

Annotated
version

Machine Learning Course - CS-433

Optimization

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minor changes by Martin Jaggi 2020,2019,2018,2017;
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Learning / Estimation / Fitting

Given a cost function $\mathcal{L}(\mathbf{w})$, we wish to find \mathbf{w}^* which minimizes the cost:

$$\min_{\mathbf{w}} \mathcal{L}(\mathbf{w}) \quad \text{subject to } \mathbf{w} \in \mathbb{R}^D$$

This means the *learning* problem is formulated as an *optimization problem*.

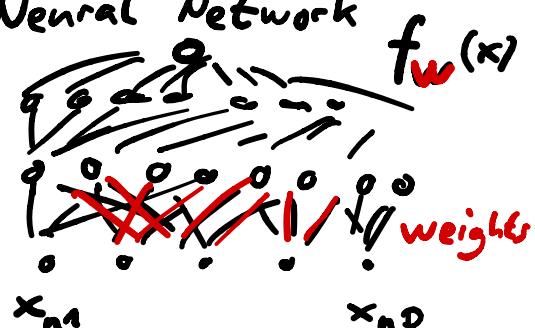
We will use an *optimization algorithm* to solve the problem (to find a good \mathbf{w}).

$$\mathcal{L}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^N (y_n - f_{\mathbf{w}}(x_n))^2$$

Examples • Linear Model

$$f_{\mathbf{w}}(\mathbf{x}) = \mathbf{w}^T \mathbf{x}$$

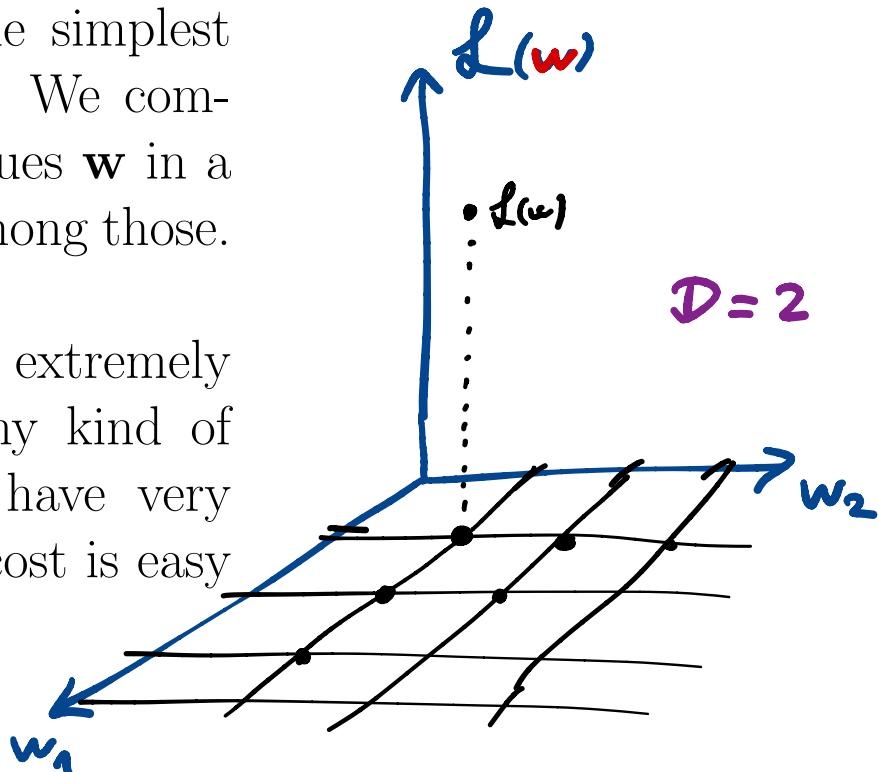
• Neural Network



Grid Search

Grid search is one of the simplest optimization algorithms. We compute the cost over all values \mathbf{w} in a grid, and pick the best among those.

This is brute-force, but extremely simple and works for any kind of cost function when we have very few parameters and the cost is easy to compute.



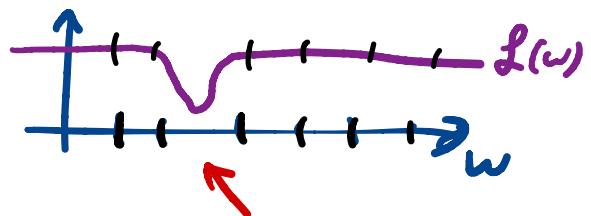
① For a large number of parameters D , however, grid search has too many “for-loops”, resulting in an exponential computational complexity:

$$\mathbf{w} \in \mathbb{R}^D$$

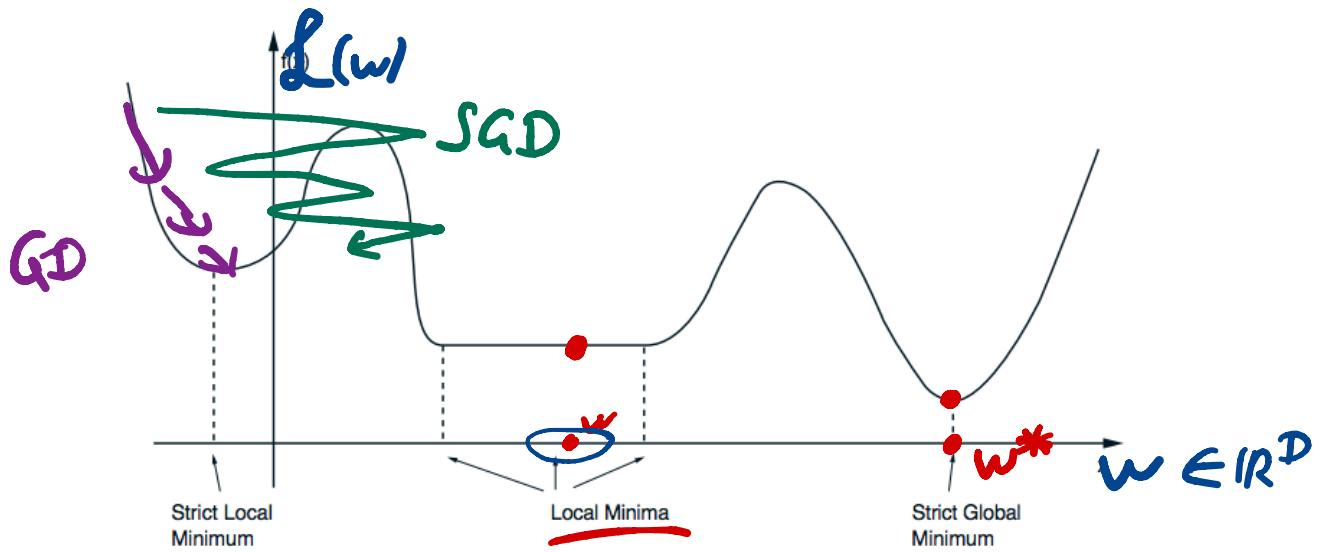
If we decide to use 10 possible values for each dimension of \mathbf{w} , then we have to check 10^D points. This is clearly impossible for most practical machine learning models, which can often have $D \approx$ millions of parameters. Choosing a good range of values for each dimension is another problem.

