Machine Learning Course - CS-433

Optimization

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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 $\mathbf{w}$).

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.

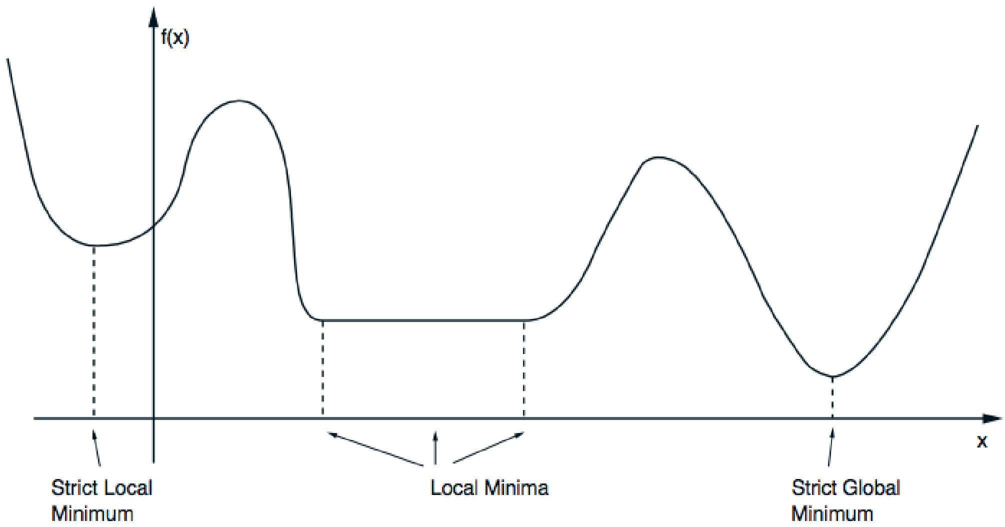
This is brute-force, but extremely simple and works for any kind of cost function when we have very few parameters and the cost is easy to compute.

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.

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,

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

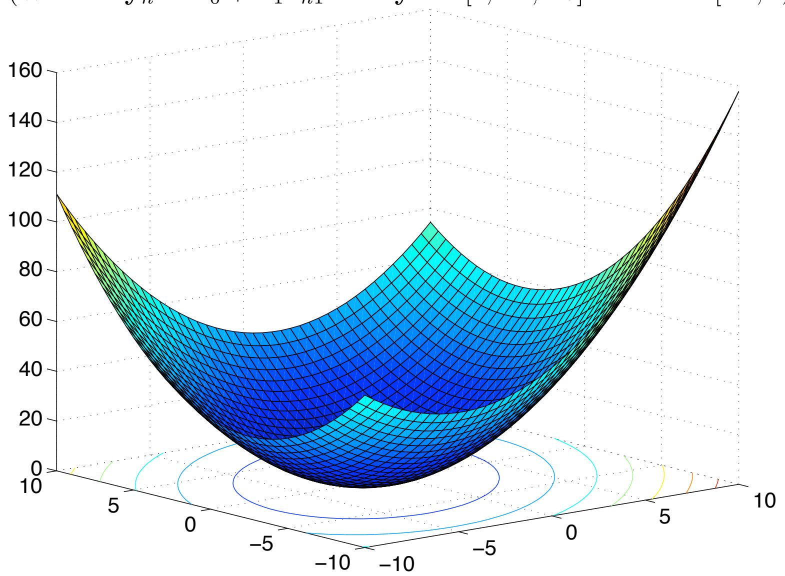
A local or global minimum is said to be strict if the corresponding inequality is strict for $\mathbf{w} \neq \mathbf{w}^\star$.

