Tight PAC-Bayes Generalisation Guarantees for Large Language Model Safety Monitoring

Tom. A. Lamb [1]   Philip H. S. Torr [1]   Tim G. J. Rudner [2]

Abstract

How can we ensure that safety oversight models used to detect safety violations in AI systems reliably generalise, and how can we understand the factors that influence their generalisation? In this paper, we formalise PAC-Bayes certification for large language model-based safety oversight and obtain non-vacuous PAC-Bayes guarantees for safety oversight models, even under limited data for safety alignment. Building on compression-based PAC-Bayes bounds, we show that highly compressed PEFT adaptations yield extremely short adaptation description lengths, enabling informative and often tight guarantees that certify both classification risk and predictive uncertainty. We introduce a global-scale quantisation method (LoRA-GT) that reduces adaptor description length while preserving model performance, tightening bounds. Our results show that certifiability is strongly linked to adaptor compressibility, with shorter adaptor description lengths yielding tighter guarantees. Empirically, highly compressed adaptations exhibit minimal degradation in performance while enabling substantially stronger certification, suggesting that certifiable large language model oversight may naturally favour low-complexity safety adaptations. We further show that functional distortion tracks both test risk and bound tightness under compression, providing a practical mechanism for selecting simple, certifiable safety adaptations. Together, these results show that compression-based PAC-Bayes analysis provides a practical framework for understanding and designing reliable safety oversight models.

[1]University of Oxford [2]University of Toronto & Vigil. Correspondence to: Tom A. Lamb <thomas.lamb@eng.ox.ac.uk>.

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1. Introduction

How can we ensure that large language models (LLMs) work as intended and are safe at deployment? Although LLMs are increasingly being deployed in generative workflows such as text generation (Brown et al., 2020) and agentic systems (Luo et al., 2025)—including in safety-critical domains—they remain vulnerable to adversarial attacks, misuse, and hallucinations (Wang et al., 2023; Zou et al., 2023) and require robust oversight to prevent harm. As human supervision does not scale, *scalable oversight* (Bowman et al., 2022), where weaker LLMs act as automated judges of more capable LLMs, is rapidly becoming a central tool for LLM monitoring (Inan et al., 2023).

In this setting, accuracy alone is insufficient: oversight models must support decisions such as blocking or escalation, which require reliable uncertainty estimates (Gneiting and Raftery, 2007; Geifman and El-Yaniv, 2017; Guo et al., 2017). However, current LLM judges are typically deployed without guarantees on their performance or predictive uncertainty, and with limited understanding of the factors governing generalisation in this setting (Zheng et al., 2023). While standard test-set bounds can certify the performance of a fixed trained model based on empirical error, they do not account for the learning process or model structure, limiting their usefulness for understanding how generalisation varies across architectures or training procedures. Classical complexity measures are similarly uninformative for modern overparameterised models (Dziugaite and Roy, 2017).

PAC-Bayes theory provides data-dependent generalisation bounds that relate empirical performance to model complexity (Catoni, 2007; Alquier et al., 2024). Recent work has applied compression-based PAC-Bayes analysis to generative LLMs (Lotfi et al., 2024a;b). However, these approaches have primarily focused on large-scale training regimes and often rely on specialised parameterisations that enforce compressibility during pre-training and diverge from standard practice.

Instead, in this paper, we focus on parameter-efficient fine-tuning (PEFT) for safety oversight models in small-data regimes. PEFT adaptations are widely used, inherently low-dimensional, and naturally compressible, yielding short

Figure 1. **Compression yields tight PAC-Bayes guarantees for safety oversight models.** Left: LoRA-T with per-tensor vs. shared global scale s^* (LoRA-GT), where global scaling reduces adaptor description length $|h|$. Right: PAC-Bayes bounds and test error on BeaverTails. Shorter $|h|$ yields tighter guarantees, with highly compressed adaptors preserving competitive performance.

description lengths without modifying the training procedure. This raises a key question: *can compression-based PAC-Bayes bounds yield non-vacuous guarantees for safety oversight models while providing insight into how adaptor simplicity influences performance and uncertainty?* To approach this question, we introduce a PAC-Bayes framework for scalable oversight by formalising certification of a judge model relative to the distribution induced by a fixed generator to enable computable guarantees and principled reasoning about certifiable safety adaptations.

We show that the compressibility induced by standard PEFT methods is sufficient to yield tight, non-vacuous PAC-Bayes guarantees for LLM-based safety oversight models, and that careful choices of PAC-Bayes bound, compressed representation, and description-length accounting can significantly tighten generalization certificates with minimal impact on performance.

In summary, our key contributions are as follows:

1. **Formalisation of LLM safety oversight certification:** We formalise PAC-Bayes certification of LLM-based safety oversight models under the joint distribution induced by a fixed generator, yielding non-vacuous and often tight guarantees for both classification risk and predictive distributions in realistic small-data safety alignment settings.

2. **Compression governs certifiability in PEFT safety alignment:** We show that standard PEFT safety adaptations already induce highly compressible, low-complexity hypothesis classes, enabling tight PAC-Bayes guarantees without modifying conventional fine-tuning pipelines. Empirically, shorter adaptor description lengths yield systematically tighter certificates, sup-

porting an Occam-style view in which certifiable generalisation depends more strongly on adaptation complexity than base model scale.

3. **Tightening compression-based PAC-Bayes guarantees:** We demonstrate that PAC-Bayes bound choice, compressed hypothesis representation, quantisation strategy, and description-length accounting affect certificate tightness. In particular, we introduce LoRA-GT, a global-scale quantisation method that reduces adaptor description length and yields tighter PAC-Bayes guarantees while preserving competitive performance.

4. **Functional distortion as a practical signal:** We show that functional distortion tracks both test risk and PAC-Bayes bound tightness under compression, providing a practical mechanism for selecting minimum-description-length adaptations that preserve both performance and certifiability.

2. Related Work

PAC-Bayes bounds. Classical generalisation bounds based on measures such as VC-dimension (Vapnik, 1998) and Rademacher complexity (Bartlett and Mendelson, 2002) are typically vacuous for modern over-parameterised models (Catoni, 2007; Dziugaite and Roy, 2017). PAC-Bayes theory instead provides data-dependent guarantees by comparing a learned posterior to a fixed prior over hypotheses (McAllester, 1999; Alquier et al., 2024), and has yielded non-vacuous bounds for deep neural networks (Dziugaite and Roy, 2017). Recent work extends this perspective to LLMs through compression-based analyses linking generalisation to the trade-off between empirical fit and compressibility (Lotfi et al., 2022; 2024a;b). However, these ap-

proaches primarily target large-data regimes and often rely on specialised parameterisations designed around compressibility (e.g., SubLoRA). In contrast, we show that standard PEFT safety adaptation already induces highly compressible, low-complexity hypothesis classes, enabling tight PAC-Bayes guarantees even in constrained small-data alignment settings.

Parameter-Efficient Fine-Tuning. Parameter-Efficient Fine-Tuning (PEFT) methods adapt LLMs through low-dimensional parameter updates (Hu et al., 2022). LoRA (Hu et al., 2022) and more compact variants such as LoRA-XS (Bałazy et al., 2024) and LoRA-T (Morris et al., 2026) enable extremely compact adaptations via structured low-rank or latent parameterisations. In contrast to full fine-tuning, these methods produce small, highly structured updates that are naturally compressible, enabling compression-based PAC-Bayes guarantees in small-data safety alignment settings.

LLMs as Safety Oversight Models. Scalable oversight has emerged as a key paradigm for supervising large models using automated evaluators (Bowman et al., 2022). The LLM-as-a-judge paradigm (Zheng et al., 2023) uses specialised models to evaluate the outputs of larger systems, forming the basis of modern safety oversight approaches. Models such as Llama Guard (Inan et al., 2023; Chi et al., 2024) and Qwen3Guard (Zhao et al., 2025) act as system-level safety filters by classifying prompts and responses according to predefined risk taxonomies. However, these systems are typically deployed without formal guarantees of generalisation (Zheng et al., 2023). Our work addresses this gap by providing non-vacuous, interpretable guarantees for LLM-based safety oversight models.

3. Preliminaries

3.1. Quantisation, Compression, and Description Length

Quantisation maps real-valued parameters to a finite discrete representation (Gersho and Gray, 2012). Given $\theta \in \mathbb{R}^p$ and bit-width $b \in \mathbb{N}$, a quantisation scheme is defined via a codebook $\mathcal{C}_b$ with $|\mathcal{C}_b| \leq 2^b$, a space of reconstruction parameters $\mathcal{S}$, and a dequantisation rule $d_b : \mathcal{C}_b^p \times \mathcal{S} \to \mathbb{R}^p$. The quantised representation is $(z, m) \in \mathcal{C}_b^p \times \mathcal{S}$, where z are discrete values and m contains reconstruction parameters (e.g., scales). The reconstructed parameters are $\hat{\theta} = d_b(z, m)$, typically via scaling or other transformations determined by the quantisation scheme. This mapping is inherently lossy, introducing quantisation error while enabling a more compact and simpler representation.

In practice, schemes differ in how $(\mathcal{C}_b, \mathcal{S}, d_b)$ are specified: data-driven methods such as GPTQ choose the discrete values $z \in \mathcal{C}_b$ to approximately minimise changes in outputs

using calibration data and second-order Hessian information (Frantar et al., 2022), while preprocessing techniques such as QuIP transform weights to improve robustness to low-bit quantisation (Tseng et al., 2024). For extremely small parameterisations, simple nearest-integer rounding is typically adequate given the limited number of trainable parameters.

Compression further reduces the number of bits required to represent $(z, m) \in \mathcal{C}_b^p \times \mathcal{S}$ by exploiting redundancy (Cover, 1999). For a hypothesis $h \in \mathcal{H}$, lossless compressors (e.g., Brotli (Google Inc., 2015)) encode the quantised representation $(z, m) \in \mathcal{C}_b^p \times \mathcal{S}$ of h's parameters as a binary string $c(h) \in \{0, 1\}^*$ without inducing reconstruction error. We define the description length as $|c(h)| \in \mathbb{N}$ and write $|h| := |c(h)|$. See implementation Section I for further details.

3.2. PAC-Bayes Bounds

Let $\mathbb{P}_\mathcal{D} \in \mathcal{P}(\mathcal{X} \times \mathcal{Y})$ denote a data distribution over example-label pairs, and let $\mathcal{H}$ denote a hypothesis class. Given a dataset $S = \{(x_i, y_i)\}_{i=1}^n \sim \mathbb{P}_\mathcal{D}^n$ of n i.i.d. samples and a loss $\ell : \mathcal{Y} \times \mathcal{Y} \to [0, 1]$, define the population and empirical risks of a hypothesis $h \in \mathcal{H}$ respectively as:

$$\mathcal{R}_\mathcal{D}(h) = \mathbb{E}_{(x,y) \sim \mathbb{P}_\mathcal{D}}[\ell(h(x), y)],$$
$$\widehat{\mathcal{R}}_S(h) = \frac{1}{n} \sum_{i=1}^n \ell(h(x_i), y_i).$$

For distributions $\mathbb{Q}, \mathbb{P} \in \mathcal{P}(\mathcal{H})$, the Kullback–Leibler (KL) divergence is defined as

$$\mathrm{KL}(\mathbb{Q}\|\mathbb{P}) = \int_\mathcal{H} \log \frac{d\mathbb{Q}}{d\mathbb{P}}(h) \, d\mathbb{Q}(h),$$

assuming $\mathbb{Q} \ll \mathbb{P}$, with $\frac{d\mathbb{Q}}{d\mathbb{P}} : \mathcal{H} \to \mathbb{R}_{\geq 0}$ the Radon–Nikodym derivative of $\mathbb{Q}$ with respect to $\mathbb{P}$ (Probability, 1995). For a posterior $\mathbb{Q}$, define the Gibbs risks as

$$\mathcal{R}_\mathcal{D}(\mathbb{Q}) = \mathbb{E}_{h \sim \mathbb{Q}}[\mathcal{R}_\mathcal{D}(h)], \quad \widehat{\mathcal{R}}_S(\mathbb{Q}) = \mathbb{E}_{h \sim \mathbb{Q}}[\widehat{\mathcal{R}}_S(h)].$$

The PAC-Bayes literature provides many bounds trading off tightness, interpretability, and ease of optimisation for Gibbs risks (Alquier et al., 2024). In this work, we adopt the following generalised Catoni-style bound (Rodriguez-Galvez et al., 2024), not explored in prior compression-based PAC-Bayes analyses of LLMs.

