Optimization in ML

Machine Learning and Data Mining

Maxim Borisyak

National Research University Higher School of Economics (HSE)

October 2, 2018

Machine Learning in a nutshell

ML algorithms

Every (supervised) ML algorithm ever:

- a model $\mathcal{A}$ - set of all possible solutions:

$$\mathcal{A} \subseteq \{f : \mathcal{X} \to \mathcal{Y}\}$$

  - $\mathcal{X}$, $\mathcal{Y}$ - sample and target spaces.
- a search procedure:

$$S : (\mathcal{X} \times \mathcal{Y})^n \to \mathcal{A}$$

ML algorithms

Decision Trees:

- model: piece-wise constant functions;
- search procedure: very sinful one.

SVM:

- linear functions (in some space);
- search procedure: margin maximization.

Logistic regression:

- linear functions;
- search procedure: $\mathrm{cross\text{-}entropy} \to \min$, any optimization method.

In Deep Learning models are often decoupled from search procedures.

ML algorithms

Often, model-search can be factorized further:

- parametrized model:

$$\mathcal{A} = \{f_\theta : \mathcal{X} \to \mathcal{Y} \mid \theta \in \Theta \subseteq \mathbb{R}^n\}$$

- optimization problem:

$$L(f_\theta, D) = \mathcal{L}(\theta) \to_\theta \min$$

  - $D \in (\mathcal{X} \times \mathcal{Y})^N$ - training set;

- optimization method O:

$$\theta^{t+1} = O\left[\theta^t, \mathcal{L}\right].$$

ML algorithms

- parametrized model:
  - heavily domain/data dependent;
- optimization problem:
  - more or less universal:

$$\mathcal{L} = \{\text{log}, \text{hinge}, \dots\}\text{-loss} + \{l_1, l_2\}\text{-regularization};$$

- optimization method O:
  - heavily-dependent on nature of $\mathcal{L}$.

Optimization in ML

Optimization methods:

- heavily restrict:
  - speed of the algorithm:
  - quality of solutions;
- some optimization methods allows for new models:
  - discreet or mixed parameters;
  - variable size models.

Gradient methods

The zoo

- SGD, SGD with momentum:
  - you have no memory;
  - you have to write optimizer in 1 minute;
- Nesterov momentum:
  - you want to fine-tune your solution.
- RMSprop:
  - you have little memory and you gradients explode/vanish;
  - you have 2 minutes before submitting your code for training;
- adagrad, adadelta, adam, adamax:
  - methods to go.

Details are likely to be considered in Deep Learning course.

Second-order methods

Flow chart

Do you have a nearly-quadratic target function?

- yes: is the problem low-dimensional?
  - yes: go Newton!
  - no: use gradient or quasi-Newton methods;
- no: use gradient or quasi-Newton methods.

Hyper-parameter optimization

Hyper-parameter optimization

Hyper-parameter optimization is a meta-algorithm that operates on union of models parametrized by ψ:

$$\mathcal{A} = \bigcup_{\psi} \mathcal{A}_{\psi} = \{ f^{\psi}_{\theta_{\psi}} \mid \theta_{\psi} \in \Theta_{\psi} \}$$

- outer loss **might differ** from inner loss:

$$\psi^* = \arg\max_{\psi} Q \left(\arg\min_{\theta_{\psi}} L(\theta_{\psi}) \right)$$

  - no sacred meaning, just for convinience:
  - example: L - cross-entropy, Q - ROC AUC.

Hyper-parameter optimization

Outer optimization is usually evaluated on a separate set:

- via train-validation-test split;
- via cross-validation;
- the main reason for split into outer and inner problems.

Alternatevely, BIC or similar can be used.

Outer optimization problem is usually non-differentiable:

- number of units, maximal depth of trees.

Grid-search

Usually, ML algorithms are designed to have **a few**, **non-sensitive** hyper-parameters:

- outer problem is mostly convex and changes slowly;
- grid-search often works perfectly fine.

Modifications, alternatives:

- randomized grid-search;
- random walk.

