Scalable Logistic Regression

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COM6012 Scalable Machine Learning, Spring 2026

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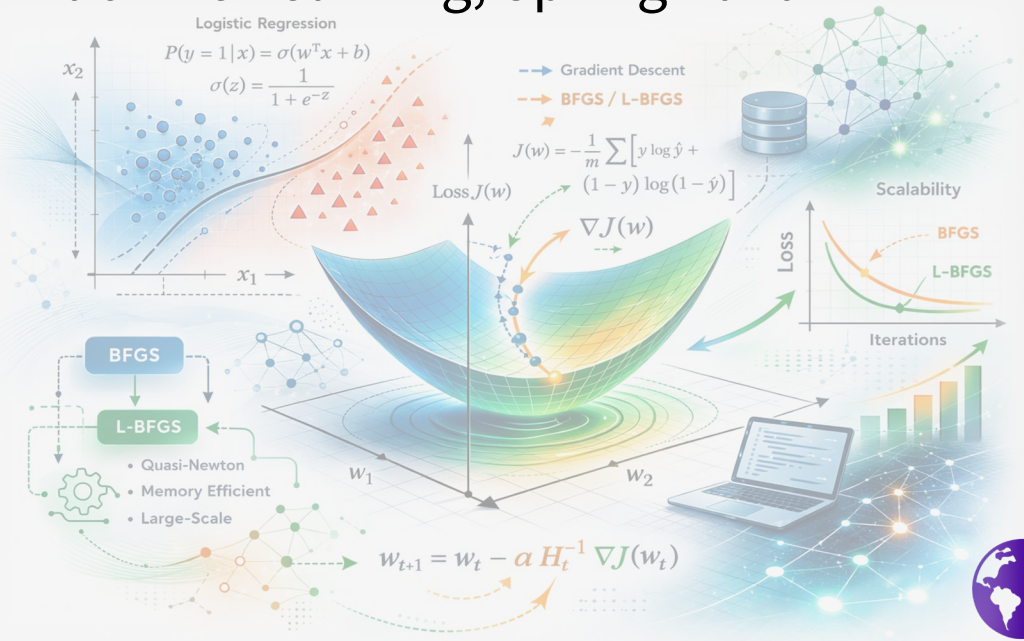

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Week 3 Objectives

- Formulate logistic regression (binary and multinomial) and define the cross-entropy loss.
- Explain **first- and second-order optimisation methods** and derive the **gradient and Hessian** for logistic regression.
- Explain how **Stochastic Gradient Descent (SGD)** and **Quasi-Newton methods (e.g., BFGS)** improve efficiency.
- Evaluate and apply ℓ_2, ℓ_1, and Elastic Net regularization.
- Train and tune scalable logistic regression models in PySpark on real-world datasets.

Content

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- **Cross-entropy error function**
- Optimization and efficient computation
  - First- and second-order optimization method
  - Quasi-Newton Methods
  - Stochastic gradient descent
- Beyond basic logistic regression
  - Regularization
  - Multi-class logistic regression
- Logistic regression in PySpark

Probabilistic classifier

- A logistic regression model is an example of a probabilistic classifier.
- Let $\mathbf{x} \in \mathbb{R}^p$ represents a feature vector and y the target value.
- $y \in \{0, 1\}$ or $y \in \{-1, +1\}$ for a binary classification problem.
- We model the relationship between y and $\mathbf{x}$ using a Bernoulli distribution.

Bernoulli distribution

- A Bernoulli random variable can only take two possible values.
- A Bernoulli distribution is a probability distribution for Y, expressed as

$$p(Y = y) = \text{Ber}(y|\mu) = \begin{cases} \mu & y = 1, \\ 1 - \mu & y = 0, \end{cases}$$

where $\mu = p(Y = 1)$.

- The expression above can be summarized in one line using

$$p(Y = y) = \text{Ber}(y|\mu) = \mu^y (1 - \mu)^{1-y}$$

How are y and x related in logistic regression?

- The target value y follows a Bernoulli distribution $p(y|\mathbf{x}) = \mathrm{Ber}(y|\mu(\mathbf{x}))$.
- Notice how the probability $\mu = P(y = 1)$ explicitly depends on $\mathbf{x}$.
- In logistic regression, the probability $\mu(\mathbf{x})$ is given as

$$\mu(\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{w}^\top \mathbf{x})} = \sigma(\mathbf{w}^\top \mathbf{x}),$$

  where $\sigma(z)$ is known as the *sigmoid function* and $\mathbf{w}$ is the coefficient vector to learn (In COM6509 the sigmoid function was denoted by $\pi(z)$).

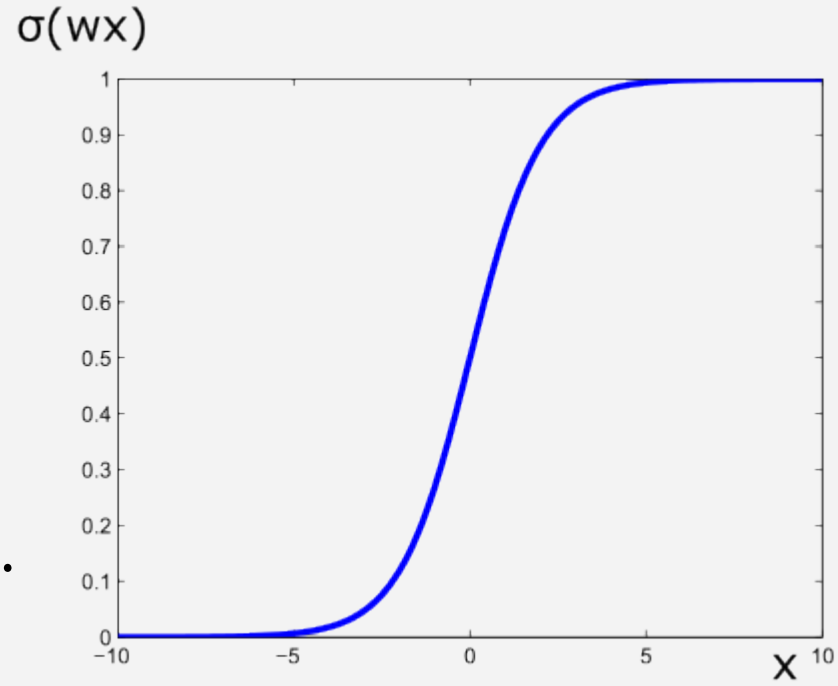
- We then have

$$p(y|\mathbf{w}, \mathbf{x}) = \mathrm{Ber}(y|\sigma(\mathbf{w}^\top \mathbf{x})).$$

The sigmoid function

- Recall $\sigma(z) = \dfrac{1}{1+\exp(-z)}$.

- If $z \to \infty$, $\sigma(z) \to 1$.
- If $z \to -\infty$, $\sigma(z) \to 0$.
- If $z = 0$, $\sigma(z) = 0.5$.
- $z = \mathbf{w}^\top \mathbf{x}$ in logistic regression.