Theorem 3.1 (Rodriguez-Galvez et al., 2024, Theorem 6)**.** *Let* $\ell : \mathcal{Y} \times \mathcal{Y} \to [0, 1]$ *and let* $\mathbb{P}$ *be independent of* $\mathcal{S}$. *For any* $\beta \in (0, 1)$, *with probability at least* $1 - \beta$ *over* $\mathcal{S} \sim \mathbb{P}_\mathcal{D}^n$,

$$\mathcal{R}_\mathcal{D}(\mathbb{Q}) \leq \inf_{\lambda > 0} \left\{ \frac{1}{1 - e^{-\lambda/n}} \left[1 - \right.\right.$$
$$\left.\left. \times \exp\left(-\frac{\lambda \widehat{\mathcal{R}}_S(\mathbb{Q}) + \mathrm{KL}(\mathbb{Q}\|\mathbb{P}) + \log \frac{2+\sqrt{2n}}{\beta}}{n}\right) \right] \right\}.$$

This bound holds simultaneously over the choice of $\lambda \in \mathbb{R}_{>0}$, avoiding the union bound penalties required when tuning λ in standard Catoni bounds used in prior work (Lotfi et al., 2022). It can be optimised directly over λ and $\mathbb{Q}$, and typically yields tighter guarantees than Hoeffding-type PAC-Bayes bounds (Lotfi et al., 2024a;b), which are generally looser in practice. We consider several alternative PAC-Bayes bounds defined in Section B and evaluate them for comparison. In our setting, the KL term is controlled by the description length of the model, linking generalisation guarantees directly to compressibility.

3.3. Compression-Based Bounds

Following prior work on compression-based PAC-Bayes bounds for LLMs (Lotfi et al., 2022; 2024b), we adopt a Solomonoff prior (Solomonoff, 1964) of the form:

$$\mathbb{P}_{\text{Sol}}(h) = 2^{-K_p(h|M)}/Z, \qquad (1)$$

where $K_p(h|M)$ denotes the prefix-free Kolmogorov complexity of $h \in \mathcal{H}$ given decoder M (Li et al., 2008), and $Z \leq 1$ (Kraft, 1949) is a normalising constant. In our setting, M corresponds to a fixed decoding scheme determined by the base model architecture and quantisation procedure, and h represents the resulting compressed parameter update. This prior assigns higher probability to simpler, more compressible hypotheses, linking tighter generalisation guarantees to high-performing, low-description-length models and thereby encoding an Occam-style notion of simplicity.

4. PAC-Bayes Certification of Large Language Model Safety Oversight

We formalise PAC-Bayes certification of LLM-based safety oversight models acting under the joint distribution induced by a fixed generator model. This formulation captures the setting of scalable oversight, where a judge evaluates responses produced by a fixed underlying model, and enables computable PAC-Bayes certificates for LLM-based oversight systems.

Let $\mathcal{V}$ be a finite vocabulary, with prompt space $\mathcal{X} \subseteq \mathcal{V}^*$ and response space $\mathcal{Y} \subseteq \mathcal{V}^*$. Let $\mathbb{P}_{\mathcal{D}} \in \mathcal{P}(\mathcal{X})$ be the marginal data distribution over prompts, and let a fixed generator G define a Markov kernel $\mathbb{P}_G(\cdot \mid x) \in \mathcal{P}(\mathcal{Y})$. This induces a joint distribution $\mathbb{P}_{\mathcal{D},G} \in \mathcal{P}(\mathcal{X} \times \mathcal{Y})$ given by:

$$\mathbb{P}_{\mathcal{D},G}(B) = \int_{\mathcal{X}} \mathbb{P}_G(B_x \mid x) \, d\mathbb{P}_{\mathcal{D}}(x),$$

where $B_x = \{y \in \mathcal{Y} : (x, y) \in B\}$. This formulation makes explicit that oversight guarantees are conditional on the response distribution induced by the underlying generator.

Let $z^* : \mathcal{X} \times \mathcal{Y} \to \{0, 1\}$ denote a deterministic ground-truth evaluation function, indicating whether a given prompt–response pair satisfies the evaluation criterion, which the judge $h \in \mathcal{H}_J$ seeks to approximate. We define the judge's risk and empirical risk with respect to $\mathbb{P}_{\mathcal{D},G}$ as:

$$\mathcal{R}_G(h) := \mathbb{E}_{(x,y) \sim \mathbb{P}_{\mathcal{D},G}}[\ell(h(x, y), z^*(x, y))],$$

$$\widehat{\mathcal{R}}_S(h) := \frac{1}{n} \sum_{i=1}^{n} \ell(h(x_i, y_i), z^*(x_i, y_i)),$$

for $S = \{(x_i, y_i)\}_{i=1}^{n} \sim (\mathbb{P}_{\mathcal{D},G})^n$.

To obtain practical generalisation guarantees for LLMs, we restrict attention to deterministic posteriors $\mathbb{Q}_h = \delta_h$, where δ_h denotes the Dirac measure at h, following prior compression-based PAC-Bayes analyses of LLMs (Lotfi et al., 2024a;b); see Section E.1 for further discussion of this pragmatic choice in our setting.

Proposition 4.1. *Assume $|\mathcal{H}_J| < \infty$ and let M be a fixed decoder. For $\mathbb{Q}_h = \delta_h$ and the Solomonoff prior $\mathbb{P}_{\text{Sol}}$ from Equation* (1)*, define*

$$\text{KL}^{\text{UB}}(\mathbb{Q}_h \| \mathbb{P}_{\text{Sol}}) := \Big(|h| + \lfloor \log_2 |h| \rfloor $$
$$+ 2\lfloor \log_2(\lfloor \log_2 |h| \rfloor + 1) \rfloor + 1 \Big) \log 2.$$

Then

$$\text{KL}(\mathbb{Q}_h \| \mathbb{P}_{\text{Sol}}) \leq \text{KL}^{\text{UB}}(\mathbb{Q}_h \| \mathbb{P}_{\text{Sol}}).$$

Proof. See Section A.1. The proof combines the Elias δ-code upper bound on $K_p(h \mid M)$ with the deterministic-posterior KL under the Solomonoff prior. $\square$

For the KL divergence to be well-defined under a Dirac posterior, it is required that the hypothesis space be finite; this condition is satisfied in practice since quantisation restricts models to finite precision.

Substituting Theorem 4.1 into the generalised Catoni bound given in Theorem 3.1 yields a computable PAC-Bayes certificate within this scalable oversight framework.

Corollary 4.2 (Oversight Model Certificate)**.** *Let $S \sim (\mathbb{P}_{\mathcal{D},G})^n$. For any $\beta \in (0, 1)$, with probability at least $1 - \beta$, for all $h \in \mathcal{H}_J$, we have*

$$\mathcal{R}_G(h) \leq \inf_{\lambda > 0} \left\{ \frac{1}{1 - e^{-\lambda/n}} \left[1 - \right. \right.$$
$$\left. \left. \times \exp\left(-\frac{\lambda \widehat{\mathcal{R}}_S(h) + \text{KL}^{\text{UB}}(\mathbb{Q}_h \| \mathbb{P}_{\text{Sol}}) + \log \frac{2 + \sqrt{2n}}{\beta}}{n} \right) \right] \right\}.$$

Proof. Immediate from combining Theorem 3.1 and Theorem 4.1. $\square$

This certificate makes explicit that certifiable generalisation is characterised by a trade-off between empirical performance and description length, providing an interpretable

link between compressibility and certifiability. These guarantees form the basis of our empirical evaluation, where we assess their tightness and explanatory power in practice.

Compression and Safety Fine-Tuning. Compression-based PAC-Bayes bounds favour simple hypotheses through the Solomonoff prior, yielding tighter guarantees for models with shorter description lengths. In safety fine-tuning, this inductive bias is particularly natural: modern oversight models are already highly capable, so adapting them to new oversight tasks typically requires only small refinements, especially given the limited availability of high-quality safety data. PEFT methods therefore provide a natural hypothesis class for certification, learning small structured updates relative to a frozen base model. Quantisation further shortens adaptor description length by selecting simpler discrete representations, and, as in Lotfi et al. (2024a), lossless compression can then be applied to obtain a still shorter representation without information loss, jointly tightening the PAC-Bayes complexity term whenever strong empirical performance is maintained.

4.1. Global-Scale Quantisation, LoRA-GT Adaptations

We instantiate compressed hypotheses using LoRA-T (Morris et al., 2026), a parameter-efficient adaptation in which weight updates are generated from a low-dimensional trainable vector via fixed projection matrices. We denote variants of LoRA-T as LoRA-TN for the non-tied version, LoRA-TT for the tied version, and LoRA-GT for the tied variant with global-scale quantisation, which we introduce in this work.

In the tied variant (LoRA-TT), a single vector is shared across all adapted modules within each transformer layer. Concretely, for a base weight $W_0 \in \mathbb{R}^{d \times k}$, the adapted weights take the form

$$W = W_0 + U\Sigma \left(\sum_{i=1}^{u} v_i P_i \right) V^\top,$$

where U, Σ, V and $\{P_i\}_{i=1}^{u}$ are fixed, and $\mathbf{v} \in \mathbb{R}^u$ is the trainable parameter vector. In the tied setting, $\mathbf{v}^{(\ell)} \in \mathbb{R}^u$ is shared within each layer ℓ. See Section D.2 for further details.

Scale Overhead in Extreme Compression. For LoRA-TT, each transformer layer $\ell \in \{1, \ldots, L\}$ is parameterised by a small vector $\mathbf{v}^{(\ell)} \in \mathbb{R}^u$. Under b-bit quantisation, storing per-layer scales in bfloat16 incurs an overhead of $16L$ bits.

For highly compressed adaptors (small u and b), this overhead dominates the hypothesis description length $|h|$ and therefore the KL penalty in Theorem 4.1. For example, with $u = 1$ and $b = 2$ on Llama-Guard-3-8B ($L = 32$), the weights require only 64 bits, while scales require 512 bits.

Global Scale Quantisation. This motivates sharing a single global quantisation scale across layers. Replacing per-layer scales with a global scale reduces the description length by

$$|h|_{\text{per-layer}} - |h|_{\text{global}} = (L-1) \times 16 \text{ bits.}$$

For the example above, this reduces the total from 576 bits to 80 bits (an 86% reduction).

Scale Selection. For LoRA-TT, each layer contains only u trainable parameters, making second-order quantisation methods such as GPTQ less critical. In this setting, nearest-integer rounding is sufficient and admits a simple analytical treatment. Given a global scale $s > 0$, parameters are quantised via

$$q_i = \text{clip}\left(\text{round}\left(\frac{v_i}{s} \right), -q_{\max}, q_{\max} \right), \quad q_{\max} = 2^{b-1} - 1,$$

with dequantisation given by $\hat{v}_i = q_i s$, where $\text{clip}(x, a, b) = \min\{b, \max\{a, x\}\}$ and $\text{round} : \mathbb{R} \to \mathbb{Z}$ denotes rounding to the nearest integer.

Let $\mathbf{v} \in \mathbb{R}^{Lu}$ denote the concatenation of all layer vectors. We set

$$s^* = \frac{\|\mathbf{v}\|_\infty}{q_{\max} + \frac{1}{2}}, \tag{2}$$

which yields the following optimality property.

