# Optimization Methods for Large-Scale Machine Learning

V. Estellers

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#### What this lectures are about

The optimization problems that result from training a large-scale machine learning model have characteristics that make the stochastic gradient (SG) method more effective than conventional gradient-based nonlinear optimization techniques.

- 1. Characteristic of optimization of large-scale machine learning models
- 2. Stochastic gradient algorithm
- 3. Analysys of SG algorithm
- 4. Improved SG convergence with noise-reduction techniques
- 5. Improved SG convergence with second-order derivatives

#### References

The lectures are organized following:

Bottou, L., Curtis, F. E., and Nocedal, J. *Optimization Methods for Large-Scale Machine Learning*. 2016.http://arxiv.org/abs/1606.04838 We will also cover some material from:

- 1. Gower, R. M., Roux, N. Le, and Bach, F. *Tracking the gradients using the Hessian: A new look at variance reducing stochastic methods.*, 2017.
- 2. Roux, N. Le, Schmidt, M., and Bach, F. A Stochastic Gradient Method with an Exponential Convergence Rate for Strongly-Convex Optimization with Finite Training Sets. 2012.

# **Optimization Problems in Machine Learning**

We illustrate how optimization problems arise in machine learning and what makes them challenging with two case studies:

- 1. linear regressor with bag-of-words features for text classification
- 2. open-ended deep neural network for speech and image recognition.

Both problems have some common characteristics:

- Large-scale: models described by a large number of parameters.
- Stochastic: models designed to make decisions on unseen data...

They differ in the optimization problem: (1) convex, (2) nonconvex.

# **Text Classification via Convex Optimization**

Text classification: assigning a predefined class to a natural language text based on its contents. For example, determine if a text discusses politics.

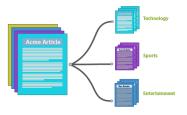


Fig.: http://blog.thedigitalgroup.com/rajendras/2015

Given a set of examples  $\{(x_1, y_1), \dots, (x_n, y_n)\}$ , where

- feature vector  $x_i$  of a text document (e.g., the words it includes).
- scalar label  $y_i$  indicating if the document belongs  $(y_i = 1)$  or not  $(y_i = 1)$  to a particular class.

Construct a classifier that predicts the class of an unseen text.

# First Solution: Minimizing Empirical Risk

Design a prediction function h s.t. h(x) predicts the text document.

- Performance measure: how often  $h(x_i)$  differs from the prediction  $y_i$ .
- Search h that minimizes the frequency of observed misclassifications:

$$R_n(h) = \frac{1}{n} \sum_{i=1}^n \mathbb{1}[h(x_i) \neq y_i], \text{ where } \mathbb{1}[A] = \begin{cases} 1 & \text{if } A \text{ is true,} \\ 0 & \text{otherwise.} \end{cases}$$

$$\tag{1.1}$$

 $R_n$  is the empirical risk of misclassification.

# Minimizing Empirical Risk is Not Enough

Rote memorization with

$$h^{\text{rote}}(x) = \begin{cases} y_i & \text{if } x = x_i \text{ for some } i \in \{1, \dots, n\}, \\ \pm 1 & \text{(arbitrarily) otherwise.} \end{cases}$$
 (1.2)

minimizes the empirical risk but has no guarantees on unseen documents.

The prediction function should generalizes the concepts learned from the examples. To this goal, we choose

- parametric functions satisfying certain smoothness conditions
- use cross-validation to choosing between classes of prediction functions

# Minimizing Expected Risk with Cross-validation

Cross-validation minimizes the expected risk by splitting examples into:

- training set to optimize the parameters of h by minimizing  $R_n$ . The selects a candidate for each class of parametric functions  $h_1, \ldots, h_k$
- validation set to estimate the performance of  $h_1, \ldots, h_k$ . This selects the best candidate  $h^*$
- testing set to estimate the performance of  $h^{st}$

Cross-validation has shown the success of **bag-of-words** approach for text classification.

# **Linear Regression with Bag-of-Words Features**

#### Bag-of-Words features:

- represents a text document by a feature vector  $x \in \mathbb{R}^d$ , where each component measures the appearance of a specific word.
- very sparse vectors of high-dimensionality.

Affine prediction function classifies the documents:

$$h(x; w, \tau) = w^T x - \tau \tag{1.3}$$



Fig.: https://www.python-kurs.eu/text\_klassifikation\_python.php

# **Optimization of the Model**

Finding  $w, \tau$  that minimize the empirical risk of misclassification

$$R_n(h) = \frac{1}{n} \sum_{i=1}^n \text{sign}(-h(x_i; w, \tau) \cdot y_i)$$
 (1.4)

is difficult because the sign is discontinuous, takes discrete values, and results in a combinatorial problem. For this reason, we approximate it by a continuous loss function that we can minimize effective like

$$\ell(h, y) = \log(1 + \exp(-h(x_i)y)).$$
 (1.5)

Classes of prediction functions  $h_{\lambda}$  are determined by a regularization term

$$\min_{(w,\tau)\in\mathbb{R}^{d+1}} \frac{1}{n} \sum_{i=1}^{n} \log(1 + \exp(-h(x_i)y_i)) + \frac{\lambda}{2} ||w||^2.$$
 (1.6)

Optimizing the model parameters with various  $\lambda_1,\ldots,\lambda_k$  on the training set gives the candidate solution  $h_{\lambda_1},\ldots,h_{\lambda_k}$ . The final solution is the candidate with best performance on the validation set.

#### Perceptual Tasks via Deep Networks

Deep/Convolutional neural networks have recently achieved spectacular success on perceptual problems such as speech and image recognition.

They are essentially the same types of networks from the 90s, but their successes is now possible due to the availability of larger datasets and computational resources.

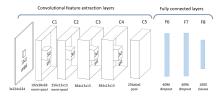


Fig.: Architecture for image recognition. The 2012 ILSVRC winner consists of eight layers: each layer performs a linear transformation followed by nonlinear transformations.

#### **Neural Networks**

DNN/CNNs construct a prediction function h whose value is computed by applying successive transformations to a given input vector  $x_i \in \mathbb{R}^{d_0}$ . These transformations are made in layers.

$$x_i^{(j)} = s(W_j x_i^{(j-1)} + b_j) \in \mathbb{R}^{d_j}, \tag{1.7}$$

where  $x_i^{(0)} = x_i$  and

- $\boldsymbol{x}_i^{(j)}$  is the input vector to layer j
- j-th layer parameters: matrix  $W_j \in \mathbb{R}^{d_j imes d_{j-1}}$  and vector  $b_j \in \mathbb{R}^{d_j}$
- s componentwise nonlinear activation/pooling function.

# **Deep Neural Networks**

Neural Networks use simple activation functions, like the sigmoid or the rectified linear unit (ReLU)

$$s(x) = 1/(1 + \exp(-x))$$
  $s(x) = \max\{0, x\}.$ 

CNNs are networks where layers have

- circulant matrices  $W_j$ , s.t.  $W_j x_i^{(j1)}$  is an image convolution.
- activation functions rectify, normalize, or subsample images.

The output vector  $x_i^{(J)}$  is the prediction function value  $h(x_i; w)$ , where  $w = \{(W_1, b_1), \dots, (W_J, b_J)\}$  collects the parameters of all the layers.

# **Optimization of Deep Neural Networks**

The optimization of DNN/CNN over the training set  $\{(x_1,y_1),\ldots,(x_n,y_n)\}$  with a loss function  $\ell$  define the problem

$$\min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n \ell(h(x_i; w), y_i). \tag{1.8}$$

This problem is nonconvex. Finding a global optimum is intractable and we look for approximate solutions with gradient-based methods.

The gradient of the objective function of (1.8) can be computed efficiently by the chain rule (back propagation).

#### Convolutional neural networks

The training process of DNNs and CNNs requires extreme care to overcome the difficulties of large, nonlinear and nonconvex problems:

- 1. initialize the optimization process with a good starting point
- 2. monitor its progress to correct conditioning issues as they appear (vanishing gradients).

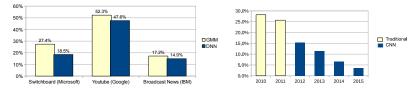


Fig.: Left:Word error rates reported by three different research groups on three standard speech recognition benchmarks. Right: Historical *top5* error rate of the annual winner of the ImageNet image classification challenge.

# Formulation of a Supervised Classification Problem

 $\textbf{Classification} \text{: choose a prediction function from an input space } \mathscr{X} \text{ to an output space } \mathscr{Y}$ 

$$h: \mathfrak{X} \to \mathfrak{Y}$$

s.t., given  $x \in \mathcal{X}$ , h(x) offers an accurate prediction about the output y.

**Supervised**: h that generalizes the properties meaningful to determine y from x that can be learned from input-output examples  $\{(x_i, y_i)\}_{i=1}^n$ .

**Problem**: avoid rote memorization by choosing a prediction function h that minimizes a risk measure over a family of prediction functions  $\mathcal{H}$ .

# **Expected Risk instead of Empirical Risk**

Let  $\{(x_i,y_i)\}_{i=1}^n$  be samples from a joint probability distribution function P(x,y). Rather than finding h that minimizes the empirical risk

$$R_n(h) = \frac{1}{n} \sum_{i=1}^n \mathbb{1}[h(x_i) = y_1] \quad \mathbb{1}[A] = \begin{cases} 1 & \text{if A is true} \\ 0 & \text{otherwise} \end{cases}, \tag{1.9}$$

we find h that minimizes the expected misclassification risk over all possible inputs, i.e., an h that minimizes

$$R(h) = \mathbb{P}[h(x) \neq y] = \mathbb{E}[\mathbb{1}[h(x) \neq y]], \tag{1.10}$$

**Stochastic** problem (objective is an expectation) is substituted by a surrogate problem constructed from  $\{(x_i, y_i)\}_{i=1}^n$  as we do not know P.

