NeuralSVD : Operator SVD with Neural Networks via Nested Low-Rank Approximation

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Joint work with

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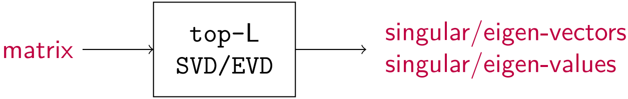
Spectral Decomposition is Extremely Versatile



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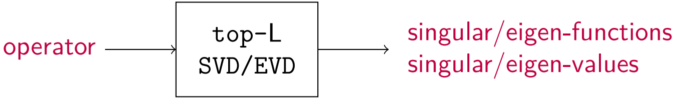

Spectral Decomposition is Extremely Versatile

1. Representation learning (low-dimensional embedding of data)

operator $\longrightarrow$ `top-L SVD/EVD` $\longrightarrow$ singular/eigen-functions, singular/eigen-values

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   PCA,

$$\underbrace{\hat{\Sigma} \triangleq \mathbb{E}_{\hat{p}(\mathbf{x})}[\mathbf{x}\mathbf{x}^{\mathsf{T}}]}_{\substack{\text{empirical covariance} \\ \in \mathbb{R}^{D\times D}}} \longrightarrow \boxed{\begin{array}{c}\texttt{top-L} \\ \texttt{EVD}\end{array}} \longrightarrow \sum_{i=1}^{L} \lambda_i \mathbf{u}_i \mathbf{u}_i^{\mathsf{T}}$$

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   PCA, **Kernel PCA**,

$$\underbrace{k(\mathbf{x}, \mathbf{x}')}_{\text{kernel}} \longrightarrow \boxed{\begin{array}{c}\texttt{top-L}\\ \texttt{EVD}\end{array}} \longrightarrow \sum_{i=1}^{L} \lambda_i \phi_i(\mathbf{x}) \phi_i(\mathbf{x}')$$

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$$\underbrace{K \triangleq \big[k(\mathbf{x}_i, \mathbf{x}_j)\big]}_{\substack{\text{kernel matrix}\\ \in \mathbb{R}^{N\times N}}} \longrightarrow \boxed{\begin{array}{c}\texttt{top-L}\\ \texttt{EVD}\end{array}} \longrightarrow \sum_{i=1}^{L} \hat{\lambda}_i \hat{\phi}_i \hat{\phi}_i^{\intercal}$$

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   PCA, **Kernel PCA**, **Laplacian eigenmaps**, ...

$$\underbrace{L \triangleq I - D^{-1/2} A D^{-1/2}}_{\substack{\text{graph Laplacian} \\ \in \mathbb{R}^{N\times N}}} \longrightarrow \boxed{\begin{array}{c}\texttt{top-L} \\ \texttt{EVD}\end{array}} \longrightarrow \sum_{i=1}^{L} \hat{\lambda}_i \hat{\phi}_i \hat{\phi}_i^{\intercal}$$

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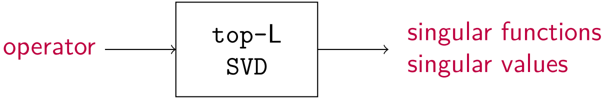

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   CCA,

$$\underbrace{\hat{\Sigma}_{\mathbf{x}}^{-1/2}\hat{\Sigma}_{\mathbf{xy}}\hat{\Sigma}_{\mathbf{y}}^{-1/2}}_{\substack{\text{cross correlation}\\ \in\mathbb{R}^{D_{\mathbf{x}}\times D_{\mathbf{y}}}}} \longrightarrow \boxed{\begin{array}{c}\texttt{top-L}\\ \texttt{SVD}\end{array}} \longrightarrow \sum_{i=1}^{L}\sigma_i \mathbf{u}_i \mathbf{v}_i^{\mathsf{T}}$$

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   CCA, **HGR maximal correlation**, ...

$$\underbrace{\frac{p(\mathbf{x},\mathbf{y})}{p(\mathbf{x})p(\mathbf{y})}-1}_{\text{canonical dependence kernel}} \longrightarrow \boxed{\begin{array}{c}\texttt{top-L}\\ \texttt{EVD}\end{array}} \longrightarrow \sum_{i=1}^{L}\sigma_i\phi_i(\mathbf{x})\psi_i(\mathbf{y})$$

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3. Solving PDEs (e.g., **quantum chemistry**)

$$\underbrace{\mathcal{H} \triangleq \mathcal{T} + \mathcal{V}}_{\text{Hamiltonian}} \longrightarrow \boxed{\begin{array}{c}\texttt{top-L}\\ \texttt{SVD/EVD}\end{array}} \longrightarrow \sum_{i=1}^{L} \lambda_i |\phi_i\rangle\langle\phi_i|$$

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$$\text{operator} \longrightarrow \boxed{\begin{array}{c}\texttt{top-L}\\ \texttt{SVD/EVD}\end{array}} \longrightarrow \begin{array}{l}\text{singular-/eigen-functions}\\ \text{singular-/eigen-values}\end{array}$$

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- **The standard approach**: decompose LARGE matrix 🤔???

