Annotated version

Machine Learning Course - CS-433

Optimization

Sep 20+26, 2023

Martin Jaggi
Last updated on: September 20, 2023

credits to Mohammad Emtiyaz Khan

EPFL

Learning / Estimation / Fitting

Given a cost function $\mathcal{L}(\mathbf{w})$, we wish to find $\mathbf{w}^\star$ 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 $\mathbf{w}$).

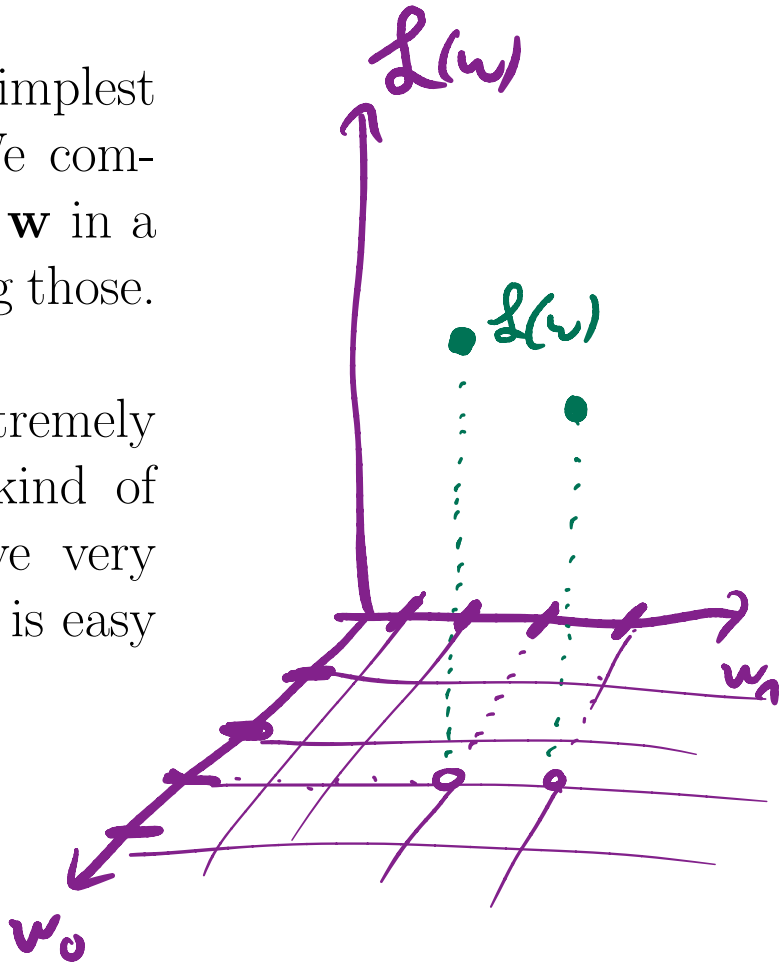
$\mathcal{L}(w) = \frac{1}{N} \sum_{n=1}^{N} \mathcal{L}_n(w)$

example: $(y_n - f_w(x_n))^2$

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.



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

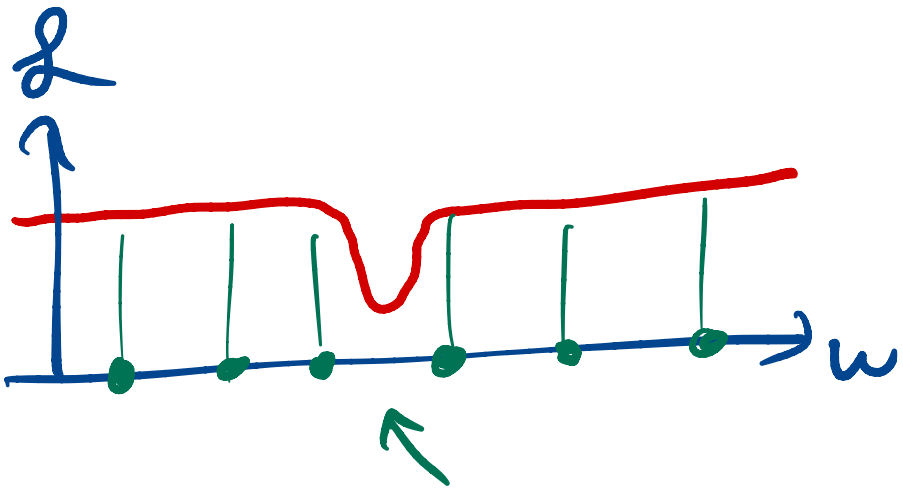
If we decide to use 10 possible values for each dimension of $\mathbf{w}$, then we have to check 10^D points. This is clearly impossible for most practical machine learning models, which can often have $D \approx$ millions of parameters. Choosing a good range of values for each dimension is another problem.

granularity

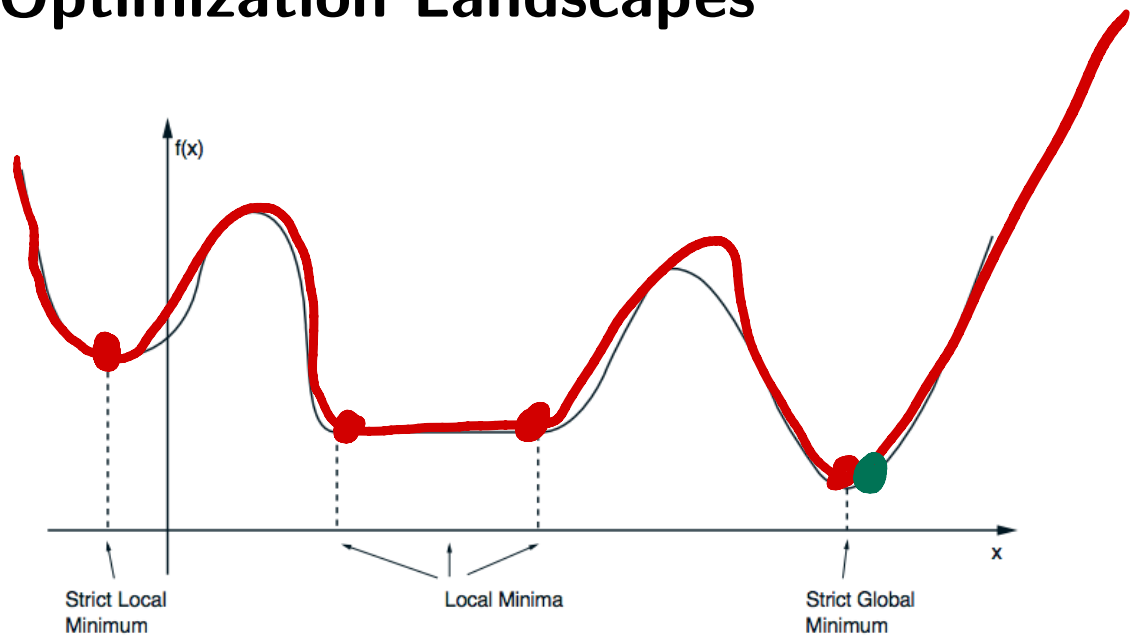
$|\text{search range}| = |\{1, \ldots, 10\}^D| = 10^D$