# **Choice of Prediction Function Family**

We choose the family of functions  $\mathcal{H}$  with three goals in mind:

- 1.  $\mathcal{H}$  should contain functions that achieve a low empirical risk to avoid underfitting the data.  $\Rightarrow$  select a rich family of functions
- 2.  ${\mathscr H}$  should be selected to make the optimization problem solvable
- 3.  $R(h)-R_n(h)$  should be small over all  $h\in \mathcal{H}$ . This gap might increase when  $\mathcal{H}$  becomes too rich and overfits the training data.

#### **Gap Between Expected and Empirical Risk**

When the expected risk represents a misclassification probability, with probability at least  $1-\eta$ ,

$$\sup_{h \in \mathcal{H}} |R(h) - R_n(h)| \le \mathcal{O}\left(\sqrt{\frac{1}{2n}\log\left(\frac{2}{\eta}\right) + \frac{d_{\mathcal{H}}}{n}\log\left(\frac{n}{d_{\mathcal{H}}}\right)}\right). \quad (1.11)$$

- $d_{\mathscr{H}}$ : Vapnik-Chervonenkis dimension measures the capacity of  $\mathscr{H}$
- fixed  $d_{\mathcal{H}}$ , the gap decreases by increasing number of examples (n).
- fixed n, the gap can widen for larger  $d_{\mathcal{H}}$  (richer function families).

Bound (1.11) is not used in practice because it is easier to estimate the gap with cross-validation than calculate the VC dimension of  $\mathcal{H}$ .

#### **Structural Risk Minimization**

Structural risk minimization: technique for choosing a prediction function. Consider a nested families of function parametrized by function  $\Omega$ 

$$H_C = \{ h \in \mathcal{H} : \Omega(h) \le C \} \Rightarrow H_C \subset H_D \text{ for } C < D$$

- 1. Increasing C reduces the  $R_n$  because it enlarges the family of functions we can optimize over.
- 2. For large C, the  $R_n-R$  increases because the prediction function overfits the training data.

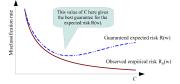


Fig.: The optimal empirical risk decreases when C increases.  $|R(w) - R_n(w)|$  is bounded above by a quantity that increases with C. The value of C that offers the best guarantee on the expected risk increases with n.

# In the following, we consider the problem...

Assume that the prediction function h is parameterized by a real vector  $w \in \mathbb{R}^d$ . This vector defines our optimization variable and the family of prediction functions

$$\mathcal{H} = \{ h(\cdot; w) \colon \mathbb{R}^d \times \mapsto \mathbb{R}^{d_y} \mid w \in \mathbb{R}^d \}.$$

Given a loss function  $\ell\colon \mathbb{R}^{d_y}\times \mathbb{R}^{d_y}\mapsto \mathbb{R}$  that measures the loss associated with the prediction h(x;w) when the true label is y with  $\ell(h(x;w),y)$ , we define:

- $\xi$ : random variable that represents a sample or a set of samples  $\{(x_i,y_i)\}_{i\in S}$ .
- $f(w;\xi) = \ell(h(w;\xi),y)$ : the loss incurred for a given  $(w,\xi)$

# **Expected and Empirical Risk**

Let P(x,y) be the probability distribution between inputs and outputs, we define  $\operatorname{\textbf{expected}}$  risk by

$$R(w) = \int_{\mathbb{R}^{d_x} \times \mathbb{R}^{d_y}} \ell(h(x; w), y) dP(x, y) = \mathbb{E}[\ell(h(x; w), y)] = \mathbb{E}[f(w; \xi)]$$

To minimize the expected risk, we need complete information about P. As this is not possible, we minimize the **empirical risk** 

$$R_n(w) = \frac{1}{n} \sum_{i=1}^n \ell(h(x_i; w), y_i) = \frac{1}{n} \sum_{i=1}^n f(w; \xi[i])$$

that estimates the expected risk ( in supervised classification) from n independently drawn input-output samples  $\{\xi[i]\}_{i=1}^n = \{(x_i,y_i)\}_{i=1}^n$ .

# Stochastic Optimization for Empirical Risk Minimization

The stochastic gradient method (SG) minimizes the empirical risk  $R_n$  with the sequence:

$$w_{k+1} = w_k - \alpha_k \nabla f_{i_k}(w_k) \quad \forall k \in \mathbb{N}, \tag{2.12}$$

where  $w_1$  is given,  $\alpha_k$  is a positive stepsize, and  $i_k$  is chosen randomly. Characteristics:

- 1. Cheap iterations that only computate one gradient  $\nabla f_{i_k}(w_k)$
- 2. The sequence is not determined uniquely by  $R_n$ ,  $w_1$ , and stepsizes, but depends also on the random sequence  $\{i_k\}$ .
- 3.  $-\nabla f_{i_k}(w_k)$  might not be a descent direction from  $w_k$ .

# **Batch Optimization for Empirical Risk Minimization**

A batch approach minimizes the Empirical Risk directly. The simplest steepest descent or gradient method defines the sequence:

$$w_{k+1} = w_k - \alpha_k \nabla R_n(w_k) = w_k - \alpha_k \frac{1}{n} \sum_{i=1}^n \nabla f_i(w_k) \quad \forall k \in \mathbb{N}, \quad (2.13)$$

#### Characteristics:

- 1. Computing  $\alpha_k \nabla R_n(w_k)$  is more expensive than  $\alpha_k \nabla f_{i_k}(w_k)$  in SG.
- 2. By iterating over all samples, batch methods compute better steps.
- 3. It can use (quasi) Newton methods to speed up optimization of  $R_n$ .
- 4. The sum structure of  $R_n$  allows parallel or distributed updates.

# Typical Performance of Stochastic and Batch Methods

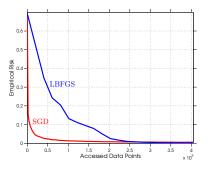


Fig.: Empirical risk  $R_n$  as a function of the number of accessed data points (ADP) for a batch L-BFGS method and the SG method on a binary classification problem with a logistic loss objective and the RCV1 dataset.

#### **Stochastic vs Batch Methods**

SG is used in machine learning when cannot afford to iterate over all samples to compute the next iterate.

SG uses the samples more efficient than a batch method. Intuitively:

- Consider a training set S with ten copies of a set  $S_s$ .
- In a batch approach, the iterations that use S as training set are ten times more expensive than iteration that only use one copy of  $S_s$ .
- In the SG method, the iterations using S and  $S_s$  as training sets cost the same.
- In reality, a training set does not consist of exact duplicates of sample data, but it has enough redundancy to make using all of the samples in every iteration inefficient.

#### Next week: Stochastic vs Batch Methods

Let  $R_n^*$  be the minimal value of  $R_n$ , then if  $R_n$  is strongly convex

- the error of a batch gradient method satisfies

$$|R_n(w_k) - R_n^*| \le \mathcal{O}(\rho^k), \quad \rho \in (0, 1).$$

The number of iterations where the training error is above  $\epsilon$  is proportional to  $\log(\frac{1}{\epsilon})$ , and the cost of  $\epsilon$ -optimality is  $\mathcal{O}(n\log(\frac{1}{\epsilon}))$ .

- the SG error for  $i_k$  is drawn uniformly from  $\{1,\dots,n\}$  is

$$\mathbb{E}[|Rn(w_k) - R_n^*|] = \mathcal{O}(\frac{1}{k})$$
(2.14)

As it does not depend on n, the cost of  $\epsilon$ -optimality is  $\mathcal{O}(\frac{1}{\epsilon})$ .

The SG cost  $\mathcal{O}(\frac{1}{\epsilon})$  is smaller than the batch cost  $\mathcal{O}(n\log(\frac{1}{\epsilon}))$  if n is large.

#### Next week: Stochastic vs Batch Methods

SG avoids overfitting in the sense that the minimizer of the empirical risk found by SG has some minimization guarantees on the expected risk.

By applying the SG iteration with  $\nabla f(w_k; x_{i_k})$  replaced by  $\nabla f(w_k; \xi_k)$  with each  $\xi_k$  drawn independently according to the distribution P,

$$\mathbb{E}[|R(w_k) - R^*|] = \mathcal{O}\left(\frac{1}{k}\right). \tag{2.15}$$

This is again a sublinear rate, but on the expected risk.

#### Other Methods

A mini-batch approach chooses a subset of samples  $S_k \subset \{1, \dots, n\}$  randomly in each iteration to improve the gradient estimate as follows:

$$w_{k+1} = w_k - \frac{\alpha_k}{|S_k|} \sum_{i \in S_k} \nabla f_i(w_k) \quad \forall k \in \mathbb{N},$$
 (2.16)

This allows some degree of parallelization and reduces the variance of the stochastic gradient estimates.

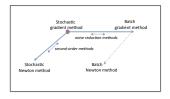


Fig.: Schematic of a two-dimensional spectrum of optimization methods for machine learning. The horizontal axis represents methods designed to control stochastic noise; the second axis, methods that deal with ill conditioning.

# **Optimization for Supervised Learning**

Given a set of examples  $(x_1, y_1), \ldots, (x_n, y_n)$ 

- each example  $\xi = (x, y)$  is a pair of an input x and a scalar output y.
- loss  $\ell(\hat{y},y)$  measures the cost of predicting  $\hat{y}$  when the answer is y
- family  $\mathcal H$  of functions  $h(\cdot;w)$  parametrized by a weight vector w.

We seek  $h \in \mathcal{H}$  that minimizes the loss  $f(\xi; w) = \ell(h(x; w), y)$ .

Although we would like to average over the unknown distribution P(x,y)

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

we must settle for computing the average over the samples

$$f(w) = R_n(w) = \frac{1}{n} \sum_{i=1}^n \ell(h(x_i; w), y_i).$$

Statistical learning theory (Vapnik and Chervonenkis, 1971) justifies minimizing  $R_n$  instead of R when  $\mathcal{H}$  is sufficiently restrictive.