🤯 **Example**: With N electrons, $\mathbf{r} \in \mathbb{R}^{3N} \to O(\epsilon^{-3N})$ samples

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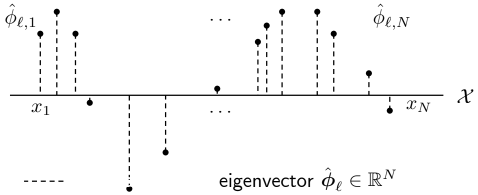
Is there an alternative to this matrix approach?

Nonparametric Approach

$\hat{\phi}_{\ell,1}$				$\cdots$	$\cdots$				$\hat{\phi}_{\ell,N}$

eigenvector $\hat{\boldsymbol{\phi}}_\ell \in \mathbb{R}^N$

Nonparametric Approach



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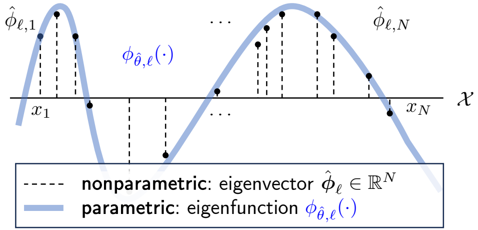

$$\phi(\cdot) \approx [\phi(x_1), \ldots, \phi(x_N)]^\intercal$$

Parametric Approach

Matrix SVD

$$T = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^T$$

where $\mathbf{u}_i^T \mathbf{u}_j = \mathbf{v}_i^T \mathbf{v}_j = \delta_{ij}$, $\sigma_1 \geq \sigma_2 \geq \ldots \geq 0$

Parametric Approach

Operator SVD

$$\mathcal{T} = \sum_{i=1}^{\infty} \sigma_i |\phi_i\rangle\langle\psi_i|$$

where $\langle\phi_i|\phi_j\rangle = \langle\psi_i|\psi_j\rangle = \delta_{ij}$, $\sigma_1 \geq \sigma_2 \geq \ldots \geq 0$

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- Hilbert space $\mathcal{F} := \mathscr{L}^2_\mu(\mathcal{X}) := \{f\colon \mathcal{X} \to \mathbb{R} \mid \|f\|^2 < \infty\}$ with inner product

$$\langle f_1|f_2\rangle := \int_{\mathcal{X}} f_1(x) f_2(x) \mu(dx) \approx \frac{1}{N} \sum_{n=1}^{N} f_1(x_n) f_2(x_n)$$

Parametric Approach

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- When $\mathcal{T}$ is symmetric PD, SVD = EVD
- Integral kernel operator: $(\mathcal{K}\phi)(y) := \int k(x, y)\phi(x)\mu(dx)$

Parametric Approach

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- To train parametric eigen- (singular-) functions (parameterized by neural networks), solve an **optimization problem** that characterizes the top-L EVD/SVD

Parametric Approach

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😎 We propose an optimization framework based on **nested low-rank approximation**!

Low-Rank Approximation (LoRA)

Theorem (Eckart–Young, 1936)

$$(\mathbf{f}_{1:L}^\star, \mathbf{g}_{1:L}^\star) \in \mathop{\arg\min}_{\substack{\mathbf{f}_1,\ldots,\mathbf{f}_L \in \mathbb{R}^M,\\ \mathbf{g}_1,\ldots,\mathbf{g}_L \in \mathbb{R}^N}} \Big\| \mathsf{T} - \sum_{i=1}^{L} \mathbf{f}_i \mathbf{g}_i^\intercal \Big\|_F^2$$

$$\textit{If } \mathsf{T} = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^\intercal, \quad \textit{then} \quad \sum_{i=1}^{L} \mathbf{f}_i^\star (\mathbf{g}_i^\star)^\intercal = \sum_{i=1}^{L} \sigma_i \mathbf{u}_i \mathbf{v}_i^\intercal$$

