Kernel Embeddings, Meta Learning and Distributional Transfer

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DeepMind
07/06/2019

Outline

1. Preliminaries on Kernel Embeddings
2. Hyperparameter Learning for Distributional Transfer
3. Meta Learning for Conditional Density Estimation

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2. Hyperparameter Learning for Distributional Transfer
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Kernels and Reproducing Kernel Hilbert Spaces

- Kernel function is as an *inner product of features*: any function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ for which there exists a Hilbert space $\mathcal{H}$ and a map $\varphi : \mathcal{X} \to \mathcal{H}$ s.t. $k(x, x') = \langle \varphi(x), \varphi(x') \rangle_{\mathcal{H}}$ for all $x, x' \in \mathcal{X}$.
- Kernel method is any method that endows a generic abstract domain $\mathcal{X}$ with an inner product structure induced by some feature transformation.
- Feature map φ and feature space $\mathcal{H}$ are not unique, but the inner product structure (kernel) is.

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Definition ([Aronszajn, 1950; Berlinet & Thomas-Agnan, 2004])

Let $\mathcal{X}$ be a non-empty set and $\mathcal{H}$ be a Hilbert space of real-valued functions defined on $\mathcal{X}$. A function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is called *a reproducing kernel* of $\mathcal{H}$ if:

1. $\forall x \in \mathcal{X}, \quad k(\cdot, x) \in \mathcal{H}$, and
2. $\forall x \in \mathcal{X}, \forall f \in \mathcal{H}, \quad \langle f, k(\cdot, x) \rangle_{\mathcal{H}} = f(x)$.

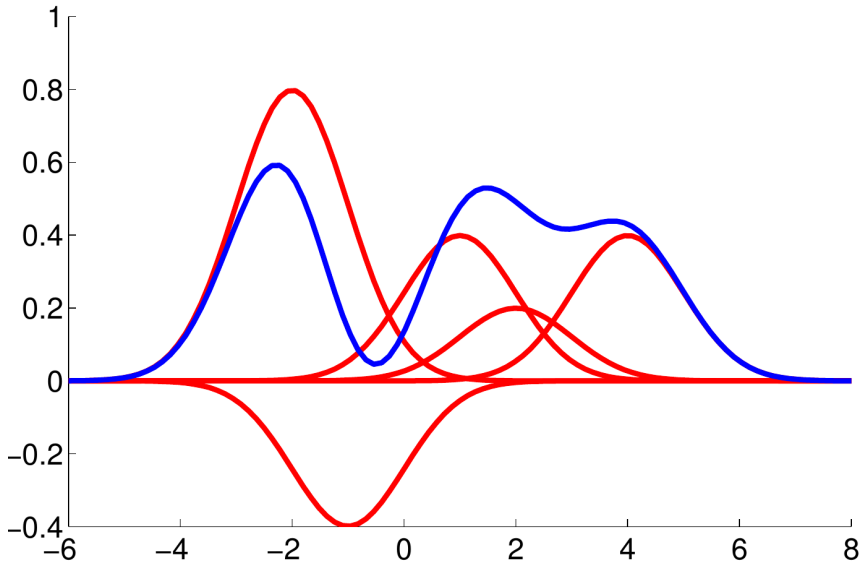
If $\mathcal{H}_k$ has a reproducing kernel, it is said to be a *reproducing kernel Hilbert space*.

In particular, for any $x, y \in \mathcal{X}$, $k(x, y) = \langle k(\cdot, y), k(\cdot, x) \rangle_{\mathcal{H}} = \langle k(\cdot, x), k(\cdot, y) \rangle_{\mathcal{H}}$. Thus, RKHS serves as a *canonical feature space* with *canonical feature map* $x \mapsto k(\cdot, x)$.

Kernels and Reproducing Kernel Hilbert Spaces

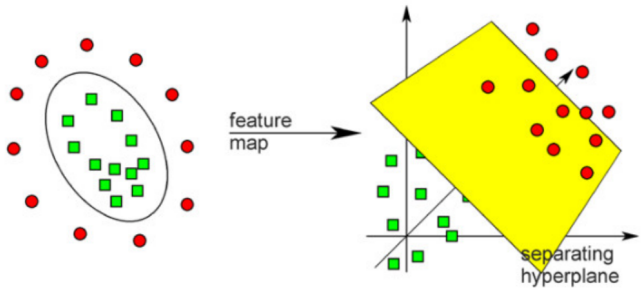
- Equivalent definition: Hilbert space of functions where evaluations $f \mapsto f(x)$ at any given point x are continuous maps (norm convergence implies pointwise convergence).
- Moore-Aronszajn Theorem: *every positive semidefinite* $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a reproducing kernel and has a *unique* RKHS $\mathcal{H}_k$.
- Example: Gaussian RBF kernel $k(x, x') = \exp\left(-\frac{1}{2\gamma^2}\left\|x - x'\right\|^2\right)$ has an infinite-dimensional $\mathcal{H}$ with elements $h(x) = \sum_{i=1}^{n} \alpha_i k(x_i, x)$ and their limits which give completion with respect to the inner product

$$\left\langle \sum_{i=1}^{n} \alpha_i k(x_i, \cdot), \sum_{j=1}^{m} \beta_j k(y_j, \cdot) \right\rangle = \sum_{i=1}^{n} \sum_{j=1}^{m} \alpha_i \beta_j k(x_i, y_j).$$



Kernel Trick and Kernel Mean Trick

- implicit feature map $x \mapsto k(\cdot, x) \in \mathcal{H}_k$
  replaces $x \mapsto [\phi_1(x), \ldots, \phi_s(x)] \in \mathbb{R}^s$
- $\langle k(\cdot, x), k(\cdot, y) \rangle_{\mathcal{H}_k} = k(x, y)$
  inner products readily available
  - nonlinear decision boundaries, nonlinear regression functions, learning on non-Euclidean/structured data



[Cortes & Vapnik, 1995; Schölkopf & Smola, 2001]

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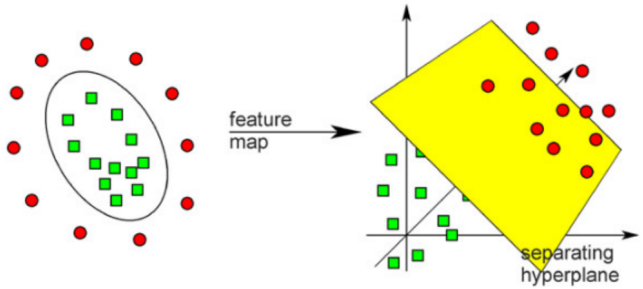
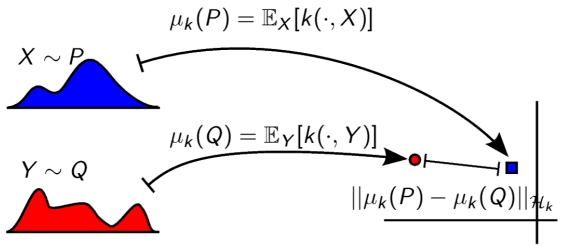


[Cortes & Vapnik, 1995; Schölkopf & Smola, 2001]

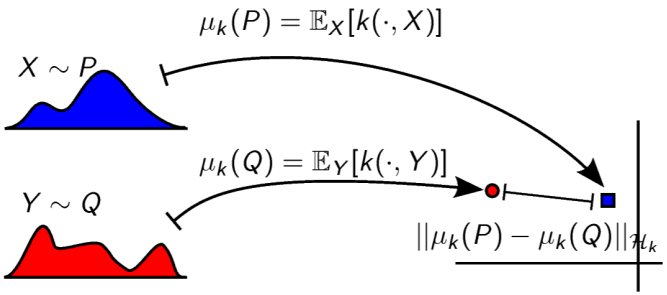
- **RKHS embedding**: implicit feature mean
  [Smola et al, 2007; Sriperumbudur et al, 2010; Muandet et al, 2017]
  $P \mapsto \mu_k(P) = \mathbb{E}_{X \sim P} k(\cdot, X) \in \mathcal{H}_k$
  replaces $P \mapsto [\mathbb{E}\phi_1(X), \dots, \mathbb{E}\phi_s(X)] \in \mathbb{R}^s$
- $\langle \mu_k(P), \mu_k(Q) \rangle_{\mathcal{H}_k} = \mathbb{E}_{X \sim P, Y \sim Q} k(X, Y)$
  inner products easy to estimate
  - nonparametric two-sample, independence, conditional independence, interaction testing, learning on distributions

