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)
2. KL
3. Intro to variational distribution
4. Mean-field approximation
5. Stochastic (Black-box) VI
6. Pathwise gradients of ELBO
7. Appendix
8. Reparameterization trick

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:

- ∇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 θ
- If $\theta > 5$, the gradient is positive $\Rightarrow$ decrease θ

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

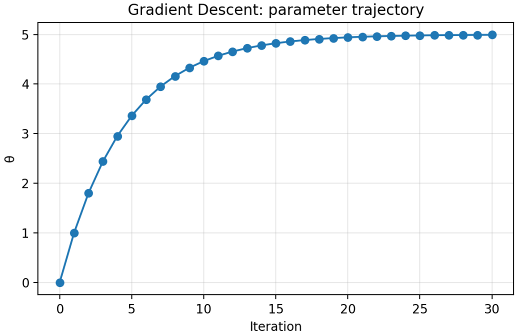
We minimize $f(\theta) = (\theta - 5)^2$.

- **Gradient descent update:**

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

- Figure shows the iterates θ_k converging to the minimizer:

$$\theta^\star = 5.$$



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

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

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

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

Mini-batch stochastic gradient (batch size k)

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

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

- **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** η 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/transformers.
- **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`.

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

```
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 $\{1, \ldots, n\}$          ▷ shuffle indices
    for $b = 1$ to $\lceil n/k \rceil$ do
        $B \leftarrow \{\pi[(b-1)k+1], \ldots, \pi[\min(bk, n)]\}$          ▷ 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

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

```
Dataset size $n$, batch size $k$, steps $T$, learning rates $\{\eta_t\}$
Initialize parameters $\theta$
for $t = 0$ to $T - 1$ do
    Sample indices $i_{t,1}, \dots, i_{t,k} \overset{i.i.d.}{\sim} \mathrm{Unif}(\{1, \dots, n\})$
    $g \leftarrow \frac{1}{k} \sum_{j=1}^{k} \nabla_\theta \ell(\theta; x_{i_{t,j}}, y_{i_{t,j}})$
    $\theta \leftarrow \theta - \eta_t \, g$
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

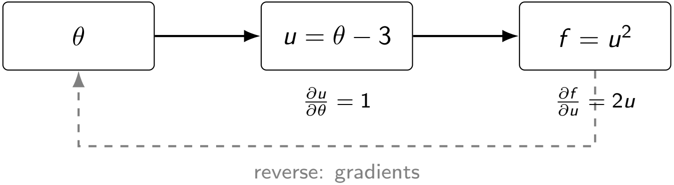
$$\nabla_\theta \left(\frac{1}{k} \sum_{i \in B} \ell(\theta; x_i, y_i) \right) = \frac{1}{k} \sum_{i \in B} \nabla_\theta \ell(\theta; x_i, y_i).$$

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.


θ
$u = \theta - 3$
$f = u^2$
$\frac{\partial u}{\partial \theta} = 1$
$\frac{\partial f}{\partial u} = 2u$
reverse: gradients

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 $x_1, \ldots, x_n$ 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 ⇒ outcomes are hard to predict.
- Low entropy ⇒ outcomes are more predictable.

Example: coin toss

- Fair coin: $p(\mathrm{H}) = p(\mathrm{T}) = 0.5$.

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

- Biased coin: $p(\mathrm{H}) = 0.9$, $p(\mathrm{T}) = 0.1$.

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

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: $p_i = 1/6$.

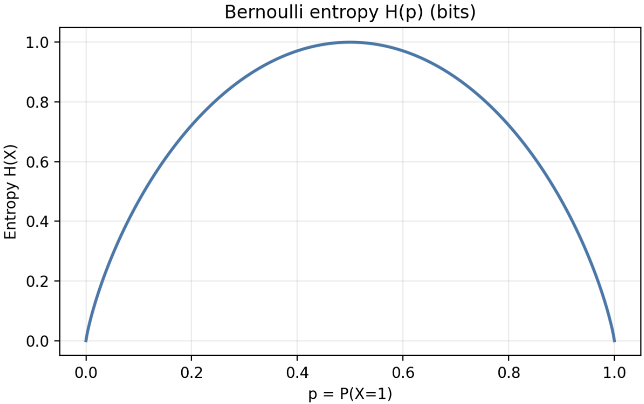
$$H(X) = -\sum_{i=1}^{6} \tfrac{1}{6} \log_2 \tfrac{1}{6} = \log_2 6 \approx 2.585 \text{ bits.}$$