exponential cost

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

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

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

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

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

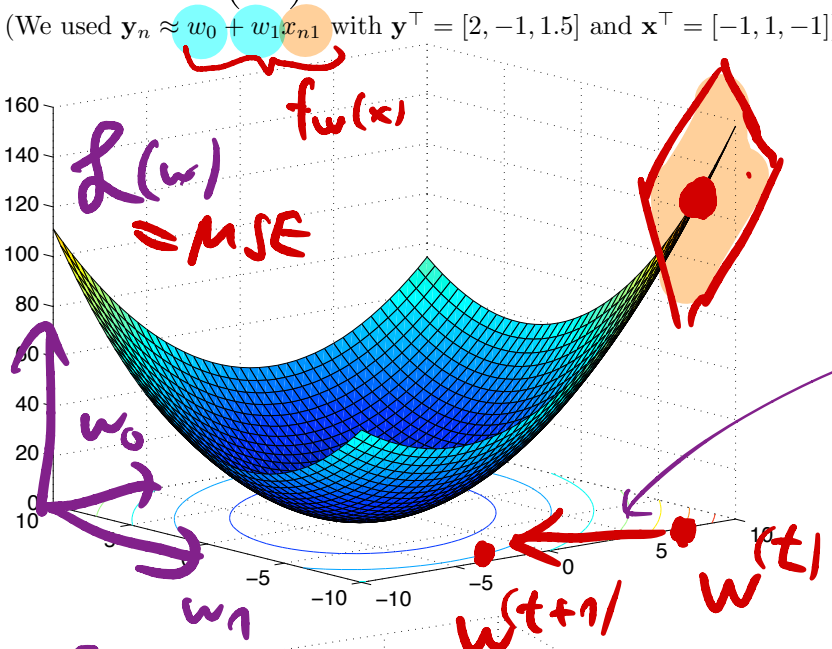
Smooth Optimization

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.

Cauchy 1848

For a 2-parameter model, MSE($\mathbf{w}$) and MAE($\mathbf{w}$) are shown below.
(We used $\mathbf{y}_n \approx w_0 + w_1 x_{n1}$ with $\mathbf{y}^\top = [2, -1, 1.5]$ and $\mathbf{x}^\top = [-1, 1, -1]$).



$f_w(x)$

$\mathcal{L}(w)$ = MSE

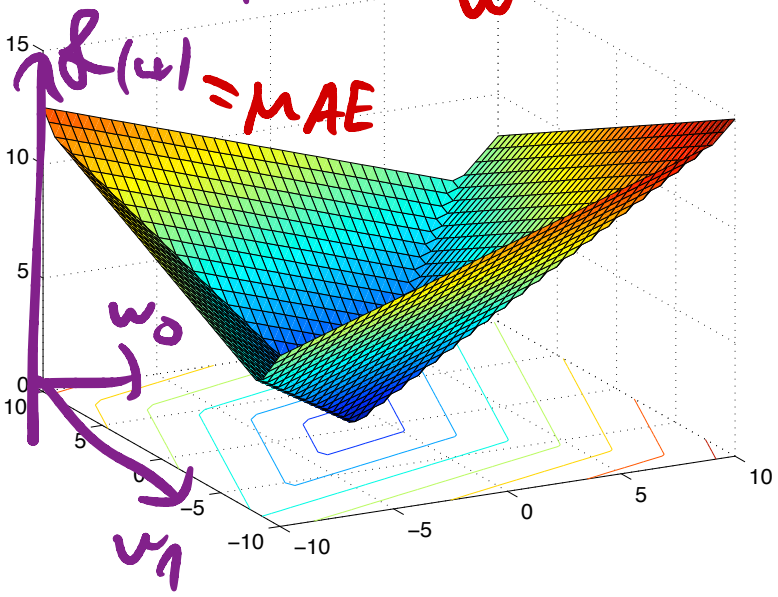
w_0

w_1

$w^{(t+1)}$

$w^{(t)}$

$-\gamma \nabla \mathcal{L}(w)$



$\mathcal{L}(w)$ = MAE

w_0

w_1

Definition of the gradient:

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

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

Gradient Descent

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

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

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

popular stepsize $\gamma := c/t$

1-param: $w = w_0$

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

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

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

$\min_w \mathcal{L}(w_0)$

$f_w(x) = w_0$

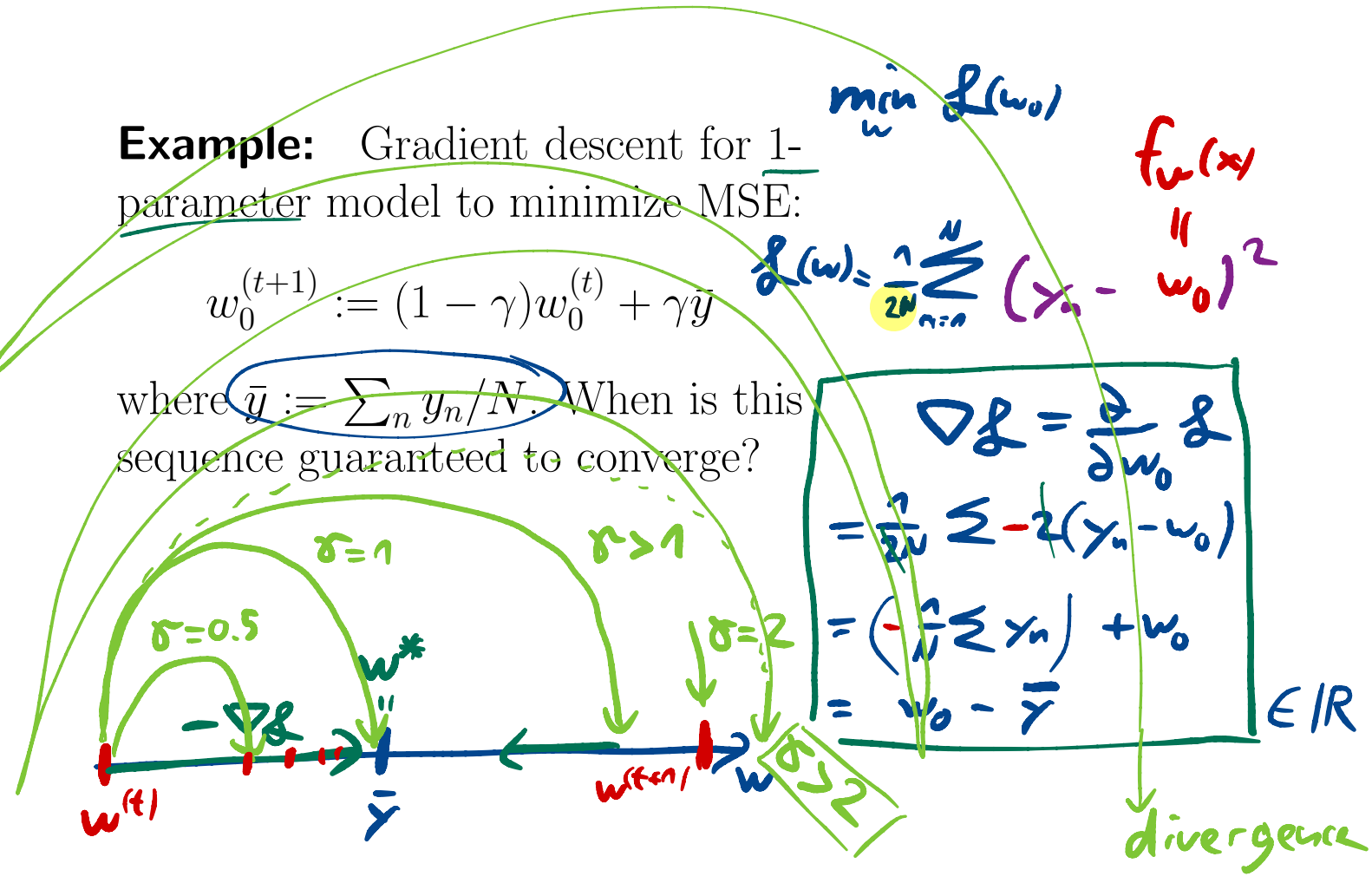
$\mathcal{L}(w) = \frac{1}{2N} \sum_{n=1}^{N} (y_n - w_0)^2$

