Gradient Descent

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Introduction to Machine Learning

Optimization in Machine Learning

- For linear regression there is an analytical solution that minimizes the RMSE.
- For logistic regression (and most other methods) there is no analytical solution.
- For many models there are specialized optimizers.
- There is a course at EPFL on Optimization for machine learning
  `https://edu.epfl.ch/coursebook/en/optimization-for-machine-learning-CS-439`
- A simple optimizer that works usually well for parametric models is

  gradient descent.

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Gradient Descent

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 $t = 1, \ldots, T$
   - $\delta_i = \eta \dfrac{\partial L}{\partial \beta_i}\left(\beta^{(t-1)}\right)$
   - $\beta_i^{(t)} = \beta_i^{(t-1)} - \delta_i$
3. Return $\beta^{(T)}$

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.

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Convex and Non-Convex Loss Functions

Globally Convex Loss Function

Loss function has a unique global minimum

From any initial condition there is a path towards the global minimum along which the loss is monotonically decreasing. The same solution is found by gradient descent independently of the initial condition.

The loss function of (multiple) (logistic) linear regression (with L1 or L2 regularization) is globally convex.

Non-Convex Loss Function

Loss function has multiple local minima

The solution of gradient descent depends on the initial condition.

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Stochastic Gradient Descent (SGD)

Computing the loss over all samples $1, \ldots, n$ can be computationally costly.

A subset of the training data may be sufficient to estimate the gradient direction.

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, batch size B.
2. For $t = 1, \ldots, T$
   - Determine batch of training indices $\mathcal{I}$
   - $\delta_i = \eta \frac{\partial L}{\partial \beta_i}\left(\beta^{(t-1)}; \mathcal{I}\right)$
   - $\beta_i^{(t)} = \beta_i^{(t-1)} - \delta_i$
3. Return $\beta^{(T)}$

where $L(\beta; \mathcal{I})$ is the loss function evaluated on the training samples with indices in $\mathcal{I}$, e.g.

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

Example $n = 20, B = 5$

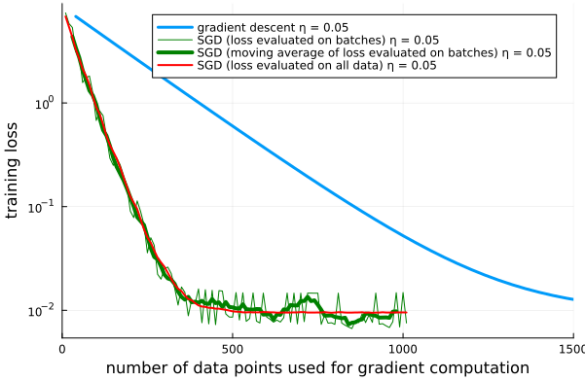
	batch 1	batch 2	batch 3	batch 4
$\mathcal{I}$	1, .., 5	6, .., 10	11, .., 15	16, .., 20

Terminology

- **batchsize** B (hyper-parameter): number of samples in each batch. Sometimes this is also called **minibatch size**.
- **epoch**: collection of update steps that go once through the entire dataset.
- **number of epochs** (hyper-parameter): number of times to go through the entire dataset.

Example: If we choose for a dataset of size $n = 1000$ a batchsize of $B = 20$ and we train for 30 epochs, there are in total $T = n/B \times 30 = 50 \times 30 = 1500$ gradient descent updated steps and each data point contributes 30 times to the computation of partial derivatives.

Example Learning Curve



- SGD is faster!
- Moving average of training loss evaluated on batches (thick green) is close to true training loss (red).

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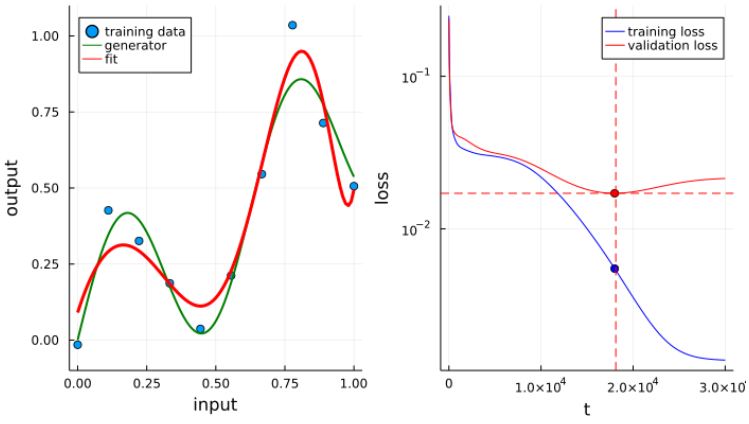
Early Stopping

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



- At the beginning of gradient descent all parameter values are small.
- Typically, the norm of the parameters increases during gradient descent.
- The parameter values found at early stopping have usually a smaller norm than the parameter values with the lowest training error.

