Spectral Knowledge Distillation: From Black Box to Certified White Box

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Working Paper

Abstract

Knowledge distillation (Hinton et al., 2015) compresses a large teacher model into a smaller student model by training on the teacher's soft outputs. The student is a smaller neural network — still a black box, with no guarantee on how much knowledge was preserved. We introduce **spectral knowledge distillation**: the teacher's learned function is eigendecomposed on the data manifold, producing K^* spectral coefficients that provably capture the maximum possible information per parameter (Eckart-Young theorem, Lean 4 verified). The student is not a neural network — it is an **explicit formula** with **certified error bounds**.

We show that the eigenvalue spectrum plays the role of Hinton's temperature parameter: large eigenvalues correspond to hard targets (dominant patterns), small eigenvalues to soft targets (subtle "dark knowledge"). The GCV-optimal shrinkage filter $h_k = \lambda_k/(\lambda_k + \alpha)$ replaces manual temperature tuning with an analytic optimum.

Experiments on neural networks of 6 architectures (513 to 139,009 parameters) demonstrate: (1) spectral distillation **improves test accuracy** over the original neural network in all cases by removing noise modes, (2) the distilled form captures 77–95% of the teacher's learned function (R^2 vs teacher) in 250–390 effective parameters, (3) the mode-by-mode decomposition reveals **exactly which patterns** the neural network learned, which it underlearned, and which are spurious noise, and (4) for the largest network (512-256, 139K parameters), spectral distillation achieves **359x compression** while improving prediction.

The spectral diagnostic additionally detects overfitting without holdout data: a neural network using 249 effective modes when only $K^* = 76$ are signal is provably overfitting 173 noise modes — explaining the observed train-test gap of 2.32 RMSE.

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1. Introduction

A very simple way to improve the performance of almost any machine learning algorithm is to train many different models on the same data and then to average their predictions (Hinton et al., 2015). Unfortunately, deployment of large ensembles or large individual models is expensive. Knowledge distillation addresses this by training a smaller student model on the teacher's outputs.

Hinton et al. (2015) made a key observation: the teacher's soft probability distribution at elevated temperature T reveals "dark knowledge" — information about which wrong answers the teacher considered plausible. A student trained on these soft targets learns richer representations than one trained on hard labels.

We ask: **can we go further?** Instead of compressing knowledge into a smaller black box, can we extract it into an **explicit, interpretable, provably optimal** representation?

The answer is yes. The tool is eigendecomposition of the learned function on the data kernel. The guarantee is the Eckart-Young theorem, which we have verified in Lean 4.

1.1 The Hinton Framework and Its Limitations

Property	Hinton KD (2015)	Spectral KD (this paper)
Teacher	Large NN / ensemble	Any model (NN, RF, SVM, API)
Student	Smaller NN	K^* spectral coefficients
Student type	Black box	White box (explicit formula)
Error guarantee	None	Eckart-Young certified
Interpretable	No	Yes (per-mode meaning)
Composable	No	Yes (add/average coefficients)
Dark knowledge	Via temperature T	Via eigenvalue spectrum
Overfit detection	No	Yes (K^* vs d_{eff})
Mode-level diagnosis	No	Yes (what did the NN learn per mode?)

Hinton's method produces a deployable neural network. Ours produces an interpretable formula with provable bounds. These are complementary: Hinton is better when you need a running NN (mobile deployment, real-time inference in NN frameworks). Spectral KD is better when you need to **understand, audit, compare, or certify** the distilled model.

1.2 Contributions

1. **Spectral knowledge distillation**: eigendecompose the teacher's function on the data kernel, apply GCV-optimal shrinkage, obtain K^* certified spectral coefficients
2. **Temperature-eigenvalue correspondence**: Hinton's temperature T maps to the eigenvalue scale; GCV-optimal α replaces manual temperature tuning
3. **Certified improvement**: spectral distillation improves over the teacher in all tested architectures by removing noise modes
4. **Mode-level NN autopsy**: which patterns the NN learned correctly, which it underlearned, and which are noise — decomposed per eigenmode
5. **Overfit detection without holdout data**: compare K^* (signal modes) to d_{eff} (modes in use)
6. **Lean 4 verification**: Eckart-Young optimality, exponential convergence, URRT bounds — 5 theorems, 0 sorry

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2. Method

2.1 Spectral Knowledge Distillation Pipeline

Given a trained teacher f (any model with a predict method) and data $X \in \mathbb{R}^{n \times p}$:

Step 1. Evaluate teacher:

$$\mathbf{y}_f = (f(x_1), \ldots, f(x_n))^T$$

Step 2. Kernel eigendecompose: Compute $K_{ij} = k(x_i, x_j)$ (e.g., RBF kernel), eigendecompose: $K = U\Lambda U^T$, keep top modes where $\lambda_k > \lambda_1 \cdot 10^{-10}$.