Gradient-free methods

Gradient-free methods

- local optimization:
  - 'traditional' methods;
- global optimization:
  - gradient and Hessian are fundamentally local properties;
  - evolutionary methods;
- black-box optimization:
  - variational optimization;
  - Bayesian optimization.

Traditional gradient-free methods

- evaluation of objective function is cheap;
- in practice, **often** can be replaced by gradient-methods:

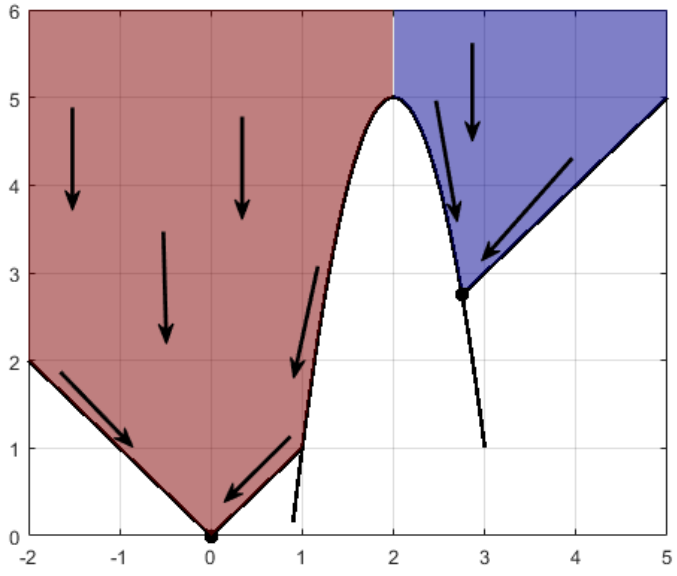
$$\text{cheap} \Rightarrow \begin{bmatrix} \text{closed-form expression} \\ \text{or} \\ \text{allow approximation} \end{bmatrix} \Rightarrow \text{differentiable.}$$

- example: Powell, Nelder-Mead.

Multi-start

Just launch local procedure multiple times with different initial guesses.

- each local optima acts like an attractor for local methods;
- effective if depth of local optima positively depend on area of attraction.



Evolution methods

There are just so many...

Basic operations:

- mutation: $x' = x + \text{noise}$;
- crossover: $x' = \text{crossover}(x_1, x_2)$;

Application:

- you have no idea how to optimize objective function;
- evolution algorithms basically can handle any parametrization:
  - e.g. DNA molecules.

Memetic algorithms

```
def memetic(global_step=evolutionary,
            locally_optimize=annealing):

  population = []
  mature_population = [ <random> ]

  while ...:
    population = global_step(mature_population)
    mature_population = [
      locally_optimize(x) for x in population
    ]
  return mature_population

multistart = lambda locally_optimize:  memetic(
```

Black-box optimization

- heavy objective;
- non-differentiable:
    - complex computer simulations (e.g. aero-dynamics);
- so multi-modal, gradient does not have sense:
    - extremely deep networks (e.g. recurrent networks);

Surrogate optimization

A type of black-box optimization.

Given known samples $\mathcal{O}^t = \{(\theta_i, L_i)\}_{i=1}^t$:

- fit regression (surrogate) model to $\{(\theta_i, L_i)\}_{i=1}^t$;
- find the most promising θ_{t+1} with conventional optimization methods;
- evaluate objective in θ_{t+1};
- $\mathcal{O}^{t+1} = \mathcal{O}^t \cup \{(\theta_{t+1}, L_{t+1})\}$;
- repeat.

Bayesian optimization

The most well-known black-box optimization method.

Surrogate model:

- must estimate: $P(y \mid D, x)$;
- usually Gaussian processes:
  - easy to handle (normal distribution everywhere);
  - computationally expensive $O(n^3)$, n - number of points.
- possible to use Random Forest or Boosting;
- the most promising point is defined by aquisition function:

$$a(x) \to \max$$

Aquisition functions

- f' - current minimum; D - observed values.

