The **Anisotropic Noise** in Stochastic Gradient Descent: Its Behavior of Escaping from Sharp Minima and Regularization Effects

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The implicit bias of stochastic gradient descent

- Compared with gradient descent (GD), stochastic gradient descent (SGD) tends to generalize better.
- This is attributed to the noise in SGD.
- In this work **we study the anisotropic structure of SGD noise and its importance for escaping and regularization**.

Stochastic gradient descent and its variants

Loss function $L(\theta) := \frac{1}{N}\sum_{i=1}^{N} \ell(x_i;\theta)$.

Gradient Langevin dynamic (GLD)

$$\theta_{t+1} = \theta_t - \eta\nabla_\theta L(\theta_t) + \eta\epsilon_t,\ \ \epsilon_t \sim \mathcal{N}\left(0, \sigma_t^2 I\right).$$

Stochastic gradient descent (SGD)

$$\theta_{t+1} = \theta_t - \eta\tilde{g}(\theta_t),\ \ \tilde{g}(\theta_t) = \frac{1}{m}\sum_{x\in B_t} \nabla_\theta \ell(x;\theta_t).$$

The structure of SGD noise

$$\tilde{g}(\theta_t) \sim \mathcal{N}\left(\nabla L(\theta_t), \Sigma^{\mathrm{sgd}}(\theta_t)\right),\ \ \Sigma^{\mathrm{sgd}}(\theta_t) \approx \frac{1}{m}\left[\frac{1}{N}\sum_{i=1}^{N} \nabla\ell(x_i;\theta_t)\nabla\ell(x_i;\theta_t)^T - \nabla L(\theta_t)\nabla L(\theta_t)^T\right].$$

SGD reformulation

$$\theta_{t+1} = \theta_t - \eta\nabla L(\theta_t) + \eta\epsilon_t,\ \ \epsilon_t \sim \mathcal{N}\left(0, \Sigma^{\mathrm{sgd}}(\theta_t)\right).$$

GD with unbiased noise

$$\theta_{t+1} = \theta_t - \eta \nabla_\theta L(\theta_t) + \epsilon_t, \quad \epsilon_t \sim \mathcal{N}(0, \Sigma_t). \tag{1}$$

Iteration (1) could be viewed as a discretization of the following continuous stochastic differential equation (SDE):

$$\mathrm{d}\theta_t = -\nabla_\theta L(\theta_t)\,\mathrm{d}t + \sqrt{\Sigma_t}\,\mathrm{d}W_t. \tag{2}$$

Next we study the role of noise structure Σ_t by analyzing the continous SDE (2).

Escaping efficiency

Definition (Escaping efficiency)

Suppose the SDE (2) is initialized at minimum θ_0, then for a fixed time t small enough, the *escaping efficiency* is defined as the increase of loss potential:

$$\mathbb{E}_{\theta_t}[L(\theta_t) - L(\theta_0)] \tag{3}$$

Under suitable approximations, we could compute the escaping efficiency for SDE (2),

$$\begin{aligned} \mathbb{E}[L(\theta_t) - L(\theta_0)] &= -\int_0^t \mathbb{E}\left[\nabla L^T \nabla L\right] + \int_0^t \frac{1}{2}\mathbb{E}\mathrm{Tr}(H_t \Sigma_t)\,\mathrm{d}t \quad (4) \\ &\approx \frac{1}{4}\mathrm{Tr}\left(\left(I - e^{-2Ht}\right)\Sigma\right) \approx \frac{t}{2}\mathrm{Tr}\left(H\Sigma\right). \quad (5) \end{aligned}$$

Thus $\mathrm{Tr}\left(\mathbf{H\Sigma}\right)$ serves as an important indicator for measuring the escaping behavior of noises with different structures.

Factors affecting the escaping behavior

The noise scale For Gaussian noise $\epsilon_t \sim \mathcal{N}(0, \Sigma_t)$, we can measure its scale by $\|\epsilon_t\|_{\text{trace}} := \mathbb{E}[\epsilon_t^T \epsilon_t] = \cdots = \text{Tr}(\Sigma_t)$. Thus based on $\text{Tr}(H\Sigma)$, we see that the larger noise scale is, the faster the escaping happens.
To eliminate the impact of noise scale, assume that

$$\textbf{given time t}, \text{Tr}(\boldsymbol{\Sigma_t}) \textbf{ is constant}. \tag{6}$$

The ill-conditioning of minima For the minima with Hessian as scalar matrix $H_t = \lambda I$, the noises in same magnitude make no difference since $\text{Tr}(H_t\Sigma_t) = \lambda \text{Tr}\Sigma_t$.

