TTIC 31230, Fundamentals of Deep Learning

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Continuous Time Models of SGD

Gradient Flow

The Diffusion SDE

The Langevin SDE

General SDEs

The SGD SDE

Gradient Flow

Gradient flow is a non-stochastic (deterministic) model of stochastic gradient descent (SGD).

Gradient flow is defined by the total gradient differential equation

$$\frac{d\Phi}{dt} = -g(\Phi) \qquad g(\Phi) = \nabla_\Phi \; E_{(x,y)\sim \mathrm{Train}} \; \mathcal{L}(\Phi, x, y)$$

We let $\Phi(t)$ be the solution to this differential equation satisfying $\Phi(0) = \Phi_{\mathrm{init}}$.

Gradient Flow

$$\frac{d\Phi}{dt} = -g(\Phi)$$

For small values of Δt this differential equation can be approximated by

$$\Delta\Phi = -g(\Phi)\Delta t$$

Time as the Sum of the Learning Rates

Consider the update.

$$\Delta\Phi = -g\Delta t$$

Here Δt has both a natural interpretation as time in a numerical simulation of the flow differential equation.

But it also has a natural interpretation as a learning rate.

This leads to interpreting the sum of the learning rates as "time" in SGD.

Gradient Flow and SGD

Consider a sequence of model parameters $\Phi_1, \ldots, \Phi_N$ produced by SGD with

$$\Phi_{i+1} = \Phi_i - \eta \hat{g}_i$$

and where $\hat{g}_i$ is the gradient of the ith randomly selected training point.

Take $\eta \to 0$ and $N \to \infty$ using $N = t/\eta$. We will show that in this limit for SGD we have that Φ_N converges to $\Phi(t)$ as defined by gradient flow.

Gradient Flow and SGD

For $\Phi_{i+1} = \Phi_i - \eta\hat{g}_i$ we divide Φ_1, …, Φ_N into $\sqrt{N}$ blocks.
$(\Phi_1, \ldots, \Phi_{\sqrt{N}})\ (\Phi_{\sqrt{N}+1}, \ldots, \Phi_{2\sqrt{N}})\ \cdots\ (\Phi_{T-\sqrt{N}+1}, \ldots, \Phi_N)$

For $\eta \to 0$ and $N = t/\eta$ we have $\eta\sqrt{N} \to 0$ which implies

$$\Phi_{\sqrt{N}} \sim \Phi_0 - \eta\sqrt{N}g$$

where g is the average (non-stochastic) gradient.

Since the gradients within each block become non-stochastic, we are back to gradient flow.

Diffusion

Consider a discrete-time process $z(0), z(1), z(2), z(3), \ldots$ with $z(n) \in \mathbb{R}^d$ defined by

$$\begin{aligned} z(0) &= y, \quad y \sim \mathrm{pop}(y) \\ z(n+1) &= z(n) + \sigma\delta, \quad \delta \sim \mathcal{N}(0, I) \end{aligned}$$

We can sample from $z(n)$ using

$$\begin{aligned} z(0) &= y, \quad y \sim \mathrm{pop}(y) \\ z(n) &= z(0) + \sigma\delta\sqrt{n}, \quad \delta \sim \mathcal{N}(0, I) \end{aligned}$$

Diffusion

Fix a numerical time step Δt and consider a discrete-time process $z(0)$, $z(\Delta t)$, $z(2\Delta t)$, ...

$$
\begin{aligned}
z(0) &= y, \quad y \sim \mathrm{pop}(y) \\
z(t + \Delta t) &= z(t) + \sigma \delta \sqrt{\Delta t}, \quad \delta \sim \mathcal{N}(0, I)
\end{aligned}
$$

We now take the limit of this numerical simulation as $\Delta t \to 0$.

This limit defines a probability measure on the space of functions $z(t)$.