#### **Stochastic Gradient Method**

The objective function  $F: \mathbb{R}^d \mapsto \mathbb{R}$  can be the expected or empirical risk:

$$F(w) = \mathbb{E}[f(w,\xi)]$$
 or  $F(w) = \frac{1}{n} \sum_{i=1}^{n} f_i(w)$ .

The analysis applies to both objectives. The only difference is the way that the stochastic gradient estimates are chosen.

- 1.  $F = R_n$ : pick samples uniformly from a finite training set with replacement (sample discrete distribution with equal weights for every sample).
- 2. F = R: pick samples in each iteration according to distribution P (online or large-scale setting).

#### **Stochastic Gradient Method**

```
Choose an initial iterate w_1 for k=1,2,... do 
 Generate a realization of the random variable \xi_k Compute a stochastic vector g(w_k,\xi_k) Choose a stepsize \alpha_k>0 
 Set the new iterate as w_{k+1}=w_k-\alpha_k g(w_k,\xi_k) end for
```

The algorithm requires three computational tools:

- 1. mechanism for generating a realization of a random variable  $\xi_k$ , where  $\{\xi_k\}$  is a sequence of jointly independent random variables.
- 2. mechanism for computing stochastic vector  $g(w_k, \xi_k) \in \mathbb{R}^d$
- 3. mechanism for computing a scalar stepsize  $\alpha_k>0$

#### **General version of Stochastic Gradient Method**

This SG algorithm generalizes many stochastic gradient-based algorithms:

$$g(w_k,\xi_k) = \begin{cases} \nabla f(w_k,\xi_k) & \text{simple or base SG} \\ \frac{1}{n_k} \sum_{i=1}^{n_k} \nabla f(w_k,\xi_{k,i}) & \text{mini-batch SG} \\ H_k \frac{1}{n_k} \sum_{i=1}^{n_k} \nabla f(w_k,\xi_{k,i}) & \text{2nd-order SG} \end{cases}$$

flexibility choosing mini-batch size  $n_k$  and symmetric positive definite  $H_k$ .

Prove convergence of SG with two assumptions:

- 1. smoothness of the objective function
- 2. bounded 1st and 2nd moments of stochastic vectors  $\{g(w_k, \xi_k)\}$

If the objective is strongly convex SG converges to the minimum, otherwise to a stationary point.

# **Assumption 1:** *L*-smooth function

The objective function  $F\colon \mathbb{R}^d \mapsto \mathbb{R}$  is continuously differentiable and the gradient function of  $F, \nabla F\colon \mathbb{R}^d \mapsto \mathbb{R}^d$ , is Lipschitz continuous with Lipschitz constant L, that is

$$\|\nabla F(w) - \nabla F(\bar{w})\| \le L\|w - \bar{w}\| \ \forall w, \bar{w} \in \mathbb{R}^d.$$

This assumption ensures that the gradient of F does not change arbitrarily quickly with respect to the parameter vector and can be used to estimate how far to move (SG stepsize) to decrease F.

An important consequence of F being L-smooth is that

$$F(w) \le F(\bar{w}) + \nabla F(\bar{w})^T (w - \bar{w}) + \frac{1}{2} L \|w - \bar{w}\|^2 \quad \forall w, \bar{w} \in \mathbb{R}^d.$$

#### First Lemma

#### Lemma

If F is an L-smooth function and  $\mathbb{E}_{\xi_k}[\cdot]$  denotes the expected value taken w.r.t the distribution of the random variable  $\xi_k$ , the iterates of SG satisfy:

$$\mathbb{E}_{\xi_k}[F(w_{k+1})] - F(w_k) \leq -\alpha_k \underbrace{\nabla F(w_k)^T \mathbb{E}_{\xi_k}[g(w_k, \xi_k)]}_{\text{expected directional derivative of } F \text{ along direction } g(w_k, \xi_k)} + \underbrace{\frac{\alpha_k^2 L}{2}}_{\text{second moment } g(w_k, \xi_k)} \underbrace{\mathbb{E}_{\xi_k}[\|g(w_k, \xi_k)\|^2]}_{\text{second moment } g(w_k, \xi_k)}$$

If  $g(w_k, \xi_k)$  is an unbiased estimate of  $\nabla F(w_k)$ , we have

$$\mathbb{E}_{\xi_k}[F(w_{k+1})] - F(w_k) \le -\alpha_k \|\nabla F(w_k)\|^2 + \frac{1}{2}\alpha_k^2 L \mathbb{E}_{\xi_k}[\|g(w_k, \xi_k)\|^2].$$

#### **Proof**

As F is L-smooth and the SG iterates  $w_{k+1} = w_k - \alpha_k g(w_k, \xi_k)$ , we have

$$F(w_{k+1}) - F(w_k) \le \nabla F(w_k)^T (w_{k+1} - w_k) + \frac{1}{2} L \|w_{k+1} - w_k\|^2$$
  
$$\le -\alpha_k \nabla F(w_k)^T g(w_k, \xi_k) + \frac{1}{2} L \alpha_k^2 \|g(w_k, \xi_k)\|^2.$$

Taking expectations on both sides w.r.t the distribution of  $\xi_k$ , and noting that only  $w_{k+1}$  and  $g(w_k, \xi_k)$  depend on  $\xi_k$ , we obtain the desired bound

$$\mathbb{E}_{\xi_k}[F(w_{k+1}) - F(w_k)] \le \mathbb{E}_{\xi_k}[-\alpha_k \nabla F(w_k)^T \ g(w_k, \xi_k) + \frac{1}{2}\alpha_k^2 L \|g(w_k, \xi_k)\|^2],$$

$$\le -\alpha_k \nabla F(w_k)^T \mathbb{E}_{\xi_k}[g(w_k, \xi_k)] + \frac{\alpha_k^2}{2} L \mathbb{E}_{\xi_k}[\|g(w_k, \xi_k)\|^2].$$

# **Assumption 2: Bounds on First and Second Moments**

The objective function and the SG Algorithm satisfy:

- 1.  $\{w_k\}$  are in an open set where F is bounded below by scalar  $F_{\text{inf}}$ .
- 2. In expectation,  $-g(w_k, \xi_k)$  is a direction of sufficient descent with a norm comparable to the norm of the gradient. There is  $\mu_G \geq \mu > 0$

$$\frac{1}{\mu} \nabla F(w_k)^T \mathbb{E}[g(w_k, \xi_k)] \ge \|\nabla F(w_k)\|^2 \|\nabla F(w_k)\| \ge \frac{1}{\mu_G} \|\mathbb{E}[g(w_k, \xi_k)]\|$$

3. There exist scalars  $M, M_V \geq 0$  such that, for all  $k \in \mathbb{N}$ 

$$\mathbb{V}_{\xi_k}[g(w_k, \xi_k)] \le M + M_V \|\nabla F(w_k)\|^2$$

# **Assumption 2: In practice**

Point 1, just means that there is no *trivial* solution  $\min_{w} F(w) = -\infty$ .

Point 2 holds if  $g(w_k, \xi_k)$  is an unbiased estimate of  $\nabla F(w_k)$  multiplied by positive definite  $H_k$  with eigenvalues in a fixed interval.

Points 2 and 3 are combined into a single inequality with  $M_G \ge \mu^2 \ge 0$ 

$$\mathbb{E}_{\xi_k}[\|g(w_k, \xi_k)\|^2] = \mathbb{V}_{\xi_k}[g(w_k, \xi_k)] + \|\mathbb{E}_{\xi_k}[g(w_k, \xi_k)]\|^2$$

$$\leq M + M_V \|\nabla F(w_k)\|^2 + \mu_G^2 \|\nabla F(w_k)\|^2$$

$$\leq M + M_G \|\nabla F(w_k)\|^2$$

## Lemma 2

#### Lemma

If F is L-smooth and Assumption 2 holds, the SG iterates satisfy

$$\mathbb{E}_{\xi_{k}}[F(w_{k+1})] - F(w_{k}) \leq -\mu \alpha_{k} \|\nabla F(w_{k})\|^{2} + \frac{1}{2} \alpha_{k}^{2} L \mathbb{E}_{\xi_{k}}[\|g(w_{k}, \xi_{k})\|^{2}]$$

$$\mathbb{E}_{\xi_{k}}[F(w_{k+1})] - F(w_{k}) \leq -\underbrace{(\mu - \frac{1}{2} \alpha_{k} L M_{G}) \alpha_{k} \|\nabla F(w_{k})\|^{2} + \frac{1}{2} \alpha_{k}^{2} L M}_{\text{deterministic}}.$$

In English, regardless of how the method arrived at  $w_k$ , the optimization continues in a Markovian manner:  $w_{k+1}$  that depends only on the iterate  $w_k$ , the seed  $\xi_k$ , and the stepsize  $\alpha_k$  and not on any past iterates.

