GHENT UNIVERSITY

FACULTY OF ENGINEERING AND ARCHITECTURE

E016350 - Artificial Intelligence

Lecture 3

Machine learning

Optimization Algorithms and Logistic Regression

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Outline

These slides are based on: Andrew Ng and Tengyu Ma: Lecture Notes (CS229) Machine learning https://cs229.stanford.edu/main_notes.pdf and Moses Charikar and Sanmi Koyejo: (CS221) Artificial Intelligence: Principles and Techniques (Stanford)

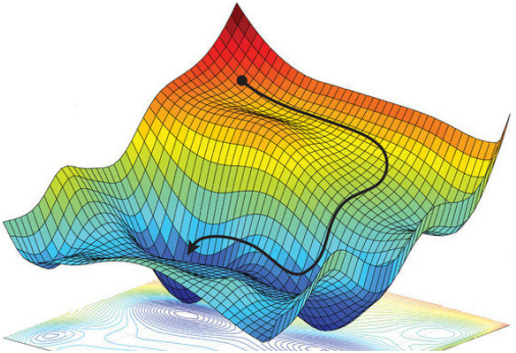
Outline

Optimization in machine learning

Our learning task: determine the parameters (weights) $\mathbf{w}$ of a hypothesis $h_{\mathbf{w}}(\mathbf{x})$ that approximates true, unknown function $y = f(\mathbf{x})$.

To find the optimal $\mathbf{w}$ we minimize a loss function.

– Why using gradient descent?

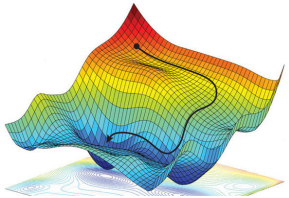


Picture credit: N. Azizan R. and B. Hassibi. Stochastic Gradient/Mirror Descent: Minimax Optimality and Implicit Regularization. ICLR 2019.

What is the Steepest Direction?

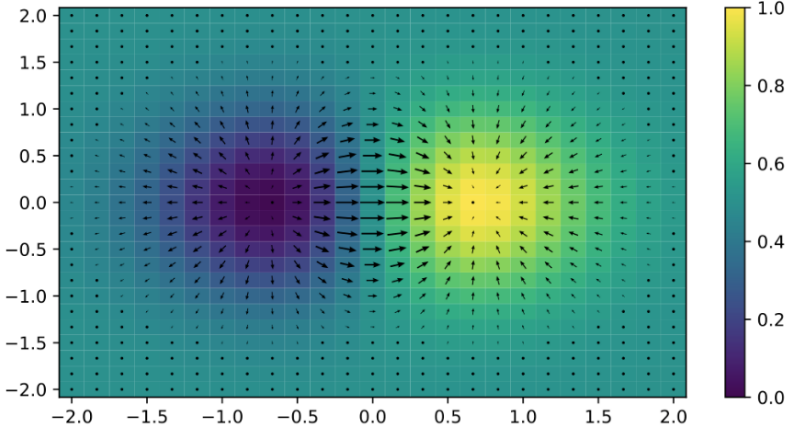
Goal: take a step $\Delta : \Delta_1^2 + \Delta_2^2 < \epsilon$ such that $Loss(\mathbf{w} + \Delta) \leq Loss(\mathbf{w})$

$$\min_{\Delta:\Delta_1^2+\Delta_2^2<\epsilon} Loss(\mathbf{w}+\Delta); \qquad \mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}; \qquad \Delta = \begin{bmatrix} \Delta_1 \\ \Delta_2 \end{bmatrix}$$



- First-order Taylor expansion
  $Loss(\mathbf{w}+\Delta) \approx Loss(\mathbf{w}) + \frac{\partial Loss}{\partial w_1}\Big|_{\mathbf{w}} \Delta_1 + \frac{\partial Loss}{\partial w_2}\Big|_{\mathbf{w}} \Delta_2 = Loss(\mathbf{w}) + \Delta^\top \nabla_{\mathbf{w}} Loss(\mathbf{w})$
- So, for maximum leverage out of moving along Δ:
  align Δ with $-\nabla_{\mathbf{w}} Loss(\mathbf{w})$
- I.e., steepest direction (down) = (negative) gradient direction in a given point

A visualization of the gradient field



The gradient of a scalar-valued differentiable function of several variables is the vector field whose value at a point p gives the direction and the rate of fastest increase at that point.
https://en.wikipedia.org/wiki/Gradient