$$\begin{aligned} \text{\# tries} & (\text{L(w) eval}) \\ = 10^D \end{aligned}$$

② Other issues: No guarantee can be given that we end up close to an optimum.



Optimization Landscapes



The above figure is taken from Bertsekas, Nonlinear programming.

A vector \mathbf{w}^* is a local minimum of \mathcal{L} if it is no worse than its neighbors; i.e. there exists an $\epsilon > 0$ such that,

$$\mathcal{L}(\mathbf{w}^*) \leq \mathcal{L}(\mathbf{w}), \quad \forall \mathbf{w} \text{ with } \|\mathbf{w} - \mathbf{w}^*\| < \epsilon$$

A vector \mathbf{w}^* is a global minimum of \mathcal{L} if it is no worse than all others,

$$\mathcal{L}(\mathbf{w}^*) \leq \mathcal{L}(\mathbf{w}), \quad \forall \mathbf{w} \in \mathbb{R}^D$$

A local or global minimum is said to be strict if the corresponding inequality is strict for $\mathbf{w} \neq \mathbf{w}^*$.

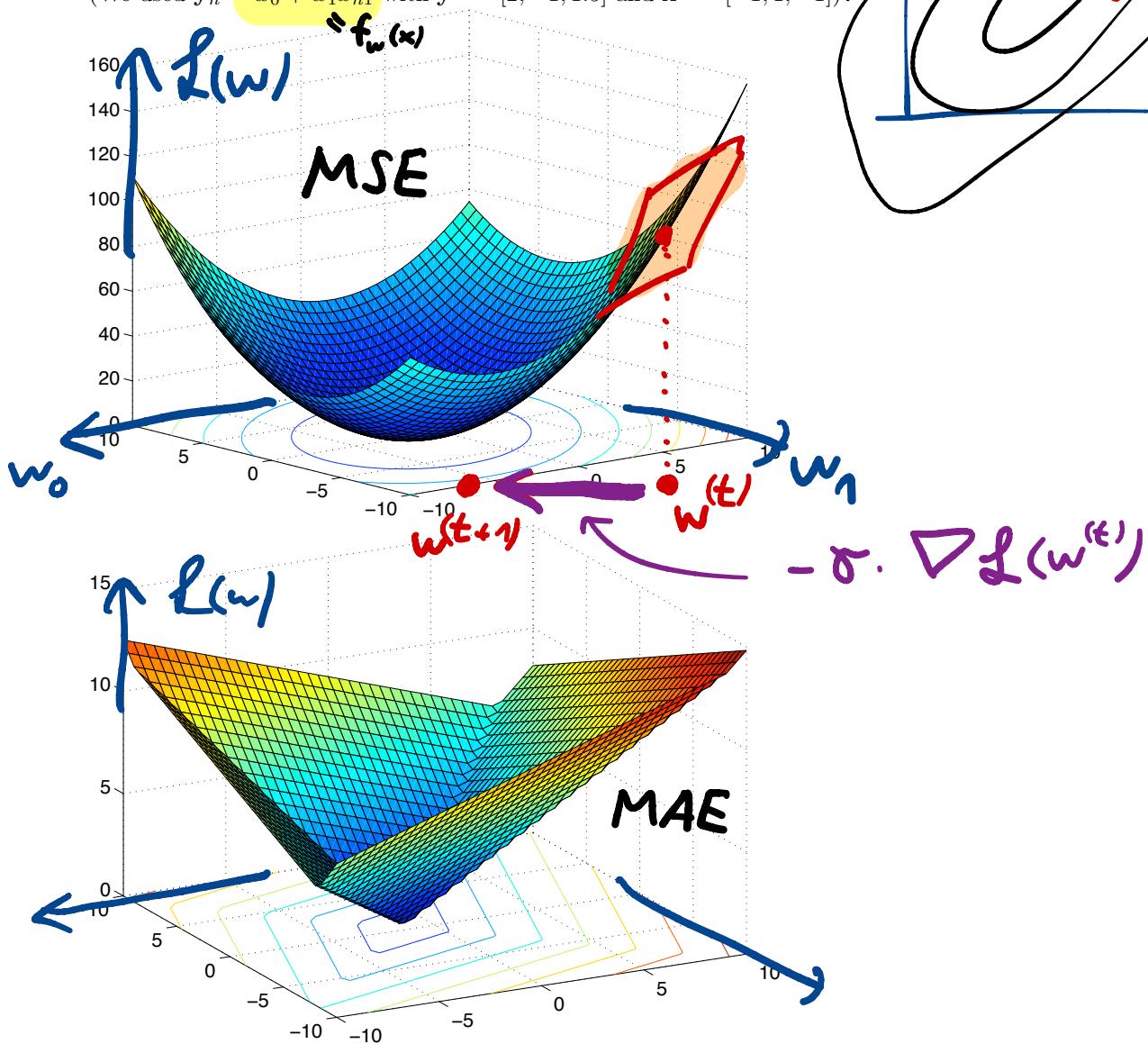
Smooth Optimization

Follow the Gradient

A gradient (at a point) is the slope of the tangent to the function (at that point). It points to the direction of largest increase of the function.

For a 2-parameter model, $\text{MSE}(\mathbf{w})$ and $\text{MAE}(\mathbf{w})$ are shown below.

(We used $\mathbf{y}_n \approx \mathbf{w}_0 + \mathbf{w}_1 \mathbf{x}_{n1}$ with $\mathbf{y}^\top = [2, -1, 1.5]$ and $\mathbf{x}^\top = [-1, 1, -1]$).