# Lemma 2, Proof

Let us prove the first inequality. As F is L-smooth, Lemma 1 states

$$\mathbb{E}_{\xi_{k}}[F(w_{k+1})] - F(w_{k}) \leq \underbrace{-\alpha_{k}\nabla F(w_{k})^{T}\mathbb{E}_{\xi_{k}}[g(w_{k},\xi_{k})]}_{\text{Assumption 2}} + \frac{1}{2}\alpha_{k}^{2}L\mathbb{E}_{\xi_{k}}[\|g(w_{k},\xi_{k})\|^{2}]$$

$$\mathbb{E}_{\xi_{k}}[F(w_{k+1})] - F(w_{k}) \leq -\mu\alpha_{k}\|\nabla F(w_{k})\|^{2} + \frac{1}{2}\alpha_{k}^{2}L\underbrace{\mathbb{E}_{\xi_{k}}[\|g(w_{k},\xi_{k})\|^{2}]}_{\text{combined assumption 2}}$$

$$\leq M + M_{G}\|\nabla F(w_{k})\|^{2}$$

$$\mathbb{E}_{\xi_{k}}[F(w_{k+1})] - F(w_{k}) \leq -\mu\alpha_{k}\|\nabla F(w_{k})\|^{2} + \frac{1}{2}\alpha_{k}^{2}L(M + M_{G}\|\nabla F(w_{k})),$$

$$\mathbb{E}_{\xi_{k}}[F(w_{k+1})] - F(w_{k}) \leq (-\mu\alpha_{k} + \frac{1}{2}\alpha_{k}^{2}LM_{G})\|\nabla F(w_{k})\|^{2} + \frac{1}{2}\alpha_{k}^{2}LM.$$

# Intuitive Convergence of SG with fixed stepsize

Consider the inequality of the second lemma

$$\mathbb{E}_{\xi_k}[F(w_{k+1})] - F(w_k) \leq \underbrace{-(\mu - \frac{1}{2}\alpha_k LM_G)\alpha_k \|\nabla F(w_k)\|^2}_{\text{tends to 0 as } \nabla F(w_k) \to 0} + \frac{1}{2}\alpha_k^2 LM.$$

For a fixes stepsize, the last term remains constant and, after some point, we cannot expect to reduce the distance between the objective iterates beyond  $\frac{1}{2}\alpha^2LM$ . That is, we converge to a neighborhood of the optimal.

 $\Rightarrow$  SG needs diminishing stepsizes  $\alpha_k \to 0$  to converge.

# Convergence of SG with fixed stepsize

#### **Theorem**

If F is an L-smooth and c-strongly convex function that satisfies Assumption 2, with  $F_{\inf} = F^*$ , and the SG method is run with a positive stepsize  $\alpha \leq \frac{\mu}{LM_G}$ , then the expected optimality gap satisfies for all k

$$\mathbb{E}[F(w_k) - F^*] \le \frac{\alpha LM}{2c\mu} + (1 - \alpha c\mu)^{k-1} \left( F(w_1) - F^* - \frac{\alpha LM}{2c\mu} \right),$$

where  $\mathbb{E}$  is the expectation w.r.t joint distribution of all random variables.

A direct result of this theorem states that the SG iterates converge to the  $\frac{\alpha LM}{2c\mu}$  neighborhood of the optimal value as  $k\to\infty.$ 

# **Strongly Convex Functions**

#### Definition

The objective function  $F:\mathbb{R}^d\mapsto\mathbb{R}$  is **strongly convex** in that there exists a constant c>0 such that

$$F(w) \ge F(\bar{w}) + \nabla F(\bar{w})^T (w - \bar{w}) + \frac{1}{2}c\|w - \bar{w}\|^2 \quad \forall w, \ \bar{w} \in \mathbb{R}^d.$$

Moreover, F has a unique minimizer  $w^* \in \mathbb{R}^d$  with  $F^* = F(w^*)$  and satisfies

$$2c(F(w) - F^*) \le \|\nabla F(w)\|^2 \quad \forall w \in \mathbb{R}^d.$$

If F is L-smooth and c-strongly convex, then  $c \leq L$ .

# **Proof**

Let us use the bound on the stepsize  $\alpha \leq \frac{\mu}{LMC}$  in Lemma 2

$$\mathbb{E}_{\xi_k}[F(w_{k+1})] - F(w_k) \le -(\mu - \frac{1}{2}\alpha L M_G)\alpha \|\nabla F(w_k)\|^2 + \frac{1}{2}\alpha_k^2 L M$$

$$\le -\frac{\mu}{2}\alpha \|\nabla F(w_k)\|^2 + \frac{1}{2}\alpha^2 L M.$$

As F is c-strongly convex,  $2c(F(w_k) - F^*) \leq ||\nabla F(w_k)||^2$  and we get

$$\mathbb{E}_{\xi_k}[F(w_{k+1})] - F(w_k) \le -\mu \alpha c(F(w_k) - F^*) + \frac{1}{2}\alpha^2 LM.$$

Subtracting  $F^*$  from both sides, taking total expectations, and rearranging

$$\mathbb{E}[F(w_{k+1}) - F^*] \le (1 - \mu \alpha c) \mathbb{E}[F(w_k) - F^*] + \frac{1}{2} \alpha^2 LM.$$

Subtracting the constant  $\frac{\alpha LM}{2cu}$  from both sides

$$\mathbb{E}[F(w_{k+1}) - F^*] - \frac{\alpha LM}{2c\mu} \le (1 - \mu\alpha c)\mathbb{E}[F(w_k) - F^*] + \frac{1}{2}\alpha^2 LM - \frac{\alpha LM}{2c\mu}$$

$$\le (1 - \mu\alpha c)\mathbb{E}[F(w_k) - F^*] + \frac{\alpha LM}{2c\mu}(\alpha c\mu - 1)$$

$$\le (1 - \mu\alpha c)\left(\mathbb{E}[F(w_k) - F^*] - \frac{\alpha LM}{2c\mu}\right).$$

# **Continuation Proof**

This inequality

$$\mathbb{E}[F(w_{k+1}) - F^*] - \frac{\alpha LM}{2c\mu} \le (1 - \mu \alpha c) \left( \mathbb{E}[F(w_k) - F^*] - \frac{\alpha LM}{2c\mu} \right).$$

is a contraction because

$$0 < \alpha c \mu \underbrace{\leq}_{\alpha \leq \frac{\mu}{LM_G}} \frac{c\mu^2}{LM_G} \underbrace{\leq}_{M_G \geq \mu^2} \frac{c\mu^2}{L\mu^2} = \frac{c}{L} \underbrace{\leq}_{L \geq c} 1$$

Applying the contraction inequality k-1 times, we obtain the desired result

$$\mathbb{E}[F(w_k) - F^*] - \frac{\alpha LM}{2c\mu} \le (1 - \alpha c\mu)^{k-1} \left( F(w_1) - F^* - \frac{\alpha LM}{2c\mu} \right)$$

$$\mathbb{E}[F(w_k) - F^*] \le \frac{\alpha LM}{2c\mu} + (1 - \alpha c\mu)^{k-1} \left( F(w_1) - F^* - \frac{\alpha LM}{2c\mu} \right).$$

# **Choice of Stepsize (Learning Rate)**

From the inequality

$$\mathbb{E}[F(w_k) - F^*] \le \frac{\alpha LM}{2c\mu} + (1 - \alpha c\mu)^{k-1} \left( F(w_1) - F^* - \frac{\alpha LM}{2c\mu} \right),$$

we see that selecting a smaller stepsize worsens the contraction constant, but ensures convergence to a smaller neighborhood of the optimal value.

We have two cases of interest:

- 1. If the noise in the gradient decays with  $\|\nabla F(w_k)\|^2$  (M=0), SG converges linearly to the optimal value.
- 2. If the gradient computation is noisy (M>0), we only have linear convergence to a neighborhood of the optimal value. After some point, the noise in the gradient prevents further progress.

# **Intuitive Approach to Decreasing Stepsizes**

Run SG with a fixed stepsize and when progress stalls halve the stepsize. For instance:

- Run SG until iteration  $k_2$  where the expected suboptimality gap is twice the asymptotic value

$$\mathbb{E}[F(w_{K_2}) - F^*] \le 2\frac{\alpha_1 LM}{2c\mu} = 2F_{\alpha_1}.$$

- - Halve the stepsize  $\{\alpha_{r+1}\}=\{\alpha_12^{-r}\}$  and repeat the process.

The sequence of optimality gaps converges to 0 and SG to a minimum.

$$\mathbb{E}[F(w_{k_{r+1}}) - F^*] \le \alpha_1 2^{-r} \le 2F_{\alpha_r} \quad \mathbb{E}[F(w_{k_r}) - F^*] \approx 2F_{\alpha_{r-1}} = 4F_{\alpha_r}$$

The speed of convergence depends on how many iterations it takes to reach each bound.

# First Approach to Decreasing Stepsizes

We can show that each time the stepsize is cut in half, we need twice as many iterations to reach the next bound. As doubling the number of iterations, halves the suboptimality gap, the convergence rate is  $\mathcal{O}(1/k)$ .

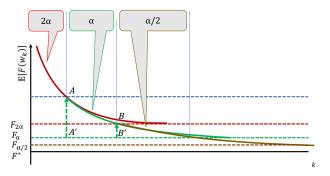


Fig.: Depiction of the strategy of halving the stepsize  $\alpha$  when the expected suboptimality gap is smaller than twice the asymptotic limit  $F_{\alpha}$ .

