

# Variational inference

ELG 5218 - Uncertainty Evaluation in Engineering Measurements and Machine Learning

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# Outline

## 1 Gradients

- Gradient Descent / SGD
- Stochastic Optimization (SGD)
- Automatic Differentiation (Autodiff)

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## 5 Stochastic (Black-box) VI

## 6 Pathwise gradients of ELBO

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Notebook: From\_entropy\_to\_Advi.ipynb

# Gradients

- Gradients: definition, geometry, and why VI needs them
- Gradient descent / ascent and stochastic gradients
- Expectations inside objectives (Monte Carlo estimation)
- Automatic differentiation intuition (computation graphs)
- Mini-VI example: optimizing an ELBO for a Gaussian variational posterior

# Gradients: the basic object

A **gradient** of a scalar function  $f(\theta)$  with respect to parameters  $\theta \in \mathbb{R}^d$  is

$$\nabla_{\theta} f(\theta) = \begin{bmatrix} \partial f / \partial \theta_1 \\ \vdots \\ \partial f / \partial \theta_d \end{bmatrix}.$$

## Key geometry:

- $\nabla f$  points in the direction of *steepest increase*
- $-\nabla f$  points in the direction of *steepest decrease*

## Quick example

Let  $f(\theta) = (\theta - 5)^2$ . Then

$$\frac{d}{d\theta} f(\theta) = 2(\theta - 5).$$

- If  $\theta < 5$ , the gradient is negative  $\Rightarrow$  increase  $\theta$
- If  $\theta > 5$ , the gradient is positive  $\Rightarrow$  decrease  $\theta$

# Gradient descent vs ascent

**Minimize**  $f(\theta)$  (gradient descent):

$$\theta \leftarrow \theta - \eta \nabla_{\theta} f(\theta)$$

**Maximize**  $\mathcal{L}(\theta)$  (gradient ascent):

$$\theta \leftarrow \theta + \eta \nabla_{\theta} \mathcal{L}(\theta)$$

In VI we usually **maximize the ELBO**, so we do **ascent** (or minimize the negative ELBO).

# Example: gradient descent trajectory

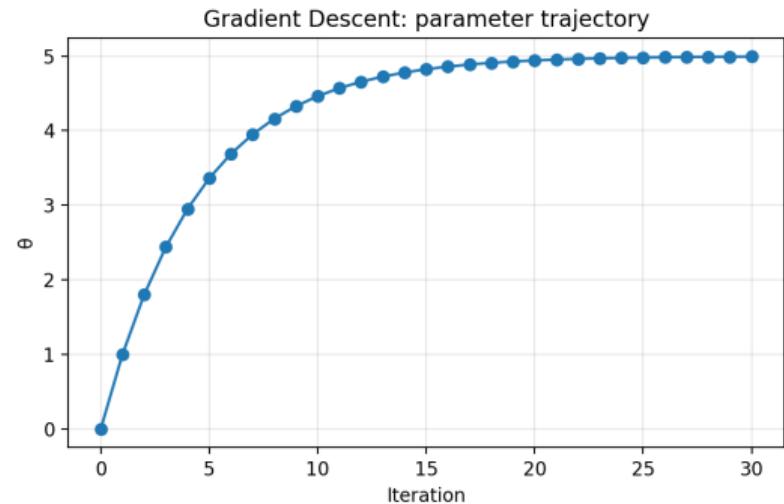
We minimize  $f(\theta) = (\theta - 5)^2$ .

- **Gradient descent update:**

$$\theta_{k+1} = \theta_k - \eta \nabla f(\theta_k) = \theta_k - \eta 2(\theta_k - 5).$$

- Figure shows the iterates  $\theta_k$  converging to the minimizer:

$$\theta^* = 5.$$



# Definition: full gradient vs. stochastic gradient

Let the empirical risk be

$$f(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(\theta; x_i, y_i).$$

**Full (batch) gradient:**

$$\nabla f(\theta) = \frac{1}{n} \sum_{i=1}^n \nabla_{\theta} \ell(\theta; x_i, y_i).$$

**Stochastic gradient (single sample):** pick  $i_t$  and use

$$g_t = \nabla_{\theta} \ell(\theta_t; x_{i_t}, y_{i_t}), \quad \theta_{t+1} = \theta_t - \eta_t g_t.$$

**Key property (typical assumption):**  $g_t$  is an *unbiased* estimator:

$$\mathbb{E}[g_t | \theta_t] = \nabla f(\theta_t) \quad (\text{true under uniform sampling with replacement}).$$

# Mini-batch stochastic gradient (batch size $k$ )

Pick a mini-batch  $B_t \subset \{1, \dots, n\}$  with  $|B_t| = k$  and use

$$g_t = \frac{1}{k} \sum_{i \in B_t} \nabla_{\theta} \ell(\theta_t; x_i, y_i), \quad \theta_{t+1} = \theta_t - \eta_t g_t.$$

- **Variance reduction:** gradient noise typically decreases as  $\approx 1/k$  (up to finite-population corrections).
- **Compute tradeoff:** each step costs  $k$  examples, but can be faster in wall-clock time on GPUs/TPUs.
- **Two common sampling modes:**
  - *With replacement:* indices i.i.d. uniform each step (clean analysis).
  - *Without replacement within an epoch:* shuffle once per epoch, then take consecutive slices of the shuffled order (common in ML code).

# What parameters do you choose in SGD?

## Core knobs

- **Batch size  $k$  (or  $B$ ):** e.g., 1, 32, 128, 1024.
- **Learning rate  $\eta$  and schedule:** constant, step decay, cosine, warmup, etc.
- **Number of epochs  $E$**  (passes through data) or total steps  $T$ .
- **Shuffling / sampling policy:** shuffle each epoch; with/without replacement; sequential windows for time series.

## Common practical knobs (often essential in deep learning)

- **Momentum / Nesterov** (SGD variants).
- **Weight decay** (L2 regularization), dropout (model-level).
- **Gradient clipping** (stability), especially with RNNs/transfomers.
- **Early stopping** based on validation performance.

# Algorithm: shuffle each epoch + mini-batches (no replacement within epoch)

This is the standard training loop used in most ML frameworks when `shuffle=True`.

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## Algorithm 1 Mini-batch SGD with epoch shuffling (typical in ML)

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Dataset  $\{(x_i, y_i)\}_{i=1}^n$ , batch size  $k$ , epochs  $E$ , learning rates  $\{\eta_t\}$

Initialize parameters  $\theta$

**for**  $e = 1$  to  $E$  **do**

    Sample a random permutation  $\pi$  of  $\{1, \dots, n\}$  ▷ shuffle indices

**for**  $b = 1$  to  $\lceil n/k \rceil$  **do**

$B \leftarrow \{\pi[(b-1)k+1], \dots, \pi[\min(bk, n)]\}$  ▷ take next slice

$$g \leftarrow \frac{1}{|B|} \sum_{i \in B} \nabla_{\theta} \ell(\theta; x_i, y_i)$$

$$\theta \leftarrow \theta - \eta_t g$$

$$t \leftarrow t + 1$$

**end for**

**end for**

# Algorithm: mini-batch sampling with replacement

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**Algorithm 2** Mini-batch SGD with replacement (clean unbiased estimator)

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Dataset size  $n$ , batch size  $k$ , steps  $T$ , learning rates  $\{\eta_t\}$

Initialize parameters  $\theta$

**for**  $t = 0$  to  $T - 1$  **do**

    Sample indices  $i_{t,1}, \dots, i_{t,k} \stackrel{i.i.d.}{\sim} \text{Unif}(\{1, \dots, n\})$

$g \leftarrow \frac{1}{k} \sum_{j=1}^k \nabla_{\theta} \ell(\theta; x_{i_{t,j}}, y_{i_{t,j}})$

$\theta \leftarrow \theta - \eta_t g$

**end for**

---

Batch size  $k = 1$

Set  $k = 1$  in either algorithm to obtain “single-sample” SGD.

