Sampling Methods: From MCMC to Generative Modeling
Bayesian learning and Langevin algorithm

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Outline

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Step 1. Compute the Likelihood:

$$p(\mathcal{D}|x) \overset{(1)}{\propto} \prod_{i=1}^{p} p(y_i|x, w_i) \overset{(2)}{\propto} \exp(-\frac{1}{2}\sum_{i=1}^{p} \|y_i - g(w_i, x)\|^2).$$

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$$p(x|\mathcal{D}) = \frac{p(\mathcal{D}|x)p_0(x)}{Z} \quad \text{where} \quad Z = \int_{\mathbb{R}^d} p(\mathcal{D}|x)p_0(x)dx$$

is called the normalization constant and is **intractable**.

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Denoting $\pi := p(\cdot|\mathcal{D})$ the posterior on parameters $x \in \mathbb{R}^d$, we have:

$$\boxed{\pi(x) \propto \exp\left(-V(x)\right), \quad V(x) = \frac{1}{2}\sum_{i=1}^{p} \|y_i - g(w_i, x)\|^2 + \frac{\|x\|^2}{2}.}$$

i.e. π's density is known "up to a normalization constant".
π is a probability distribution over parameters of a model.

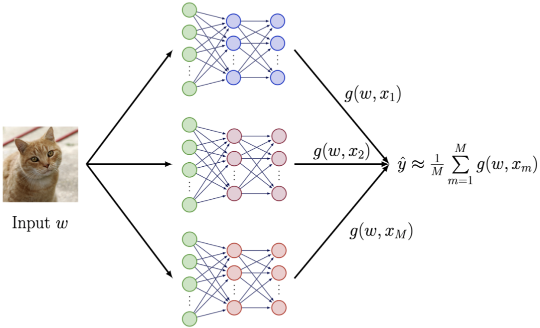
The posterior π is interesting for

- measuring uncertainty on prediction through the distribution of $g(w, \cdot)$, $x \sim \pi$.
- prediction for a new input w:

$$\hat{y} = \underbrace{\int_{\mathbb{R}^d} g(w, x) d\pi(x)}_{\text{"Bayesian model averaging"}}$$

i.e. predictions of models parametrized by $x \in \mathbb{R}^d$ are reweighted by $\pi(x)$.

Here, Sampling methods construct an approximation $\mu_M = \frac{1}{M}\sum_{m=1}^{M}\delta_{x_m}$ of π.



Sampling as Optimization

Actually, in many cases (e.g. it is underlying many algorithms), the sampling problem (approximating π) can be viewed as optimization over $\mathcal{P}(\mathbb{R}^d)$:

$$\min_{\mu \in \mathcal{P}(\mathbb{R}^d)} \mathrm{D}(\mu|\pi)$$

where D is a divergence or distance, hence that is minimized for $\mu = \pi$.

The Kullback-Leibler divergence

D could be the (reverse) Kullback-Leibler (KL) divergence:

$$\mathrm{KL}(\mu|\pi) = \begin{cases} \int_{\mathbb{R}^d} \log\left(\frac{\mu}{\pi}(x)\right) d\mu(x) & \text{if } \mu \ll \pi \\ +\infty & \text{otherwise.} \end{cases}$$

We recognize a f-divergence $\int f\left(\frac{\mu}{\pi}\right) d\pi$ where $f(x) = x\log(x)$. Taking $f(x) = -\log(x)$ yields the (forward) KL i.e. $\mathrm{KL}(\pi|\mu)$.

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The (reverse) KL as an objective is convenient when the unnormalized density of π is known since it **does not depend on the normalization constant!**

Indeed writing $\pi(x) = e^{-V(x)}/Z$ we have:

$$\mathrm{KL}(\mu|\pi) = \int_{\mathbb{R}^d} \log\left(\frac{\mu}{e^{-V}}(x)\right) d\mu(x) + \log(Z).$$

But, it is not convenient when μ or π are discrete, because the KL is $+\infty$ unless $supp(\mu) \subset supp(\pi)$.