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

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

- 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

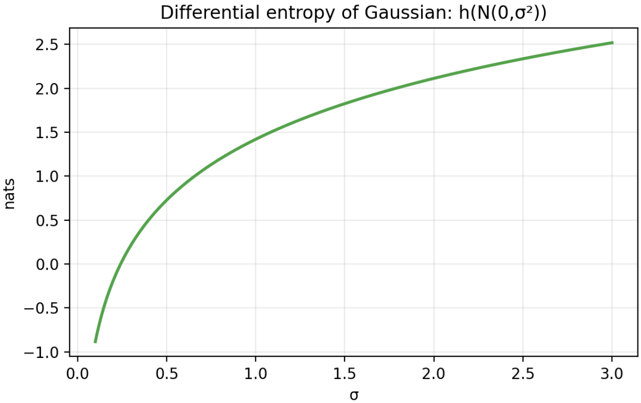
$$h(X) = \frac{1}{2} \log \left(2\pi e \sigma^2\right).$$

Maximum entropy principle (continuous case)

Among all real-valued random variables with a given mean μ and variance σ^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 σ 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 $\{x_1, \ldots, x_n\}$ with

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

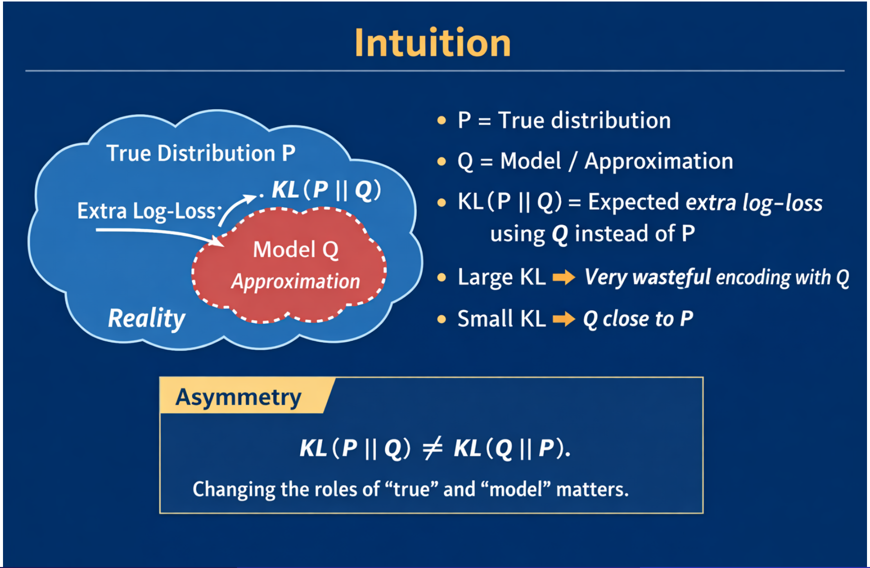
Kullback–Leibler divergence

The KL divergence from Q to P is

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

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

Intuition



Intuition

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

Asymmetry

$$KL(P \,||\, Q) \neq KL(Q \,||\, P).$$

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)

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

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

Example: Bernoulli Distributions

Let $P = \mathrm{Ber}(p)$ and $Q = \mathrm{Ber}(q)$ 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

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

- If $p = q$ then $\mathrm{KL}(P\|Q) = 0$.
- 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

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

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

Three-outcome example

Let

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

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

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

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

Why order matters (intuition)