Low-Rank Approximation (LoRA)

Theorem (Schmidt, 1907)

$$(\mathbf{f}^\star_{1:L}, \mathbf{g}^\star_{1:L}) \in \operatorname*{arg\,min}_{\substack{f_1,\ldots,f_L \in \mathcal{F},\\ g_1,\ldots,g_L \in \mathcal{G}}} \left\| \mathcal{T} - \sum_{i=1}^{L} |f_i\rangle\langle g_i| \right\|_{HS}^2$$

$$\textit{If } \mathcal{T} = \sum_{i=1}^{\infty} \sigma_i |\phi_i\rangle\langle\psi_i|, \ \textit{then} \ \sum_{i=1}^{L} |f_i^\star\rangle\langle g_i^\star| = \sum_{i=1}^{L} \sigma_i |\phi_i\rangle\langle\psi_i|$$

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$$\boxed{\mathcal{L}_{\mathrm{LoRA}}(\mathbf{f}_{1:L}, \mathbf{g}_{1:L}) := \Big\| \mathcal{T} - \sum_{i=1}^{L} |f_i\rangle\langle g_i| \Big\|_{\mathrm{HS}}^2 - \|\mathcal{T}\|_{\mathrm{HS}}^2}$$

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$$\boxed{\mathcal{L}_{\mathrm{LoRA}}(\mathbf{f}_{1:L}, \mathbf{g}_{1:L}) := -2\sum_{i=1}^{L} \langle g_i | \mathcal{T} f_i\rangle + \sum_{i=1}^{L}\sum_{i'=1}^{L} \langle f_i | f_{i'}\rangle\langle g_i | g_{i'}\rangle}$$

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☺️ Unconstrained optimization with computable objective!

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If $\mathcal{T} = \sum_{i=1}^{\infty} \sigma_i |\phi_i\rangle\langle\psi_i|$, *then* $\sum_{i=1}^{L} |f_i^\star\rangle\langle g_i^\star| = \sum_{i=1}^{L} \sigma_i |\phi_i\rangle\langle\psi_i|$

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- ☺️ Unconstrained optimization with computable objective!
- 🤨 But, the optimal solution only captures the top-L subspaces (i.e., not ordered)

Nesting for Symmetry Breaking

- **High-level idea**: minimize $\mathcal{L}_{\mathsf{LoRA}}(\mathbf{f}_{1:i}, \mathbf{g}_{1:i})$ for $i = 1, \ldots, L$

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- **Why does this work?**

$$
\begin{aligned}
(f_1^\star, g_1^\star) &\in \arg\min_{f_1, g_1} \mathcal{L}_{\mathsf{LoRA}}(f_1, g_1) \\
(\mathbf{f}_{1:2}^\star, \mathbf{g}_{1:2}^\star) &\in \arg\min_{\mathbf{f}_{1:2}, \mathbf{g}_{1:2}} \mathcal{L}_{\mathsf{LoRA}}(\mathbf{f}_{1:2}, \mathbf{g}_{1:2}) \\
&\vdots \\
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$$|f_1^\star\rangle\langle g_1^\star| = \sigma_1|\phi_1\rangle\langle\psi_1|$$

$$|f_1^\star\rangle\langle g_1^\star| + |f_2^\star\rangle\langle g_2^\star| = \sigma_1|\phi_1\rangle\langle\psi_1| + \sigma_2|\phi_2\rangle\langle\psi_2|$$

$$\vdots$$

$$|f_1^\star\rangle\langle g_1^\star| + \ldots + |f_L^\star\rangle\langle g_L^\star| = \sigma_1|\phi_1\rangle\langle\psi_1| + \ldots + \sigma_L|\phi_L\rangle\langle\psi_L|$$

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$\Longrightarrow$ $|f_i^\star\rangle\langle g_i^\star| = \sigma_i|\phi_i\rangle\langle\psi_i|$ for all $i \in [L]$ $\square$

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- How can we **implement** this idea?