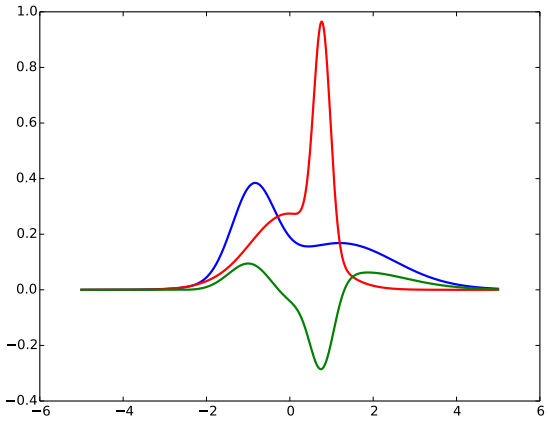


[Gretton et al, 2005; Gretton et al, 2006; Fukumizu et al, 2007; DS et al, 2013; Muandet et al, 2012; Szabo et al, 2015]

Maximum Mean Discrepancy

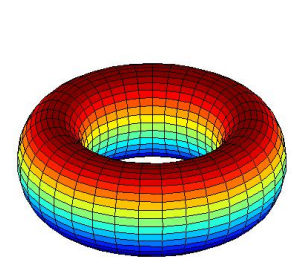
- **Maximum Mean Discrepancy (MMD)** [Borgwardt et al, 2006; Gretton et al, 2007] between P and Q:

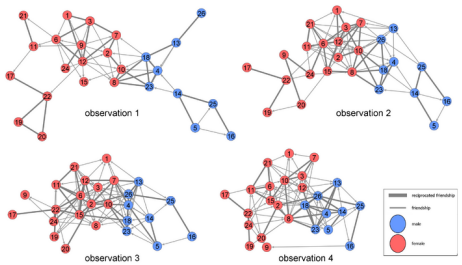




$$\mathrm{MMD}_k(P, Q) = \|\mu_k(P) - \mu_k(Q)\|_{\mathcal{H}_k} = \sup_{f \in \mathcal{H}_k : \|f\|_{\mathcal{H}_k} \leq 1} |\mathbb{E} f(X) - \mathbb{E} f(Y)|$$

- Characteristic kernels: $\mathrm{MMD}_k(P, Q) = 0$ iff $P = Q$ (also metrizes weak* [Sriperumbudur,2010]).
  - Gaussian RBF $\exp(-\frac{1}{2\sigma^2}\|x - x'\|_2^2)$, Matérn family, inverse multiquadrics.
- Can encode structural properties in the data: kernels on non-Euclidean domains, networks, images, text...





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Some uses of MMD

within-sample average similarity

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between-sample average similarity

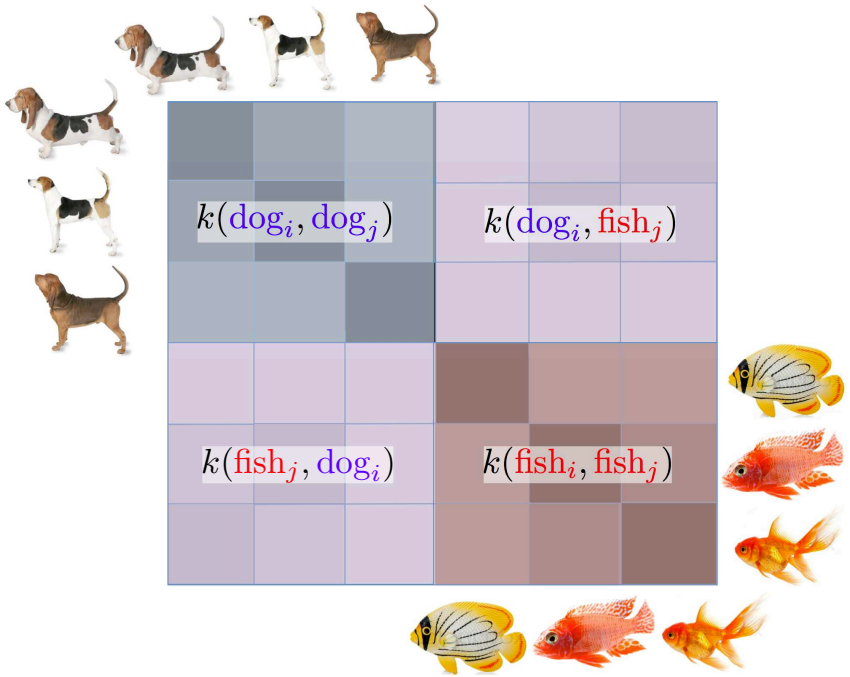

Figure by Arthur Gretton

MMD has been applied to:

- two-sample tests and independence tests (on graphs, text, audio...) [Gretton et al, 2009, Gretton et al, 2012]
- model criticism and interpretability [Lloyd & Ghahramani, 2015; Kim, Khanna & Koyejo, 2016]
- analysis of Bayesian quadrature [Briol et al, 2018]
- ABC summary statistics [Park, Jitkrittum & DS, 2015; Mitrovic, DS & Teh, 2016]
- summarising streaming data [Paige, DS & Wood, 2016]
- traversal of manifolds learned by convolutional nets [Gardner et al, 2015]
- MMD-GAN: training deep generative models [Dziugaite, Roy & Ghahramani, 2015; Sutherland et al, 2017; Li et al, 2017]

$$\text{MMD}_k^2(P, Q) = \mathbb{E}_{X, X' \overset{i.i.d.}{\sim} P} k(X, X') + \mathbb{E}_{Y, Y' \overset{i.i.d.}{\sim} Q} k(Y, Y') - 2\mathbb{E}_{X \sim P, Y \sim Q} k(X, Y).$$

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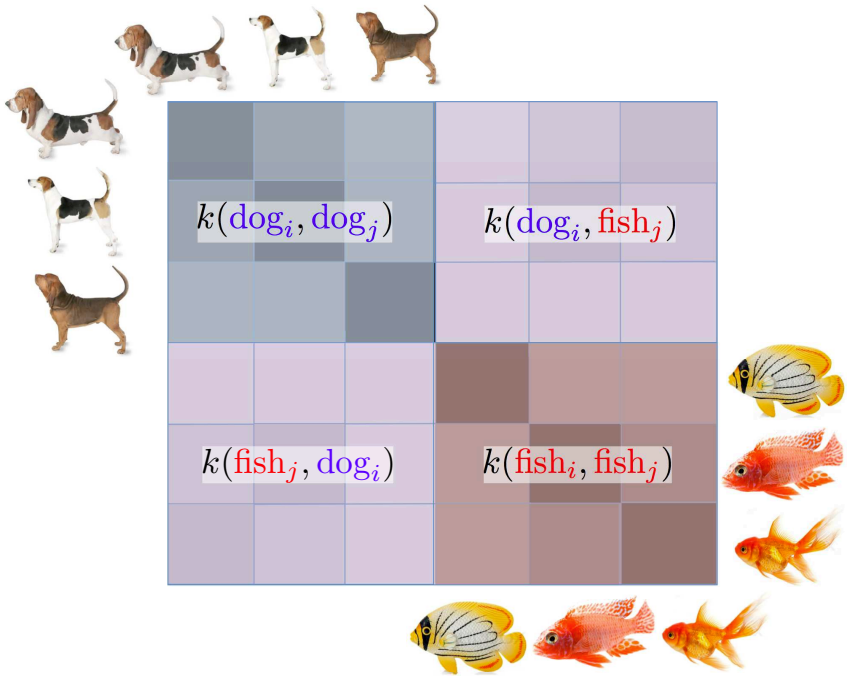