The Diffusion SDE

$$z(t + \Delta t) = z(t) + \sigma\delta\sqrt{\Delta t}, \quad \delta \sim \mathcal{N}(0, I)$$

For simple diffusion (Brownian motion) this equation holds for any continuous $t \geq 0$ and $\Delta t \geq 0$.

The Langevin SDE

Consider gradient flow.

$$\frac{d\Phi(t)}{dt} = -g(\Phi)$$

$$g(\Phi) = \nabla_\Phi \, \mathcal{L}(\Phi)$$

$$\mathcal{L}(\Phi) = E_{(x,y)\sim\mathrm{Pop}} \, \mathcal{L}(\Phi, x, y)$$

The Langevin SDE

In the Langevin SDE we add Gaussian noise to gradient flow.

$$\Phi(t + \Delta t) = \Phi(t) - g\Delta t + \sigma\delta\sqrt{\Delta t}, \quad \delta \sim \mathcal{N}(0, I)$$

We will show that the stationary distribution of Langevin Dynamics models a Bayesian posterior probability distrbution on the model parameters where σ acts as a temperature parameter.

The Langevin SDE

$$\Phi(t + \Delta t) \;=\; \Phi(t) - g(\Phi)\Delta t + \sigma\delta\sqrt{\Delta t}, \quad \delta \sim \mathcal{N}(0, I)$$

Let $p(\Phi)$ be a probability density on the parameter space Φ. The density $p(\Phi)$ defines a gradient flow and a diffusion flow.

$$\text{gradient flow} \;=\; -p(\Phi)g(\Phi)$$

$$\text{diffusion flow} \;=\; -\frac{1}{2}\,\sigma^2\,\nabla_\Phi\,p(\Phi)$$

The expression for the diffusion flow follows from the Fokker-Planck equation. A derivation of the diffusion flow expression from first princple is given in the appendix.

The Langevin SDE

$$\text{gradient flow} \;=\; -p(\Phi)g(\Phi)$$

$$\text{diffusion flow} \;=\; -\frac{1}{2}\,\sigma^2\;\nabla_\Phi(p(\Phi))$$

For the stationary distribution these two flows cancel each other out. In one dimension we have

$$\frac{1}{2}\sigma^2\nabla_\Phi\, p = -p\nabla_\Phi\mathcal{L}$$

The Langevin Stationary Distribution

$$\frac{1}{2}\sigma^2 \nabla_\Phi\, p = -p \nabla_\Phi \mathcal{L}$$

$$\frac{1}{2}\sigma^2 \frac{\nabla_\Phi\, p}{p} = -\nabla_\Phi \mathcal{L}$$

$$\frac{1}{2}\sigma^2 \left(\nabla_\Phi \ln p\right) = \nabla_\Phi(-\mathcal{L})$$

$$\frac{1}{2}\sigma^2 \ln p = -\mathcal{L} + C$$

$$p(\Phi) = \frac{1}{Z} \exp\left(\frac{-2\mathcal{L}(\Phi)}{\sigma^2}\right)$$

A Bayesian Interpretation of Langevin Dynamics

$$\text{Train} = (x_1, y_1), \ldots, (x_n, y_n)$$

The parameters Φ determine $P_\Phi(y|x)$.

$$\begin{aligned} p(\Phi|\text{Train}) &= \frac{p(\Phi)p(\text{Train}|\Phi)}{p(\text{Train})} \\ &= \frac{p(\Phi)p(x_1, \ldots, x_n)P_\Phi(y_1, \ldots, y_n|x_1, \ldots, x_n)}{p(x_1, \ldots, x_n)P(y_1, \ldots y_n|x_1, \ldots x_n)} \\ &= \frac{p(\Phi)P_\Phi(y_1, \ldots, y_n|x_1, \ldots, x_n)}{P(y_1, \ldots y_n|x_1, \ldots x_n)} \end{aligned}$$