Probability of improvement:

$$a_{pi}(x) = \mathbb{E}\left[\mathbb{I}[f(x) > f'] \mid D\right] \underbrace{= \Phi(f', \mu(x), K(x,x))}_{GP}$$

Expected improvement:

$$a_{ei}(x) = \mathbb{E}\left[\max(0, f' - f(x)) \mid D\right] =$$
$$\underbrace{(f' - \mu(x))\Phi(f', \mu(x), K(x,x)) + K(x,x)\phi(f', \mu(x), K(x,x))}_{GP}$$

Lower confidence bound:

$$a_{lcb}(x) = \mu(x) + \beta\sigma(x)$$

Variational optimization

$$\min_x f(x) \leq \mathop{\mathbb{E}}_{x \sim \pi_\psi} f(x) = J(\psi)$$

- π_ψ - search distribution;

$$\nabla J(\psi) = \nabla \mathop{\mathbb{E}}_{x \sim \pi_\psi} f(x) =$$

$$\int_x f(x) \left(\nabla \pi(x \mid \psi)\right) \frac{\pi(x \mid \psi)}{\pi(x \mid \psi)} dx =$$

$$\int_x f(x) \nabla \log \pi(x \mid \psi) \pi(x \mid \psi) dx =$$

$$\mathop{\mathbb{E}}_{x \sim \pi_\psi} f(x) \nabla \log \pi(x \mid \psi) \approx$$

$$\frac{1}{n} \sum_{i=1}^{n} f(x_i) \nabla \log \pi(x_i \mid \psi)$$

Evolution Strategies

Evolution Strategies - is a subset of variational optimization (?).

- Repeat:
  - sample $\{x_i\}_{i=1}^n$ from $\pi(\cdot \mid \psi)$;
  - evaluate $f_i = f(x_i)$;
  - compute:

$$\nabla J(\psi) \approx \frac{1}{n} \sum_{i=1}^{n} f_i \nabla \log \pi(x_i \mid \psi)$$

  - update ψ, e.g.

$$\psi \leftarrow \mathrm{adamax}(\nabla J(\psi))$$

Evolution Strategies

- d - dimensionality of the problem;
- π_ψ - Gaussian:
  - $\dim(\psi) = O(d^2)$: covariance matrix and mean vector;
  - $O(d^3)$ operations per step;
- π_ψ - Gaussian with independent components:
  - $|\psi| = O(d)$: diagonal covariance matrix and mean vector;
  - $O(d)$ operations per step;
- π_ψ - scaled normal:
  - $|\psi| = O(d)$: variance σ and mean vector;
  - $O(d)$ operations per step;
  - less samples for estimating gradient.

Summary

Summary

Known your optimization algorithms:

- differentiable $\Rightarrow$ gradient methods;
- super heavy objective $\Rightarrow$ Bayesian;
- non-differentiable $\Rightarrow$ Variational Optimization;
- wierd model $\Rightarrow$ evolutionary optimization.

Don't blindly follow this.

References, gradient-methods

- Bottou, L., 2012. Stochastic gradient descent tricks. In Neural networks: Tricks of the trade (pp. 421-436). Springer Berlin Heidelberg.
- Kingma, D. and Ba, J., 2014. Adam: A method for stochastic optimization. arXiv preprint arXiv:1412.6980.
- Zeiler, M.D., 2012. ADADELTA: an adaptive learning rate method. arXiv preprint arXiv:1212.5701.

References, quasi-Newton

- Fletcher, R., 2013. Practical methods of optimization. John Wiley Sons.

References, gradient-free

- Back, T., 1996. Evolutionary algorithms in theory and practice: evolution strategies, evolutionary programming, genetic algorithms. Oxford university press.
- Kennedy, J., 2011. Particle swarm optimization. In Encyclopedia of machine learning (pp. 760-766). Springer US.
- Wierstra, D., Schaul, T., Glasmachers, T., Sun, Y., Peters, J. and Schmidhuber, J., 2014. Natural evolution strategies. Journal of Machine Learning Research, 15(1), pp.949-980.
- Snoek, J., Larochelle, H. and Adams, R.P., 2012. Practical bayesian optimization of machine learning algorithms. In Advances in neural information processing systems (pp. 2951-2959).