$\nabla \mathcal{L} = \frac{\partial}{\partial w_0} \mathcal{L}$

$= \frac{1}{2N} \sum -2(y_n - w_0)$

$= \left(-\frac{1}{N} \sum y_n \right) + w_0$

$= w_0 - \bar{y}$ $\in \mathbb{R}$



MatrixCalculus.org

Gradient Descent for Linear MSE

For linear regression

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

We define the error vector $\mathbf{e}$:

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

and MSE as follows:

$$\mathcal{L}(\mathbf{w}) := \frac{1}{2N} \sum_{n=1}^{N} (y_n - \mathbf{x}_n^\top \mathbf{w})^2 = \frac{1}{2N} \mathbf{e}^\top \mathbf{e}$$

then the gradient is given by

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

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 $O(N \cdot D) + O(N)$

② compute $\nabla \mathcal{L}$, given $\mathbf{e}$, $\mathbf{w}$
$O(N \cdot D) + O(D)$

$O(N \cdot D)$

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

artificial feature

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

$w \in \mathbb{R}^{D+1}$

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

Stochastic Gradient Descent

SGD

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

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

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 a datapoint $n \in \{1, \dots, N\}$ u.a.r.
2. $\mathbf{w}^{(t+1)} := \mathbf{w}^{(t)} - \gamma \nabla \mathcal{L}_n(\mathbf{w}^{(t)})$.

stochastic gradient $= g$

Theoretical Motivation. *Idea:* Cheap but unbiased estimate of the gradient!

In expectation over the random choice of n, we have

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

which is the true gradient direction. (check!)

$$\mathbb{E}_n\left[\nabla \mathcal{L}_n(w)\right] = \frac{1}{n}\sum_{n=1}^{N} \nabla \mathcal{L}_n(w) = \nabla\left(\frac{1}{n}\sum \ldots\right) = \nabla \mathcal{L}(w) \quad \square$$

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 $\mathbf{w}^{(t)}$.

$B \subseteq \{1, \ldots, N\}$ sample of size $|B|$

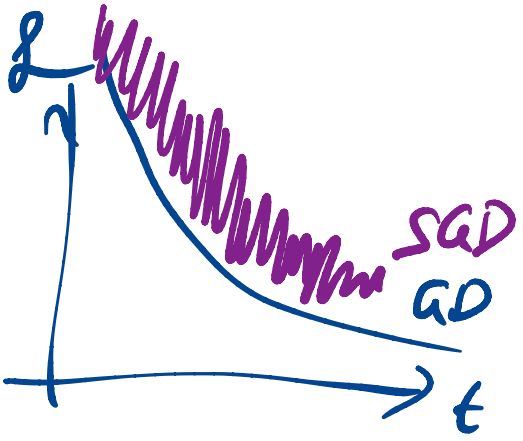
- $|B| = 1$ → pure SGD
- $|B| = 128$ → mini-batch
- $|B| = N$ → full GD

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.

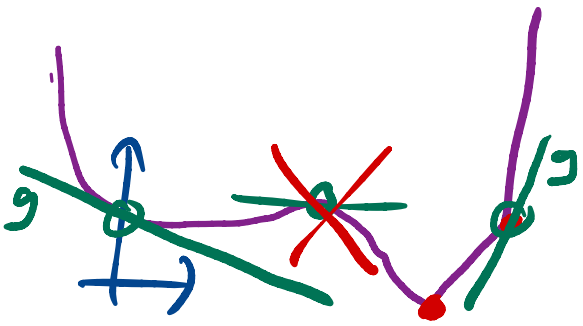


Computational cost. For linear MSE, what is the complexity (# operations) of computing the stochastic gradient?
(using only $|B| = 1$ data examples)

cost per step	$\mathcal{L}_n = \frac{1}{2}(y_n - x_n^T w)^2$
SGD	$\nabla \mathcal{L}_n = -x_n^T (y_n - x_n^T w)$
$\mathcal{O}(D)$	$e_n \in \mathbb{R}$
N times cheaper	$\mathcal{L} = \frac{1}{2N} \sum_{n=1}^{N} (y_n - x_n^T w)^2$
GD	$\nabla \mathcal{L} = -\frac{1}{N} X^T (y - Xw)$
$\mathcal{O}(N \cdot D)$	$e \in \mathbb{R}^N$

non-differentiable

Non-Smooth Optimization

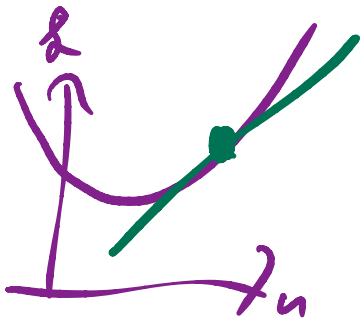


An alternative characterization of *convexity*, for differentiable functions is given by

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

1st-order Taylor exp.

meaning that the function must always lie above its linearization.