# Convergence of SG with decaying stepsizes

#### **Theorem**

If F is an L-smooth and c-strongly convex function that satisfies Assumption 2, with  $F_{\inf} = F^*$ , and the SG method is run with a fixed stepsize sequence satisfying

$$\alpha_k = \frac{\beta}{\gamma + k} \quad \text{for some} \quad \beta > \frac{1}{c\mu}, \ \gamma > 0 \quad \text{such that} \quad \alpha_1 \leq \frac{\mu}{LM_G}.$$

Then, for all  $k \in \mathbb{N}$  the expected optimality gap satisfies the inequality

$$\mathbb{E}[F(w_k) - F^*] \le \frac{\eta}{\gamma + k} \qquad \eta = \max \left\{ \frac{\beta^2 LM}{2(\beta c\mu - 1)}, (\gamma + 1)(F(w_1) - F^*) \right\}.$$

# **Proof**

As the step size decays  $\alpha_k LM \leq \alpha_1 LM \leq \mu$ , which in Lemma 2 gives

$$\mathbb{E}_{\xi_k}[F(w_{k+1})] - F(w_k) \le -(\mu - \frac{1}{2}\alpha_k L M_G)\alpha_k \|\nabla F(w_k)\|^2 + \frac{1}{2}\alpha_k^2 L M$$

$$\le -\frac{\mu}{2}\alpha_k \|\nabla F(w_k)\|^2 + \frac{1}{2}\alpha_k^2 L M.$$

As F is strongly convex,  $2c(F(w_k) - F^*) \leq \|\nabla F(w_k)\|^2$  and

$$\mathbb{E}_{\xi_k}[F(w_{k+1})] - F(w_k) \le -\mu \alpha_k c(F(w_k) - F^*) + \frac{1}{2} \alpha_k^2 LM$$

Subtracting  $F^{*}$  from both sides, taking total expectations, and rearranging,

$$\mathbb{E}[F(w_{k+1}) - F^*] \le (1 - \mu \alpha_k c) \mathbb{E}[F(w_k) - F^*] + \frac{1}{2} \alpha_k^2 LM.$$

## **Proof**

We prove

$$\mathbb{E}[F(w_k) - F^*] \le \frac{\eta}{\gamma + k} \qquad \eta = \max \left\{ \frac{\beta^2 LM}{2(\beta c\mu - 1)}, (\gamma + 1)(F(w_1) - F^*) \right\}.$$

by induction. The definition of  $\eta$  ensures that it is true for k=1. We assume that the inequality holds for some  $k\geq 1$  and use it in the inequality from the previous slide

$$\mathbb{E}[F(w_{k+1}) - F^*] \le (1 - \mu \alpha_k c) \mathbb{E}[F(w_k) - F^*] + \frac{1}{2} \alpha_k^2 LM$$

$$\le (1 - \mu \alpha_k c) \frac{\eta}{\gamma + k} + \frac{1}{2} \alpha_k^2 LM.$$
(3.18)

Let  $\hat{k} = \gamma + k$  and write  $\alpha_k = \frac{\beta}{\hat{k}}$ , the previous expression becomes

$$\begin{split} \mathbb{E}[F(w_{k+1}) - F^*] &\leq (1 - \frac{\beta \mu c}{\hat{k}}) \frac{\eta}{\hat{k}} + \frac{1}{2} \frac{\beta^2 L M}{\hat{k}^2} = \frac{\hat{k} - \beta \mu c}{\hat{k}^2} \eta + \frac{1}{2} \frac{\beta^2 L M}{\hat{k}^2} \\ &= \frac{\hat{k} - 1}{\hat{k}^2} \eta - \frac{\beta \mu c - 1}{\hat{k}^2} \eta + \frac{1}{2} \frac{\beta^2 L M}{\hat{k}^2} \\ &\leq \frac{\hat{k} - 1}{\hat{k}^2} \eta + \underbrace{\frac{-2(\beta \mu c - 1) \eta + \beta^2 L M}{2\hat{k}^2}}_{\text{non positive, by definition of } \eta \leq \frac{\hat{k} - 1}{\hat{k}^2 - 1} \eta \leq \frac{\eta}{\hat{k} + 1}, \end{split}$$

# As we promised last week

Let the objective function  $F \colon \mathbb{R}^d \mapsto \mathbb{R}$  be the expected or empirical risk:

$$F(w) = \mathbb{E}[f(w,\xi)]$$
 or  $F(w) = \frac{1}{n} \sum_{i=1}^{n} f_i(w)$ .

1. If we pick samples uniformly from a finite training set with replacement, the SG iterates satisfy

$$\mathbb{E}[|R_n(w_k) - R_n^*|] = \mathcal{O}(\frac{1}{k})$$

2. If we pick samples in each iteration according to distribution P, the SG iterates satisfy

$$\mathbb{E}[|R(w_k) - R^*|] = \mathcal{O}(\frac{1}{k}).$$

# Trade-Offs of mini-batch SG method

Compare simple SG to mini-batch SG with mini-batches of size  $n_{mb} \ll n$ 

$$g(w_k, \xi_k) = \nabla f_{i_k}(w_k) \qquad g(w_k, \xi_k) = \frac{1}{|S_k|} \sum_{i \in S_k} \nabla f_i(w_k)$$

#### Observe that

- minibatch iterations are  $n_{mb}$  times more expensive than SG
- $\mathbb{V}[g(w_k,\xi_k)]$ , M and  $M_V$  (assumption 2) are  $n_{mb}$  times smaller

Does the variance reduction pay for higher iteration cost?

## Trade-Offs of mini-batch SG method

Assume we run minibatch SG with stepsize  $\alpha$  and SG with  $\alpha/n_{mb}$  and compare the number of iterations to reach the same optimality gap

$$\begin{split} \text{mbSG} & \quad \mathbb{E}[F(w_k) - F^*] \leq \frac{\alpha LM}{2c\mu n_{mb}} + (1 - \alpha c\mu)^{k-1} \left(F(w_1) - F^* - \frac{\alpha LM}{2c\mu n_{mb}}\right) \\ \text{SG} & \quad \mathbb{E}[F(w_k) - F^*] \leq \frac{\alpha LM}{2c\mu n_{mb}} + (1 - \frac{\alpha c\mu}{n_{mb}})^{k-1} \left(F(w_1) - F^* - \frac{\alpha LM}{2c\mu n_{mb}}\right) \end{split}$$

SG needs  $n_{mb}$  times more iterations to obtain the optimality gap of minibatch SG, but each SG iteration is  $n_{mb}$  times cheaper.

 $\Rightarrow$  The cost of SG and minibatch are the same if we can run minibatch SG with a stepsize  $n_{mb}$  times larger than the SG stepsize, which might not be possible because of the bound  $\alpha < \frac{\mu}{LMG} \underbrace{\qquad \qquad }_{M_G>\mu^2}$ 

# **SG** for General Objectives

This is not part of the convex class, it is here to relate SG to the algorithms that some of you use in the deep learning lecture.

- Many important machine learning models lead to nonconvex optimization problems.
- Analyzing the SG method when minimizing nonconvex objectives is more challenging because functions may possess multiple local minima and other stationary points.
- Two results: one for employing a fixed positive stepsize and one for diminishing stepsizes.

# Fixed Stepsize SG for General Objectives

## **Theorem**

If F is an L-smooth function that satisfies Assumption 2, with  $F_{inf}$  the lower bound on the sequence of function values  $\{F(w_k)\}$ , and the SG method is run with positive stepsize  $\alpha \leq \frac{\mu}{LM_G}$ , then for all  $K \in \mathbb{N}$ :

$$\mathbb{E}\left[\frac{1}{K}\sum_{k=1}^{K}\|\nabla F(w_k)\|^2\right] \leq \frac{\alpha LM}{\mu} + 2\frac{F(w_1) - F_{inf}}{K\mu\alpha} \xrightarrow{K \to \infty} \frac{\alpha LM}{\mu}.$$

#### Observe

- 1. the asymptotic behavior illustrates that noise in the gradients inhibits further progress, as happens with the convex case.
- 2. The average norm of the gradients can be made arbitrarily small by selecting a small stepsize, but doing so reduces the speed at which the norm of the gradient approaches its limiting distribution.

# **Proof**

Taking the total expectation in Lemma 2 and using the bound  $0<\alpha \leq \frac{\mu}{LMG}$ 

$$\mathbb{E}[F(w_{k+1})] - \mathbb{E}[F(w_k)] \le -(\mu - \frac{1}{2}\alpha L M_G)\alpha \mathbb{E}[\|\nabla F(w_k)\|^2] + \frac{1}{2}\alpha^2 L M$$

$$\le -\frac{1}{2}\mu\alpha \mathbb{E}[\|\nabla F(w_k)\|^2] + \frac{1}{2}\alpha^2 L M,$$

Summing the inequality for  $k \in \{1, \dots, K\}$  and recalling  $F_{\mathsf{inf}} \leq F(w_k)$ ,

$$F_{\mathsf{inf}} - F(w_1) \le \mathbb{E}[F(w_{K+1})] - F(w_1) \le -\frac{1}{2}\mu\alpha \sum_{k=1}^K \mathbb{E}[\|\nabla F(w_k)\|^2] + \frac{1}{2}K\alpha^2 LM.$$

Re-arranging terms we obtain the desired result

$$\sum_{k=1}^{K} \mathbb{E}[\|\nabla F(w_k)\|^2] \le \frac{K\alpha LM}{\mu} + 2\frac{F(w_1) - F_{\text{inf}}}{\mu\alpha}.$$

# **Interesting Cases**

1. if the noise reduces proportionally to  $\|\nabla F(w_k)\|^2$  (M=0)

$$\sum_{k=1}^K \mathbb{E}[\|\nabla F(w_k)\|^2] \leq \underbrace{\frac{K\alpha LM}{\mu}}_{0} + 2\frac{F(w_1) - F_{\mathsf{inf}}}{\mu\alpha}.$$

the sum of squared gradients remains finite and  $\{\|\nabla F(w_k)\|^2\} \to 0$ .

2. in the presence of noise (M > 0) the rhs of

$$\mathbb{E}\left[\frac{1}{K}\sum_{k=1}^{K}\|\nabla F(w_k)\|^2\right] \leq \frac{\alpha LM}{\mu} + 2\frac{F(w_1) - F_{\mathsf{inf}}}{K\mu\alpha} \xrightarrow{K \to \infty} \frac{\alpha LM}{\mu}.$$

gets smaller as K increases and the SG method spends increasingly more time in regions where the objective has a small gradient.