Definition of the gradient:

$$\nabla \mathcal{L}(\mathbf{w}) = \frac{\partial \mathcal{L}(\mathbf{w})}{\partial w_1}, \dots, \frac{\partial \mathcal{L}(\mathbf{w})}{\partial w_D}$$

$$\nabla \mathcal{L}(\mathbf{w}) := \left[\frac{\partial \mathcal{L}(\mathbf{w})}{\partial w_1}, \dots, \frac{\partial \mathcal{L}(\mathbf{w})}{\partial w_D} \right]^\top$$

This is a vector, $\nabla \mathcal{L}(\mathbf{w}) \in \mathbb{R}^D$.

Gradient Descent

$$t = 1, 2, \dots, T$$

To minimize the function, we iteratively take a step in the (opposite) direction of the gradient

$$\underline{\mathbf{w}}^{(t+1)} := \underline{\mathbf{w}}^{(t)} - \gamma \nabla \mathcal{L}(\mathbf{w}^{(t)})$$

common step size

$$\sigma = \sigma(\epsilon) = \frac{c}{\epsilon}$$

where $\gamma > 0$ is the step-size (or learning rate). Then repeat with the next t .

$\mathcal{D}=1$

Example: Gradient descent for 1-parameter model to minimize MSE:

$$w_0^{(t+1)} := w_0^{(t)} - \sigma \cdot \nabla \mathcal{L}(w_0^{(t)})$$

$$w_0^{(t+1)} := (1 - \gamma)w_0^{(t)} + \gamma \bar{y}$$

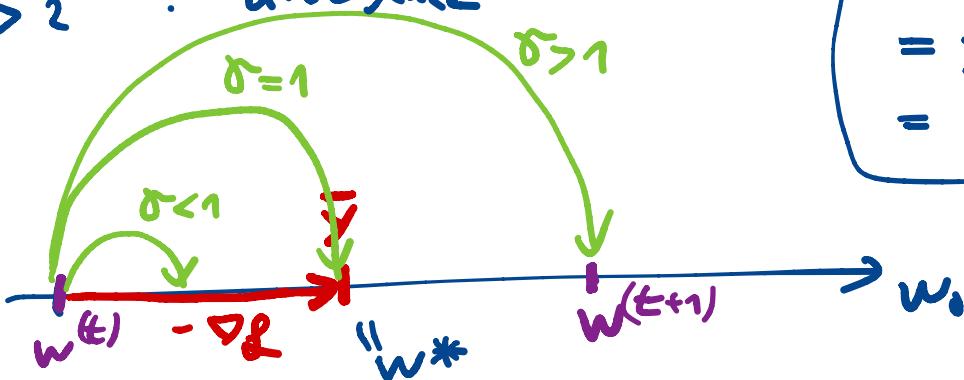
where $\bar{y} := \sum_n y_n / N$. When is this sequence guaranteed to converge?

$\sigma \in (0, 2)$: convergence to w^*

$\sigma > 2$: divergence

$$\mathcal{L}(\mathbf{w}) = f_{\mathbf{w}}(\mathbf{x})$$

$$\frac{1}{N} \sum_{n=1}^N \frac{1}{2} (x_n - w_0)^2$$



$$\begin{aligned} \nabla \mathcal{L}(\mathbf{w}) &= \frac{\partial}{\partial w_0} \mathcal{L} \\ &= \frac{1}{N} \sum_{n=1}^N \frac{1}{2} (y_n - w_0)^2 \\ &= w_0 - \bar{y} \end{aligned}$$

Gradient Descent for Linear MSE

For linear regression

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}, \mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1D} \\ x_{21} & x_{22} & \dots & x_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N1} & x_{N2} & \dots & x_{ND} \end{bmatrix}$$

← data point 1

We define the error vector \mathbf{e} :

matrixcalculus.org

$$\mathbf{e} = \mathbf{y} - \mathbf{X}\mathbf{w}$$

and MSE as follows:

$$\begin{aligned} \mathcal{L}(\mathbf{w}) &:= \frac{1}{2N} \sum_{n=1}^N (y_n - \mathbf{x}_n^\top \mathbf{w})^2 \\ &= \frac{1}{2N} \mathbf{e}^\top \mathbf{e} \\ &= \frac{1}{2N} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 \end{aligned}$$

then the gradient is given by

$$\nabla \mathcal{L}(\mathbf{w}) = -\frac{1}{N} \mathbf{X}^\top \mathbf{e}$$

$$\begin{array}{c} f_{\mathbf{w}}(\mathbf{x}) \\ \parallel \end{array}$$

$$\begin{aligned} \frac{\partial}{\partial w_1} \mathcal{L} &= \frac{1}{2N} \sum_{n=1}^N -2(y_n - \mathbf{x}_n^\top \mathbf{w}) \mathbf{x}_{n1} \\ &= -\frac{1}{N} (\mathbf{X}_{:,1})^\top \mathbf{e} \\ &\vdots \\ \frac{\partial}{\partial w_D} \mathcal{L} &= -\frac{1}{N} (\mathbf{X}_{:,D})^\top \mathbf{e} \end{aligned}$$

Computational cost. What is the complexity (# operations) of computing the gradient?

- a) starting from \mathbf{w} and
- b) given \mathbf{e} and \mathbf{w} ?

① compute \mathbf{e}

cost: $\mathcal{O}(N \cdot D) + \mathcal{O}(N)$
 for $\mathbf{X}\mathbf{w}$ for $\mathbf{y} - \mathbf{X}\mathbf{w}$

② compute $\nabla \mathcal{L}$ given \mathbf{e}

cost: $\mathcal{O}(N \cdot D) + \mathcal{O}(D)$

for $\mathbf{X}^\top \mathbf{e}$ for $\frac{1}{N}$

total: $\mathcal{O}(N \cdot D)$

Variant with offset. Recall: Alternative trick when also incorporating an offset term for the regression:

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} \quad \tilde{\mathbf{X}} = \begin{bmatrix} 1 & x_{11} & x_{12} & \dots & x_{1D} \\ 1 & x_{21} & x_{22} & \dots & x_{2D} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{N1} & x_{N2} & \dots & x_{ND} \end{bmatrix}$$

$w = (w_0, w_1, \dots, w_D)$

artificial feature per datapoint

Exercise :

compute $\nabla \mathcal{L}(w)$

Stochastic Gradient Descent

Sum Objectives. In machine learning, most cost functions are formulated as a sum over the training examples, that is

$$\mathcal{L}(w) = \frac{1}{N} \sum_{n=1}^N \mathcal{L}_n(w),$$

cost of one datapoint n

where \mathcal{L}_n is the cost contributed by the n -th training example.