Proposition 4.3 (Error-Minimising Clipping-Free Scale). *Let $\mathbf{v} \in \mathbb{R}^{Lu}$. The scale s^* is the minimal scale that avoids clipping under nearest-integer quantisation, i.e., ensures that $|\text{round}(v_i/s^*)| \leq q_{\max}$ for all i, and minimises the worst-case rounding error among clipping-free scales:*

$$\left\| \mathbf{v} - \hat{\mathbf{v}}(s^*) \right\|_\infty \leq \frac{s^*}{2}. \tag{3}$$

Proof. See Section A.2. □

5. Empirical Evaluation

Models and Datasets. We evaluate our framework on three safety oversight models of varying scales: Llama Guard 3 1B (Grattafiori et al., 2024), Llama Guard 3 8B (Grattafiori et al., 2024), and Qwen-3-Guard (Zhao et al., 2025) 0.4B, 4B and 8B variants. Experiments are conducted across four safety benchmarks: Egida (Garcia-Gasulla et al., 2025), OpenAI Content Moderation (Markov et al., 2023), Aegis (Ghosh et al., 2025), and BeaverTails (Ji et al., 2023). Full dataset details are provided in Section C. While evaluating binary safety, our judges operate generatively; predictive distribution over safety categories in this regard for Brier scores are discussed in Section G

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Figure 2. **Non-vacuous PAC-Bayes guarantees for safety oversight models.** PAC-Bayes bounds and test risk for 0–1 and Brier losses across models, datasets, and adaptor families (LoRA, LoRA-XS, LoRA-T), showing the tightest bounds per adaptor family for each dataset and model. Highly compressed adaptors consistently achieve the tightest non-vacuous guarantees while preserving competitive predictive performance.

Fine-Tuning Setup. We fine-tune models using PEFT to analyse the relationship between description length and generalisation. Specifically, we use LoRA with ranks $r \in \{1, 2, 4\}$, LoRA-XS with $r \in \{2, 4\}$, and all three LoRA-T variants introduced in Section 4.1: the non-tied LoRA-TN, the tied variant LoRA-TT, and our global-scale variant LoRA-GT, with $(r, u) \in \{(2,1), (4,1), (4,2), (4,4)\}$. Models are trained autoregressively via supervised fine-tuning (SFT) using the standard log-loss objective. All linear layers are adapted. Further details given in Section D.2.

Quantisation and Compression. Following Section 3.1, we quantise adapter parameters post-training at 2-bit and 4-bit precision. All adaptor variants use QuIP preprocessing (Tseng et al., 2024) to reduce quantisation sensitivity to outliers. LoRA, LoRA-XS, and LoRA-TN additionally use GPTQ (Frantar et al., 2022), implemented via `llm-compressor` (Red Hat AI and vLLM Project, 2024), while the tied LoRA-T variants (LoRA-TT and LoRA-GT) use nearest-integer rounding. Only adapter parameters are quantised and encoded; the frozen base model is excluded from the description length. This reflects the transfer-learning setting considered here, where certification concerns the complexity of the learned safety adaptation relative to a fixed pre-trained model. The resulting adapter bitstream, including reconstruction metadata, is compressed losslessly using Brotli (Alakuijala et al., 2015; Syed and Soomro, 2018), which we find yields strictly shorter description lengths than the compressor used in prior compression-based PAC-Bayes work (Lotfi et al., 2024b) (see Table 1).

Figure 3. **Generalised Catoni yields the tightest PAC-Bayes bounds.** Mean difference in bound tightness relative to the gen. Catoni bound, aggregated across non-vacuous runs with 95% bootstrap confidence intervals.

The full certification pipeline is summarised in Figure 7.

5.1. Non-Vacuous and Tight PAC-Bayes Guarantees for LLM-Based Safety Oversight Models

We obtain non-vacuous PAC-Bayes guarantees for LLM-based safety oversight models, even in practically relevant small-data regimes not addressed by prior compression-based work. As shown in Figure 2, these guarantees hold for both misclassification error (0–1 loss) and probabilistic prediction error (Brier loss), certifying both predictive accuracy and uncertainty estimates.

The bounds are non-vacuous for sufficiently compressed adaptations (e.g. LoRA-T) across datasets and model scales (1B–8B), vary primarily with adaptor complexity rather than

Figure 4. **Compression strongly influences certifiability in safety oversight models.** (a) Bound vs. description length across models and datasets, showing that smaller, more compressed adaptations yield tighter PAC-Bayes guarantees. (b) LoRA-T variants, where tying and global-scale quantisation reduce description length and tighten bounds with only modest changes in test risk.

model size, and tighten as dataset size increases. In contrast, larger adaptors such as standard LoRA often achieve only modest improvements in test risk while producing substantially looser, and frequently vacuous, guarantees. This suggests that simple adaptations are often sufficient to preserve oversight performance while enabling stronger certification.

In several settings, the bounds closely track test risk (e.g. BeaverTails), suggesting that they are informative for model selection. Finally, as shown in Figure 3, the generalised Catoni bound consistently outperforms alternatives such as McAllester, Rivasplata, and Thiemann, as well as bounds used in prior work (Lotfi et al., 2024a), indicating that commonly used formulations can be unnecessarily loose in this regime. Notably, for highly compressed adaptations such as LoRA-GT, the resulting certificates are often informative and in several settings closely track observed test risk.

5.2. Adaptor Compression Yields the Tightest PAC-Bayes Guarantees

As shown in Figure 2, tighter PAC-Bayes guarantees are consistently achieved by smaller, more compressed adaptor families, with LoRA-T variants yielding the strongest certificates. Figure 4 (a) shows a monotonic relationship between adaptor description length and bound tightness, indicating that compression strongly influences certifiability. Further compression through tying and global-scale quantisation tightens bounds within the LoRA-T family (Figure 4 (b)), with LoRA-GT achieving the tightest guarantees relative to test error across methods.

Crucially, these substantial reductions in description length induce only modest degradation in predictive performance. In particular, larger adaptors such as standard LoRA often achieve only small reductions in test error while producing substantially looser, and frequently vacuous, guarantees. In contrast, highly compressed LoRA-T variants preserve competitive performance while enabling dramatically tighter certification. Overall, these results suggest that reducing adaptor description length is an effective mechanism for improving certifiability in safety oversight models.

5.3. Functional Distortion for Understanding Generalisation Under Compression

We examine how compression affects generalisation through functional distortion, defined as the expected loss difference between compressed LoRA-GT adaptors and their corresponding uncompressed base adaptors (see Section F). To trace the compression frontier, we progressively quantise adaptors at 2, 3, 4, 8, and 16-bit precision. As shown in Figure 5, low-distortion models consistently concentrate near low-error, tight-bound regimes across both BeaverTails and Aegis, while increasing distortion aligns with progressively looser PAC-Bayes certificates and higher test error.

The figures reveal a clear compression–distortion trade-off. Smaller, more compressed adaptations can maintain tight certificates and competitive performance provided distortion remains low, while highly distorted compressed models drift away from the low-risk, tight-bound frontier. This suggests a practical selection principle: progressively compress a fine-tuned model while monitoring distortion, and select the

Figure 5. **Functional distortion tracks certifiability under compression.** Test error versus PAC-Bayes bound for LoRA-GT across Aegis and BeaverTails, coloured by functional distortion and scaled by adaptor description length. Low-distortion models concentrate near low-error, tight-bound regimes, while increasing distortion corresponds to looser certificates and higher test error.

minimum-description-length adaptation that remains within the low-distortion regime.

6. Discussion

We introduced a PAC-Bayes framework for scalable oversight under generator-induced distributions, enabling computable certification of LLM-based judge systems. Within this framework, we obtained non-vacuous PAC-Bayes guarantees for safety oversight models, a practically important setting where such guarantees are largely absent. We showed that compression-based PAC-Bayes analysis yields tight and practical certificates in this regime without modifying standard safety alignment pipelines or introducing specialised parameterisations. Moreover, PAC-Bayes bound choice, compressed model representation, and description-length accounting substantially affect certificate tightness, enabling markedly stronger guarantees for both classification risk and predictive uncertainty. Taken together, these results show that seemingly minor design choices in compression-based PAC-Bayes pipelines can materially affect practical certifiability for LLMs.

Across models and datasets, shorter description lengths yield systematically tighter bounds, indicating that certifiability is governed primarily by adaptation complexity rather than base model scale. This suggests that highly capable models can often be adapted through extremely low-complexity PEFT updates while remaining practically certifiable, supporting an Occam-style view in which effective safety adaptations minimally modify strong pre-trained models. LoRA-GT parameterisation sharpens this effect through global-scale quantisation, reducing adaptor description length while preserving competitive performance. Empirically, highly compressed PEFT adaptations often match substantially larger adaptors in performance while yielding dramatically tighter PAC-Bayes certificates.

We further identified functional distortion as a practical proxy for certifiable generalisation. Distortion jointly tracks test error and bound tightness under compression, suggesting a simple design principle: select the minimum-description-length adaptation that remains within the low-distortion regime. This provides a principled alternative to heuristic model selection in safety-critical settings.

Our work relies on deterministic posteriors and compression-based certificates over learnable adapters relative to a fixed pre-trained model. Alternative priors or stochastic posteriors may yield tighter certificates, though potentially at increased computational cost for deployment-scale oversight systems. Finally, further work is needed to understand how extreme compression affects more complex reasoning capabilities, which may be less robust to aggressive compression than zero-shot judgments.

7. Conclusion

We presented non-vacuous PAC-Bayes guarantees for LLM-based safety oversight models, a setting where such guarantees have been largely absent, covering both classification risk and predictive distributions via the Brier score. We showed that bound tightness is governed by the compressibility of the learned adaptation, and that refining compression-based methodology and reducing adaptor description length yields substantially tighter guarantees without modifying standard fine-tuning. Empirically, compressed adaptations often preserve performance while enabling stronger certification, providing a practical basis for selecting simple, certifiable models.

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Appendix

A. Proofs of Statements Used

A.1. Proof of Theorem 4.1

Proof. The prefix-free Kolmogorov complexity $K_p(h \mid M)$ is defined as the length of the shortest program that outputs h under a fixed decoder M, where M captures the shared decoding procedure and model specification, and is therefore independent of the data and the learned adaptation defining the hypothesis. Consequently, the length of any valid prefix-free encoding of h provides an upper bound on $K_p(h \mid M)$.

We construct such an encoding by concatenating two components: the length $|h|$, encoded using the Elias δ-code (Elias, 2003), followed by the binary string h itself. This forms a valid prefix-free program for h. The Elias δ-code for an integer x has length

$$\lfloor \log_2 x \rfloor + 2\lfloor \log_2(\lfloor \log_2 x \rfloor + 1) \rfloor + 1,$$

and hence

$$K_p(h \mid M) \le |h| + \lfloor \log_2 |h| \rfloor + 2\lfloor \log_2(\lfloor \log_2 |h| \rfloor + 1) \rfloor + 1. \tag{A.4}$$

Note that, as shown in Table 2, Elias δ coding yields a tighter description-length upper bound than the Elias γ coding used in prior work (Lotfi et al., 2024a), revealing an additional source of looseness in prior methodology that can be exploited to improve bound tightness.