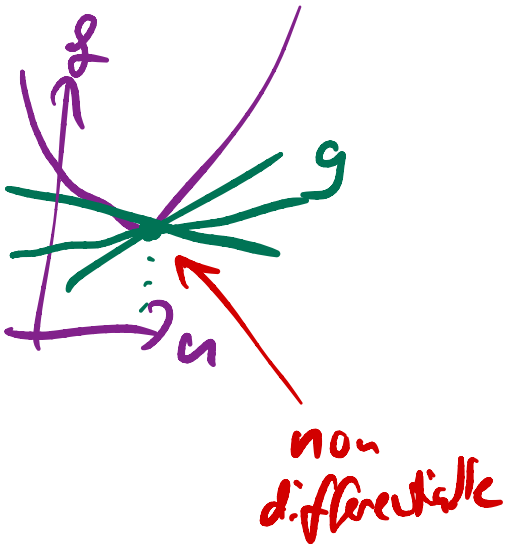


Subgradients

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

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

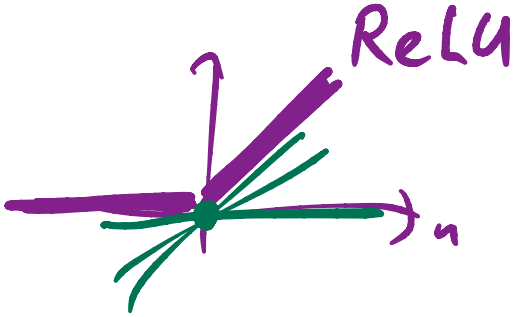
is called a subgradient to the function $\mathcal{L}$ at $\mathbf{w}$.



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 $\mathbf{g} = \nabla\mathcal{L}(\mathbf{w})$.

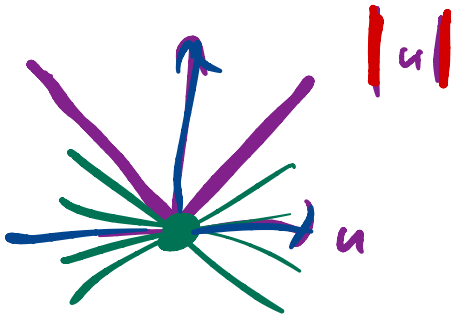
Subgradient Descent



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 $\mathbf{w}^{(t)}$.



Example: Optimizing Linear MAE

1. Compute a subgradient of the absolute value function

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

$$g = \begin{cases} -1 & \text{if } e<0 \\ [-1,1] & \text{if } e=0 \\ 1 & \text{if } e>0 \end{cases}$$

2. Recall the definition of the mean absolute error:

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

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

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

$$\ell(w) = h(q(w))$$

h: non-differentiable
q: differentiable

See Exercise Sheet 2.

Subgradient of ℓ at w

$$g \in \partial h(q(w)) \cdot \nabla q(w)$$

∂h = set of subgradients of h

Stochastic (Sub)gradient Descent

Stochastic SubGradient Descent (still abbreviated SGD commonly).

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

Exercise: Compute the SGD update for linear MAE.

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

potentially not differentiable

g : take a subgradient of $\mathcal{L}_n$

Linear model training

	smooth MSE	non-smooth MAE
GD	gradient $\nabla\mathcal{L}$ $\mathcal{O}(N \cdot D)$	subgradient $g \in \partial\mathcal{L}$ $\mathcal{O}(N \cdot D)$
SGD	gradient $\nabla\mathcal{L}_n$ $\mathcal{O}(D)$	subgradient $g \in \partial\mathcal{L}_n$ $\mathcal{O}(D)$

per iteration

Variants of SGD

SGD with Momentum

$\beta_1 = 0.9$

pick a stochastic gradient $\mathbf{g}$

$$\mathbf{m}^{(t+1)} := \beta_1 \mathbf{m}^{(t)} + (1-\beta_1)\mathbf{g} \quad \text{(momentum term)}$$

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

g in standard SGD

- momentum from previous gradients (acceleration)

Adam

pick a stochastic gradient $\mathbf{g}$

$$\mathbf{m}^{(t+1)} := \beta_1 \mathbf{m}^{(t)} + (1-\beta_1)\mathbf{g} \quad \text{(momentum term)}$$

$$\mathbf{v}_i^{(t+1)} := \beta_2 \mathbf{v}_i^{(t)} + (1-\beta_2)(\mathbf{g}_i)^2 \quad \forall i \quad \text{(2nd-order statistics)}$$

$$\mathbf{w}_i^{(t+1)} := \mathbf{w}_i^{(t)} - \frac{\gamma}{\sqrt{\mathbf{v}_i^{(t+1)}}} \mathbf{m}_i^{(t+1)} \quad \forall i$$

- faster forgetting of older weights
- is a momentum variant of Adagrad
- momentum from previous gradients (acceleration)
- strong performance in practice, e.g. for self-attention networks

$$\frac{m}{\sqrt{v}} = \frac{g_i}{\sqrt{g_i^2}} = \frac{g_i}{|g_i|} = sign(g_i)$$

SignSGD

pick a stochastic gradient $\mathbf{g}$

$$\mathbf{w}_i^{(t+1)} := \mathbf{x}_i^{(t)} - \gamma \, sign(\mathbf{g}_i) \quad \forall i$$

- only use the sign (one bit) of each gradient entry -¿ communication efficient for distributed training
- convergence issues

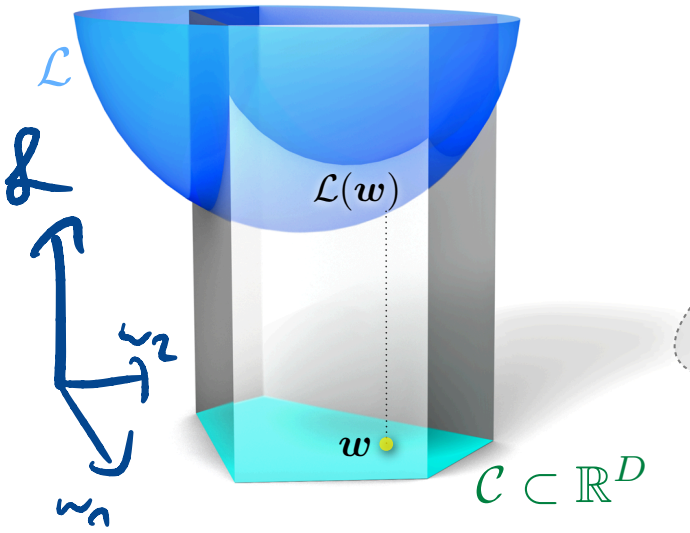
special case of Adam with $\beta_1 = 0$, $\beta_2 = 0$