Q: What are the \mathcal{L}_n for linear MSE?

The SGD Algorithm. The stochastic gradient descent (SGD) algorithm is given by the following update rule, at step t :

- ① Sample one datapoint $n \in \{1, \dots, N\}$ uniformly at random
- ② $w^{(t+1)} := w^{(t)} - \gamma \nabla \mathcal{L}_n(w^{(t)})$.

"g" „stochastic gradient“

Theoretical Motivation. Idea:

Cheap but unbiased estimate of the gradient!

In expectation over the random choice of n , we have

$$\mathbb{E} [\nabla \mathcal{L}_n(\mathbf{w})] = \nabla \mathcal{L}(\mathbf{w})$$

which is the true gradient direction.
(check!)

Mini-batch SGD. There is an intermediate version, using the update direction being

$$\mathbf{g} := \frac{1}{|B|} \sum_{n \in B} \nabla \mathcal{L}_n(\mathbf{w}^{(t)})$$

again with

$$\mathbf{w}^{(t+1)} := \mathbf{w}^{(t)} - \gamma \mathbf{g}.$$

In the above gradient computation, we have randomly chosen a subset $B \subseteq [N]$ of the training examples. For each of these selected examples n , we compute the respective gradient $\nabla \mathcal{L}_n$, at the same current point $\mathbf{w}^{(t)}$.

$$\begin{aligned} & \mathbb{E} [\nabla \mathcal{L}_n(\omega)] \\ &= \frac{1}{N} \sum_{n=1}^N \nabla \mathcal{L}_n(\omega) \\ &= \nabla \frac{1}{N} \sum_n \mathcal{L}_n \\ &= \nabla \mathcal{L}(\omega) \\ &\Rightarrow \text{unbiased} \end{aligned}$$

Randomly select
 $|B|$ datapoints
 $B \subseteq \{1, \dots, N\}$

Example:

- $B = \{n\}$ $|B|=1$
⇒ SGD
- $B = \{1, 2, \dots, N\}$
⇒ (full) gradient descent
- $|B|=5$
⇒ mini-batch SGD

The computation of \mathbf{g} can be parallelized easily. This is how current deep-learning applications utilize GPUs (by running over $|B|$ threads in parallel).

Note that in the extreme case $B := [N]$, we obtain (batch) gradient descent, i.e. $\mathbf{g} = \nabla \mathcal{L}$.

SGD for Linear MSE

See Exercise Sheet 2.

Computational cost. For linear MSE, what is the complexity (# operations) of computing the stochastic gradient?

(using only $|B| = 1$ data examples)

a) starting from \mathbf{w} ?

$$\text{(GD)} : \quad \mathcal{L}(\mathbf{w}) = \frac{1}{n} \sum_{n=1}^N \frac{1}{2} (\mathbf{y}_n - \mathbf{x}_n^\top \mathbf{w})^2$$

$$\nabla \mathcal{L}(\mathbf{w}) = -\frac{1}{n} \mathbf{x}^\top (\mathbf{y} - \mathbf{x} \mathbf{w})$$

cost: $\Theta(N \cdot D)$

$$\mathbf{e} \in \mathbb{R}^n$$

$$\text{(SGD)} : \quad \mathcal{L}_n(\mathbf{w}) = \frac{1}{2} (\mathbf{y}_n - \mathbf{x}_n^\top \mathbf{w})^2$$

$$\nabla \mathcal{L}_n(\mathbf{w}) = -\mathbf{x}_n^\top (\mathbf{y}_n - \mathbf{x}_n^\top \mathbf{w})$$

cost: $\Theta(D)$

N times
cheaper

per iteration

Non-differentiable Optimization

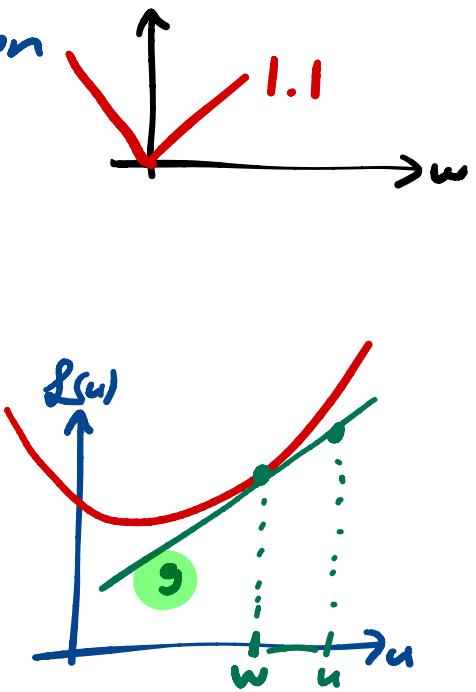
Non-Smooth Optimization

An alternative characterization of convexity, for differentiable functions is given by

$$\underline{\mathcal{L}(\mathbf{u})} \geq \underline{\mathcal{L}(\mathbf{w}) + \nabla \mathcal{L}(\mathbf{w})^\top (\mathbf{u} - \mathbf{w})} \quad \forall \mathbf{u}, \mathbf{w}$$

1st order Taylor

meaning that the function must always lie above its linearization.