# **Decreasing Stepsize SG for General Objectives**

#### Theorem

If F is an L-smooth function that satisfies Assumption 2 and the SG method is run with a fixed stepsize sequence satisfying

$$\sum_{k=1}^{\infty} \alpha_k = \infty \qquad \qquad \sum_{k=1}^{\infty} \alpha_k^2 < \infty$$

Then, with  $A_K = \sum_{k=1}^K \alpha_k$ 

$$\mathbb{E}\left[\sum_{k=1}^{K} \alpha_k \|\nabla F(w_k)\|^2\right] < \infty \Rightarrow \mathbb{E}\left[\frac{1}{A_K} \sum_{k=1}^{K} \alpha_k \|\nabla F(w_k)\|^2\right] \xrightarrow{K \to \infty} 0.$$

#### Proof.

We proof the implication. The condition  $\sum_{k=1}^{\infty} \alpha_k = \infty$  ensures that

$$A_K \to \infty \text{ as } K \to \infty \text{ and } \mathbb{E}\left[\frac{1}{A_K} \sum_{k=1}^K \alpha_k \|\nabla F(w_k)\|^2\right] \xrightarrow{K \to \infty} 0.$$

## **Proof**

The condition  $\sum_{k=1}^{\infty} \alpha_k^2 < \infty$  ensures that  $\{\alpha_k\} \to 0$ , and we can assume without loss of generality that  $\alpha_k LM_G \le \mu$  for all  $k \in \mathbb{N}$ . Taking the total expectation in Lemma 2 we have

$$\mathbb{E}[F(w_{k+1})] - \mathbb{E}[F(w_k)] \le -(\mu - \frac{1}{2}\alpha_k L M_G)\alpha_k \mathbb{E}[\|\nabla F(w_k)\|^2] + \frac{1}{2}\alpha_k^2 L M$$

$$\le -\frac{1}{2}\mu\alpha_k \mathbb{E}[\|\nabla F(w_k)\|^2] + \frac{1}{2}\alpha^2 L M.$$

Summing the inequality for  $k \in \{1, ..., K\}$  and recalling  $F_{\mathsf{inf}} \leq F(w_k)$ 

$$F_{\inf} - F(w_1) \le \mathbb{E}[F(w_{K+1})] - F(w_1) \le -\frac{1}{2}\mu \sum_{k=1}^K \alpha_k \mathbb{E}[\|\nabla F(w_k)\|^2] + \frac{1}{2}LM \sum_{k=1}^K \alpha_k^2.$$

Dividing by  $\frac{\mu}{2}$  and rearranging the terms, we obtain

$$\sum_{k=1}^{K} \alpha_k \mathbb{E}[\|\nabla F(w_k)\|^2] \le 2 \frac{F(w_1) - F_{\inf}}{\mu} + \frac{LM}{\mu} \sum_{k=1}^{K} \alpha_k^2.$$
 (4.19)

As  $\sum_{k=1}^{\infty} \alpha_k^2 < \infty$ , the right-hand side converges to a finite limit when  $K \to \infty$ , which proves  $\mathbb{E}\left[\sum_{k=1}^K \alpha_k \|\nabla F(w_k)\|^2\right] < \infty$ .

# Consequences of Decreasing Stepsize SG for General Objectives

Under the theorem's assumptions, the weighted average norm of the squared gradients converges to zero even if the gradients are noisy because

$$\mathbb{E}\left[\frac{1}{A_K} \sum_{k=1}^K \alpha_k \|\nabla F(w_k)\|^2\right] \xrightarrow{K \to \infty} 0$$

#### Theorem

If F is an L-smooth function that satisfies Assumption 2 and the SG method is run with a fixed stepsize sequence satisfying

$$\sum_{k=1}^{\infty} \alpha_k = \infty \qquad \qquad \sum_{k=1}^{\infty} \alpha_k^2 < \infty$$

Then, the expected optimality gap satisfies the following inequality

$$\liminf_{k \to \infty} \mathbb{E}[\|\nabla F(w_k)\|^2] = 0.$$

# **Recall: Learning Problem**

Given a set of examples  $(x_1, y_1), \ldots, (x_n, y_n)$ 

- each example  $\xi = (x, y)$  is a pair of an input x and a scalar output y.
- loss  $\ell(\hat{y}, y)$  measures the cost of predicting  $\hat{y}$  when the answer is y
- family  $\mathcal{H}$  of functions  $h(\cdot; w)$  parametrized by a weight vector w.

We seek  $h \in \mathcal{H}$  that minimizes the loss  $f(\xi; w) = \ell(h(x; w), y)$ .

Although we would like to average over the unknown distribution P(x,y)

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

we must settle for computing the average over the samples

$$f(w) = R_n(w) = \frac{1}{n} \sum_{i=1}^n \ell(h(x_i; w), y_i).$$

Statistical learning theory (Vapnik and Chervonenkis, 1971) justifies minimizing  $R_n$  instead of R when  $\mathcal{H}$  is sufficiently restrictive.

#### Recall: Stochastic Gradient Method

As an optimization problem, we consider an objective function F

$$F(w) = \mathbb{E}[f(w,\xi)]$$
 or  $F(w) = \frac{1}{n} \sum_{i=1}^{n} f_i(w)$ .

The stochastic gradient method applies to the expected or empirical risk, depending on how the stochastic gradients are chosen.

#### Stochastic Gradient Method

Choose an initial iterate  $w_1$ 

for  $k=1,2,\ldots$  do

Generate a realization of the random variable  $\xi_k$ 

Compute a stochastic vector  $g(w_k, \xi_k)$  that samples the gradient

Choose a stepsize  $\alpha_k > 0$ 

Set the new iterate as  $w_{k+1} = w_k - \alpha_k g(w_k, \xi_k)$ 

end for

## **Noise-Reduction Methods**

# Recall the fundamental inequality

$$\mathbb{E}_{\xi_k}[F(w_{k+1})] - F(w_k) \le -\alpha_k \nabla F(w_k)^T \mathbb{E}_{\xi_k}[g(w_k, \xi_k)] + \frac{1}{2} \alpha_k^2 L \mathbb{E}_{\xi_k}[\|g(w_k, \xi_k)\|^2]$$

Which is the rate of decrease in noise that allows a SG method to converge at a linear rate?

- if  $-g(w_k, \xi_k)$  is a descent direction in expectation  $\Rightarrow$  first term < 0
- the term  $\alpha_k^2 L \mathbb{E}_{\xi_k}[\|g(w_k,\xi_k)\|^2] > 0$  determines the convergence rate
- with constant  $\mathbb{E}[\|g(w_k,\xi_k)\|^2]$  and constant  $\alpha$ , SG converges to a neighborhood of the solution of size proportional to  $\mathbb{E}[\|g(w_k,\xi_k)\|^2]$
- with constant  $\mathbb{E}[\|g(w_k, \xi_k)\|^2]$  and diminishing  $\alpha \sim \frac{1}{k}$ , SG converges to the solution with rate  $\mathcal{O}(\frac{1}{k})$
- with constant  $\alpha$  and diminishing  $\mathbb{E}[\|g(w_k, \xi_k)\|^2]$ , can we improve the convergence rate?

# Noise Reduction and Convergence Rate

# **Theorem**

Let F be an L-smooth and c-strongly convex function satisfying a **modified** Assumption 2

$$\mathbb{V}_{\xi_k}[g(w_k, \xi_k)] \le M + M_V \|\nabla F(w_k)\|^2 \le M\zeta^{k-1} \quad \text{for } M \ge 0, \ \zeta \in (0, 1)$$

Then the SG method with positive stepsize  $\alpha \leq \min\{\frac{\mu}{L\mu_G^2}, \frac{1}{c\mu}\}$  satisfies

$$\mathbb{E}[F(w_k) - F^*] \le \omega \rho^{k-1} \quad \text{where} \quad \begin{cases} \omega &= \max\{\frac{\alpha LM}{c\mu}, F(w_1) - F^*\} \\ \rho &= \max\{1 - \frac{\alpha c\mu}{2}, \zeta\} < 1 \end{cases}$$

# **Proof**

#### Recall Lemma 2

$$\mathbb{E}_{\xi_{k}}[F(w_{k+1})] - F(w_{k}) \leq -\mu\alpha \|\nabla F(w_{k})\|^{2} + \frac{\alpha^{2}}{2} L \mathbb{E}_{\xi_{k}}[\|g(w_{k}, \xi_{k})\|^{2}] \\
\leq -\mu\alpha \|\nabla F(w_{k})\|^{2} + \frac{\alpha^{2}}{2} L \left(\mathbb{V}_{\xi_{k}}[g(w_{k}, \xi_{k})] + \|\mathbb{E}_{\xi_{k}}[g(w_{k}, \xi_{k})]\|^{2}\right) \\
\leq -\mu\alpha \|\nabla F(w_{k})\|^{2} + \frac{\alpha^{2}}{2} L \left(M\zeta^{k-1} + \mu_{G}^{2}\|\nabla F(w_{k})\|^{2}\right) \\
\leq -(\mu - \frac{1}{2}\alpha L\mu_{G}^{2})\alpha \|\nabla F(w_{k})\|^{2} + \frac{1}{2}\alpha^{2} LM\zeta^{k-1} \\
\leq -\frac{1}{2}\mu\alpha \|\nabla F(w_{k})\|^{2} + \frac{1}{2}\alpha^{2} LM\zeta^{k-1} \\
\leq -\mu\alpha c(F(w) - F^{*}) + \frac{1}{2}\alpha^{2} LM\zeta^{k-1}.$$

#### where in

- line 3, we have used Assumption 2
- line 5,  $\alpha \leq \min\{\frac{\mu}{LM_G^2},\frac{1}{c\mu}\}$
- line 6, F is c-strongly convex  $2c(F(w)-F^*) \leq \|\nabla F(w_k)\|^2 \ \forall w \in \mathbb{R}^d$

## Proof'

From

$$\mathbb{E}_{\xi_k}[F(w_{k+1})] - F(w_k) \le -\mu \alpha c(F(w) - F^*) + \frac{1}{2}\alpha^2 LM\zeta^{k-1},$$

we add and substract  $F^*$  and take total expectations to obtain

$$\mathbb{E}[F(w_{k+1}) - F^*] \le (1 - \alpha c\mu) \mathbb{E}[F(w_k) - F^*] + \frac{1}{2} \alpha^2 LM \zeta^{k-1}$$

We now use induction to prove the bound on the gap

$$\mathbb{E}[F(w_k) - F^*] \le \omega \rho^{k-1} \quad \text{where} \quad \begin{cases} \omega &= \max\{\frac{\alpha LM}{c\mu}, F(w_1) - F^*\} \\ \rho &= \max\{1 - \frac{\alpha c\mu}{2}, \zeta\} < 1 \end{cases}.$$

By definition of  $\omega = \max\{\frac{\alpha LM}{c\mu}, F(w_1) - F^*\}$ , it holds for k = 1.

