

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: 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

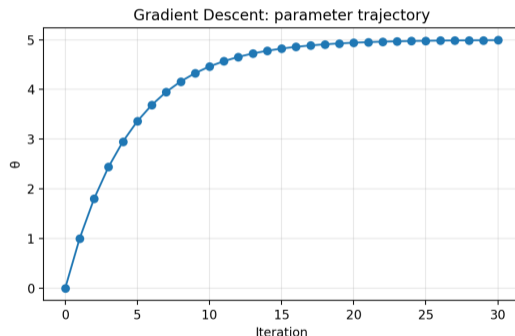
We minimize $f(\theta) = (\theta - 5)^2$.

- **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:

$$\theta^* = 5.$$



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:

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

Mini-batch stochastic gradient (batch size k)

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

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

- **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** 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 θ

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

 Sample a random permutation π 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

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

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

Initialize parameters θ

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

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

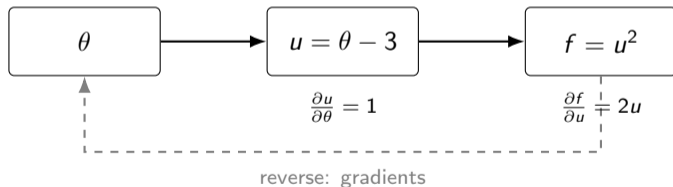
Key takeaway: Autodiff computes gradients; batching controls **which** data points contribute to the gradient estimate. 

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.

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: $p_i = 1/6$.

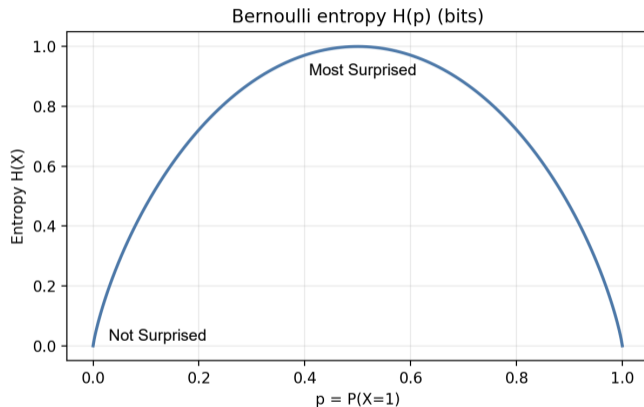
$$H(X) = -\sum_{i=1}^6 \frac{1}{6} \log_2 \frac{1}{6} = \log_2 6 \approx 2.585 \text{ bits.}$$

- 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

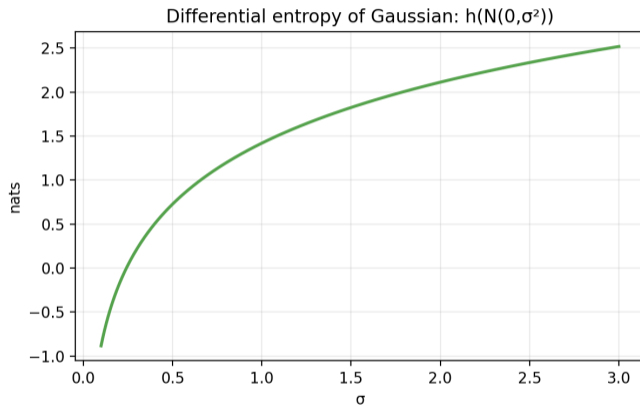
$$h(X) = \frac{1}{2} \log (2\pi e \sigma^2).$$

Maximum entropy principle (continuous case)

Among all real-valued random variables with a given mean 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 $\{x_1, \dots, x_n\}$ with

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

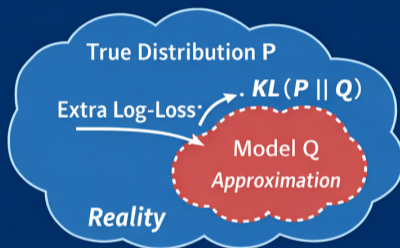
Kullback–Leibler divergence

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
- $KL(P || Q)$ = 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

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

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)

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

- $\text{KL}(P\|Q)$: **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.

