Learning using Large Datasets

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Abstract. This contribution develops a theoretical framework that takes into account the effect of approximate optimization on learning algorithms. The analysis shows distinct tradeoffs for the case of small-scale and large-scale learning problems. Small-scale learning problems are subject to the usual approximation–estimation tradeoff. Large-scale learning problems are subject to a qualitatively different tradeoff involving the computational complexity of the underlying optimization algorithms in non-trivial ways. For instance, a mediocre optimization algorithms, stochastic gradient descent, is shown to perform very well on large-scale learning problems.

Keywords. Large-scale learning. Optimization. Statistics.

Introduction

The computational complexity of learning algorithms has seldom been taken into account by the learning theory. Valiant [1] states that a problem is "learnable" when there exists a probably approximatively correct learning algorithm *with polynomial complexity*. Whereas much progress has been made on the statistical aspect (e.g., [2,3,4]), very little has been told about the complexity side of this proposal (e.g., [5].)

Computational complexity becomes the limiting factor when one envisions large amounts of training data. Two important examples come to mind:

- Data mining exists because competitive advantages can be achieved by analyzing the masses of data that describe the life of our computerized society. Since virtually every computer generates data, the data volume is proportional to the available computing power. Therefore one needs learning algorithms that scale roughly linearly with the total volume of data.
- Artificial intelligence attempts to emulate the cognitive capabilities of human beings. Our biological brains can learn quite efficiently from the continuous streams of perceptual data generated by our six senses, using limited amounts of sugar as a source of power. This observation suggests that there are learning algorithms whose computing time requirements scale roughly linearly with the total volume of data.

This contribution finds its source in the idea that approximate optimization algorithms might be sufficient for learning purposes. The first part proposes new decomposition of the test error where an additional term represents the impact of approximate optimization. In the case of small-scale learning problems, this decomposition reduces to the well known tradeoff between approximation error and estimation error. In the case of

large-scale learning problems, the tradeoff is more complex because it involves the computational complexity of the learning algorithm. The second part explores the asymptotic properties of the large-scale learning tradeoff for various prototypical learning algorithms under various assumptions regarding the statistical estimation rates associated with the chosen objective functions. This part clearly shows that the best optimization algorithms are not necessarily the best learning algorithms. Maybe more surprisingly, certain algorithms perform well regardless of the assumed rate for the statistical estimation error. Finally, the final part presents some experimental results.

1. Approximate Optimization

Following [6,2], we consider a space of input-output pairs $(x, y) \in \mathcal{X} \times \mathcal{Y}$ endowed with a probability distribution $P(x, y)$. The conditional distribution $P(y|x)$ represents the unknown relationship between inputs and outputs. The discrepancy between the predicted output $\hat{y}$ and the real output y is measured with a loss function $\ell(\hat{y}, y)$. Our benchmark is the function f^* that minimizes the expected risk

$$E(f) = \int \ell(f(x), y)\, dP(x, y) = \mathbb{E}\,[\ell(f(x), y)],$$

that is,

$$f^*(x) = \arg\min_{\hat{y}} \mathbb{E}\,[\,\ell(\hat{y}, y)|\, x].$$

Although the distribution $P(x, y)$ is unknown, we are given a sample $\mathcal{S}$ of n independently drawn training examples (x_i, y_i), $i = 1 \ldots n$. We define the empirical risk

$$E_n(f) = \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i) = \mathbb{E}_n[\ell(f(x), y)].$$

Our first learning principle consists in choosing a family $\mathcal{F}$ of candidate prediction functions and finding the function $f_n = \arg\min_{f \in \mathcal{F}} E_n(f)$ that minimizes the empirical risk. Well known combinatorial results (e.g., [2]) support this approach provided that the chosen family $\mathcal{F}$ is sufficiently restrictive. Since the optimal function f^* is unlikely to belong to the family $\mathcal{F}$, we also define $f^*_{\mathcal{F}} = \arg\min_{f \in \mathcal{F}} E(f)$. For simplicity, we assume that f^*, $f^*_{\mathcal{F}}$ and f_n are well defined and unique.