A Bayesian Interpretation of Langevin Dynamics

$$\mathrm{Train} = (x_1, y_1), \ldots, (x_n, y_n)$$

$$p(\Phi|\mathrm{Train}) \;=\; \frac{p(\Phi)P_\Phi(y_1,\ldots,y_n|x_1,\ldots,x_n)}{P(y_1,\ldots y_n|x_1,\ldots x_n)}$$

The denominator does does not depend on Φ which implies

$$p(\Phi|\mathrm{Train}) \propto p(\Phi)\prod_i P_\Phi(y_i|x_i)$$

A Bayesian Interpretation of Langevin Dynamics

$$
\begin{aligned}
p(\Phi|\mathrm{Train}) &\propto p(\Phi) \prod_i P_\Phi(y_i|x_i) \\
\ln p(\Phi|\mathrm{Train}) &= \sum_i \ln P_\Phi(y_i|x_i) + \ln p(\Phi) + C
\end{aligned}
$$

$$
\begin{aligned}
\text{Define } \ \mathcal{L}(\Phi) &= \frac{1}{n} \sum_i - \ln P_\Phi(y_i|x_i) - \frac{1}{n} \ln p(\Phi) \\
&= E_{(x,y)\sim \mathrm{Train}} \left[- \ln P_\Phi(y|x)\right] - \frac{1}{n} \ln p(\Phi)
\end{aligned}
$$

This Gives $\quad p(\Phi|\mathrm{Train}) = \frac{1}{Z} \exp\left(-n\mathcal{L}(\Phi)\right)$

A Bayesian Interpretation of Langevin Dynamics

$$p(\Phi|\mathrm{Train}) = \frac{1}{Z} e^{-n\mathcal{L}(\Phi)}$$

$$p_{\mathrm{Langevin}}(\Phi) = \frac{1}{Z} \exp\left(\frac{-2\mathcal{L}(\Phi)}{\sigma^2}\right)$$

Setting $\sigma^2 = \frac{1}{2n}$ gives

$$p_{\mathrm{Langevin}}(\Phi) = p(\Phi|\mathrm{Train})$$

A General SDE

$$x(t + \Delta t) \;=\; x(t) + \mu(x,t)\Delta t + \sigma(x,t)\delta\sqrt{\Delta t}, \quad \delta \sim \mathcal{N}(0, I) \quad (1)$$

Here $\sigma(x,t)$ is a matrix.

This is conventionally written as

$$dx = \mu(x,t)dt + \sigma(x,t)dB \quad (2)$$

where B denotes a Weiner process (simple diffusion, aka Brownian motion)

I find (1) more intuitive than (2) but they are the same thing.

The SGD SDE

We now consider SGD

$$\Phi_{i+1} = \Phi_i - \eta \hat{g}_i$$

We consider Φ_i and Φ_{i+N} with N small enough that

$$\Phi_{i+N} \approx \Phi_i$$

.

Gradient Noise

$$\hat{g} = g(\Phi) + (\hat{g} - g(\Phi))$$

$\hat{g} - g(\Phi)$ has zero mean.

$$\Phi_{i+N} \approx \Phi_i - \eta N g(\Phi) - \eta \sum_{j=1}^{N} (\hat{g}_i - g(\Phi))$$

We pick N large enough that $\sum_{j=1}^{N} (\hat{g}_i - g(\Phi))$ is approximately Gaussian.