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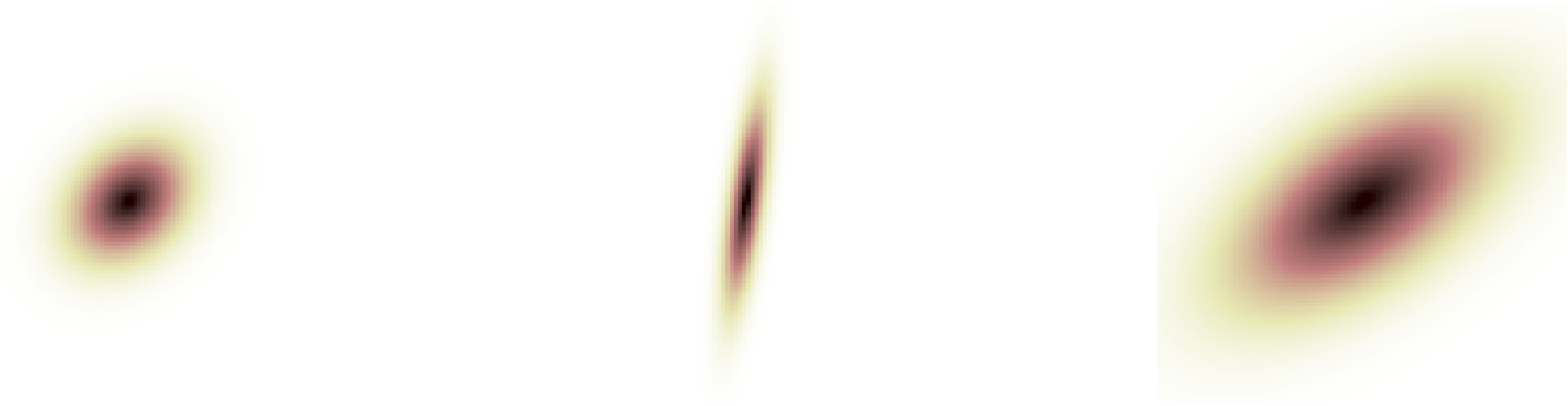
$$\widehat{\text{MMD}}_k^2(P, Q) = \frac{1}{n_x(n_x-1)} \sum_{i \neq j} k(X_i, X_j) + \frac{1}{n_y(n_y-1)} \sum_{i \neq j} k(Y_i, Y_j) - \frac{2}{n_x n_y} \sum_{i,j} k(X_i, Y_j).$$

Kernel Embeddings for Learning on Distribution Inputs



- Labels $y_i = f(P_i)$ but observe only $\{x_i^j\}_{j=1}^{N_i} \sim P_i$.
- The goal: build a predictive model $\hat{y}_\star = f(\{x_\star^j\}_{j=1}^{N_\star})$ for a new sample $\{x_\star^j\}_{j=1}^{N_\star} \sim P_\star$.
- Represent each sample with the empirical mean embedding $\hat{\mu}_i = \frac{1}{N_i} \sum_{j=1}^{N_i} k(\cdot, x_i^j) \in \mathcal{H}_k$.
- Now can use the induced inner product structure on empirical measures to build a regression model:
  - Linear kernel on the RKHS: $K\left(\hat{\mu}_i, \hat{\mu}_j\right) = \langle \hat{\mu}_i, \hat{\mu}_j \rangle_{\mathcal{H}_k} = \frac{1}{N_i N_j} \sum_{r,s} k(x_i^r, x_j^s)$
  - Gaussian kernel on the RKHS: $K\left(\hat{\mu}_i, \hat{\mu}_j\right) = \exp(-\gamma \|\hat{\mu}_i - \hat{\mu}_j\|_{\mathcal{H}_k}^2) = \exp\left(-\gamma \widehat{\mathrm{MMD}}_k^2\left(P_i, P_j\right)\right)$

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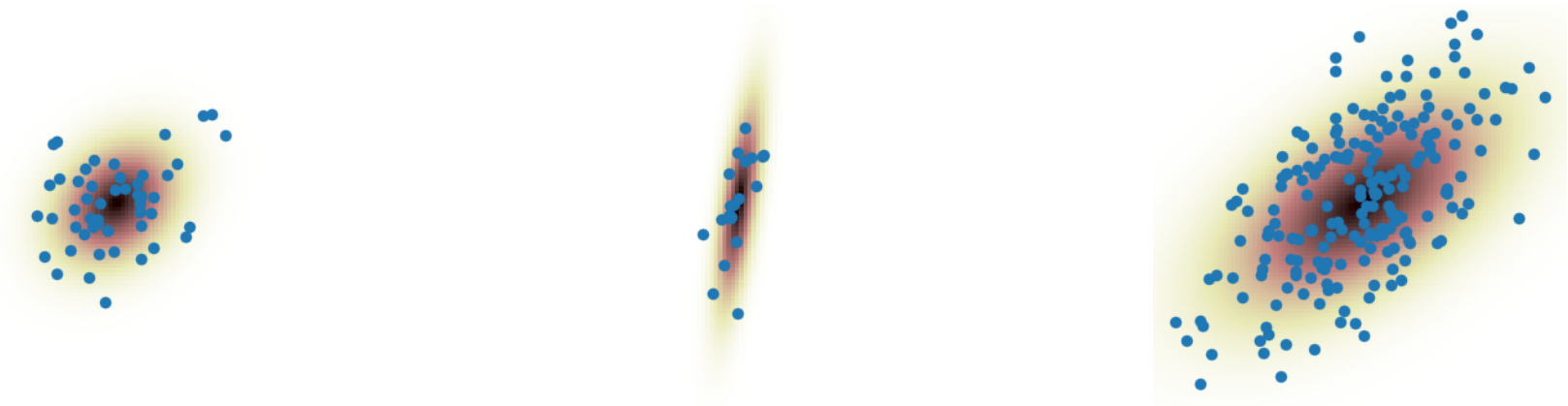

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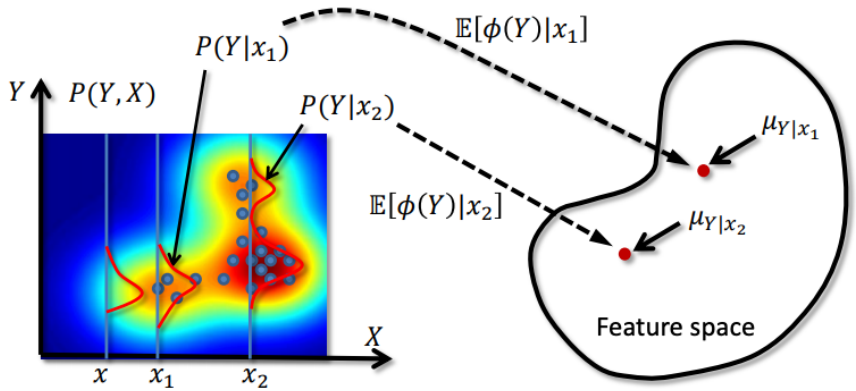
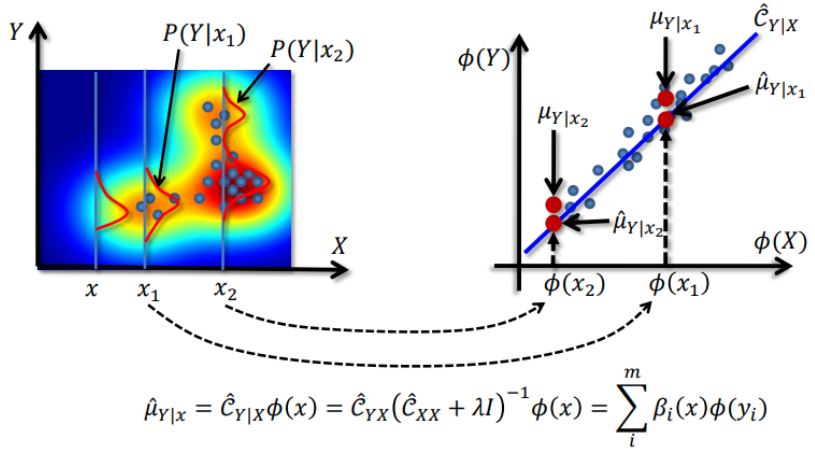
Conditional Embeddings