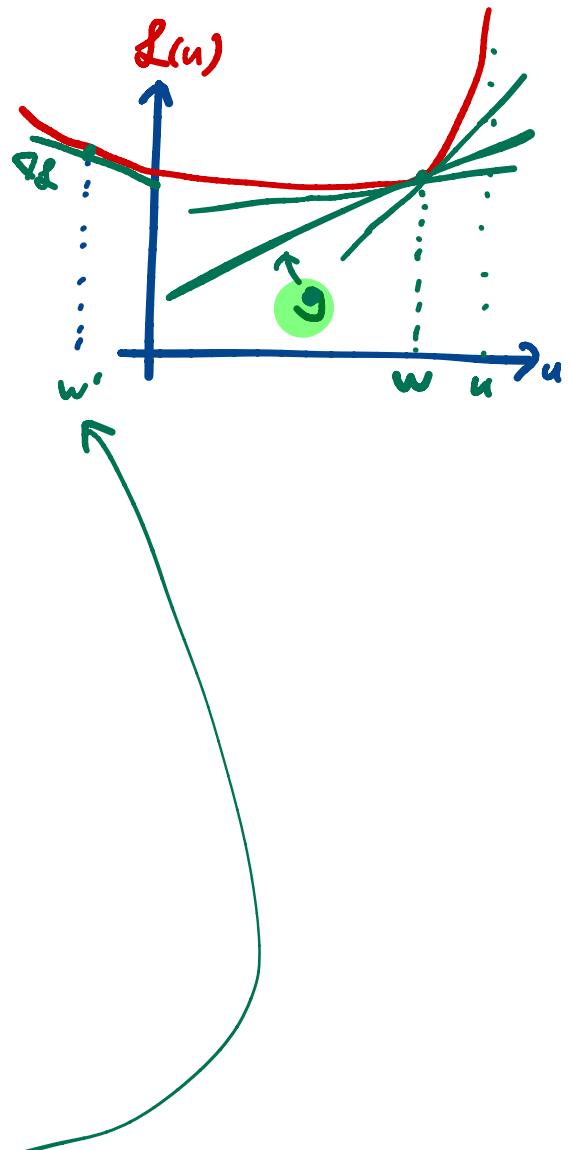


Subgradients

A vector $\mathbf{g} \in \mathbb{R}^D$ such that

$$\underline{\mathcal{L}(\mathbf{u})} \geq \underline{\mathcal{L}(\mathbf{w}) + \mathbf{g}^\top (\mathbf{u} - \mathbf{w})} \quad \forall \mathbf{u}$$

is called a **subgradient** to the function \mathcal{L} at \mathbf{w} .



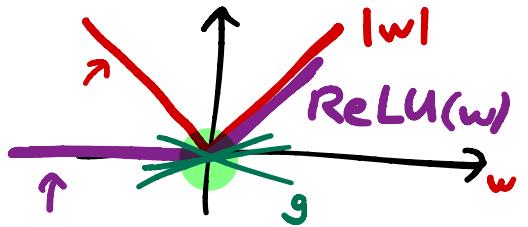
This definition makes sense for objectives \mathcal{L} which are not necessarily differentiable (and not even necessarily convex).

If \mathcal{L} is convex and differentiable at \mathbf{w} , then the only subgradient at \mathbf{w} is $\mathbf{g} = \nabla \mathcal{L}(\mathbf{w})$.

Subgradient Descent

Identical to the gradient descent algorithm, but using a **subgradient** instead of **gradient**. Update rule

$$\mathbf{w}^{(t+1)} := \mathbf{w}^{(t)} - \gamma \mathbf{g}$$



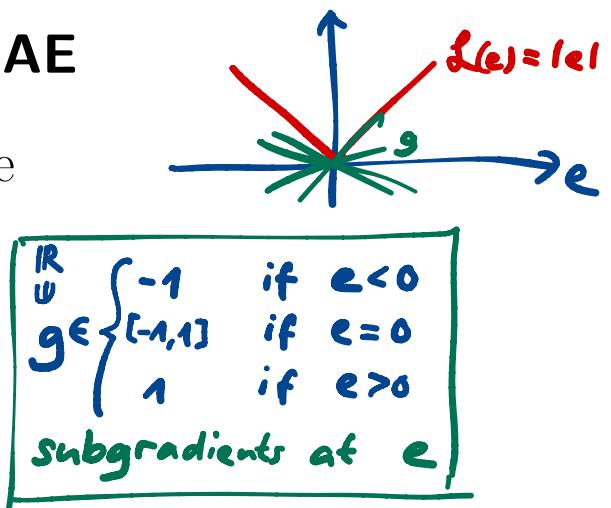
for \mathbf{g} being a subgradient to \mathcal{L} at the current iterate $\underline{\mathbf{w}^{(t)}}$.

Example: Optimizing Linear MAE

1. Compute a subgradient of the absolute value function

$$h : \mathbb{R} \rightarrow \mathbb{R}, h(e) := |e|.$$

toy example



2. Recall the definition of the mean absolute error:

$$\mathcal{L}(\mathbf{w}) = \text{MAE}(\mathbf{w}) := \frac{1}{N} \sum_{n=1}^N |y_n - f_{\mathbf{w}}(\mathbf{x}_n)|$$

For linear regression, its (sub)gradient is easy to compute using the **chain rule**.
Compute it!

*for
subgradients*

$$\mathcal{L}(\mathbf{w}) = h(q(\mathbf{w}))$$

*h: non-differentiable
q: differentiable*

\Rightarrow subgradient of $\mathcal{L}(\mathbf{w})$

$$g \in \underbrace{\partial h(q(\mathbf{w}))}_{\text{set of subgradients of } h \text{ at } q(\cdot)} \cdot \nabla q(\mathbf{w})$$

set of subgradients of h at q(.)

See Exercise Sheet 2.

Stochastic Subgradient Descent

Stochastic SubGradient Descent
(still abbreviated SGD commonly).

$$L(w) = \frac{1}{N} \sum_{n=1}^N L_n(w)$$

possibly non-differentiable

Same, \mathbf{g} being a subgradient to the randomly selected L_n at the current iterate $\mathbf{w}^{(t)}$.

Exercise: Compute the SGD update for linear MAE.

