Adaptively Preconditioned Stochastic Gradient Langevin Dynamics

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Abstract
Stochastic Gradient Langevin Dynamics infuses isotropic gradient noise to SGD to help navigate pathological curvature in the loss landscape for deep networks. Isotropic nature of the noise leads to poor scaling, and adaptive methods based on higher order curvature information such as Fisher Scoring have been proposed to precondition the noise in order to achieve better convergence. In this paper, we describe an adaptive method to estimate the parameters of the noise and conduct experiments on well-known model architectures to show that the adaptively preconditioned SGLD method achieves convergence with the speed of adaptive first order methods such as Adam, AdaGrad etc. and achieves generalization equivalent of SGD in the test set.

1. Introduction
Generalizability is the ability of a model to perform well on unseen examples (Jiang et al., 2019). Neural networks are known to overfit the data, and mechanisms such as regularization are employed to constrain a model’s ability to learn in order to reduce the generalization gap.

Various schemes such as dropout (Srivastava et al., 2014), weight decay (Krogh & Hertz, 1992) and early stopping (Prechelt, 1998; Caruana et al., 2001; Yao et al., 2007) have been proposed to regularize neural network models. Regularization in neural networks can be roughly categorized into implicit methods (Neyshabur et al., 2014) and explicit methods (Neyshabur et al., 2018). The ability of Stochastic Gradient Descent (SGD) to generalize better than other adaptive optimization methods is often attributed to its role as an implicit regularization mechanism.

Various adaptive optimization methods such as RMSProp (Tieleman & Hinton, 2012), Adam (Kingma & Ba, 2014), AdaGrad (Duchi et al., 2011) and AMSGrad (Reddi et al., 2019) have been proposed to speed up the training of deep networks. First order adaptive methods typically have a faster training speed, but Stochastic Gradient Descent is often found to achieve better generalization on the test set (Wilson et al., 2017; Luo et al., 2019).

Stochastic Gradient Langevin Dynamics (SGLD) (Welling & Teh, 2011) adds an isotropic noise to SGD to help it navigate out of saddle points and suboptimal local minima. SGLD has a powerful Bayesian interpretation, and is often used in Monte Carlo Markov Chains to sample the posterior for inference (Mandt et al., 2017).

The slow convergence of SGD while training is due to the uniform scaling in the parameter space. Adaptive methods conventionally speed up training by applying an element wise scaling scheme. Various approaches to pre-condition the noise in SGLD on the basis of higher order information such as Fisher Scoring (Ahn et al., 2012) have been shown to achieve better generalizability than SGD, but such higher order methods have a high computational complexity and hence not scalable to very deep networks.

In this paper, we propose a method to adaptively estimate the parameters of noise in SGLD using first order information in order to achieve high training speed and better generalizability.

2. Related Work
Adding noise to the input, the model structure or the gradient updates itself is a well-studied topic (An, 1996). The success of mini-batch gradient descent over batch gradient descent is attributed to the variance brought due to constraint in the sampling procedure.

Methods such as weight noise (Steijvers & Grünwald, 1996) and adaptive weight noise (Graves, 2011; Blundell et al., 2015) infuses noise by perturbing the weights with a Gaussian Noise. Dropout randomly drops neurons with a probability, and it mimics training an ensemble of neural networks.

Hamiltonian Monte Carlo (Duane et al., 1987; Neal et al., 2011) works by sampling a posterior using noise to explore the state space. A mini-batch variant of Hamiltonian Monte Carlo
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We propose a method to scale the noise proportionally to the noise in SGLD help it better explore the loss landscape and also helps it navigate out of malformed curved such as saddle points and sub-optimal local minima.

Various adaptive optimization algorithms have been proposed to improve the speed of training of neural networks such as Adam, AdaGrad and AMSGrad. The adaptive methods apply an element wise scaling on the gradients to allow for faster convergence. The adaptive algorithms perform incredibly well for convex settings, but are not able to generalize as well as SGD for non-convex problems.

Similar to SGD, the slow convergence in SGLD is attributed to uniform scaling in the parameter space. The speed of convergence and generalizability of the method can be improved using an adaptive preconditioner on the noise.

