

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

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

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

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 Φ_1, \dots, 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 i th randomly selected training point.

Take $\eta \rightarrow 0$ and $N \rightarrow \infty$ 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, \dots, Φ_N into \sqrt{N} blocks.

$$(\Phi_1, \dots, \Phi_{\sqrt{N}}) (\Phi_{\sqrt{N}+1}, \dots, \Phi_{2\sqrt{N}}) \cdots (\Phi_{T-\sqrt{N}+1}, \dots, \Phi_N)$$

For $\eta \rightarrow 0$ and $N = t/\eta$ we have $\eta\sqrt{N} \rightarrow 0$ 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 $z(0), z(1), z(2), z(3), \dots$ with $z(n) \in \mathbb{R}^d$ defined by

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

We can sample from $z(n)$ using

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

Diffusion

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

$$z(0) = y, \quad y \sim \text{pop}(y)$$

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

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

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.

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

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

$$\mathcal{L}(\Phi) = E_{(x,y) \sim P_{\text{op}}} \mathcal{L}(\Phi, x, y)$$

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 distribution 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 principle 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

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

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

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

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

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

A Bayesian Interpretation of Langevin Dynamics

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

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

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

A Bayesian Interpretation of Langevin Dynamics

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

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

The denominator 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

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

$$\ln p(\Phi|\text{Train}) = \sum_i \ln P_{\Phi}(y_i|x_i) + \ln p(\Phi) + C$$

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

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

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

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

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 Wiener 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.

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

We pick N large enough that $\sum_{j=1}^N (\hat{g}_j - g(\Phi))$ 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 update direction 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

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

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

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

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

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

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

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

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

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

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

The Gibbs distribution

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

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

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

This equation is independent of coordinates.

The Gibbs Distribution

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

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

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 cumulative 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 $\Delta t \rightarrow 0$ 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 analysis 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.

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

α can be calculated using integration by parts.

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

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