## Proof"

Assume that it holds for  $k \geq 1$  and use  $\mathbb{E}[F(w_k) - F^*] \leq \omega \rho^{k-1}$  in

$$\begin{split} \mathbb{E}[F(w_{k+1}) - F^* &\leq (1 - \alpha c \mu) \mathbb{E}[F(w_k) - F^*] + \frac{1}{2} \alpha^2 L M \zeta^{k-1} \\ &\leq (1 - \alpha c \mu) \omega \rho^{k-1} + \frac{1}{2} \alpha^2 L M \zeta^{k-1} \\ &\leq \omega \rho^{k-1} \left( 1 - \alpha c \mu + \frac{\alpha^2 L M}{2 \omega} \left( \frac{\zeta}{\rho} \right)^{k-1} \right) \\ &\leq \omega \rho^{k-1} \left( 1 - \alpha c \mu + \frac{\alpha^2 L M}{2 \omega} \right) & \text{because } \rho > \zeta \\ &\leq \omega \rho^{k-1} \left( 1 - \alpha c \mu + \frac{\alpha c \mu}{2} \right) & \text{because } \omega > \frac{\alpha L M}{c \mu} \\ &\leq \omega \rho^{k-1} \left( 1 - \frac{\alpha c \mu}{2} \right) \\ &\leq \omega \rho^k & \text{because } \rho > 1 - \frac{\alpha c \mu}{2}. \end{split}$$

# **Dynamic Sample Size Methods**

Let F be an L-smooth and c-strongly convex function and  $\{w_k\}$  be the iterates generated by the **dynamic sample size method** with increasing minibatches of size  $|S_k| = \lceil \tau^{k-1} \rceil$  for  $\tau > 1$ 

$$g(w_k, \xi_k) = \frac{1}{|S_k|} \sum_{i \in S_k} \nabla f(w_k; \xi_{k,i})$$
$$w_{k+1} = w_k - \alpha g(w_k, \xi_k)$$

with unbiased gradient estimates with a variance bounded by M, then the variance of the dynamic sample size method satisfies

$$\mathbb{V}_{\xi_k}[g(w_k, \xi_k)] \le \frac{\mathbb{V}_{\xi_k}[\nabla f(w_k; \xi_{k,i})]}{n_k} \le \frac{M}{n_k} \le \frac{M}{\lceil \tau^{k-1} \rceil} \le M\zeta^{k-1}.$$

and the expected optimality gap vanishes linearly.

# **Dynamic Sample Size Methods**

**Question**: Is the method really linearly convergent if the per-iteration cost increases without bound with the minibatch size?

#### **Theorem**

Let F be an L-smooth and c-strongly convex function satisfying Assumption 2, with  $F_{\inf} = F^*$ , and run the dynamic sampling SG method with a positive stepsize  $\alpha \leq \min\{\frac{\mu}{L\mu_G^2}, \frac{1}{c\mu}\}$  and  $\tau \in (1, (1-\frac{\alpha c\mu}{2})^{-1})$ . Then, the total number of evaluations of a stochastic gradient of the form  $\nabla f(w_k; \xi_{k,i})$  required to obtain  $\mathbb{E}[F(w_k) - F^*] \leq \epsilon$  is  $\emptyset(\frac{1}{\epsilon})$ .

# **Proof**

With minibatches of size  $\lceil \tau^{k-1} \rceil$ , the variance condition  $\mathbb{V}_{\xi_k}[g(w_k,\psi_k)] \leq M\zeta^{k-1}$  holds with  $\zeta = \frac{1}{\tau}$  and SG with stepsize  $\alpha \leq \min\{\frac{\mu}{L\mu_G^2},\frac{1}{c\mu}\}$  satisfies

$$\mathbb{E}[F(w_k) - F^*] \le \omega \rho^{k-1} \quad \text{where} \quad \begin{cases} \omega &= \max\{\frac{\alpha LM}{c\mu}, F(w_1) - F^*\} \\ \rho &= \max\{1 - \frac{\alpha c\mu}{2}, \zeta\} < 1 \end{cases}$$

Therefore, there is  $k_0 \in \mathbb{N}$  such that

$$\begin{split} \mathbb{E}[F(w_{k_0}) - F^*] &\leq \omega \rho^{k_0 - 1} \leq \epsilon \\ (k_0 - 1)\log \rho &\leq \log(\frac{\epsilon}{\omega}) \quad \text{as } \rho \in (0, 1) \\ k_0 - 1 &\geq \left\lceil \frac{\log(\frac{\epsilon}{\omega})}{\log \rho} \right\rceil = \left\lceil \frac{\log(\frac{\omega}{\epsilon})}{-\log \rho} \right\rceil. \end{split}$$

# Proof'

Assume  $\frac{\log(\frac{\omega}{\epsilon})}{-\log \rho} \in \mathbb{N}$  and the inequality is tight,

$$\begin{split} \tau^{k_0-1} &= \tau^{\frac{\log(\frac{\omega}{\epsilon})}{-\log\rho}} \\ &= \exp(\log(\tau^{\frac{\log(\frac{\omega}{\epsilon})}{-\log\rho}})) \\ &= \exp(\frac{\log(\frac{\omega}{\epsilon})}{-\log\rho}\log(\tau)) \\ &= \exp(\log(\frac{\omega}{\epsilon})\frac{\log(\tau)}{-\log\rho}) \\ &= (\exp(\log(\frac{\omega}{\epsilon}))^{\frac{\log(\tau)}{-\log\rho}} \\ &= \left(\frac{\omega}{\epsilon}\right)^{\theta} \quad \text{where} \quad \theta = \frac{\log(\tau)}{-\log\rho}. \end{split}$$

The number of sample gradient evaluations for the first  $k_0$  iterations is

$$\sum_{k=1}^{k_0} \lceil \tau^{k-1} \rceil \leq 2 \sum_{k=1}^{k_0} \tau^{k-1} = 2 \frac{\tau^{k_0} - \tau}{\tau - 1} = 2 \frac{\tau \left(\frac{\omega}{\epsilon}\right)^{\theta} - \tau}{\tau - 1} \leq 2 \frac{\tau \left(\frac{\omega}{\epsilon}\right)^{\theta}}{\tau - 1} = 2 \left(\frac{\omega}{\epsilon}\right)^{\theta} \frac{\tau}{\tau - 1}.$$

### Proof"

We have that  $\rho=\zeta=\frac{1}{\tau}$  and  $\theta=\frac{\log(\tau)}{-\log\rho}=1$  because

- the variance rate  $\zeta=\frac{1}{ au}$
- the theorem's assumption  $\tau \leq (1-\frac{\alpha c \mu}{2})^{-1} \Rightarrow 1-\frac{\alpha c \mu}{2} \leq \frac{1}{\tau}=\zeta$
- the convergence rate  $\rho = \max\{1 \frac{\alpha c \mu}{2}, \zeta\} = \zeta$

Let  $\sigma\in(0,1]$  parametrize  $\tau=(1-\sigma\frac{\alpha c\mu}{2})^{-1}$ , then the number of sample gradient evaluations for the first  $k_0$  iterations is

$$\sum_{k=1}^{k_0} \lceil \tau^{k-1} \rceil \leq 2 \frac{\omega}{\epsilon} \frac{\tau}{\tau-1} = 2 \frac{\omega}{\epsilon} \frac{1}{1-\frac{1}{\tau}} = 2 \frac{\omega}{\epsilon} \frac{2}{\sigma \alpha c \mu} = \frac{4\omega}{\epsilon \sigma \alpha c \mu} = \mathcal{O}\left(\frac{1}{\epsilon}\right).$$

And the cost of reaching  $\mathbb{E}[F(w_k) - F^*] \leq \epsilon$  is  $\mathcal{O}\left(\frac{1}{\epsilon}\right)$ , the same as SG.

# **Advanced Stochastic Techniques**

Other methods come with few guarantees but work well in practice:

- Gradient Methods with Momentum
- Accelerated Gradient Method
- Adaptive Methods: adagrad, adadelta, adam

They tend to be studied in a case by case matter.

### **Gradient Methods with Momentum**

Each step is chosen as a combination of the steepest descent direction and the most recent iterate displacement:

$$w_{k+1} = w_k - \alpha_k \nabla F(w_k) + \beta_k \underbrace{(w_k - w_{k-1})}_{\text{momentum}}.$$

The momentum term  $\beta_k(w_k-w_{k-1})$  maintains the movement along previous directions. If we use fixed  $\alpha$ 

$$w_{k+1} = w_k - \alpha \nabla F(w_k) + \beta(w_k - w_{k-1})$$

$$w_{k+1} = w_k - \alpha \nabla F(w_k) - \alpha \beta \nabla F(w_{k-1}) + \beta^2(w_{k-1} - w_{k-2})$$

$$w_{k+1} = w_k - \alpha \nabla F(w_k) - \alpha \beta \nabla F(w_{k-1}) - \alpha \beta^2 \nabla F(w_{k-2}) + \beta^3(w_{k-1} - w_{k-2})$$

$$\cdots$$

$$w_{k+1} = w_k - \alpha \sum_{k=1}^{k} \beta^{k-j} \nabla F(w_j).$$

Each step is an exponentially decaying average of past gradients.