Examples

- (Parametric methods) Variational Inference : Restrict the search space to a parametric families $\{\mu_\theta,\ \theta \in \mathbb{R}^p\}$. The problem rewrites as a finite-dimensional optimization problem (i.e. over $\mathbb{R}^p$):

$$\min_{\theta \in \mathbb{R}^p} \mathrm{D}(\mu_\theta | \pi)$$

- Example: Gaussians with diagonal covariance matrices can be parametrized by $\theta = (m, \sigma) \in \mathbb{R}^{2d}$ (see Bayes by Backprop in the last section)
- Example: use normalizing flows to construct a family $\mu_\theta = f_{\theta\#}p$ and optimize the previous objective[1]. [1] Rezende, D., Mohamed, S. (2015, June). Variational inference with normalizing flows. In International conference on machine learning.

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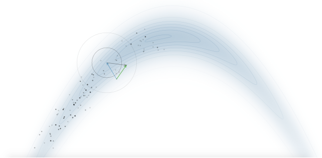
- (Non parametric methods) Markov Chain Monte Carlo (MCMC) methods, Sequential Monte Carlo (SMC)...: generate a Markov chain in $\mathbb{R}^d$ whose law converges to $\pi \propto \exp(-V)$
- Example: Langevin (next section)

Langevin Monte Carlo

Langevin Monte Carlo (LMC) [Roberts and Tweedie (1996)]

$$x_{m+1} = x_m + \gamma \nabla \log \pi(x_m) + \sqrt{2\gamma}\eta_m, \quad \eta_m \sim \mathcal{N}(0, \mathrm{Id}).$$



Picture from `https://chi-feng.github.io/mcmc-demo/app.html`.

Note that in the Bayesian inference setting, where $\pi = \frac{\exp(-V)}{Z}$, it is easily implementable since the **score** $\nabla_x \log \pi(x) = -\nabla_x(V(x) + \log(Z)) = -\nabla V(x)$ since $\nabla_x \log(Z) = 0$.

Outline

Langevin diffusion

Langevin diffusion is the Stochastic Differential Equation (SDE):

$$\mathrm{d}x_t = -\nabla V(x_t)dt + \sqrt{2}\mathrm{d}B_t, \quad x_t \sim p_t$$

where B_t denotes the standard Brownian motion in $\mathbb{R}^d$, defined as:

- $B_0 = 0$ almost surely;
- For any $t_0 < t_1 < \cdots < t_N$, the increments $B_{t_n} - B_{t_{n-1}}$ are independent, $n = 1, 2, \ldots, N$;
- The difference $B_t - B_s$ and B_{t-s} have the same distribution: $\mathcal{N}(0, (t-s)\,\mathrm{Id})$ for $s < t$;
- B_t is continuous almost surely.

Langevin diffusion defines a *Markov process* as follows:

$$x_t = x_0 - \int_0^t \nabla V(x_s)ds + \sqrt{2}B_t,$$

where x_0 is some initialization.

Time-discretization

An Euler-Maruyama time-discretization of Langevin diffusion yields:

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Proof:

$$\begin{aligned} x_\gamma &\approx x_0 - \int_0^\gamma \nabla V(x_0)\, dt + \sqrt{2\gamma}\, \eta \\ &= x_0 - \left(\int_0^\gamma dt \right) \nabla V(x_0) + \sqrt{2\gamma}\, \eta \\ &= x_0 - \gamma \nabla V(x_0) + \sqrt{2\gamma}\, \eta. \end{aligned}$$

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We can now iterate this approach k times, which gives us a recursion, which can be easily implementable on a computer:

$$x_{k\gamma} \approx x_{(k-1)\gamma} - \gamma \nabla V(x_{(k-1)\gamma}) + \sqrt{2\gamma}\, \eta_k,$$

where $\eta_k \sim \mathcal{N}(0, \mathrm{Id})$ for all k. Dropping the dependency on γ in the indices yields the scheme (1).

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(continuous time) **Langevin diffusion** $=$ Ornstein-Uhlenbeck process:

$$\mathrm{d}x_t = -x_t + \mathrm{d}B_t.$$

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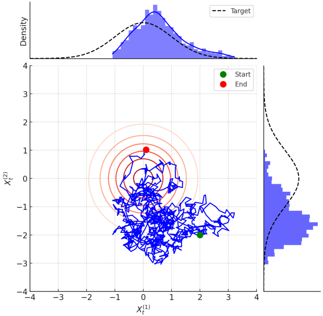

Recall above we plot $x_{t+1} = x_t + \gamma \nabla \log \pi(x_t) + \sqrt{2\gamma}\eta_t$ for $\pi \propto \exp(-\frac{\|x\|^2}{2})$.