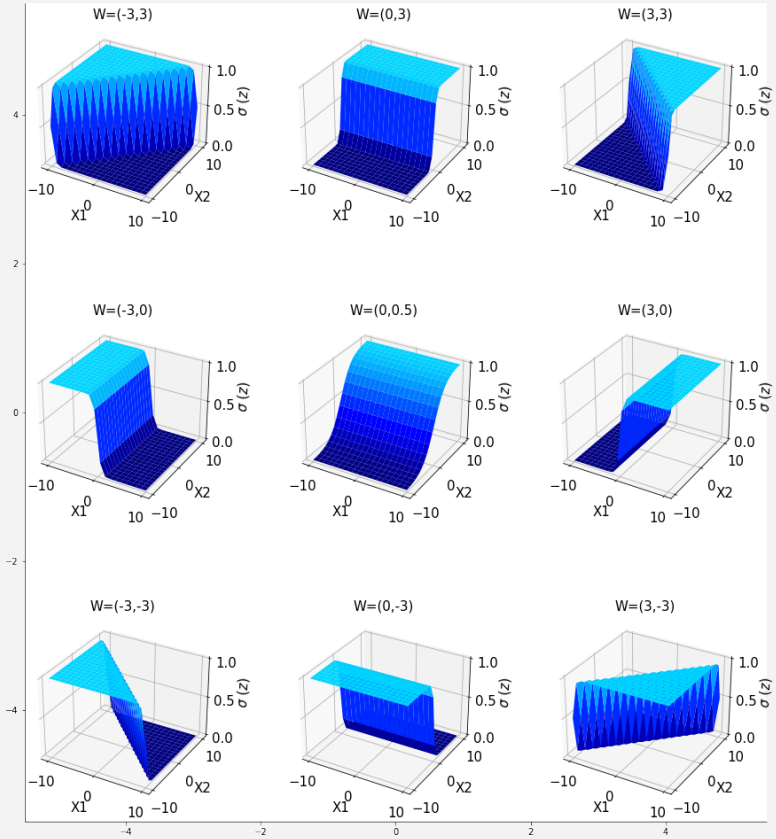
The sigmoid function in 2d

Plot of $\sigma(w_1 x_1 + w_2 x_2)$

Here $\mathbf{w} = [w_1, w_2]^\top$

Figure generated by code at:

https://github.com/probml/pyprobml/blob/master/notebooks/book1/10/sigmoid_2d_plot.ipynb



Decision boundary

- After the training phase, we will have an estimation for $\mathbf{w}$.
- For a test input vector $\mathbf{x}_*$, we compute

$$p(y = 1|\mathbf{w}, \mathbf{x}_*) = \sigma(\mathbf{w}^\top \mathbf{x}_*).$$

- This will give us a value between 0 and 1.
- We define a threshold of 0.5 to decide to which class we assign $\mathbf{x}_*$.
- With this threshold we induce a linear decision boundary in the input space.

Cross-entropy error function

- Let $\mathcal{D} = \{\mathbf{x}_n, y_n\}_{n=1}^N$.
- We write $\mathbf{X} = [\mathbf{x}_1 \cdots \mathbf{x}_N]^\top$, and $\mathbf{y} = [y_1 \cdots y_N]^\top$.
- Assuming IID observations

$$p(\mathbf{y}|\mathbf{w}, \mathbf{X}) = \prod_{n=1}^N p(y_n|\mathbf{w}, \mathbf{x}_n) = \prod_{n=1}^N \mathrm{Ber}(y_n|\sigma(\mathbf{w}^\top \mathbf{x}_n)).$$

- The cross-entropy function or negative log-likelihood is given as

$$\begin{aligned} NLL(\mathbf{w}) &= -\log p(\mathbf{y}|\mathbf{w}, \mathbf{X}) \\ &= -\sum_{n=1}^N \{y_n \log[\sigma(\mathbf{w}^\top \mathbf{x}_n)] + (1 - y_n) \log[1 - \sigma(\mathbf{w}^\top \mathbf{x}_n)]\}, \end{aligned}$$

which can be minimized with respect to $\mathbf{w}$.

Content

- Cross-entropy error function
- **Optimization and efficient computation**
  - First- and second-order optimization method
  - Quasi-Newton Methods
  - Stochastic gradient descent
- Beyond basic logistic regression
  - Regularization
  - Multi-class logistic regression
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General problem

- We are given a function $\mathcal{L}(\mathbf{w})$, where $\mathbf{w} \in \mathbb{R}^p$.
- Aim: to find value(s) for $\mathbf{w}$ that minimizes $\mathcal{L}(\mathbf{w})$.
- Use an iterative procedure

$$\mathbf{w}_{k+1} = \mathbf{w}_k + \eta \mathbf{d}_k,$$

  where $\mathbf{d}_k$ is known as the search direction in the kth step and it is such that

$$\mathcal{L}(\mathbf{w}_{k+1}) < \mathcal{L}(\mathbf{w}_k).$$

- The parameter η is known as the **step size** or **learning rate**.

First-order method: gradient descent

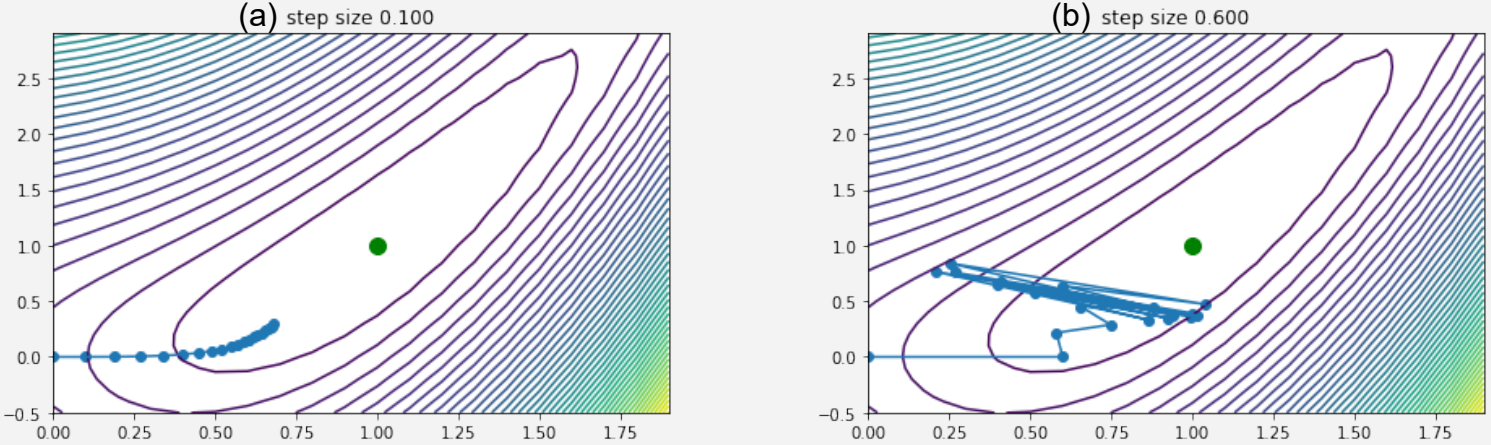
- Perhaps, the simplest algorithm for unconstrained optimization.
- It assumes that $\mathbf{d}_k = -\mathbf{g}_k,$ where $\mathbf{g}_k = \nabla \mathcal{L}(\mathbf{w}_k)$.
- It can be written like $\mathbf{w}_{k+1} = \mathbf{w}_k - \eta \mathbf{g}_k$.
- The gradient $\mathbf{g}(\mathbf{w})$ of $NLL(\mathbf{w})$ is given as

