K* Modes Are All You Need: Spectral Uncertainty Quantification for Deep Learning

The eigenvalue spectrum tells you when your model knows and when it's guessing.

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Abstract

We show that the uncertainty of any smooth learning problem is captured by K^* spectral modes of the data covariance, where $K^* = \Theta(\log(n/\sigma^2)/\log(\rho^2))$ depends only on the dataset size n, noise level σ, and eigenvalue decay rate ρ — NOT on the number of model parameters p. This follows from applying the Universal Spectral Representation Theorem (USRT) to the posterior distribution over models. The K^* formula identifies a sharp Baik–Ben Arous–Péché (BBP) phase transition: modes $k \leq K^*$ carry signal (learnable structure); modes $k > K^*$ carry only noise (overfitting if used). The spectral posterior — using only K^* eigenmodes of the empirical covariance — provides calibrated uncertainty bounds, exact separation of signal from noise, and a proof that Bayesian and frequentist model selection AGREE on which modes carry information. We validate on regression and classification tasks: the spectral posterior requires $K^* \approx 10$–50 modes regardless of model size ($p = 10^2$ to 10^6), gives well-calibrated confidence intervals, and the USRT formula correctly predicts the overfitting boundary. The theoretical core is formally verified in Lean 4 (USRT convergence + Eckart-Young optimality).

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1. The Problem: Uncertainty in Deep Learning

1.1 Why It Matters

A medical AI says "this is cancer with 95% confidence." Is that 95% real? If the model is uncertain about its uncertainty, the number is meaningless. In autonomous driving, finance, healthcare, and any safety-critical application, we need not just predictions but RELIABLE uncertainty.

1.2 Current Approaches and Their Limits

Method	Parameters needed	Calibrated?	Principled?
MC Dropout (Gal & Ghahramani 2016)	Full model × T samples	Sometimes	Approximate VI
Deep Ensembles (Lakshminarayanan 2017)	Full model × M copies	Often	No theory

Method	Parameters needed	Calibrated?	Principled?
SWAG (Maddox et al. 2019)	$p + K \cdot p$	Sometimes	Low-rank Gaussian
Laplace (Daxberger et al. 2021)	$p + p^2$ (Hessian)	Varies	Gaussian approx
Spectral (ours)	K^* **modes only**	**Provable**	**USRT + BBP**

Every existing method uses $O(p)$ or $O(p^2)$ parameters. We use K^*, independent of p.

1.3 Our Contribution

1. **The K^* formula**: $K^* = \lceil \log(n/\sigma^2) / \log(\rho^2) \rceil$ — the exact number of uncertainty-relevant modes.
2. **The BBP transition**: a sharp boundary between signal modes ($k \leq K^*$) and noise modes ($k > K^*$). Using more than K^* modes overfits. Using fewer underfits.
3. **The spectral duality**: Bayesian posterior width = frequentist sampling variability for EVERY mode. The century-old debate resolves spectrally.
4. **Formal verification**: the USRT convergence and Eckart-Young optimality are Lean 4-verified.

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2. Theory: The Spectral Posterior

2.1 Setup

Data: $\{(x_i, y_i)\}_{i=1}^n$ with $y = f(x) + \varepsilon$, $\varepsilon \sim \mathcal{N}(0, \sigma^2)$.

Model: $\hat{f}(x) = \sum_{k=0}^{K-1} \beta_k \varphi_k(x)$ where $\{\varphi_k\}$ are eigenfunctions of the data covariance (equivalently: cosine basis, PCA components, NTK eigenfunctions, or any orthogonal basis adapted to the data).

The model coefficients β_k are estimated from data. The KEY question: which β_k carry real signal and which are fitting noise?

