Deep Sketched Output Kernel Regression for Structured Prediction

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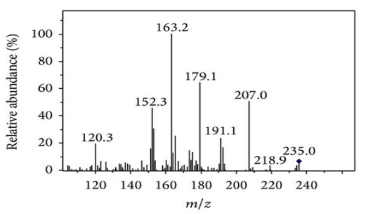
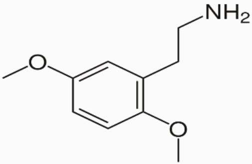
Structured Prediction

Goal: learn a mapping $f : \mathcal{X} \longrightarrow \mathcal{Y}$ with $\mathcal{Y}$ a space of structured objects (graphs, rankings, sequences, binary vectors, etc.).

MS/MS spectra



$f \; = \; ?$ $\longrightarrow$



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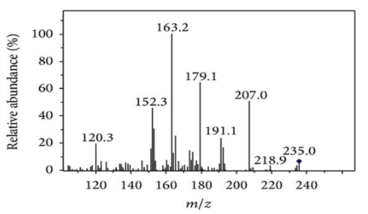
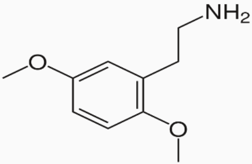


$$\xrightarrow{\quad f \;=\; ? \quad}$$



Existing works: Energy-based models (Lafferty et al., 2001; Taskar et al., 2003; Tsochantaridis et al., 2004; LeCun et al., 2007; Belanger and McCallum, 2016):

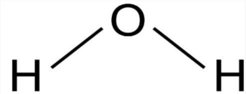
$$f(x) = \arg\min_{y \in \mathcal{Y}} E(x, y) \tag{1}$$

Structured Prediction with complex inputs

Goal of this work: solve structured prediction tasks with **complex inputs** such as texts

Water is an oxygen hydride consisting of an oxygen atom that is covalently bonded to two hydrogen atoms.

$$\xrightarrow{f \;=\; ?}$$



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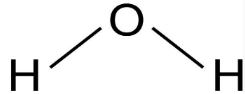

$\implies$ need of **expressive** models such as **deep neural networks**

Motivation

Build a versatile and expressive estimator able to tackle a wide variety of structured prediction tasks and learn representations from complex inputs.

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Output Kernel Regression

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Given a p.d. kernel $k : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ **defining a relevant similarity measure** and $\psi : y \in \mathcal{Y} \mapsto k(\cdot, y) \in \mathcal{H}$,

we define $\Delta(y, y') = \|\psi(y) - \psi(y')\|^2_{\mathcal{H}} = k(y, y) - 2k(y, y') + k(y', y')$ (Weston et al., 2003; Cortes et al., 2005), and solve

$$\min_{\theta \in \Theta} \ \mathbb{E}_{(X,Y)\sim\rho}[\|\psi(f_\theta(X)) - \psi(Y)\|^2_{\mathcal{H}}] \tag{2}$$

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How to learn f_θ through ψ?

Output Kernel Regression

$$\mathcal{X} \xrightarrow[f_{\hat{\theta}} \approx \underset{f_\theta,\, \theta \in \Theta}{\arg\inf}\ \mathbb{E}_{x,y}\left[\|\psi(f_\theta(x)) - \psi(y)\|^2_{\mathcal{H}}\right]]{} \mathcal{Y}$$

Output Kernel Regression

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\begin{tikzcd}
 & \mathcal{H} \arrow[d, bend left=60, "d"] \\
\mathcal{X} \arrow[ur, "h_{\widehat{\theta}} \approx \underset{h_\theta,\, \theta\in\Theta}{\arg\inf}\ \mathbb{E}_{x,y}\left[\|h_\theta(x) - \psi(y)\|_{\mathcal{H}}^2\right]"] \arrow[r, "f_{\widehat{\theta}} = d \circ h_{\widehat{\theta}} = \underset{y\in\mathcal{Y}}{\arg\min}\ \underbrace{\|h_{\widehat{\theta}}(\,\cdot\,) - \psi(y)\|_{\mathcal{H}}^2}_{E(\cdot,\, y)}"'] & \mathcal{Y} \arrow[u, "\psi"']
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\end{tikzcd}$$

How to deal with implicit or infinite-dimensional output feature maps while using an input neural network?