Compare

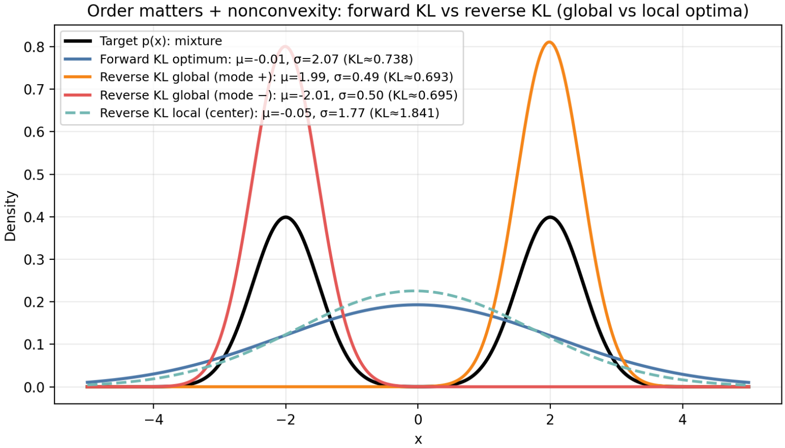
$$\mathrm{KL}(p\|q) = \mathbb{E}_p[\log p - \log q] \quad \text{vs} \quad \mathrm{KL}(q\|p) = \mathbb{E}_q[\log q - \log p].$$

- $\mathrm{KL}(p\|q)$: expectation under $p \Rightarrow$ penalizes q for missing any region where p has mass (**mass-covering**).
- $\mathrm{KL}(q\|p)$: 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 $\mathrm{KL}(q\|p(z \mid x))$

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

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

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 $p_\theta(y \mid x)$.
- Per-example negative log-likelihood (NLL):

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

Expected NLL under the true distribution:

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

We can write this as a two-step expectation:

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

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

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

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

For each fixed x, we have the identity

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

where

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

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

Taking expectation over x:

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

where

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

Interpretation and generality

- $H_{p_{\text{data}}}(Y \mid X)$: intrinsic label uncertainty (Bayes error).
- The KL term: how far the model $p_\theta(y \mid x)$ is from the true conditional $p_{\text{data}}(y \mid x)$.
- 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 $p(z \mid x)$

Key quantities

- **Posterior:**
$$p(z \mid x) = \frac{p(x, z)}{p(x)}.$$
- **Evidence (marginal likelihood):**
$$p(x) = \int p(x, z)\, dz.$$

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

Introducing a Variational Distribution

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

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

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 $X \sim \mathrm{LogNormal}(m, s^2)$, i.e.

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

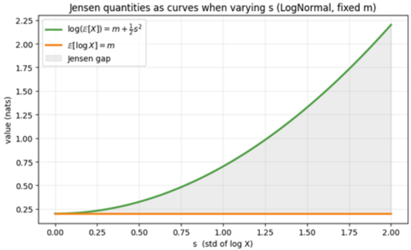
Closed-form expectations (fix m).

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

Jensen gap.

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

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),

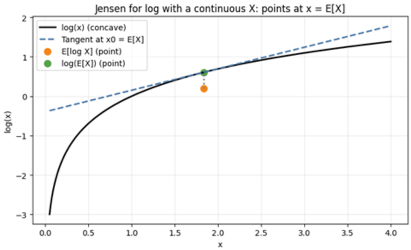
$$\log(\mathbb{E}[X]) \;\geq\; \mathbb{E}[\log X].$$

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

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

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 $\log(\mathbb{E}[X]) - \mathbb{E}[\log X] \geq 0$.



- E[X] = 1.83
- E[log X] = 0.2
- log(E[X]) = 0.61
- gap = 0.41

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

Derivation

Start from the KL divergence to the true posterior:

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

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

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

Rearrange:

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

Key takeaway

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

Alternative Form of the ELBO

Decompose the joint:

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

Plug into the ELBO:

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

Interpretation

- Minimizing L(q) will give a q that explains data well ($\mathbb{E}_{q(z)}[\log p(x \mid z)]$) and is close to the prior ($\mathrm{KL}(q(z) \| p(z))$).
- $\mathbb{E}_{q(z)}[\log p(x \mid z)]$ is the expected log-likelihood under the variational posterior.
- $\mathrm{KL}(q(z) \| p(z))$ 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.

Optimal update for factor q_i:

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

This is a *closed-form* solution: it directly gives the best q_i given the current values of q_{-i}. vspace0.7em Intuition: mean field approximates the influence of all other variables by their expected value $\mathbb{E}_{q_{-i}}[\log p(x,z)]$

Mean-Field VI: Coordinate Ascent Update

Why this form? Mean-field VI solves

$$\min_q \mathrm{KL}\big(q(z) \,\|\, p(z \mid x)\big) \qquad \text{s.t.} \qquad q(z) = \prod_i q_i(z_i).$$

Taking the functional derivative of the ELBO w.r.t. q_i yields:

$$q_i^*(z_i) \;\propto\; \exp\big(\mathbb{E}_{q_{-i}}[\log p(x,z)]\big)\,.$$

Meaning: q_i mimics the conditional $p(z_i \mid x, z_{-i})$ but with z_{-i} replaced by its variational expectation under q_{-i}.