Consider a joint distribution P_{XY} over the random variables (X, Y) taking values in $\mathcal{X} \times \mathcal{Y}$. The conditional mean embedding (CME) of $Y|X = x$ is defined as:

$$\mu_{Y|X=x} := \mathbb{E}_{Y|X=x}[k_y(\cdot, Y)] = \int_{\mathcal{Y}} k_y(\cdot, y) dP(y|x) \in \mathcal{H}_{k_y}$$





To model conditional embeddings as functions of x, we associate them with a linear operator $\mathcal{C}_{Y|X} : \mathcal{H}_{k_x} \to \mathcal{H}_{k_y}$, which satisfies

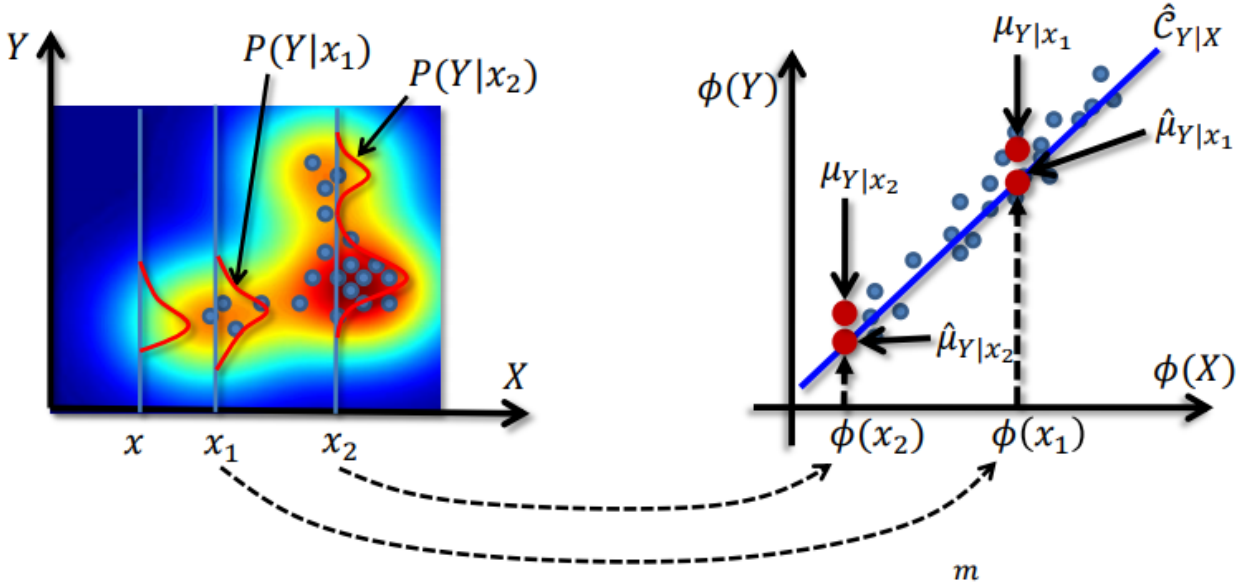
$$\mu_{Y|X=x} = \mathcal{C}_{Y|X} k_x(\cdot, x).$$

Estimation of Conditional Embeddings

Considering finite-dimensional feature maps ϕ_x and ϕ_y, the finite sample estimator of $\mathcal{C}_{Y|X}$ based on dataset $\{(x_i, y_i)\}_{i=1}^n$ is given by feature-to-feature regression coefficients:

$$\widehat{\mathcal{C}}_{Y|X} = \Phi_y (K_{xx} + \lambda I)^{-1} \Phi_x^T,$$

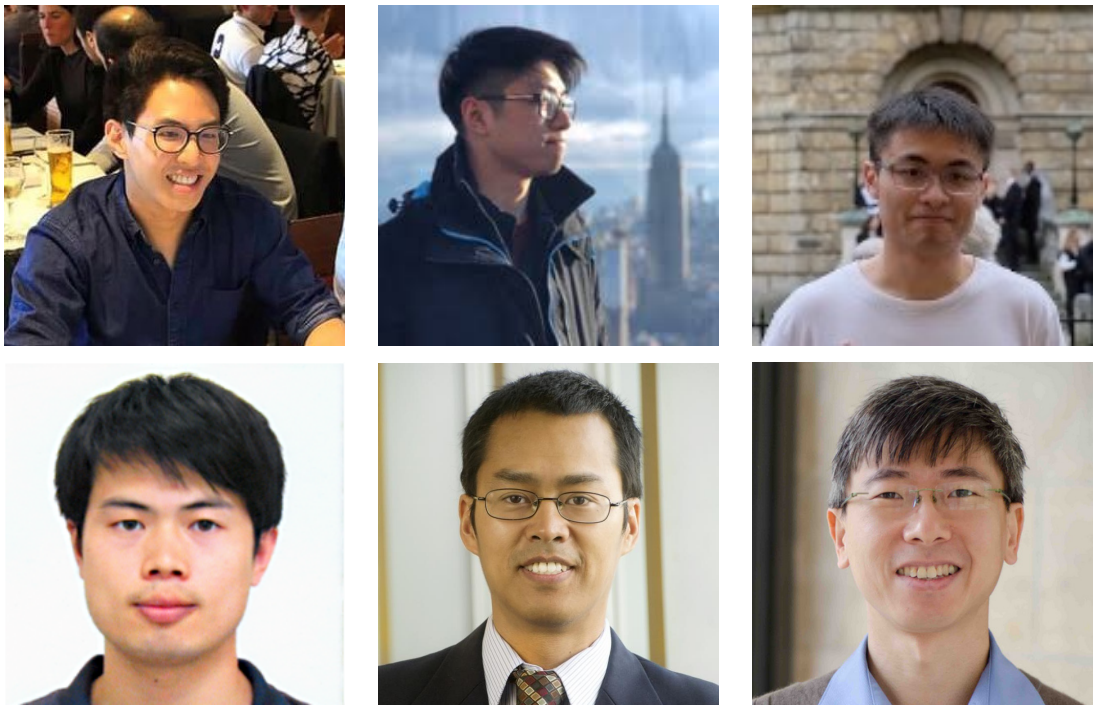
where $\Phi_y := (\phi_y(y_1), \ldots, \phi_y(y_n))$ and $\Phi_x := (\phi_x(x_1), \ldots, \phi_x(x_n))$ are the feature matrices, $K_{xx} := \Phi_x \Phi_x^T$ is the kernel matrix with entries $[K_{xx}]_{i,j} = k_x(x_i, x_j) := \langle \phi_x(x_i), \phi_x(x_j) \rangle$, and $\lambda > 0$ is a regularization parameter of feature-to-feature regression.



$$\hat{\mu}_{Y|x} = \hat{\mathcal{C}}_{Y|X}\phi(x) = \hat{\mathcal{C}}_{YX}\left(\hat{\mathcal{C}}_{XX} + \lambda I\right)^{-1}\phi(x) = \sum_i^m \beta_i(x)\phi(y_i)$$

Kernel Embeddings for Meta Learning

- Ho Chung Leon Law, Peilin Zhao, Lucian Chan, Junzhou Huang, and DS. **Hyperparameter Learning via Distributional Transfer**. *ArXiv e-prints:1810.06305*, 2018.
- Jean-Francois Ton, Lucian Chan, Yee Whye Teh, and DS. **Noise Contrastive Meta Learning for Conditional Density Estimation using Kernel Mean Embeddings**. *ArXiv e-prints:1906.02236*, 2019.