Output Kernel Regression with Deep Learning: a basis approach

$$
\begin{tikzcd}[column sep=huge, row sep=huge]
 & \mathrm{span}\Big((e_i)_{i=1}^{p}\Big) \subsetneq \mathcal{H} \arrow[d, bend left, "d"] \\
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How to build this base $\mathrm{span}\left((e_i)_{i=1}^{p}\right)$?

Deep Sketched Output Kernel Regression

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Let $m \ll n$, $R \in \mathbb{R}^{m \times n}$ be a random matrix and n data $(y_i)_{i=1}^n \in \mathcal{Y}$

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Basic idea: The linear subspace of $\mathcal{H}$ is obtained by

$$\operatorname{span}\left(\left(\sum_{j=1}^{n} R_{ij}\psi(y_j)\right)_{i=1}^{m}\right) \tag{4}$$

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What is its orthonormal basis?

Construction of the orthonormal basis

- $\widehat{C} = \frac{1}{n} \sum_{i=1}^{n} \psi(y_i) \otimes \psi(y_i) \in \mathcal{H}^{\mathcal{H}}$

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Related work on Nyström: Yang et al. (2012); Rudi et al. (2015)

Solving the surrogate problem

$$\min_{W \in \mathcal{W}} \frac{1}{n} \sum_{i=1}^{n} \| g_{\widetilde{E}} \circ g_W(x_i) - \psi(y_i) \|_{\mathcal{H}}^2 \tag{5}$$

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$$\left\|g_{\widetilde{E}} \circ g_W(x) - \psi(y)\right\|_{\mathcal{H}}^2 = \left\|\sum_{i=1}^{p} g_W(x)_j \tilde{e}_j - \psi(y)\right\|_{\mathcal{H}}^2$$

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&= \| g_W(x) \|_2^2 - 2 g_W(x)^\top \tilde{\psi}(y) + k(y,y) \,,
\end{aligned}$$

where $\tilde{\psi}(y) = (\langle \tilde{e}_1, \psi(y) \rangle_{\mathcal{H}}, \dots, \langle \tilde{e}_p, \psi(y) \rangle_{\mathcal{H}})^\top = \widetilde{D}_p^{-1/2} \widetilde{U}_p^\top R k^Y \in \mathbb{R}^p$, $\widetilde{U}_p = (\tilde{\mathbf{u}}_1, \dots, \tilde{\mathbf{u}}_p)$, $\widetilde{D}_p = \operatorname{diag}(\sigma_1(\widetilde{K}), \dots, \sigma_p(\widetilde{K}))$, and $k^Y = (k(y, y_1), \dots, k(y, y_n))$.

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&= \|g_W(x)\|_2^2 - 2 g_W(x)^\top \tilde{\psi}(y) + k(y,y) \\
&= \left\|g_W(x) - \tilde{\psi}(y)\right\|_2^2 - \left\|\tilde{\psi}(y)\right\|_2^2 + k(y,y)\,,
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Deep Sketched Output Kernel Regression: Inference

$$f_{\hat{\theta}}(x) = d \circ h_{th\hat{e}ta}(x) = \underset{y \in \mathcal{Y}}{\arg\min} \; \left\| h_{\hat{\theta}}(x) - \psi(y) \right\|_{\mathcal{H}}^2 =$$

$$\underset{y \in \mathcal{Y}}{\arg\min} \; k(y, y) - 2 g_{\hat{W}}(x)^\top \tilde{\psi}(y) = \underset{y \in \mathcal{Y}}{\arg\max} \; g_{\hat{W}}(x)^\top \tilde{\psi}(y)$$