# Automatic Differentiation (autodiff) and its relation to SGD

**Definition (autodiff).** Automatic differentiation is a set of techniques that compute *exact derivatives* (of a function implemented as code) by applying the chain rule to the program's computational graph. Unlike:

- *symbolic differentiation* (manipulates formulas), and
- *numerical differentiation* (finite differences, approximate),

autodiff produces derivatives accurate up to floating-point rounding.

## Forward and reverse mode.

- **Forward-mode:** efficient when #inputs is small.
- **Reverse-mode (backpropagation):** efficient when #outputs is small (e.g., scalar loss).

**How autodiff connects to batch vs. stochastic gradients.** Let the empirical risk be

$$f(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(\theta; x_i, y_i).$$

Autodiff is the engine that computes  $\nabla_{\theta} \ell(\theta; x_i, y_i)$  for whatever data you feed in.

- **Full-batch GD:** feed all  $n$  points, autodiff returns  $\nabla f(\theta)$ .
- **Mini-batch SGD:** feed a batch  $B$  of size  $k$ , autodiff returns

$$\nabla_{\theta} \left( \frac{1}{k} \sum_{i \in B} \ell(\theta; x_i, y_i) \right) = \frac{1}{k} \sum_{i \in B} \nabla_{\theta} \ell(\theta; x_i, y_i).$$

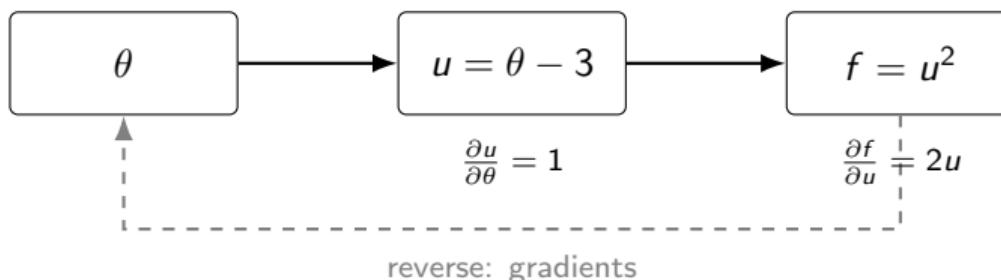
**Key takeaway:** Autodiff computes gradients; batching controls which data points contribute to the gradient estimate.

# Autodiff (reverse-mode): forward values + reverse gradients on a computation graph

**What we want.** Compute  $\nabla_{\theta} f(\theta)$  automatically.

**Idea.** Autodiff builds a *computation graph* of elementary operations.

- **Forward pass:** compute and store intermediate values.
- **Reverse pass (backprop):** propagate sensitivities using the chain rule.



**Example.**  $f(\theta) = (\theta - 3)^2$ .

**Forward:**  $u = \theta - 3$ , then  $f = u^2$ .

**Reverse:**

$$\frac{df}{d\theta} = \frac{df}{du} \frac{du}{d\theta} = (2u) \cdot 1 = 2(\theta - 3).$$

**Takeaway.** Reverse-mode autodiff computes gradients efficiently by reusing stored forward values and applying the chain rule backward.

# Shannon Entropy: Definition

## Discrete random variable

Let  $X$  be a discrete random variable taking values  $x_1, \dots, x_n$  with probabilities  $p_i = \mathbb{P}(X = x_i)$  and  $\sum_{i=1}^n p_i = 1$ .

The **Shannon entropy** of  $X$  (in base  $b$ ) is

$$H_b(X) = - \sum_{i=1}^n p_i \log_b p_i.$$

- If we use  $\log_2$ , the units are **bits**.
- If  $X$  is deterministic (one outcome has probability 1), then  $H(X) = 0$ .
- Entropy measures the **average uncertainty** about  $X$ .

# Entropy as Uncertainty

- High entropy  $\Rightarrow$  outcomes are hard to predict.
- Low entropy  $\Rightarrow$  outcomes are more predictable.

## Example: coin toss

- Fair coin:  $p(H) = p(T) = 0.5$ .

$$H(X) = -[0.5 \log_2 0.5 + 0.5 \log_2 0.5] = 1 \text{ bit.}$$

- Biased coin:  $p(H) = 0.9$ ,  $p(T) = 0.1$ .

$$H(X) = -[0.9 \log_2 0.9 + 0.1 \log_2 0.1] \approx 0.47 \text{ bits.}$$

The biased coin is more predictable, so its entropy is smaller.

# Discrete Examples

## Fair die and non-uniform distribution

- Fair 4-sided die:  $p_i = 0.25$  for  $i = 1, \dots, 4$ .

$$H(X) = -4 \cdot 0.25 \log_2 0.25 = 2 \text{ bits.}$$

- Fair 6-sided die:  $p_i = 1/6$ .

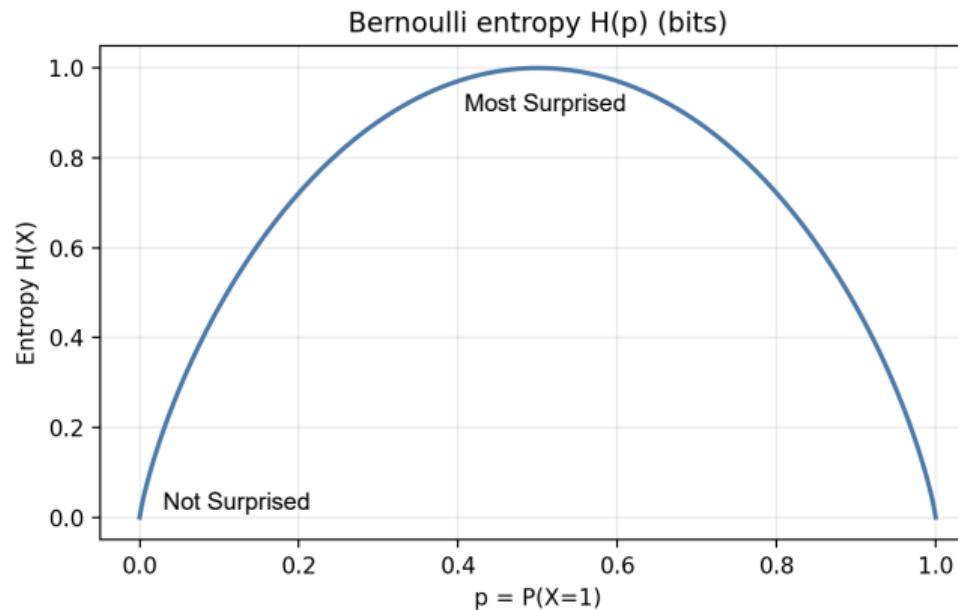
$$H(X) = -\sum_{i=1}^6 \frac{1}{6} \log_2 \frac{1}{6} = \log_2 6 \approx 2.585 \text{ bits.}$$

- Non-uniform (0.5, 0.25, 0.25):

$$H(X) = -[0.5 \log_2 0.5 + 0.25 \log_2 0.25 + 0.25 \log_2 0.25] = 1.5 \text{ bits.}$$

- More spread-out distributions (for fixed support) have higher entropy.
- More “peaked” distributions have lower entropy.

# Bernoulli entropy example



Entropy is maximal at  $p = 0.5$  (most uncertain).