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To understand how $p(x,t)$ evolves, we will use the Fokker–Planck equation, which governs the evolution of $p(x,t)$ through the following partial differential equation (PDE):

$$\partial_t p(x,t) = \partial_x\left[\partial_x V(x) p(x,t)\right] + \partial_x^2 p(x,t).$$

This equation characterizes how the “change” in $p(\cdot,t)$ behaves, i.e., $\partial_t p(x,t)$.

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Remark: for $d > 1$, the Fokker-Planck equation writes:

$$\partial_t p(x,t) = \nabla \cdot (\nabla V(x) p(x,t)) + \Delta(p(x,t)).$$

(where $\nabla\cdot$ and Δ are the divergence and Laplacian operators: analog to above but summing all partial derivatives for $x_1, \ldots, x_d$).

The Fokker-Planck equation

Now, the idea is: if $p(\cdot, t)$ converges to a distribution as $t \to \infty$, then whenever this limit is reached, there should not be any more changes in p. In other words, whenever $p(\cdot, t)$ hits its limit, $\partial_t p(x, t)$ has to be equal to 0.

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Therefore, we can simply "check" if $\pi \propto \exp(-V)$ is a limit of $p(\cdot, t)$ by replacing $p(x, t)$ with $\pi(x)$ in the Fokker–Planck equation and observing whether the right-hand side is equal to 0 or not. Let us apply this procedure:

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$$\begin{aligned}\partial_x \left[\partial_x V(x)\pi(x)\right] + \partial_x^2 \pi(x) &= \partial_x \left[\partial_x V(x)\pi(x) + \partial_x \pi(x)\right] \\ &= \partial_x \left[\partial_x V(x)\pi(x) - \partial_x V(x)\pi(x)\right] \\ &= 0,\end{aligned}$$

where we used the fact that

$$\partial_x V(x) = -\partial_x \log \pi(x) = -\frac{1}{\pi(x)} \partial_x \pi(x),$$

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Conclusion: π is an equilibrium for the FP equation !

Ornstein–Uhlenbeck Process

We now focus on a specific case of a Langevin diffusion and we will prove that:

For the SDE:

$$dX_t = -\beta X_t\, dt + \sigma\, dB_t$$

The solution is:

$$X_t = e^{-\beta t} X_0 + \sigma e^{-\beta t} \int_0^t e^{\beta s}\, dB_s$$

with stationary/limiting distribution $\pi = \mathcal{N}(0, \frac{\sigma^2}{2\beta})$
and we have:

$$X_t \mid X_0 \sim \mathcal{N}\left(e^{-\beta t} X_0, \frac{\sigma^2}{2\beta}(1 - e^{-2\beta t})\right)$$

Observe that:

- The farther into the future, the more the initial value gets "forgotten"

Proof

Step 1 (Multiply by the integrating factor)
Multiply both sides of the SDE by $\mu(t) = e^{\beta t}$:

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Rewriting:

$$X_t = e^{-\beta t} X_0 + \sigma e^{-\beta t} \int_0^t e^{\beta s} \, dB_s$$

Proof (continued)

Step 3 (Distribution of the integral term)
Let: $I_t := \int_0^t e^{\beta s}\, dB_s$. This is an Itô integral of a deterministic function $\Rightarrow$ it's a **Gaussian random variable** with:

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- Variance :

$$\begin{aligned}\mathrm{Var}(I_t) &= \mathbb{E}\left[\left(\int_0^t e^{\beta s}\, dB_s\right)^2\right] = \int_0^t \left(e^{\beta s}\right)^2 ds \quad \text{(using } \textbf{Itô isometry}\text{)} \\ &= \int_0^t e^{2\beta s}\, ds = \left[\frac{1}{2\beta} e^{2\beta s}\right]_0^t = \frac{1}{2\beta}(e^{2\beta t} - 1).\end{aligned}$$

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Therefore:

$$\sigma e^{-\beta t} I_t \sim \mathcal{N}\left(0,\ \sigma^2 e^{-2\beta t} \cdot \frac{1}{2\beta}(e^{2\beta t} - 1)\right) = \mathcal{N}\left(0,\ \frac{\sigma^2}{2\beta}(1 - e^{-2\beta t})\right).$$