For the deterministic posterior $\mathbb{Q}_h = \delta_h$, and assuming $|\mathcal{H}| < \infty$, the KL divergence simplifies to

$$\mathrm{KL}(\mathbb{Q}_h \| \mathbb{P}_{\mathrm{Sol}}) = \sum_{g \in \mathcal{H}} \delta_h(g) \log \frac{\delta_h(g)}{\mathbb{P}_{\mathrm{Sol}}(g)} = -\log \mathbb{P}_{\mathrm{Sol}}(h). \tag{A.5}$$

Using the definition of the Solomonoff prior in Equation (1),

$$-\log \mathbb{P}_{\mathrm{Sol}}(h) = -\log \left(\frac{2^{-K_p(h|M)}}{Z} \right) = K_p(h \mid M) \log 2 + \log Z \le K_p(h \mid M) \log 2, \tag{A.6}$$

where the inequality follows from $Z \le 1$ by Kraft's inequality (Kraft, 1949). Substituting the bound from Equation (A.4) yields

$$\mathrm{KL}(\mathbb{Q}_h \| \mathbb{P}_{\mathrm{Sol}}) \le (|h| + \lfloor \log_2 |h| \rfloor + 2\lfloor \log_2(\lfloor \log_2 |h| \rfloor + 1) \rfloor + 1) \log 2,$$

which coincides with $\mathrm{KL}^{\mathrm{UB}}(\mathbb{Q}_h \| \mathbb{P}_{\mathrm{Sol}})$. $\square$

A.2. Proof of Theorem 4.3

Proof. Let $M = \|\mathbf{v}\|_\infty$ and define $q_{\max} = 2^{b-1} - 1$ as the maximum representable signed integer under b-bit quantisation. Avoiding clipping under nearest-integer quantisation requires

$$\left| \mathrm{round}\left(\frac{v_i}{s} \right) \right| \le q_{\max} \quad \text{for all } i,$$

which is satisfied whenever

$$\frac{|v_i|}{s} \le q_{\max} + \frac{1}{2}.$$

Thus, the minimal scale avoiding clipping is given by

$$s^* = \frac{M}{q_{\max} + \frac{1}{2}}.$$

For such $s \in \mathbb{R}_{>0}$, the quantisation error is governed by rounding:

$$|v_i - \hat{v}_i| = \left| v_i - s \cdot \mathrm{round}\left(\frac{v_i}{s} \right) \right| = s \left| \frac{v_i}{s} - \mathrm{round}\left(\frac{v_i}{s} \right) \right| \le \frac{s}{2},$$

since rounding to the nearest integer incurs error at most $1/2$. Since the bound $s/2$ increases with s, the minimal valid scale s^* yields the tightest bound. $\square$

B. Alternative PAC-Bayes Risk Certificates

While the main text focuses on the generalised Catoni bound, we also evaluate several variants of PAC-Bayes certificates from the literature, which we apply in the setting of LLM safety oversight as shown in Figure 3. This comparison situates our work relative to existing approaches applied to LLMs in alternative settings (Lotfi et al., 2024a;b), and allows us to assess the empirical tightness of our proposed method against established baselines.

Proposition B.1 (Lotfi Finite Hypothesis Certificate). *For discrete, finite hypothesis spaces (Lotfi et al., 2024a) with a deterministic posterior $h \in \mathcal{H}_J$, the true risk is bounded by:*

$$\mathcal{R}(h) \leq \widehat{\mathcal{R}}_S(h) + \sqrt{\frac{\mathrm{KL}^{UB}(\mathbb{Q}_h \| \mathbb{P}_{Sol}) + \log(1/\beta)}{2n}} .$$

Proposition B.2 (McAllester Certificate). *The classic PAC-Bayes generalisation bound (McAllester, 1999), incorporating the distribution-free overhead $\xi(n) = 2 + \sqrt{2n}$ (Maurer, 2004), provides the following certificate:*

$$\mathcal{R}(h) \leq \widehat{\mathcal{R}}_S(h) + \sqrt{\frac{\mathrm{KL}^{UB}(\mathbb{Q}_h \| \mathbb{P}_{Sol}) + \log(\xi(n)/\beta)}{2n}} .$$

Proposition B.3 (Seeger-Langford Certificate). *Based on the PAC-Bayes theorem for Bernoulli random variables (Seeger, 2002), the true risk satisfies the following relative entropy inequality:*

$$KL\left(\widehat{\mathcal{R}}_S(h) \,\middle\|\, \mathcal{R}(h)\right) \leq \frac{\mathrm{KL}^{UB}(\mathbb{Q}_h \| \mathbb{P}_{Sol}) + \log(\xi(n)/\beta)}{n} ,$$

where $\mathrm{KL}(q\|p) = q \log \frac{q}{p} + (1-q) \log \frac{1-q}{1-p}$ *is the binary Kullback-Leibler divergence. The bound on $\mathcal{R}(h)$ is found by taking the largest $p \in (\widehat{\mathcal{R}}, 1)$ satisfying the inequality.*

Proposition B.4 (Thiemann Certificate). *Utilising the strongly quasiconvex bound from Thiemann et al. (2017), the risk is bounded for any $\lambda \in (0, 2)$:*

$$\mathcal{R}(h) \leq \inf_{\lambda \in (0,2)} \left\{ \frac{\widehat{\mathcal{R}}}{1 - \lambda/2} + \frac{\mathrm{KL}^{UB}(\mathbb{Q}_h \| \mathbb{P}_{Sol}) + \log(\xi(n)/\beta)}{n\lambda(1 - \lambda/2)} \right\} .$$

Proposition B.5 (Rivasplata Certificate). *The empirical risk inversion bound (Rivasplata et al., 2019) yields a certificate that avoids square roots of the complexity term in the dominant part of the bound:*

$$\mathcal{R}(h) \leq \widehat{\mathcal{R}}_S(h) + \frac{C}{n} + \sqrt{2\widehat{\mathcal{R}}_S(h)\frac{C}{n} + \left(\frac{C}{n}\right)^2} ,$$

where $C = \mathrm{KL}^{UB}(\mathbb{Q}_h \| \mathbb{P}_{Sol}) + \log(\xi(n)/\beta)$.

C. Dataset Details and Prompt Templates

Our work evaluates methods over four safety benchmarks, encompassing a diverse range of unsafe categories.

C.1. Dataset Descriptions

Egida. The Egida dataset (Garcia-Gasulla et al., 2025) focuses on evaluating the safety of agent responses to potentially harmful user queries. We use the Egida-HSafe configuration, drawing from the dataset's test split of 1,000 high quality, manually labelled samples. As no pre-defined training partition is provided, we apply a fixed 80/20 train–test split, yielding 800 training samples and 200 test samples. Safety labels are derived by majority vote over five independent human annotators, with each annotator assigning a "safe" or "unsafe" label to the agent response; a sample is classified as unsafe if the majority vote is "unsafe". The taxonomy covers 9 hazard categories: Cybercrime, Non-Violent Crimes, Violent Crimes, Sexual Crimes and Erotic Content, Illegal Weapons and Substances, Hate and Harassment, Fake News and Misinformation, Dangerous Acts and Self-Harm, and Health.

OpenAI Moderation. The OpenAI Moderation evaluation set (Markov et al., 2023) provides labelled standalone user prompts drawn from interactions with the OpenAI API, with no accompanying agent response; only the user prompt is evaluated for harm. The full dataset comprises 1,680 samples in a single split. As no pre-defined training partition is provided, we once again apply a fixed 80/20 train–test split, yielding 1,344 training samples and 336 test samples. A sample is classified as unsafe if any of 8 binary moderation flags is positive. The taxonomy covers 8 hazard categories: Sexual Content, Hate Speech, Violence, Harassment, Self-Harm, Sexual Content Involving Minors, Hate Speech with Threats, and Graphic Violence.

Aegis 2.0. Aegis 2.0 (Ghosh et al., 2025) tasks the judge with jointly evaluating both the user prompt and the agent response for safety violations. We use the pre-defined train and test splits, filtering out entries marked as "REDACTED" and applying length constraints (prompts exceeding 5,000 characters and responses exceeding 10,000 characters) for more efficient training and inference. After filtering, this yields approximately 28,984 training samples and 1,900 test samples. Each sample carries separate "safe" or "unsafe" labels for the prompt and response; a conversation is deemed unsafe if either the prompt label or the response label is "unsafe". The benchmark taxonomy covers 12 hazard categories: Hate/Identity Hate, Sexual Content, Suicide/Self-Harm, Violence, Guns/Illegal Weapons, Threats, PII/Privacy, Sexual Content (Minors), Criminal Planning, Harassment, Controlled Substances, and Profanity.

BeaverTails. The BeaverTails dataset (Ji et al., 2023) is designed to assess the safety of generated responses from an agent in response to a user query; only the agent response is evaluated for harm. We use the pre-defined 330k_train and 330k_test splits, comprising 300,567 training samples and 33,396 test samples respectively. A sample is classified as unsafe if the is_safe field evaluates to False. The taxonomy of unsafe categories covers 14 distinct hazards, including: Animal Abuse, Child Abuse, Controversial Topics/Politics, Discrimination/Stereotype, Drug Abuse/Weapons, Financial/Property Crime, Hate Speech, Misinformation, Non-Violent Unethical Behaviour, Privacy Violation, Self-Harm, Sexually Explicit, Terrorism/Organised Crime, and Violence/Incitement.

C.2. Prompt Templates

All evaluations rely on a standardised prompt structure: `[Task Instruction]` → `[Safety Categories]` → `[Conversation]` → `[Assessment Instruction]` → `[Output]`. The specific instructions vary depending on the target being assessed. The general prompt templates for each of the safety datasets that we consider in this work are included in Figure 6.

Figure 6. **Safety Fine-Tuning and Evaluation Prompts.** Prompts applied for both PEFT and evaluation, shown separately for each for the four safety datasets and corresponding tasks that we consider in this work.

C.3. Connection to the Oversight Framework

Within the context of Section 4, these datasets instantiate the setting where prompts are drawn from an underlying data distribution and responses are generated by a fixed generator model, with accompanying safety evaluations defining the target oversight labels. In this setting, our guarantees certify the generalisation of an oversight model relative to the generator underlying the collected prompt–response pairs. More broadly, however, the framework applies generally to certifying oversight models for arbitrary fixed generators.

D. Parameter-Efficient Fine-Tuning – LoRA Variants

D.1. LoRA Adaptor Variants

Low-Rank Adaptation (LoRA). LoRA (Hu et al., 2022) parametrises weight updates for a frozen, pre-trained linear transformation $W_0 \in \mathbb{R}^{d \times k}$ through a low-rank perturbation. The adapted weights $W \in \mathbb{R}^{d \times k}$ are defined as:

$$W = W_0 + BA \tag{D.7}$$

where $B \in \mathbb{R}^{d \times r}$ and $A \in \mathbb{R}^{r \times k}$ are trainable matrices with rank $r \leq \min(d, k)$.

LoRA-XS. LoRA-XS (Bałazy et al., 2024) enhances the parameter efficiency of LoRA by performing latent editing within the SVD-transformed space of the original weights. The update is formulated as:

$$W = W_0 + U\Sigma R V^\top \tag{D.8}$$

where U, Σ, and V are obtained via singular value decomposition (SVD) of W_0 and remain frozen during training. By training only the small latent mapping matrix $R \in \mathbb{R}^{r \times r}$, LoRA-XS significantly reduces the number of trainable parameters by decoupling them from the model's hidden dimensionality.

LoRA-T. TinyLoRA (denoted LoRA-T in this work) (Morris et al., 2026) further compresses the LoRA-XS architecture by replacing the trainable matrix R with a low-dimensional trainable vector $v \in \mathbb{R}^u$ projected through fixed matrices. The update rule is defined as:

$$W = W_0 + U\Sigma \left(\sum_{i=1}^{u} v_i P_i \right) V^\top \tag{D.9}$$

where $P_i \in \mathbb{R}^{r \times r}$ are fixed random matrices and only the vector $v \in \mathbb{R}^u$ is updated. For further parameter reduction, LoRA-T offers a weight-tied variant, denoted *LoRA-T Tied* (LoRA-TT as introduced in the main body of the paper). In this configuration, a single trainable vector v is shared across all targeted modules within a given transformer layer (e..g all MLP and attention modules), whilst each individual module retains its own independent set of frozen projection matrices P_i.

These parameterisations produce highly compact updates whose complexity can be quantified via their description length after quantisation and compression, making them well-suited to compression-based PAC-Bayes analyses.

D.2. PEFT Fine-Tuning Details

All models are fine-tuned using the `SFTTrainer` from the Hugging Face Transformers library (Wolf et al., 2020). We perform supervised-fine tuning (SFT) via PEFT on safe vs unsafe completion judgements of input examples according to each individual dataset's own taxonomy of hazards.

Shared Hyperparameters across Adaptor Methods. We utilise the AdamW optimiser with learning rate decay implemented via a cosine learning rate scheduler with a 3% linear warm-up period. Weight decay is set per method as specified below. All training operations are performed in bfloat16 precision. The maximum sequence length for training is set dynamically per dataset to the 99th percentile of tokenised prompt lengths (rounded up to the nearest 64 tokens), ensuring fewer than 1% of training examples are truncated for training efficiency. For inference, we use dataset-appropriate context windows: 2048 tokens for BeaverTails, 4096 for OpenAI Moderation, and 6000 for Aegis and Egida, matching training.