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- **Test set:** X_{te} of size n_{te}
- **Candidate set:** $\mathcal{Y}_c \subseteq \mathcal{Y}$ of size n_c

$$\underbrace{g_{\hat{W}}(X^{te})}_{n_{te} \times p} \underbrace{\tilde{\psi}(Y^c)^\top}_{p \times n_c} \tag{6}$$

DSOKR Inference: Ensemble Approach

Let $T > 1$, and for $1 \leq t \leq T$, let R_t be a randomly drawn sketching matrix, $h_{\hat{\theta}_t} = g_{\tilde{E}_t} \circ g_{\hat{W}_t}$ denotes the trained DSOKR neural network based on R_t

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$$f_{\hat{\theta}}^{\text{mean}}(x) = \underset{y \in \mathcal{Y}_c}{\arg\max} \sum_{t=1}^{T} \omega_t \, g_{\hat{W}_t}(x)^\top \tilde{\psi}_t(y) \quad \text{with} \quad \sum_{t=1}^{T} \omega_t = 1 \tag{7}$$

or

$$f_{\hat{\theta}}^{\max}(x) = \underset{y \in \mathcal{Y}_c}{\arg\max} \ \underset{1 \leq t \leq T}{\arg\max} \ g_{\hat{W}_t}(x)^\top \tilde{\psi}_t(y) \tag{8}$$

DSOKR: summary

1. Training. a. Computations for the basis $\widetilde{E}$.
   - SVD of $\widetilde{K} = RKR^\top \to \left\{\left(\sigma_i(\widetilde{K}), \tilde{\mathbf{u}}_i\right), i \in [m]\right\}$
   - $\widetilde{\Omega} = \widetilde{D}_p^{-1/2}\widetilde{U}_p^\top \in \mathbb{R}^{p\times m}$, where $\widetilde{U}_p = (\tilde{\mathbf{u}}_1, \ldots, \tilde{\mathbf{u}}_p)$, $\widetilde{D}_p = \mathrm{diag}(\sigma_1(\widetilde{K}), \ldots, \sigma_p(\widetilde{K}))$

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1. Training. b. Solving the surrogate problem.

- $\{(x_i, y_i)\}_{i=1}^n \leftarrow \{(x_i, \tilde{\psi}(y_i))\}_{i=1}^n$, $\{(x_i^{\mathrm{val}}, y_i^{\mathrm{val}})\}_{i=1}^{n_{\mathrm{val}}} \leftarrow \{(x_i, \tilde{\psi}(y_i^{\mathrm{val}}))\}_{i=1}^{n_{\mathrm{val}}}$, where $\tilde{\psi}(y) = \widetilde{\Omega} R k^y$
- $g_{\hat{W}} = \underset{g_W, W \in \mathcal{W}}{\arg\min} \frac{1}{n} \sum_{i=1}^n \left\| g_{\hat{W}}(x_i) - \tilde{\psi}(y_i) \right\|_2^2$

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1. Training. b. Solving the surrogate problem.

- $\{(x_i, y_i)\}_{i=1}^n \leftarrow \{(x_i, \tilde{\psi}(y_i))\}_{i=1}^n$, $\{(x_i^{\mathrm{val}}, y_i^{\mathrm{val}})\}_{i=1}^{n_{\mathrm{val}}} \leftarrow \{(x_i, \tilde{\psi}(y_i^{\mathrm{val}}))\}_{i=1}^{n_{\mathrm{val}}}$, where $\tilde{\psi}(y) = \widetilde{\Omega} R k^y$
- $g_{\hat{W}} = \underset{g_W, W \in \mathcal{W}}{\arg\min} \frac{1}{n} \sum_{i=1}^n \left\| g_{\hat{W}}(x_i) - \tilde{\psi}(y_i) \right\|_2^2$