We can then decompose the excess error as

$$\begin{aligned} \mathbb{E}\,[E(f_n) - E(f^*)] &= \underbrace{\mathbb{E}\,[E(f^*_{\mathcal{F}}) - E(f^*)]}_{\mathcal{E}_{\rm app}} + \underbrace{\mathbb{E}\,[E(f_n) - E(f^*_{\mathcal{F}})]}_{\mathcal{E}_{\rm est}}, \\ &= \mathcal{E}_{\rm app} + \mathcal{E}_{\rm est} \end{aligned} \tag{1}$$

where the expectation is taken with respect to the random choice of training set. The *approximation error* $\mathcal{E}_{\rm app}$ measures how closely functions in $\mathcal{F}$ can approximate the optimal solution f^*. The *estimation error* $\mathcal{E}_{\rm est}$ measures the effect of minimizing the empirical risk $E_n(f)$ instead of the expected risk $E(f)$. The estimation error is determined by the number of training examples and by the capacity of the family of functions [2]. Large

families[1] of functions have *smaller approximation errors* but lead to *higher estimation errors*. This tradeoff has been extensively discussed in the literature [2,3] and lead to excess error that scale between the inverse and the inverse square root of the number of examples [7,8].

1.1. Optimization Error

Finding f_n by minimizing the empirical risk $E_n(f)$ is often a computationally expensive operation. Since the empirical risk $E_n(f)$ is already an approximation of the expected risk $E(f)$, it should not be necessary to carry out this minimization with great accuracy. For instance, we could stop an iterative optimization algorithm long before its convergence.

Let us assume that our minimization algorithm returns an approximate solution $\tilde{f}_n$ that minimizes the objective function up to a predefined tolerance $\rho \geq 0$.

$$E_n(\tilde{f}_n) < E_n(f_n) + \rho$$

We can then decompose the excess error $\mathcal{E} = \mathbb{E}\big[E(\tilde{f}_n) - E(f^*)\big]$ as

$$\begin{aligned} \mathcal{E} &= \underbrace{\mathbb{E}\left[E(f^*_{\mathcal{F}}) - E(f^*)\right]}_{\mathcal{E}_{\text{app}}} + \underbrace{\mathbb{E}\left[E(f_n) - E(f^*_{\mathcal{F}})\right]}_{\mathcal{E}_{\text{est}}} + \underbrace{\mathbb{E}\big[E(\tilde{f}_n) - E(f_n)\big]}_{\mathcal{E}_{\text{opt}}} . \\ &= \mathcal{E}_{\text{app}} + \mathcal{E}_{\text{est}} + \mathcal{E}_{\text{opt}} \end{aligned} \tag{2}$$

We call the additional term $\mathcal{E}_{\text{opt}}$ the *optimization error*. It reflects the impact of the approximate optimization on the generalization performance. Its magnitude is comparable to ρ (see section 2.1.)

1.2. The Approximation–Estimation–Optimization Tradeoff

This decomposition leads to a more complicated compromise. It involves three variables and two constraints. The constraints are the maximal number of available training example and the maximal computation time. The variables are the size of the family of functions $\mathcal{F}$, the optimization accuracy ρ, and the number of examples n. This is formalized by the following optimization problem.

$$\min_{\mathcal{F},\rho,n} \quad \mathcal{E} = \mathcal{E}_{\text{app}} + \mathcal{E}_{\text{est}} + \mathcal{E}_{\text{opt}} \quad \text{subject to} \begin{cases} n \leq n_{\max} \\ T(\mathcal{F},\rho,n) \leq T_{\max} \end{cases} \tag{3}$$

The number n of training examples is a variable because we could choose to use only a subset of the available training examples in order to complete the optimization within the alloted time. This happens often in practice. Table 1 summarizes the typical evolution of the quantities of interest with the three variables $\mathcal{F}$, n, and ρ increase.

The solution of the optimization program (3) depends critically of which budget constraint is active: constraint $n < n_{\max}$ on the number of examples, or constraint $T < T_{\max}$ on the training time.

[1] We often consider nested families of functions of the form $F_c = \{f \in \mathcal{H},\ \Omega(f) \leq c\}$. Then, for each value of c, function f_n is obtained by minimizing the regularized empirical risk $E_n(f) + \lambda\Omega(f)$ for a suitable choice of the Lagrange coefficient λ. We can then control the estimation-approximation tradeoff by choosing λ instead of c.

Table 1. Typical variations when $\mathcal{F}$, n, and ρ increase.