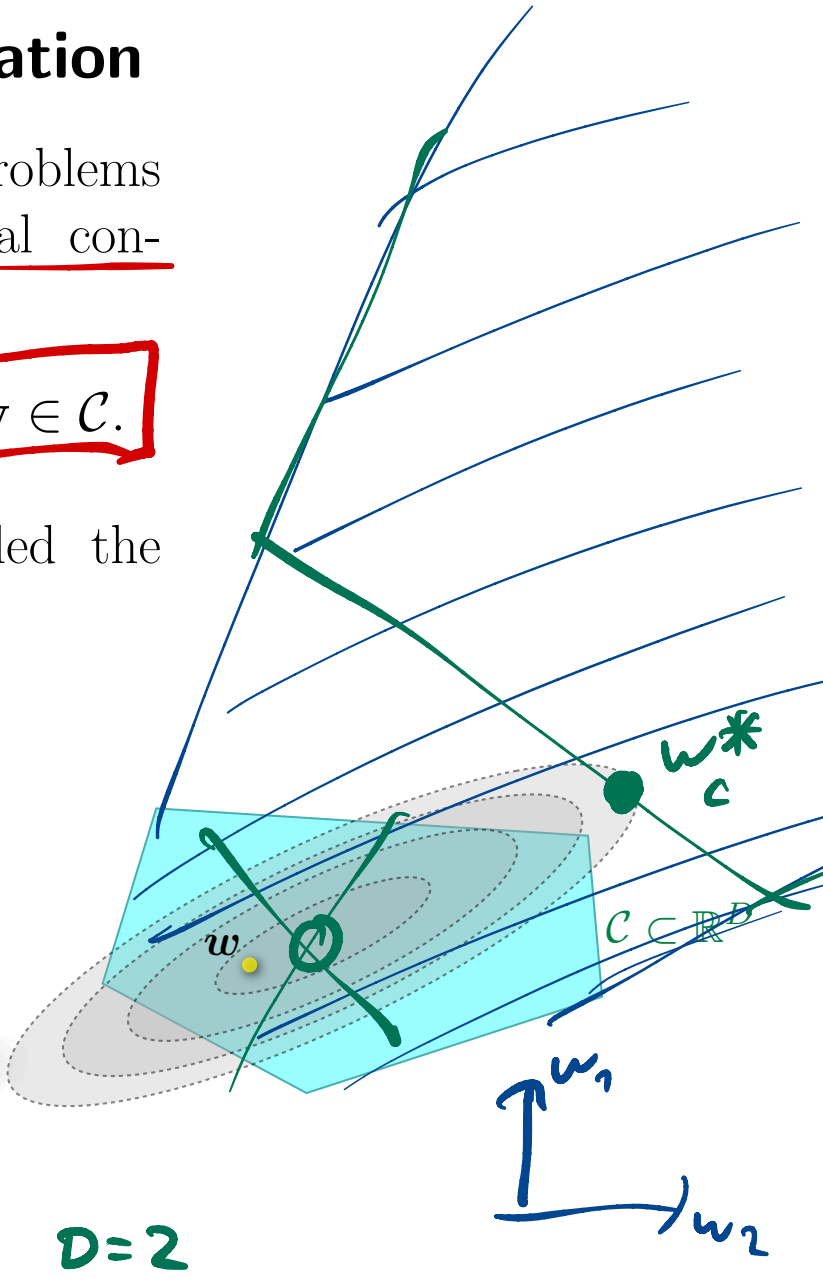
Constrained Optimization

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

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

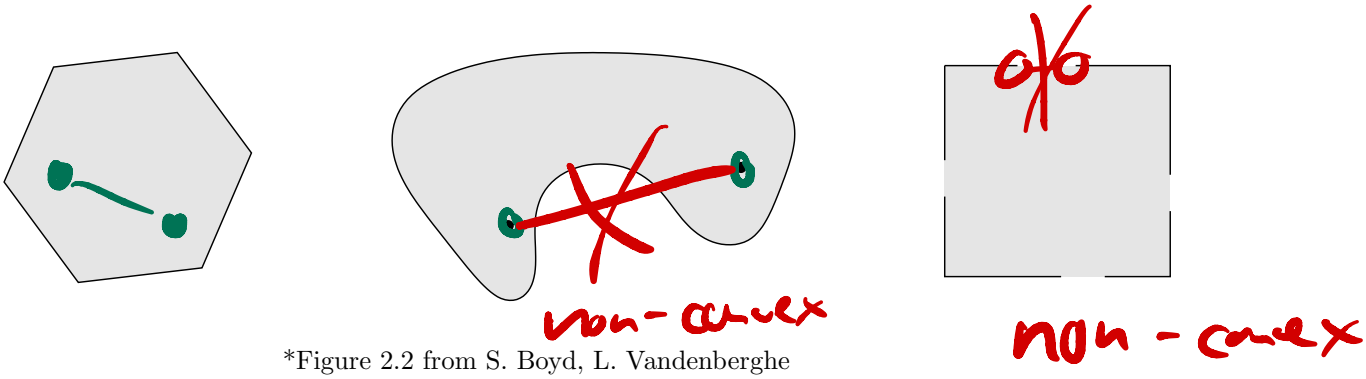
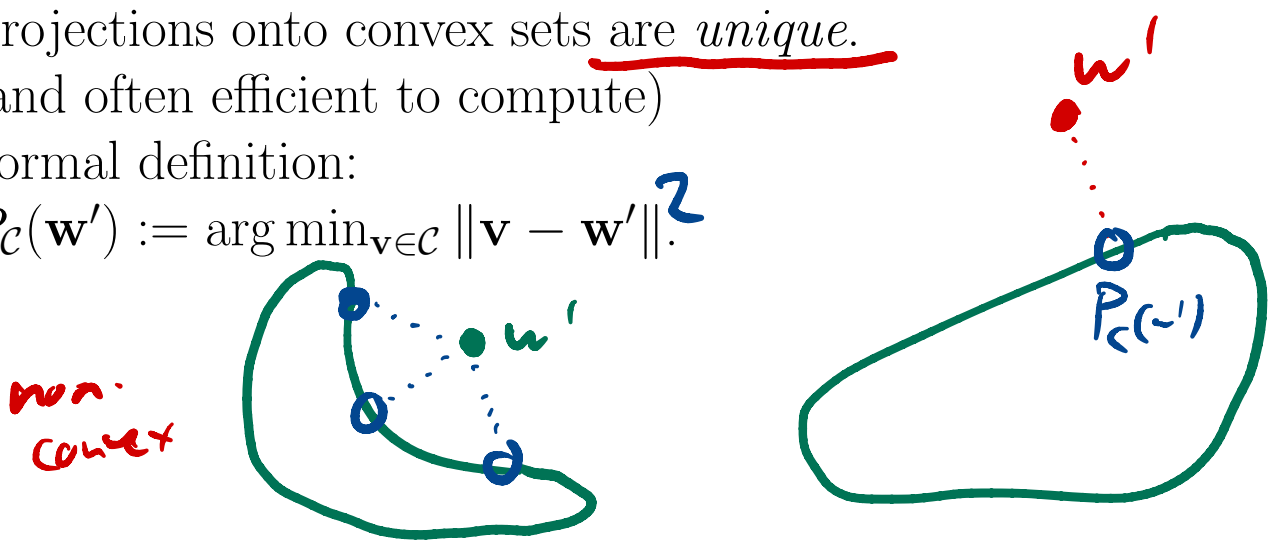