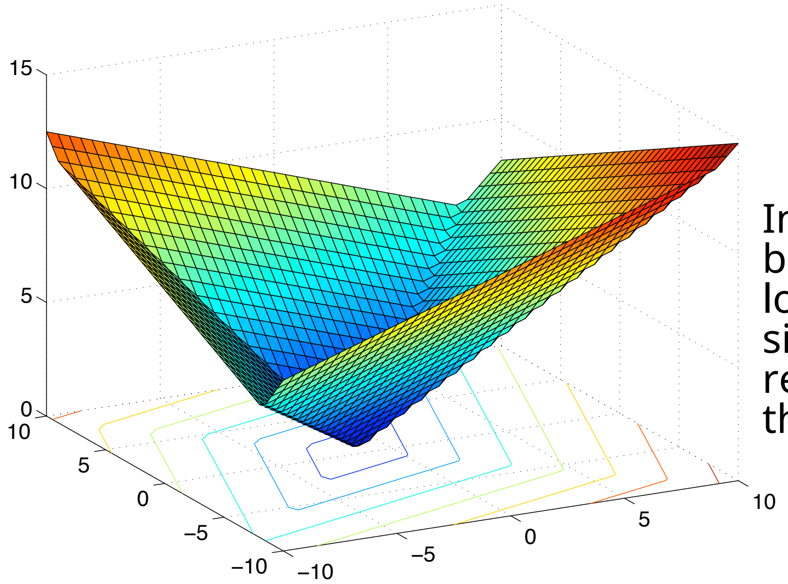
Smooth Optimization

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.

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 $\mathbf{x}^\top = [-1, 1, -1]$).





In this case it can happen that you bounce between each side of the loss function, reducing the step size could be a solution, but reducing it too much might stop the process entirely

Estimate of how much I would go up the loss function if I were to go along the D dimension in the tangent plane

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.

remember that this is a vector that points towards the direction where the loss function grows the most when a set of certain set of weights are used to calculate results. So flipping the gradient of the loss function with the current weight and adding it to the current weights brings us closer to the optimum weights. Which are the ones that when used to calculate results we have the lowest loss function across data

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?

the loss function is just MSE (1/n sum of (y_n - w_0)^2)

to get the gradient we just compute the derivative of MSE:
1/n sum of (2 * (y_n - w_0) * -1) =
2/n sum of (w_0 - y_n) =
(dropping the 2 as it's useless)
1/n sum of (w_0 - y_n) =
1/n (N * w_0 - sum of (y_n)) =
w_0 - 1/n * sum of (y_n) = (second part is y¬)
w_0 - y¬

this means that y¬ was picked correctly in the exercise

having verified the correctness of y¬ we just need to pick a step size below 2, as if we were to pick 2 we would stay at the same distance from the optimum but on the other side, the next does the same but in the opposite direction and you end up in an endless loop

Gradient Descent for Linear MSE

X_n belongs to R_D
w belongs to R_D

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:

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

2N so that when you compute the gradient you dont have to drop the 2 (see two pages before)

$$= \tfrac{1}{2N} \mathbf{e}^\top \mathbf{e}$$

Vector i..n V
N sum of V_i ^ 2 = V_T * V

then the gradient is given by

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

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

a) starting from $\mathbf{w}$ and

b) given $\mathbf{e}$ and $\mathbf{w}$?

Computing e:
Xw = O(N * D) (dot product of N rows of dimension D)
Compute L:
O(N * D) (summing N times a multiplication of two D-sized vectors)

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

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

Stochastic Gradient Descent

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:

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

Instead of computing the Loss function and applying Gradient Descent to all data points every time, you just do it for a random data point. It still makes sense because over many iterations you would still achieve the optimum weights, because taking a random point is an unbiased estimate. All points must converge eventually, it might just take more iterations but each iteration is N times faster (O(D) instead of O(ND))

Theoretical Motivation. *Idea:* Cheap but unbiased estimate of the gradient!
In expectation over the random choice of n, we have

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

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

This is the perfect trade off, can be customized per computers/systems

The calculation of g for each data point in B can be parallelized

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)

mostly trying not to get stuck in local minimums

Variants of SGD

momentum can be initialized with 0 or whatever

it's basically a way to have a moving average of the gradient (it works nicely with stochastic gradients as the moving average softens possible discrepancies between the single data points picked for SGD)

SGD with Momentum

pick a stochastic gradient $\mathbf{g}$

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

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

- momentum from previous gradients (acceleration)

Adam

pick a stochastic gradient $\mathbf{g}$

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

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

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

this moving average helps soften big variations in the gradient's coordinates (we square them as we don't care about the sign, just the magnitude)

- faster forgetting of older weights
- is a momentum variant of Adagrad
- coordinate-wise adjusted learning rate
- strong performance in practice, e.g. for self-attention networks

go slowly around cliffs, or accellerate in smooth valleys (dynamic adjustments)