for linear models

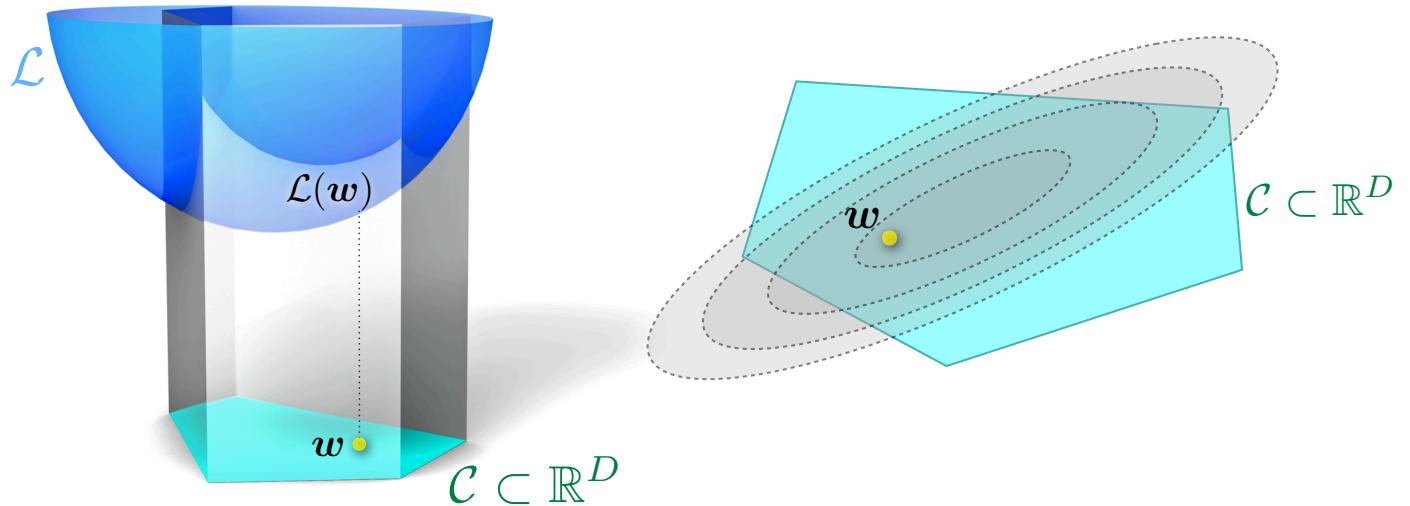
computational cost		smooth MSE	non-smooth MAE
GD	L	gradient ∇L $\Theta(N \cdot D)$	subgradient of L $\Theta(N \cdot D)$
SGD	L_n	stoch. grad. ∇L_n $\Theta(D)$	stoch. subgradient of L_n $\Theta(D)$

Constrained Optimization

Sometimes, optimization problems come posed with additional constraints:

$$\min_{\mathbf{w}} \mathcal{L}(\mathbf{w}), \quad \text{subject to } \mathbf{w} \in \mathcal{C}.$$

The set $\mathcal{C} \subset \mathbb{R}^D$ is called the constraint set.



Solving Constrained Optimization Problems

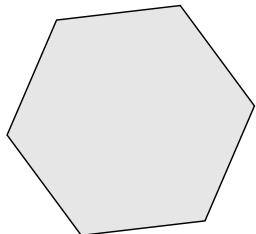
- A) Projected Gradient Descent
- B) Transform it into an *unconstrained* problem

Convex Sets

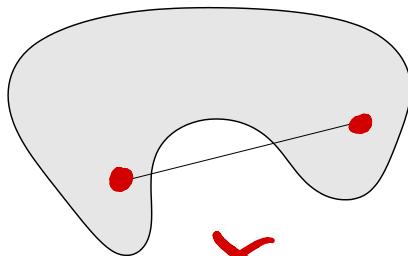
A set \mathcal{C} is convex iff

the line segment between any two points of \mathcal{C} lies in \mathcal{C} , i.e., if for any $\mathbf{u}, \mathbf{v} \in \mathcal{C}$ and any θ with $0 \leq \theta \leq 1$, we have

$$\theta\mathbf{u} + (1 - \theta)\mathbf{v} \in \mathcal{C}.$$



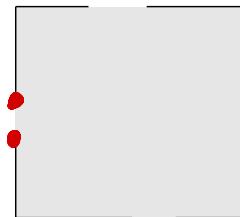
Convex



X

*Figure 2.2 from S. Boyd, L. Vandenberghe

not convex



X

not convex

Properties of Convex Sets

- Intersections of convex sets are convex
- Projections onto convex sets are *unique*.
(and often efficient to compute)
Formal definition:
$$P_{\mathcal{C}}(\mathbf{w}') := \arg \min_{\mathbf{v} \in \mathcal{C}} \|\mathbf{v} - \mathbf{w}'\|.$$

1

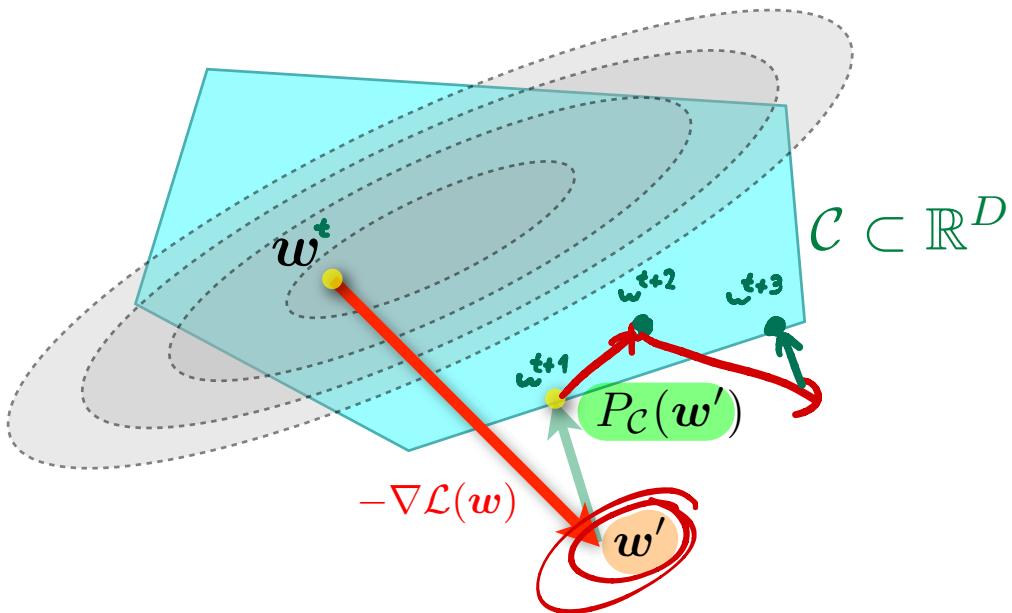
Projected Gradient Descent

Idea: add a projection onto \mathcal{C} after every step:

$$P_{\mathcal{C}}(\mathbf{w}') := \arg \min_{\mathbf{v} \in \mathcal{C}} \|\mathbf{v} - \mathbf{w}'\|.$$

Update rule:

$$\mathbf{w}^{(t+1)} := P_{\mathcal{C}}[\mathbf{w}^{(t)} - \gamma \nabla \mathcal{L}(\mathbf{w}^{(t)})].$$



Projected SGD. Same SGD step, followed by the projection step, as above. Same convergence properties.

Computational cost of projection? // Crucial!

depends on geometry of set \mathcal{C}

Turning Constrained into Unconstrained Problems

(Alternatives to projected gradient methods)

Use penalty functions instead of directly solving $\min_{\mathbf{w} \in \mathcal{C}} \mathcal{L}(\mathbf{w})$.