Gradient in d dimensions

Same reasoning in arbitrary number of directions

In d dimensions, $\mathbf{w} \in \mathbb{R}^d$ and the gradient of the loss function in particular $\mathbf{w}$ point:

$$\nabla_{\mathbf{w}} Loss(\mathbf{w}) = \begin{bmatrix} \frac{\partial Loss}{\partial w_1}(\mathbf{w}) \\ \frac{\partial Loss}{\partial w_2}(\mathbf{w}) \\ . \\ . \\ . \\ \frac{\partial Loss}{\partial w_d}(\mathbf{w}) \end{bmatrix}$$

Weight optimization

We optimize the $\mathbf{w} \in \mathbb{R}^d$ by applying the gradient descent to the training loss:

$$w_j \leftarrow w_j - \alpha \frac{\partial}{\partial w_j} TrainLoss(w_1, ..., w_d)$$

Sometimes we write this more compactly as

$$w_j \leftarrow w_j - \alpha \frac{\partial}{\partial w_j} TrainLoss(\mathbf{w})$$

or in a vector form

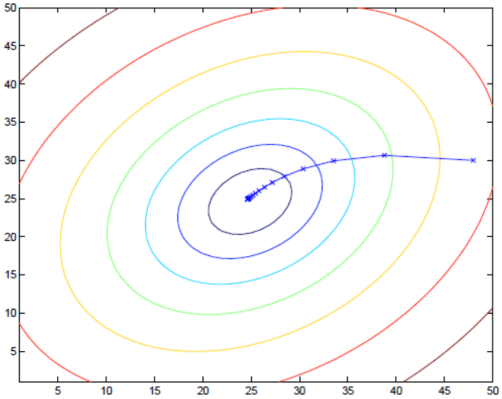
$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \nabla_{\mathbf{w}} TrainLoss(\mathbf{w})$$

- Perform update in downhill direction for each coordinate
- The steeper the slope (i.e. the larger the magnitude of the derivative) the bigger the step for that coordinate.

Gradient descent algorithm

Idea:

- Start somewhere
- Repeat: Take a step in the gradient direction



Credit: Stanford CS229 Course Notes. Trajectory for gradient descent is like climbing down into a valley

Optimization procedure: Gradient Descent (GD)

$$TrainLoss(\mathbf{w}) = \frac{1}{|\mathcal{D}_{train}|} \sum_{(x,y)\in\mathcal{D}_{train}} L(x, y, \mathbf{w})$$

- init $\mathbf{w} = [0, \ldots, 0]$
- for iter $1, 2, ...$

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \nabla_{\mathbf{w}} TrainLoss(\mathbf{w})$$

- α: learning rate — tweaking parameter that needs to be chosen carefully
- How? Try multiple choices
  - Crude rule of thumb: update changes $\mathbf{w}$ about 0.1–1%

Influence of the learning rate

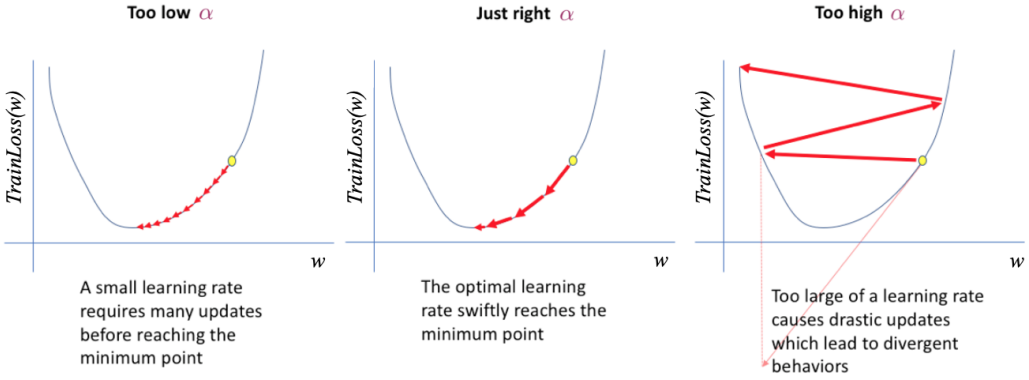


Illustration Credit: Edouard Duchesnay, NeuroSpin CEA Université Paris-Saclay, France.