$$\mathbf{g}(\mathbf{w}) = \nabla_{\mathbf{w}} NLL(\mathbf{w}) = \sum_{n=1}^{N} [\sigma(\mathbf{w}^\top \mathbf{x}_n) - y_n]\mathbf{x}_n = \mathbf{X}^\top (\boldsymbol{\sigma} - \mathbf{y}),$$

where $\boldsymbol{\sigma} = [\sigma(\mathbf{w}^\top \mathbf{x}_1) \cdots \sigma(\mathbf{w}^\top \mathbf{x}_N)]^\top$.

Step size

- Main issue: If it is too small, convergence will be very slow. If it is too large, the method can fail to converge at all.
- Steepest descent on function $f(w_1, w_2) = 0.5(w_1^2 - w_2)^2 + 0.5(w_1 - 1)^2$. Start from $(0, 0)$ for 20 steps. The minimum is at $(1, 1)$. In (a) $\eta = 0.1$. In (b) $\eta = 0.6$.



Figures generated by code at https://github.com/probml/pyprobml/blob/master/notebooks/book1/08/steepestDescentDemo.ipynb

Second-order method: Newton's method

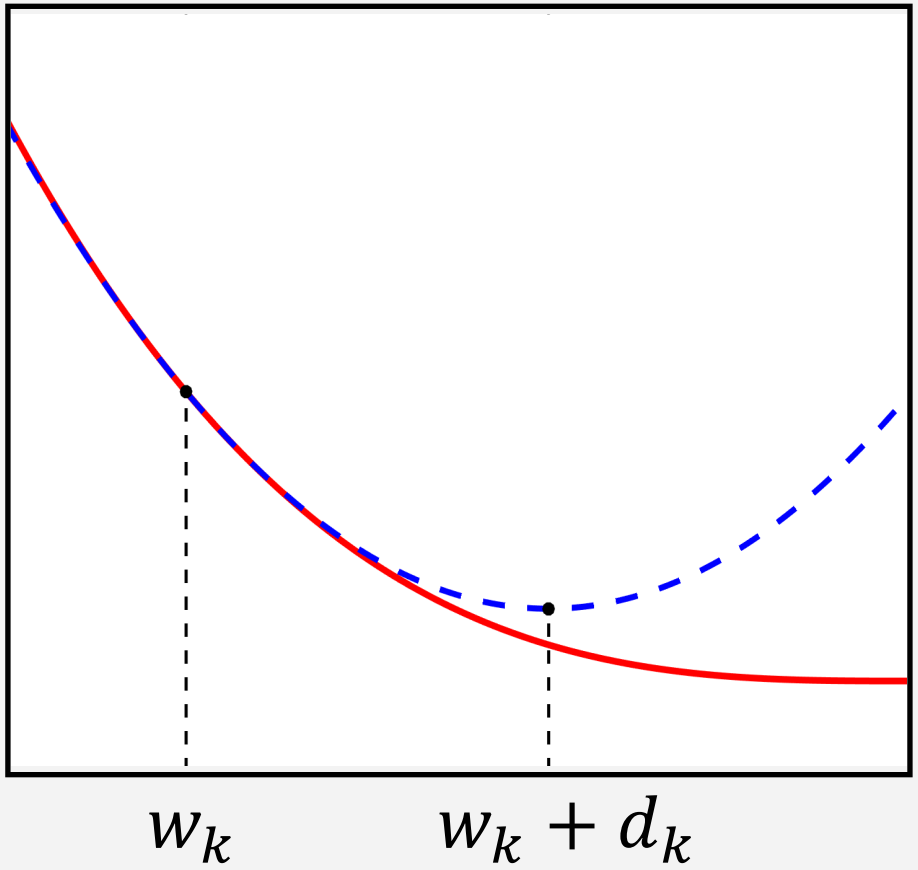
- Newton's algorithm $\mathbf{w}_{k+1} = \mathbf{w}_k - \eta \mathbf{H}_k^{-1} \mathbf{g}_k,$

  Where $\mathbf{g}_k = \nabla \mathcal{L}(\mathbf{w}_k)$ and $\mathbf{H}_k = \nabla^2 \mathcal{L}(\mathbf{w}_k)$ is a **Hesslian matrix**.

- Usually $\eta = 1$, and $\mathbf{d}_k = -\mathbf{H}_k^{-1} \mathbf{g}_k$.

- It derives a faster optimization algorithm by taking the curvature of the space (i.e., the Hessian) into account.

Newton's method



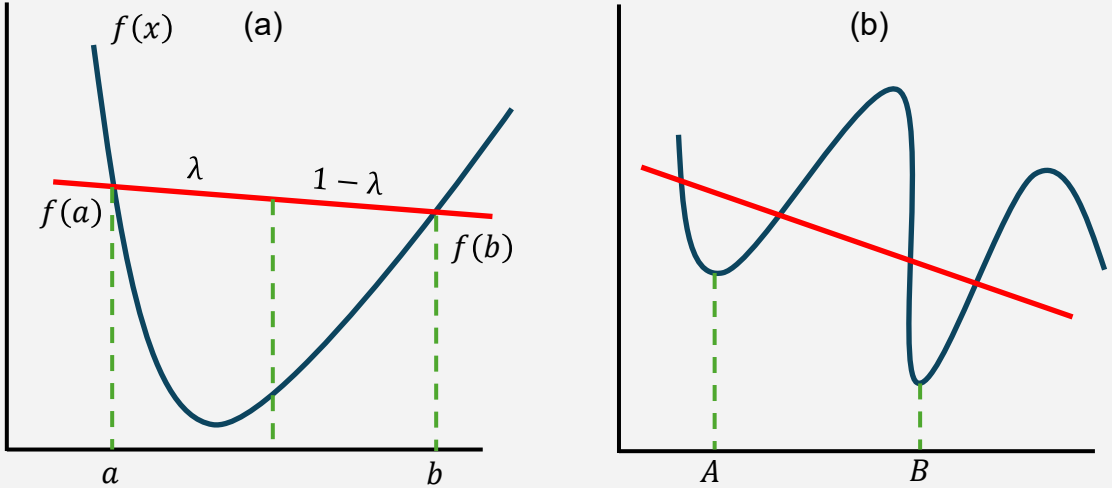
The solid curve is the function $\mathcal{L}(x)$.

The dotted line $\mathcal{L}_{quad}(w)$ is its second-order approximation at w_k.

The Newton step d_k is what must be added to w_k to get to the minimum of $\mathcal{L}_{quad}(w)$.