- “brick wall” (indicator function)

$$I_C(\mathbf{w}) := \begin{cases} 0 & \mathbf{w} \in \mathcal{C} \\ \infty & \mathbf{w} \notin \mathcal{C} \end{cases}$$

$$\Rightarrow \min_{\mathbf{w} \in \mathbb{R}^D} \mathcal{L}(\mathbf{w}) + I_C(\mathbf{w})$$

(disadvantage: non-continuous objective)

original cost



penalty function

- Penalize error. Example:

$$\mathcal{C} = \{\mathbf{w} \in \mathbb{R}^D \mid A\mathbf{w} = \mathbf{b}\}$$

$$\Rightarrow \min_{\mathbf{w} \in \mathbb{R}^D} \mathcal{L}(\mathbf{w}) + \lambda \underbrace{\|A\mathbf{w} - \mathbf{b}\|^2}_{\text{trade-off parameter } \lambda}$$

trade-off parameter λ

- Linearized Penalty Functions
(see Lagrange Multipliers)

$$\boxed{A} \boxed{\mathbf{w}} = \boxed{\mathbf{b}}$$

Implementation Issues

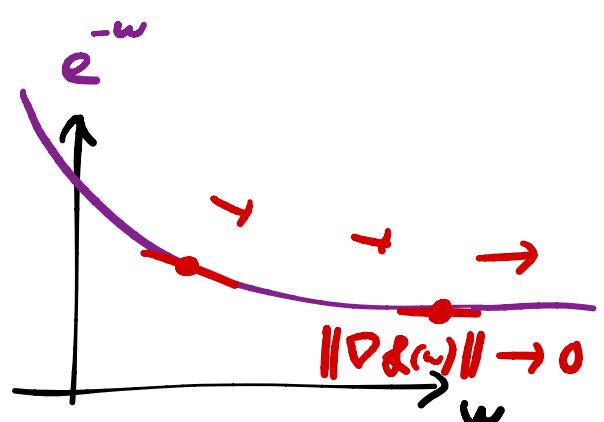
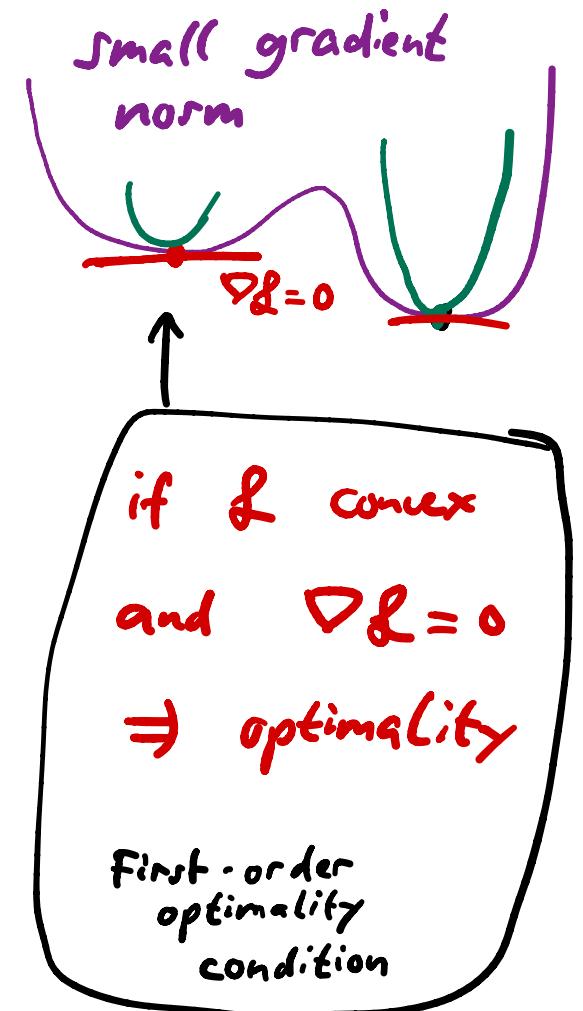
For gradient methods:

Stopping criteria: When $\|\nabla \mathcal{L}(\mathbf{w})\|$ is (close to) zero, we are (often) close to the optimum value.

2nd-order optimality

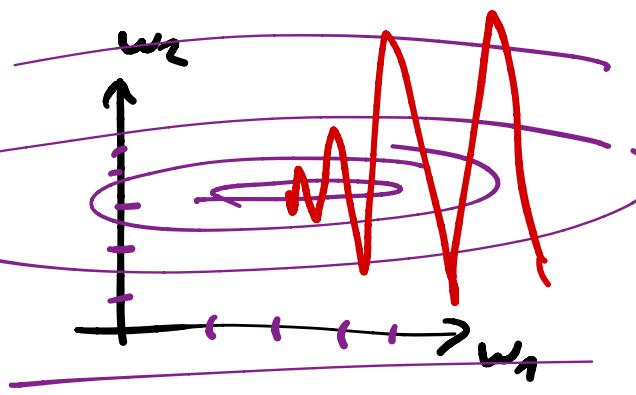
Optimality: If the second-order derivative is positive (positive semi-definite to be precise), then it is a (possibly local) minimum. If the function is also convex, then this condition implies that we are at a global optimum. See the supplementary section on **Optimality Conditions**.

Step-size selection: If γ is too big, the method might diverge. If it is too small, convergence is slow. Convergence to a local minimum is guaranteed only when $\gamma < \gamma_{min}$ where γ_{min} is a fixed constant that depends on the problem.