# Uniform Distribution and Maximum Entropy

Consider all discrete distributions on a finite set  $\{x_1, \dots, x_n\}$ :

$$\mathcal{P} = \left\{ (p_1, \dots, p_n) : p_i \geq 0, \sum_{i=1}^n p_i = 1 \right\}.$$

## Maximum entropy principle (discrete case)

Among all  $(p_1, \dots, p_n) \in \mathcal{P}$ , entropy

$$H(X) = - \sum_{i=1}^n p_i \log p_i$$

is **maximized** when

$$p_i = \frac{1}{n}, \quad i = 1, \dots, n.$$

In this case,  $H(X) = \log n$  (in the same log base).

- The uniform distribution represents **maximal uncertainty** when only the support size  $n$  is known.
- Any deviation from uniformity makes outcomes more predictable and reduces entropy.

# Differential Entropy and the Normal Distribution

For a continuous random variable  $X$  with density  $p(x)$ , the **differential entropy** (in nats meaning that the  $\log = \ln$ ) is

$$h(X) = - \int_{-\infty}^{\infty} p(x) \log p(x) dx.$$

## Entropy of a normal distribution

If  $X \sim \mathcal{N}(\mu, \sigma^2)$ , then

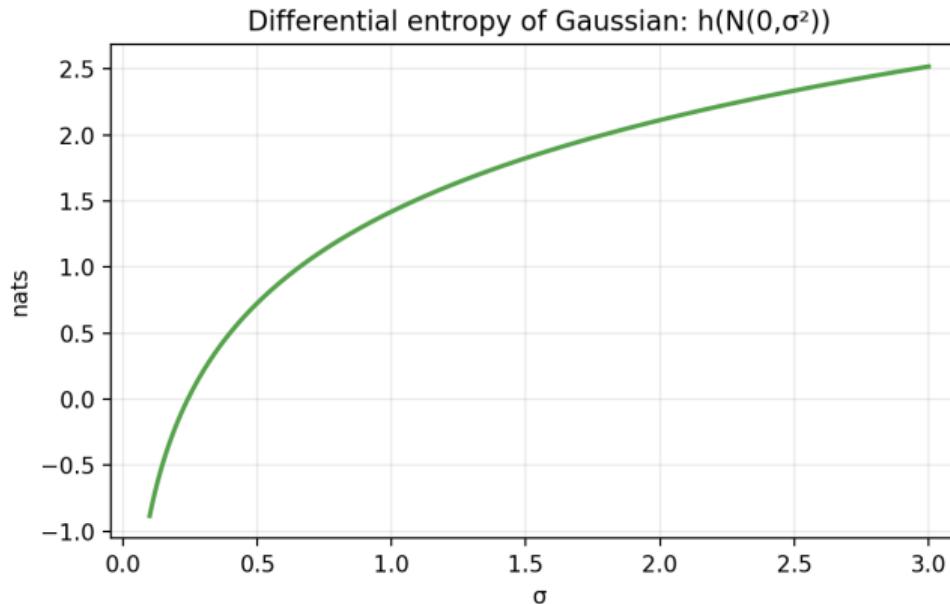
$$h(X) = \frac{1}{2} \log (2\pi e \sigma^2).$$

## Maximum entropy principle (continuous case)

Among all real-valued random variables with a given mean  $\mu$  and variance  $\sigma^2$ , the normal distribution  $\mathcal{N}(\mu, \sigma^2)$  has the **largest** differential entropy.

- The normal distribution is the “most spread out” shape compatible with the specified mean and variance.

# Gaussian differential entropy



Larger  $\sigma$  means a more spread-out distribution and higher entropy.

# Kullback–Leibler divergence Definition (Discrete Case)

Let  $P$  and  $Q$  be two discrete probability distributions on the same support  $\{x_1, \dots, x_n\}$  with

$$p_i = P(x_i), \quad q_i = Q(x_i), \quad \sum_{i=1}^n p_i = \sum_{i=1}^n q_i = 1.$$

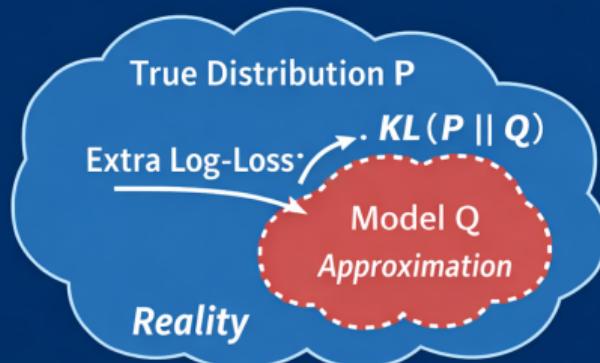
## Kullback–Leibler divergence

The KL divergence from  $Q$  to  $P$  is

$$\text{KL}(P\|Q) = \sum_{i=1}^n p_i \log \frac{p_i}{q_i}.$$

- Usually computed with  $\log_2$  (bits) or natural log (nats).
- $\text{KL}(P\|Q) \geq 0$  and equals 0 iff  $P = Q$ .
- Measures how different  $Q$  is from  $P$  when  $P$  is the *true* distribution.

## Intuition



- $P$  = True distribution
- $Q$  = Model / Approximation
- $KL(P \parallel Q)$  = Expected extra *log-loss* using  $Q$  instead of  $P$
- Large  $KL \rightarrow$  *Very wasteful encoding with  $Q$*
- Small  $KL \rightarrow$   *$Q$  close to  $P$*

### Asymmetry

$$KL(P \parallel Q) \neq KL(Q \parallel P).$$

Changing the roles of “true” and “model” matters.

# Entropy, Cross-Entropy, and KL as *Expected Log-Loss*

**Setup.** Reality generates outcomes  $i$  from the true distribution  $P$  (probabilities  $p_i$ ). We predict using a model  $Q$  (probabilities  $q_i$ ). Consider the **log-loss** (negative log-likelihood) for outcome  $i$ :  $\ell_Q(i) = -\log q_i$ .

## Interpretations

- **Entropy:**

$$H(P) = - \sum_i p_i \log p_i = \mathbb{E}_{i \sim P}[-\log p_i]$$

is the *irreducible average uncertainty/surprise* in outcomes drawn from  $P$ .

- **Cross-entropy:**

$$H(P, Q) = - \sum_i p_i \log q_i = \mathbb{E}_{i \sim P}[-\log q_i]$$

is the *average log-loss you incur* when using model  $Q$  on data from  $P$ .

## Decomposition (mismatch penalty)

$$\text{KL}(P\|Q) = \sum_i p_i \log \frac{p_i}{q_i} = H(P, Q) - H(P).$$

- $\text{KL}(P\|Q)$ : **extra expected log-loss** due to using the wrong probabilities  $Q$ .

# Example: Bernoulli Distributions

Let  $P = \text{Ber}(p)$  and  $Q = \text{Ber}(q)$  on  $\{0, 1\}$ :

$$P(X = 1) = p, \quad P(X = 0) = 1 - p,$$

$$Q(X = 1) = q, \quad Q(X = 0) = 1 - q.$$

## Closed form

$$\text{KL}(P\|Q) = p \log \frac{p}{q} + (1 - p) \log \frac{1 - p}{1 - q}.$$

- If  $p = q$  then  $\text{KL}(P\|Q) = 0$ .
- If  $q$  is far from  $p$  (e.g.  $p = 0.9, q = 0.1$ ), the divergence becomes large.
- If  $q = 0$  but  $p > 0$  (or vice versa), the divergence is *infinite*:  $Q$  assigns probability 0 to an event that actually occurs.

# Discrete Examples

## Two-outcome example

Let

$$P = (0.6, 0.4), \quad Q = (0.5, 0.5).$$

Then

$$\text{KL}(P\|Q) = 0.6 \log \frac{0.6}{0.5} + 0.4 \log \frac{0.4}{0.5}.$$

Numerically (base 2):  $\text{KL}(P\|Q) \approx 0.029$  bits.