Adaptor Method-Specific Settings. For each of the three different PEFT LoRA-based adaptor methods, we experiment over the following specific hyperparameter settings:

- **LoRA:** For standard LoRA, we evaluate ranks $r \in \{1, 2, 4\}$. The scaling hyperparameter α is set equal to the rank ($\alpha = r$), resulting in a constant adapter scaling factor of $\alpha/r = 1$. We employ a learning rate of 2×10^{-4} with weight decay 0.01, training for 4 epochs on smaller datasets (Egida and OpenAI Moderation) and 1 epoch on larger datasets (Aegis and BeaverTails).

- **LoRA-XS:** The base adapter matrices A and B are initialised via Singular Value Decomposition (SVD) of the base weights using 10 power iterations, and are subsequently frozen prior to training. Only the $r \times r$ latent mapping matrix R is updated during fine-tuning. We evaluate SVD ranks $r \in \{2, 4\}$, again setting $\alpha = r$ to maintain a scaling factor of 1. We utilise a learning rate of 8×10^{-4} with no weight decay, training for 6 epochs on smaller datasets and 2 epochs on larger datasets.

- **LoRA-T:** Similar to LoRA-XS, the base matrices for LoRA-T are SVD-initialised and completely frozen. The trainable parameters are restricted strictly to a u-dimensional vector v, which modifies the latent space via fixed random projection matrices. We evaluate the following pairings of the SVD rank r and trainable vector dimension u: $(r = 2, u = 1)$, $(r = 4, u = 1)$, $(r = 4, u = 2)$, and $(r = 4, u = 4)$. The scaling parameter α is matched to the SVD rank, again giving a scaling factor of 1. We apply a learning rate of 1×10^{-3} with no weight decay, training for 6 epochs on smaller datasets and 2 epochs on larger datasets.

For each LoRA-based adaptation method, we target all linear layers within the transformer blocks. Specifically we target all attention and MLP projections within each transformer block layer of models.

Model-Specific Hyperparameters. Training batch sizes are adjusted based on model scale to accommodate GPU memory constraints. For Llama-Guard-3-1B, a batch size of 8 is used across all four datasets. For the larger models, Llama-Guard-3-8B and Qwen3Guard-Gen-8B, a batch size of 4 is used across all four datasets.

E. Risk Functions

We consider the two bounded risk functionals induced by losses $\ell : \mathcal{Y} \times \mathcal{Y} \to [0, 1]$, used in the main body of this work. We follow the notation for applying PAC-Bayes theory to LLMs-as-judges introduced in Section 4.

0–1 Risk. For binarised correctness-based evaluation of LLM safety oversight models, we consider the standard 0–1 loss, measuring safety misclassification, which induces the risk:

$$\mathcal{R}_{0\text{-}1}(h) = \mathbb{E}_{(x,y) \sim \mathbb{P}_{\mathcal{D},G}} \left[\mathbf{1}\big(h(x, y) \neq z^*(x, y)\big) \right],$$

where $z^*(x, y) \in \{0, 1\}$ denotes the ground-truth evaluation of a prompt–response pair and $h(x, y)$ is the prediction of the judge. Equivalently, this risk can be interpreted as the probability that the judge makes an error:

$$\mathcal{R}_{0\text{-}1}(h) = \mathbb{P}_{(x,y) \sim \mathbb{P}_{\mathcal{D},G}}\big(h(x, y) \neq z^*(x, y)\big).$$

Brier Risk. To evaluate probabilistic predictions, we use the Brier score, a strictly proper scoring rule that captures both accuracy and calibration (Murphy, 1973). For predictions $h(x, y) \in [0, 1]$, this induces the Brier risk defined as

$$\mathcal{R}_{\text{Brier}}(h) = \mathbb{E}_{(x,y) \sim \mathbb{P}_{\mathcal{D},G}} \left[\big(h(x, y) - z^*(x, y)\big)^2 \right],$$

where $c := z^*(x, y) \in \{0, 1\}$.

Conditioning on the predicted probability $h(x, y)$ yields the classic Murphy (1973) decomposition (with expectations taken over $(x, y) \sim \mathbb{P}_{\mathcal{D},G}$):

$$\mathcal{R}_{\text{Brier}}(h) = \underbrace{\mathbb{E}\big[(h(x, y) - \mathbb{E}[c \mid h(x, y)])^2\big]}_{\text{Calibration}} - \underbrace{\mathbb{E}\big[\mathbb{V}(c \mid h(x, y))\big]}_{\text{Resolution}} + \underbrace{\mathbb{V}(c)}_{\text{Uncertainty}}.$$

The calibration term measures the discrepancy between predicted probabilities and true conditional frequencies, the resolution term captures how informative predictions are about the label, and the uncertainty term reflects the intrinsic variability of the labels. This decomposition is provided for interpretability; our analysis operates directly on the Brier risk.

E.1. Deterministic Posteriors for LLM Certification

In our setting, the object being certified is the deployed compressed oversight model itself rather than a sampled Gibbs classifier. Deterministic posteriors of the form $Q_h = \delta_h$ are therefore particularly natural for deployment-scale LLM oversight systems, where the objective is to certify the behaviour of a single deployed adaptation.

More broadly, our use of the PAC-Bayes framework is primarily as a mechanism for deriving data-dependent, complexity-sensitive generalisation certificates over compressed hypotheses. Under deterministic posteriors, the KL term reduces directly to a complexity penalty determined by the description length of the deployed adaptation under the Solomonoff prior, yielding an interpretable trade-off between empirical fit and compressibility. This perspective is especially natural in compression-based settings, where complexity accounting is fundamentally defined at the level of individual compressed hypotheses.

This formulation also aligns with prior compression-based PAC-Bayes analyses for LLMs (Lotfi et al., 2024a;b), enabling direct comparison with existing methodologies while isolating the effects of our proposed refinements, including PAC-Bayes bound choice, description-length accounting, and compressed hypothesis representations.

More specifically, in our setting the compressed adaptor itself constitutes the learned object of interest: the PAC-Bayes complexity term is induced directly by the compressed representation used to reconstruct the deployed hypothesis. This makes deterministic posteriors particularly well aligned with the Solomonoff-style compression framework adopted in this work.

While optimised stochastic posteriors may in principle yield tighter certificates, such approaches require repeated sampling and evaluation in order to approximate Gibbs risks. For deployment-scale LLM oversight systems, this introduces substantial inference and latency overhead, making stochastic certification objectives less aligned with the practical certification setting considered in this work.

F. Functional Distortion under Compression

To quantify the effect of compression on a learned predictor, we define *functional distortion* as the expected difference in loss between a fine-tuned model and its compressed counterpart.

Let $h \in \mathcal{H}$ denote the fine-tuned model and $\tilde{h} \in \mathcal{H}$ its compressed version. For a loss function $\ell : \mathcal{Y} \times \mathcal{Y} \to [0, 1]$, we define the population functional distortion as:

$$\Delta(h, \tilde{h}) := \mathbb{E}_{(x,y) \sim \mathbb{P}_{\mathcal{D},G}} \big[\ell(\tilde{h}(x, y), z^*(x, y)) - \ell(h(x, y), z^*(x, y)) \big]. \tag{F.10}$$

In practice, this expectation is not directly computable, and we estimate it using a Monte Carlo average over a sample

$$S = \{(x_i, y_i)\}_{i=1}^n \sim (\mathbb{P}_{\mathcal{D},G})^n,$$

yielding the *empirical functional distortion*:

$$\delta_n(h, \tilde{h}) := \frac{1}{n} \sum_{i=1}^n \big(\ell(\tilde{h}(x_i, y_i), z^*(x_i, y_i)) - \ell(h(x_i, y_i), z^*(x_i, y_i)) \big). \tag{F.11}$$

In our experiments, the sample S is taken from the training set used for fine-tuning, and thus $\delta_n(h, \tilde{h})$ can be computed directly as the difference in empirical risk between the compressed and fine-tuned models:

$$\delta_n(h, \tilde{h}) = \hat{R}_S(\tilde{h}) - \hat{R}_S(h). \tag{F.12}$$

G. Deriving Predictive Distributions Over Safety Categories from Token Probabilities

In our setting, the safety oversight model $h \in \mathcal{H}_J$ is generative and outputs a sequence of tokens. To obtain a predictive distribution over output categories (e.g., safe, unsafe), we extract probabilities from the model's token-level conditional distribution.

Let $\mathcal{C}$ denote the finite set of output categories, and let each $c \in \mathcal{C}$ correspond to a token sequence $w_{1:T_c}^{(c)} \in \mathcal{V}^*$. For an input $(x, y) \in \mathcal{X} \times \mathcal{Y}$, the judge model $h \in \mathcal{H}_J$ induces an autoregressive distribution over token sequences, yielding the following likelihood for each category:

$$s_h(c \mid x, y) = \prod_{t=1}^{T_c} p_h\big(w_t^{(c)} \mid x, y, w_{<t}^{(c)} \big).$$

We then obtain a predictive distribution over categories by normalising across $\mathcal{C}$:

$$p_h(c \mid x, y) = \frac{s_h(c \mid x, y)}{\sum_{c' \in \mathcal{C}} s_h(c' \mid x, y)}.$$

This induces a distribution over $\mathcal{C}$ derived directly from the model's token-level probabilities. In the common case where each category corresponds to a single token (e.g., safe, unsafe), this reduces to extracting the next-token probabilities and renormalising over $\mathcal{C}$.

This allows us to get judge confidence scores over safety categories, allowing for the investigation of generalisation guarantees on model prediction probabilities via Brier score.

H. Computational Resources

Experiments involving the lightweight Llama-Guard-3-1B model were conducted on a single NVIDIA L40S GPU equipped with 48 GB of VRAM. Experiments for the larger 8B models utilised either single NVIDIA H100 GPUs (80 GB VRAM) or two L40s GPUs.

I. Quantisation and Compression Details

To minimise the complexity penalty in our PAC-Bayesian certificates, we subject the fine-tuned trainable adapter weights to post-training quantisation and compression pipeline. This procedure is implemented using the llmcompressor library (Red Hat AI and vLLM Project, 2024). In particular, we sequentially apply Quantisation with Incoherence Processing (QuIP#) (Tseng et al., 2024) followed by Generalised Post-Training Quantisation (GPTQ) (Frantar et al., 2022).

I.1. Quantisation Pipeline

QuIP (Hadamard Rotation).   To mitigate the impact of outlier features and reduce overall quantisation error, we first apply QuIP# (Tseng et al., 2024). This involves multiplying the weights by deterministic Hadamard matrices (Sylvester, 1867). For the standard LoRA and LoRA-XS adapters, this rotation is applied to both the input (v) and output (u) dimensions. However, for LoRA-T, the rotation is applied exclusively to the input side, as the output dimension of the trainable vector is simply 1. Following the subsequent GPTQ step, these rotations are mathematically inverted (de-rotated), and the quantised weights are restored in-place.

GPTQ Calibration and Configuration.   We perform second-order quantisation leveraging Hessian information via the GPTQ algorithm (Frantar et al., 2022). The calibration data consists of the identical subsample used during the fine-tuning phase, tokenised using the same prompt formatting. To ensure numerical stability during the Hessian inversion, we apply a damping factor of 0.05. The block size for the algorithm is aligned with the structural rank of the adapter: r for LoRA and LoRA-XS, and u for LoRA-T. The quantisation target is strictly symmetric, mapping the parameters to either b-bit precision. For weight-tied LoRA-T, we use nearest-integer rounding with a single max-abs scale per layer (or a single global scale when a global quantisation scheme is adopted); all other adapters use GPTQ throughout. Nearest-integer rounding suffices here given the extremely small number of quantised parameters ($u \leq 4$ scalars per layer), where the second-order Hessian correction provided by GPTQ yields negligible benefit.