Gradient Noise

$$
\begin{aligned}
\Phi_{i+N} &\approx \Phi_i - \eta N g(\Phi) - \eta \sum_{j=1}^{N} (\hat{g}_i - g(\Phi)) \\
&\approx \Phi_i - \eta N g(\Phi) - \eta \sqrt{N}\delta, \quad \delta \sim \mathcal{N}(0, \Sigma)
\end{aligned}
$$

Now define $\Delta t = N\eta$ or $N = \Delta t/\eta$.

$$
\begin{aligned}
\Phi(t + \Delta t) &\approx \Phi(t) - g(\Phi)\Delta t + \eta\delta\sqrt{\Delta t/\eta}, \quad \delta \sim \mathcal{N}(0, \Sigma) \\
&= \Phi(t) - g(\Phi)\Delta t + \sqrt{\eta}\delta\sqrt{\Delta t}, \quad \delta \sim \mathcal{N}(0, \Sigma)
\end{aligned}
$$

The SGD SDE

$$\Phi(t+\Delta t) \approx \Phi(t) - g(\Phi)\Delta t + \sqrt{\eta}\delta\sqrt{\Delta t}, \quad \delta \sim \mathcal{N}(0,\Sigma)$$

$$= \Phi(t) - g(\Phi)\Delta t + \sqrt{\eta}\sigma(\Phi)\delta\sqrt{\Delta t}, \quad \delta \sim \mathcal{N}(0,I)$$

Here the matrix $\sigma(\Phi)$ is the square root of the covariance matrix $\Sigma(\Phi)$.

The SGD SDE in One Dimension

$$\Phi(t+\Delta t) \;=\; \Phi(t) - g(\Phi)\Delta t + \sqrt{\eta}\sigma(\Phi)\delta\sqrt{\Delta t}$$

In one dimension, if the gradient noise $\sigma(\Phi)$ is constant, then the SGD SDE has the same form as Langevin dynamics and we get.

$$p(x) \;=\; \frac{1}{Z}\exp\left(\frac{-2\mathcal{L}(x)}{\eta\sigma^2}\right)$$

This is Gibbs and provides an interpretation of the learning rate as temperature.

The SGD SDE in Higher Dimension

$$\Phi(t + \Delta t) \;=\; \Phi(t) - g(\Phi)\Delta t + \sqrt{\eta}\sigma(\Phi)\delta\sqrt{\Delta t}$$

This is almost the general case of an SDE.

Here $g(\Phi)$ is the gradient of a scalar function. This is not true for a general SDE.

But the matrix $\sigma(\Phi)$ is arbitrary.

Here the learning rate η controls the level of noise but we do not in general have a Gibbs distribution.

The SGD SDE, A Counter Example

If we have two dimensions x and y where the loss separates as $\mathcal{L}(x,y) = \mathcal{L}(x) + \mathcal{L}(y)$, and the matrix $\sigma(\Phi)$ is constant and diagonal, each dimension behaves as an independent one dimensional SGD and we get.

$$p(x,y) = \frac{1}{Z}\exp\left(\frac{-2\mathcal{L}(x)}{\eta\sigma_x^2} + \frac{-2\mathcal{L}(y)}{\eta\sigma_y^2}\right)$$

This is not Gibbs.

Langevin-Adaptive SGD

Consider SGD where the upde dirction is determined by an arbitrary inner-product (symmtetric and positive-definite) matrix D.

$$\Phi_{i+1} = \Phi_i + \eta D \hat{g}_i$$

D defines a linear map from dual vectors to primal vectrors.

The function has a meaning indepent of the choice of coordinates.

Coordinate Independent Formulation of Gradient Noise

We can define the covariance matrix of the noise as

$$\Sigma(\Phi) = E_{\hat{g}}\ \hat{g}\hat{g}_i^\top$$

The gradient noise covariance matrix $\Sigma(\Phi)$ defines a linear map from the primal vectors to dual vectors.

$$\Sigma(\Phi)\Delta\Phi = E_{\hat{g}}\ \hat{g}(\hat{g}^\top\Delta\Phi)$$

Solving for D to Get Langevin

$$\Phi_{i+1} = \Phi_i + \eta D \hat{g}_i$$

Setting $\Delta t = N\eta$ we get

$$\Phi(t + \Delta t) = \Phi(t) - Dg\Delta t + \sqrt{\eta} D \delta \sqrt{\Delta t}, \quad \delta \sim \mathcal{N}(0, \Sigma(\Phi))$$

Here the noise vector δ is a dual vector.