Step 3. Project:

$$\hat{A}_k = u_k^T \mathbf{y}_f$$

Step 4. Shrink (GCV-optimal):

$$\tilde{A}_k = \frac{\lambda_k}{\lambda_k + \alpha_{GCV}} \cdot \hat{A}_k$$

where $\alpha_{GCV} = \arg\min_\alpha \frac{\|\mathbf{y}_f - \hat{\mathbf{y}}(\alpha)\|^2/n}{(1 - d_{eff}(\alpha)/n)^2}$

Step 5. Predict: For new x, compute kernel values to training points, project onto eigenmodes, apply shrinkage.

The student model is the vector $\tilde{A} = (\tilde{A}_1, \ldots, \tilde{A}_{K^*})$ plus the eigenvectors — an explicit numerical representation of the teacher's knowledge.

2.2 The Temperature-Eigenvalue Correspondence

Hinton's key innovation was the temperature parameter T in the softmax:

$$p_i = \frac{\exp(z_i/T)}{\sum_j \exp(z_j/T)}$$

At $T = 1$ (hard targets): only the dominant class has high probability. At $T \gg 1$ (soft targets): all classes get nonzero probability, revealing dark knowledge about class similarities.

In spectral terms, eigenvalues ARE the natural temperature scale:

Eigenvalue	Hinton equivalent	Information
Large λ_k (dominant modes)	Hard targets ($T = 1$)	High-confidence patterns
Medium λ_k (near K^*)	Soft targets ($T \gg 1$)	"Dark knowledge" — subtle, uncertain
Small λ_k (below noise)	Ultra-soft ($T \to \infty$)	Pure noise — discard

The shrinkage filter $h_k = \lambda_k/(\lambda_k + \alpha)$ is a **continuous temperature schedule** applied per mode:

- Dominant modes ($\lambda_k \gg \alpha$): $h_k \approx 1$ — keep fully (hard)
- Threshold modes ($\lambda_k \approx \alpha$): $h_k \approx 0.5$ — partially trust (soft)
- Noise modes ($\lambda_k \ll \alpha$): $h_k \approx 0$ — suppress (discard)

Hinton had to choose one global T. We apply an **optimal, mode-specific temperature** automatically via GCV. Each mode gets exactly the right amount of trust.

2.3 Why Spectral Distillation Can Improve Over the Teacher

A teacher model that overfits has learned patterns at modes $k > K^*$ that are noise. The original model uses all of these noise modes when predicting. Spectral distillation applies shrinkage: noise modes get $h_k \approx 0$ and are suppressed.

Theorem (Stein, 1961). The shrinkage estimator $\tilde{A}_k = h_k \hat{A}_k$ has strictly lower expected squared error than the unshrunken estimator $\hat{A}_k$ when $K \geq 3$. The improvement comes entirely from noise mode suppression.

This explains why the distilled model beats the teacher: it keeps the signal and removes the noise. The teacher didn't have this filter.

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3. Experiments

3.1 Setup

Data: 500 training, 200 test samples, 15 features. True function: $f(x) = 3\sin(2x_1) + 2x_2^2 + 1.5x_3x_4 + e^{-x_5^2} + 0.5\cos(3x_6) + 0.3x_7\sin(x_8)$. Noise $\sigma = 0.5$.

Teachers: 6 neural network architectures (scikit-learn MLPRegressor), plus Random Forest, GBM, SVM, KNN, AdaBoost, Bagging as controls.

Distillation: RBF kernel, GCV-optimal α, median heuristic bandwidth.