Sequential **Nesting**

- **Idea**: for each $i \in [L]$,

$$\text{update } (f_i, g_i) \text{ as if } (\mathbf{f}_{1:i-1}, \mathbf{g}_{1:i-1}) \text{ were perfectly matched}$$

- **Implementation**: for each $i \in [L]$,

$$\text{update } (f_i^{(t)}, g_i^{(t)}) \text{ using gradient } \partial_{(f_i, g_i)} \mathcal{L}_{\mathsf{LoRA}}(\mathbf{f}_{1:i}^{(t)}, \mathbf{g}_{1:i}^{(t)})$$

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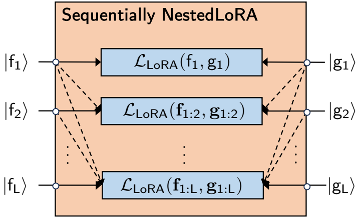

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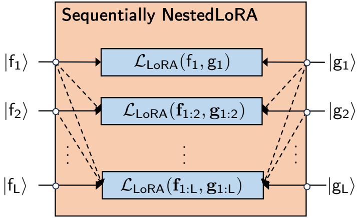

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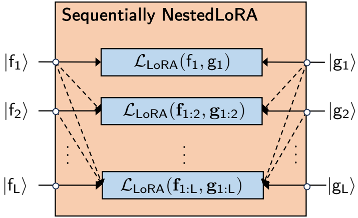

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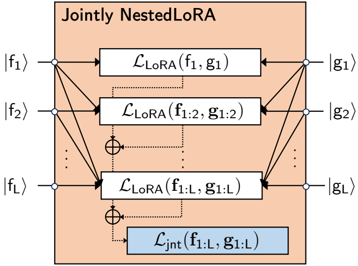

NeuralSVD = NestedLoRA + Neural Networks

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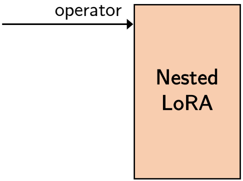

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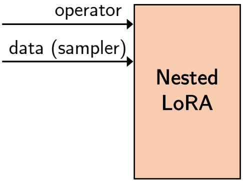

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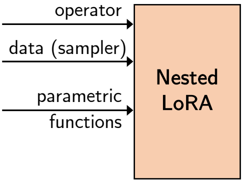

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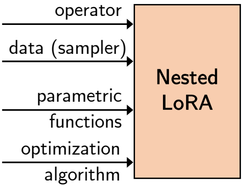

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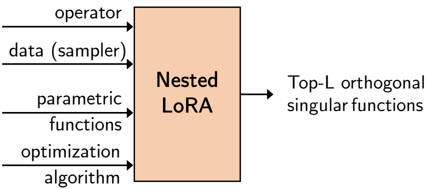

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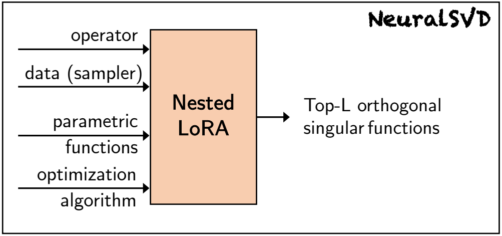

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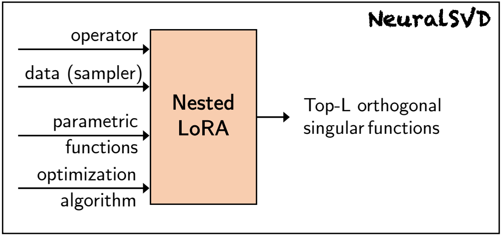

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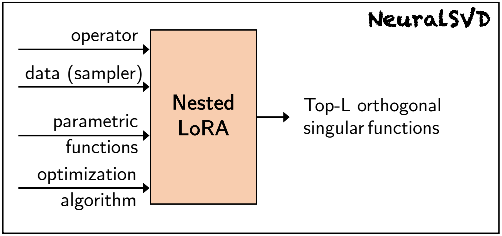

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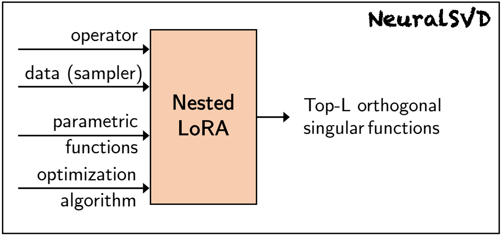

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- **Practical considerations**: NN architecture / optimization algorithm

Experiment 1. Schrödinger Equation (2D Hydrogen atom)

- Time-independent Schrödinger equation: for Hamiltonian $\mathcal{H} := -\nabla^2 + \mathcal{V}$,

