Stochastic gradient descent

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Gradient

- For any function $f(x)$, depending from $x=(x_1,...x_D)^T$ gradient

$$\nabla f(x) := \begin{pmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \cdots \\ \frac{\partial f(x)}{\partial x_D} \end{pmatrix}$$

- If function $f(x,y)$ depends on other variables y gradient ∇_x considers only derivatives with respect to x:

$$\nabla_x f(x,y) := \begin{pmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \cdots \\ \frac{\partial f(x)}{\partial x_D} \end{pmatrix}$$

Directional derivative

Definition 1

Consider differentiable function $f : \mathbb{R}^D \to \mathbb{R}$. A derivative along direction d, $\|d\| = 1$ is defined as

$$f'(x, d) = \lim_{\lambda \to 0} \frac{f(x + \lambda d) - f(x)}{\lambda}$$

Theorem 2

$f'(x, d) = \nabla f(x)^T d$

Proof. Using 1-st order Taylor expansion we have

$$f(x + \lambda d) = f(x) + \nabla f(x)^T (\lambda d) + o(\lambda)$$

$$\frac{f(x + \lambda d) - f(x)}{\lambda} = \nabla f(x)^T d + o(1) \xrightarrow{\lambda \to 0} \nabla f(x)^T d$$

$\square$

Direction of maximal growth/decrease

Theorem 3

For differentiable function $f(x)$ locally at point x:

- $\frac{\nabla f(x)}{\|\nabla f(x)\|}$ *is the direction of maximum growth*
- $-\frac{\nabla f(x)}{\|\nabla f(x)\|}$ *is the direction of maximal decrease.*

Proof. From Cauchi-Schwartz inequality, using that $\|d\| = 1$:

$$\left|\nabla f(x)^T d\right| \le \|\nabla f(x)\| \, \|d\| = \|\nabla f(x)\|$$

Equality is achieved when $d \propto \nabla f(x)$, i.e. $d = \pm \nabla f(x) / \|\nabla f(x)\|$.
Theorem follows from 1-st order Taylor expansion

$$f(x + \lambda d) = f(x) + \nabla f(x)^T (\lambda d) + o(\lambda)$$

$\square$

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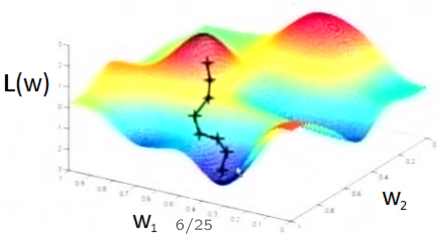
Gradient descend optimization

- Optimization task to obtain the weights:

$$L(w) = \sum_{n=1}^{N} \mathcal{L}(x_n, y_n, w) \to \min_w$$

- For convex $\mathcal{L}(u)$ $L(w)$ will also be convex => method will converge to global optimum from any starting conditions.
- Gradient descend - iterative movement in direction of $-\nabla_w F(w)$.
- Example for $w \in \mathbb{R}^2$:



Gradient descend optimization

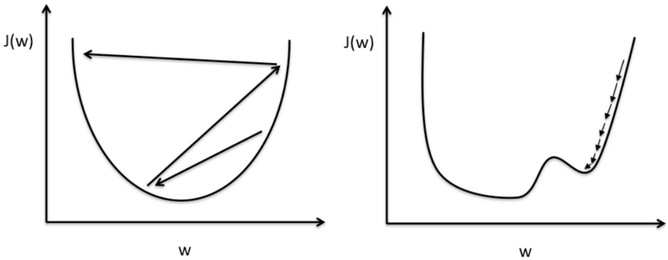
INPUT:
* ε: parameter, controlling the speed of convergence
* stopping rule

ALGORITHM:
initialize $t = 0$, w_0 randomly
WHILE stopping rule is not satisfied:
    $w_{t+1} := w_t - \varepsilon \nabla_w L(w_t)$
    $t := t + 1$

RETURN w_n

Learning rate selection[1]

ε should be selected carefully based on $L(w_t)$ dynamics.



Large learning rate: Overshooting.

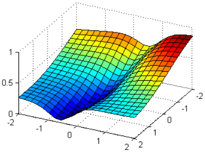
Small learning rate: Many iterations until convergence and trapping in local minima.

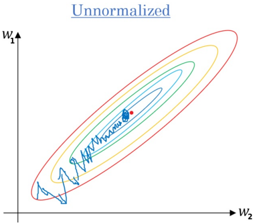
[1] Picture source.