Solving for D

For a given probability density $p(\Phi)$ over the parameters Φ the flows are

$$\begin{aligned} \text{gradient flow} &= -pDg \\ \text{diffusion flow} &= -\frac{1}{2}\eta D \Sigma(\Phi) D \nabla_\Phi p \end{aligned}$$

These are vectors in parameter space that are independent of the choice of coordinates.

Solving for D

$$\text{gradient flow} = -pDg$$

$$\text{diffusion flow} = -\frac{1}{2}\eta D\Sigma(\Phi)D\nabla_\Phi p$$

Detailed Balance:

$$\frac{1}{2}\eta D\Sigma(\Phi)D\nabla_\Phi\, p = -pD\nabla_\Phi\mathcal{L}$$

Solving for D

$$\frac{1}{2}\eta D\Sigma(\Phi)D\nabla_\Phi\, p \;=\; -pD\nabla_\Phi\mathcal{L}$$

$$\frac{1}{2}\eta D\Sigma(\Phi)D\frac{\nabla_\Phi\, p}{p} \;=\; -D\nabla_\Phi\mathcal{L}$$

$$\frac{1}{2}\eta D\Sigma(\Phi)D\left(\nabla_\Phi \ln p\right) \;=\; D\nabla_\Phi\mathcal{L}$$

Setting $D = \Sigma(\Phi)^{-1}$ gives

$$\frac{1}{2}\eta\Sigma(\Phi)^{-1}\left(\nabla_\Phi \ln p\right) = \Sigma(\Phi)^{-1}\nabla_\Phi\mathcal{L}$$

The Gibbs distribution

$$\frac{1}{2}\eta\Sigma(\Phi)^{-1}\left(\nabla_\Phi \ln p\right) = \Sigma(\Phi)^{-1}\nabla_\Phi \mathcal{L}$$

The facors of $\Sigma(\Phi)^{-1}$ now cancel (we can multiply both sides by $\Sigma(\Phi)$) and we get

$$\frac{1}{2}\eta\left(\nabla_\Phi \ln p\right) = \nabla_\Phi \mathcal{L}$$

This equation is independent of corrdinates.

The Gibbs Distribution

$$\frac{1}{2}\eta\left(\nabla_\Phi \ln p\right) = \nabla_\Phi \mathcal{L}$$

$$p(\Phi) = \frac{1}{Z}\exp\left(\frac{-2\mathcal{L}(\Phi)}{\eta}\right)$$

The Gibbs Distribution

For the adaptive update

$$\Phi_{i+1} = \Phi i + \eta \Sigma(\Phi)^{-1} \hat{g}_i$$

we have a stationary distribution

$$p(\Phi) = \frac{1}{Z} \exp\left(\frac{-2\mathcal{L}}{\eta}\right)$$

END

Appendix: Diffusion Flow

We consider the one dimensional case where we have a function $x(t) \in \mathbb{R}$. We consider a very small time step Δt and consider only the diffusion flow.

$$x(t + \Delta t) \;=\; x(t) + \sigma\delta\sqrt{\Delta t}, \quad \delta \sim \mathcal{N}(0,1)$$

We assume a density p_x of values of x and let $p_\delta(\delta)$ be the normal distribution $\mathcal{N}(0,1)$ on δ.

The quantity of mass transfer in the time interval Δt from values above x to values below x is

$$\begin{aligned}
& \int_{z=0}^{\infty} p_x(x+z)\; p_\delta(\sigma\delta\sqrt{\Delta t} \leq -z) dz \\
= & \int_{z=0}^{\infty} p_x(x+z)\; p_\delta\left(\delta \leq \frac{-z}{\sigma\sqrt{\Delta t}}\right) dz \\
= & \int_{z=0}^{\infty} p_x(x+z)\; \Phi\left(\frac{-z}{\sigma\sqrt{\Delta t}}\right) dz
\end{aligned}$$

where Φ is the cummulative function of the Gaussian.