I.2. Compression Certificate Construction

For a PAC-Bayes certificate to remain theoretically valid, the prior must be constructed strictly independently of the training data. When employing the Solomonoff prior, the KL divergence between this data-independent prior and the deterministic posterior is upper-bounded by an expression involving the model's description length. We empirically measure this description length via the size of an encoded file storing trained adaptor weights. Consequently, to preserve the theoretical validity of the bound, this file must encode strictly and exclusively the data-dependent information required to perfectly reconstruct the posterior hypothesis.

Components Included in the Certificate.   The encoded bit-stream strictly includes:

1. **Packed Quantised Weights:** The trainable weight parameters of all LoRA-based adaptation methods, symmetrically quantised to the target bit-width and tightly packed at exactly b bits per value into a contiguous bitstream.

2. **Quantisation Scales:** The scaling factors required to de-quantise the weights back into the continuous parameter space. These are strictly stored per-tensor, retaining their original precision (e.g., `bfloat16`).

3. **Random Seed:** The scalar random seed used to initialise all stochastic components of the pipeline (e.g., SVD initialisation of frozen adapter matrices, generation of LoRA-T projection matrices, data shuffling) is stored alongside the certificate; its Elias delta code length is added as a theoretical overhead to the total hypothesis description length $|h|$, ensuring the description-length accounting is complete.

Components Excluded from the Certificate.   Several components of the network are excluded from the encoded file because they are either strictly data-independent (forming part of the fixed prior/decoder M) or unnecessary for weight reconstruction:

1. **Base LLM Weights:** The pre-trained weights of the generator model are frozen and shared between the prior and the posterior.

2. **Frozen Adapter and Projection Matrices:** In architectures like LoRA-XS and LoRA-T, the base adapter matrices (A and B) are initialised via singular value decomposition and subsequently frozen before any training occurs. Furthermore, for LoRA-T specifically, the full projection matrices (P) are excluded. Because these matrices are fixed prior to observing the training data, and the P matrices can be perfectly reconstructed from the explicitly stored scalar seed, the matrices themselves do not contribute to the complexity penalty.

3. **QuIP Rotation Matrices:** The Hadamard transform matrices (U and V) used during QuIP quantisation are deterministically generated based on the matrix dimensions. Because they contain no information derived from the training set, they are treated as part of the fixed decoding scheme and excluded from the description length.

4. **Zero-Points and Group Indices:** Because we strictly employ symmetric quantisation without activation order permutations, zero-points are trivially zero and data-dependent column permutations are non-existent. Therefore, no bits are required to encode them.

Configuration Selection Overhead.   Several results in the main text report the tightest PAC-Bayes certificate obtained within an adaptor family across a finite set of PEFT configurations. To compare certificates across configurations, these models may be viewed as elements of a common enlarged hypothesis class. Under the coding interpretation of the Solomonoff prior, the index of the selected configuration (e.g. the choice of LoRA-T variant, (r, u) setting, or quantisation scheme) forms part of the hypothesis description and contributes an additional complexity cost of at most $\lceil \log_2 K \rceil$ bits when selecting among K candidate configurations. Since this overhead grows only logarithmically in K, it is small relative to the adaptor description lengths considered in this work (e.g. selecting among all 24 LoRA-T configurations contributes at most $\lceil \log_2 24 \rceil = 5$ additional bits).

Compression. By perfectly isolating the data-dependent latent mappings from the data-independent prior structures, we ensure the theoretical validity of the certificate. To further compress the model's description length $|h|$, we apply strong lossless Brotli compression (Google Inc., 2015) at its maximum setting (`quality=11`) to this isolated bit-stream. As demonstrated in Table 1, we conducted an empirical comparison of Brotli against LZMA (`preset=9`) (Python Software Foundation, 2026b) and gzip (`preset=9`) (Python Software Foundation, 2026a), two popular lossless compression algorithms, with gzip being the standard choice in prior compression-based PAC-Bayes work on LMs (Lotfi et al., 2024b). Brotli consistently achieves the tightest description length across all evaluated adapter configurations. Crucially, this superior compression ratio demonstrates that the complexity penalties, and consequently the generalisation bounds, reported in prior work (Lotfi et al., 2024b) could be systematically tightened simply by adopting more advanced compression mechanisms, highlighting a suboptimality in their methodology for which we provide a simple and readily available solution.

Table 1. **Compression Algorithm Comparison.** Compression certificate size (in bits) under three lossless compressors for LoRA-based adapter configurations on Llama-Guard-3-1B (BeaverTails, 2-bit quantisation).

Adapter	Raw (B)	LZMA-9	gzip-9	Brotli-11
LoRA-TN ($u=1$, $r=4$)	336	2,432	2,192	**1,752**
LoRA-TN ($u=4$, $r=4$)	336	3,104	2,696	**2,560**
LoRA-XS ($r=2$)	336	2,976	2,736	**2,648**
LoRA-XS ($r=4$)	672	5,376	5,056	**4,576**
LoRA ($r=1$)	176,576	859,040	925,264	**828,672**
LoRA ($r=4$)	704,960	2,067,584	2,406,144	**1,994,400**

J. Full Pipeline

Figure Figure 7 summarises the full training and evaluation pipeline used in our experiments. The training set is used for supervised fine-tuning (SFT) of safery oversight models, as well as for post-training quantisation and computation of the empirical risk. The resulting quantised models are then compressed to obtain their description length. Finally, evaluation is performed using the quantised models, reporting both empirical test risk and PAC-Bayes bounds to assess the tightness of the resulting certificates.

Figure 7. **Training and certification pipeline.** Models are trained via SFT, quantised using QuIP preprocessing with either GPTQ (LoRA/LoRA-XS/LoRA-TN) or nearest-integer rounding (LoRA-TT/LoRA-GT), compressed to obtain description lengths, and evaluated using empirical test risk and PAC-Bayes certificates.

K. Adaptor Description Lengths

To make the compression story explicit, Figure 8 reports the compressed description lengths $|h|$ for all adaptor families and quantisation settings considered in this work. Across models, tying and global-scale quantisation consistently reduce description length, with LoRA-GT achieving the shortest codes, and as Figure 4 shows, the tightest bounds with minimal trade-off in performance.

Figure 8. **Adaptor Description Lengths.** Description lengths $|h|$ (log scale) for all adaptor families and quantisation settings considered in this work. Across guardrail models, 2-bit and 4-bit LoRA, LoRA-XS, LoRA-T, LoRA-T-Tied, and LoRA-GT exhibit progressively shorter codes as compression increases, with tying and global-scale quantisation yielding the smallest description lengths.

L. Coding Scheme Comparison

Table 2 compares hypothesis description lengths under different integer coding schemes for Llama-Guard-4 12B (2-bit quantisation). We report the raw compressed size $|h|$ and the resulting complexities under Elias-γ and Elias-δ coding. The differences are negligible, and we use Elias-δ in all reported bounds.

M. Detailed Results

We report the full per-model, per-stage results from Section 5 for all datasets and losses. Tables 3 and 10 give test risks and Catoni PAC-Bayes bounds ($\delta = 0.05$) for zero-shot, fine-tuned (FT), and quantised models (Q2, Q4). For each adapter family and base model, we report a single configuration, chosen as the one achieving the tightest bound across Q2 and Q4, and report its FT, Q2, and Q4 results. Within each table, underlining marks the lowest test risk per model and **bold** marks the tightest bound.

N. Comparison to Validation-Based Bounds

N.1. Validation-Based Generalisation Bounds

A seemingly simpler approach to certifying generalisation is to reserve a held-out validation set and apply concentration inequalities to bound the true risk in terms of the empirical validation error. Let $S_{\text{val}} = \{(x_i, y_i)\}_{i=1}^{n_{\text{val}}} \sim \mathcal{D}^{n_{\text{val}}}$ denote an i.i.d. validation sample, and let $\hat{R}_{\text{val}}(h)$ denote the empirical risk of a hypothesis $h \in \mathcal{H}$ on the validation set.

Classical bounds such as Hoeffding's (Hoeffding, 1963) inequality yield guarantees of the form:

$$R(h) \leq \hat{R}_{\text{val}}(h) + \sqrt{\frac{\log(1/\beta)}{2n_{\text{val}}}}, \tag{N.13}$$

Table 2. **Coding scheme ablation, Llama-Guard-3 1B** (BeaverTails, $b=2$): Elias-δ vs. Elias-γ coding of the hypothesis description length (bits).

Adapter	KL_δ	KL_γ	$\Delta\,\mathrm{KL}$
LoRA ($r=4$)	1,974,975	1,974,987	+12
LoRA-XS ($r=2$)	2,588	2,593	+5
LoRA-XS ($r=4$)	4,501	4,507	+6
LoRA-T ($r=4,\ u=1$)	1,691	1,695	+4
LoRA-T ($r=4,\ u=2$)	2,108	2,113	+5

Table 3. **Complete results on Egida (0–1 loss).** Test risk and Catoni PAC-Bayes bound ($\delta = 0.05$) at each pipeline stage (zero-shot, fine-tuned, and quantised at 2/4 bits). The chosen variant per cell is given in parentheses beside the FT entry. Per model, the lowest test risk across FT/Q2/Q4 is underlined and the lowest non-vacuous Catoni bound across Q2/Q4 is **bolded**.

		Qwen 0.6B			LG3-1B			Qwen-4B			LG3-8B			Qwen-8B		
Zero-shot	Risk	.179			.173			.189			.133			.158		
Adapter		FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4
LoRA	Risk	.087 (r=4)	.092	.087	.112 (r=1)	.128	.112	.087 (r=2)	.092	.087	.112 (r=2)	.117	.112	.092 (r=1)	.102	.102
	Bound		1.000	1.000		1.000	1.000		1.000	1.000		1.000	1.000		1.000	1.000
LoRA-XS	Risk	.153 (r=2)	.158	.148	.158 (r=2)	.163	.158	.158 (r=2)	.158	.153	.133 (r=2)	.138	.138	.138 (r=2)	.143	.143
	Bound		.991	.998		.961	.989		.995	1.000		.994	.999		.996	.999
LoRA-T	Risk	.158 (r=4,u=1)	.163	.158	.168 (r=4,u=1)	.153	.158	.153 (r=4,u=1)	.148	.153	.163 (r=2,u=1)	.163	.163	.153 (r=2,u=1)	.153	.158
	Bound		.967	.970		.925	.939		.985	.984		.979	.985		.981	.987
LoRA-T-Tied	Risk	.173 (r=4,u=1)	.173	.179	.194 (r=4,u=1)	.209	.194	.163 (r=2,u=1)	.163	.163	.148 (r=4,u=1)	.143	.153	.153 (r=4,u=1)	.163	.153
	Bound		.632	.662		.594	.607		.695	.717		.670	.680		.679	.704
LoRA-GT	Risk	.173 (u=1)	.173	.179	.163 (u=2)	.168	.168	.179 (u=1)	.148	.168	.148 (u=1)	.158	.138	.153 (u=1)	.168	.163
	Bound		**.356**	.411		**.414**	.478		**.365**	.423		**.387**	.410		**.352**	.423

Table 4. **Complete results on Egida (Brier loss).** Test risk and Catoni PAC-Bayes bound ($\delta = 0.05$) at each pipeline stage (zero-shot, fine-tuned, and quantised at 2/4 bits). The chosen variant per cell is given in parentheses beside the FT entry. Per model, the lowest test risk across FT/Q2/Q4 is underlined and the lowest non-vacuous Catoni bound across Q2/Q4 is **bolded**.