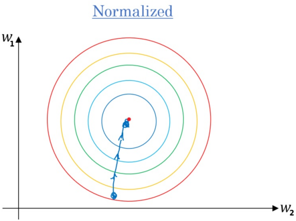
Feature normalization

Convergence is faster for normalized features:

- feature normalization solves the problem of «elongated valleys»







Gradient descend (GD)

INPUT:
* η: parameter, controlling the speed of convergence
* stopping rule

ALGORITHM:
initialize $t=0$, w_0 randomly
WHILE stopping rule is not satisfied:

$$w_{t+1} := w_t - \varepsilon \frac{1}{N} \sum_{i=1}^{N} \nabla_w \mathcal{L}(x_i, y_i | w_n)$$

$$t := t+1$$

RETURN w_n

Gradient calculation requires $O(N)$ operations!

Stochastic gradient descent (SGD)

```
INPUT:
* ε: parameter, controlling the speed of convergence
* stopping rule

ALGORITHM:
initialize t = 0, w_0 randomly
WHILE stopping rule is not satisfied:
    randomly sample I = {n_1, ...n_K} from {1, 2, ...N}
    w_{t+1} := w_t − ε (1/K) Σ_{n∈I} ∇_w L(x_n, y_n | w_t)
    t := t + 1

RETURN w_t
```

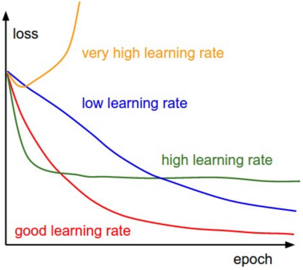
Main idea: $\frac{1}{N}\sum_{n=1}^{N}\mathcal{L}(x_n, y_n|w) \approx \frac{1}{K}\sum_{n\in I}\mathcal{L}(x_n, y_n|w)$, one step takes $O(K)$, $K \ll N$.

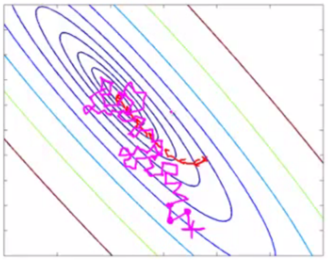
SGD comments

- Indices generation: before each pass through the training set, it is randomly shuffled and then passed sequentially.
- Works even for $K = 1$ and small ε.
- $\frac{1}{K}\sum_{i\in I}\nabla_w\mathcal{L}(x_i, y_i|w_n)$ can be computed in $O(1)$ for small K because processors internally perform vector arithmetics.

Learning rate selection

- $\varepsilon \equiv const$:





- Convergence requirements:

$$\sum_t \varepsilon_t = +\infty \qquad \text{SGD should reach any point}$$

$$\sum_t \varepsilon_t^2 < +\infty \qquad \varepsilon_t \text{ should converge to 0 fast}$$

Gradient descend optimization

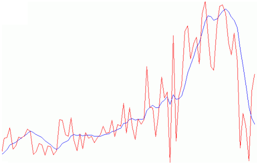
- Possible stopping rules:
    - $|w_{n+1} - w_n| < \varepsilon$
    - $|L(w_{n+1}) - L(w_n)| < \varepsilon$
    - $n > n_{max}$
- Linear regression loss $\mathcal{L}(w^T x_n - y_n)$
- Binary linear classification loss $\mathcal{L}(w^T x_n y_n)$.

Tracking convergence of SGD

- Estimation of $L(w_n) = \frac{1}{N}\sum_{i=1}^{N}\mathcal{L}(x_i, y_i|w_n)$ on each iteration takes $O(N)$ and is impractical.
- Use rolling window scheme with window K.
- For series $z_1, ...z_N$ exponentially smoothed series is obtained by

$$\begin{cases} s_1 = z_1 & \alpha \in (0,1) \text{ - hyperparameter} \\ s_{n+1} = \alpha z_{n+1} + (1-\alpha)s_n & \text{recalculation takes } O(1) \end{cases}$$

Example: original (red) and exp-smoother (blue) time series:



Tracking convergence of SGD

Exponential smoothing of loss enables loss reestimation in $O(1)$:

$$L_0^{smooth} = \sum_{i=1}^{N} \mathcal{L}(x_i, y_i)$$
$$L_{n+1}^{smooth} = \alpha \mathcal{L}(x_i, y_i) + (1-\alpha) L_n^{smooth}$$

where i is sampled object in SGD.