Coordinate Ascent Algorithm:

$$q_1^{(t+1)}(z_1) \propto \exp\left(\mathbb{E}_{q_{-1}^{(t)}}[\log p(x,z)]\right),$$

$$q_2^{(t+1)}(z_2) \propto \exp\left(\mathbb{E}_{q_{-2}^{(t)}}[\log p(x,z)]\right), \quad \dots$$

Repeat cyclically until convergence.

Intuition: Each factor updates by matching the model's conditional structure, averaged over the remaining latent variables according to $q(z)$.

Mean-Field VI: A Simple Gaussian Example

Model:

$$x_n \sim \mathcal{N}(\mu, \tau^{-1}), \qquad p(\mu \mid \tau) = \mathcal{N}(\mu_0, (\lambda_0 \tau)^{-1}), \qquad p(\tau) = \mathrm{Gamma}(a_0, b_0).$$

Goal: Illustrate coordinate ascent VI (even though the true posterior is conjugate).

Mean-field assumption:

$$q(\mu, \tau) = q_\mu(\mu)\, q_\tau(\tau).$$

Coordinate ascent updates:

$$\boxed{\log q_\mu^*(\mu) = \mathbb{E}_{q_\tau}[\log p(X, \mu, \tau)] + \text{const}}$$

$$\boxed{\log q_\tau^*(\tau) = \mathbb{E}_{q_\mu}[\log p(X, \mu, \tau)] + \text{const}}$$

Idea: Each factor matches the model's conditional distribution, averaged over the other variational factors.

Updating $q_\mu(\mu)$

Log-joint terms involving μ:

$$\log p(X, \mu, \tau) = -\frac{\tau}{2} \sum_{n=1}^{N} (x_n - \mu)^2 - \frac{\lambda_0 \tau}{2} (\mu - \mu_0)^2 + C.$$

Apply MF update:

$$\log q_\mu^*(\mu) = -\frac{\mathbb{E}_{q_\tau}[\tau]}{2} \left[\sum_{n=1}^{N} (x_n - \mu)^2 + \lambda_0 (\mu - \mu_0)^2 \right] + \text{const.}$$

Recognize a Gaussian:

$$q_\mu^*(\mu) = \mathcal{N}(\mu_N, \tau_N^{-1}),$$

$$\mu_N = \frac{\lambda_0 \mu_0 + N\bar{x}}{\lambda_0 + N}, \qquad \tau_N = (\lambda_0 + N)\, \mathbb{E}_{q_\tau}[\tau].$$

Note: q_μ depends on $\mathbb{E}[\tau]$, so we alternate updates.

Updating $q_\tau(\tau)$ and Summary

Log-joint terms involving τ:

$$\log p(X,\mu,\tau) = \left(a_0 - 1 + \frac{N+1}{2}\right)\log\tau - \tau\left[b_0 + \frac{1}{2}\left(\sum_{n=1}^{N}(x_n-\mu)^2 + \lambda_0(\mu-\mu_0)^2\right)\right] + C.$$

Apply MF update:

$$q_\tau^*(\tau) = \mathrm{Gamma}(a_N, b_N),$$

$$a_N = a_0 + \frac{N+1}{2}, \qquad b_N = b_0 + \frac{1}{2}\,\mathbb{E}_{q_\mu}\left[\sum_{n=1}^{N}(x_n-\mu)^2 + \lambda_0(\mu-\mu_0)^2\right].$$

Summary:

- q_μ and q_τ have closed-form Gaussian and Gamma updates.
- Updates depend on each other ⇒ run *cyclic* coordinate ascent.
- This example shows the classic MFVI pattern: exponentiate expected log-joint and normalize.