Scaling of noise in SGLD can be performed by using a pre-conditioner (Li et al., 2016). Second order pre-conditioners encoding inverse Hessians (Martin et al., 2012) and Fisher Information (Marceau-Caron & Ollivier, 2017; Nado et. al, 2018) have been used to establish better generalizability but suffer from high computational complexity. First order methods based on RMSProp (Li et al., 2016) use the second order moments of the gradients to inversely scale the noise, thereby increasing noise in sensitive dimensions and dampening noise in dimensions with large gradients.

We propose a method to scale the noise proportional to the second order moment of the gradients in order to achieve a higher training speed by increasing the noise for dimensions with larger gradients. In this paper we describe a method to create a pre-conditioner for SGLD which possess the training speed of adaptive methods and the generalizability of SGD with minimal computational overhead.

3. Adaptively Preconditioned SGLD

Consider a supervised learning problem, where we have identically distributed data and label pairs $(x_1, y_1), \ldots, (x_n, y_n) \in \mathbb{R}^{d+1}$. Our goal is to optimize the distribution $p(y|x)$ by minimizing an approximate loss function $L(y, x; \Theta)$ with respect to $\Theta$, where the distribution $p(y|x)$ is parametrized by $\Theta$.

Finding the optimal parameters for a Neural Network is a known NP-hard problem (Neyshabur et al., 2014; Allen-Zhu, 2018). The parameters of a probability distribution occupy a Riemannian Manifold (Amari, 1998), and greedy optimization methods such as Stochastic Gradient Descent exploit curvature information in the manifold to find the most optimal parameters of the distribution in a convex case. Stochastic Gradient Descent optimizes the loss function using gradients of the loss function with respect to the parameter at each step

$$\hat{g}_s(\Theta_t) \leftarrow \nabla_{\Theta} \hat{L}_s(\Theta_t)$$

where $\hat{L}_s(\Theta)$ is the stochastic estimate of the loss function computed over a mini-batch of size $s$ sampled uniformly from the data. The parameter updates can be written as

$$\Theta_{t+1} \leftarrow \Theta_t - \eta(\hat{g}_s(\Theta_t))$$

SGD with decreasing step sizes provably converges to the optimum of a convex function, and to the local optimum in case of a non-convex function (Robbins & Monro, 1951).

The loss landscape of very deep neural networks is often ill-behaved and non-convex in nature. To navigate out of sub-optimal local minima, strategies such as momentum (Polyak, 1964; Sutskever et al., 2013) are employed

$$\mu_t \leftarrow \rho \mu_{t-1} + (1-\rho)\hat{g}_s(\Theta_t)$$

$$\Theta_{t+1} \leftarrow \Theta_t - \eta(\mu_t)$$

Stochastic Gradient Langevin Dynamics (SGLD) further extends SGD by adding additional Gaussian noise to help it escape sub-optimal minima. We can approximate SGLD using

$$\xi_t \sim N(0, \epsilon)$$

$$\Theta_{t+1} \leftarrow \Theta_t - \eta(\hat{g}_s(\Theta_t) + \xi_t)$$

SGLD can also be provably shown to converge to the optimal minima in a convex case when limit $\epsilon, \eta \rightarrow 0$ holds. (Mandt et al., 2017). Stochastic Gradient Hamiltonian Monte Carlo Stochastic Gradient (Chen et al., 2014) adds momentum to SGLD

$$\Theta_{t+1} \leftarrow \Theta_t - \eta(\mu_t + \xi_t)$$

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**Algorithm 1** Adaptively Preconditioned SGLD

| Input : $\Theta_0$, step size $\eta$, momentum $\rho$, noise $\psi$ |
| Set $\mu_0 = 0$ and $\sigma_0 = 0$ |
| for $t = 1$ to $T$ do |
| $\hat{g}_s(\Theta_t) \leftarrow \nabla_{\Theta} \hat{L}_s(\Theta_t)$ |
| $\mu_t \leftarrow \rho \mu_{t-1} + (1-\rho)\hat{g}_s(\Theta_t)$ |
| $C_t \leftarrow \rho C_{t-1} + (1-\rho)(\hat{g}_s(\Theta_t) - \mu_t)(\hat{g}_s(\Theta_t) - \mu_{t-1})$ |
| $\xi_t \sim N(\mu_t, C_t)$ |
| $\Theta_{t+1} \leftarrow \Theta_t - \eta(\hat{g}_s(\Theta_t) + \psi \xi_t)$ |
| end for |
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The equi-scaled nature of noise leads to poor scaling of parameter updates, leading to a slower training speed and risk of converging to a sub-optimal minima (Luo et al., 2019). Noise can be adaptively pre-conditioned to help traverse pathological curvature

\[ \xi_t \sim N(0, C) \]  \hspace{1cm} (8)

Preconditioners based on higher order information use the inverse of Hessian or Fisher Information matrix to help traverse the curvature better. Unfortunately, such higher order approaches are computationally infeasible for large and deep networks. Adaptive pre-conditioners based on popular adaptive methods such as RMSProp use a diagonal approximation of the inverse of second order moments of the gradient updates.