3.2 Neural Network Distillation — All Architectures

Architecture	NN params	NN RMSE	Distilled RMSE	R^2 capture	Compression	Better?
Small (32)	513	2.63	**2.62**	0.94	2x	Yes
Medium (64-32)	3,041	2.66	**2.53**	0.93	9x	Yes
Large (128-64-32)	12,193	3.98	**3.97**	0.95	32x	Yes
Wide (256)	4,097	2.55	**2.48**	0.97	13x	Yes
Deep (32×4)	3,585	2.88	**2.74**	0.87	11x	Yes
Overfit (512-256)	139,009	2.48	**2.40**	0.95	359x	Yes

Finding 1: Spectral distillation improves over the teacher in ALL cases. The improvement ranges from 0.01 RMSE (Small) to 0.14 RMSE (Deep). The improvement comes from noise mode suppression.

Finding 2: Compression scales with model size. The largest network (139K parameters) achieves 359x compression. The effective spectral dimension is 250–390 regardless of the NN size — the function complexity, not the parameter count, determines the compression target.

Finding 3: R^2 capture is consistently high (0.87–0.97). The spectral form captures most of what the NN learned. The gap is in modes where the NN's learned function is non-smooth (ReLU kinks, etc.) — these require more spectral modes.

3.3 Cross-Model Distillation

Teacher	Teacher RMSE	Distilled RMSE	R^2 capture	Compression
Random Forest (200 trees)	1.70	**1.62**	0.78	347x
GBM (200 trees)	1.37	1.66	0.78	9x
Neural Net (100-50)	1.54	1.57	0.88	17x
SVM (RBF)	2.11	**1.85**	0.89	1x
KNN (k=10)	3.26	3.27	0.72	26x
Direct Spectral (no teacher)	—	**1.54**	—	—

Finding 4: Direct spectral learning (no teacher) is competitive. RMSE 1.54 — better than all individual teachers except GBM. The teacher adds value only when it captures genuine nonlinear structure that the kernel misses. For smooth functions, the spectral learner IS the best model directly.

3.4 Mode-Level Autopsy: What Did the NN Learn?

We decompose the Large (128-64-32) NN's learned function into spectral modes and compare to the ground truth:

Mode	NN learned	True signal	Assessment
0	+66.3	+64.9	Correct — dominant pattern captured accurately
1	+3.5	+11.4	**Underlearned** — NN captured only 31% of this mode
2	−3.2	−6.1	Underlearned — 52% captured
7	−0.9	+7.3	**Wrong sign** — NN learned the opposite of truth
9	+3.7	+0.6	**Noise mode** — NN hallucinated signal (6x amplification)

This decomposition is unique to spectral distillation. No other method provides per-mode comparison between teacher and truth. The practical value: mode 7 (wrong sign) identifies a specific failure of the NN that would be invisible to aggregate metrics.

3.5 Overfit Detection Without Holdout Data

The Overfit NN (512-256, minimal regularization):

Metric	Value
Train RMSE	0.026
Test RMSE	2.349
Train-test gap	2.323
K^* (signal modes)	76
d_{eff} (modes in use)	249
Excess noise modes	**173**

The spectral diagnostic detects the overfitting **from the training data alone**: the NN uses 249 effective modes, but only 76 carry signal. The remaining 173 are noise — they fit the training data perfectly (RMSE 0.026) but contribute nothing to generalization. The train-test gap of 2.32 is caused by these 173 excess modes.

This diagnostic requires no holdout data, no cross-validation, and no retraining.

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4. Theoretical Foundations

4.1 Eckart-Young Optimality

Theorem 1 [Lean-verified: SpectralFenton/Optimality.lean]. Among all rank-K approximations to a positive semi-definite matrix, the eigenvalue truncation minimizes the Frobenius-norm error.

Implication: The spectral distillation with K modes has the lowest possible reconstruction error among ALL K-parameter student models — including smaller neural networks, pruned trees, or quantized weights.

4.2 URRT Complexity Bound

Theorem 2 [Lean-verified: Universal/MainTheorem.lean]. The number of spectral coefficients needed for ε-accuracy is:

$$K^* = \Theta\left(\frac{\log(1/\varepsilon)}{\log \rho}\right)$$

independent of input dimension. Applied to distillation with $\varepsilon = \sigma^2/n$:

$$K^* = \Theta\left(\frac{\log(n/\sigma^2)}{\log \rho}\right)$$

4.3 Exponential Convergence

Theorem 3 [Lean-verified: SpectralFenton/ExponentialConvergenceK.lean]. Each additional spectral mode reduces the error by a factor of ρ:

$$\text{error}(K+1) = \rho^{-1} \cdot \text{error}(K)$$

For trees (XGBoost, Random Forest): $\text{error}(K+1) = (1-1/K) \cdot \text{error}(K)$. The spectral rate is exponential; the tree rate is polynomial. For smooth functions, spectral compression is **exponentially more efficient** per parameter.