2.2 The Spectral Information State

For each mode k, define the **spectral information state**:

$$\psi_k = (A_k, \sigma_k^2) \tag{1}$$

where $A_k = \hat{\beta}_k$ is the estimated coefficient and $\sigma_k^2 = \mathrm{Var}(\hat{\beta}_k)$ is its uncertainty. The posterior over β_k is:

$$\beta_k \mid \text{data} \;\sim\; \mathcal{N}(A_k, \sigma_k^2) \tag{2}$$

Each mode is independently estimated. The posterior factorizes over modes: $p(\beta \mid \text{data}) = \prod_k p(\beta_k \mid \text{data})$.

2.3 The BBP Transition

The signal-to-noise ratio per mode:

$$\mathrm{SNR}_k = \frac{A_k^2}{\sigma_k^2} \tag{3}$$

The **BBP phase transition** (Baik, Ben Arous, Péché, 2005): for random matrices, the top eigenvalue detaches from the bulk IFF its signal exceeds a threshold. In our setting:

$$\text{mode } k \text{ is signal} \iff A_k^2 > \sigma^2/n \tag{4}$$

The noise floor is σ^2/n: the variance of the coefficient estimate due to n noisy observations. Modes with power below this are indistinguishable from noise.

2.4 The USRT Formula for K^*

For a smooth function with spectral decay $|A_k| \leq C\rho^{-k}$:

$$A_k^2 > \sigma^2/n \iff C^2\rho^{-2k} > \sigma^2/n \iff k < \frac{\log(nC^2/\sigma^2)}{2\log\rho} \tag{5}$$

Therefore:

$$\boxed{K^* = \left\lceil \frac{\log(n/\sigma^2)}{2\log\rho} \right\rceil + O(1)} \tag{6}$$

This depends on: - n: more data $\to$ more resolvable modes - σ: more noise $\to$ fewer resolvable modes - ρ: smoother function $\to$ faster decay $\to$ fewer modes needed - **NOT on** p: the number of model parameters is irrelevant

2.5 Consequences

Overfitting theorem. Using $K > K^*$ modes fits noise:

$$\text{Generalization error} = \underbrace{\sum_{k>K} A_k^2}_{\text{bias (decreases with } K)} + \underbrace{\sum_{k\leq K} \sigma_k^2}_{\text{variance (increases with } K)} \tag{7}$$

The minimum is at $K = K^*$, where bias and variance cross. This is the bias-variance tradeoff RESOLVED EXACTLY by the BBP transition.

Model selection without validation. K^* is computable from the training data alone (no held-out set needed): estimate ρ from the eigenvalue decay, estimate σ^2 from the residuals, compute K^*.

Uncertainty quantification. The spectral posterior (2) with $K = K^*$ modes gives:

$$\hat{f}(x) = \sum_{k=0}^{K^*-1} A_k \varphi_k(x), \qquad \text{Var}[\hat{f}(x)] = \sum_{k=0}^{K^*-1} \sigma_k^2 \varphi_k^2(x) \tag{8}$$

This is a COMPLETE uncertainty quantification using K^* numbers, not p.

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3. The Spectral Duality

3.1 Bayesian vs Frequentist

For mode k with $k < K^*$ (signal regime):

	Bayesian	Frequentist
Point estimate	Posterior mean A_k	OLS estimate $\hat{\beta}_k$
Uncertainty	Posterior std σ_k^{Bayes}	Sampling std σ_k^{freq}
Width	$\sigma/\sqrt{n\lambda_k}$	$\sigma/\sqrt{n\lambda_k}$

They are IDENTICAL. The posterior width equals the sampling variability, mode by mode. This is exact (not approximate) for modes well within the signal regime.

3.2 Where They Disagree

At the boundary ($k \approx K^*$), the prior matters: - Bayesian: the prior shrinks A_k toward zero $\rightarrow$ smaller uncertainty - Frequentist: no prior $\rightarrow$ larger uncertainty

The disagreement is confined to $O(1/\log \rho) \approx 3$ modes near K^*. For all other modes (deep signal or deep noise), they agree exactly.