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Towards End-to-End Learning

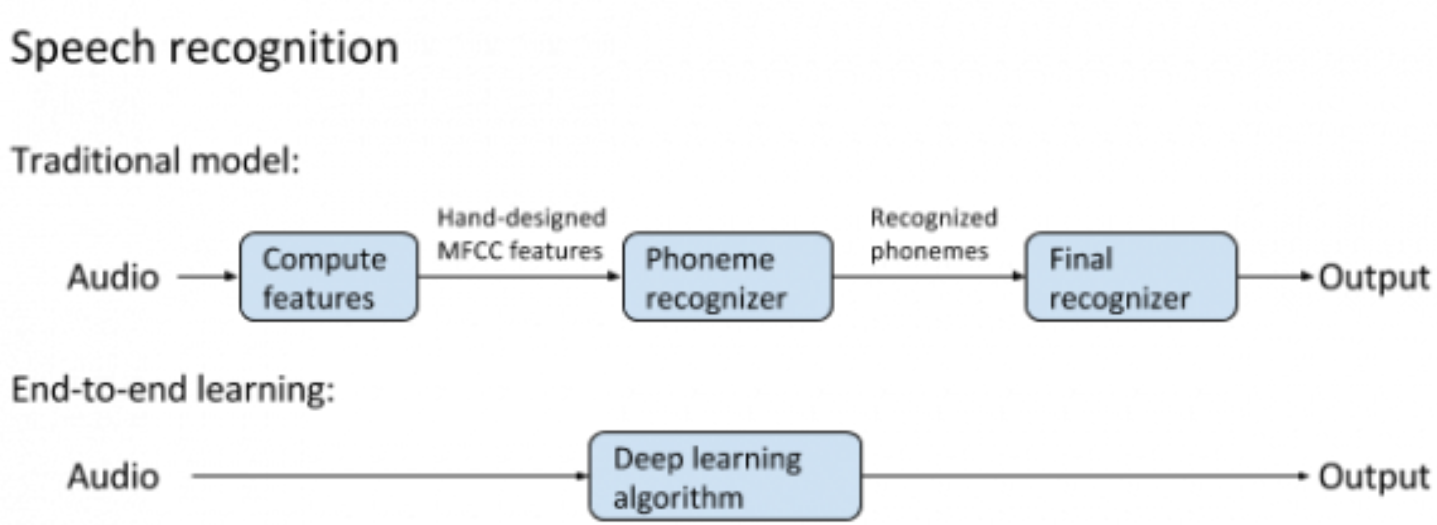
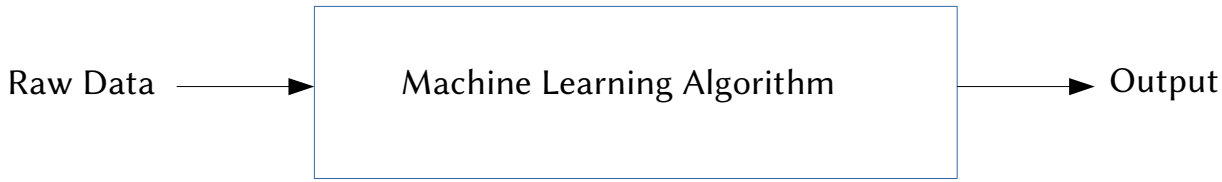


figure from https://blog.easysol.net/building-ai-applications/

Towards End-to-End Learning



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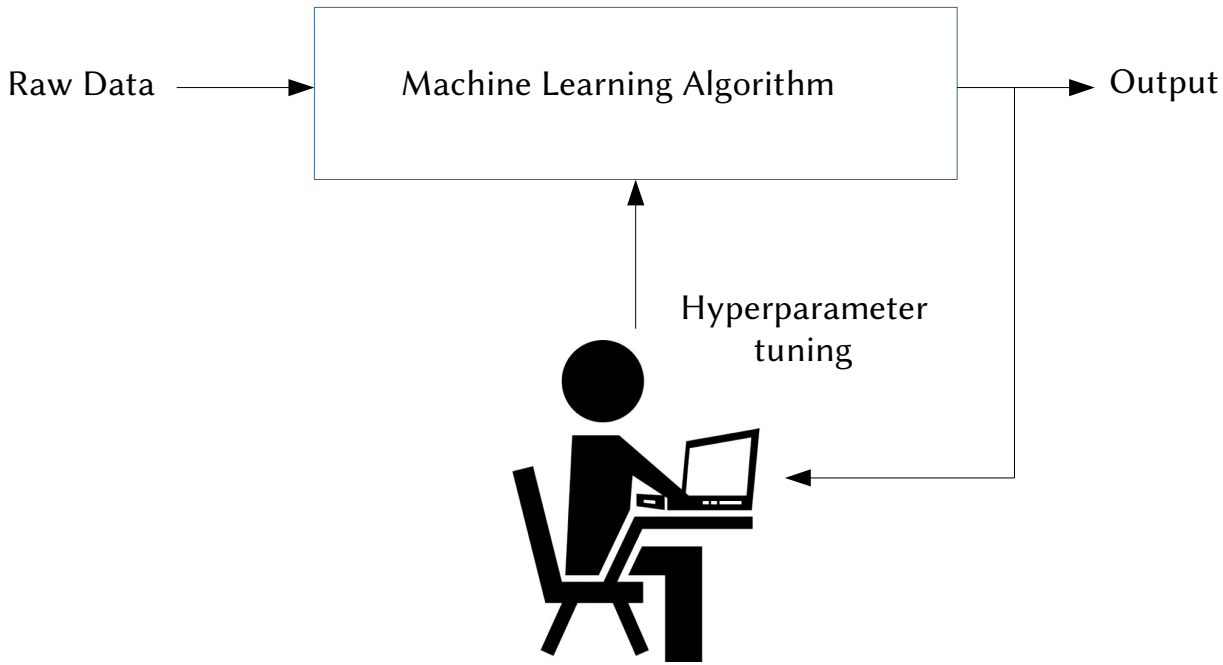

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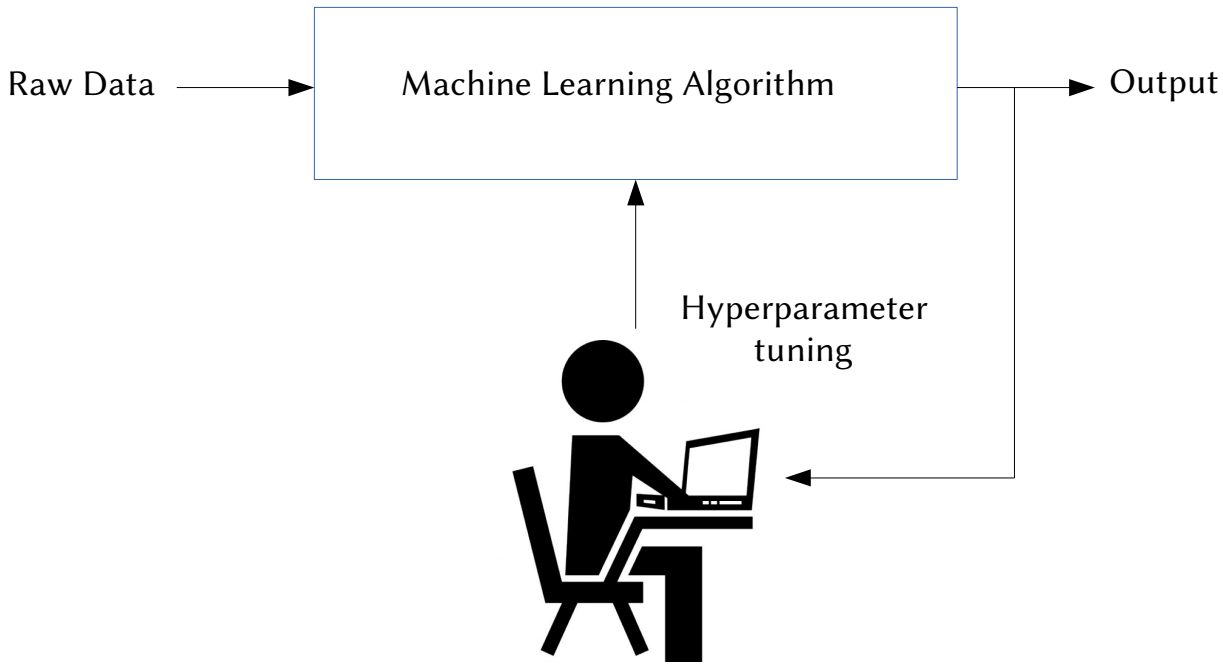


Grid search, random search, trial-and-error, graduate student descent,...