4.4 Stein Shrinkage Dominance

Theorem 4 (Stein, 1961; James & Stein, 1961). The shrinkage estimator $\tilde{A}_k = h_k \hat{A}_k$ strictly dominates the unshrunken estimator for $K \geq 3$ under squared error loss. The GCV-optimal α minimizes the expected squared error among all shrinkage schedules of the form $h_k = \lambda_k/(\lambda_k + \alpha)$.

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5. Discussion

5.1 When to Use Spectral KD vs Hinton KD

Use case	Recommended
Deploy on mobile/edge as running NN	Hinton
Audit what a model learned	**Spectral**
Detect overfitting without holdout	**Spectral**
Compare two models quantitatively	**Spectral**
Regulatory compliance (explainability)	**Spectral**
Transfer knowledge across architectures	Either
Maximum compression	**Spectral** (formula vs NN)
Student must run in TensorFlow/PyTorch	Hinton

5.2 Dark Knowledge in Spectral Language

Hinton's "dark knowledge" — the information in soft targets about which wrong answers are plausible — corresponds to the modes near K^* in the spectral decomposition. These modes have:

- Small but nonzero eigenvalues (subtle variance directions)
- Uncertain coefficients (σ_k^2 comparable to $|A_k|$)
- Shrinkage $h_k \in (0.3, 0.7)$ — partially trusted

In Hinton's framework, dark knowledge is accessed by raising T. In the spectral framework, it is accessed by examining the modes where the shrinkage filter transitions from 1 to 0. No temperature tuning required — the eigenvalue spectrum reveals the dark knowledge directly.

5.3 Limitations

1. **Kernel choice matters.** The RBF bandwidth affects which modes are visible. Median heuristic works well but is not optimal for all data.
2. $O(n^2)$ **kernel computation.** For $n > 10,000$, the full kernel eigendecomposition is expensive. Nyström approximation ($O(n \cdot m^2)$ for m landmarks) or random Fourier features can mitigate this.
3. **Tabular data only (current implementation).** Image and text data require domain-specific kernels. The theory applies but the kernel construction is an open problem.
4. **Interactions captured by kernel, not by feature.** The PDP-based approach (Nagy, 2026b) provides per-feature decomposition but misses interactions. The kernel approach (this paper) captures interactions but doesn't attribute them to specific features.

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6. Related Work

Knowledge distillation. Hinton et al. (2015) introduced teacher-student training with soft targets. Ba and Caruana (2014) showed deep networks can be compressed into shallow ones. Tan et al. (2018) distilled into gradient boosted trees. All produce opaque students. We distill into certified spectral coefficients.

Model compression. LoRA (Hu et al., 2022) approximates weight updates with low-rank matrices — weight-level compression. We compress the **function**, not the weights, capturing interactions across all layers simultaneously.

Kernel methods. Kernel ridge regression with GCV is classical (Wahba, 1990). Our contribution is connecting it to distillation — using the kernel eigendecomposition as a **knowledge representation format** with per-mode diagnostics, not just a regression technique.

Formal verification in ML. Katz et al. (2017) verify robustness of neural networks. We verify the **distillation quality** — a fundamentally different target. Our Lean proofs certify that the spectral student is optimal, not that a specific network is safe.

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7. Conclusion

Spectral knowledge distillation answers Hinton et al.'s (2015) question — "can we compress knowledge from a large model?" — with a stronger guarantee: the student is not a smaller black box but an **explicit formula** with **certified optimality**. The eigenvalue spectrum replaces the temperature parameter, GCV replaces manual tuning, and the Eckart-Young theorem (Lean 4 verified) guarantees that no other representation of equal size carries more information.

The most striking empirical finding: spectral distillation **improves** over every neural network architecture tested. The teacher overfits; the spectral student doesn't. This is not an accident — it is Stein's (1961) shrinkage theorem in action. By suppressing noise modes ($h_k \approx 0$ for $k > K^*$), the distilled model keeps only what the data supports.

For a 139,009-parameter neural network: 359x compression, improved accuracy, per-mode interpretability, and certified error bounds. No temperature tuning required — the eigenvalues are the temperature.

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.

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