The structure of noise For the ill-conditioned minima, the structure of noise plays an important role on the escaping!

The impact of noise structure

Proposition

Let $H_{D\times D}$ and $\Sigma_{D\times D}$ be semi-positive definite. If

1. **H is ill-conditioned.** *Let $\lambda_1, \lambda_2 \dots \lambda_D$ be the eigenvalues of H in descent order, and for some constant $k \ll D$ and $d > \frac{1}{2}$, the eigenvalues satisfy*

$$\lambda_1 > 0, \ \lambda_{k+1}, \lambda_{k+2}, \dots, \lambda_D < \lambda_1 D^{-d}; \tag{7}$$

2. **$\boldsymbol{\Sigma}$ is "aligned" with H.** *Let u_i be the corresponding unit eigenvector of eigenvalue λ_i, for some projection coefficient $a > 0$, we have*

$$u_1^T \Sigma u_1 \geq a\lambda_1 \frac{Tr\Sigma}{TrH}. \tag{8}$$

Then for such anisotropic Σ and its isotropic equivalence $\bar{\Sigma} = \frac{Tr\Sigma}{D} I$ under constraint (6), we have the follow ratio describing their difference in term of escaping efficiency,

$$\frac{Tr(H\Sigma)}{Tr(H\bar{\Sigma})} = \mathcal{O}\left(aD^{(2d-1)}\right), \quad d > \frac{1}{2}. \tag{9}$$

Analyze the noise of SGD via Proposition 1

By Proposition 1, The anisotropic noises satisfying the two conditions indeed help escape from the ill-conditioned minima. Thus to see the importance of SGD noise, we only need to show it meets the two conditions.

- Condition 1 is naturally hold for neural networks, thanks to their over-parameterization!
- See the following Proposition 2 for the second condition.

SGD noise and Hessian

Proposition

Consider a binary classification problem with data $\{(x_i, y_i)\}_{i \in I}, y \in \{0, 1\}$*, and mean square loss,* $L(\theta) = \mathbb{E}_{(x,y)} \left\| \phi \circ f(x; \theta) - y \right\|^2$*, where* f *denotes the network and* ϕ *is a threshold activation function,*

$$\phi(f) = \min\{\max\{f, \delta\}, 1 - \delta\}, \tag{10}$$

δ *is a small positive constant.*
Suppose the network f *satisfies:*

1. *it has one hidden layer and piece-wise linear activation;*
2. *the parameters of its output layer are fixed during training.*

Then there is a constant $a > 0$*, for* θ *close enough to minima* θ^**,*

$$u(\theta)^T \Sigma(\theta) u(\theta) \geq a \lambda(\theta) \frac{Tr\Sigma(\theta)}{TrH(\theta)} \tag{11}$$

holds almost everywhere, for $\lambda(\theta)$ *and* $u(\theta)$ *being the maximal eigenvalue and its corresponding eigenvector of Hessian* $H(\theta)$*.*

Examples of different noise structures

Table: Compared dynamics defined in Eq. (1).

Dynamics	Noise ϵ_t	Remarks
SGD	$\epsilon_t \sim \mathcal{N}\left(0, \Sigma_t^{\text{sgd}}\right)$	Σ_t^{sgd} is the gradient covariance matrix.
GLD constant	$\epsilon_t \sim \mathcal{N}\left(0, \varrho_t^2 I\right)$	ϱ_t is a tunable constant.
GLD dynamic	$\epsilon_t \sim \mathcal{N}\left(0, \sigma_t^2 I\right)$	σ_t is adjusted to force the noise share the same magnitude with SGD noise, similarly hereinafter.
GLD diagonal	$\epsilon_t \sim \mathcal{N}\left(0, \text{diag}(\Sigma_t^{\text{sgd}})\right)$	$\text{diag}(\Sigma_t^{\text{sgd}})$ is the diagonal of the covariance of SGD noise Σ_t^{sgd}.
GLD leading	$\epsilon_t \sim \mathcal{N}\left(0, \sigma_t \tilde{\Sigma}_t\right)$	$\tilde{\Sigma}_t$ is the best low rank approximation of Σ_t^{sgd}.
GLD Hessian	$\epsilon_t \sim \mathcal{N}\left(0, \sigma_t \tilde{H}_t\right)$	$\tilde{H}_t$ is the best low rank approximation of the Hessian.
GLD 1st eigven(H)	$\epsilon_t \sim \mathcal{N}\left(0, \sigma_t \lambda_1 u_1 u_1^T\right)$	λ_1, u_1 are the maximal eigenvalue and its corresponding unit eigenvector of the Hessian.