Appendix: Diffusion Flow

The quantity of mass transfer in the time interval Δt from values above x to values below x is

$$\int_{z=0}^{\infty} p_x(x+z)\ \Phi\left(\frac{-z}{\sigma\sqrt{\Delta t}}\right) dz$$

By a change of variables $u = z/(\sigma\sqrt{\Delta t})$ we get

$$\int_{u=0}^{\infty} p_x(x+\sigma\sqrt{\Delta t}\ u)\ \Phi(-u)\sigma\sqrt{\Delta t}\ du$$

As $\Delta t \to 0$ we can use the first order Taylor expansion of the density.

$$\sigma\sqrt{\Delta t}\int_{u=0}^{\infty}\left(p_x(x)+\sigma\sqrt{\Delta t}\ u\frac{dp_x(x)}{dx}\right)\ \Phi(-u)\ du$$

Appendix: Diffusion Flow

$$
\begin{aligned}
& \sigma\sqrt{\Delta t}\int_{u=0}^{\infty}\left(p_x(x)+\sigma\sqrt{\Delta t}\; u\frac{dp_x(x)}{dx}\right)\;\Phi(-u)\;du \\
= \;& \sigma\sqrt{\Delta t}\;p_x(x)\left(\int_{u=0}^{\infty}\Phi(-u)\;du\right)+\sigma^2\Delta t\frac{dp_x(x)}{dx}\left(\int_{u=0}^{\infty}u\Phi(-u)du\right)
\end{aligned}
$$

A similar alanysis shows that the mass transfer from lower values to higher values is

$$
= \;\sigma\sqrt{\Delta t}\;p_x(x)\left(\int_{u=0}^{\infty}\Phi(-u)\;du\right)-\sigma^2\Delta t\frac{dp_x(x)}{dx}\left(\int_{u=0}^{\infty}u\Phi(-u)du\right)
$$

The net mass transfer in the positive x direction is the second minus the first or

$$
= \;-2\sigma^2\Delta t\frac{dp_x(x)}{dx}\left(\int_{u=0}^{\infty}u\Phi(-u)du\right)
$$

Appendix: Diffusion Flow

The net mass transfer in the positive x direction is

$$-2\sigma^2 \Delta t \frac{dp_x(x)}{dx} \left(\int_{u=0}^{\infty} u\Phi(-u)du \right)$$

Note that the mass transfer is proportional to Δt. Dividing by Δt gives the flow per unit time.

$$\text{Diffusion flow} \quad = -\alpha\sigma^2 \frac{dp_x(x)}{dx} \qquad \alpha = 2\int_{u=0}^{\infty} u\Phi(-u)du$$

α can be calculated using integration by parts.

$$\begin{aligned}
\alpha &= 2\int_0^{\infty} u\Phi(-u)du \\
&= \int_0^{\infty} \Phi(-u)du^2 \\
&= u^2\Phi(-u)|_0^{\infty} + \int_0^{\infty} u^2\phi(-u)du \ \text{ where } \phi \text{ is the Gaussian density} \\
&= \int_0^{\infty} u^2\phi(-u)du \\
&= \frac{1}{2}
\end{aligned}$$

Appendix: Diffusion Flow

We now have that the diffusion flow is

$$\text{Diffusion flow} \;\; = -\frac{1}{2}\,\sigma^2 \frac{dp_x(x)}{dx}$$

For dimension larger than 1 we have

$$\text{Diffusion flow} \;\; = -\frac{1}{2}\,\Sigma \nabla_x p_x$$

Where $\Sigma = E\;(\hat{g} - g)(\hat{g} - g)^\top$ is the covariance matrix of the gradient noise.

Here we have derived this from first principle but it also follows from the Fokker–Planck equation (see Wikipedia).

END