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So the full solution is : $X_t = e^{-\beta t} X_0 + \sigma e^{-\beta t} I_t$, where
$X_t \mid X_0 \sim \mathcal{N}\left(e^{-\beta t} X_0, \frac{\sigma^2}{2\beta}(1 - e^{-2\beta t})\right)$. **Done!**

(Very) Important remarks

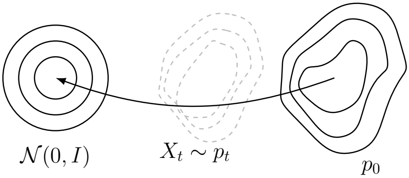

Figure: Representing X_t an OU process (with $\beta = 1$, $\sigma = \sqrt{2}$), and p_t its (time) marginals

- We know that the full solution :

$$X_t = e^{-\beta t} X_0 + \text{Gaussian noise} \tag{2}$$

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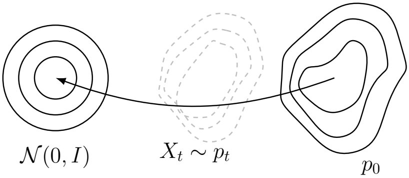

Figure: Representing X_t an OU process (with $\beta = 1$, $\sigma = \sqrt{2}$), and p_t its (time) marginals

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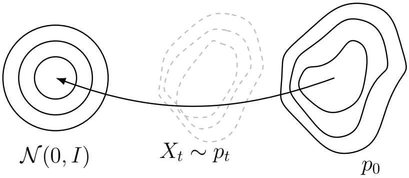

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- but the **conditional laws** in (3) are Gaussian

Introducing some initial Condition

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Proof: Recall $X_t = A + B$ where $A = e^{-\beta t} X_0, \quad B = \sigma e^{-\beta t} \int_0^t e^{\beta s} dW_s$.

- $A \sim \mathcal{N}(0, e^{-2\beta t} \cdot \frac{\sigma^2}{2\beta})$
- $B \sim \mathcal{N}(0, \frac{\sigma^2}{2\beta}(1 - e^{-2\beta t}))$
- $A \perp B \Rightarrow A + B \sim \mathcal{N}(0, \text{sum of variances})$

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Above, the law of X_t does not depend on time, because we have started the process at the stationary distribution $\pi(x) = \mathcal{N}\left(0, \frac{\sigma^2}{2\beta}\right)$:

$$\text{If: } X_0 \sim \pi(x) \Rightarrow X_t \sim \pi(x) \quad \text{for all } t$$

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In general, for a $X_0 \sim \mathcal{N}(0, \sigma_0^2)$, we would have

$$X_t \sim \mathcal{N}\left(0,\ e^{-2\beta t}\sigma_0^2 + \frac{\sigma^2}{2\beta}(1 - e^{-2\beta t})\right).$$

Back to general Langevin diffusion

- We have spent quite a lot of time on Ornstein-Uhlenbeck (OU):

$$dx_t = -\beta x_t \, dt + \sigma \, dB_t$$

Solution:

$$x_t = e^{-\beta t} x_0 + \sigma e^{-\beta t} \int_0^t e^{\beta s} \, dB_s$$

Distribution:

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- Let's go back to a general Langevin diffusion :

$$\mathrm{d}x_t = -\nabla V(x_t) dt + \sqrt{2} \mathrm{d}B_t, \quad x_t \sim p_t$$

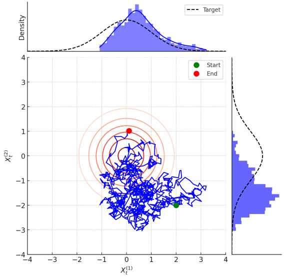
Solution:

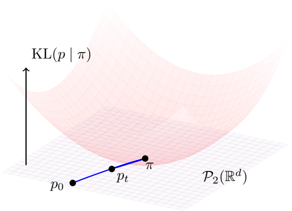
$$x_t = x_0 - \int_0^t \nabla V(x_s) ds + \sqrt{2} B_t,$$

- Remember that OU is a specific case of Langevin, where the target/stationary distribution is: $\pi = \mathcal{N}(0, \frac{\sigma^2}{2\beta})$, where $\pi(x) \propto \exp(-\frac{\beta \|x\|^2}{\sigma^2})$
- **for general Langevin, the stationary distribution is** $\pi \propto \exp(-V)$.