2-D toy example

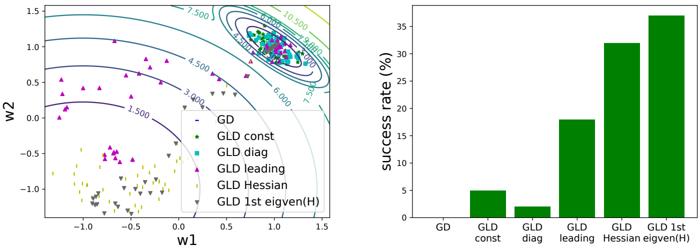

Figure: 2-D toy example. Compared dynamics are initialized at the sharp minima. **Left**: The trajectory of each compared dynamics for escaping from the sharp minimum in one run. **Right**: Success rate of arriving the flat solution in 100 repeated runs

One hidden layer network

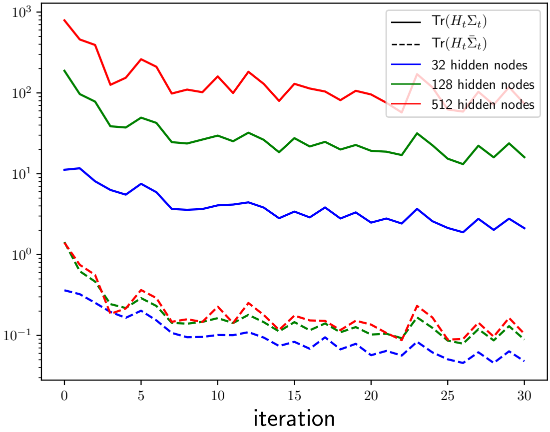

Figure: One hidden layer neural networks. The solid and the dotted lines represent the value of $\text{Tr}(H\Sigma)$ and $\text{Tr}(H\bar{\Sigma})$, respectively. The number of hidden nodes varies in $\{32, 128, 512\}$.

FashionMNIST experiments

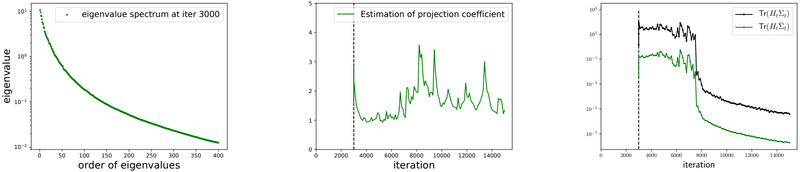

Figure: FashionMNIST experiments. **Left**: The first 400 eigenvalues of Hessian at θ^*_{GD}, the sharp minima found by GD after 3000 iterations. **Middle**: The projection coefficient estimation $\hat{a} = \frac{u_1^T \Sigma u_1 \mathrm{Tr} H}{\lambda_1 \mathrm{Tr} \Sigma}$ in Proposition 1. **Right**: $\mathrm{Tr}(H_t\Sigma_t)$ versus $\mathrm{Tr}(H_t\bar{\Sigma}_t)$ during SGD optimization initialized from θ^*_{GD}, $\bar{\Sigma}_t = \frac{\mathrm{Tr}\Sigma_t}{D} I$ denotes the isotropic equivalence of SGD noise.

FashionMNIST experiments

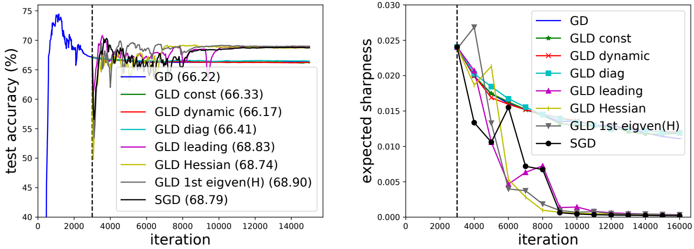

Figure: FashionMNIST experiments. Compared dynamics are initialized at θ^*_{GD} found by GD, marked by the vertical dashed line in iteration 3000. **Left**: Test accuracy versus iteration. **Right**: Expected sharpness versus iteration. Expected sharpness (the higher the sharper) is measured as $\mathbb{E}_{\nu\sim\mathcal{N}(0,\delta^2 I)}\left[L(\theta+\nu)\right]-L(\theta)$, and $\delta=0.01$, the expectation is computed by average on 1000 times sampling.

Conclusion

- We explore the escaping behavior of SGD-like processes through analyzing their continuous approximation.
- We show that thanks to the anisotropic noise, SGD could escape from sharp minima efficiently, which leads to implicit regularization effects.
- Our work raises concerns over studying the structure of SGD noise and its effect.
- Experiments support our understanding.

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$06:30 \sim 09:00$ PM @
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