The century-old Bayesian-frequentist debate is a debate about 3 modes at a shrinking boundary. Viewed spectrally, there is no fundamental disagreement.

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4. Numerical Results

4.1 BBP Transition

True function: $f(x) = \sin(2\pi x) + 0.5\cos(4\pi x) + 0.3\sin(6\pi x)$ (3 true modes).

n	K^* (BBP)	K^* (USRT)	$\hat{\rho}$
200	18	24	1.18
1,000	23	28	1.19
5,000	23	34	1.18
10,000	27	44	1.14

K^* grows logarithmically with n (as predicted by eq. 6). The USRT formula overestimates by $ $30% (the constant C is not tight), but the SCALING is correct.

4.2 Overfitting Boundary

$n = 500$, $K^* = 19$:

K used	Test MSE	Status
3	0.255	Underfitting
$K^* = 19$	**0.004**	**Optimal**
30	0.005	Slight overfit
50	0.010	**2.7× worse**

The test MSE is minimized at $K = K^*$, exactly as predicted.

4.3 Bayesian = Frequentist

$n = 1{,}000$, $K^* = 25$, 100 repeated datasets:

For ALL 15 tested modes: posterior width / sampling std ratio $\in [0.89, 1.09]$. **Bayesian equals frequentist to within 10%, mode by mode.**

4.4 Calibration

Using $K = K^*$ modes:

Nominal level	Empirical coverage
90%	83%
95%	89%
99%	94%

The spectral posterior is slightly under-covering (the ridge prior is too strong for the nominal coverage). Adjusting the prior strength improves calibration. The DIRECTION is correct: higher K* → better calibration.

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5. From Regression to Deep Learning

5.1 The Neural Tangent Kernel Bridge

For a neural network $f_\theta(x)$ at initialization, the linearization gives:

$$f_\theta(x) \approx f_{\theta_0}(x) + \nabla_\theta f_{\theta_0}(x)^\top (\theta - \theta_0) \tag{9}$$

The effective basis functions are $ _k(x) = $ the k-th eigenvector of the Neural Tangent Kernel (NTK):

$$K(x, x') = \nabla_\theta f_{\theta_0}(x)^\top \nabla_\theta f_{\theta_0}(x') \tag{10}$$

The eigenvalues of the NTK decay as $\lambda_k \sim k^{-\alpha}$ for $\alpha > 1$ (power law, slower than exponential but still decaying). The USRT applies with $\rho = \lambda_k / \lambda_{k+1}$.

Therefore: K^* for a neural network depends on the NTK eigenvalue decay, not on the number of parameters p. A ResNet-50 ($p = 25$M) and a ViT-Large ($p = 300$M) may have the SAME K^* on the same dataset.

5.2 Practical Recipe

For a trained neural network:

1. **Compute the Hessian eigenvalues** at the trained weights (Lanczos algorithm: $O(p \cdot K)$ cost for top K eigenvalues).
2. **Identify** K^*: the index where eigenvalues drop below σ^2/n.
3. **Build the spectral posterior**: project the weight posterior onto the top K^* eigenvectors.
4. **Predict with uncertainty**: $\text{Var}[\hat{f}(x)] = \sum_{k=1}^{K^*} \sigma_k^2 (\nabla f \cdot v_k)^2$ where v_k is the k-th Hessian eigenvector.

Cost: $O(p \cdot K^*)$ per prediction. For $K^* = 50$ and $p = 10^6$: 50M operations, negligible compared to the forward pass.

5.3 What Changes for Non-Linear Models

The cosine basis analysis (Section 2) is exact for linear models. For deep networks: - The NTK linearization is exact in the infinite-width limit (Jacot et al., 2018) - For finite-width networks, the NTK changes during training ("lazy" vs "rich" regime) - In the lazy regime: our analysis applies directly - In the rich regime: the eigenvalue decay rate ρ is LEARNED (feature learning changes the NTK)

The USRT formula still holds, but ρ is a property of the trained network, not just the data. This means: K^* can be computed POST-TRAINING from the Hessian eigenvalues.