## Three-outcome example

Let

$$P = (0.6, 0.3, 0.1), \quad Q = (0.5, 0.25, 0.25).$$

Then  $\text{KL}(P\|Q) \approx 0.066$  bits, while  $\text{KL}(Q\|P) \approx 0.084$  bits.

These values are small:  $Q$  is reasonably close to  $P$ , but not identical.

## Continuous Case (Briefly)

For continuous distributions with densities  $p(x)$  and  $q(x)$ , the KL divergence is

$$\text{KL}(P\|Q) = \int p(x) \log \frac{p(x)}{q(x)} dx.$$

- The same basic interpretation holds: difference in log-likelihood between the true density  $p$  and the model density  $q$ .
- For example, KL between two normal distributions has a closed-form expression.
- In practice, continuous KL is often approximated via Monte Carlo.

# Core properties

- **Non-negativity (Gibbs):**  $\text{KL}(p\|q) \geq 0$  and equals 0 iff  $p = q$  (a.e.).
- **Asymmetry:** generally  $\text{KL}(p\|q) \neq \text{KL}(q\|p)$ .
- **Support sensitivity:** if  $q(z) = 0$  where  $p(z) > 0$  then  $\text{KL}(p\|q) = \infty$ .

# Why order matters (intuition)

Compare

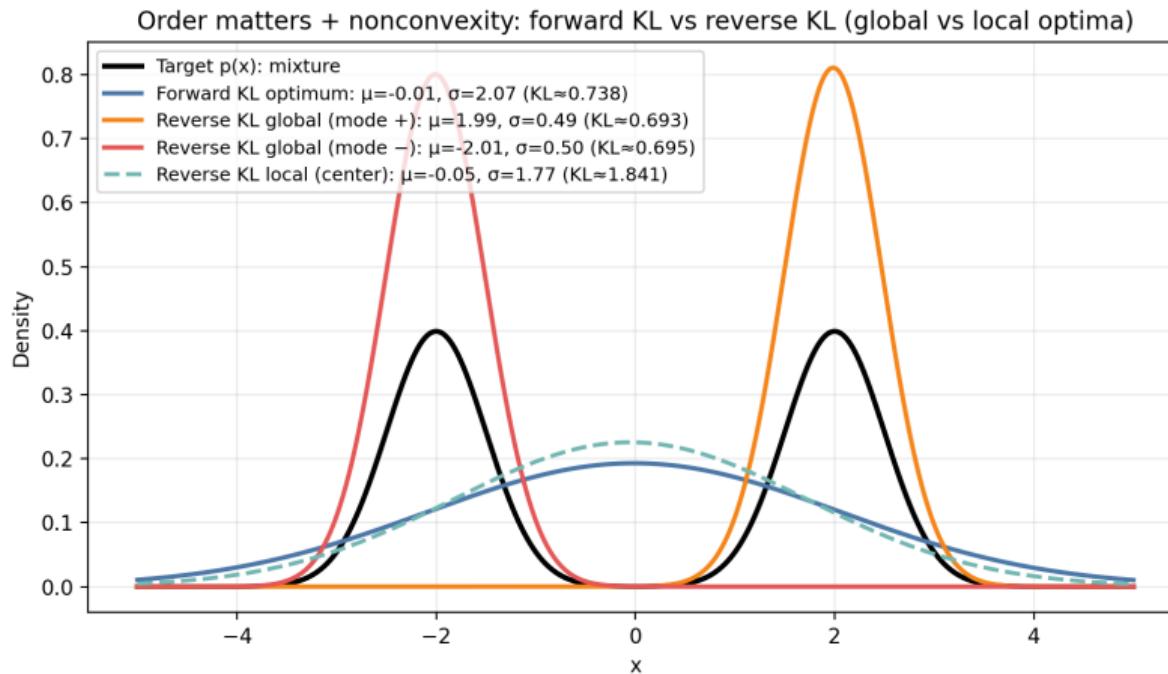
$$\text{KL}(p\|q) = \mathbb{E}_p[\log p - \log q] \quad \text{vs} \quad \text{KL}(q\|p) = \mathbb{E}_q[\log q - \log p].$$

- $\text{KL}(p\|q)$ : expectation under  $p \Rightarrow$  penalizes  $q$  for missing any region where  $p$  has mass (**mass-covering**).
- $\text{KL}(q\|p)$ : expectation under  $q \Rightarrow$  penalizes  $q$  for placing mass where  $p$  is tiny (**mode-seeking**).

**Rule of thumb (global optima):** forward KL tends to *cover modes*; reverse KL tends to *choose a mode*.

**Example:** Target:  $p(x) = 0.5 \mathcal{N}(-2, 0.5^2) + 0.5 \mathcal{N}(2, 0.5^2)$ . Approximation family:  $q(x) = \mathcal{N}(\mu, \sigma^2)$ . We'll optimize forward and reverse KL.

# Bimodal example (corrected): global vs local optima



Reverse KL has two global minima (one per mode) and a higher-cost local optimum near the center.

# Why VI uses reverse KL $\text{KL}(q\|p(z | x))$

Variational inference chooses  $q_\lambda(z)$  and minimizes

$$\text{KL}(q_\lambda(z)\|p(z | x)).$$

This direction is convenient because the expectation is under  $q$ :

- we can sample from  $q$  and evaluate  $\log p$  up to a constant,
- this yields the ELBO objective.

**Consequence:** mode-seeking behavior can cause *mode dropping* for multi-modal posteriors.

# Cross-Entropy and NLL in Classification (Derivation)

## Setup.

- True data distribution:  $p_{\text{data}}(x, y)$ .
- Model: conditional probabilities  $p_\theta(y | x)$ .
- Per-example negative log-likelihood (NLL):  
Minimize Log Likelihood

$$\text{NLL}(x, y) = -\log p_\theta(y | x).$$

## Expected NLL under the true distribution:

$$\mathbb{E}_{(X, Y) \sim p_{\text{data}}} [\text{NLL}(X, Y)] = \mathbb{E}_{p_{\text{data}}(x, y)} [-\log p_\theta(y | x)].$$

We can write this as a two-step expectation:

$$\begin{aligned}\mathbb{E}_{p_{\text{data}}(x, y)} [-\log p_\theta(y | x)] &= \mathbb{E}_{p_{\text{data}}(x)} \left[ \mathbb{E}_{p_{\text{data}}(y|x)} [-\log p_\theta(y | x)] \right] \\ &= \mathbb{E}_{p_{\text{data}}(x)} \left[ H(p_{\text{data}}(\cdot | x), p_\theta(\cdot | x)) \right],\end{aligned}$$

where for each fixed  $x$  we define the *cross-entropy*

$$H(p_{\text{data}}(\cdot | x), p_\theta(\cdot | x)) = - \sum_y p_{\text{data}}(y | x) \log p_\theta(y | x).$$

# Cross-Entropy, Entropy, KL and NLL (General Case)

For each fixed  $x$ , we have the identity

$$H(p_{\text{data}}(\cdot | x), p_{\theta}(\cdot | x)) = H(p_{\text{data}}(\cdot | x)) + \text{KL}(p_{\text{data}}(\cdot | x) \| p_{\theta}(\cdot | x)),$$

where

$$H(p_{\text{data}}(\cdot | x)) = - \sum_y p_{\text{data}}(y | x) \log p_{\text{data}}(y | x)$$

is the (conditional) entropy of the true labels given  $x$ .