Newton's method and convex functions

- Newton's method requires $\mathbf{H}_k$ that be positive definite (p.d.)
- The condition holds if the function is strictly convex.



In (a), an illustration of a convex function. The chord joining $(a, f(a))$ and $(b, f(b))$ lies above the function. In (b), a function that is neither convex nor concave.

Hessian of $NLL(\mathbf{w})$

- Recall the gradient $\mathbf{g}(\mathbf{w})$ of $NLL(\mathbf{w})$

$$\mathbf{g}(\mathbf{w}) = \nabla_{\mathbf{w}} NLL(\mathbf{w}) = \sum_{n=1}^{N} [\sigma(\mathbf{w}^\top \mathbf{x}_n) - y_n]\mathbf{x}_n$$

- Derive the Hessian

$$\mathbf{H}(\mathbf{w}) = \frac{d}{d\mathbf{w}} \mathbf{g}(\mathbf{w})^\top$$

Quasi-Newton methods

- The main drawback of the Newton direction is the need for the Hessian.
- Explicit computation of this matrix of second derivatives can sometimes be a cumbersome, error-prone, and expensive process.
- Quasi-Newton search directions provide an attractive alternative to Newton's method.
- They do not require computation of the Hessian and yet still attain a faster rate of convergence.
- In place of the true Hessian $\mathbf{H}_k$, they use an approximation $\mathbf{B}_k$, which is updated after each step to take account of the additional knowledge gained during the step.

BFGS formula

Image source: https://aria42.com/blog/2014/12/understanding-lbfgs

BFGS formula for $\mathbf{H}_k$

- In the Broyden, Fletcher, Goldfarb, and Shanno (BFGS) formula

$$\mathbf{B}_{k+1} = \mathbf{B}_k + \frac{\mathbf{z}_k \mathbf{z}_k^\top}{\mathbf{z}_k^\top \mathbf{s}_k} - \frac{(\mathbf{B}_k \mathbf{s}_k)(\mathbf{B}_k \mathbf{s}_k)^\top}{\mathbf{s}_k^\top \mathbf{B}_k \mathbf{s}_k},$$

  where $\mathbf{s}_k = \mathbf{w}_k - \mathbf{w}_{k-1}$ and $\mathbf{z}_k = \mathbf{g}_k - \mathbf{g}_{k-1}$.

- This is a rank-two update to the matrix and ensures that the matrix remains positive definite.
- Usually $\mathbf{B}_0 = \mathbf{I}$.
- The search direction is then $\mathbf{d}_k = -\mathbf{B}_k^{-1} \mathbf{g}_k$.

BFGS formula for $\mathbf{H}_k^{-1}$

- BFGS can alternatively update $\mathbf{C}_k = \mathbf{H}_k^{-1}$

$$\mathbf{C}_{k+1} = \left(\mathbf{I} - \frac{\mathbf{s}_k \mathbf{z}_k^\top}{\mathbf{z}_k^\top \mathbf{s}_k}\right) \mathbf{C}_k \left(\mathbf{I} - \frac{\mathbf{z}_k \mathbf{s}_k^\top}{\mathbf{z}_k^\top \mathbf{s}_k}\right) + \frac{\mathbf{s}_k \mathbf{s}_k^\top}{\mathbf{z}_k^\top \mathbf{s}_k}.$$

- The search direction is then $\mathbf{d}_k = -\mathbf{C}_k \mathbf{g}_k$.

Limited memory BFGS (L-BFGS)

- Since storing the Hessian takes $O(p^2)$ space, for very large problems, one can use limited memory BFGS, or L-BFGS.
- In L-BFGS, $\mathbf{H}_k$ or $\mathbf{H}_k^{-1}$ is approximated by a diagonal plus low rank matrix.
- In particular, the product $\mathbf{B}_k^{-1}$ can be obtained by performing a sequence of inner products with $\mathbf{s}_k$ and $\mathbf{z}_k$, using only the m most recent $(\mathbf{s}_k, \mathbf{z}_k)$ pairs, and ignoring older information.
- The storage requirements are therefore $O(mp)$. Typically, $m \sim 20$ suffices for good performance.

Exercise

An implementation of L-BFGS uses the **10** most recent values of differences in gradients, $\mathbf{z}_k = \mathbf{g}_k - \mathbf{g}_{k-1}$, and the **10** most recent values of differences in the weight vector, $\mathbf{s}_k = \mathbf{w}_k - \mathbf{w}_{k-1}$. If the number of features is 100, what percentage of storage is saved by L-BFGS compared to full BFGS? [Enter the integer percentage without the % sign]

Hint: Use $O(2mp)$ for the storage complexity of L-BFGS

Stochastic gradient descent (SGD)

- Traditionally in machine learning, the gradient $\mathbf{g}_k$ and the Hessian $\mathbf{H}_k$ are computed using the whole dataset $\mathcal{D} = \{\mathbf{x}_n, y_n\}_{n=1}^N$.
- **Large datasets**: computing the exact $\mathbf{g}_k$ and $\mathbf{H}_k$ for $\mathcal{D}$ would be expensive.
- **Stochastic gradient descent (SGD):**

$$\mathbf{w}_{k+1} = \mathbf{w}_k - \eta_k \nabla \mathcal{L}(\mathbf{w}_k, \mathbf{x}_k) = \mathbf{w}_k - \eta_t \mathbf{g}_k.$$

- **Online learning**: the instances $(\mathbf{x}_n, y_n)$ appear one at a time.

Stochastic gradient descent (II)

- In the stochastic setting, a better estimate can be found if the gradient is computed using

$$\mathbf{g}_k \approx \frac{1}{|S_k|} \sum_{i \in S_k} \nabla \mathcal{L}_i(\mathbf{w}_k),$$

- where $S_k \in \mathcal{D}$, $|S_k|$ is the cardinality of S_k and $\nabla \mathcal{L}_i(\mathbf{w}_k)$ is the gradient at iteration k computed using the instance $(\mathbf{x}_i, y_i)$.
- This setting is called **Mini-batch gradient descent**
- For logistic regression, $\nabla \mathcal{L}_i(\mathbf{w}_k)$ would be the gradient computed for $NLL(\mathbf{x}_i)$

Step size in SGD

Choosing the value of η is important in SGD since there is no easy way to compute it. It should follow the **Robbins-Monro conditions**:

$$\eta_k \to 0, \frac{\sum_{k=1}^{\infty} \eta_k^2}{\sum_{k=1}^{\infty} \eta_k} \to 0. \qquad \sum_{k=1}^{\infty} \eta_k^2 < \infty, \sum_{k=1}^{\infty} \eta_k = \infty.$$