Optimizing "black-box" functions

Most machine learning models have hyperparameters to be tuned:

- *deep neural networks*: number of layers, regularization parameters, dropout parameters, layer size, batch size, learning rate, momentum,...
- *kernel methods*: kernel lengthscale parameters, regularization parameters, number and type of random features,...
- *variational methods*: prior parameters, variational family, choice of divergence, type of the variational bound, batch size, learning rate,...

An objective function: a measure of generalization performance for a given set of hyperparameters obtained using held-out dataset or cross-validation.

Optimizing "black-box" functions

We are interested in optimizing a 'well behaved' function $f : \Theta \to \mathbb{R}$ over some bounded domain $\Theta \subset \mathbb{R}^d$, i.e. in solving

$$\theta_\star = \operatorname{argmin}_{\theta \in \Theta} f(\theta).$$

However, f is not known explicitly, i.e. it is a black-box function and we can only ever obtain noisy and expensive evaluations of f.

Goal: Find θ such that $f(\theta) \approx f(\theta_\star)$ while minimizing the number of evaluations of f.

Probabilistic model for the objective f

Assuming that f is well behaved, we build a surrogate probabilistic model for it (Gaussian Process).

1. Compute the posterior predictive distribution of f using all evaluations so far.
2. Optimize a cheap proxy / acquisiton function instead of f which takes into account predicted values of f at new points as well as the *uncertainty in those predictions*: this proxy is typically much cheaper to evaluate than the actual objective f.
3. Evaluate the objective f at the optimum of the proxy and go to 1.

The proxy / acquisiton function should balance exploration against exploitation.

Surrogate Gaussian Process model

Assume that the *noise* in the evaluations of the black-box function is i.i.d. $\mathcal{N}\left(0, \tau^2\right)$. Having evaluated the objective at locations $\boldsymbol{\theta} = \{\theta_i\}_{i=1}^m$, we denote the observed values by $\mathbf{y} = [y_1, \ldots, y_m]^\top$ and the true function values by $\mathbf{f} = [f(\theta_1), \ldots, f(\theta_m)]^\top$. Then

$$\mathbf{f} \sim \mathcal{N}(0, \mathbf{K}),$$
$$\mathbf{y}|\mathbf{f} \sim \mathcal{N}(\mathbf{f}, \tau^2 I).$$

GP model gives the *posterior predictive mean* $\mu(\theta)$ and the *posterior predictive variance* $\sigma^2(\theta) = \kappa(\theta, \theta)$ at any new location θ, i.e.

$$f(\theta)|\mathbf{y} \sim \mathcal{N}\left(\mu(\theta), \kappa(\theta, \theta)\right),$$

where

$$\begin{aligned} \mu(\theta) &= \mathbf{k}_{\theta\boldsymbol{\theta}}(\mathbf{K} + \tau^2 I)^{-1}\mathbf{y}, \\ \kappa(\theta, \theta) &= k(\theta, \theta) - \mathbf{k}_{\theta\boldsymbol{\theta}}(\mathbf{K} + \tau^2 I)^{-1}\mathbf{k}_{\boldsymbol{\theta}\theta} \end{aligned}$$

- Exploitation: seeking locations with low posterior mean $\mu(\theta)$,
- Exploration: seeking locations with high posterior variance $\kappa(\theta, \theta)$.

Acquisition functions

- GP-LCB. "optimism in the phase of uncertainty"; minimize the lower $(1-\alpha)$-credible bound of the posterior of the unknown function values $f(\theta)$, i.e.

$$\alpha_{LCB}(\theta) = \mu(\theta) - z_{1-\alpha}\sigma(\theta),$$

  where $z_{1-\alpha} = \Phi^{-1}(1-\alpha)$ is the desired quantile of the standard normal distibution.

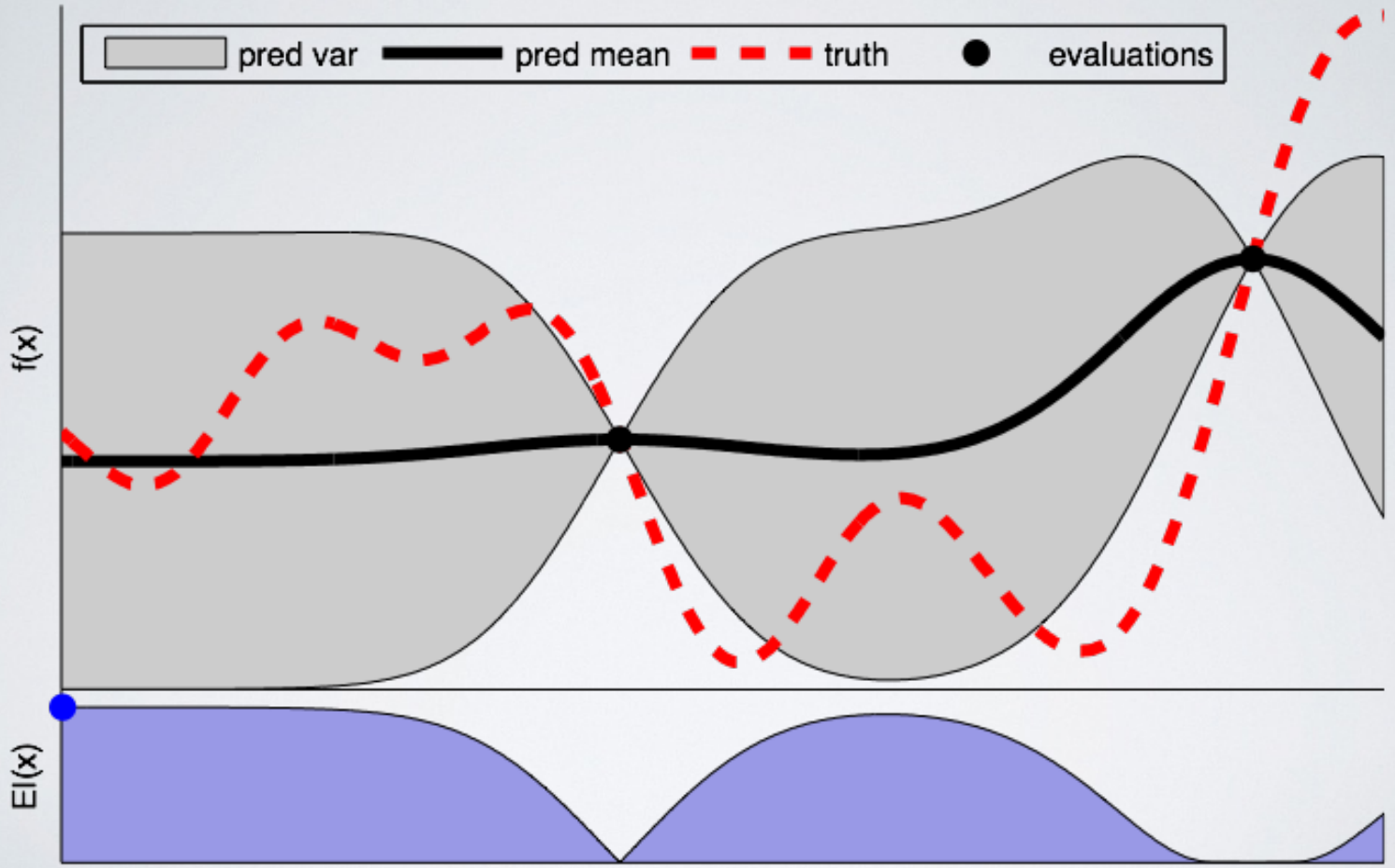
- PI (probability of improvement). $\tilde{\theta}$: the optimal location so far, $\tilde{y}$: the observed minimum. Let $u(\theta) = \mathbf{1}\{f(\theta) < \tilde{y}\}$,

$$\alpha_{PI}(\theta) = \mathbb{E}[u(\theta)|\mathcal{D}] = \Phi(\gamma(\theta)), \quad \gamma(\theta) = \frac{\tilde{y} - \mu(\theta)}{\sigma(\theta)}$$