Taking expectation over  $x$ :

$$\mathbb{E}_{p_{\text{data}}(x,y)}[-\log p_{\theta}(y | x)] = H_{p_{\text{data}}}(Y | X) + \mathbb{E}_{p_{\text{data}}(x)}[\text{KL}(p_{\text{data}}(\cdot | x) \| p_{\theta}(\cdot | x))],$$

where

$$H_{p_{\text{data}}}(Y | X) = \mathbb{E}_{p_{\text{data}}(x)}[H(p_{\text{data}}(\cdot | x))].$$

## Interpretation and generality

- $H_{p_{\text{data}}}(Y | X)$ : intrinsic label uncertainty (Bayes error).
- The KL term: how far the model  $p_{\theta}(y | x)$  is from the true conditional  $p_{\text{data}}(y | x)$ .
- This derivation is valid for *any discrete label space*: binary, multi-class, or any finite set.

# Setup and Notation for Variational Inference

We consider a probabilistic model with:

- Latent variable  $z$
- Observed data  $x$
- Joint distribution  $p(x, z)$
- Posterior distribution  $p(z | x)$

## Key quantities

- **Posterior:**

$$p(z | x) = \frac{p(x, z)}{p(x)}.$$

- **Evidence (marginal likelihood):**

$$p(x) = \int p(x, z) dz.$$

In many interesting models,  $p(z | x)$  is intractable. **Variational inference (VI)** approximates  $p(z | x)$  with a simpler distribution  $q(z)$  and finds the best  $q$  by optimization.

# Introducing a Variational Distribution

We want to approximate the posterior  $p(z | x)$ .

- Choose a variational family  $\mathcal{Q} = \{q(z; \lambda)\}$ , e.g. Gaussians with parameters  $\lambda$ .
- Goal: find  $q^*(z) \in \mathcal{Q}$  that is as close as possible to the true posterior by finding the optimal value of  $\lambda$ :  $q^*(z) = \arg \min_{\lambda} \text{KL}(q_{\lambda}(z) \| p(z | x))$

Start from the marginal likelihood:

$$\log p(x) = \log \int p(x, z) dz.$$

Multiply and divide by any density  $q(z)$ :

$$\log p(x) = \log \int q(z) \frac{p(x, z)}{q(z)} dz = \log \mathbb{E}_{q(z)} \left[ \frac{p(x, z)}{q(z)} \right].$$

Next: apply Jensen's inequality.

# Deriving the ELBO via Jensen's Inequality

Recall Jensen's inequality for a concave function  $f$ :

$$f(\mathbb{E}[Y]) \geq \mathbb{E}[f(Y)].$$

For  $f = \log$  (concave) and

$$Y = \frac{p(x, z)}{q(z)},$$

we obtain

$$\log \mathbb{E}_{q(z)} \left[ \frac{p(x, z)}{q(z)} \right] \geq \mathbb{E}_{q(z)} \left[ \log \frac{p(x, z)}{q(z)} \right].$$

Therefore

$$\begin{aligned} \log p(x) &= \log \mathbb{E}_{q(z)} \left[ \frac{p(x, z)}{q(z)} \right] \\ &\geq \mathbb{E}_{q(z)} [\log p(x, z) - \log q(z)]. \end{aligned}$$

## Evidence Lower Bound (ELBO)

$$\mathcal{L}(q) := \mathbb{E}_{q(z)} [\log p(x, z)] - \mathbb{E}_{q(z)} [\log q(z)],$$

so that

$$\log p(x) \geq \mathcal{L}(q).$$

# LogNormal example: Jensen quantities as functions of the parameter $s$

**Distribution.** Let  $X \sim \text{LogNormal}(m, s^2)$ , i.e.

$$\log X \sim \mathcal{N}(m, s^2), \quad X > 0.$$

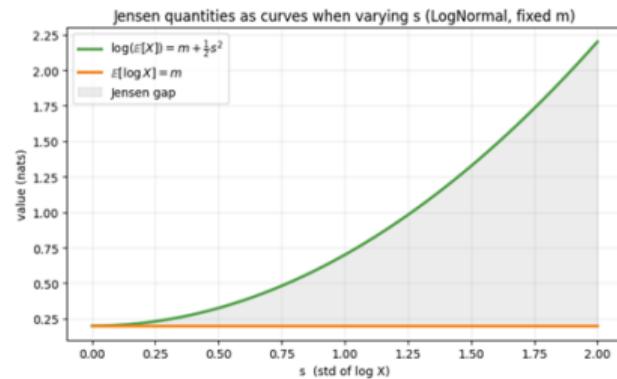
**Closed-form expectations (fix  $m$ ).**

- $\mathbb{E}[\log X] = m$  *(flat line in  $s$ )*
- $\mathbb{E}[X] = \exp(m + \frac{1}{2}s^2)$
- $\log(\mathbb{E}[X]) = m + \frac{1}{2}s^2$  *(curves upward in  $s$ )*

**Jensen gap.**

$$\log(\mathbb{E}[X]) - \mathbb{E}[\log X] = \frac{1}{2}s^2 \geq 0,$$

with equality only when  $s = 0$  (degenerate case).



# Jensen geometry for log: points at $x = \mathbb{E}[X]$ (as $x$ varies)

For any positive random variable  $X$  (with finite expectations),

$$\log(\mathbb{E}[X]) \geq \mathbb{E}[\log X].$$

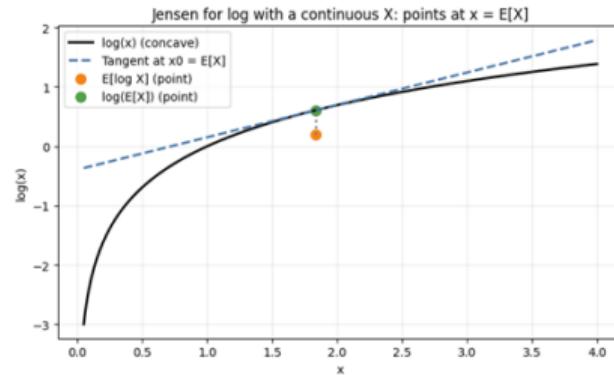
**Geometric proof idea (concavity).** Because  $\log$  is concave, the tangent line at  $x_0 = \mathbb{E}[X]$  lies above the curve:

$$\log(x) \leq \log(x_0) + \frac{1}{x_0}(x - x_0), \quad x_0 = \mathbb{E}[X].$$

Taking expectations of both sides gives Jensen's inequality. How

to read the plot.

- Both quantities are **single numbers** once the distribution is fixed.
- They are shown as two **points** at the same  $x = \mathbb{E}[X]$ :  $(\mathbb{E}[X], \mathbb{E}[\log X])$  and  $(\mathbb{E}[X], \log(\mathbb{E}[X]))$ .
- The vertical gap is  $\log(\mathbb{E}[X]) - \mathbb{E}[\log X] \geq 0$ .



- $\mathbb{E}[X] = 1.83$
- $\mathbb{E}[\log X] = 0.2$
- $\log(\mathbb{E}[X]) = 0.61$
- gap = 0.41

# Gap to evidence: $\log p(x) = \mathcal{L}(q) + \text{KL}(q(z) \| p(z | x))$

## Derivation

Start from the KL divergence to the true posterior:

$$\text{KL}(q(z) \| p(z | x)) = \mathbb{E}_q \left[ \log \frac{q(z)}{p(z | x)} \right] = \mathbb{E}_q[\log q(z)] - \mathbb{E}_q[\log p(z | x)].$$

Use Bayes' rule  $p(z | x) = \frac{p(x, z)}{p(x)}$ , so  $\log p(z | x) = \log p(x, z) - \log p(x)$ . Plug in:

$$\text{KL}(q \| p(\cdot | x)) = \mathbb{E}_q[\log q(z)] - \mathbb{E}_q[\log p(x, z) - \log p(x)] = \mathbb{E}_q[\log q(z)] - \mathbb{E}_q[\log p(x, z)] + \log p(x).$$

Rearrange:

$$\log p(x) = \underbrace{\mathbb{E}_q[\log p(x, z)] - \mathbb{E}_q[\log q(z)]}_{\mathcal{L}(q)} + \text{KL}(q(z) \| p(z | x)).$$

## Key takeaway

Since  $\text{KL}(\cdot) \geq 0$ , we have  $\log p(x) \geq \mathcal{L}(q)$ , and maximizing the ELBO is equivalent to minimizing  $\text{KL}(q(z) \| p(z | x))$ .