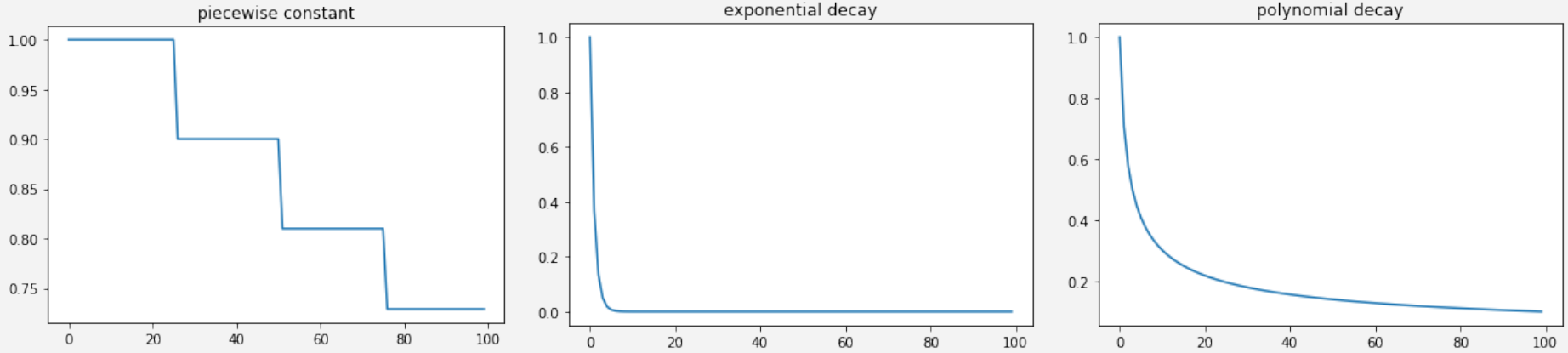


Illustration of some common learning rate schedules: Stepwise decay, exponential decay, and polynomial decay. Generated by code at https://github.com/probml/pyprobml/blob/master/notebooks/book1/08/learning_rate_plot.ipynb

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What is regularization?

- It refers to a technique used for preventing overfitting in a predictive model.
- It consists in adding a term (a regularizer) to the objective function that encourages simpler solutions.
- With regularization, the objective function for logistic regression would be

$$\mathcal{L}(\mathbf{w}) = NLL(\mathbf{w}) + \lambda R(\mathbf{w}),$$

  where $R(\mathbf{w})$ is the regularization term and λ the regularization parameter.
- If $\lambda = 0$, we get $\mathcal{L}(\mathbf{w}) = NLL(\mathbf{w})$.

ℓ_2 regularization

- Prior of $\mathbf{w}$: zero-mean normal distribution

$$f(w|0,\sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(w-0)^2}{2\sigma^2}\right),$$

where σ is the standard deviation of the distribution.

- Likelihood:

$$p(\mathbf{y}|\mathbf{w},\mathbf{X})p(\mathbf{w}) = \prod_{n=1}^{N} p(y_n|\mathbf{w},\mathbf{x}_n) \prod_{m=1}^{p} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{w_m^2}{2\sigma^2}\right)$$

- Negative log-likelihood:

$$NLL(\mathbf{w}) + \frac{1}{2\sigma^2} \sum_{m=1}^{p} w_m^2 \rightarrow NLL(\mathbf{w}) + \lambda \sum_{m=1}^{p} w_m^2$$

- Convex, smooth

ℓ_1 regularization

- Prior of $\mathbf{w}$: zero-mean Laplace distribution

$$f(w|0,b) = \frac{1}{2b}\exp\left(-\frac{|w-0|}{b}\right),$$

where $b > 0$ is a scale parameter of the distribution.

- Likelihood:

$$p(\mathbf{y}|\mathbf{w},\mathbf{X})p(\mathbf{w}) = \prod_{n=1}^{N} p(y_n|\mathbf{w},\mathbf{x}_n) \prod_{m=1}^{p} \frac{1}{2b}\exp\left(-\frac{|w_m|}{b}\right)$$

- Negative log-likelihood:

$$NLL(\mathbf{w}) + \frac{1}{b}\sum_{m=1}^{p}|w_m| \rightarrow NLL(\mathbf{w}) + \lambda\sum_{m=1}^{p}|w_m|$$

- Convex, nonsmooth, sparse

Smooth vs nonsmooth optimization

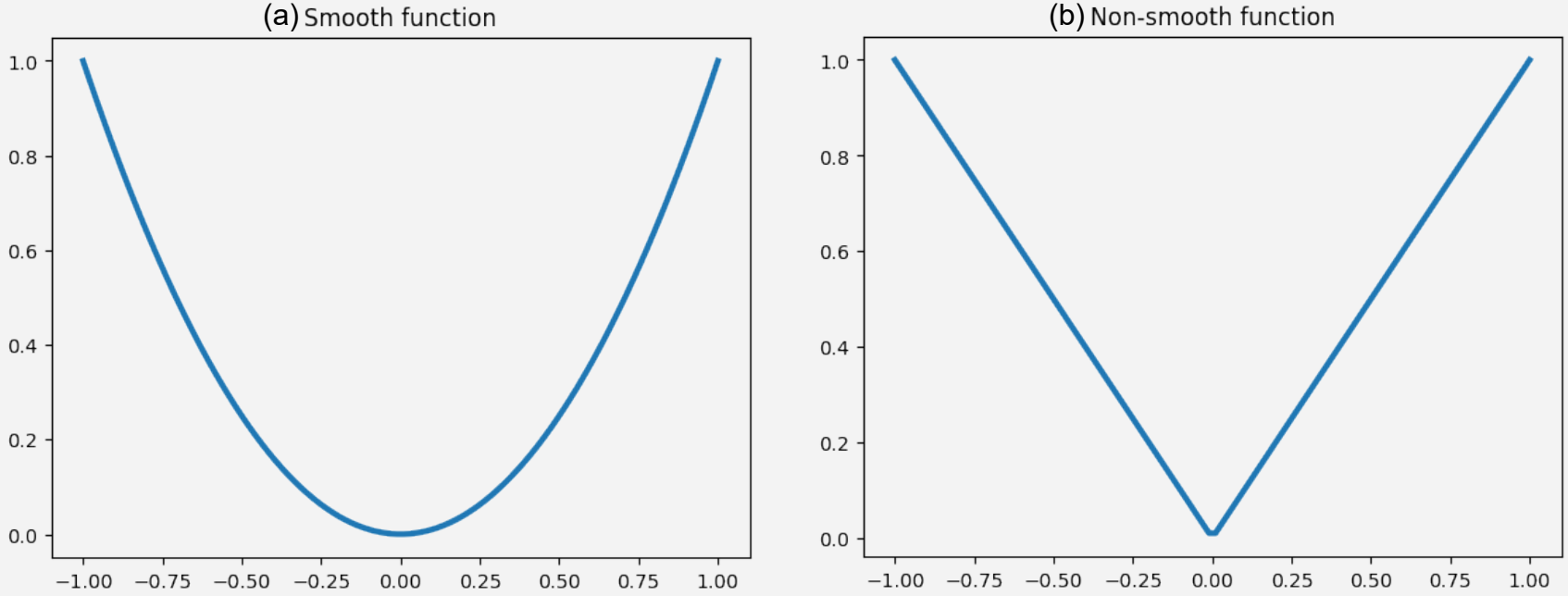

Figure generated by code at:
https://github.com/probml/pyprobml/blob/master/notebooks/book1/08/smooth-vs-nonsmooth-1d.ipynb

Elastic net regularization

- The objective function for logistic regression with a regularization term

$$\mathcal{L}(\mathbf{w}) = NLL(\mathbf{w}) + \lambda R(\mathbf{w}),$$

  where $R(\mathbf{w})$ in elastic net regularization follows as

$$R(\mathbf{w}) = \alpha \|\mathbf{w}\|_1 + (1-\alpha)\frac{1}{2}\|\mathbf{w}\|_2^2,$$

  where $\|\mathbf{w}\|_1 = \sum_{m=1}^{p} |w_m|$ and $\|\mathbf{w}\|_2^2 = \sum_{m=1}^{p} w_m^2$.