SignSGD

ADAM with B_1 = 0 and B_2 = 0

pick a stochastic gradient $\mathbf{g}$

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

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

Non-Smooth Optimization

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

this gradient is just the tangent of L function (needed for the "linearization")

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

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 $\mathbf{w}$.

any plane lying under the L function is a subgradient (useful when L is not differentiable because there are multiple subgradients)

in convex and differentiable functions you only have one gradient (tangent plane) at each point

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

this means we can apply SGD by just picking a subgradient as gradient

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

with e < 0 the only gradient is -1
with e = 0 the only gradients are all numbers in [-1, 1]
with e > 0 the only gradient is 1

Example: Optimizing Linear MAE

1. Compute a subgradient of the absolute value function

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

Loss

e

2. Recall the definition of the mean absolute error:

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

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

See Exercise Sheet 2.

Stochastic Subgradient 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.

Implementation Issues

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 the step-size γ follows a schedule becoming small enough, where 'small enough' depends on the problem (landscape) parameters.

Feature normalization and pre-conditioning: Gradient descent is very sensitive to ill-conditioning, that is the phenomenon when some coordinates (directions) have change rates vastly different from others.

Therefore, it is typically advised to normalize input features if possible, and also normalize each layer in a neural network (we will get to this in the later chapters on neural networks). Without this, step-size selection is much more difficult since different "directions" might converge (or fail to do so) at different speed. Rescaling the space in this sense is also known as *pre-conditioning* the optimization problem.

Epoch: sets of iterations that loop through the whole dataset

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

or if the loss changes very slightly after each iteration

Optimality Conditions

For a *smooth* optimization problem, the first-order *necessary* condition says that at *an* optimum the gradient is equal to zero. Points of zero gradient are called critical points.

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

If $\mathcal{L}$ is convex and $\mathbf{w}^\star$ is a critical point, then $\mathbf{w}^\star$ is a global optimum.

the second derivative in a a candidate point is positive if the loss afterwards increases (meaning the candidate point is a local minimum)
the opposite happens if the second derivative is negative

We can use the second derivative to study if a candidate point is a local minimum (not a local maximum or saddle-point) using the Hessian matrix,

$$\nabla^2\mathcal{L}(\mathbf{w}) := \frac{\partial^2\mathcal{L}}{\partial\mathbf{w}\partial\mathbf{w}^\top}(\mathbf{w})$$

this is because the second derivative to a point is the tangent plane to the derivative in that same point, and the derivative is just the slopes at each point of the tangent plane to the original function

The second-order *sufficient* condition states that if

- $\nabla\mathcal{L}(\mathbf{w}) = \mathbf{0}$ (critical point)
- and $\underline{\nabla^2\mathcal{L}(\mathbf{w}) \succ 0}$ (positive definite),

Hessian matrix

then $\mathbf{w}$ is a local minimum.

s_T H s > 0 for each s

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.