Langevin diffusion (and its discretized versions) is an example of a non-parametric method: we built a process $x_t \in \mathbb{R}^d$, whose distribution p_t converges to π as $t \to \infty$

- The law $(p_t)_{t \geq 0}$ of Langevin diffusion $(x_t)_{t \geq 0}$ is known to follow a gradient flow to minimize $\mathrm{D}(p|\pi) = \mathrm{KL}(p|\pi)$: $\mathrm{d}p_t = -\nabla_{W_2} \mathrm{KL}(p_t|\pi)\mathrm{d}t$ (see [1])



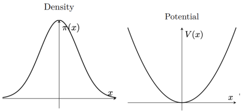


Recall above we plot $x_{t+1} = x_t + \gamma \nabla \log \pi(x_t) + \sqrt{2\gamma}\eta_t$ for $\pi \propto \exp(-\frac{\|x\|^2}{2})$, $x_0 \sim p_0$.

[1] Jordan, R., Kinderlehrer, D., & Otto, F. (1998). The variational formulation of the Fokker–Planck equation. SIAM journal on mathematical analysis.

When does Langevin diffusion's law converges (fast) to π?

- Consider a standard Gaussian distribution $\pi(x) \propto \exp(-\frac{\|x\|^2}{2})$, i.e. $\pi \propto \exp(-V)$ with V 1-strongly convex, i.e. π is (1-)strongly log-concave.



Then $\mathrm{KL}(p_t|\pi) = \exp(-2t)\,\mathrm{KL}(p_0|\pi)$.

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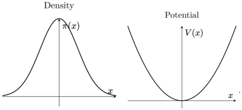

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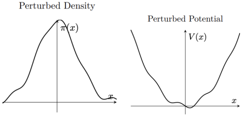
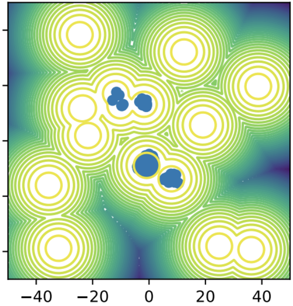
- If π is a perturbation of a strongly-log-concave distribution, then the rate degrades with the size of the perturbation.



(see Holley–Stroock theorem and log-Sobolev inequalities, (Bakry et al., 2014)).

Langevin in the multimodal case



Mixture of equally weighted 16 Gaussians with unit variance and uniformly chosen centers in $[-40, 40]^2$, a standard sampling benchmark. ULA was initialized with $\mathcal{N}(0, I_2)$, step-size $h = 0.01$. ULA was run with 5.10^4 steps (one minute run).

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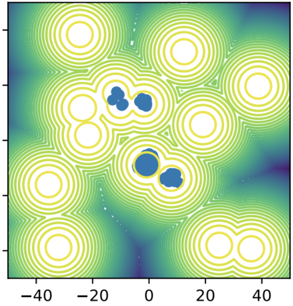

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The theoretical convergence is so slow, that in practice Langevin gets stuck for infinite time the modes close to its initialization !

Outline

Bayesian learning

Langevin

Bayesian deep learning

Recall Bayesian inference

Given labelled data $(w_i, y_i)_{i=1}^p$, we want to sample from the posterior distribution over the parameters of a model $g(\cdot, x)$

$$\pi(x) \propto \exp\left(-V(x)\right), \quad V(x) = \underbrace{\sum_{i=1}^{p} \|y_i - g(w_i, x)\|^2}_{\text{loss on labeled data } (w_i,\, y_i)_{i=1}^p} + \underbrace{\frac{\|x\|^2}{2}}_{\text{prior reg.}} .$$

I.e., $\pi(x) = \frac{\exp(-V(x))}{Z}$, $V(x) = -\log p(\mathcal{D}|x) - \log p_0(x)$ with Z intractable.