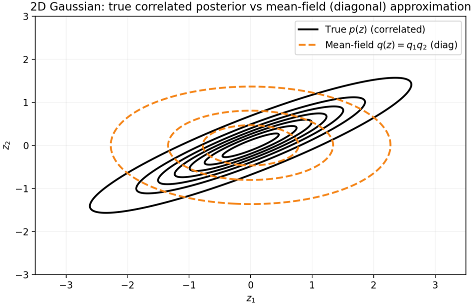
Correlated posterior vs mean-field: geometry of uncertainty (contours)

Setup. True posterior: $p(z) = \mathcal{N}(0, \Sigma)$ with correlation. Mean-field Gaussian: $q(z) = \mathcal{N}(0, \Sigma_q)$ with Σ_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 ⇒ **tilted ellipses** (off-axis principal components),
- diagonal covariance ⇒ **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 ⇒ 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 λ.
- Optimize the approximation by solving

$$\lambda^\star \in \arg\min_{\lambda} \; \mathrm{KL}(q_\lambda(z) \,\|\, p(z \mid x))\,.$$

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

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

Objective (ELBO). Define

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

Gradient ascent

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

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

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

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

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

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

Define

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

Derivation sketch (log-derivative trick)

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

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,

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

VI via stochastic gradient ascent (Monte Carlo estimate)

From the previous slide,

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

Monte Carlo estimator

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

Basic fixed-form VI algorithm (SGA)

1. Initialize $\lambda^{(0)}$, choose step sizes $\{a_t\}_{t\geq 0}$ and MC size S.
2. For $t = 0, 1, 2, \ldots$:
    1. Sample $z^{(1)},\ldots,z^{(S)} \sim q_{\lambda^{(t)}}(z)$.
    2. Compute $\widehat{\nabla_\lambda \mathcal{L}}(\lambda^{(t)})$ using the MC estimator above.
    3. Update $\lambda^{(t+1)} = \lambda^{(t)} + a_t\,\widehat{\nabla_\lambda \mathcal{L}}(\lambda^{(t)})$.
3. 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:

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

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_λ), we can optimize $\mathcal{L}(q_\lambda)$ using stochastic gradients.

Pathwise (Reparameterization) Estimator: Assumptions

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

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

Assume we can reparameterize the variational sample:

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

Example (Gaussian q_λ):

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

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:

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

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

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

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

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

This is the reparameterization gradient / pathwise estimator.

From Formula to Algorithm

We want to maximize the ELBO:

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

Stochastic gradient ascent step:

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

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

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

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

Worked Example: 1D Gaussian VI

Model:

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

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:

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

Pathwise gradients:

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

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

SG estimator (single sample):

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

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

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_λ (no reparameterization needed).
- **Downside:** variance can be large (often needs baselines/control variates).

Pathwise (reparameterization) estimator

- Rewrite sampling as

$$z = g(\epsilon; \lambda), \qquad \epsilon \sim p(\epsilon)$$

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

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

$$\nabla_\lambda \Big[\log p\big(x, g(\epsilon; \lambda)\big) - \log q_\lambda\big(g(\epsilon; \lambda)\big) \Big].$$

- Requires **(reparameterizable) continuous** q_λ 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`.

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*.

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Appendix

Problem: gradients of expectations

In VI and VAEs we optimize objectives of the form:

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

We need $\nabla_\lambda \mathcal{L}(\lambda)$, 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

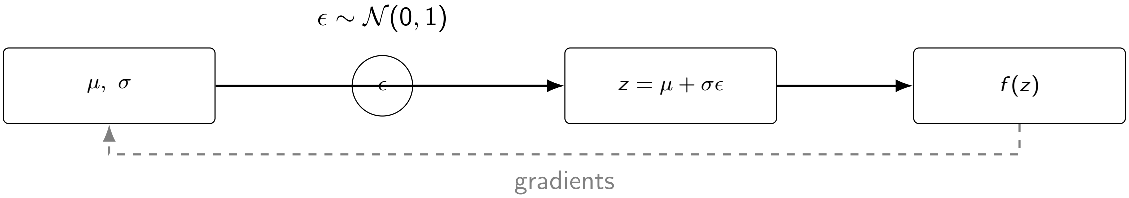
$$\nabla_\lambda \mathbb{E}_{q_\lambda}[f(z)] = \mathbb{E}_\epsilon\big[\nabla_\lambda f(g(\lambda, \epsilon))\big].$$

Gaussian case:

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

This lets gradients flow through the computation graph.

Reparameterization computation graph



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

Intuition. Move randomness to ϵ and make z a deterministic function of (μ, σ, ϵ).
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:

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

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)