- **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

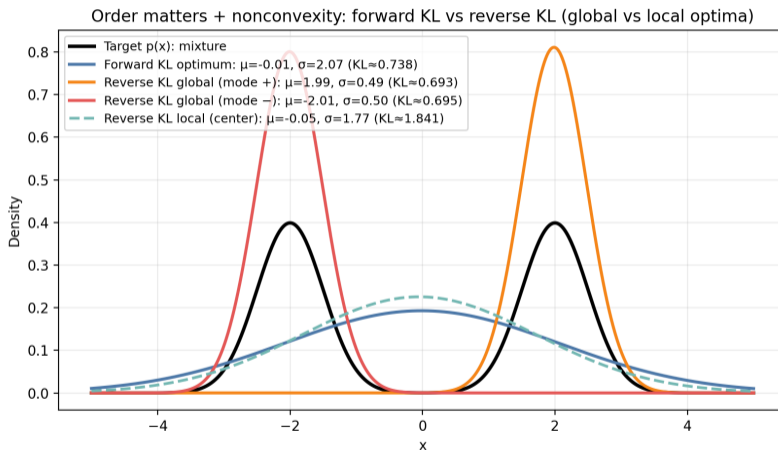
$$\text{KL}(p\|q) = \mathbb{E}_p[\log p - \log q] \quad \text{vs} \quad \text{KL}(q\|p) = \mathbb{E}_q[\log q - \log p].$$

- $\text{KL}(p\|q)$: 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 $p(z \mid x)$.

- 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 : $q^*(z) = \arg \min_{\lambda} \text{KL}(q_{\lambda}(z) \parallel p(z \mid x))$

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

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

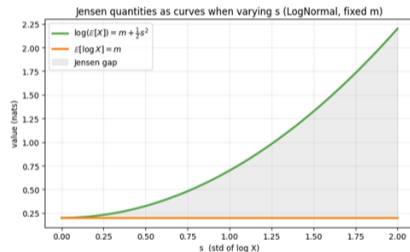
Closed-form expectations (fix m).

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

Jensen gap.

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

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),

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

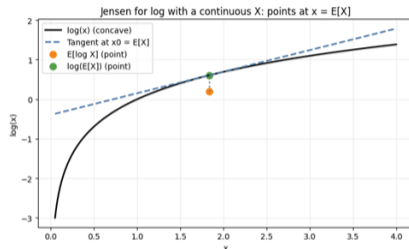
Geometric proof idea (concavity). Because log is concave, the tangent line at $x_0 = \mathbb{E}[X]$ lies above the curve:

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

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



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

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.

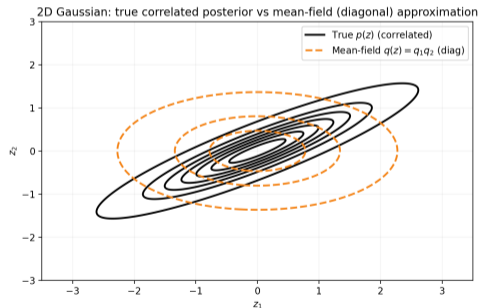
Correlated posterior vs mean-field: geometry of uncertainty (contours)

Setup. True posterior: $p(z) = \mathcal{N}(0, \Sigma)$ with correlation. Mean-field Gaussian: $q(z) = \mathcal{N}(0, \Sigma_q)$ with 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 \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 λ .
- Optimize the approximation by solving

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

- 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:** $q_\lambda(z) = \mathcal{N}(z \mid \mu, \Sigma)$, $\lambda = (\mu, L)$ with $\Sigma = LL^\top$ (Cholesky).
- **Low-rank + diagonal:** $q_\lambda(z) = \mathcal{N}(z \mid \mu, aa^\top + D)$, $\lambda = (\mu, a, d)$, $D = \text{Diag}(d)$.
- **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 $\widehat{\nabla_{\lambda} \mathcal{L}(\lambda)} = \frac{1}{S} \sum_{s=1}^S \left(h_{\lambda}(z^{(s)}) \nabla_{\lambda} \log q_{\lambda}(z^{(s)}) \right)$.

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 $\lambda^{(t+1)} = \lambda^{(t)} + a_t \widehat{\nabla_{\lambda} \mathcal{L}(\lambda^{(t)})}$.
- 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:

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

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_{λ}), 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_{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:

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

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_{λ} (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_{λ} and a differentiable model.
- **Upside:** typically much lower-variance gradients.

References for Variational Inference and Reparameterization

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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

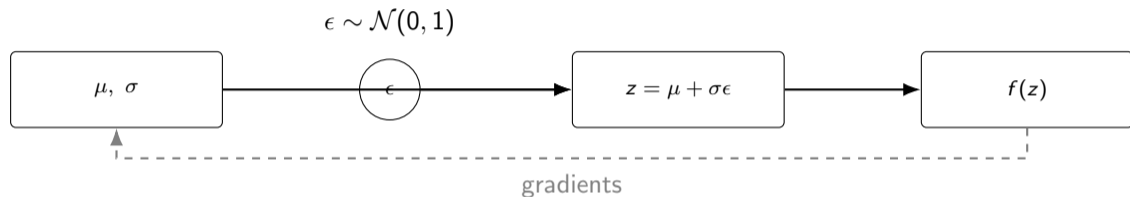
$$\nabla_{\lambda} \mathbb{E}_{q_{\lambda}}[f(z)] = \mathbb{E}_{\epsilon}[\nabla_{\lambda} f(g(\lambda, \epsilon))].$$

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 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:

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

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

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)