2. Inference.

- $\{y_i^{\mathrm{c}}\}_{i=1}^{n_{\mathrm{c}}} \leftarrow \{\tilde{\psi}(y_i^{\mathrm{c}})\}_{i=1}^{n_{\mathrm{c}}}$
- $f_{\hat{\theta}}(x_i^{\mathrm{te}}) = y_j^{\mathrm{c}}$ where $j = \underset{1 \le j \le n_{\mathrm{c}}}{\arg\max} \, [g_{\hat{W}}(X^{\mathrm{te}}) \tilde{\psi}(Y^{\mathrm{c}})^\top]_{ij}$

Experiments

Sketching size selection strategy

Goal: set the minimal value of m s.t. it captures the information contained in the empirical covariance operator $\widehat{C} = \frac{1}{n}\sum_{i=1}^{n} \psi(y_i) \otimes \psi(y_i)$

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1. Approximate leverage scores of $\widehat{C}$

2. Set the optimal m according to the performance of the *perfect h* estimator on the validation set, i.e.

$$h : (x, y) \mapsto \sum_{j=1}^{p} \langle \tilde{e}_j, \psi(y) \rangle_{\mathcal{H}} \, \tilde{e}_j = \sum_{j=1}^{p} \tilde{\psi}(y)_j \, \tilde{e}_j \,. \tag{9}$$

$\Longrightarrow$ allows to cope with the neural net training phase

Synthetic Least Squares Regression

1) $n = 50,000$, $\mathcal{X} = \mathbb{R}^{2,000}$, $\mathcal{Y} = \mathbb{R}^{1,000}$, k linear kernel $\implies$ $\mathcal{H} = \mathcal{Y} = \mathbb{R}^{1,000}$

Goal: build this dataset such that the outputs lie in a subspace of $\mathcal{Y}$ of dimension $d = 50 < 1,000$

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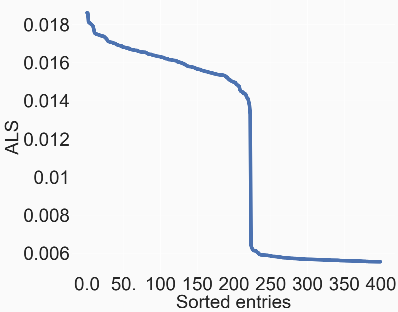
2) Draw $H = (H_{ij})_{1 \leq i \leq d, 1 \leq j \leq 2,000} \in \mathbb{R}^{d \times 2,000}$ s.t. $H_{ij} \sim \mathcal{N}(0,1)$, $x_i \sim \mathcal{N}(0, C)$, where $(\sigma_j(C) = j^{-1/2})_{j=1}^{2,000}$, $\varepsilon_i \sim \mathcal{N}(0, \sigma^2 I_{1,000})$ with $\sigma^2 = 0.01$,

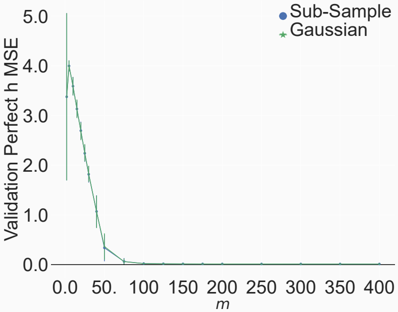
$$y_i = UHx_i + \varepsilon_i\,, \tag{10}$$

where $U = (u_1, \ldots, u_d) \in \mathbb{R}^{1,000 \times d}$ and $(u_j)_{j=1}^{d}$ are d randomly drawn orthonormal vectors

Synthetic Least Squares Regression: Sketching Size Selection



(a) Sorted 400 highest ALS.



(b) Validation MSE of *Perfect h* w.r.t. *m*.