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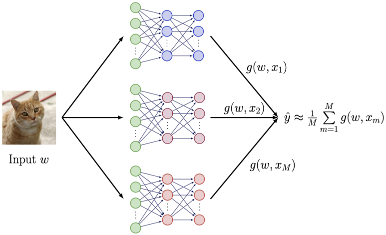
Ensemble prediction for an input w:

$$\hat{y} = \underbrace{\int_{\mathbb{R}^d} g(w, x) d\pi(x)}_{\text{"Bayesian model averaging"}}$$

Predictions of models parametrized by $x \in \mathbb{R}^d$ are reweighted by $\pi(x)$.



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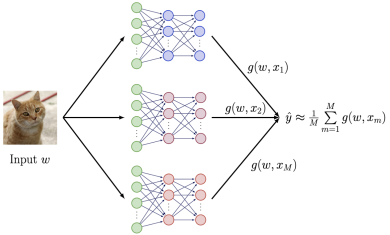

recall that a frequentist NN would predict $\hat{y} = g(w, x^*)$ where $x^* = \arg\max_{x \in \mathbb{R}^d} \log p(\mathcal{D}|x)$

Langevin for (Bayesian) deep NN?

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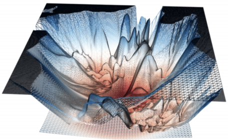


A highly nonconvex loss surface, as is common in deep neural nets. From `https://www.telesens.co/2019/01/16/neural-network-loss-visualization`.

Different strategies in practice/in the literature

Close to what we've seen previously:

- Stochastic Langevin dynamics: approximate $\nabla V(x) = \nabla \left(\sum_{i=1}^{p} \|y_i - g(w_i, x)\|^2 + \frac{\|x\|^2}{2} \right)$ by a batch of data samples $(w_i, y_i)_{i=1}^{m}$ with $m << p$
- Variational Inference

$$\text{find } q_\theta = \arg\min_{p \in P_\theta} \mathrm{KL}(p|\pi)$$

where P_θ is a family of parametric distributions (upcoming in few slides).

Different strategies in practice/in the literature

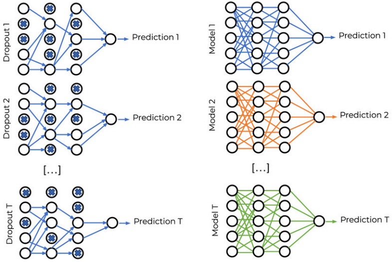
More heuristic:

- Monte Carlo Dropout

  Gal, Y., & Ghahramani, Z. (2016). Dropout as a bayesian approximation: Representing model uncertainty in deep learning. In international conference on machine learning.

- Deep ensembles

  Lakshminarayanan, B., Pritzel, A., & Blundell, C. (2017). Simple and scalable predictive uncertainty estimation using deep ensembles. Advances in neural information processing systems.



(a) MC Dropout (b) Ensemble Method

Variational Inference for BNN - Bayes by Backprop example

Variational Inference

$$\text{find } q_\theta = \arg\min_{p \in P_\theta} \mathrm{KL}(p|\pi)$$

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where P_θ is a family of parametric distributions.

A typical neural network of depth L (with non-linearity $h(\cdot)$) for input w and parameter x writes:

$$g(w,x) = A^L h\left(A^{L-1} h\left(\dots h\left(A^1 w + b^1\right)\right) + b^{L-1}\right) + b^L,$$

$$h^l = h(A^l h^{l-1} + b^l), \quad h^1 = h(A^1 w + b^1).$$

Neural network parameters: $x = \{A^l, b^l\}_{l=1}^L$.

We will describe the approach of "**Bayes by Backprop**"[1].

Blundell, C., Cornebise, J., Kavukcuoglu, K., & Wierstra, D. (2015). Weight uncertainty in neural network. In International conference on machine learning.

