

Discriminative Embeddings of Latent Variable Models for Structured Data

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What is a kernel?

A feature map transforms the input space to a feature space:

$$\varphi : \overbrace{\mathbb{R}^n}^{\text{Input space}} \rightarrow \overbrace{\mathbb{R}^m}^{\text{Feature space}} \quad (1)$$

A kernel function k is a real-valued function with two inputs:

$$k : \Omega \times \Omega \rightarrow \mathbb{R} \quad (2)$$

Kernel functions generalize the notion of inner products to feature maps:

$$k(x, y) = \varphi(x)^\top \varphi(y) \quad (3)$$

Gives us $\varphi(x)^\top \varphi(y)$ without directly computing $\varphi(x)$ or $\varphi(y)$.

What is a kernel?

Consider the univariate polynomial regression algorithm:

$$\hat{f}(x; \beta) = \beta \varphi(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \dots + \beta_m x^m = \sum_{j=0}^m \beta_j x^j \quad (4)$$

Where $\varphi(x) = [1, x, x^2, x^3, \dots, x^m]$. We seek β minimizing the error:

$$\beta^* = \underset{\beta}{\operatorname{argmin}} ||Y - \hat{f}(X; \beta)||^2 \quad (5)$$

Can solve for β^* using the normal equation or gradient descent:

$$\beta^* = (X^T X)^{-1} X^T Y \quad (6)$$

$$\beta' \leftarrow \beta - \alpha \nabla_{\beta} ||Y - \hat{f}(X; \beta)||^2 \quad (7)$$

What happens if we want to approximate a multivariate polynomial?

$$z(x, y) = 1 + \beta_x x + \beta_y y + \beta_{xy} xy + \beta_{x^2} x^2 + \beta_{y^2} y^2 + \beta_{xy^2} xy^2 + \dots \quad (8)$$

What is a kernel?

Consider the polynomial kernel $k(x, y) = (1 + x^T y)^2$ with $x, y \in \mathbb{R}^2$.

$$k(x, y) = (1 + x^T y)^2 = (1 + x_1 y_1 + x_2 y_2)^2 \quad (9)$$

$$= 1 + x_1^2 y_1^2 + x_2^2 y_2^2 + 2x_1 y_1 + 2x_2 y_2 + 2x_1 x_2 y_1 y_2 \quad (10)$$

This gives us the same result as computing the 6 dimensional feature map:

$$k(x, y) = \varphi(x)^T \varphi(y) \quad (11)$$

$$= [1, x_1^2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1 x_2]^T \begin{bmatrix} 1 \\ y_1^2 \\ y_2^2 \\ \sqrt{2}y_1 \\ \sqrt{2}y_2 \\ \sqrt{2}y_1 y_2 \end{bmatrix} \quad (12)$$

But does not require computing $\varphi(x)$ or $\varphi(y)$.

Examples of common kernels

Popular kernels

Polynomial	$k(x, y) := (x^T y + r)^n$	$x, y \in \mathbb{R}^d, n \in \mathbb{N}, r \geq 0$
Laplacian	$k(x, y) := \exp\left(-\frac{\ x-y\ }{\sigma}\right)$	$x, y \in \mathbb{R}^d, \sigma > 0$
Gaussian RBF	$k(x, y) := \exp\left(-\frac{\ x-y\ ^2}{2\sigma^2}\right)$	$x, y \in \mathbb{R}^d, \sigma > 0$

Popular Graph Kernels

RW	$k_{\times}(G, H) := \sum_{i,j=1}^{ V_{\times} } \left[\sum_{n=1}^{\infty} \lambda^n A_{\times}^n \right]_{ij} = \mathbf{e}^T (\mathbf{I} - \lambda A_{\times})^{-1} \mathbf{e}$	$\mathcal{O}(n^6)$
SP	$k_{SP}(G, H) := \sum_{s_1 \in SD(G)} \sum_{s_2 \in SD(H)} k(s_1, s_2)$	$\mathcal{O}(n^4)$
WL	$l^{(i)}(G) := \begin{cases} \deg_v, \forall v \in G & i = 1 \\ \text{HASH}(\{\{l^{(i-1)}(u), \forall u \in \mathcal{N}(v)\}\}) & i > 1 \end{cases}$ $k_{WL}(G, H) := \langle \psi_{WL}(G), \psi_{WL}(H) \rangle$	$\mathcal{O}(hm)$

<https://people.mpi-inf.mpg.de/~mehlhorn/ftp/genWLPaper.pdf>

Positive definite kernels

Positive Definite Matrix

A symmetric matrix $K \in \mathbb{R}^{N^2}$ is **positive definite** if $x^T K x > 0, \forall x \in \mathbb{R}^N \setminus 0$.