- If $0 < \alpha < 1$, we get the elastic net regularization.
- If $\alpha = 1$, we get ℓ_1 regularization.
- If $\alpha = 0$, we get ℓ_2 regularization.

Categorical distribution

- Imagine a random experiment where the output can only take 1 of K outputs.
- The result of the experiment can be coded using a vector $\boldsymbol{y}$ of dimension K, where only one of its entries is 1, and the rest is zero.
- Each of the K outputs of the experiment has a probability μ_k with $\sum_{k=1}^{K} \mu_k = 1$.
- We say that the vector $\boldsymbol{y}$ follows a categorical distribution

$$p(\mathbf{y}|\boldsymbol{\mu}) = \prod_{k=1}^{K} \mu_k^{y_k},$$

where $\mathbf{y} = [y_1, y_2, \cdots, y_K]^\top$, and $\boldsymbol{\mu} = [\mu_1, \mu_2, \cdots, \mu_K]^\top$.

Multinomial logistic regression (I)

- The categorical distribution is a particular case of the multinomial distribution.
- The categorical distribution can be used for multi-class logistic regression.
- Each instance in a multi-class classification problem is made of $(\mathbf{x}, \mathbf{y})$.
- In multinomial logistic regression, each probability μ_k is represented as

$$\mu_k = \frac{\exp(\mathbf{w}_k^\top \mathbf{x})}{\sum_{j=1}^{K} \exp(\mathbf{w}_j^\top \mathbf{x})},$$

where $\{\mathbf{w}_k\}_{k=1}^{K}$ is a set of weights, that we jointly refer to as $\mathbf{W}$.

Multinomial logistic regression (II)

- In this way, we can model $p(\mathbf{y}|\mathbf{W}, \mathbf{x})$ using

$$p(\mathbf{y}|\mathbf{W}, \mathbf{x}) = \prod_{k=1}^{K} \mu_k^{y_k} = \prod_{k=1}^{K} \left[\frac{\exp(\mathbf{w}_k^\top \mathbf{x})}{\sum_{j=1}^{K} \exp(\mathbf{w}_j^\top \mathbf{x})} \right]^{y_k}.$$

- Suppose we have a dataset $\mathcal{D} = \{\mathbf{x}_n, \mathbf{y}_n\}_{n=1}^{N}$.
- We write $\mathbf{X} = [\mathbf{x}_1 \cdots \mathbf{x}_N]^\top$, and $\mathbf{Y} = [\mathbf{y}_1 \cdots \mathbf{y}_N]^\top$.

Multinomial logistic regression (III)

- The parameters $\mathbf{W}$ could be estimated by minimizing

$$NLL(\mathbf{W}) = -\log p(\mathbf{Y}|\mathbf{W}, \mathbf{X}) = -\log \prod_{n=1}^{N} \prod_{k=1}^{K} \mu_{n,k}^{y_{n,k}} = -\sum_{n=1}^{N} \sum_{k=1}^{K} y_{n,k} \log \mu_{n,k},$$

  where $\mu_{n,k} = \frac{\exp(\mathbf{w}_k^\top \mathbf{x}_n)}{\sum_{j=1}^{K} \exp(\mathbf{w}_j^\top \mathbf{x}_n)}$.

- We could also add a regularization term to $\mathbf{W}$, and minimize

$$f(\mathbf{W}) = NLL(\mathbf{W}) + \lambda R(\mathbf{W}),$$

  with respect to $\mathbf{W}$.

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`LogisticRegression()`

- `LogisticRegression()` work with DataFrames.
- It is possible to use regularization ℓ_2, ℓ_1, or Elastic Net.
- L-BFGS is used as a solver for `LogisticRegression()`, with ℓ_2.
- When ℓ_1, or Elastic Net is used, a variant of L-BFGS, known as Orthant-Wise Limited-memory Quasi-Newton (OWL-QN) is used instead.