- EI (expected improvement). Let $u(\theta) = \max(0, \tilde{y} - f(\theta))$

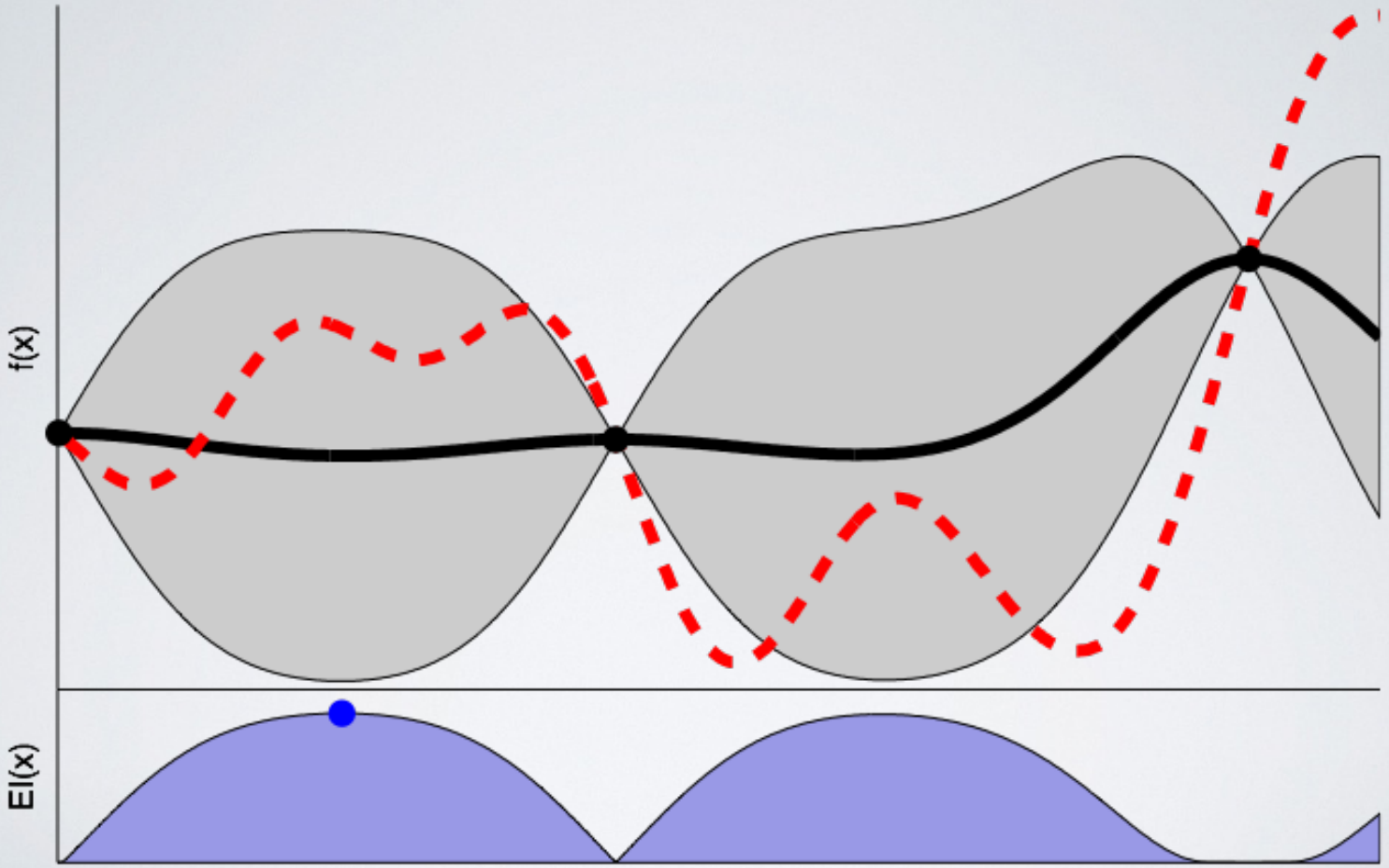
$$\alpha_{EI}(\theta) = \mathbb{E}[u(\theta)|\mathcal{D}] = \sigma(\theta)(\gamma(\theta)\Phi(\gamma(\theta)) + \phi(\gamma(\theta))).$$

Illustrating Bayesian Optimization



figures from *A Tutorial on Bayesian Optimization for Machine Learning* by Ryan Adams

Illustrating Bayesian Optimization



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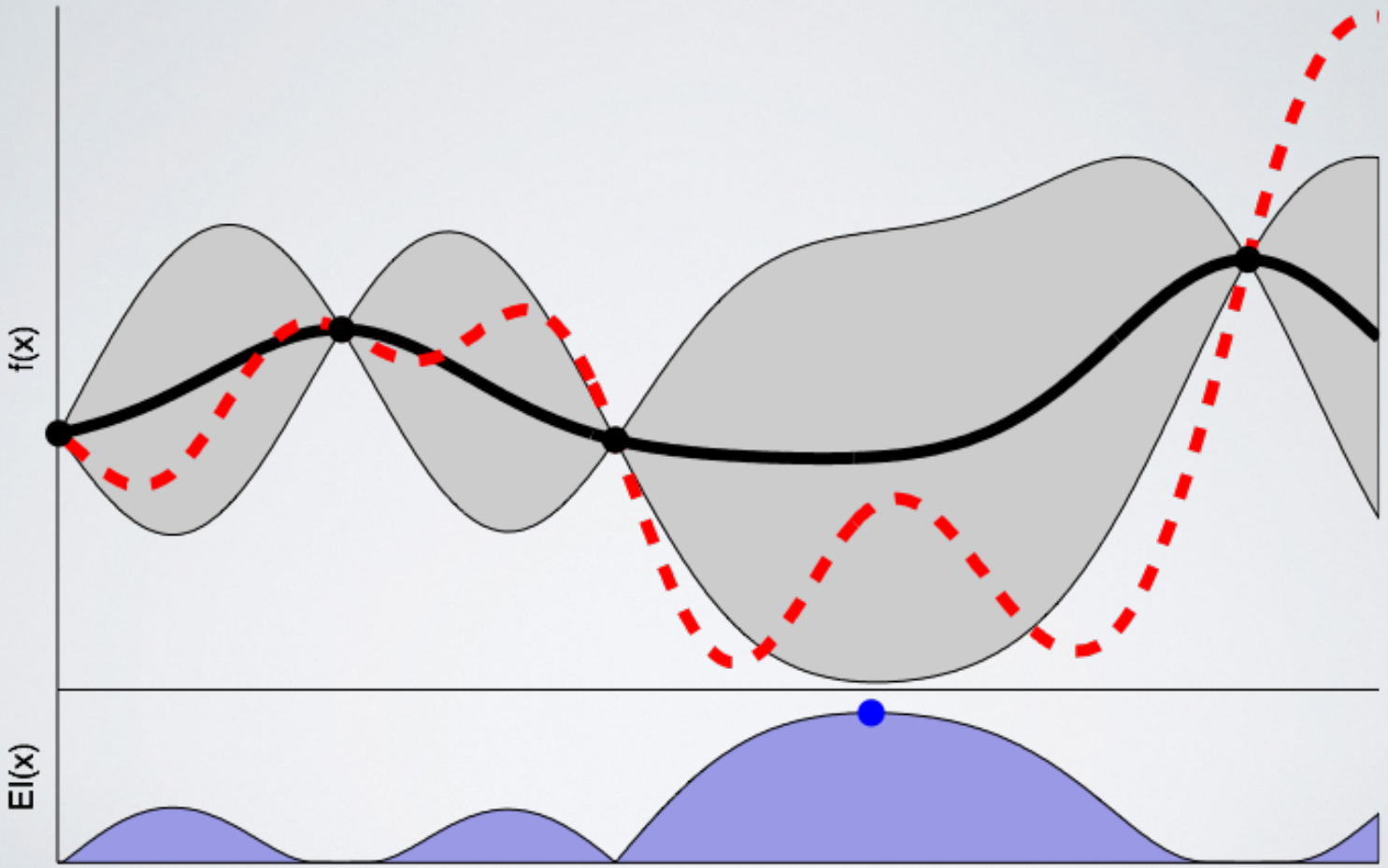