Positive Definite Kernel

A symmetric kernel k is called positive definite on Ω if its associated kernel matrix $K = [k(x_i, x_j)]_{i,j=0}^N$ is positive definite $\forall N \in \mathbb{N}, \forall \{x_1, \dots, x_N\} \subset \Omega$.

<http://www.math.iit.edu/~fass/PDKernels.pdf>

What is an inner product space?

Linear function

Let X be a vector space over \mathbb{R} . A function $f : X \rightarrow \mathbb{R}$ is **linear** iff $f(\alpha x) = \alpha f(x)$ and $f(x + z) = f(x) + f(z)$ for all $\alpha \in \mathbb{R}, x, z \in X$.

Inner product space

X is an **inner product space** if there exists a symmetric bilinear map $\langle \cdot, \cdot \rangle : X \times X \rightarrow \mathbb{R}$ if $\forall x \in X, \langle x, x \rangle > 0$ (i.e. is positive definite).

Cauchy-Schwartz Inequality

If X is an inner product space, then $\forall u, v \in \mathcal{X}, |\langle u, v \rangle|^2 \leq \langle u, u \rangle \cdot \langle v, v \rangle$.

Scalar Product

$$\langle x, y \rangle := xy$$

Vector Dot Product

$$\left\langle \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}, \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \right\rangle := x^T y$$

Random Variable

$$\langle X, Y \rangle := \mathbb{E}(XY)$$

What is a Hilbert space?

Let $d : X \times X \rightarrow \mathbb{R}^{\geq 0}$ be a metric on the space X .

Cauchy sequence

A sequence $\{x_n\}$ is called a **Cauchy sequence** if

$\forall \varepsilon > 0, \exists N \in \mathbb{N}$, such that $\forall n, m \geq N, d(x_n, x_m) \leq \varepsilon$.

Completeness

X is called **complete** if every Cauchy sequence converges to a point in X .

Separability

X is called **separable** if there exists a sequence $\{x_n\}_{n=1}^{\infty} \in X$ s.t. every nonempty open subset of X contains at least one element of the sequence.

Hilbert space

A Hilbert space \mathcal{H} is an inner product space that is complete and separable.

Properties of Hilbert Spaces

Hilbert space inner products are kernels

The inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}} : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{R}$ is a positive definite kernel:

$$\sum_{i,j=1}^n c_i c_j \langle x_i, x_j \rangle_{\mathcal{H}} = \left\langle \sum_{i=1}^n c_i x_i, \sum_{j=1}^n c_j x_j \right\rangle_{\mathcal{H}} = \left\| \sum_{i=1}^n c_i x_i \right\|_{\mathcal{H}}^2 \geq 0$$

Reproducing Kernel Hilbert Space (RKHS)

Any continuous, symmetric, positive definite kernel $k : X \times X \rightarrow \mathbb{R}$ has a corresponding Hilbert space, which induces a feature map $\varphi : X \rightarrow \mathcal{H}$ satisfying $k(x, y) = \langle \varphi(x), \varphi(y) \rangle_{\mathcal{H}}$.

<http://jmlr.csail.mit.edu/papers/volume11/vishwanathan10a/vishwanathan10a.pdf>
https://marcocuturi.net/Papers/pdk_in_ml.pdf

Hilbert Space Embedding of Distributions

Maps distributions into potentially infinite dimensional feature spaces:

$$\mu_X := \mathbb{E}_X[\phi(X)] = \int_{\mathcal{X}} \phi(x)p(x)dx : \mathcal{P} \mapsto \mathcal{F} \quad (13)$$

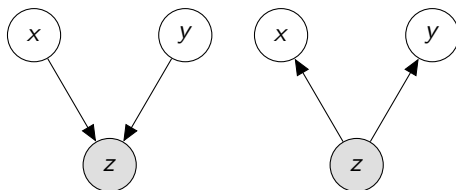
By choosing the right kernel, we can make this mapping injective.