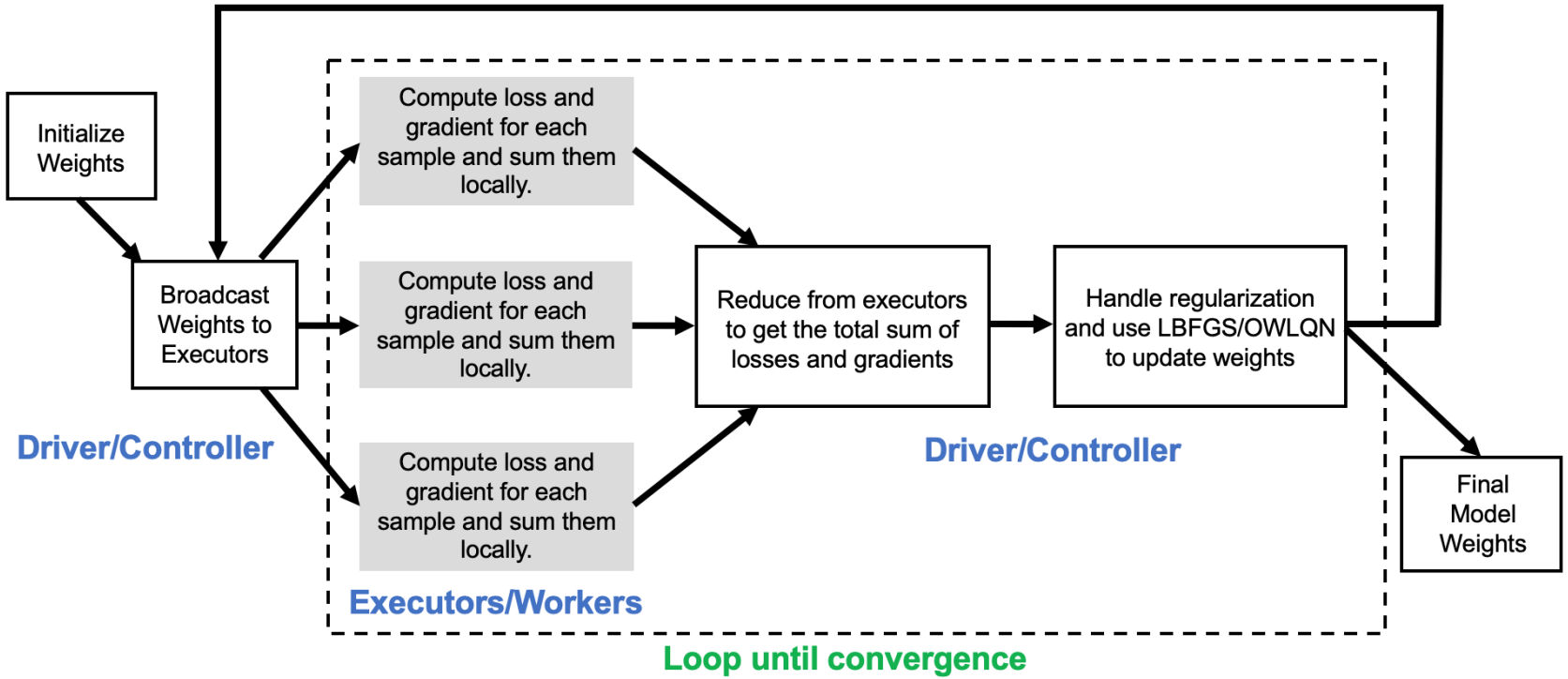
Parameters to adjust

- `maxIter`: max number of iterations.
- `regParam`: regularization parameter (≥ 0).
- `elasticNetParam`: the ElasticNet mixing parameter, in range $[0, 1]$. For $\alpha = 0$, the penalty is an ℓ_2 penalty. For $\alpha = 1$, it is an ℓ_1 penalty.
- `family`: the name of the family which describes the label distribution to be used in the model. Supported options: auto, binomial, multinomial.
- `standardization`: whether to standardize the training features before fitting the model. It can be true or false.

Algorithms in summation form

- When an algorithm sums over the data, we can easily distribute the calculations over multiple workers (e.g. cores).
- We just divide the dataset into as many pieces as there are workers, give each worker its share of the data to sum the equations over, and aggregate the result at the end.
- Both the gradient and Hessian in the optimization algorithms we saw before have a summation form.
- Notice that the summation form does not change the underlying algorithm: it is not an approximation but an exact implementation.

Update of w in Apache Spark

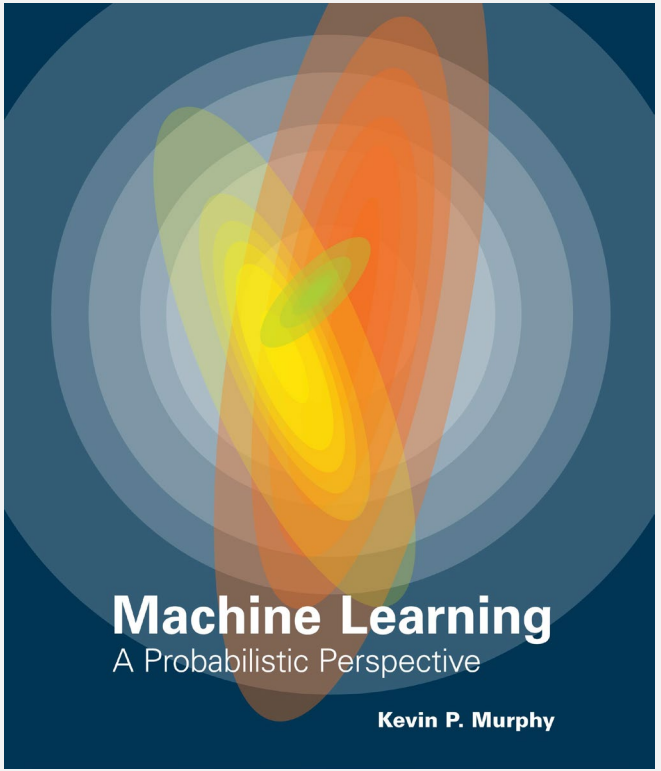


References and recommended reading

Machine Learning: a Probabilistic Perspective

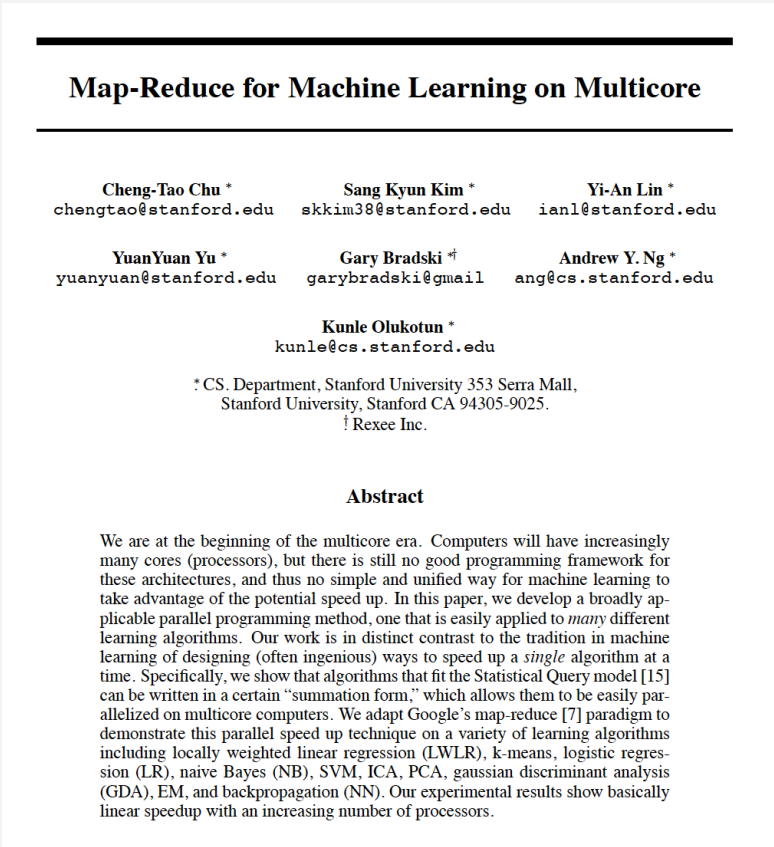
Sections 8.1-8.3 and 8.5.1-8.5.3

The eBook is available via the University Library and can be accessed through the reading list on Blackboard.



References and recommended reading

Map-Reduce for Machine Learning on Multicore
by C-T Chu et al. (2006).