# Alternative Form of the ELBO

Decompose the joint:

$$\log p(x, z) = \log p(x | z) + \log p(z).$$

Plug into the ELBO:

$$\begin{aligned}\mathcal{L}(q) &= \mathbb{E}_{q(z)}[\log p(x, z)] - \mathbb{E}_{q(z)}[\log q(z)] \\ &= \mathbb{E}_{q(z)}[\log p(x | z)] + \mathbb{E}_{q(z)}[\log p(z)] - \mathbb{E}_{q(z)}[\log q(z)] \\ &= \mathbb{E}_{q(z)}[\log p(x | z)] - \text{KL}(q(z) \| p(z)).\end{aligned}$$

## Interpretation

- Minimizing  $\mathcal{L}(q)$  will give a  $q$  that explains data well ( $\mathbb{E}_{q(z)}[\log p(x | z)]$ ) and is close to the prior ( $\text{KL}(q(z) \| p(z))$ ).
- $\mathbb{E}_{q(z)}[\log p(x | z)]$  is the expected log-likelihood under the variational posterior.
- $\text{KL}(q(z) \| p(z))$  penalizes deviation from the prior.
- VI trades off data fit vs. regularization toward the prior.

# Mean-field approximation (independence)

**Mean-field** assumes independence among latent components:

$$q(z) = \prod_{i=1}^m q_i(z_i).$$

**Why it matters:**

- Makes expectations under  $q$  easier (breaks high-dimensional integrals).
- Enables **coordinate ascent** updates with closed forms in conjugate models.
- Scales to large latent spaces.

**Cost:** ignores posterior dependencies/correlations  $\Rightarrow$  can underestimate uncertainty.

# Coordinate ascent update (mean-field VI)

If  $q(z) = \prod_i q_i(z_i)$ , the ELBO is maximized by updating one factor at a time:

$$\log q_i^*(z_i) = \mathbb{E}_{q_{-i}}[\log p(x, z)] + \text{const},$$

where  $q_{-i}$  denotes all factors except  $i$ .

**Intuition:** each factor matches the conditional structure of the model, averaged over the other variables.

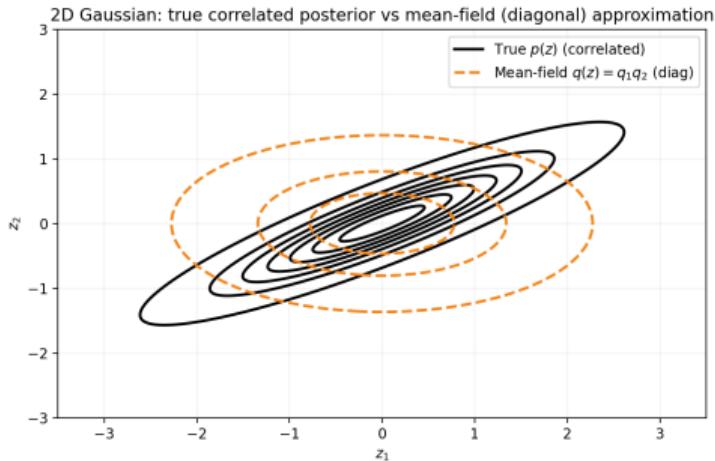
# Correlated posterior vs mean-field: geometry of uncertainty (contours)

**Setup.** True posterior:  $p(z) = \mathcal{N}(0, \Sigma)$  with correlation. Mean-field Gaussian:  $q(z) = \mathcal{N}(0, \Sigma_q)$  with  $\Sigma_q$  diagonal (equivalently  $q(z) = q_1(z_1)q_2(z_2)$ ).

**What we expect.** Correlation rotates the principal axes of uncertainty:

- correlated Gaussian  $\Rightarrow$  **tilted ellipses** (off-axis principal components),
- diagonal covariance  $\Rightarrow$  **axis-aligned ellipses** (no tilt).

- **Observed:** black contours (true  $p$ ) are tilted.
- **Observed:** dashed contours (mean-field  $q$ ) are axis-aligned.
- **Meaning:**  $q$  cannot “rotate” to match  $p$  because independence forbids correlation.



**Takeaway.** Mean-field captures some spread but misses joint structure  $\Rightarrow$  biased uncertainty and wrong dependence.

# Fixed-form variational inference (beyond mean-field)

- The independence assumption in *mean-field* VI can be restrictive.
- **Fixed-form VI:** choose a parametric family  $q_\lambda(z)$  with variational parameters  $\lambda$ .
- Optimize the approximation by solving

$$\lambda^* \in \arg \min_{\lambda} \text{KL}(q_\lambda(z) \| p(z | x)).$$

- In practice we maximize a tractable lower bound (the ELBO) instead of working directly with  $\log p(x)$ .

## Examples of fixed-form families $q_\lambda(z)$

- **Full Gaussian:**  $q_\lambda(z) = \mathcal{N}(z | \mu, \Sigma)$ ,  $\lambda = (\mu, L)$  with  $\Sigma = LL^\top$  (Cholesky).
- **Low-rank + diagonal:**  $q_\lambda(z) = \mathcal{N}(z | \mu, aa^\top + D)$ ,  $\lambda = (\mu, a, d)$ ,  $D = \text{Diag}(d)$ .
- **Richer:** mixtures of Gaussians, flows, etc.

# Fixed-form VI: gradient-based optimization of the ELBO

**Objective (ELBO).** Define

$$\mathcal{L}(\lambda) \equiv \mathcal{L}(q_\lambda) := \mathbb{E}_{q_\lambda(z)}[\log p(x, z)] - \mathbb{E}_{q_\lambda(z)}[\log q_\lambda(z)] = \mathbb{E}_{q_\lambda(z)}\left[\log \frac{p(x, z)}{q_\lambda(z)}\right].$$

## Gradient ascent

For  $t = 0, 1, 2, \dots$  until convergence:

$$\lambda^{(t+1)} = \lambda^{(t)} + a_t \nabla_\lambda \mathcal{L}(\lambda^{(t)}), \quad a_t > 0.$$

Stop e.g. when the change in the objective is small:

$$|\mathcal{L}(\lambda^{(t+1)}) - \mathcal{L}(\lambda^{(t)})| < \varepsilon.$$

**Link to your “gap” slide:**  $\log p(x) = \mathcal{L}(q_\lambda) + \text{KL}(q_\lambda(z) \| p(z | x))$ , so maximizing  $\mathcal{L}$  is equivalent to minimizing the KL gap.