$$f(p(x)) = \tilde{f}(\mu_x), f : \mathcal{P} \mapsto \mathbb{R} \quad (14)$$

$$\mathcal{T} \circ p(x) = \tilde{\mathcal{T}} \circ \mu_x, \tilde{\mathcal{T}} : \mathcal{F} \mapsto \mathbb{R}^d \quad (15)$$

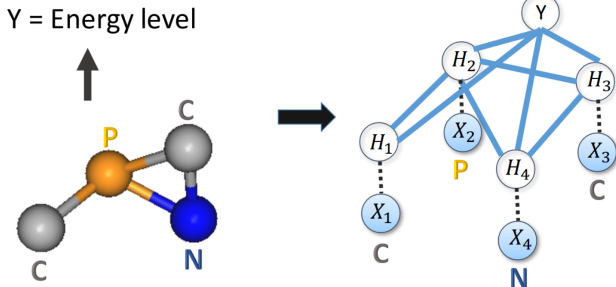
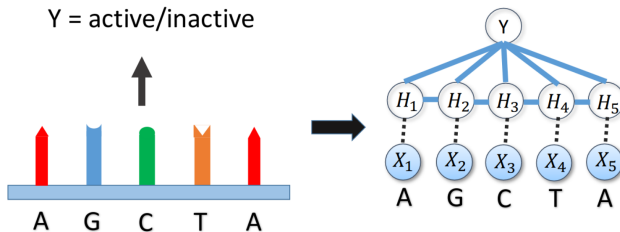
Belief network is a distribution of the form:

$$P(x_1, \dots, x_D) = \prod_{i=1}^D P(x_i | pa(x_i)) \quad (16)$$



$$P(X, Y|Z) \propto P(Z|X, Y)P(X)P(Y) \quad P(X, Y|Z) = P(X|Z)P(Y|Z)$$

Latent Variable Models



Algorithm 1 Embedded Mean Field

- 1: **Input:** parameter \mathbf{W} in $\tilde{\mathcal{T}}$
 - 2: Initialize $\tilde{\mu}_i^{(0)} = \mathbf{0}$, for all $i \in \mathcal{V}$
 - 3: **for** $t = 1$ **to** T **do**
 - 4: **for** $i \in \mathcal{V}$ **do**
 - 5: $l_i = \sum_{j \in \mathcal{N}(i)} \tilde{\mu}_j^{(t-1)}$
 - 6: $\tilde{\mu}_i^{(t)} = \sigma(W_1 x_i + W_2 l_i)$
 - 7: **end for**
 - 8: **end for** {fixed point equation update}
 - 9: return $\{\tilde{\mu}_i^T\}_{i \in \mathcal{V}}$
-

Algorithm 2 Embedding Loopy BP

```
1: Input: parameter  $\mathbf{W}$  in  $\tilde{\mathcal{T}}_1$  and  $\tilde{\mathcal{T}}_2$ 
2: Initialize  $\tilde{\nu}_{ij}^{(0)} = \mathbf{0}$ , for all  $(i, j) \in \mathcal{E}$ 
3: for  $t = 1$  to  $T$  do
4:   for  $(i, j) \in \mathcal{E}$  do
5:      $\tilde{\nu}_{ij}^t = \sigma(W_1 x_i + W_2 \sum_{k \in \mathcal{N}(i) \setminus j} \tilde{\nu}_{ki}^{(t-1)})$ 
6:   end for
7: end for
8: for  $i \in \mathcal{V}$  do
9:    $\tilde{\mu}_i = \sigma(W_3 x_i + W_4 \sum_{k \in \mathcal{N}(i) \setminus j} \tilde{\nu}_{ki}^{(T)})$ 
10: end for
11: return  $\{\tilde{\mu}_i\}_{i \in \mathcal{V}}$ 
```

Algorithm 3 Discriminative Embedding

Input: Dataset $\mathcal{D} = \{\chi_n, y_n\}_{n=1}^N$, loss function $l(f(\chi), y)$.

Initialize $\mathbf{U}^0 = \{\mathbf{W}^0, \mathbf{u}^0\}$ randomly.

for $t = 1$ **to** T **do**

 Sample $\{\chi_t, y_t\}$ uniform randomly from \mathcal{D} .

 Construct latent variable model $p(\{H_i^t\}|\chi_n)$ as (5).