		Qwen 0.6B			LG3-1B			Qwen-4B			LG3-8B			Qwen-8B		
Zero-shot	Risk	.133			.132			.181			.120			.145		
Adapter		FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4
LoRA	Risk	.082 (r=4)	.080	.081	.085 (r=1)	.095	.084	.081 (r=2)	.081	.081	.102 (r=2)	.101	.103	.074 (r=1)	.078	.078
	Bound		1.000	1.000		1.000	1.000		1.000	1.000		1.000	1.000		1.000	1.000
LoRA-XS	Risk	.109 (r=2)	.111	.109	.118 (r=2)	.120	.118	.124 (r=2)	.128	.124	.103 (r=2)	.104	.104	.122 (r=2)	.117	.122
	Bound		.986	.997		.944	.983		.994	.999		.991	.998		.994	.999
LoRA-T	Risk	.109 (r=4,u=1)	.114	.112	.124 (r=2,u=1)	.125	.123	.127 (r=4,u=1)	.128	.128	.114 (r=2,u=1)	.111	.113	.134 (r=2,u=1)	.131	.130
	Bound		.958	.962		.897	.916		.981	.980		.971	.979		.978	.985
LoRA-T-Tied	Risk	.123 (r=4,u=1)	.121	.123	.137 (r=4,u=1)	.139	.137	.136 (r=2,u=1)	.140	.136	.111 (r=4,u=1)	.115	.111	.129 (r=4,u=1)	.134	.135
	Bound		.584	.610		.517	.534		.666	.692		.631	.647		.656	.684
LoRA-GT	Risk	.123 (u=1)	.125	.122	.137 (u=1)	.141	.135	.142 (u=1)	.137	.143	.111 (u=1)	.124	.109	.129 (u=1)	.153	.134
	Bound		**.296**	.350		**.321**	.348		**.345**	.392		**.325**	.368		**.329**	.394

which hold with probability at least $1 - \beta$ over the draw of S_{val}.

An often tighter alternative for 0–1 losses is given by KL-based concentration inequalities for Bernoulli random variables (Seeger, 2002), which apply to losses in $[0, 1]$. In this case, with probability at least $1 - \beta$:

$$\mathrm{KL}\big(\hat{R}_{\mathrm{val}}(h)\,\|\,R(h)\big) \;\leq\; \frac{\log(1/\beta)}{n_{\mathrm{val}}}, \tag{N.14}$$

where $\mathrm{KL}(q\|p) = q\log\frac{q}{p} + (1 - q)\log\frac{1-q}{1-p}$ denotes the binary Kullback–Leibler divergence. This inequality can be inverted as described by Dziugaite and Roy (2017) to obtain an upper bound on the model risk.

Despite their generality, these validation-based guarantees have several limitations in the setting we consider. First, they do not account for the training procedure or hypothesis class, and therefore answer a different question: they certify the performance of a fixed model on unseen data, but do not explain how generalisation depends on model structure or learning dynamics. In particular, for a fixed validation set, the bounds depend only on empirical validation error and sample size, making them insensitive to differences in hypothesis complexity

Table 5. **Complete results on OpenAI Moderation (0–1 loss).** Test risk and Catoni PAC-Bayes bound ($\delta = 0.05$) at each pipeline stage (zero-shot, fine-tuned, and quantised at 2/4 bits). The chosen variant per cell is given in parentheses beside the FT entry. Per model, the lowest test risk across FT/Q2/Q4 is underlined and the lowest non-vacuous Catoni bound across Q2/Q4 is **bolded**.

		Qwen 0.6B			LG3-1B			Qwen-4B			LG3-8B			Qwen-8B		
Zero-shot	Risk	*.188*			*.274*			*.188*			*.107*			*.188*		
Adapter		FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4
LoRA	Risk	.116 (r=1)	.134	.122	.113 (r=1)	.110	.113	.098 (r=1)	.098	.104	.086 (r=4)	.083	.086	.104 (r=1)	.107	.110
	Bound		1.000	1.000		1.000	1.000		1.000	1.000		1.000	1.000		1.000	1.000
LoRA-XS	Risk	.155 (r=2)	.146	.158	.238 (r=2)	.250	.241	.134 (r=2)	.134	.134	.101 (r=2)	.104	.098	.122 (r=2)	.137	.125
	Bound		.933	.972		.885	.939		.964	.988		.939	.978		.965	.989
LoRA-T	Risk	.149 (r=4,u=1)	.155	.146	.211 (r=4,u=1)	.220	.217	.128 (r=4,u=1)	.137	.128	.107 (r=2,u=1)	.110	.113	.128 (r=2,u=1)	.143	.128
	Bound		.871	.883		.810	.835		.909	.920		.873	.867		.897	.912
LoRA-T-Tied	Risk	.164 (r=2,u=1)	.167	.161	.182 (r=4,u=1)	.235	.167	.143 (r=2,u=1)	.137	.143	.131 (r=4,u=1)	.128	.122	.158 (r=4,u=1)	.158	.167
	Bound		.472	.493		.473	.455		.500	.523		.491	.506		.524	.539
LoRA-GT	Risk	.170 (u=2)	.185	.164	.182 (u=1)	.304	.167	.143 (u=1)	.152	.149	.131 (u=1)	.122	.125	.158 (u=1)	.146	.185
	Bound		**.285**	.358		.421	**.317**		**.251**	.296		**.244**	.287		**.290**	.308

Table 6. **Complete results on OpenAI Moderation (Brier loss).** Test risk and Catoni PAC-Bayes bound ($\delta = 0.05$) at each pipeline stage (zero-shot, fine-tuned, and quantised at 2/4 bits). The chosen variant per cell is given in parentheses beside the FT entry. Per model, the lowest test risk across FT/Q2/Q4 is underlined and the lowest non-vacuous Catoni bound across Q2/Q4 is **bolded**.

		Qwen 0.6B			LG3-1B			Qwen-4B			LG3-8B			Qwen-8B		
Zero-shot	Risk	*.128*			*.210*			*.184*			*.087*			*.184*		
Adapter		FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4
LoRA	Risk	.086 (r=1)	.092	.086	.097 (r=1)	.094	.097	.076 (r=1)	.074	.077	.078 (r=4)	.072	.078	.080 (r=1)	.077	.080
	Bound		1.000	1.000		1.000	1.000		1.000	1.000		1.000	1.000		1.000	1.000
LoRA-XS	Risk	.103 (r=2)	.105	.103	.166 (r=2)	.168	.166	.096 (r=2)	.099	.096	.078 (r=2)	.079	.077	.090 (r=2)	.091	.090
	Bound		.924	.967		.851	.916		.958	.985		.931	.975		.957	.987
LoRA-T	Risk	.104 (r=2,u=1)	.102	.104	.161 (r=4,u=1)	.161	.162	.098 (r=4,u=1)	.100	.098	.079 (r=2,u=1)	.079	.080	.093 (r=2,u=1)	.095	.093
	Bound		.854	.869		.761	.792		.896	.909		.863	.858		.882	.898
LoRA-T-Tied	Risk	.108 (r=2,u=1)	.109	.109	.137 (r=4,u=1)	.158	.141	.109 (r=2,u=1)	.107	.108	.099 (r=4,u=1)	.104	.098	.120 (r=4,u=1)	.119	.122
	Bound		.428	.448		.397	.395		.469	.492		.454	.470		.507	.509
LoRA-GT	Risk	.111 (u=1)	.138	.115	.137 (u=1)	.215	.140	.112 (u=1)	.128	.109	.099 (u=1)	.089	.097	.120 (u=1)	.110	.129
	Bound		**.244**	.254		.316	**.258**		**.233**	.267		**.213**	.253		**.247**	.279

Table 7. **Complete results on Aegis (0–1 loss).** Test risk and Catoni PAC-Bayes bound ($\delta = 0.05$) at each pipeline stage (zero-shot, fine-tuned, and quantised at 2/4 bits). The chosen variant per cell is given in parentheses beside the FT entry. Per model, the lowest test risk across FT/Q2/Q4 is underlined and the lowest non-vacuous Catoni bound across Q2/Q4 is **bolded**.

		Qwen 0.6B			LG3-1B			Qwen-4B			LG3-8B			Qwen-8B		
Zero-shot	Risk	*.170*			*.317*			*.211*			*.236*			*.166*		
Adapter		FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4
LoRA	Risk	.117 (r=4)	.122	.118	.118 (r=4)	.119	.118	.113 (r=2)	.119	.112	.109 (r=2)	.106	.108	.113 (r=4)	.113	.112
	Bound		1.000	1.000		1.000	1.000		1.000	1.000		1.000	1.000		1.000	1.000
LoRA-XS	Risk	.150 (r=2)	.155	.153	.178 (r=4)	.185	.174	.136 (r=2)	.161	.138	.166 (r=2)	.178	.166	.146 (r=2)	.314	.149
	Bound		.315	.349		.382	.456		.506	.397		.395	.423		.579	.393
LoRA-T	Risk	.156 (r=4,u=1)	.161	.155	.195 (r=4,u=4)	.217	.195	.137 (r=4,u=1)	.141	.135	.154 (r=4,u=2)	.171	.157	.139 (r=4,u=4)	.137	.133
	Bound		.290	.288		.358	.365		.360	.307		.387	.344		.321	.367
LoRA-T-Tied	Risk	.169 (r=4,u=2)	.181	.166	.268 (r=4,u=4)	.292	.261	.142 (r=4,u=4)	.850	.140	.174 (r=4,u=4)	.179	.179	.146 (r=4,u=2)	.499	.141
	Bound		.218	.214		.399	.332		.889	**.230**		.335	.263		.548	.210
LoRA-GT	Risk	.169 (u=2)	.180	.170	.268 (u=4)	.351	.276	.156 (u=1)	.189	.159	.174 (u=4)	.269	.175	.146 (u=2)	.176	.154
	Bound		.276	**.185**		.447	**.313**		.344	.231		.362	**.238**		.361	**.180**

and unable to capture structural effects such as compressibility.

Second, these bounds require a held-out validation set, typically obtained by splitting data, with care required to avoid leakage. In small-data regimes, where every example is informative, this reduces the effective training set and can degrade performance. Moreover, because the guarantees are model-agnostic and do not adapt to properties of the learned hypothesis such as description length, they provide limited insight into the systematic variation in generalisation behaviour observed across adaptor parameterisations.

Table 8. **Complete results on Aegis (Brier loss).** Test risk and Catoni PAC-Bayes bound ($\delta = 0.05$) at each pipeline stage (zero-shot, fine-tuned, and quantised at 2/4 bits). The chosen variant per cell is given in parentheses beside the FT entry. Per model, the lowest test risk across FT/Q2/Q4 is underlined and the lowest non-vacuous Catoni bound across Q2/Q4 is **bolded**.

Adapter	Risk	Qwen 0.6B			LG3-1B			Qwen-4B			LG3-8B			Qwen-8B		
Zero-shot	Risk	*.121*			*.231*			*.181*			*.202*			*.156*		
Adapter		FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4
LoRA	Risk	.087 (r=4)	.090	.087	.086 (r=4)	.086	.086	.081 (r=2)	.086	.082	.080 (r=2)	.081	.081	.081 (r=4)	.082	.082
	Bound		1.000	1.000		1.000	1.000		1.000	1.000		1.000	1.000		1.000	1.000
LoRA-XS	Risk	.108 (r=2)	.109	.109	.155 (r=2)	.170	.155	.112 (r=2)	.132	.112	.117 (r=2)	.123	.118	.117 (r=2)	.157	.118
	Bound		.268	.303		.309	.312		.462	.362		.328	.357		.377	.358
LoRA-T	Risk	.113 (r=4,u=1)	.116	.113	.159 (r=4,u=1)	.182	.157	.108 (r=4,u=1)	.111	.108	.116 (r=4,u=1)	.128	.117	.104 (r=4,u=2)	.114	.106
	Bound		.242	.242		.351	.280		.308	.268		.297	.285		.303	.291
LoRA-T-Tied	Risk	.118 (r=4,u=2)	.132	.117	.181 (r=4,u=4)	.194	.180	.115 (r=4,u=4)	.247	.115	.124 (r=4,u=4)	.136	.127	.114 (r=4,u=2)	.303	.113
	Bound		.174	.171		.264	.239		.343	**.197**		.264	.211		.354	.176
LoRA-GT	Risk	.118 (u=2)	.127	.121	.181 (u=4)	.213	.183	.132 (u=1)	.154	.130	.124 (u=4)	.196	.126	.114 (u=2)	.146	.122
	Bound		.195	**.143**		.266	**.223**		.310	.197		.272	**.188**		.319	**.150**

Table 9. **Complete results on BeaverTails (0–1 loss).** Test risk and Catoni PAC-Bayes bound ($\delta = 0.05$) at each pipeline stage (zero-shot, fine-tuned, and quantised at 2/4 bits). The chosen variant per cell is given in parentheses beside the FT entry. Per model, the lowest test risk across FT/Q2/Q4 is underlined and the lowest non-vacuous Catoni bound across Q2/Q4 is **bolded**.