		$\mathcal{F}$	n	ρ
$\mathcal{E}_{\rm app}$	(approximation error)	$\searrow$		
$\mathcal{E}_{\rm est}$	(estimation error)	$\nearrow$	$\searrow$	
$\mathcal{E}_{\rm opt}$	(optimization error)	$\cdots$	$\cdots$	$\nearrow$
T	(computation time)	$\nearrow$	$\nearrow$	$\searrow$

- We speak of *small-scale learning problem* when (3) is constrained by the maximal number of examples $n_{\max}$. Since the computing time is not limited, we can reduce the optimization error $\mathcal{E}_{\rm opt}$ to insignificant levels by choosing ρ arbitrarily small. The excess error is then dominated by the approximation and estimation errors, $\mathcal{E}_{\rm app}$ and $\mathcal{E}_{\rm est}$. Taking $n = n_{\max}$, we recover the approximation-estimation tradeoff that is the object of abundant literature.
- We speak of *large-scale learning problem* when (3) is constrained by the maximal computing time $T_{\max}$. Approximate optimization, that is choosing $\rho > 0$, possibly can achieve better generalization because more training examples can be processed during the allowed time. The specifics depend on the computational properties of the chosen optimization algorithm through the expression of the computing time $T(\mathcal{F}, \rho, n)$.

2. The Asymptotics of Large-scale Learning

In the previous section, we have extended the classical approximation-estimation tradeoff by taking into account the optimization error. We have given an objective criterion to distiguish small-scale and large-scale learning problems. In the small-scale case, we recover the classical tradeoff between approximation and estimation. The large-scale case is substantially different because it involves the computational complexity of the learning algorithm. In order to clarify the large-scale learning tradeoff with sufficient generality, this section makes several simplifications:

- We are studying upper bounds of the approximation, estimation, and optimization errors (2). It is often accepted that these upper bounds give a realistic idea of the actual convergence rates [9,10,11,12]. Another way to find comfort in this approach is to say that we study guaranteed convergence rates instead of the possibly pathological special cases.
- We are studying the asymptotic properties of the tradeoff when the problem size increases. Instead of carefully balancing the three terms, we write $\mathcal{E} = \mathcal{O}(\mathcal{E}_{\rm app}) + \mathcal{O}(\mathcal{E}_{\rm est}) + \mathcal{O}(\mathcal{E}_{\rm opt})$ and only need to ensure that the three terms decrease with the same asymptotic rate.
- We are considering a fixed family of functions $\mathcal{F}$ and therefore avoid taking into account the approximation error $\mathcal{E}_{\rm app}$. This part of the tradeoff covers a wide spectrum of practical realities such as choosing models and choosing features. In the context of this work, we do not believe we can meaningfully address this without discussing, for instance, the thorny issue of feature selection. Instead we focus on the choice of optimization algorithm.
- Finally, in order to keep this paper short, we consider that the family of functions $\mathcal{F}$ is linearly parametrized by a vector $w \in \mathbb{R}^d$. We also assume that x, y and w

are bounded, ensuring that there is a constant B such that $0 \leq \ell(f_w(x), y) \leq B$ and $\ell(\cdot, y)$ is Lipschitz.

We first explain how the uniform convergence bounds provide convergence rates that take the optimization error into account. Then we discuss and compare the asymptotic learning properties of several optimization algorithms.

2.1. Convergence of the Estimation and Optimization Errors

The optimization error $\mathcal{E}_{\rm opt}$ depends directly on the optimization accuracy ρ. However, the accuracy ρ involves the empirical quantity $E_n(\tilde{f}_n) - E_n(f_n)$, whereas the optimization error $\mathcal{E}_{\rm opt}$ involves its expected counterpart $E(\tilde{f}_n) - E(f_n)$. This section discusses the impact on the optimization error $\mathcal{E}_{\rm opt}$ and of the optimization accuracy ρ on generalization bounds that leverage the uniform convergence concepts pioneered by Vapnik and Chervonenkis (e.g., [2].)

In this discussion, we use the letter c to refer to any positive constant. Multiple occurences of the letter c do not necessarily imply that the constants have identical values.

2.1.1. Simple Uniform Convergence Bounds

Recall that we assume that $\mathcal{F}$ is linearly parametrized by $w \in \mathbb{R}^d$. Elementary uniform convergence results then state that

$$\mathbb{E}\left[\sup_{f\in\mathcal{F}} |E(f) - E_n(f)|\right] \leq c\sqrt{\frac{d}{n}}\,,$$

where the expectation is taken with respect to the random choice of the training set.[2] This result immediately provides a bound on the estimation error:

$$\begin{aligned}\mathcal{E}_{\rm est} &= \mathbb{E}\,\big[\,\big(E(f_n) - E_n(f_n)\big) + \big(E_n(f_n) - E_n(f_{\mathcal{F}}^*)\big) + \big(E_n(f_{\mathcal{F}}^*) - E(f_{\mathcal{F}}^*)\big)\,\big] \\ &\leq 2\,\mathbb{E}\left[\sup_{f\in\mathcal{F}} |E(f) - E_n(f)|\right] \;\leq\; c\sqrt{\frac{d}{n}}.\end{aligned}$$