Non-Convex Optimization

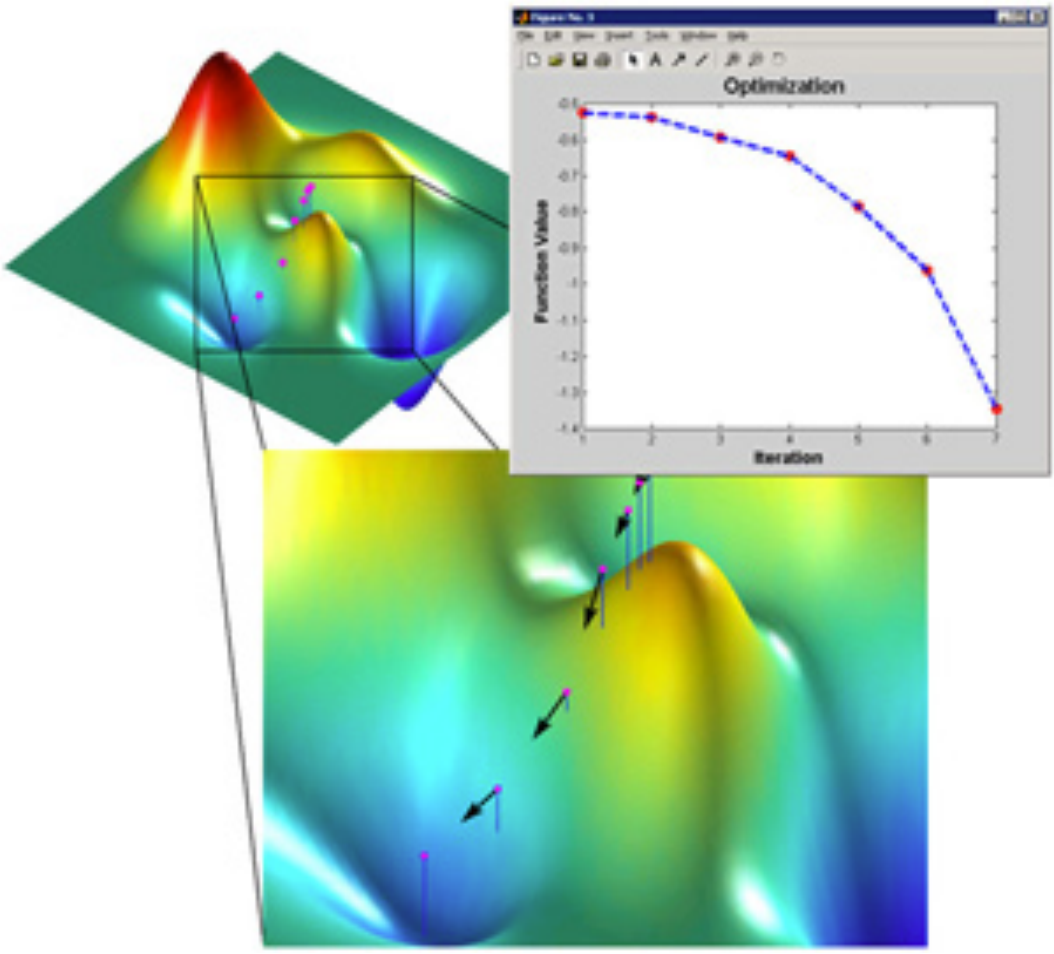


*image from mathworks.com

Real-world problems are not convex!

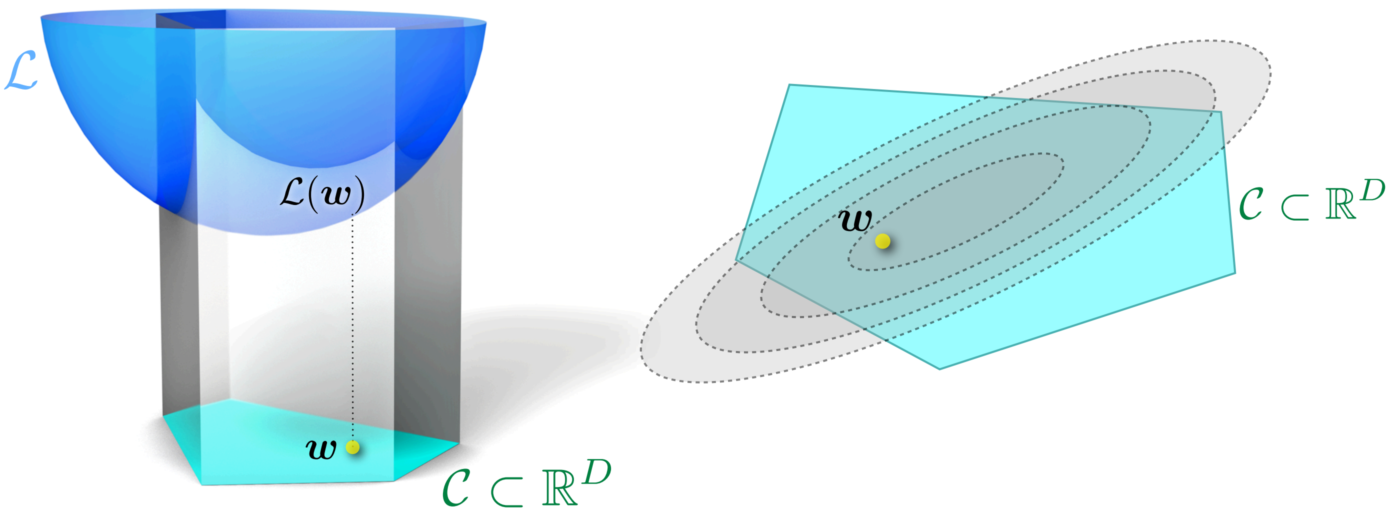
All we have learnt on algorithm design and performance of convex algorithms still helps us in the non-convex world.