Map-Reduce for Machine Learning on Multicore

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Abstract

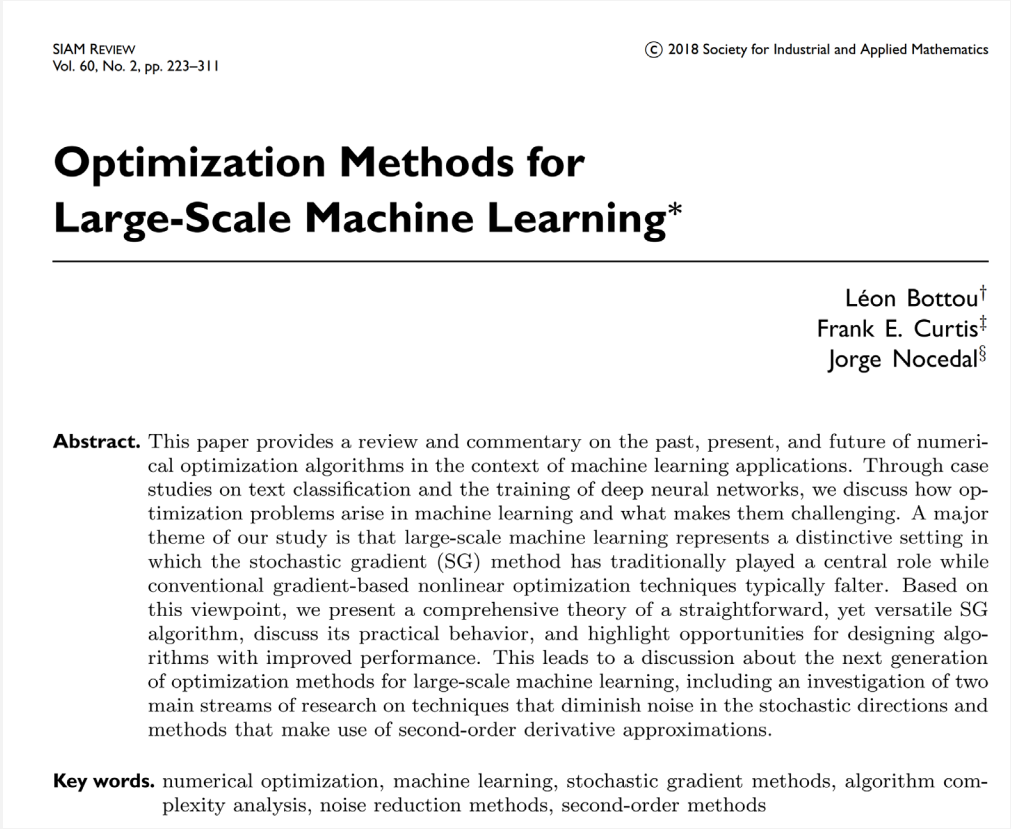
We are at the beginning of the multicore era. Computers will have increasingly many cores (processors), but there is still no good programming framework for these architectures, and thus no simple and unified way for machine learning to take advantage of the potential speed up. In this paper, we develop a broadly applicable parallel programming method, one that is easily applied to *many* different learning algorithms. Our work is in distinct contrast to the tradition in machine learning of designing (often ingenious) ways to speed up a *single* algorithm at a time. Specifically, we show that algorithms that fit the Statistical Query model [15] can be written in a certain "summation form," which allows them to be easily parallelized on multicore computers. We adapt Google's map-reduce [7] paradigm to demonstrate this parallel speed up technique on a variety of learning algorithms including locally weighted linear regression (LWLR), k-means, logistic regression (LR), naive Bayes (NB), SVM, ICA, PCA, gaussian discriminant analysis (GDA), EM, and backpropagation (NN). Our experimental results show basically linear speedup with an increasing number of processors.

References and recommended reading

Optimization Methods for Large Scale Machine Learning by L. Bottou et al. (2018).

- ❑ Chapter 3-4 pp. 235 -258
- ❑ Chapter 6 pp. 270-284
- ❑ Chapter 8 pp. 293-298

The full paper is available via the University Library and can be accessed through the reading list on Blackboard.



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Optimization Methods for Large-Scale Machine Learning*

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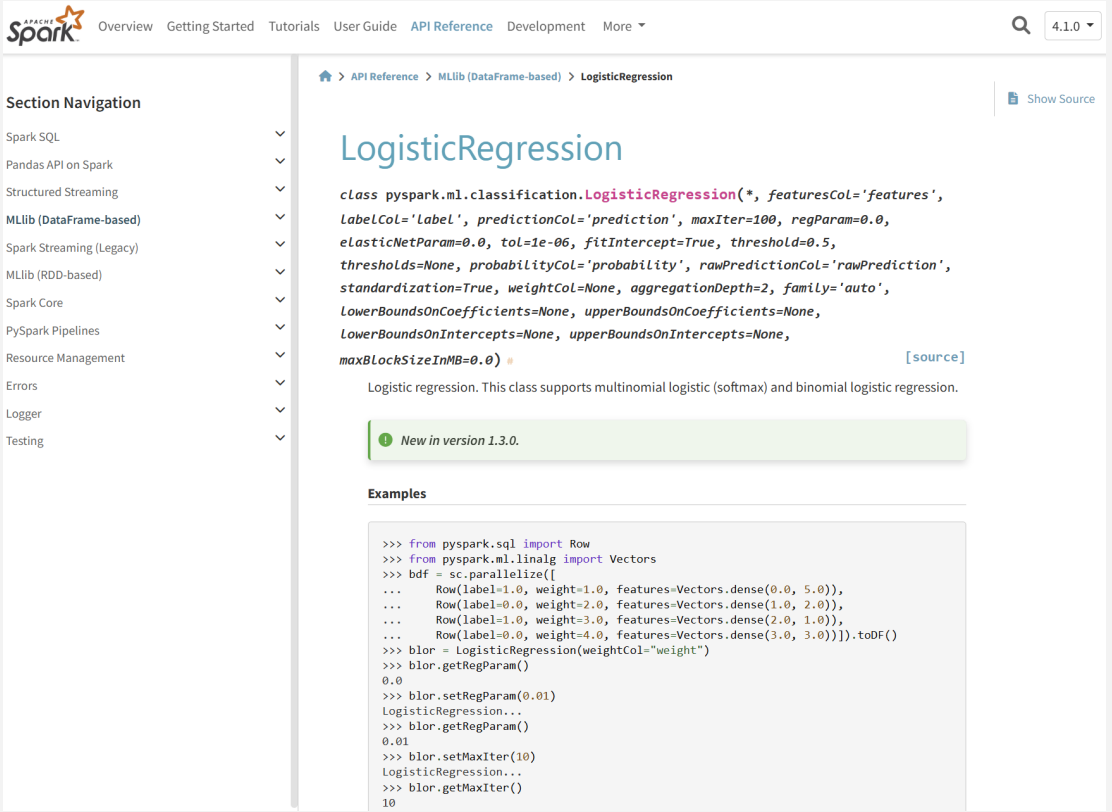
Abstract. This paper provides a review and commentary on the past, present, and future of numerical optimization algorithms in the context of machine learning applications. Through case studies on text classification and the training of deep neural networks, we discuss how optimization problems arise in machine learning and what makes them challenging. A major theme of our study is that large-scale machine learning represents a distinctive setting in which the stochastic gradient (SG) method has traditionally played a central role while conventional gradient-based nonlinear optimization techniques typically falter. Based on this viewpoint, we present a comprehensive theory of a straightforward, yet versatile SG algorithm, discuss its practical behavior, and highlight opportunities for designing algorithms with improved performance. This leads to a discussion about the next generation of optimization methods for large-scale machine learning, including an investigation of two main streams of research on techniques that diminish noise in the stochastic directions and methods that make use of second-order derivative approximations.

Key words. numerical optimization, machine learning, stochastic gradient methods, algorithm complexity analysis, noise reduction methods, second-order methods

References and recommended reading

Spark Python API Documentation for logistic regression: https://spark.apache.org/docs/4.1.0/api/python/reference/api/pyspark.ml.classification.LogisticRegression.html



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