This same result also provides a combined bound for the estimation and optimization errors:

$$\begin{aligned}\mathcal{E}_{\rm est} + \mathcal{E}_{\rm opt} &= \mathbb{E}\big[E(\tilde{f}_n) - E_n(\tilde{f}_n)\big] + \mathbb{E}\big[E_n(\tilde{f}_n) - E_n(f_n)\big] \\ &\quad + \mathbb{E}\,[E_n(f_n) - E_n(f_{\mathcal{F}}^*)] + \mathbb{E}\,[E_n(f_{\mathcal{F}}^*) - E(f_{\mathcal{F}}^*)] \\ &\leq c\sqrt{\frac{d}{n}} + \rho + 0 + c\sqrt{\frac{d}{n}} \;=\; c\left(\rho + \sqrt{\frac{d}{n}}\right).\end{aligned}$$

Unfortunately, this convergence rate is known to be pessimistic in many important cases. More sophisticated bounds are required.

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[2] Although the original Vapnik-Chervonenkis bounds have the form $c\sqrt{\frac{d}{n}\log\frac{n}{d}}$, the logarithmic term can be eliminated using the "chaining" technique (e.g., [10].)

2.1.2. Faster Rates in the Realizable Case

When the loss functions $\ell(\hat{y}, y)$ is positive, with probability $1 - e^{-\tau}$ for any $\tau > 0$, relative uniform convergence bounds state that

$$\sup_{f \in \mathcal{F}} \frac{E(f) - E_n(f)}{\sqrt{E(f)}} \leq c\sqrt{\frac{d}{n} \log \frac{n}{d} + \frac{\tau}{n}} \,.$$

This result is very useful because it provides faster convergence rates $\mathcal{O}(\log n/n)$ in the *realizable case*, that is when $\ell(f_n(x_i), y_i) = 0$ for all training examples (x_i, y_i). We have then $E_n(f_n) = 0$, $E_n(\tilde{f}_n) \leq \rho$, and we can write

$$E(\tilde{f}_n) - \rho \leq c\sqrt{E(\tilde{f}_n)} \sqrt{\frac{d}{n} \log \frac{n}{d} + \frac{\tau}{n}} \,.$$

Viewing this as a second degree polynomial inequality in variable $\sqrt{E(\tilde{f}_n)}$, we obtain

$$E(\tilde{f}_n) \leq c \left(\rho + \frac{d}{n} \log \frac{n}{d} + \frac{\tau}{n} \right) .$$

Integrating this inequality using a standard technique (see, e.g., [13]), we obtain a better convergence rate of the combined estimation and optimization error:

$$\mathcal{E}_{\text{est}} + \mathcal{E}_{\text{opt}} = \mathbb{E}\left[E(\tilde{f}_n) - E(f^*_{\mathcal{F}}) \right] \leq \mathbb{E}\left[E(\tilde{f}_n) \right] = c \left(\rho + \frac{d}{n} \log \frac{n}{d} \right) .$$

2.1.3. Fast Rate Bounds

Many authors (e.g., [10,4,12]) obtain fast statistical estimation rates in more general conditions. These bounds have the general form

$$\mathcal{E}_{\text{app}} + \mathcal{E}_{\text{est}} \leq c \left(\mathcal{E}_{\text{app}} + \left(\frac{d}{n} \log \frac{n}{d} \right)^{\alpha} \right) \quad \text{for } \frac{1}{2} \leq \alpha \leq 1 \,. \tag{4}$$

This result holds when one can establish the following variance condition:

$$\forall f \in \mathcal{F} \quad \mathbb{E}\left[\left(\ell(f(X), Y) - \ell(f^*_{\mathcal{F}}(X), Y) \right)^2 \right] \leq c \left(E(f) - E(f^*_{\mathcal{F}}) \right)^{2 - \frac{1}{\alpha}} . \tag{5}$$

The convergence rate of (4) is described by the exponent α which is determined by the quality of the variance bound (5). Works on fast statistical estimation identify two main ways to establish such a variance condition.