Adapter	Risk	Qwen 0.6B			LG3-1B			Qwen-4B			LG3-8B			Qwen-8B		
Zero-shot	Risk	*.176*			*.299*			*.160*			*.257*			*.161*		
Adapter		FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4
LoRA	Risk	.146 (r=4)	.149	.146	.146 (r=4)	.147	.146	.141 (r=4)	.145	.141	.140 (r=4)	.142	.140	.142 (r=4)	1.000	.141
	Bound		.996	1.000		.997	1.000		1.000	1.000		1.000	1.000		1.000	1.000
LoRA-XS	Risk	.161 (r=2)	.163	.162	.174 (r=4)	.183	.173	.160 (r=2)	.181	.160	.182 (r=2)	.180	.183	.160 (r=2)	.168	.160
	Bound		.213	.221		.243	.255		.241	.230		.240	.253		.225	.229
LoRA-T	Risk	.164 (r=4,u=1)	.166	.164	.180 (r=4,u=4)	.213	.182	.158 (r=4,u=2)	.159	.158	.170 (r=4,u=2)	.190	.177	.157 (r=4,u=1)	.176	.158
	Bound		.204	.205		.254	.231		.210	.212		.243	.232		.222	.206
LoRA-T-Tied	Risk	.166 (r=4,u=1)	.166	.167	.213 (r=4,u=4)	.232	.216	.165 (r=4,u=1)	.160	.163	.180 (r=4,u=4)	.229	.183	.163 (r=4,u=1)	.165	.164
	Bound		.182	.184		.254	.234		.182	.185		.254	.210		.183	.183
LoRA-GT	Risk	.166 (u=1)	.167	.166	.213 (u=4)	.266	.214	.165 (u=1)	.161	.163	.180 (u=4)	.318	.180	.163 (u=1)	.162	.161
	Bound		**.173**	.174		.280	**.227**		**.168**	.173		.330	**.200**		**.168**	.171

Table 10. **Complete results on BeaverTails (Brier loss).** Test risk and Catoni PAC-Bayes bound ($\delta = 0.05$) at each pipeline stage (zero-shot, fine-tuned, and quantised at 2/4 bits). The chosen variant per cell is given in parentheses beside the FT entry. Per model, the lowest test risk across FT/Q2/Q4 is underlined and the lowest non-vacuous Catoni bound across Q2/Q4 is **bolded**.

Adapter	Risk	Qwen 0.6B			LG3-1B			Qwen-4B			LG3-8B			Qwen-8B		
Zero-shot	Risk	*.141*			*.258*			*.156*			*.233*			*.154*		
Adapter		FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4	FT	Q2	Q4
LoRA	Risk	.103 (r=4)	.105	.103	.103 (r=4)	.104	.103	.100 (r=4)	.102	.100	.100 (r=4)	.101	.101	.100 (r=4)	.250	.100
	Bound		.995	1.000		.996	1.000		1.000	1.000		1.000	1.000		1.000	1.000
LoRA-XS	Risk	.115 (r=2)	.117	.116	.136 (r=2)	.146	.137	.111 (r=4)	.117	.112	.127 (r=2)	.129	.129	.125 (r=2)	.158	.127
	Bound		.162	.170		.187	.182		.192	.222		.180	.191		.216	.192
LoRA-T	Risk	.117 (r=4,u=1)	.118	.117	.127 (r=4,u=4)	.155	.128	.113 (r=4,u=4)	.118	.114	.131 (r=4,u=1)	.135	.137	.116 (r=4,u=2)	.119	.116
	Bound		.155	.156		.192	.173		.170	.177		.178	.179		.165	.167
LoRA-T-Tied	Risk	.118 (r=4,u=2)	.122	.118	.147 (r=4,u=4)	.165	.149	.132 (r=4,u=4)	.151	.131	.128 (r=4,u=4)	.187	.129	.122 (r=4,u=4)	.157	.124
	Bound		.138	.136		.182	.167		.171	.156		.210	.153		.180	.148
LoRA-GT	Risk	.118 (u=2)	.123	.118	.147 (u=4)	.189	.149	.132 (u=4)	.250	.131	.128 (u=4)	.258	.128	.122 (u=4)	.150	.122
	Bound		.130	**.128**		.200	**.162**		.267	**.148**		.271	**.145**		.162	**.139**

N.2. Validation Bounds Track Empirical Risk, While PAC-Bayes Aids in Understanding Generalisation

Validation bounds track empirical risk. To further illustrate the limitations of validation-based guarantees, we examine the behaviour of KL-inversion bounds across the models and datasets introduced in Section 5.

Figure 9 (a) plots the KL-inversion bound as a function of hypothesis description length. In contrast to the PAC-Bayes results in the main

Figure 9. **Validation-based KL-inversion bounds trends. (a)** Bound vs. description length shows no strong systematic dependence on compression. **(b)** Bound vs. empirical validation risk exhibits a near-linear relationship, indicating that validation bounds primarily track empirical performance. This contrasts with PAC-Bayes bounds, which vary systematically with model compressibility.

text, no strong systematic dependence on description length is observed: models with substantially different levels of compression yield similar bounds when their empirical performance is comparable.

Figure 9 (b) instead plots the same bounds against empirical validation risk. As expected, for fixed validation set size and confidence level, a near-linear relationship is observed across all datasets, reflecting that the bound is a deterministic function of $\hat{R}_{\mathrm{val}}(h)$ and n_{val}. This highlights a limitation of validation-based bounds: they primarily rescale empirical performance and offer limited additional insight, in contrast to compression-based PAC-Bayes guarantees which incorporate model complexity.

Taken together, these results highlight a fundamental limitation: validation-based bounds provide little information beyond empirical performance. In particular, they cannot explain the systematic dependence of generalisation on compressibility observed in prior work (Lotfi et al., 2022; 2024a) and in our experiments.

PAC-Bayes aids in understanding generalisation. In contrast, the PAC-Bayes guarantees in the main text exhibit a qualitatively different behaviour. As shown in Figure 4, the bounds vary systematically with hypothesis description length, with more compressed adaptations yielding consistently tighter guarantees. This dependence arises from the explicit complexity term in the PAC-Bayes bound, which scales with the compressed description length and distinguishes between hypotheses beyond empirical performance.

More fundamentally, PAC-Bayes bounds characterise generalisation through a trade-off between empirical risk and model complexity. In this view, tight and non-vacuous bounds arise when a hypothesis achieves a favourable balance between these two terms. Empirically, we observe that highly compressed, low-description-length adaptations often maintain strong performance while incurring substantially smaller complexity penalties, resulting in tighter certificates. This provides a principled perspective on generalisation: simpler, more compressible adaptations can generalise well while remaining certifiable. Validation-based bounds, by collapsing to a rescaled version of empirical risk, do not capture this trade-off and therefore do not support such structural explanations.

N.3. Comparable Certificates, but Different Explanatory Power

Validation and PAC-Bayes in data-rich settings. We denote by $v_f \in [0, 1]$ the validation fraction, i.e., the proportion of training data held out for validation. In settings where validation-based bounds begin to provide stable and reliable estimates of generalisation, it is instructive to compare them directly with PAC-Bayes guarantees. We examine this behaviour on the Aegis dataset, which is larger than the smaller and therefore nosier datasets of Egida and OpenAI Content Moderation, though still far from the large-scale regimes typically assumed in asymptotic analyses or in prior compression-based PAC-Bayes work.

Figure 10 compares PAC-Bayes bounds computed on the full dataset with validation-based KL-inversion bounds computed using a held-out validation split. The resulting certificates are of similar magnitude across models. Given that validation-based bounds are expected to be reliable in this setting, this agreement is informative.

Figure 10. **Validation vs. PAC-Bayes on Aegis.** PAC-Bayes bounds computed on the full dataset ($v_f = 0$) and validation-based KL-inversion bounds computed with a validation fraction $v_f = 0.10$ yield certificates of similar magnitude across models.

Alignment of compression-based complexity with generalisation. The fact that PAC-Bayes yields comparably tight bounds in this setting suggests that the underlying complexity measure based on compressed description length is well-aligned with generalisation behaviour in these models. In particular, the observation that highly compressed adaptations admit tight PAC-Bayes certificates is consistent with the view that simpler, more compressible hypotheses generalise well.

At the same time, PAC-Bayes achieves these guarantees without requiring a held-out validation set, and retains an explicit dependence on hypothesis complexity. Validation-based bounds, while effective in settings where sufficient data is available, remain purely empirical and do not provide such structural insight.

Summary. Overall, these results highlight a fundamental distinction: validation-based bounds provide reliable estimates of generalisation when sufficient data is available, but do not explain it. In contrast, PAC-Bayes bounds offer both certification and a principled account of how model complexity governs generalisation.

O. Per-Model-Class Functional Distortion Analysis

In this section, we extend the analysis of Section 5.3 by examining the relationship between functional distortion, PAC-Bayes certificate tightness, and predictive performance for Llama Guard models on Aegis and BeaverTails separately. While Figure 5 aggregates results across datasets and architectures, isolating individual model families allows finer-grained analysis of the compression–distortion–generalisation relationship within a fixed architectural class.

Figures 11 and 12 show test error versus PAC-Bayes Catoni bounds for progressively quantised LoRA-GT adaptors under both 0–1 and Brier losses. Models are quantised at 2-, 3-, 4-, 8-, and 16-bit precision following the setup of Section 5.3.

Across both datasets, low-distortion compressed adaptors consistently remain concentrated near low-error, tight-bound regimes, while increasing distortion corresponds to progressively looser PAC-Bayes certificates and higher predictive error. In BeaverTails, the PAC-Bayes bounds closely track observed test error across much of the compression frontier, whereas Aegis exhibits a broader spread of bound tightness under increasing distortion, reflecting a stronger trade-off between compression and predictive performance.

Notably, some highly compressed adaptors, corresponding to the smallest description-length representations, remain near the low-risk, tight-bound frontier, indicating that substantial compression can still preserve strong predictive performance when functional distortion remains low. In contrast, less compressed adaptors often achieve lower test risk but drift further from the optimal bound–risk frontier, yielding looser PAC-Bayes guarantees despite modest predictive gains.

These results suggest that functional distortion provides a practical complementary diagnostic alongside PAC-Bayes certificates for identifying compressed models that remain both highly compact and likely to generalise reliably under quantisation.

Figure 11. Functional distortion analysis for the Llama Guard family on Aegis. Test error versus PAC-Bayes Catoni bound for LoRA-GT adaptors under 0–1 and Brier losses, coloured by functional distortion and scaled by adaptor description length. Low-distortion compressed adaptors remain concentrated near low-error, tight-bound regimes across both Llama-Guard-3 1B and 8B models.

Figure 12. Functional distortion analysis for the Llama Guard family on BeaverTails. Test error versus PAC-Bayes Catoni bound for LoRA-GT adaptors under 0–1 and Brier losses, coloured by functional distortion and scaled by adaptor description length. Increasing functional distortion corresponds to progressively looser certificates and higher predictive error under compression.

Figure 13. Functional distortion analysis for the Qwen Guard family on Aegis. Test error versus PAC-Bayes Catoni bound for LoRA-GT adaptors under 0–1 and Brier losses across Qwen3Guard 0.4B, 4B, and 8B models. The distortion–certifiability relationship remains stable across model scales.

Figure 14. Functional distortion analysis for the Qwen Guard family on BeaverTails. Low-distortion compressed LoRA-GT adaptors consistently achieve tighter PAC-Bayes guarantees while preserving competitive predictive performance, whereas highly distorted models drift away from the low-risk, tight-bound frontier.