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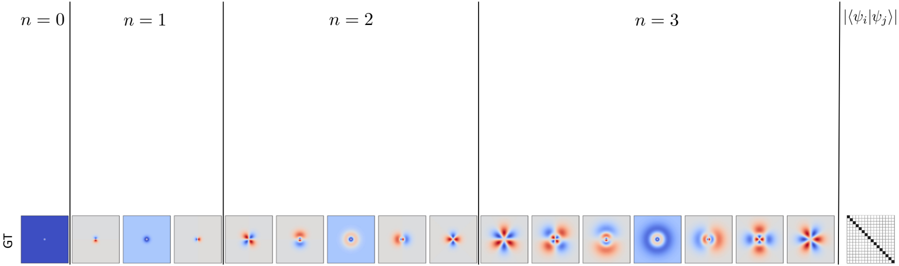
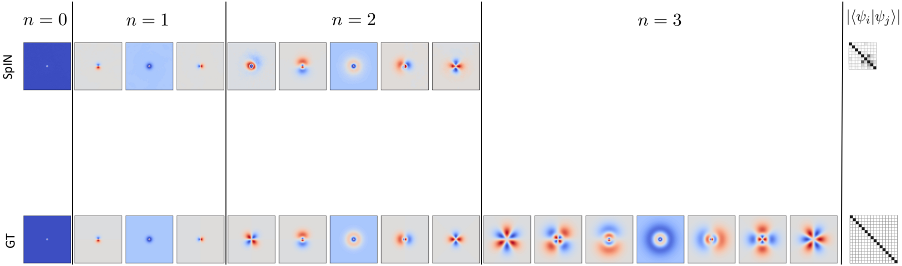


Figure: Learned eigenfunctions from SpIN, NeuralEF, and NeuralSVD.



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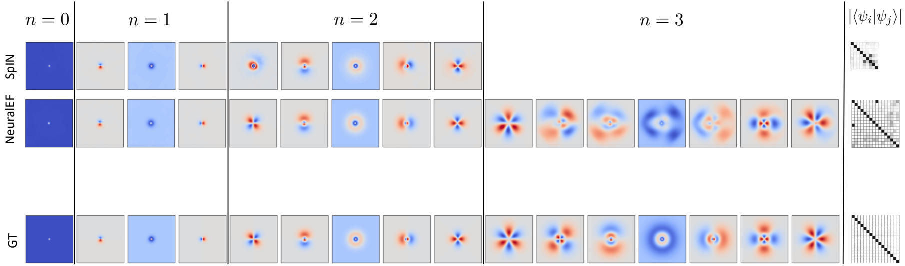

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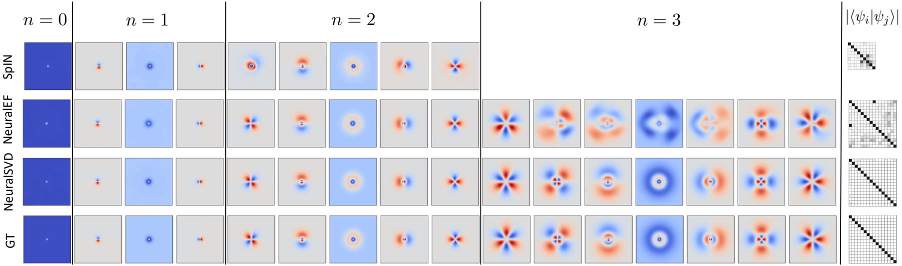

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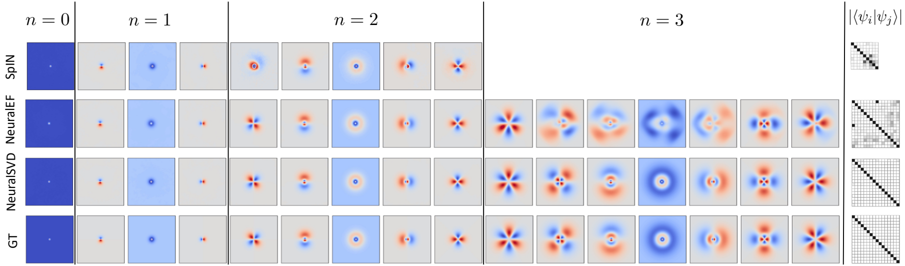

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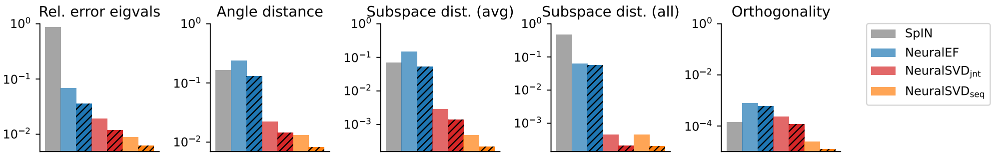
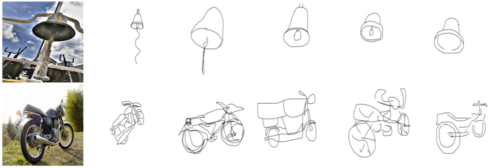


Figure: Summary of quantitative evaluations for solving TISE of 2D hydrogen atom. Non-hatched, light-colored bars represent batch size of 128, while hatched bars indicate batch size of 512.