- Exploiting the strict convexity of certain loss functions [12, theorem 12]. For instance, Lee et al. [14] establish a $\mathcal{O}(\log n/n)$ rate using the squared loss $\ell(\hat{y}, y) = (\hat{y} - y)^2$.
- Making assumptions on the data distribution. In the case of pattern recognition problems, for instance, the "Tsybakov condition" indicates how cleanly the posterior distributions $P(y|x)$ cross near the optimal decision boundary [11,12]. The realizable case discussed in section 2.1.2 can be viewed as an extreme case of this.

Despite their much greater complexity, fast rate estimation results can accomodate the optimization accuracy ρ using essentially the methods illustrated in sections 2.1.1 and 2.1.2. We then obtain a bound of the form

$$\mathcal{E} = \mathcal{E}_{\rm app} + \mathcal{E}_{\rm est} + \mathcal{E}_{\rm opt} = \mathbb{E}\left[E(\tilde{f}_n) - E(f^*)\right] \leq c\left(\mathcal{E}_{\rm app} + \left(\frac{d}{n}\log\frac{n}{d}\right)^{\alpha} + \rho\right). \quad (6)$$

For instance, a general result with $\alpha = 1$ is provided by Massart [13, theorem 4.2]. Combining this result with standard bounds on the complexity of classes of linear functions (e.g., [10]) yields the following result:

$$\mathcal{E} = \mathcal{E}_{\rm app} + \mathcal{E}_{\rm est} + \mathcal{E}_{\rm opt} = \mathbb{E}\left[E(\tilde{f}_n) - E(f^*)\right] \leq c\left(\mathcal{E}_{\rm app} + \frac{d}{n}\log\frac{n}{d} + \rho\right). \quad (7)$$

See also [15,4] for more bounds taking into account the optimization accuracy.

2.2. Gradient Optimization Algorithms

We now discuss and compare the asymptotic learning properties of four gradient optimization algorithms. Recall that the family of function $\mathcal{F}$ is linearly parametrized by $w \in \mathbb{R}^d$. Let $w^*_{\mathcal{F}}$ and w_n correspond to the functions $f^*_{\mathcal{F}}$ and f_n defined in section 1. In this section, we assume that the functions $w \mapsto \ell(f_w(x), y)$ are convex and twice differentiable with continuous second derivatives. Convexity ensures that the empirical const function $C(w) = E_n(f_w)$ has a single minimum.

Two matrices play an important role in the analysis: the Hessian matrix H and the gradient covariance matrix G, both measured at the empirical optimum w_n.

$$H = \frac{\partial^2 C}{\partial w^2}(w_n) \;=\; \mathbb{E}_n\left[\frac{\partial^2 \ell(f_{w_n}(x), y)}{\partial w^2}\right], \quad (8)$$

$$G = \mathbb{E}_n\left[\left(\frac{\partial \ell(f_{w_n}(x), y)}{\partial w}\right)\left(\frac{\partial \ell(f_{w_n}(x), y)}{\partial w}\right)'\right]. \quad (9)$$

The relation between these two matrices depends on the chosen loss function. In order to summarize them, we assume that there are constants $\lambda_{\max} \geq \lambda_{\min} > 0$ and $\nu > 0$ such that, for any $\eta > 0$, we can choose the number of examples n large enough to ensure that the following assertion is true with probability greater than $1 - \eta$:

$$\mathrm{tr}(G\,H^{-1}) \leq \nu \qquad \text{and} \qquad \mathrm{EigenSpectrum}(H) \subset [\,\lambda_{\min}\,,\,\lambda_{\max}\,] \quad (10)$$

The condition number $\kappa = \lambda_{\max}/\lambda_{\min}$ is a good indicator of the difficulty of the optimization [16].

The condition $\lambda_{\min} > 0$ avoids complications with stochastic gradient algorithms. Note that this condition only implies strict convexity around the optimum. For instance, consider the loss function ℓ is obtained by smoothing the well known hinge loss $\ell(z, y) = \max\{0, 1 - yz\}$ in a small neighborhood of its non-differentiable points. Function $C(w)$ is then piecewise linear with smoothed edges and vertices. It is not strictly convex. However its minimum is likely to be on a smoothed vertex with a non singular Hessian. When we have strict convexity, the argument of [12, theorem 12] yields fast estimation rates $\alpha \approx 1$ in (4) and (6). This is not necessarily the case here.

The four algorithm considered in this paper use information about the gradient of the cost function to iteratively update their current estimate $w(t)$ of the parameter vector.