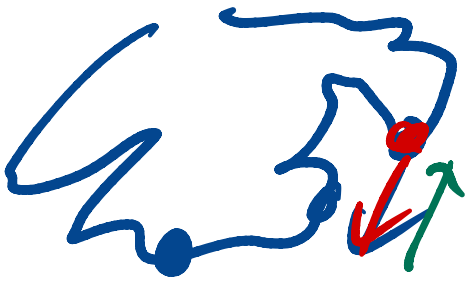
*Figure 2.2 from S. Boyd, L. Vandenberghe

Properties of Convex Sets

- Intersections of convex sets are convex
- Projections onto convex sets are *unique*.
  (and often efficient to compute)
  Formal definition:
  $P_{\mathcal{C}}(\mathbf{w}') := \arg\min_{\mathbf{v}\in\mathcal{C}} \|\mathbf{v} - \mathbf{w}'\|^2$



Projected Gradient Descent



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

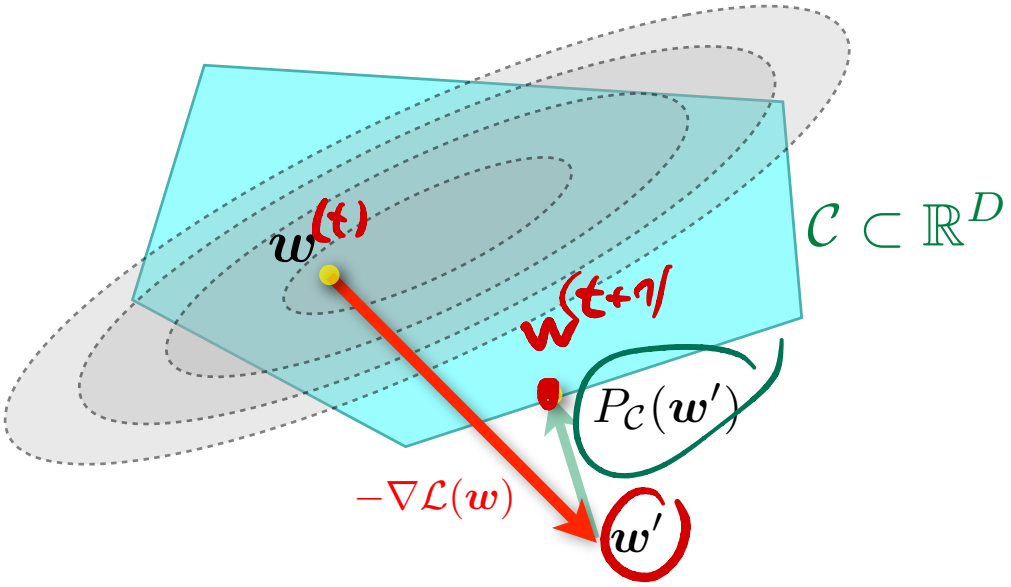
$$P_{\mathcal{C}}(\mathbf{w}') := \arg\min_{\mathbf{v}\in\mathcal{C}} \|\mathbf{v} - \mathbf{w}'\| \ .$$

Update rule:

traditional GD step $= w'$

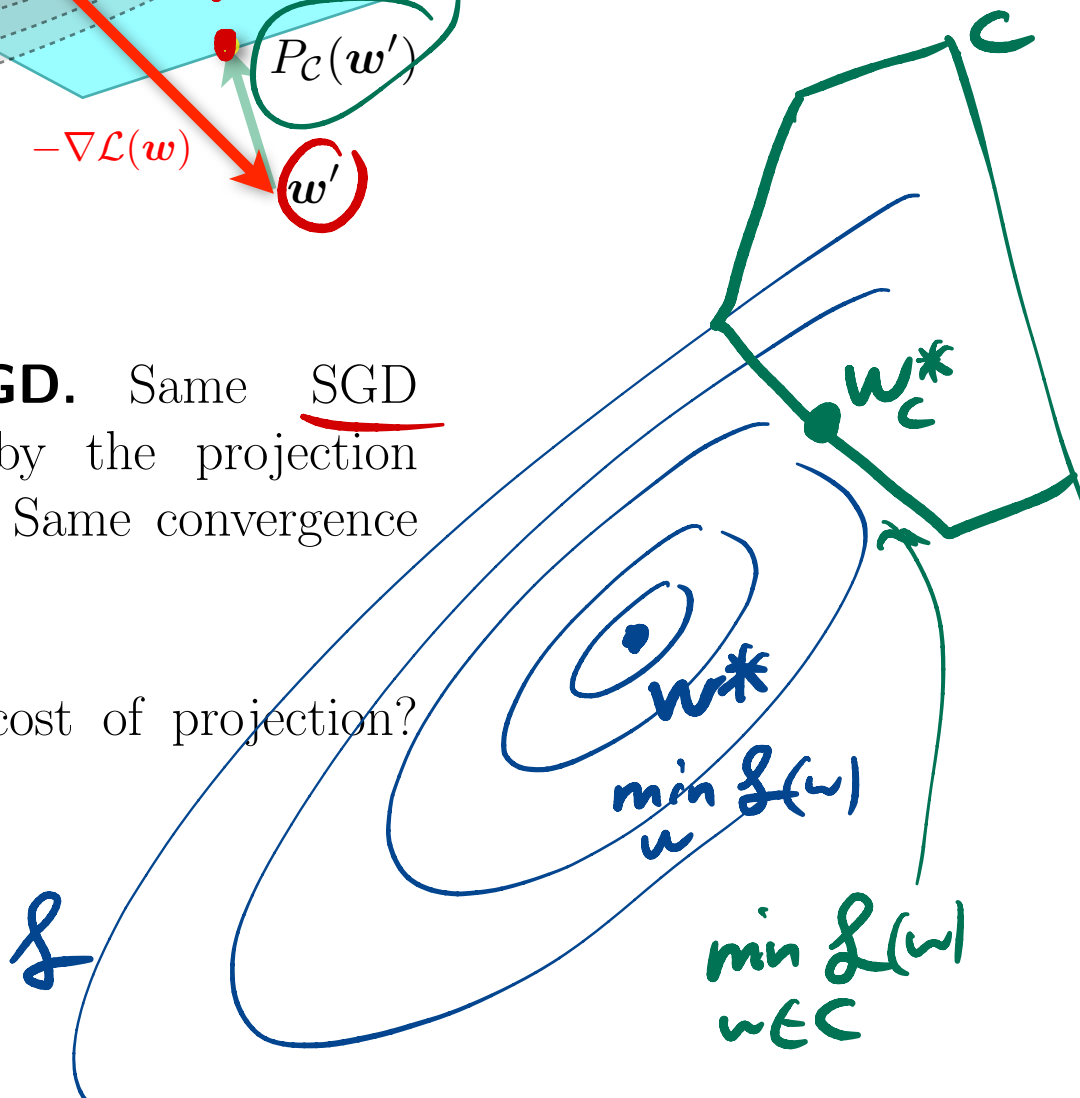
$$\mathbf{w}^{(t+1)} := P_{\mathcal{C}}\left[\mathbf{w}^{(t)} - \gamma\, \nabla\mathcal{L}(\mathbf{w}^{(t)})\right] \ .$$