Synthetic Least Squares Regression

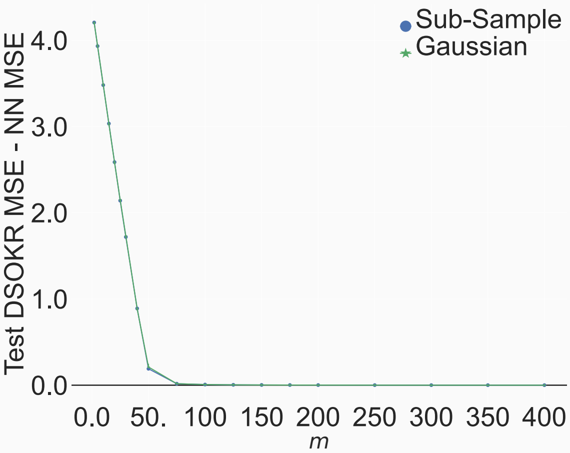


Figure 2: Difference between test MSE of DSOKR and NN w.r.t. m.

Smiles to Molecule

QM9 molecule dataset (Ruddigkeit et al., 2012; Ramakrishnan et al., 2014), containing around 130,000 small organic molecules

O=C1CC2NC2CC1O $\xrightarrow{f\ =\ ?}$

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Input neural network: Transformer (Vaswani et al., 2017)

Output kernel: core Weisfeiler-Lehman subtree kernel (CORE-WL) (Nikolentzos et al., 2018)

Sketching: Sub-Sample

Smiles to Molecule: Results

Table 1: Edit distance of different methods on SMI2Mol test set

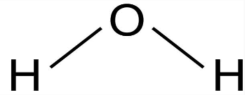
	GED w/o edge feature ↓	GED w/ edge feature ↓
SISOKR	3.330 ± 0.080	4.192 ± 0.109
NNBary-FGW	5.115 ± 0.129	-
Sketched ILE-FGW	2.998 ± 0.253	-
DSOKR	$\mathbf{1.951} \pm \mathbf{0.074}$	$\mathbf{2.960} \pm \mathbf{0.079}$

Text to Molecule

ChEBI-20 dataset (Edwards et al., 2021), containing 33,010 pairs of compounds and descriptions, compounds from PubChem (Kim et al., 2016, 2019) and their descriptions from the Chemical Entities of Biological Interest (ChEBI) database (Hastings et al., 2016). 80% for training, 10% for validation, and 10% for testing

Water is an oxygen hydride consisting of an oxygen atom that is covalently bonded to two hydrogen atoms.

$$\xrightarrow{\quad f \;=\; ? \quad}$$



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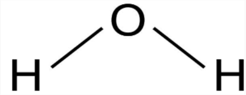

Input neural network: SciBERT (transformer) (Beltagy et al., 2019)

Output kernel: Mol2vec (Jaeger et al., 2018)

Sketching: Sub-Sample and Gaussian

Text to Molecule: Results

	Hits@1 ↑	Hits@10 ↑	MRR ↑
SISOKR	0.4%	2.8%	0.015
SciBERT Regression	16.8%	56.9%	0.298
CMAM - MLP	34.9%	84.2%	0.513
CMAM - GCN	33.2%	82.5%	0.495
CMAM - Ensemble (MLP×3)	39.8%	87.6%	0.562
CMAM - Ensemble (GCN×3)	39.0%	87.0%	0.551
CMAM - Ensemble (MLP×3 + GCN×3)	44.2%	**88.7**%	0.597
DSOKR - SubSample Sketch	48.2%	87.4%	0.624
DSOKR - Gaussian Sketch	49.0%	87.5%	0.630
DSOKR - Ensemble (SubSample×3)	**51.0**%	88.2%	**0.642**
DSOKR - Ensemble (Gaussian×3)	50.5%	87.9%	**0.642**
DSOKR - Ensemble (SubSample×3 + Gaussian×3)	50.0%	88.3%	0.640