Experiment 2. Cross-Domain Retrieval with CDK



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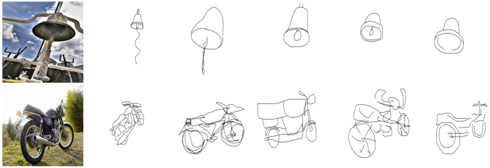

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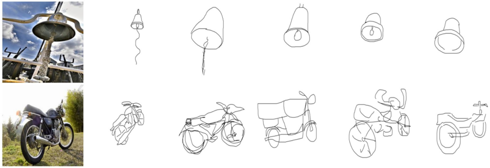

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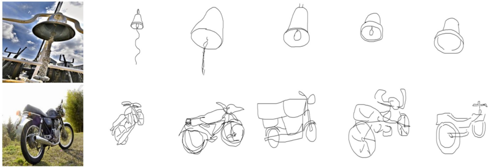

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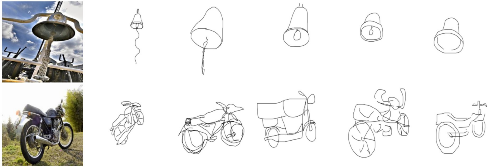

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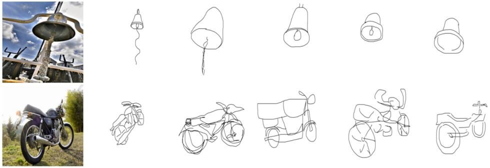

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☺️ **Structured representation**: coordinates are ordered in the order of importance

Table: Evaluation of the ZS-SBIR task with the Sketchy Extended dataset [4].

Model	Gen. model	Ext. knowledge	P@100	mAP	Split
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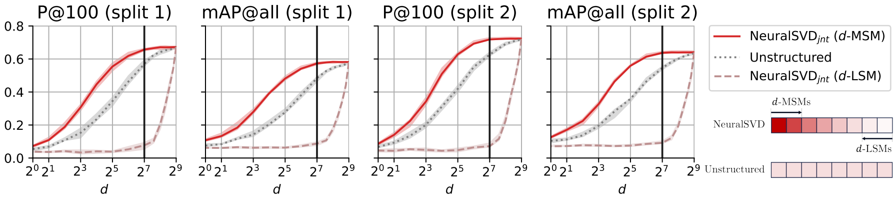
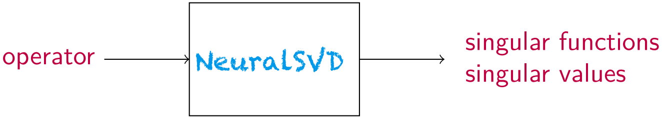


Figure: The mAP performance of NeuralSVD on ZS-SBIR task, when varying dimensions.

Postscript



Postscript

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  - ✓ Unbiased gradient estimates
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☺️ Way a lot more to come!

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😉 Check out our preprint and implementation: jongharyu.github.io

Unified Implementation: **Gradient Masking**

- A unified gradient expression:

$$|\,\partial_{f_i}\mathcal{L}\rangle = 2\Big\{-m_i|\mathcal{T}^*g_i\rangle + \sum_{i'=1}^{L} M_{ii'}|f_{i'}\rangle\langle g_{i'}|g_i\rangle\Big\}$$

- For sequential nesting:

$$\mathbf{m} \leftarrow \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}, \quad M \leftarrow \begin{bmatrix} 1 & 1 & \dots & 1 \\ 0 & 1 & \dots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 \end{bmatrix}$$

- For joint nesting:

$$\mathbf{m} \leftarrow \begin{bmatrix} w_1 + w_2 + \ldots + w_L \\ w_2 + \ldots + w_L \\ \vdots \\ w_L \end{bmatrix}, \quad M \leftarrow \begin{bmatrix} w_1 & w_2 & \dots & w_L \\ w_2 & w_2 & \dots & w_L \\ \vdots & \vdots & \ddots & \vdots \\ w_L & w_L & \dots & w_L \end{bmatrix}$$

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