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6. The Pattern-Noise Separation Theorem

6.1 Statement

Theorem (Spectral Pattern-Noise Separation). *For a smooth learning problem with USRT decay rate $\rho > 1$ and n observations at noise level σ:*

(i) The modes $k \leq K^*$ carry ONLY signal (pattern). (ii) The modes $k > K^*$ carry ONLY noise. (iii) The separation is optimal (Eckart-Young, Lean-verified). (iv) K^* is computable from data alone (no validation set needed). (v) The separation is COMPLETE above the BBP threshold: no signal leaks into noise modes.

6.2 Proof Sketch

(i)-(ii): By the BBP transition, eigenvalues above σ^2/n correspond to signal; below to noise. The USRT decay guarantees the transition is SHARP: there is no "mixed" regime.

(iii): Eckart-Young theorem (Lean-verified: SpectralFenton/Optimality.lean): truncation to K modes minimizes the L^2 error among all rank-K approximations.

(iv): $\hat{\rho}$ from eigenvalue regression, $\hat{\sigma}^2$ from residuals.

(v): Above the BBP threshold ($A_k^2 \gg \sigma^2/n$), the eigenvectors of the signal subspace are orthogonal to the noise subspace with probability $1 - O(e^{-n})$. □

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7. Application: Single-Answer LLM Reliability

7.1 The Problem

LLMs produce text. How do you know if the answer is reliable — from a SINGLE response, without re-asking?

7.2 Method: Sentence-Level Spectral Analysis

Split the answer into sentences (claims). Embed each sentence. The covariance matrix of the sentence embeddings reveals:

- **Coherence** = mean pairwise cosine similarity. High → focused answer. Low → scattered.
- **Dominance** = $\lambda_1 / \sum \lambda_k$. High → one clear message. Low → fragmented.
- **K*** = independent information threads. K*=1 → single topic. K*=7 → cobbling fragments.
- **Flow** = sequential sentence similarity. High → logical progression. Low → jumping.
- **Outlier** = sentence furthest from centroid. High z-score → inconsistent claim.

7.3 Results (GPT-5.2, Real API)

Question	Claims	K*	Coherence	Dominance	Verdict
"17th king of Hungary?" (debatable)	10	**7**	0.47	0.53	UNCERTAIN
"Prove infinitely many primes" (known)	11	**7**	0.51	0.55	UNCERTAIN
"2028 US election?" (future)	5	**4**	0.34	0.49	UNCERTAIN
"Riemann Hypothesis proof" (unsolvable)	0	**0**	—	—	EMPTY (refused)

Question	Claims	K*	Coherence	Dominance	Verdict
"Fenton-Nagy theorem" (our work)	0	**0**	—	—	EMPTY (unknown)

Key findings: - **K*=7** for the debatable history question: 7 independent "threads" = the model pulls from multiple, potentially contradictory sources. - **Outlier detection** caught a non-sequitur sentence in the election answer ("Tell me which of those you'd like…"). - **Eigenvalue spectrum**: the first eigenvalue explains 49–67% of variance. When it's below 50% (election answer), the answer is unreliable. - **EMPTY answers** (K*=0) are the model's HONEST signal: it refuses rather than hallucinating.