Quiz

- With a constant learning rate and a non-zero gradient, the training loss in gradient decent is decreasing in every step.
- In every step of gradient descent one can choose a learning rate larger than zero such that the training loss is decreasing, unless the gradient is zero.
- In every step of stochastic gradient descent one can choose a learning rate larger than zero such that the training loss is decreasing, unless the gradient is zero.
- For a training set of size n, computing the gradient in (standard) gradient descent takes n/B times longer than computing the gradient in stochastic gradient descent with batch size B.
- Models found with early stopping tend to have a lower bias but a higher variance (when fitted on different training sets from the same data generator) than models found without early stopping.

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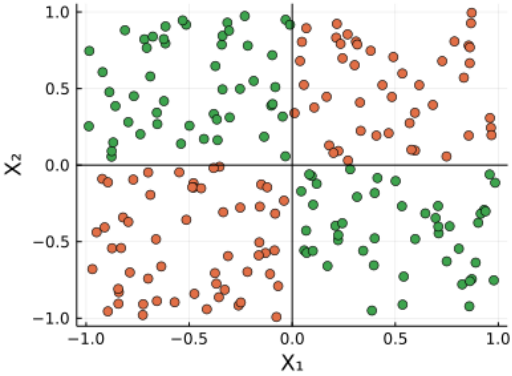
Vector Features

XOR-Problem
Training Data

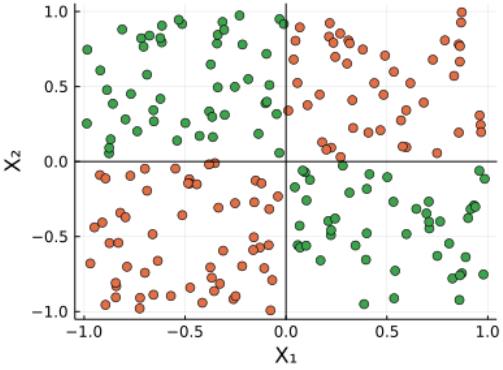


Logistic Regression fails:

There is no linear decision boundary.

Vector Features

Project data to a higher dimensional space by computing the scalar products between feature vectors $w_1, \ldots, w_q$ and input vectors x_i and thresholding.



For example $h_{21} = \max(0, w_1^T x_2)$.

Logistic Regression on the features works.

Feature Engineering is great, but couldn't it be automatized?

With smart features basically any problem can be solved by a linear method.

How should we find the smart features?

Idea: Let us take a more flexible function family and find "features" and "regression coefficients" at the same time with gradient descent.

Solving the XOR Problem without Feature Engineering

Logistic Regression: $P(Y = 1|x, \beta) = \sigma(\beta_0 + \beta_1 x_1 + \cdots \beta_p x_p)$

Logistic Regression on features:

$$P(Y = 1|x, \beta) = \sigma\big(\beta_0 + \beta_1 \underbrace{g(w_1^T x)}_{h_1} + \cdots \beta_q \underbrace{g(w_q^T x)}_{h_q}\big)$$

with hand-picked feature vectors $w_1, \ldots, w_q$ and activation function $g(x) = \text{relu}(x) = \max(0, x)$.

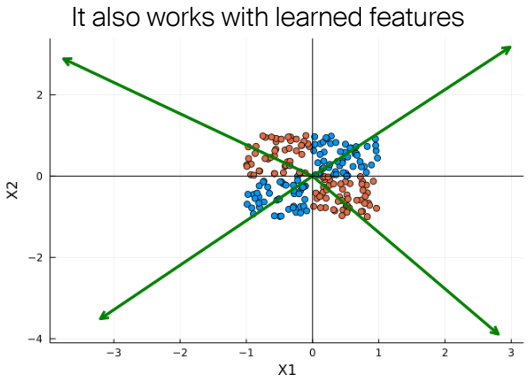
Idea

Why don't we learn the features with gradient descent?

$$P(Y = 1|x, \beta, w_1, \ldots, w_q) = \sigma\big(\beta_0 + \beta_1 g(w_1^T x) + \cdots \beta_q g(w_q^T x)\big)$$

$$\Rightarrow \quad \hat{\beta}, \hat{w} = \arg \min_{\beta, w_1, \ldots, w_q} -\sum_{i=1}^{n} \log P(y_i|x_i, \beta, w_1, \ldots, w_q)$$

Solving the XOR Problem without Feature Engineering



- We just fitted our first neural network ☺.
- The loss function has local minima; gradient descent does not find for all initial guesses a good solution.
- With more than 4 feature vectors, gradient descent finds good solutions for most initial guesses.

Suggested Reading

- 10.7 Fitting a Neural Network (skip parts 10.7.1, 10.7.3 and 10.7.4)
- 10.7.2 Regularization and Stochastic Gradient Descent