1}{B} \sum_{i \in \mathcal{I}} \left(y_i - x_i^T \beta\right)^2$$

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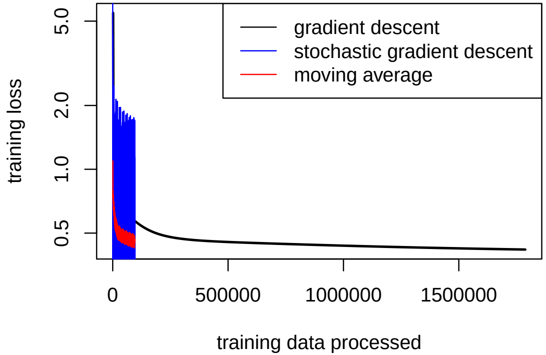
Example $B = 5$

	batch 1	batch 2	batch 3	ba
$\mathcal{I}$	1 8 3 13 93	9 14 2 26 31	$\cdots$	

Example Learning Curve



The training loss on batches of size 32 is very variable. But if we look at the moving average over the training loss of 50 subsequent batches, we see that stochastic gradient descent drops to a fairly low loss after processing far less training data than gradient descent.

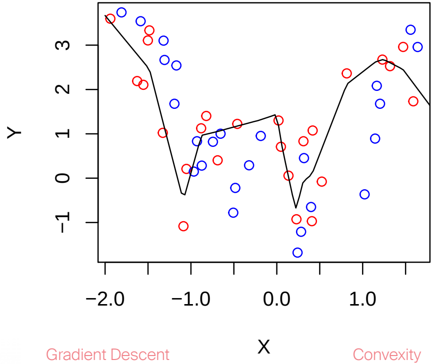
Table of Contents

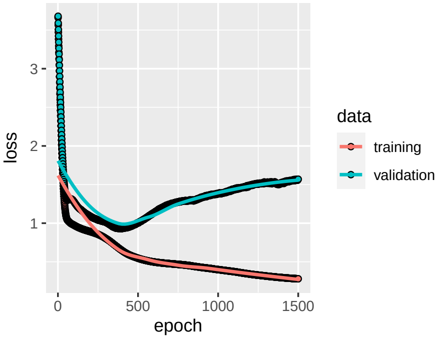
Early Stopping

Start with small weights and stop gradient descent when validation loss starts to increase.

training data validation data

black line: a flexible neural network trained with gradient descent





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- Early stopping im Gradientenabstieg führt zu Modellen mit kleinerem Bias aber grösserer Varianz, verglichen mit Gradientenabstieg ohne early stopping.