# Gradient of the ELBO is an expectation (score-function form)

Define

$$h_\lambda(z) := \log p(x, z) - \log q_\lambda(z) \implies \mathcal{L}(\lambda) = \int q_\lambda(z) h_\lambda(z) dz.$$

## Derivation sketch (log-derivative trick)

$$\begin{aligned}\nabla_\lambda \mathcal{L}(\lambda) &= \nabla_\lambda \int q_\lambda(z) h_\lambda(z) dz = \int \nabla_\lambda (q_\lambda(z) h_\lambda(z)) dz \\ &= \int \left( (\nabla_\lambda q_\lambda(z)) h_\lambda(z) + q_\lambda(z) \nabla_\lambda h_\lambda(z) \right) dz.\end{aligned}$$

Since  $\nabla_\lambda h_\lambda(z) = -\nabla_\lambda \log q_\lambda(z)$  and  $\nabla_\lambda q_\lambda(z) = q_\lambda(z) \nabla_\lambda \log q_\lambda(z)$ , the second term cancels because

$$\int \nabla_\lambda q_\lambda(z) dz = \nabla_\lambda \int q_\lambda(z) dz = \nabla_\lambda 1 = 0.$$

Therefore,

$$\nabla_\lambda \mathcal{L}(\lambda) = \int q_\lambda(z) h_\lambda(z) \nabla_\lambda \log q_\lambda(z) dz = \mathbb{E}_{q_\lambda(z)} [h_\lambda(z) \nabla_\lambda \log q_\lambda(z)].$$

# VI via stochastic gradient ascent (Monte Carlo estimate)

From the previous slide,

$$\nabla_{\lambda} \mathcal{L}(\lambda) = \mathbb{E}_{q_{\lambda}(z)}[h_{\lambda}(z) \nabla_{\lambda} \log q_{\lambda}(z)], \quad h_{\lambda}(z) = \log p(x, z) - \log q_{\lambda}(z).$$

## Monte Carlo estimator

Draw  $z^{(1)}, \dots, z^{(S)} \sim q_{\lambda}(z)$  and estimate  $\widehat{\nabla}_{\lambda} \mathcal{L}(\lambda) = \frac{1}{S} \sum_{s=1}^S (h_{\lambda}(z^{(s)}) \nabla_{\lambda} \log q_{\lambda}(z^{(s)}))$ .

## Basic fixed-form VI algorithm (SGA)

- ① Initialize  $\lambda^{(0)}$ , choose step sizes  $\{a_t\}_{t \geq 0}$  and MC size  $S$ .
- ② For  $t = 0, 1, 2, \dots$ :
  - ① Sample  $z^{(1)}, \dots, z^{(S)} \sim q_{\lambda^{(t)}}(z)$ .
  - ② Compute  $\widehat{\nabla}_{\lambda} \mathcal{L}(\lambda^{(t)})$  using the MC estimator above.
  - ③ Update  $\lambda^{(t+1)} = \lambda^{(t)} + a_t \widehat{\nabla}_{\lambda} \mathcal{L}(\lambda^{(t)})$ .
- ④ Stop when a convergence criterion is met (e.g., stabilized  $\mathcal{L}$  or parameter changes).

# The requirements for inference (score-function / black-box VI)

Noisy (Monte Carlo) gradient of the ELBO:

$$\widehat{\nabla_{\lambda} \mathcal{L}}(\lambda) = \frac{1}{S} \sum_{s=1}^S \nabla_{\lambda} \log q_{\lambda}(z^{(s)}) \left( \log p(x, z^{(s)}) - \log q_{\lambda}(z^{(s)}) \right), \quad z^{(s)} \sim q_{\lambda}(z).$$

To compute the noisy gradient of the ELBO we need:

- Sampling from  $q_{\lambda}(z)$  (draw  $z^{(s)}$ ).
- Evaluating  $\nabla_{\lambda} \log q_{\lambda}(z)$  (score function of the variational family).
- Evaluating  $\log p(x, z)$  and  $\log q_{\lambda}(z)$  (joint density and variational density).

## Black-box criterion

There is no model-specific inference work: as long as we can evaluate  $\log p(x, z)$  (and sample / score  $q_{\lambda}$ ), we can optimize  $\mathcal{L}(q_{\lambda})$  using stochastic gradients.

# Pathwise (Reparameterization) Estimator: Assumptions

**Goal:** Compute  $\nabla_{\lambda} \mathcal{J}(\lambda)$  for

$$\mathcal{J}(\lambda) = \mathbb{E}_{z \sim q_{\lambda}} [f(z)].$$

**Assume** we can reparameterize the variational sample:

$$z = g(\lambda, \epsilon), \quad \epsilon \sim p(\epsilon) \text{ independent of } \lambda.$$

**Example (Gaussian  $q_{\lambda}$ ):**

$$q_{\lambda}(z) = \mathcal{N}(z; \mu, \sigma^2), \quad \epsilon \sim \mathcal{N}(0, 1), \quad z = g(\lambda, \epsilon) = \mu + \sigma \epsilon.$$

**Smoothness:** Assume  $f(z)$ ,  $\log p(x, z)$ , and  $\log q_{\lambda}(z)$  are differentiable in  $z$  so that gradients can flow through  $z = g(\lambda, \epsilon)$ .

# Pathwise (Reparameterization) Estimator: Gradient Formula

Rewrite the expectation using the reparameterization:

$$\mathcal{J}(\lambda) = \mathbb{E}_{z \sim q_\lambda}[f(z)] = \mathbb{E}_{\epsilon \sim p(\epsilon)}[f(g(\lambda, \epsilon))].$$

Differentiate under the expectation (valid by dominated convergence / smoothness):

$$\nabla_\lambda \mathcal{J}(\lambda) = \mathbb{E}_{\epsilon \sim p(\epsilon)}[\nabla_\lambda f(g(\lambda, \epsilon))] = \mathbb{E}_\epsilon[\nabla_z f(z)|_{z=g(\lambda, \epsilon)} \nabla_\lambda g(\lambda, \epsilon)].$$

**In VI (ELBO):** If  $f(z) = \log p(x, z) - \log q_\lambda(z)$ , then

$$\nabla_\lambda \mathbb{E}_{q_\lambda}[\log p(x, z) - \log q_\lambda(z)] = \mathbb{E}_\epsilon[(\nabla_z \log p(x, z) - \nabla_z \log q_\lambda(z)) \nabla_\lambda g(\lambda, \epsilon)].$$

This is the reparameterization gradient / pathwise estimator.

# From Formula to Algorithm

We want to maximize the ELBO:

$$\mathcal{L}(\lambda) = \mathbb{E}_{z \sim q_\lambda} [\log p(x, z) - \log q_\lambda(z)].$$

**Stochastic gradient ascent step:**

- ① Sample noise  $\epsilon^{(m)} \sim p(\epsilon)$  for  $m = 1, \dots, M$ .
- ② Reparameterize  $z^{(m)} = g(\lambda, \epsilon^{(m)})$ .
- ③ Compute

$$g_\lambda \approx \frac{1}{M} \sum_{m=1}^M \left( \nabla_z \log p(x, z^{(m)}) - \nabla_z \log q_\lambda(z^{(m)}) \right) \nabla_\lambda g(\lambda, \epsilon^{(m)}).$$

- ④ Update  $\lambda \leftarrow \lambda + \eta g_\lambda$ .