- **Gradient Descent (GD)** iterates

$$w(t+1) \;=\; w(t) - \eta \frac{\partial C}{\partial w}(w(t)) \;=\; w(t) - \eta \frac{1}{n} \sum_{i=1}^{n} \frac{\partial}{\partial w} \ell\big(f_{w(t)}(x_i), y_i\big)$$

  where $\eta > 0$ is a small enough gain. GD is an algorithm with linear convergence [16]. When $\eta = 1/\lambda_{\max}$, this algorithm requires $\mathcal{O}(\kappa \log(1/\rho))$ iterations to reach accuracy ρ. The exact number of iterations depends on the choice of the initial parameter vector.

- **Second Order Gradient Descent (2GD)** iterates

$$w(t+1) \;=\; w(t) - H^{-1} \frac{\partial C}{\partial w}(w(t)) \;=\; w(t) - \frac{1}{n} H^{-1} \sum_{i=1}^{n} \frac{\partial}{\partial w} \ell\big(f_{w(t)}(x_i), y_i\big)$$

  where matrix H^{-1} is the inverse of the Hessian matrix (8). This is more favorable than Newton's algorithm because we do not evaluate the local Hessian at each iteration but simply assume that we know in advance the Hessian at the optimum. 2GD is a superlinear optimization algorithm with quadratic convergence [16]. When the cost is quadratic, a single iteration is sufficient. In the general case, $\mathcal{O}(\log\log(1/\rho))$ iterations are required to reach accuracy ρ.

- **Stochastic Gradient Descent (SGD)** picks a random training example (x_t, y_t) at each iteration and updates the parameter w on the basis of this example only,

$$w(t+1) \;=\; w(t) - \frac{\eta}{t} \frac{\partial}{\partial w} \ell\big(f_{w(t)}(x_t), y_t\big).$$

  Murata [17, section 2.2], characterizes the mean $\mathbb{E}_{\mathcal{S}}[w(t)]$ and variance $\mathbb{V}\mathrm{ar}_{\mathcal{S}}[w(t)]$ with respect to the distribution implied by the random examples drawn from the training set $\mathcal{S}$ at each iteration. Applying this result to the discrete training set distribution for $\eta = 1/\lambda_{\min}$, we have $\delta w(t)^2 = \mathcal{O}(1/t)$ where $\delta w(t)$ is a shorthand notation for $w(t) - w_n$.
  We can then write

$$\begin{aligned} \mathbb{E}_{\mathcal{S}}[\,C(w(t)) - \inf C\,] &= \mathbb{E}_{\mathcal{S}}\big[\mathrm{tr}\big(H\,\delta w(t)\,\delta w(t)'\big)\big] + \mathrm{o}\big(\tfrac{1}{t}\big) \\ &= \mathrm{tr}\,\big(\,H\,\mathbb{E}_{\mathcal{S}}[\delta w(t)]\,\mathbb{E}_{\mathcal{S}}[\delta w(t)]' + H\,\mathbb{V}\mathrm{ar}_{\mathcal{S}}[w(t)]\,\big) + \mathrm{o}\big(\tfrac{1}{t}\big) \\ &\le \tfrac{\mathrm{tr}(GH)}{t} + \mathrm{o}\big(\tfrac{1}{t}\big) \;\le\; \tfrac{\nu\kappa^2}{t} + \mathrm{o}\big(\tfrac{1}{t}\big)\,. \end{aligned} \tag{11}$$

  Therefore the SGD algorithm reaches accuracy ρ after less than $\nu\kappa^2/\rho + \mathrm{o}(1/\rho)$ iterations on average. The SGD convergence is essentially limited by the stochastic noise induced by the random choice of one example at each iteration. Neither the initial value of the parameter vector w nor the total number of examples n appear in the dominant term of this bound! When the training set is large, one could reach the desired accuracy ρ measured on the whole training set without even visiting all the training examples. This is in fact a kind of generalization bound.

Table 2. Asymptotic results for gradient algorithms (with probability 1). Compare the second last column (time to optimize) with the last column (time to reach the excess test error ϵ).
Legend: n number of examples; d parameter dimension; κ, ν see equation (10).