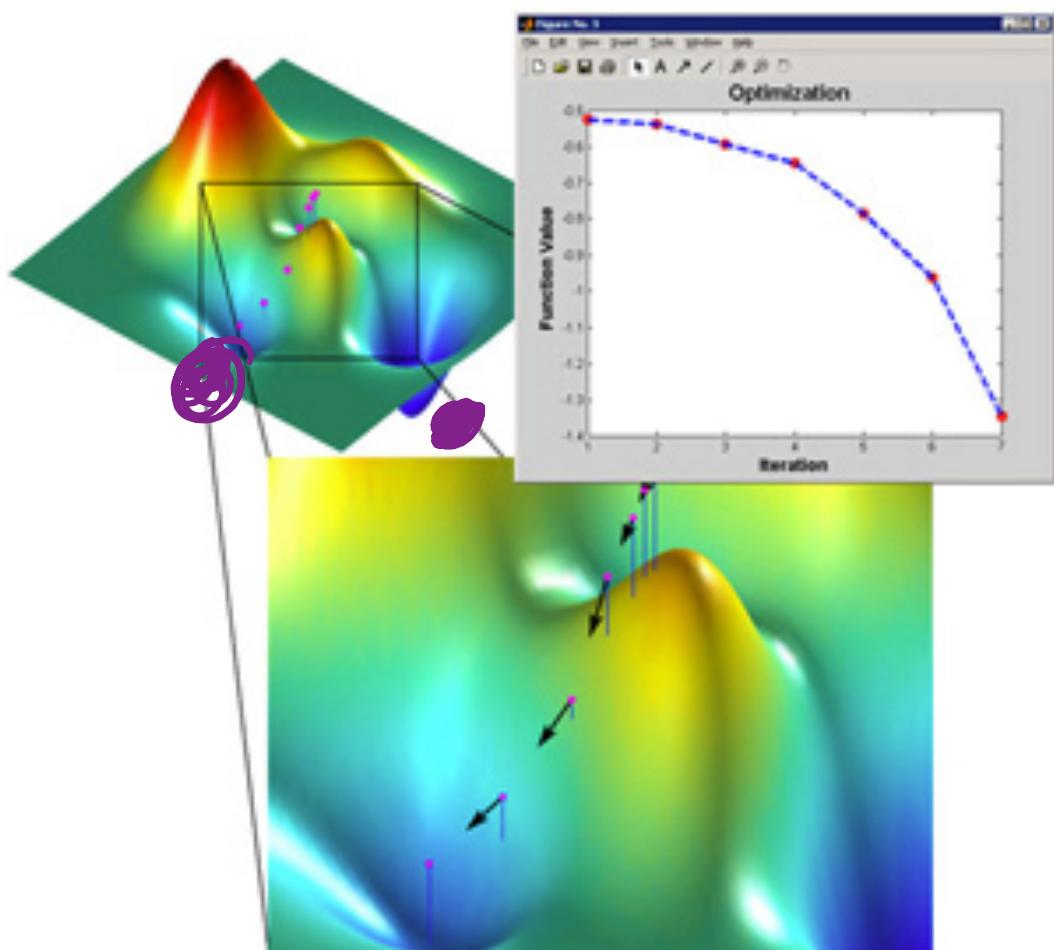


Line-search methods: For some objectives \mathcal{L} , we can set step-size automatically using a line-search method. More details on “backtracking” methods can be found in Chapter 1 of Bertsekas’ book on “nonlinear programming”.

Feature normalization and pre-conditioning: Gradient descent is very sensitive to ill-conditioning. Therefore, it is typically advised to normalize your input features. In other words, we pre-condition the optimization problem. Without this, step-size selection is more difficult since different “directions” might converge at different speed.



Non-Convex Optimization



*image from mathworks.com

Real-world problems are **not convex!**

All we have learnt on algorithm design and performance of convex algorithms still helps us in the non-convex world.



Additional Notes

Grid Search and Hyper-Parameter Optimization

Read more about grid search and other methods for “hyperparameter” setting:

en.wikipedia.org/wiki/Hyperparameter_optimization#Grid_search.

Computational Complexity

The computation cost is expressed using the [big-O](#) notation. Here is a definition taken from Wikipedia. Let f and g be two functions defined on some subset of the real numbers. We write $f(x) = \mathcal{O}(g(x))$ as $x \rightarrow \infty$, if and only if there exists a positive real number c and a real number x_0 such that $|f(x)| \leq c|g(x)|$, $\forall x > x_0$.

Please read and learn more from this page in Wikipedia:

en.wikipedia.org/wiki/Computational_complexity_of_mathematical_operations#Matrix_algebra .

- What is the computational complexity of matrix multiplication?
- What is the computational complexity of matrix-vector multiplication?

Optimality Conditions

For a *convex* optimization problem, the first-order *necessary* condition says that at *an* optimum the gradient is equal to zero.

$$\nabla \mathcal{L}(\mathbf{w}^*) = \mathbf{0} \quad (1)$$

The second-order *sufficient* condition ensures that the optimum is a minimum (not a maximum or saddle-point) using the [Hessian](#) matrix,

which is the matrix of second derivatives:

$$\mathbf{H}(\mathbf{w}^*) := \frac{\partial^2 \mathcal{L}(\mathbf{w}^*)}{\partial \mathbf{w} \partial \mathbf{w}^\top} \quad \text{is positive semi-definite.} \quad (2)$$

The Hessian is also related to the convexity of a function: a twice-differentiable function is convex if and only if the Hessian is positive semi-definite at all points.

SGD Theory

As we have seen above, when N is large, choosing a random training example (\mathbf{x}_n, y_n) and taking an SGD step is advantageous:

$$\mathbf{w}^{(t+1)} := \mathbf{w}^{(t)} - \gamma^{(t)} \nabla \mathcal{L}_n(\mathbf{w}^{(t)})$$

For convergence, $\gamma^{(t)} \rightarrow 0$ “appropriately”. One such condition called the Robbins-Monroe condition suggests to take $\gamma^{(t)}$ such that:

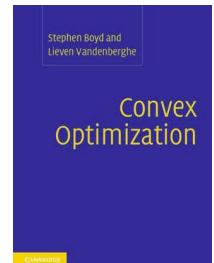
$$\sum_{t=1}^{\infty} \gamma^{(t)} = \infty, \quad \sum_{t=1}^{\infty} (\gamma^{(t)})^2 < \infty \quad (3)$$

One way to obtain such sequences is $\gamma^{(t)} := 1/(t+1)^r$ where $r \in (0.5, 1)$.

More Optimization Theory

If you want, you can gain a deeper understanding of several optimization methods relevant for machine learning from this survey:

Convex Optimization: Algorithms and Complexity
- by Sébastien Bubeck



And also from the book of Boyd & Vandenberghe
(both are free online PDFs)

(> 35 000
citations)

Exercises

1. Chain-rule



If it has been a while, familiarize yourself with it again.

2. Revise computational complexity (also see the Wikipedia link in Page 6 of lecture notes).
3. Derive the computational complexity of grid-search, gradient descent and stochastic gradient descent for linear MSE (# steps and cost per step).
4. Derive the gradients for the linear MSE and MAE cost functions.
5. Implement gradient descent and gain experience in setting the step-size.
6. Implement SGD and gain experience in setting the step-size.