#### Intuition behind stochastic Momentum Methods

When we introduce randomness, each step is an exponentially decaying average of stochastic gradients

$$w_{k+1} = w_k - \alpha \sum_{j=1}^k \beta^{k-j} \nabla f(w_j, \xi_j).$$
 (5.20)

- accumulates persistent directions of stochastic gradients
- limits directions where stochastic gradients cancel each other out

Not many theoretical guarantees, but momentum methods work well in practice.

### **Accelerated Gradient Method**

Recall: for F convex and L-smooth, steepest descent converges as  $\mathcal{O}(\frac{1}{k})$ , while the accelerated gradient method of Nesterov

$$\begin{split} \tilde{w}_k \leftarrow w_k + \beta_k (w_k - w_{k-1}) \\ \text{and} \quad w_{k+1} \leftarrow \tilde{w}_k - \alpha_k \nabla F(\tilde{w}_k), \end{split}$$

with  $\alpha_k, \beta_k$  properly chosen converges as  $\mathcal{O}(\frac{1}{k^2})$ .

We can write Nesterov's update as first taking the momentum direction and then the steepest descent one

$$w_{k+1} \leftarrow w_k - \alpha_k \nabla F(w_k + \beta_k (w_k - w_{k-1})) + \beta_k (w_k - w_{k-1}).$$

With stochastic gradients instead of full gradients, the accelerated gradient method only improves the constants in the convergence rate.

#### Second-Order Stochastic Gradient

Second-order methods multiply the gradient by matrix  $H_k > 0$  approximating the inverse of the Hessian:

$$w_{k+1} = w_k - \alpha H_k \nabla f(\xi_{i_k}, w_k).$$

This does not reduce the stochastic noise (variance of  $w_t$ ) and has the convergence rate  $\mathcal{O}(\epsilon^{-1})$  of SG but with improved constant.

2nd-order methods fill  $H_k$  with estimates of the 2nd-order derivatives of F. As derivative estimates are very noisy, large batches are required to improve over SG and 2nd-order methods are not widely used.

A full  $H_k$  is unfeasible for problem with many parameters, and usually a diagonal matrix  $H_k$  is enough. The diagonal structure correspond to adaptive learning rates for each feature.

# **Adaptive Gradient Method (Adagrad)**

Adagrad adapts the learning rate of SG to the frequency of the parameters: larger/smaller updates for infrequent/frequent parameters.

$$w_{t+1}[i] = w_t[i] - \frac{\alpha}{\sqrt{G_t[i] + \epsilon}} \nabla f(h(x_{i_t}; w_t), y_{i_t})$$

where the frequency is measured by  $G_t[i]$ , the sum of the squared gradients w.r.t parameter i up to time t.

- Adagrad is designed for sparse features
- Adagrad eliminates the need to manually tune the learning rate
- As the squared gradients  $G_t[i]$  accumulates during training, the learning rate eventually becomes too small and Adagrad stagnates.

# **Adaptive Moment Estimation (Adam)**

Instead of accumulating all past squared gradients, Adam restricts the window of accumulated past gradients to some fixed size.

$$w_{t+1} = w_t + \frac{\alpha}{\sqrt{v_t + \epsilon}} m_t$$

To avoid storing all the gradients in the window, the sum of gradients is computed as a decaying average of all past squared gradients

$$v_t[i] = \beta_2 v_{t-1}[i] + (1 - \beta_2) \left( \frac{\partial}{\partial w[i]} f(h(x_{i_t}; w_t), y_{i_t}) \right)^2$$

Adam also keeps an exponentially decaying average of past gradients  $(m_t)$  similar to momentum methods.

$$m_t = \beta_1 m_{t-1} + (1 - \beta_1) \nabla f(h(x_{i_t}; w_t), y_{i_t})$$

# **Practical recommendations for SG Implementations**

Recommendations seem trivial, but they are often overlooked.

- Randomly shuffle the training examples. It is faster to iterate sequentially through the shuffled training set than randomly pick a sample each iteration.
- Use preconditioning techniques. Stochastic gradient descent is a first-order algorithm that performs poorly when it reaches an area where the Hessian is ill-conditioned.
- Monitor the training cost periodically compute to ensure it is generally decreasing.
- Monitor the validation error. Spare some training examples to build a validation set and periodically evaluate the validation error during training to stop when it stagnates.

### **Practical recommendations for SG Implementations**

- As SG learning rate is independent of the sample size, use a small
  portion of the training set to determine the correct learning rates.
   The validation error reaches a plateau after a similar number of
  epochs to reach this point on the small training set.
- Check the gradients using finite differences to discover errors in the gradient computation. For **many**  $(x_i, y_i)$ ,  $\delta$ , and w, do:
  - Pick an example  $(x_i, y_i)$ .
  - Compute the loss for the current w.
  - Compute the gradient  $g = \nabla \ell(h(x_i; w), y_i)$ .
  - Apply a slight perturbation  $\tilde{w} = w + \delta$ .
  - Compute the new loss and verify that  $\ell(h(x_i; \tilde{w}), y_i) \approx \ell(h(x_i; w), y_i) + \langle \delta, g \rangle$ .

# **Summary: Learning Problem**

Given a set of examples  $(x_1, y_1), \ldots, (x_n, y_n)$ 

- each example  $\xi = (x, y)$  is a pair of an input x and a scalar output y.
- loss  $\ell(\hat{y},y)$  measures the cost of predicting  $\hat{y}$  when the answer is y
- family  $\mathcal{H}$  of functions  $h(\cdot; w)$  parametrized by a weight vector w.

We seek  $h \in \mathcal{H}$  that minimizes the loss  $f(\xi; w) = \ell(h(x; w), y)$ .

Although we would like to average over the unknown distribution  $P(\boldsymbol{x},\boldsymbol{y})$ 

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

we must settle for computing the average over the samples

$$f(w) = R_n(w) = \frac{1}{n} \sum_{i=1}^n \ell(h(x_i; w), y_i).$$

Statistical learning theory (Vapnik and Chervonenkis, 1971) justifies minimizing  $R_n$  instead of R when  $\mathcal{H}$  is sufficiently restrictive.

### **Stochastic Gradient Method**

The objective function  $F \colon \mathbb{R}^d \mapsto \mathbb{R}$  can be the expected or empirical risk:

$$F(w) = \mathbb{E}[f(w,\xi)]$$
 or  $F(w) = \frac{1}{n} \sum_{i=1}^{n} f_i(w)$ .

The analysis applies to both objectives, depending on how the stochastic gradient estimates are chosen.

#### Stochastic Gradient Method

```
Choose an initial iterate w_1
```

for 
$$k=1,2,...$$
 do

Generate a realization of the random variable  $\xi_k$ 

Compute a stochastic vector  $g(w_k, \xi_k)$ 

Choose a stepsize  $\alpha_k > 0$ 

Set the new iterate as  $w_{k+1} = w_k - \alpha_k g(w_k, \xi_k)$ 

#### end for

### **Fundamental Lemmas**

#### Lemma

If F is an L-smooth function, the iterates of SG satisfy:

$$\mathbb{E}_{\xi_k}[F(w_{k+1})] - F(w_k) \leq -\alpha_k \underbrace{\nabla F(w_k)^T \mathbb{E}_{\xi_k}[g(w_k, \xi_k)]}_{\text{expected directional derivative of } F \text{ along direction } g(w_k, \xi_k)} + \frac{\alpha_k^2 L}{2} \underbrace{\mathbb{E}_{\xi_k}[\|g(w_k, \xi_k)\|^2]}_{\text{second moment } g(w_k, \xi_k)}$$

#### Lemma

If F is L-smooth and there are  $M \leq 0$  and  $M_G \geq \mu^2 \geq 0$  such that

$$\mathbb{E}_{\xi_k}[\|g(w_k, \xi_k)\|^2] \le M + M_G \|\nabla F(w_k)\|^2,$$

then the SG iterates satisfy

$$\mathbb{E}_{\xi_k}[F(w_{k+1})] - F(w_k) \le -\underbrace{(\mu - \frac{1}{2}\alpha_k LM_G)\alpha_k \|\nabla F(w_k)\|^2 + \frac{1}{2}\alpha_k^2 LM}_{\text{deterministic}}.$$

# Convergence of SG

#### **Theorem**

If F is L-smooth and c-strongly convex and satisfies Assumption 2, then the SG method run with a positive stepsize  $\alpha \leq \frac{\mu}{LMG}$  satisfies

$$\mathbb{E}[F(w_k) - F^*] \le \frac{\alpha LM}{2c\mu} + (1 - \alpha c\mu)^{k-1} \left( F(w_1) - F^* - \frac{\alpha LM}{2c\mu} \right),$$

#### **Theorem**

If F is L-smooth and c-strongly convex and satisfies Assumption 2, then SG method with stepsizes  $\alpha_k = \frac{\beta}{\gamma + k}$  for some  $\beta > \frac{1}{c\mu}$ ,  $\gamma > 0$  such that  $\alpha_1 \leq \frac{\mu}{LM_G}$  satisfies

$$\mathbb{E}[F(w_k) - F^*] \le \frac{\eta}{\gamma + k} \qquad \eta = \max \left\{ \frac{\beta^2 LM}{2(\beta c\mu - 1)}, (\gamma + 1)(F(w_1) - F^*) \right\}.$$

### **Noise-Reduction Methods**

Noise-Reduction Methods: instead of decreasing the learning rate to converge to the optimum, reduce variance of the stochastic gradients. They achieve a linear convergence rate at a higher per-iteration cost.

Other methods come with few guarantees but work well in practice:

- Gradient Methods with Momentum
- Accelerated Gradient Method
- Adaptive Methods: adagrad, adadelta, adam