Algorithm	**Cost of one iteration**	**Iterations to reach ρ**	**Time to reach accuracy ρ**	**Time to reach $\mathcal{E} \leq c\,(\mathcal{E}_{\mathrm{app}} + \varepsilon)$**
GD	$\mathcal{O}(nd)$	$\mathcal{O}\Big(\kappa \log \frac{1}{\rho}\Big)$	$\mathcal{O}\Big(nd\kappa \log \frac{1}{\rho}\Big)$	$\mathcal{O}\Big(\frac{d^2\,\kappa}{\varepsilon^{1/\alpha}} \log^2 \frac{1}{\varepsilon}\Big)$
2GD	$\mathcal{O}\big(d^2 + nd\big)$	$\mathcal{O}\Big(\log\log \frac{1}{\rho}\Big)$	$\mathcal{O}\Big(\big(d^2 + nd\big) \log\log \frac{1}{\rho}\Big)$	$\mathcal{O}\Big(\frac{d^2}{\varepsilon^{1/\alpha}} \log \frac{1}{\varepsilon} \log\log \frac{1}{\varepsilon}\Big)$
SGD	$\mathcal{O}(d)$	$\frac{\nu\kappa^2}{\rho} + \mathrm{o}\Big(\frac{1}{\rho}\Big)$	$\mathcal{O}\Big(\frac{d\nu\kappa^2}{\rho}\Big)$	$\mathcal{O}\Big(\frac{d\,\nu\,\kappa^2}{\varepsilon}\Big)$

The first three columns of table 2 report for each algorithm the time for a single iteration, the number of iterations needed to reach a predefined accuracy ρ, and their product, the time needed to reach accuracy ρ. These asymptotic results are valid with probability 1, since the probability of their complement is smaller than η for any $\eta > 0$.

The fourth column bounds the time necessary to reduce the excess error $\mathcal{E}$ below $c\,(\mathcal{E}_{\mathrm{app}} + \varepsilon)$ where c is the constant from (6). This is computed by observing that choosing $\rho \sim \big(\frac{d}{n} \log \frac{n}{d}\big)^{\alpha}$ in (6) achieves the fastest rate for ε, with minimal computation time. We can then use the asymptotic equivalences $\rho \sim \varepsilon$ and $n \sim \frac{d}{\varepsilon^{1/\alpha}} \log \frac{1}{\varepsilon}$. Setting the fourth column expressions to $T_{\max}$ and solving for ϵ yields the *best excess error achieved by each algorithm* within the limited time $T_{\max}$. This provides the asymptotic solution of the Estimation–Optimization tradeoff (3) for large scale problems satisfying our assumptions.

These results clearly show that the generalization performance of *large-scale learning systems* depends on both the statistical properties of the estimation procedure and the computational properties of the chosen optimization algorithm. Their combination leads to surprising consequences:

- *The SGD result does not depend on the estimation rate* α. When the estimation rate is poor, there is less need to optimize accurately. That leaves time to process more examples. A potentially more useful interpretation leverages the fact that (11) is already a kind of generalization bound: its fast rate trumps the slower rate assumed for the estimation error.
- *Superlinear optimization brings little asymptotical improvements in* ε. Although the superlinear 2GD algorithm improves the logarithmic term, the learning performance of all these algorithms is dominated by the polynomial term in $(1/\varepsilon)$. This explains why improving the constants d, κ and ν using preconditioning methods and sensible software engineering often proves more effective than switching to more sophisticated optimization techniques [18].
- *The SGD algorithm yields the best generalization performance despite being the worst optimization algorithm.* This had been described before [19] in the case of a second order stochastic gradient descent and observed in experiments.

In contrast, since the optimization error $\mathcal{E}_{\mathrm{opt}}$ of *small-scale learning systems* can be reduced to insignificant levels, their generalization performance is solely determined by the statistical properties of their estimation procedure.

Table 3. Results with linear SVM on the RCV1 dataset.

Model	Algorithm	Training Time	Objective	Test Error
Hinge loss, $\lambda = 10^{-4}$ *See [21,22].*	SVMLight	23,642 secs	0.2275	6.02%
	SVMPerf	66 secs	0.2278	6.03%
	SGD	**1.4 secs**	0.2275	6.02%
Logistic loss, $\lambda = 10^{-5}$ *See [23].*	LibLinear ($\rho = 10^{-2}$)	30 secs	0.18907	5.68%
	LibLinear ($\rho = 10^{-3}$)	44 secs	0.18890	5.70%
	SGD	**2.3 secs**	0.18893	5.66%

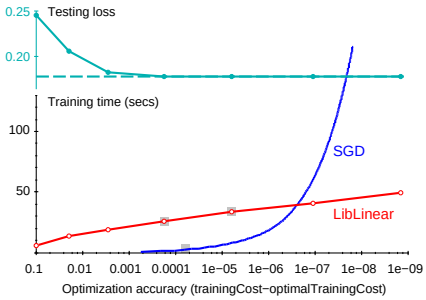

Figure 1. Training time and testing loss as a function of the optimization accuracy ρ for SGD and LibLinear [23].

