

Advance Stochastic Gradient with Variance Reduction

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Introductions

Optimization problems

$$\min f(w), \quad f(w) := \frac{1}{n} \sum_{i=1}^n f_i(w)$$

Stochastic gradient descent

At each iteration $t = 1, 2, \dots$, draw i_t randomly from $\{1, \dots, n\}$

$$w^t = w^t - \eta_t \nabla f_{i_t}(w^t)$$

Unified formulation

ζ is a random variable.

$$w^{t+1} = w^t - \eta_t g(w^t, \zeta_t)$$

Stochastic gradient

$$\nabla f_{i_t}(w^t) \rightarrow \frac{1}{n} \sum_{i=1}^n f_i(w^t)$$

Unbiased

$$\mathbb{E} \{ \nabla f_{i_t}(w^t) \} = \frac{1}{n} \sum_{i=1}^n f_i(w^t)$$

Variance Reduce(VR)

control variates	antithetic variates
important sampling	stratified sampling

Control Variates

Introduction

Unknown parameter μ , assume we have a static $X : \mathbb{E}X = \mu$, another r.v. Y , such that $\mathbb{E}Y = \tau$ is a known value, define a new r.v.

$$\bar{X} = X + c(Y - \tau)$$

Properties

- Unbias: $\mathbb{E}\bar{X} = \mathbb{E}X = \mu$
- Variance: $Var(\bar{X}) = Var(X) + c^2 Var(Y) + 2cCov(X, Y)$
Optimal coefficient: $c^* = -\frac{Cov(X, Y)}{Var(Y)}$
- Simply:
 - $\bar{X} = X - Y + \tau$, if $cov(X, Y) > 0$
 - $\bar{X} = X + Y - \tau$, if $cov(X, Y) < 0$

Control variates for stochastic gradient

VR gradient

- Former: $v_k = \nabla f_{i_k}(w_{k-1})$
- Case 1: $v_k = \nabla f_{i_k}(w_{k-1}) - \nabla h_{i_k}(w_{k-1}) + \mathbb{E} \nabla h_{i_k}(w_{k-1})$
- Case 2: $v_k = \nabla f_{i_k}(w_{k-1}) - \nabla f_{i_k}(\tilde{w}) + \tilde{v}$

Methods

- SAGA: $\nabla f_{i_k}(\tilde{w})$ is stored in the table.
- SVRG: $\nabla f_{i_k}(\tilde{w})$ is calculated after a specific number of iterations.
- $\lim_{k \rightarrow \infty} \mathbb{E} \|v_k\|^2 = 0$
- SAGA. SVRG will convergence under fixed stepsize.

Antithetic Sampling

Two r.v. X_i, X_j id, $\mathbb{E}X_i = \mu, \mathbb{E}X_j = \mu$.

As $\mathbb{E} \left\{ \frac{1}{2}(X_i + X_j) \right\} = \mu$ use $\frac{1}{2}(X_i + X_j)$ to estimate μ

Formulations

- if X and Y are independent,

$$\begin{aligned} \text{Var}\left(\frac{1}{2}(X_i + X_j)\right) &= \frac{1}{4} \text{Var}(X_i + X_j) = \frac{1}{4} \{ \text{Var}(X_i) + \text{Var}(X_j) \} \\ &= \frac{1}{4} \times 2 \text{Var}(X_i) = \frac{1}{2} \text{Var}(X_i) \end{aligned}$$

- if X and Y are negative correlation,

$$\text{Var}\left(\frac{1}{2}(X_i + X_j)\right) = \frac{1}{4} \{ \text{Var}(X_i) + \text{Var}(X_j) + 2 \text{Cov}(X_i, X_j) \} \leq \frac{1}{2} \text{Var}(X_i)$$

- if $X_j = 2\mu - X_i$, then $\text{Var}\left(\frac{1}{2}(X_i + X_j)\right) = \text{Var}(\mu) = 0$

antithetic variates for stochastic gradient

logistic regression

$$\nabla f_i(w) = \frac{e^{-y_i \cdot x_i' w}}{1 + e^{-y_i \cdot x_i' w}} y_i x_i'$$

Formulations

$$\mathbb{E} \|\nabla f_i(w) + \nabla f_j(w)\|^2 = \mathbb{E} \|\nabla f_i(w)\|^2 + \mathbb{E} \|\nabla f_j(w)\|^2 + 2\mathbb{E} \langle \nabla f_i(w), \nabla f_j(w) \rangle$$

$$\begin{aligned} \mathbb{E} \langle \nabla f_i(w), \nabla f_j(w) \rangle &= \mathbb{E} \left\langle \frac{e^{-y_i \cdot x_i' w}}{1 + e^{-y_i \cdot x_i' w}} y_i x_i', \frac{e^{-y_j \cdot x_j' w}}{1 + e^{-y_j \cdot x_j' w}} y_j x_j' \right\rangle \\ &\geq -\mathbb{E} \left\| \frac{e^{-y_i \cdot x_i' w}}{1 + e^{-y_i \cdot x_i' w}} y_i x_i' \right\| \left\| \frac{e^{-y_j \cdot x_j' w}}{1 + e^{-y_j \cdot x_j' w}} y_j x_j' \right\| \end{aligned}$$

if and only if $y_i x_i' \parallel y_j x_j'$, equal hold.