repeat



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

Computational cost of projection? Crucial!



(2)

Turning Constrained into Unconstrained Problems

(Alternatives to projected gradient methods)

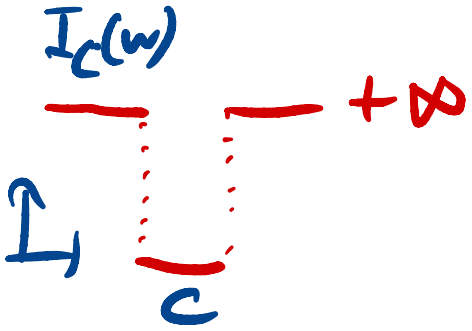
Use penalty functions instead of directly solving $\min_{\mathbf{w}\in\mathcal{C}} \mathcal{L}(\mathbf{w})$.

- "*brick wall*" (indicator function)

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

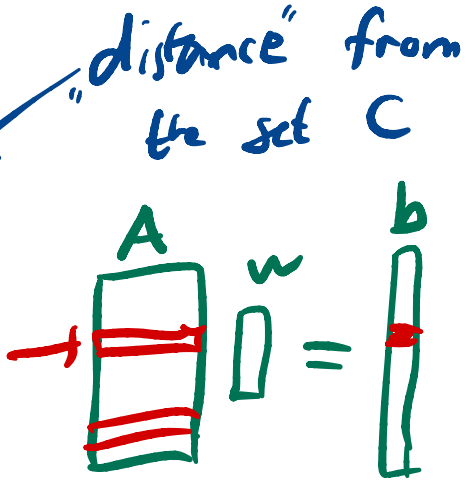
$$\Rightarrow \min_{\mathbf{w}\in\mathbb{R}^D} \mathcal{L}(\mathbf{w}) + I_{\mathcal{C}}(\mathbf{w})$$

(disadvantage: non-continuous objective)



- Penalize error. *Example:* $\mathcal{C} = \{\mathbf{w} \in \mathbb{R}^D \mid A\mathbf{w} = \mathbf{b}\}$

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



- Linearized Penalty Functions (see Lagrange Multipliers)

- Sparsity

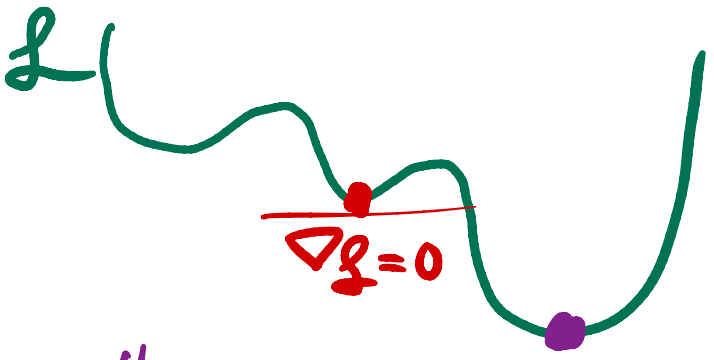
Implementation Issues

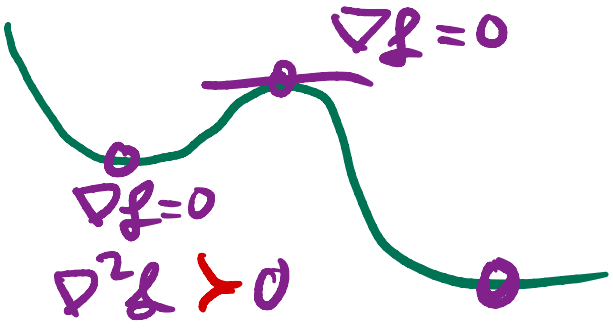
For gradient methods:

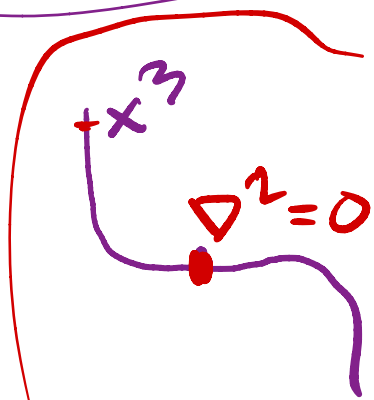
Stopping criteria: When $\|\nabla \mathcal{L}(\mathbf{w})\|$ is (close to) zero, we are (often) close to the optimum value.

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.