Adaptive pre-conditioning methods yield similar or better generalization performance versus SGD, but still possess a rather slower speed of convergence with respect to adaptive first order methods (Palacci & Hess, 2018).

We propose an adaptive preconditioner based on a diagonal approximation of second order moment of gradient updates, which posses the generalizability of SGD and the training speed of adaptive first order methods. Adaptively Preconditioned SGLD (ASGLD) method scales the noise in a directly proportional manner to allow for faster training speed

\[ C_t \leftarrow \rho C_{t-1} + (1 - \rho)(\hat{g}_s(\Theta_t) - \mu_t)(\hat{g}_s(\Theta_t) - \mu_{t-1}) \]  \hspace{1cm} (9)
\[ \xi_t \sim N(\mu_t, C_t) \]  

(10)

\[ \Theta_{t+1} \leftarrow \Theta_t - \eta (\hat{g}_s(\Theta_t) + \psi \xi_t) \]  

(11)

where \( \psi \) is the noise parameter.

The noise covariance preconditioner scales the noise proportionally in dimensions with larger gradients, essentially helping it escape suboptimal minima and saddle points better and thus helping it converge faster and to a better solution. As the algorithm approaches a wide minima, the dampened second order moment starts shrinking, allowing for convergence to the optimum.

### 4. Experiments

In this section, we examine the impact of using ASGLD method on Resnet 34 (He et al., 2016) and Densenet 121 (Huang et al., 2017) architectures on CIFAR 10 dataset (Krizhevsky et al., 2014). CIFAR 10 dataset contains 60,000 images for ten classes sampled from tiny images dataset.

Training was performed for a fixed schedule of 200 runs over the training set, and we plot the training and test accuracy in fig 1. and fig 2. We reduce the learning rate by a factor of 10 at the 150th epoch.

We performed hyperparameter tuning in accordance with methods defined in (Wilson et al., 2017) and (Luo et al., 2019). For learning rate tuning, we implement a logarithmically spaced grid with five step sizes, and we try new grid points if the best performing parameter setting is found at one end of the grid. We match the settings for other hyperparameters such as batch size, weight decay and dropout probability with the respective base architectures.

In Resenet 34 architecture, we observe in fig 1.a) that ASGLD performs better in terms of training speed than SGD and achieves similar accuracy on the held out set. We also observe in fig 1.b) that ASGLD has similar training speed as first order adaptive methods early in training, but ASGLD begins to significantly outperform adaptive methods in generalization error by the time the learning rate is decayed. We also observe that ASGLD is more stable as compared to SGD at the end of the training.

We see similar trends for Densenet 121 architecture, as evident in fig 2. We also observe that ASGLD has a lower generalization error than SGD at the end of the training.

### 5. Discussion

To investigate the ability of our method, we conducted experiments on CIFAR 10 using well known neural network architectures such as Resnet 34 and Densenet 121. Based on the results obtained in the experiment section, we can observe that ASGLD performs as well as adaptive methods and much better than SGD early in training, but by the time the learning rate is decayed we observe that the ASGLD method performs as well as SGD and significantly outperforms first order adaptive methods.

Furthermore, we also observed similar wall clock times for training with the ASGLD method versus adaptive methods.

### 6. Future Work

Future work would include exploring the impact of ASGLD on other regularization mechanisms such as Batch Normalization etc.

We would also like to investigate the effectiveness of ASGLD on other domains such as Natural Language Processing, Speech etc.

### 7. Conclusion

We propose a new method ASGLD based on adaptively preconditioning noise covariance matrix in SGLD using estimated second order moments of gradient updates for optimizing a non-convex function, and demonstrate its effectiveness over well-known datasets using popular neural network architectures.

We observe that ASGLD method significantly outperforms adaptive methods in generalizability and SGD in terms of speed of convergence and stability. We also observe the increased effectiveness of ASGLD in deeper networks.

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