Derivation

$f(w) = \frac{1}{n} \sum_{i=1}^n f_i(w) + \frac{\lambda}{2} \|w\|^2$ equals to

$$\begin{aligned} P(y, z) &= \frac{1}{n} \sum_{i=1}^n f_i(z_i) + \frac{\lambda}{2} \|y\|^2 \\ \text{s.t.} \quad &y = z_i, i = 1, 2, \dots, n \end{aligned}$$

$$L(y, z, \alpha) = P(y, z) + \frac{1}{n} \sum_{i=1}^n \alpha_i (y - z_i)$$

$$\begin{aligned} D(\alpha) &= \inf_{y, z} L(y, z, \alpha) \\ &= \frac{1}{n} \sum_{i=1}^n \inf_{z_i} \{f_i(z_i) - \alpha_i z_i\} + \inf_y \left\{ \frac{\lambda}{2} \|y\|^2 + \frac{1}{n} \sum_{i=1}^n \alpha_i y \right\} \\ &= \frac{1}{n} \sum_{i=1}^n -f_i^*(-\alpha_i) - \frac{\lambda}{2} \left\| \frac{1}{\lambda n} \sum_{i=1}^n \alpha_i \right\|^2 \end{aligned}$$

Formulation and relationships

$$\min f(w) = \frac{1}{n} \sum_{i=1}^n f_i(w) + 0.5\lambda w'w$$

$$\alpha_i^* = -\frac{1}{\lambda n} \nabla f_i(w^*) \quad w^t = \sum_{i=1}^n \alpha_i^t$$

Update

$$\alpha_l^t = \begin{cases} \alpha_l^{t-1} - \eta_t(\nabla f_l(w^{t-1}) + \lambda n \alpha_l^{t-1}) & l = i \\ \alpha_l^{t-1} & l \neq i \end{cases}$$

$$\begin{aligned} w^t &= w^{t-1} + (\alpha_i^t - \alpha_i^{t-1}) \\ &= w^{t-1} - \eta_t(\nabla f_i(w^{t-1}) + \lambda n \alpha_i^{t-1}) \end{aligned}$$

$\lambda n \alpha_i^{t-1}$ is antithetic to $\nabla f_i(w^{t-1})$, $\nabla f_i(w^{t-1}) + \lambda n \alpha_i^{t-1} \rightarrow 0$ as $t \rightarrow \infty$

Stratified Sampling

Stratified sampling

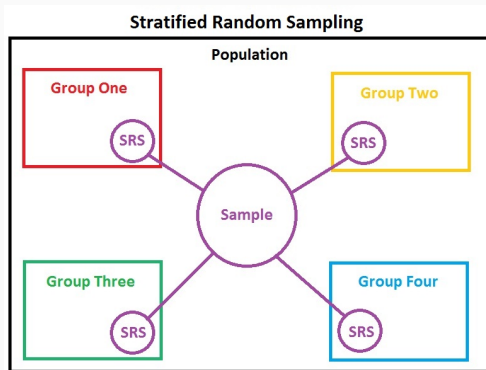


Figure 1: Stratified sampling

Group 1	Group 2	Group 3	Group 4
$\nabla f_{11}, \dots, \nabla f_{1n_1}$	$\nabla f_{21}, \dots, \nabla f_{2n_2}$	\dots	$\nabla f_{L1}, \dots, \nabla f_{Ln_L}$

Stratified sampling

Principles

- homogenous within-groups.
- heterogenous between the groups.