Conclusion

Take-home messages

- *Deep Sketched Output Kernel Regression* is a family of **deep neural architectures** whose last layer predicts a **data-dependent finite-dimensional representation of the outputs**, that lies in the possibly infinite-dimensional feature space deriving from the kernel-induced loss

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- This last layer is computed **beforehand**, and is the **eigenbasis of the sketched empirical covariance operator** $\implies$ we can use **gradient-based techniques** to learn the weights of the previous layers **for any neural architecture**

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- This last layer is computed **beforehand**, and is the **eigenbasis of the sketched empirical covariance operator** $\implies$ we can use **gradient-based techniques** to learn the weights of the previous layers **for any neural architecture**
- We provide a **strategy to select the sketching size**
- We show that DSOKR performs well on **two text-to-molecule datasets**

Future work

- Excess risk bound for DSOKR
- End-to-end version of DSOKR
- Extension to the auto-encoder architecture

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Reminder: positive definite kernels and Reproducing Kernel Hilbert Space

Positive definite kernel: $k_{\mathcal{Z}} : \mathcal{Z} \times \mathcal{Z} \to \mathbb{R}$ such that

- for all $(z, z') \in \mathcal{Z}^2$, $k_{\mathcal{Z}}(z, z') = k_{\mathcal{Z}}(z', z)^\top$
- for all $n \in \mathbb{N}$ and any $(z_i, \alpha_i)_{i=1}^n \in (\mathcal{Z} \times \mathbb{R})^n$, $\sum_{i,j=1}^n \alpha_i \alpha_j k_{\mathcal{Z}}\left(z_i, z_j\right) \geqslant 0$

RKHS (Aronszajn, 1950): Hilbert space $\mathcal{H}_{\mathcal{Z}}$ of functions $f : \mathcal{Z} \to \mathbb{R}$ s. t. for all $f \in \mathcal{H}_{\mathcal{Z}}$ and $z \in \mathcal{Z}$

1. $z' \mapsto k_{\mathcal{Z}}(z, z') \in \mathcal{H}_{\mathcal{Z}}$,
2. $\langle f, k_{\mathcal{Z}}(\cdot, z) \rangle_{\mathcal{H}_{\mathcal{Z}}} = f(z)$ **(reproducing property)**.

Fisher consistency and excess risk bound

Lemma 1 and Theorem 3 from Ciliberto et al. (2020). Let $\mathcal{Y}$ be compact, $k_{\mathcal{Y}} : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ be a p.d. kernel and $\psi_{\mathcal{Y}} : y \mapsto k_{\mathcal{Y}}(\cdot, y)$ s.t. $\|\psi_{\mathcal{Y}}(y)\|_{\mathcal{H}_{\mathcal{Y}}} = 1, \forall y \in \mathcal{Y}$, and

$$f^* = \operatorname*{arg\,inf}_{f:\mathcal{X}\to\mathcal{Y}} \mathcal{R}(f) = \operatorname*{arg\,inf}_{f:\mathcal{X}\to\mathcal{Y}} \mathbb{E}_{(x,y)\sim\rho}[\|\psi_{\mathcal{Y}}(f(x)) - \psi_{\mathcal{Y}}(y)\|^2_{\mathcal{H}_{\mathcal{Y}}}] .$$

Then,

$$f^*(x) = \operatorname*{arg\,min}_{y\in\mathcal{Y}} \|h^*(x) - \psi_{\mathcal{Y}}(y)\|^2_{\mathcal{H}_{\mathcal{Y}}} = d \circ h^*(x) , \quad h^*(x) = \mathbb{E}_y[\psi_{\mathcal{Y}}(y)|x] ,$$

almost surely with respect to $\rho_{\mathcal{X}}$.

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almost surely with respect to $\rho_{\mathcal{X}}$.