Stochastic Gradient Descent (SGD)

$$TrainLoss(\mathbf{w}) = \frac{1}{|\mathcal{D}_{train}|} \sum_{(x,y)\in\mathcal{D}_{train}} L(x, y, \mathbf{w})$$

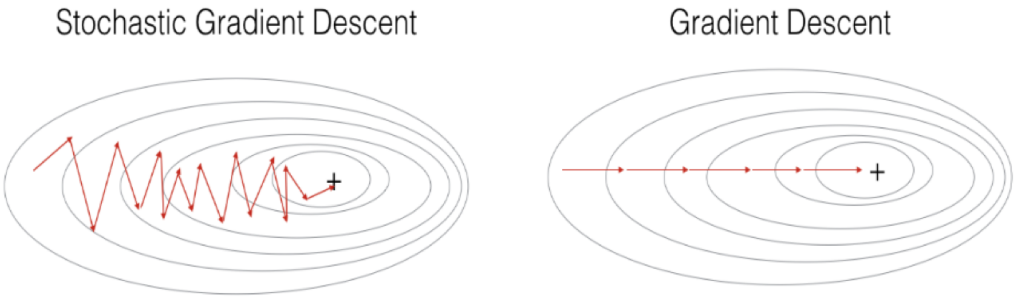
- init $\mathbf{w} = [0, \ldots, 0]$
- for iter $1, 2, \ldots$
  - For $(x, y) \in \mathcal{D}_{train}$:

$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \nabla_{\mathbf{w}} L(x, y, \mathbf{w})$$

Motivation:

- Gradient descent algorithm is slow: going over all the training examples in each iteration is expensive when lots of data!
- Rather than looping through all the training examples to compute a single gradient, update the weights based on each example $\rightarrow$ SGD

SGD vs. GD



"+" denotes a minimum of the cost. SGD leads to many oscillations to reach convergence. But each step is a lot faster to compute for SGD than for GD, as it uses only one training example (vs. the whole batch for GD).

Illustration Credit: Ankit-AI - Sharing AI: Optimization Algorithms for Machine Learning.

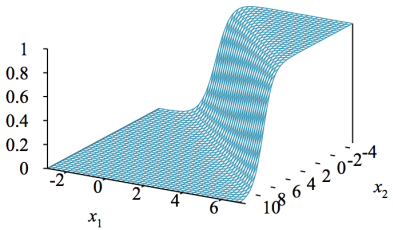
Outline

Logistic regression - Reminder

We consider binary classification: to each input data point $\mathbf{x} \in \mathbb{R}^d$ we assign a class label $y \in \{0, 1\}$.

Let $g(z)$ denote the logistic (sigmoid) function:

$$g(z) = Logistic(z) = \frac{1}{1 + e^{-z}}$$



For some weight vector $\mathbf{w} \in \mathbb{R}^d$, the hypothesis

$$h_{\mathbf{w}}(\mathbf{x}) = g(\mathbf{w} \cdot \mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w} \cdot \mathbf{x}}}$$

can be interpreted as the probability that $\mathbf{x}$ belongs to class 1, i.e., the probability that $y = 1$.

Logistic regression - Probabilistic interpretation formally

We said: $h_{\mathbf{w}}(\mathbf{x}) = g(\mathbf{w} \cdot \mathbf{x})$ can be interpreted as the probability that $y = 1$. Formally:

$$\begin{aligned} P(y = 1|\mathbf{x}, \mathbf{w}) &= h_{\mathbf{w}}(\mathbf{x}) \\ P(y = 0|\mathbf{x}, \mathbf{w}) &= 1 - h_{\mathbf{w}}(\mathbf{x}) \end{aligned}$$

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Or, more compactly:

$$P(y|\mathbf{x}, \mathbf{w}) = (h_{\mathbf{w}}(\mathbf{x}))^{y}(1 - h_{\mathbf{w}}(\mathbf{x}))^{(1-y)}$$

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If the training examples were generated independently, the likelihood of the weights is:

$$\mathcal{L}(\mathbf{w}) = \prod_{i=1}^{N} P(y^{(i)}|\mathbf{x}^{(i)}, \mathbf{w}) = \prod_{i=1}^{N} \left(h_{\mathbf{w}}(\mathbf{x}^{(i)}) \right)^{y^{(i)}} \left(1 - h_{\mathbf{w}}(\mathbf{x}^{(i)}) \right)^{1-y^{(i)}}$$

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it is easier to maximize the log likelihood:

$$\ell(\mathbf{w}) = \log \mathcal{L}(\mathbf{w}) = \sum_{i=1}^{N} y^{(i)} \log h_{\mathbf{w}}(\mathbf{x}^{(i)}) \; + \; (1 - y^{(i)}) \log(1 - h_{\mathbf{w}}(\mathbf{x}^{(i)})$$

Logistic regression under the maximum likelihood optimization

Now we can determine the update rule for the logistic regression by maximizing the log-likelihood of the weights. This is the most common form of the logistic regression.