Stratified sample size

- Proportional: $\frac{b_h}{b} = \frac{n_h}{n} = W_h$
- Neyman: $b_h = b \frac{W_h S_h}{\sum_{h=1}^L W_h S_h} = b \frac{N_h S_h}{\sum_{h=1}^L N_h S_h}$

Apply to stochastic gradient

- for the same labels y , cluster x , to stratify.
- $(x_i, y_i) \rightarrow \nabla f_i(w; x_i, y_i)$

Important Sampling

Important Sampling

- Uniform sampling: $\nabla f(w^t) = \sum_{i=1}^n \left[\frac{1}{n} \right] \nabla f_i(w^t)$
- Important sampling: $\nabla f(w^t) = \sum_{i=1}^n \frac{\nabla f_i(w)}{np_i^t} \left[p_i^t \right],$
 $\sum_{i=1}^n p_i^t = 1 \quad t = 1, 2, \dots$

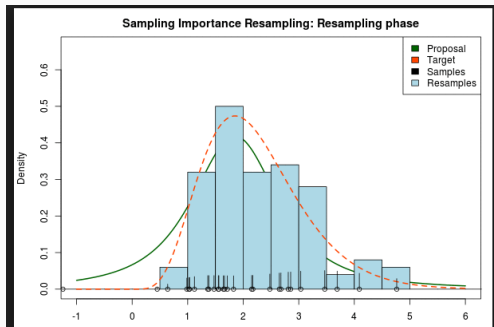


Figure 2: Important sampling

Important Sampling for Stochastic Gradient

$$\min_{p^t} E \left\| \frac{\nabla f_i(w^t)}{np_i^t} \right\|^2 = \min_{p^t} \frac{1}{n^2} \sum_{i=1}^n \frac{\|\nabla f_i(w^t)\|^2}{p_i^t} \geq \frac{1}{n^2} \left(\sum_{i=1}^n \|\nabla f_i(w^t)\| \right)^2$$

$$p_i^t = \frac{\|\nabla f_i(w^t)\|}{\sum_{j=1}^n \|\nabla f_j(w^t)\|}$$

if $f_i(w)$ is L_i -Lipschitz, then $\|\nabla f_i(w)\| \leq L_i$,

$$p_i^t = \frac{L_i}{\sum_{j=1}^n L_j}$$

Experiments

Stratified Sampling

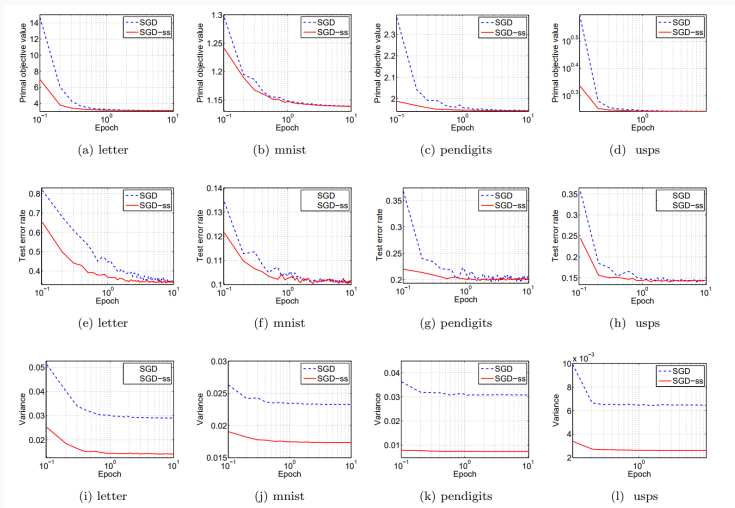


Figure 3: multi-class logistic regression (convex) on letter, mnist, pendigits, and usps.

Important sampling

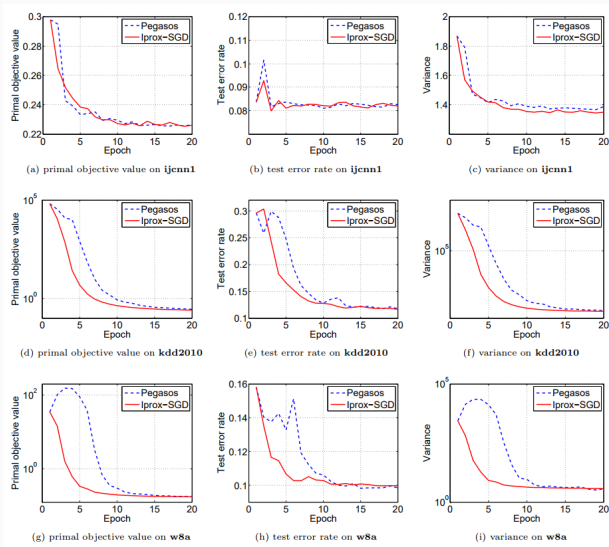


Figure 4: SVM on several datasets

Conclusions

- VR base on optimize variables, such as SDCA. SVRG, can make the variance convergence to 0.
- VR base on samples, can significantly reduce the variance.
- Constructing related variates is crucial.
- Different VR methods can be combined, but how to need our efforts.

Q & A