**Gaussian case:**

$$z = \mu + \sigma \epsilon, \quad \nabla_\mu g = 1, \quad \nabla_\sigma g = \epsilon.$$

Thus

$$\nabla_\mu \mathcal{L} \approx \frac{1}{M} \sum_m \left( \nabla_z \log p - \nabla_z \log q_\lambda \right) \Big|_{z^{(m)}}, \quad \nabla_\sigma \mathcal{L} \approx \frac{1}{M} \sum_m \left( \nabla_z \log p - \nabla_z \log q_\lambda \right) \Big|_{z^{(m)}} \epsilon^{(m)}.$$

# Worked Example: 1D Gaussian VI

Model:

$$p(z) = \mathcal{N}(0, 1), \quad p(x | z) = \mathcal{N}(x; z, 1), \quad \text{observed } x.$$

Variational family:  $q_\lambda(z) = \mathcal{N}(z; \mu, \sigma^2)$  with  $\lambda = (\mu, \sigma)$  and

$$z = g(\lambda, \epsilon) = \mu + \sigma\epsilon, \quad \epsilon \sim \mathcal{N}(0, 1).$$

ELBO integrand:

$$f(z) = \log p(x, z) - \log q_\lambda(z) = -\frac{1}{2}(x - z)^2 - \frac{1}{2}z^2 - \left( -\frac{1}{2}\log(2\pi\sigma^2) - \frac{1}{2}\frac{(z - \mu)^2}{\sigma^2} \right) + C.$$

Pathwise gradients:

$$\nabla_z \log p(x, z) = (x - z) - z = x - 2z, \quad \nabla_z \log q_\lambda(z) = -\frac{z - \mu}{\sigma^2}.$$

$$\nabla_\mu g = 1, \quad \nabla_\sigma g = \epsilon.$$

SG estimator (single sample):

$$\widehat{\nabla_\mu \mathcal{L}} = \left[ x - 2z + \frac{z - \mu}{\sigma^2} \right] \Big|_{z=\mu+\sigma\epsilon}, \quad \widehat{\nabla_\sigma \mathcal{L}} = \left[ x - 2z + \frac{z - \mu}{\sigma^2} \right] \Big|_{z=\mu+\sigma\epsilon} \cdot \epsilon.$$

Update:  $\mu \leftarrow \mu + \eta \widehat{\nabla_\mu \mathcal{L}}, \quad \sigma \leftarrow \sigma + \eta \widehat{\nabla_\sigma \mathcal{L}}.$

# Score-function estimator vs. pathwise estimator (reparameterization)

## Score-function (REINFORCE) estimator

- Differentiates the **variational density**:

$$\nabla_{\lambda} \log q_{\lambda}(z).$$

- Works for **discrete and continuous** latent variables.
- Applies to a **large class** of variational families  $q_{\lambda}$  (no reparameterization needed).
- **Downside:** variance can be large (often needs baselines/control variates).

## Pathwise (reparameterization) estimator

- Rewrite sampling as

$$z = t(\epsilon; \lambda), \quad \epsilon \sim p(\epsilon)$$

(e.g.,  $\epsilon \sim \mathcal{N}(0, I)$  for Gaussians).

- Differentiate the **sample path** (the integrand) through  $z$ :

$$\nabla_{\lambda} \left[ \log p(x, t(\epsilon; \lambda)) - \log q_{\lambda}(t(\epsilon; \lambda)) \right].$$

- Requires **(reparameterizable) continuous**  $q_{\lambda}$  and a differentiable model.
- **Upside:** typically much lower-variance gradients.

# References for Variational Inference and Reparameterization

## Core Textbook References

- D. MacKay (2003), *Information Theory, Inference, and Learning Algorithms*, Chapter 33: "Variational Methods",  
<https://www.inference.org.uk/itprnn/book.pdf>

## Key Review Articles

- D. Blei, A. Kucukelbir, and J. McAuliffe (2017), "Variational Inference: A Review for Statisticians", *JASA*,  
<https://arxiv.org/abs/1601.00670>.

## Advanced Tutorials

- T. Broderick (2018), "Variational Bayes and Beyond: Bayesian Inference for Big Data", ICML Tutorial  
[https://tamarabroderick.com/tutorial\\_2018\\_icml.html](https://tamarabroderick.com/tutorial_2018_icml.html).

## Online Course

- P. Huijse et al., *Bayesian Learning and Neural Networks*, available at:  
<https://phuijse.github.io/BLNNbook/README.html>

## Course Slide Reference

- M. Villani (2024), *Advanced Bayesian Learning, Lecture 6: Beyond Mean-Field VI.*

# Acknowledgements/ Document preparation

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# Appendix

# Problem: gradients of expectations

In VI and VAEs we optimize objectives of the form:

$$\mathcal{J}(\lambda) = \mathbb{E}_{z \sim q_\lambda} [f(z)].$$

We need  $\nabla_\lambda \mathcal{J}(\lambda)$ , but  $z$  is random.

Two main unbiased estimators:

- **Reparameterization (pathwise)**: differentiate through  $z = g(\lambda, \epsilon)$
- **Score-function (REINFORCE)**: use  $\nabla_\lambda \log q_\lambda(z)$

# What it is

If we can write

$$z = g(\lambda, \epsilon), \quad \epsilon \sim p(\epsilon) \text{ independent of } \lambda,$$

then

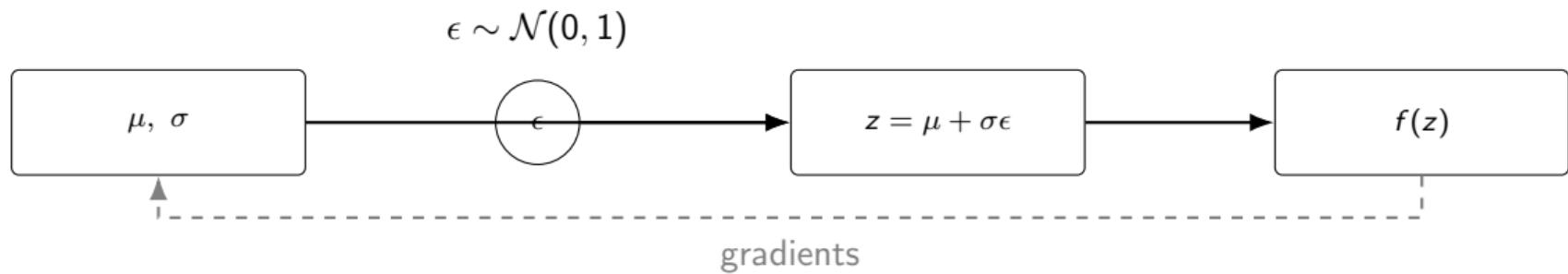
$$\nabla_\lambda \mathbb{E}_{q_\lambda} [f(z)] = \mathbb{E}_\epsilon [\nabla_\lambda f(g(\lambda, \epsilon))].$$

**Gaussian case:**

$$z = \mu + \sigma \epsilon, \quad \epsilon \sim \mathcal{N}(0, 1).$$

This lets gradients flow through the computation graph.

# Reparameterization computation graph



Backprop flows through  $z = \mu + \sigma\epsilon$ ; randomness is isolated in  $\epsilon$ .

**Intuition.** Move randomness to  $\epsilon$  and make  $z$  a deterministic function of  $(\mu, \sigma, \epsilon)$ .

**Why it helps.** Backprop can compute  $\partial f / \partial \mu$  and  $\partial f / \partial \sigma$  through  $z$ .

**Result.** Typically much lower-variance gradients than REINFORCE.

# Score-function estimator

Using the log-derivative identity:

$$\nabla_{\lambda} \mathbb{E}_{q_{\lambda}}[f(z)] = \mathbb{E}_{q_{\lambda}}[f(z) \nabla_{\lambda} \log q_{\lambda}(z)].$$

Monte Carlo:

$$\hat{g} = \frac{1}{S} \sum_{s=1}^S f(z^{(s)}) \nabla_{\lambda} \log q_{\lambda}(z^{(s)}), \quad z^{(s)} \sim q_{\lambda}.$$

**Pros:** works for discrete  $z$ .    **Cons:** often high variance.

# Control variates / baselines

Subtract a baseline  $b$  (independent of  $z$ ):

$$\mathbb{E}[(f(z) - b)\nabla_\lambda \log q_\lambda(z)] = \mathbb{E}[f(z)\nabla_\lambda \log q_\lambda(z)].$$

So the estimator stays unbiased but can have much lower variance.

- Common choice:  $b \approx \mathbb{E}[f(z)]$  (running mean)
- More advanced: learned baseline / critic (RL)