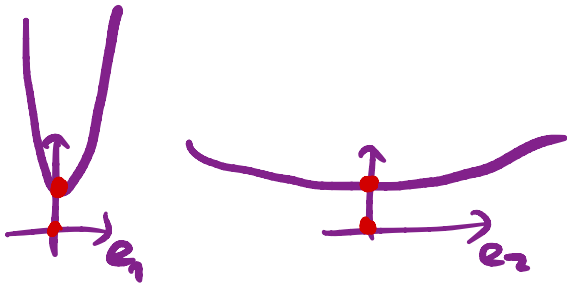


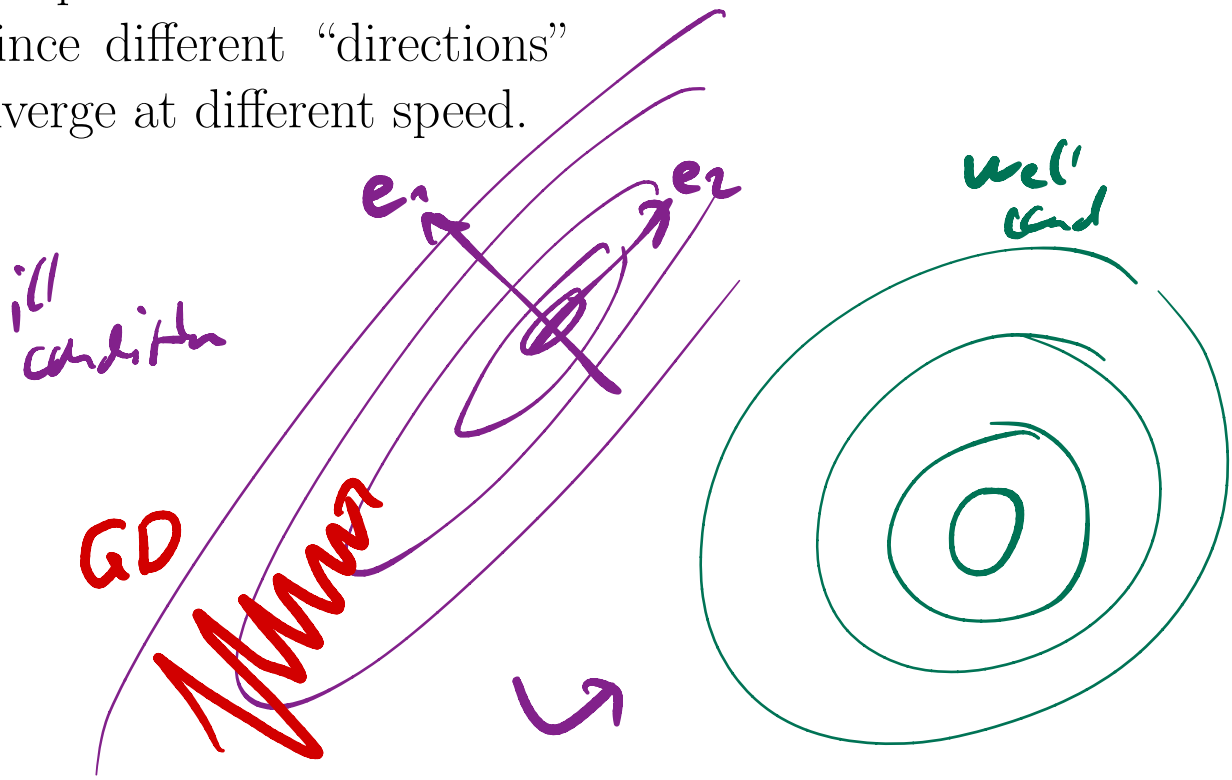


Adam is using coordinate-wise learning-rate

Line-search methods: For some objectives $\mathcal{L}$, we can set step-size automatically using a line-search method. More details on "back-tracking" 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

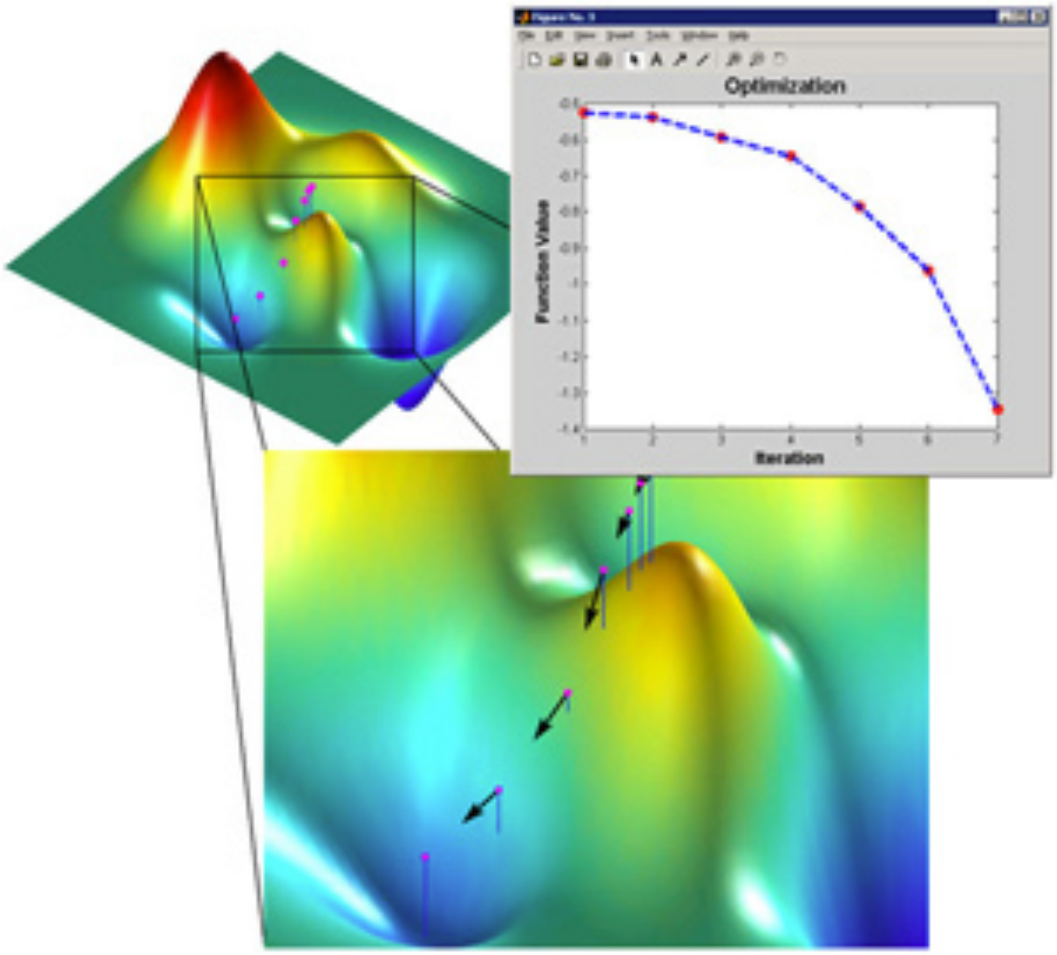


*image from mathworks.com

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-$\mathcal{O}$ 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 $x \to \infty$, if and only if there exists a positive real number c and a real number x_0 such that $|f(x)| \leq c|g(x)|, \quad \forall x > x_0$.

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.

$$\nabla \mathcal{L}(\mathbf{w}^\star) = \mathbf{0} \tag{1}$$

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:

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

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

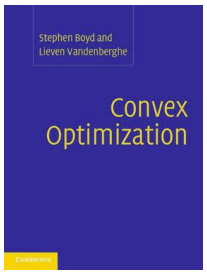
$$\sum_{t=1}^{\infty} \gamma^{(t)} = \infty, \qquad \sum_{t=1}^{\infty} (\gamma^{(t)})^2 < \infty \tag{3}$$

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)

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.