Constrained Optimization

Sometimes, optimization problems come posed with additional constraints:

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

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

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

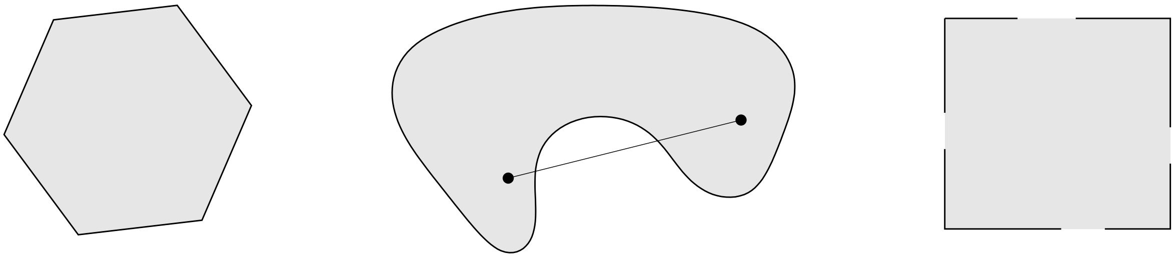


*Figure 2.2 from S. Boyd, L. Vandenberghe

Properties of Convex Sets

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

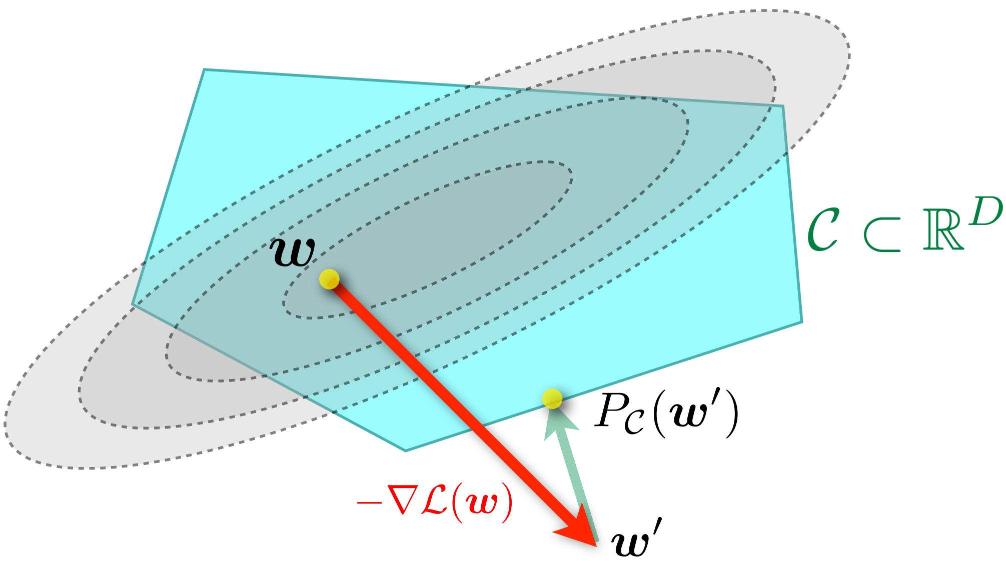
Projected Gradient Descent

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:

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



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

Computational cost of projection? Crucial!

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)

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

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

  makes sense but you make the loss function non differentiable and continuous

  (disadvantage: non-continuous objective)

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

  relax

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

- Linearized Penalty Functions (see Lagrange Multipliers)

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?

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:

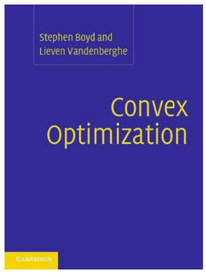
$$\sum_{t=1}^{\infty} \gamma^{(t)} = \infty, \qquad \sum_{t=1}^{\infty} (\gamma^{(t)})^2 < \infty \tag{1}$$

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 ($\mathcal{O}$-notation).

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.