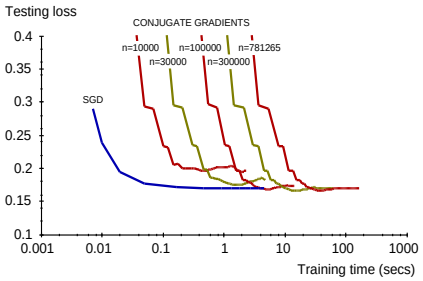

Figure 2. Testing loss versus training time for SGD, and for Conjugate Gradients running on subsets of the training set.

3. Experiments

This section empirically compares the SGD algorithm with other optimization algorithms on a well-known text categorization task, the classification of documents belonging to the CCAT category in the RCV1-v2 dataset [20]. Refer to `http://leon.bottou.org/projects/sgd` for source code and for additional experiments that could not fit in this paper because of space constraints.

In order to collect a large training set, we swap the RCV1-v2 official training and test sets. The resulting training sets and testing sets contain 781,265 and 23,149 examples respectively. The 47,152 TF/IDF features were recomputed on the basis of this new split. We use a simple linear model with the usual hinge loss SVM objective function

$$\min_w \; C(w,b) \;=\; \frac{\lambda}{2} + \frac{1}{n}\sum_{i=1}^{n} \ell(y_t(wx_t+b)) \quad \text{with} \;\; \ell(z) = \max\{0, 1-z\}\,.$$

The first two rows of table 3 replicate earlier results [21] reported for the same data and the same value of the hyper-parameter λ.

The third row of table 3 reports results obtained with the SGD algorithm

$$w_{t+1} = w_t - \eta_t \left(\lambda w + \frac{\partial \ell(y_t(wx_t+b))}{\partial w} \right) \quad \text{with} \;\; \eta_t = \frac{1}{\lambda(t+t_0)}\,.$$

The bias b is updated similarly. Since λ is a lower bound of the smallest eigenvalue of the hessian, our choice of gains η_t approximates the optimal schedule (see section 2.2).

The offset t_0 was chosen to ensure that the initial gain is comparable with the expected size of the parameter w. The results clearly indicate that SGD offers a good alternative to the usual SVM solvers. Comparable results were obtained in [22] using an algorithm that essentially amounts to a stochastic gradient corrected by a projection step. Our results indicates that the projection step is not an essential component of this performance.

Table 3 also reports results obtained with the logistic loss $\ell(z) = \log(1 + e^{-z})$ in order to avoid the issues related to the nondifferentiability of the hinge loss. Note that this experiment uses a much better value for λ. Our comparison points were obtained with a state-of-the-art superlinear optimizer [23], for two values of the optimization accuracy ρ. Yet the very simple SGD algorithm learns faster.

Figure 1 shows how much time each algorithm takes to reach a given optimization accuracy. The superlinear algorithm reaches the optimum with 10 digits of accuracy in less than one minute. The stochastic gradient starts more quickly but is unable to deliver such a high accuracy. However the upper part of the figure clearly shows that the testing set loss stops decreasing long before the moment where the superlinear algorithm overcomes the stochastic gradient.

Figure 2 shows how the testing loss evolves with the training time. The stochastic gradient descent curve can be compared with the curves obtained using conjugate gradients[3] on subsets of the training examples with increasing sizes. Assume for instance that our computing time budget is 1 second. Running the conjugate gradient algorithm on a random subset of 30000 training examples achieves a much better performance than running it on the whole training set. How to guess the right subset size a priori remains unclear. Meanwhile running the SGD algorithm on the full training set reaches the same testing set performance much faster.

4. Conclusion

Taking in account budget constraints on both the number of examples and the computation time, we find *qualitative differences* between the generalization performance of small-scale learning systems and large-scale learning systems. The generalization properties of large-scale learning systems depend on both the statistical properties of the estimation procedure and the computational properties of the optimization algorithm. We illustrate this fact by deriving asymptotic results on gradient algorithms supported by an experimental validation.

Considerable refinements of this framework can be expected. Extending the analysis to regularized risk formulations would make results on the complexity of primal and dual optimization algorithms [21,24] directly exploitable. The choice of surrogate loss function [7,12] could also have a non-trivial impact in the large-scale case.

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[3] This experimental setup was suggested by Olivier Chapelle (personal communication). His specialized variant of the conjugate gradients algorithm works nicely in this context because it converges superlinearly with very limited overhead.

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