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.

$$
\begin{aligned}
d\Phi &= -g(\Phi)dt && \text{Gadient Flow} \\
\Phi_{t+\Delta t} &\approx \Phi_t - g\Delta t && \\
\Phi_{t+\eta} &\approx \Phi_t - \eta_t \, \hat{g} && \text{SGD}
\end{aligned}
$$

We will show that as $\eta_t \to 0$ we have that SGD converges to Gradient Flow.

Gradient Flow and SGD

Consider a sequence of model parameters Φ_1, …, Φ_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.

Stochastic Differential Equations (SDEs)

SDEs are important in deep learning for understanding SGD, incorporating Bayesian priors into SGD, and in modern diffusion models.

We will start with the simplest SDE: Brownian motion. Brownian motion is the SDE used in diffusion models.

Diffusion Models: Brownian Motion

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

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

We can sample from $z(n)$ using

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

Brownian Motion

Fix a numerical time step Δt and consider a discrete-time process $z(0)$, $z(\Delta t)$, $z(2\Delta t)$, $z(3\Delta t)$ ...

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

We now take the limit of this numerical simulation as $\Delta t \to 0$. In this limit we can sample directly from $z(t)$ using

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

Brownian Motion

We can sample directly from $z(t + \Delta t)$ given $z(t)$ using

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

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

Sampling from a Bayesian Posterior: 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

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

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

The denominator does does not depend on Φ which implies

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

A Bayesian Interpretation of Langevin Dynamics

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

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

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

Sampling from a Bayesian Posterior: Langevin Dynamics

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.

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

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

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

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

$$\begin{aligned}
\frac{1}{2}\sigma^2 \nabla_\Phi \, p &= -p \nabla_\Phi \mathcal{L} \\
\frac{1}{2}\sigma^2 \frac{\nabla_\Phi \, p}{p} &= -\nabla_\Phi \mathcal{L} \\
\frac{1}{2}\sigma^2 \left(\nabla_\Phi \ln p\right) &= \nabla_\Phi(-\mathcal{L}) \\
\frac{1}{2}\sigma^2 \ln p &= -\mathcal{L} + C \\
p(\Phi) &= \frac{1}{Z} \exp\left(\frac{-2\mathcal{L}(\Phi)}{\sigma^2}\right)
\end{aligned}$$

A Bayesian Interpretation of Langevin Dynamics

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

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

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

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

A General SDE

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

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

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

$$\approx \Phi_i - \eta N g(\Phi) - \eta \sqrt{N} \epsilon, \quad \epsilon \sim \mathcal{N}(0, \Sigma)$$

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

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

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

The SGD SDE

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

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

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

The SGD SDE in One Dimension

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

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

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

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 update dirction is determined by a matrix D.

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

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

The function defined by D 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

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

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

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

Solving for D to Get Langevin

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

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

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

Here the noise vector ϵ is a dual vector.

Solving for D

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

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

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

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 factors 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 coordinates.

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.

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

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

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

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

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