Step 1: Construct the $q_\theta(x) \approx p(x \mid \mathcal{D}) = \pi(x)$ Distribution

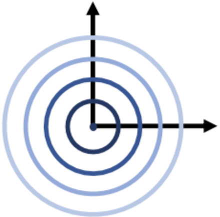
Example: Mean-field (="factorized") Gaussian distribution:

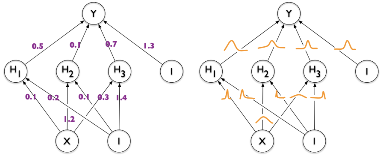
$$q_\theta = \prod_{l=1}^{L} q(A^l)\, q(b^l)$$

$$q(A_l) = \prod_{ij} q(A^l_{ij}), \quad q(A^l_{ij}) = \mathcal{N}(A^l_{ij}; M^l_{ij}, V^l_{ij})$$

$$q(b^l) = \prod_{i} q(b^l_{i}), \quad q(b^l_{i}) = \mathcal{N}(b^l_{i}; m^l_{i}, v^l_{i})$$

Variational parameters: $\theta = \left\{M^l_{ij}, V^l_{ij}, m^l_i, v^l_i\right\}_{l=1}^{L}$





In dimension two, a simple example of q_θ is a factorized Gaussian:

$$q_\theta(A^1_{11}, A^1_{12}) = \mathcal{N}(A^1_{11}; 0, 1) \cdot \mathcal{N}(A^1_{12}; 0, 1),$$

where q_θ is the product of two independent standard normal distributions over the parameters A^1_{11} and A^1_{12}.

Note that the "factor" assumption in mean-field decorrelates variables.

Step 2: Fit the q_θ Distribution

Variational inference: $\theta^* = \arg\max L(\theta)$ where L is the ELBO

$$L(\theta) = \mathbb{E}_{q_\theta}[\log p(D \mid x)] - \mathrm{KL}[q_\theta \parallel p_0(x)]$$

First scalable technique: Stochastic optimization

- i.i.d. assumption: $\log p(D \mid x) = \sum_{i=1}^{N} \log p(y_i \mid w_i, x)$
- Mini-batch training: $\{(w_m, y_m)\}_{m=1}^{M} \sim D^M$

$$L(\theta) \approx \frac{N}{M} \sum_{i=1}^{M} \mathbb{E}_{q_\theta}[\log p(y_i \mid w_i, x)] - \mathrm{KL}[q_\theta \parallel p_0(x)]$$

Reweighting to ensure calibrated posterior concentration.

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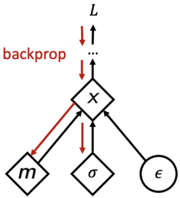
2nd Scalable Technique: Monte Carlo Sampling

- $\mathbb{E}_{q_\theta}[\log p(y \mid w, x)]$ is intractable even with Gaussian q_θ
- Solution: Monte Carlo estimate:

$$\mathbb{E}_{q_\theta}[\log p(y \mid w, x)] \approx \frac{1}{K}\sum_{k=1}^{K} \log p(y \mid w, x_k), \quad x_k \sim q_\theta$$



- Reparameterization trick to sample from mean-field Gaussians:

$$x_k = m_\theta + \sigma_\theta \odot \epsilon_k, \quad \epsilon_k \sim \mathcal{N}(0, I)$$

- Therefore:

$$\mathbb{E}_{q_\theta}[\log p(y \mid w, x)] \approx \frac{1}{K}\sum_{k=1}^{K} \log p(y \mid w, x_k), \; x_k = m_\theta + \sigma_\theta \epsilon_k$$

Combining both steps and final prediction

Full ELBO approximation:

$$L(\theta) \approx \frac{N}{M} \sum_{m=1}^{M} \frac{1}{K} \sum_{k=1}^{K} \log p(y_m \mid w_m, x_k) - \mathrm{KL}[q_\theta \,\|\, p(x)], \quad x_k \sim q_\theta$$

analytic between two Gaussians (if not, can also be estimated with Monte Carlo)

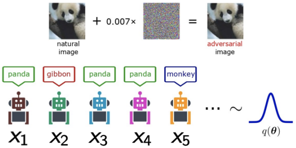
In regression: $p(y \mid w, x) = \mathcal{N}(f_x(w), \sigma^2)$,

In classification: $p(y \mid w, x) = \mathrm{Categorical}(\mathrm{logit} = f_x(w))$

Step 3: Compute Prediction with Monte Carlo Approximations

$$p(y^* \mid w^*, D) \approx \frac{1}{K} \sum_{k=1}^{K} p(y^* \mid w^*, x_k), \quad x_k \sim q_\theta$$

Mean-field Gaussian case: $x_k = m_\theta + \sigma_\theta \odot \epsilon_k, \quad \epsilon_k \sim \mathcal{N}(0, I)$



References I

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