Moreover, let $h : \mathcal{X} \to \mathcal{H}_{\mathcal{Y}}$ be measurable and $f : \mathcal{X} \to \mathcal{Y}$ such that, for any $x \in \mathcal{X}$,

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Then,

$$\mathcal{R}(f) - \mathcal{R}(f^*) \leq 12\sqrt{\mathcal{E}(h) - \mathcal{E}(h^*)}\,,$$

where $\mathcal{E}(h) = \mathbb{E}_{(x,y)\sim\rho}[\|h(x) - \psi_{\mathcal{Y}}(y)\|^2_{\mathcal{H}_{\mathcal{Y}}}]$.

Background: Scalability to large datasets

1) Random Fourier Features (Rahimi and Recht, 2007; Rudi and Rosasco, 2017; Sriperumbudur and Szabó, 2015; Brault et al., 2016; Li et al., 2021)

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2) **Sketching (Mahoney et al., 2011; Woodruff, 2014):** dimension reduction approach based on random linear projections

- Nyström approximation ($\iff$ sub-sampling sketch) (Williams and Seeger, 2001; Drineas et al., 2005; Bach, 2013; Rudi et al., 2017; Meanti et al., 2020)
- Gaussian, Randomized Orthogonal Systems, sparse sketches etc. (Yang et al., 2017; Lacotte et al., 2019; Kpotufe and Sriperumbudur, 2020; Lacotte and Pilanci, 2020; Chen and Yang, 2021; Gazagnadou et al., 2021)

Example: Sketching for scalar Kernel Ridge Regression ($\mathcal{Y} = \mathbb{R}$)

Representer theorem: $\hat{f} = \sum_{i=1}^{n} \hat{\alpha}_i k_x(\cdot, x_i)$, where

$$\hat{\alpha} = (\hat{\alpha}_1, \ldots, \hat{\alpha}_n)^\top = \underset{\alpha \in \mathbb{R}^n}{\arg\min}\ \alpha^\top \left(K_X^2 + n\lambda K_X\right) \alpha - 2Y^\top K_X \alpha$$

$$= \underbrace{(K_X + n\lambda I_n)}_{n \times n}{}^{-1} Y$$

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$\hat{f} \leftarrow \tilde{f} = \sum_{i=1}^{n} [R^\top \tilde{\gamma}]_i k_x(\cdot, x_i)$, where

$$\tilde{\gamma} = (\tilde{\gamma}_1, \dots, \tilde{\gamma}_m)^\top = \underset{\gamma \in \mathbb{R}^m}{\arg\min}\ \gamma^\top \left(RK_X^2R^\top + n\lambda RK_XR^\top\right) \gamma - 2Y^\top K_X R^\top \gamma$$
$$= \underbrace{(RK_X^2R^\top + n\lambda RK_XR^\top)}_{m \times m}{}^{\dagger} RK_X Y$$

Smiles to Molecule: some nice figures

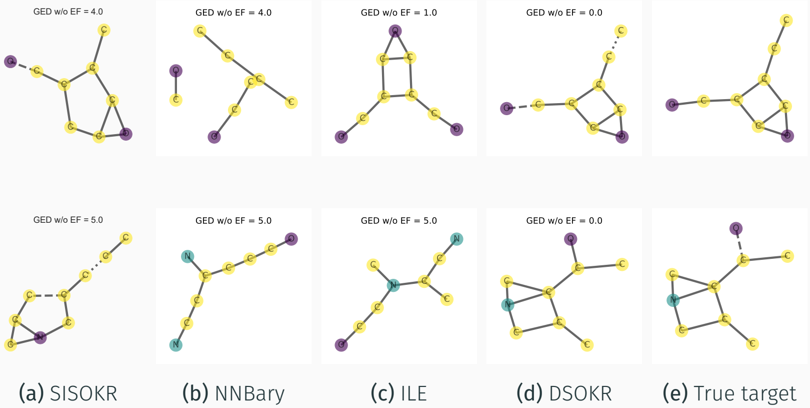

Figure 3: Predicted molecules on the SMI2Mol dataset.