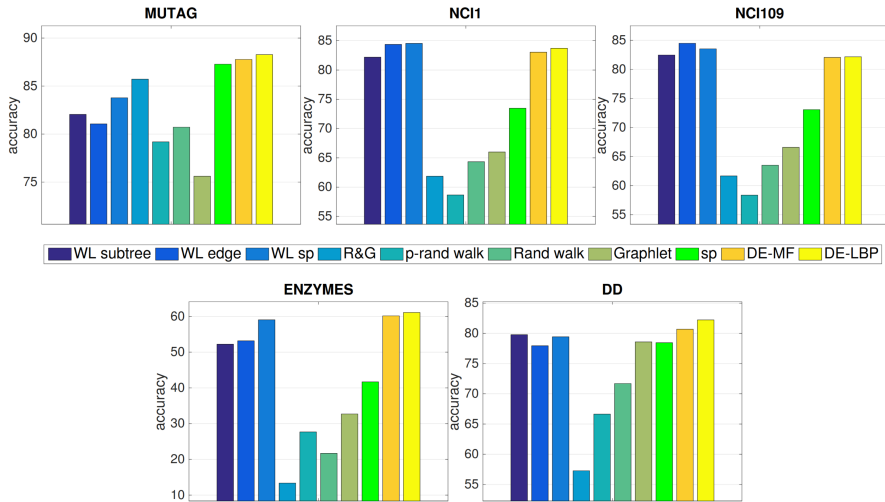
 Embed $p(\{H_i^t\}|\chi_n)$ as $\{\tilde{\mu}_i^n\}_{i \in \mathcal{V}_n}$ by Algorithm 1 or 2 with \mathbf{W}^{t-1} .

 Update $\mathbf{U}^t = \mathbf{U}^{t-1} + \lambda_t \nabla_{\mathbf{U}^{t-1}} l(f(\tilde{\mu}^n; \mathbf{U}^{t-1}), y_n)$.

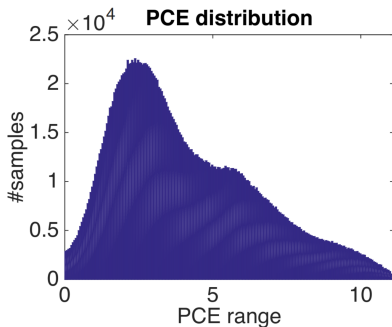
end for

return $\mathbf{U}^T = \{\mathbf{W}^T, \mathbf{u}^T\}$

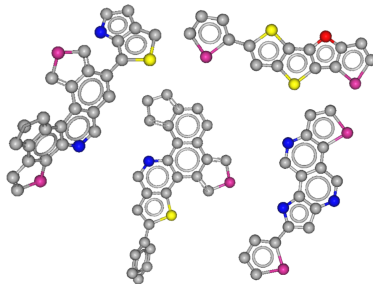
Graph Dataset Results



Harvard Clean Energy Project (CEP)



(a) PCE distribution



(b) Sample molecules

CEP Results

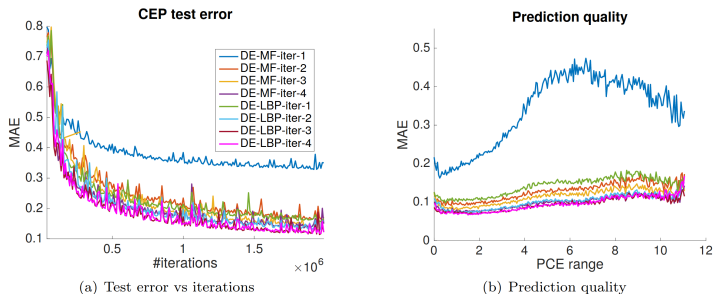


Figure 4: Details of training and prediction results for DE-MF and DE-LBP with different number of fixed point iterations.

	test MAE	test RMSE	# params
Mean Predictor	1.9864	2.4062	1
WL lv-3	0.1431	0.2040	1.6m
WL lv-6	0.0962	0.1367	1378m
DE-MF	0.0914	0.1250	0.1m
DE-LBP	0.0850	0.1174	0.1m

Table 3: Test prediction performance on CEP dataset. WL lv- k stands for Weisfeiler-lehman with degree k .

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- Fasshauer, *Positive Definite Kernels: Past, Present and Future*
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- Gormley and Eisner, *Structured Belief Propagation for NLP*
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- Görtler, et al. *A Visual Exploration of Gaussian Processes*