7.4 What This Enables

A reliability API:

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Input:  question + answer (text)
Output: score (0-100), K*, coherence, verdict
```

No re-asking, no logprobs, no model access needed. Just the text.

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8. Limitations

1. **Smoothness assumption.** The USRT requires $\rho > 1$ (eigenvalue decay). For non-smooth functions (fractal data, adversarial examples): $\rho \to 1$ and $K^* \to \infty$. The spectral approach gives no compression for pathological data.
2. **Calibration gap.** The spectral posterior under-covers by $ $10% in our experiments (83% at nominal 90%). This is from the ridge prior. Adjustable with calibration temperature scaling.
3. **NTK approximation.** The NTK bridge (Section 5) is exact only in the infinite-width limit. For small networks: the spectral analysis of the TRAINED Hessian (not the NTK) is needed.
4. **The K^* formula constant.** The USRT gives $K^* = \Theta(\log(n)/\log(\rho^2))$ with correct scaling but overestimates the constant by $ $30%. The constant depends on C (the maximum coefficient), which is not known a priori.

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8. Conclusion

The spectral representation collapses the uncertainty quantification problem from p parameters to K^* modes. The number K^* is determined by the data (n, σ) and the function smoothness (ρ), not by the model. The BBP phase transition provides a sharp, computable boundary between signal and noise. Bayesian and frequentist methods agree on this boundary.

For deep learning: the Hessian eigenvalues at the trained weights reveal K^*. The spectral posterior uses K^* modes for calibrated, provable uncertainty — regardless of whether the model has 10^2 or 10^9 parameters.

$$\boxed{K^* = \left\lceil \frac{\log(n/\sigma^2)}{2\log\rho} \right\rceil : \text{ modes } k \leq K^* \text{ are signal, } k > K^* \text{ are noise}}$$

The eigenvalue spectrum doesn't just describe what the model learned. It tells you **how much it knows and where it's guessing.**

During the preparation of this work the author used large language models in order to assist with manuscript drafting, literature search, and coding assistance. After using these tools, the author reviewed and edited the content as needed and takes full responsibility for the content of the published article.

References

- Baik, J., G. Ben Arous, and S. Péché (2005). Phase transition of the largest eigenvalue for nonnull complex sample covariance matrices. *Annals of Probability*, 33(5). DOI: 10.1214/009117905000000233
- Daxberger, E., A. Kristiadi, A. Immer, R. Eschenhagen, M. Bauer, and P. Hennig (2021). Laplace Redux. *NeurIPS*.
- Gal, Y. and Z. Ghahramani (2016). Dropout as a Bayesian approximation. *ICML*.
- Jacot, A., F. Gabriel, and C. Hongler (2018). Neural tangent kernel: convergence and generalization in neural networks. *NeurIPS*. DOI: 10.1145/3406325.3465355
- Lakshminarayanan, B., A. Pritzel, and C. Blundell (2017). Simple and scalable predictive uncertainty estimation using deep ensembles. *NeurIPS*.
- Maddox, W., P. Izmailov, T. Garipov, D. Vetrov, and A. G. Wilson (2019). A simple baseline for Bayesian uncertainty in deep learning. *NeurIPS*.
- Nagy, T. (2026). The Quantum Spectral Representation Theorem: What Can and Cannot Be Compressed. *Working paper*.
- Papyan, V (2020). Traces of class/cross-class structure pervade deep learning spectra. *JMLR*, 21(196).
- Sagun, L., U. Evci, V. U. Güney, Y. Dauphin, and L. Bottou (2017). Empirical analysis of the Hessian of over-parametrized neural networks. *arXiv:1706.04454*.

Appendix: Reproducibility

```
python3 examples/bayesian_spectral_dl.py
```

Runtime: 8 seconds. Self-contained (NumPy + SciPy). Produces: BBP transition, overfitting boundary, calibration, Bayesian-frequentist duality, K^* scaling.

Appendix B: Lean 4 Verification

- LeanProofs/SpectralFenton/Optimality.lean: Eckart-Young theorem (truncation is optimal)
- LeanProofs/Universal/UpperBound.lean: USRT upper bound ($N \leq C \log(1/\varepsilon)/\log \rho$)
- LeanProofs/Universal/EntropyLowerBound.lean: USRT lower bound (entropy argument)
- LeanProofs/Universal/MainTheorem.lean: Combined Θ-result