SGD reformulated

INPUT:
* ε: parameter, controlling the speed of convergence
* stopping rule

ALGORITHM:
initialize $t = 0$, w_0 randomly, $\Delta w_0 = 0$
WHILE stopping rule is not satisfied:
  randomly sample $I = \{n_1, ...n_K\}$ from $\{1, 2, ...N\}$
  $\Delta w_{t+1} = -\frac{1}{K}\sum_{n\in I}\nabla_w\mathcal{L}(x_n, y_n|w_t)$
  $w_{t+1} := w_t + \varepsilon\Delta w_{t+1}$
  $t := t + 1$

RETURN w_n

SGD with momentum

INPUT:
* ε: speed of convergence
* $\alpha \in (0, 1]$: speed of change direction update (typically $\alpha = 0.1$)
* stopping rule

ALGORITHM:
initialize $t = 0$, w_0 randomly, $\Delta w_0 = 0$
WHILE stopping rule is not satisfied:
    randomly sample $I = \{n_1, ...n_K\}$ from $\{1, 2, ...N\}$
    $\Delta w_{t+1} = \alpha \Delta w_t - (1 - \alpha) \frac{1}{K} \sum_{n \in I} \nabla_w \mathcal{L}(x_n, y_n | w_t)$
    $w_{t+1} := w_t + \varepsilon \Delta w_{t+1}$
    $t := t + 1$

RETURN w_n

- Intuition: $\uparrow$speed by removing noisy gradients by aggregation over longer history.
- Typically $\alpha = 0.9$.

Other improvements

Other improvements of SGD exist:

- use 2nd order derivative
- Adam, RMSProp, AdaGrad, Adadelta
  - adjust ε_t for each dimension individually.
  - important dimensions get $\downarrow \varepsilon_t$
  - unimportant dimensions get $\uparrow \varepsilon_t$

Discussion of SGD

Advantages

- Simple
- Works online
- A small subset of learning objects may be sufficient for accurate estimation

Discussion of SGD

Advantages

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Drawbacks

- Optimization using 2nd order derivatives converges faster.
- Needs selection of ε_t:
  - too big: divergence
  - too small: very slow convergence

- If $\mathcal{L}(\cdot)$ is convex => convergence to global min from any starting point.
- If $\mathcal{L}(\cdot)$ is non-convex => convergence to different local min, depending on starting point.

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Regularization

In ML we solve:

$$L(w)=\sum_{n}\mathcal{L}_{w}(x_n,y_n)\to\min_{w}$$

- linear regression: $\mathcal{L}_w(x_n,y_n)=\mathcal{L}(x_n^T w-y_n)$
- binary linear classification: $\mathcal{L}(w^T x_n y_n)$

Task is replaced with

$$\tilde{L}(w)=\sum_{n}\mathcal{L}_{w}(x_n,y_n)+\lambda R(w)=L(w)+\lambda R(w)\to\min_{w}$$

where $R(w)$ penalizes model complexity and $\lambda\geq 0$ controls strength of regularization.

L_1 regularization

- $||w||_1$ regularizer will do feature selection.
- Consider

$$\tilde{L}(w) = L(w) + \lambda \sum_{d=1}^{D} |w_d|$$

$$\frac{\partial \tilde{L}(w)}{\partial w_i} = \frac{\partial L(w)}{\partial w_i} + \lambda \operatorname{sign} w_i$$

$$\lambda \operatorname{sign} w_i \nrightarrow 0 \text{ when } w_i \to 0$$

- If $\lambda > \max_w \left| \frac{\partial L(w)}{\partial w_i} \right|$, then it becomes optimal to set $w_i = 0$
- For higher λ more weights become zero.

L_2 regularization

$$\tilde{L}(w) = L(w) + \lambda \sum_{d=1}^{D} w_d^2$$

$$\frac{\partial L(w)}{\partial w_i} = \frac{\partial L(w)}{\partial w_i} + 2\lambda w_i$$

$$2\lambda w_i \to 0 \text{ when } w_d \to 0$$

- Strength of regularization $\to 0$ as weights $\to 0$.
- So L_2 regularization will not set weights exactly to 0.

Summary

- Gradient descent iteratively optimizes $L(w)$ in the direction of maximum descent.
    - step takes $O(N)$
    - ε should be carefully chosen
- Stochastic gradient descent applies gradient descent to approximation of $L(w)$.
    - step takes $O(K)$
    - requires $\varepsilon_t \to 0$ for convergence.
- Feature normalization & momentum speeds up convergence.