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Note that now $TrainLoss(\mathbf{w}) = -\ell(\mathbf{w})$, so we are applying the gradient descent algorithm to $-\ell(\mathbf{w})$, or equivalently, we are applying the **gradient ascent** to $\ell(\mathbf{w})$:

$$\mathbf{w} \leftarrow \mathbf{w} + \alpha \nabla_{\mathbf{w}} \ell(\mathbf{w})$$

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$$\frac{\partial}{\partial w_j}\ell(\mathbf{w}) = \Big(y\frac{1}{g(\mathbf{w}\cdot\mathbf{x})} - (1-y)\frac{1}{1-g(\mathbf{w}\cdot\mathbf{x})}\Big)\frac{\partial}{\partial w_j}g(\mathbf{w}\cdot\mathbf{x})$$

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&= (y(1-g(\mathbf{w}\cdot\mathbf{x})) \;-\; (1-y)g(\mathbf{w}\cdot\mathbf{x}))x_j
\end{aligned}$$

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&= (y(1-g(\mathbf{w}\cdot\mathbf{x})) \;-\; (1-y)g(\mathbf{w}\cdot\mathbf{x}))x_j \\
&= (y - h_{\mathbf{w}}(\mathbf{x}))x_j
\end{aligned}$$

Logistic regression under the maximum likelihood optimization

The maximum likelihood estimation gives us the following update rule

$$\mathbf{w} \leftarrow \mathbf{w} + \alpha \nabla_{\mathbf{w}} \ell(\mathbf{w})$$

where for one training example we derived

$$\frac{\partial}{\partial w_j} \ell(\mathbf{w}) \quad = \quad (y - h_{\mathbf{w}}(\mathbf{x})) x_j$$

Hence, the MLE update rule for the logistic regression, with one example, is

$$w_j \leftarrow w_j + \alpha (y - h_{\mathbf{w}}(\mathbf{x})) x_j$$

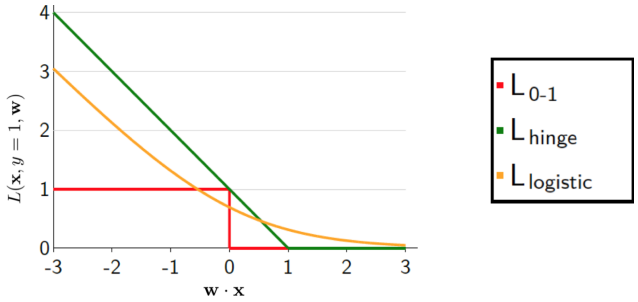
and with all training examples

$$w_j \leftarrow w_j + \alpha \sum_{(\mathbf{x},y) \in \mathcal{D}_{train}} (y - h_{\mathbf{w}}(\mathbf{x})) x_j$$

Note: Looks exactly the same as for the least-squares linear regression ($h_{\mathbf{w}}$ is different)

Classification losses

Some common losses for binary classification (shown for $y = 1$).



- **Logistic** loss:
  $L_{\text{logistic}}(\mathbf{x}, y, \mathbf{w}) = -\ell(\mathbf{w}) = -y \log h_{\mathbf{w}}(\mathbf{x}) - (1 - y) \log(1 - h_{\mathbf{w}}(\mathbf{x}))$
  - For $y = 1$, this becomes: $L_{\text{logistic}}(\mathbf{x}, y = 1, \mathbf{w}) = \log(1 + e^{-\mathbf{w} \cdot \mathbf{x}})$
- **Hinge** loss:
  - $L_{\text{hinge}}(\mathbf{x}, y = 1, \mathbf{w}) = \max(1 - \mathbf{w} \cdot \mathbf{x}, 0)$ (and $L_{\text{hinge}}(\mathbf{x}, 0, \mathbf{w}) = \max(1 + \mathbf{w} \cdot \mathbf{x}, 0)$)
  - This loss is often used with support vector machines (SVM)

Next time

- Multiclass logistic regression
- Learning with non-linear features
- Decision trees