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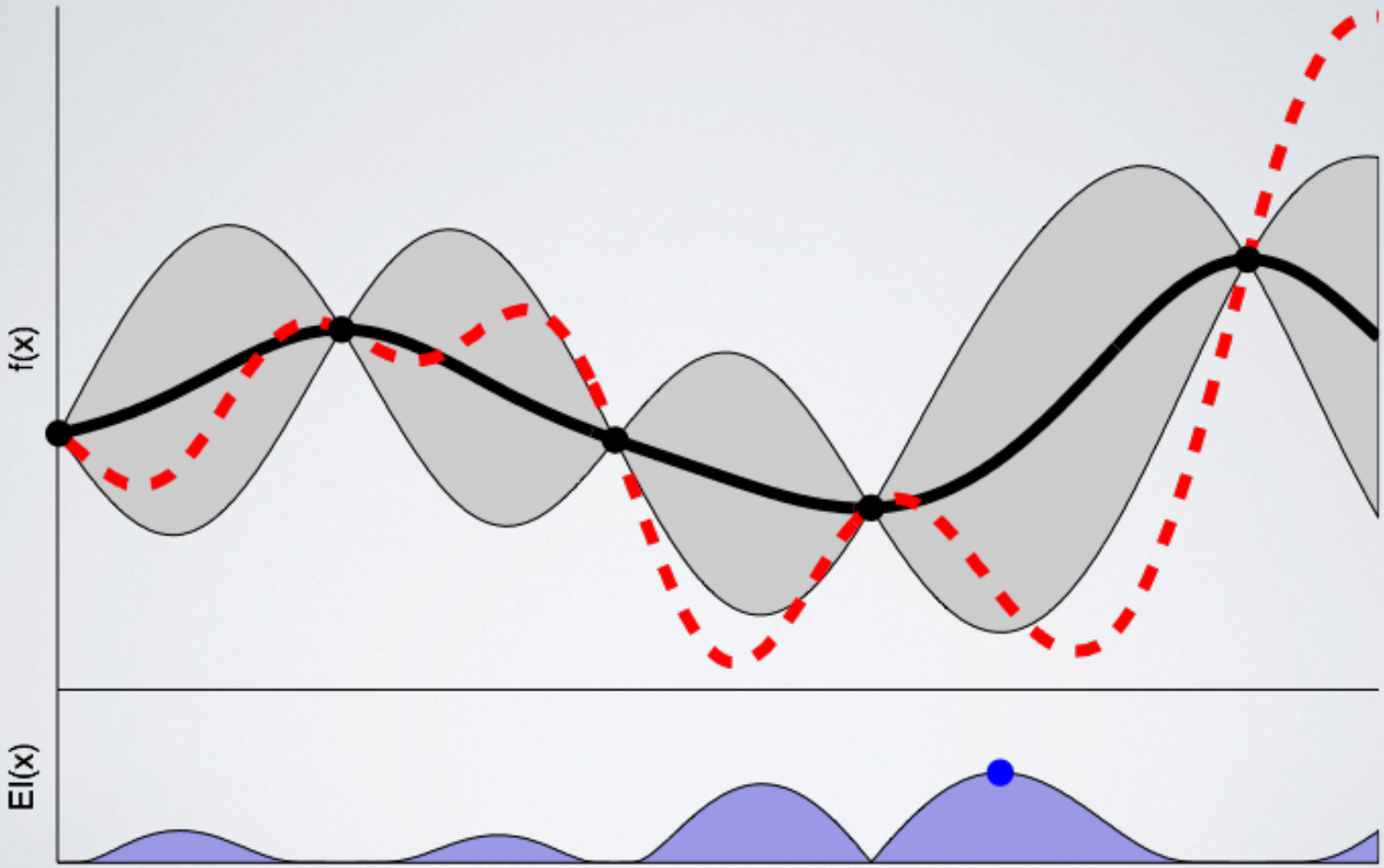

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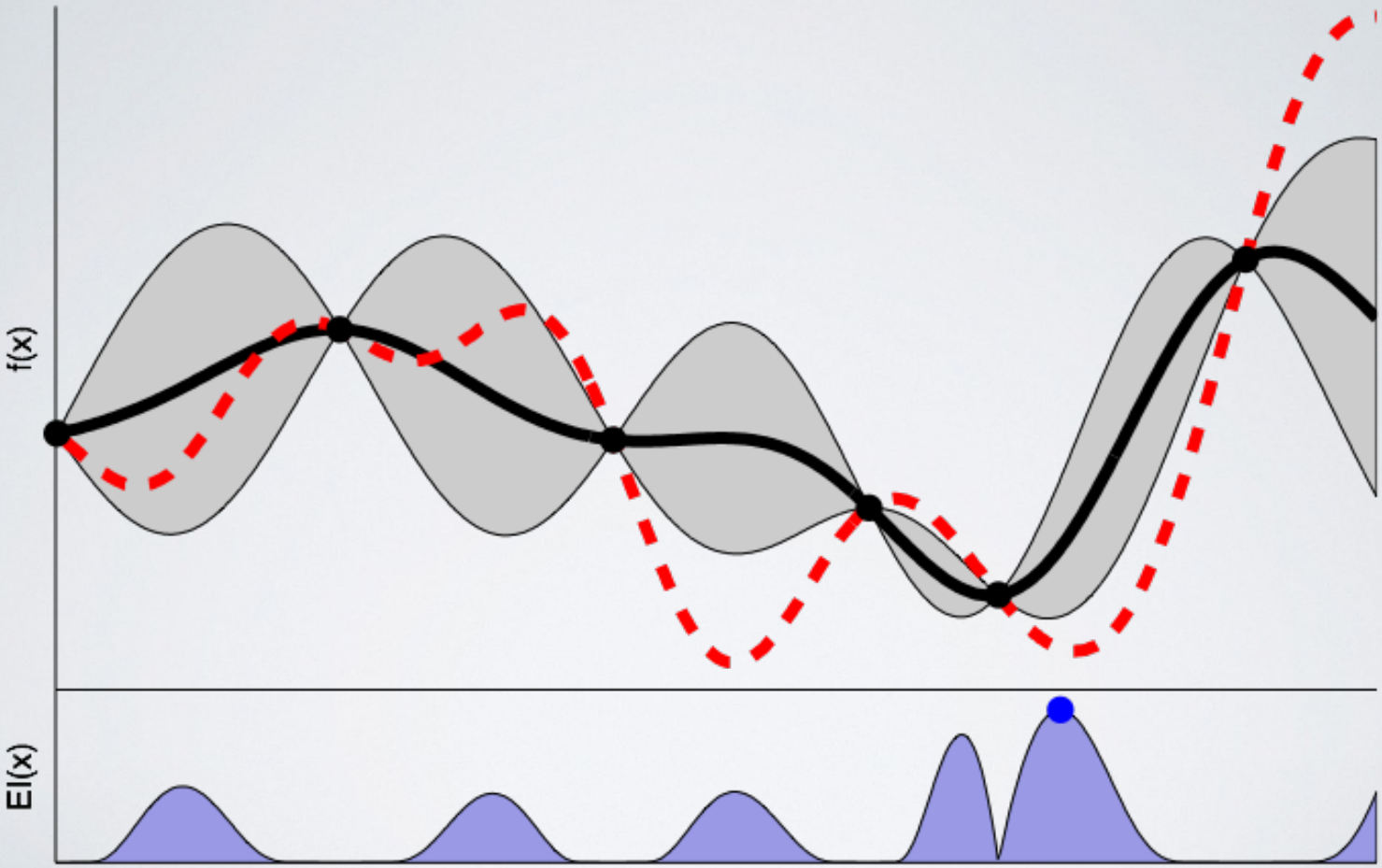

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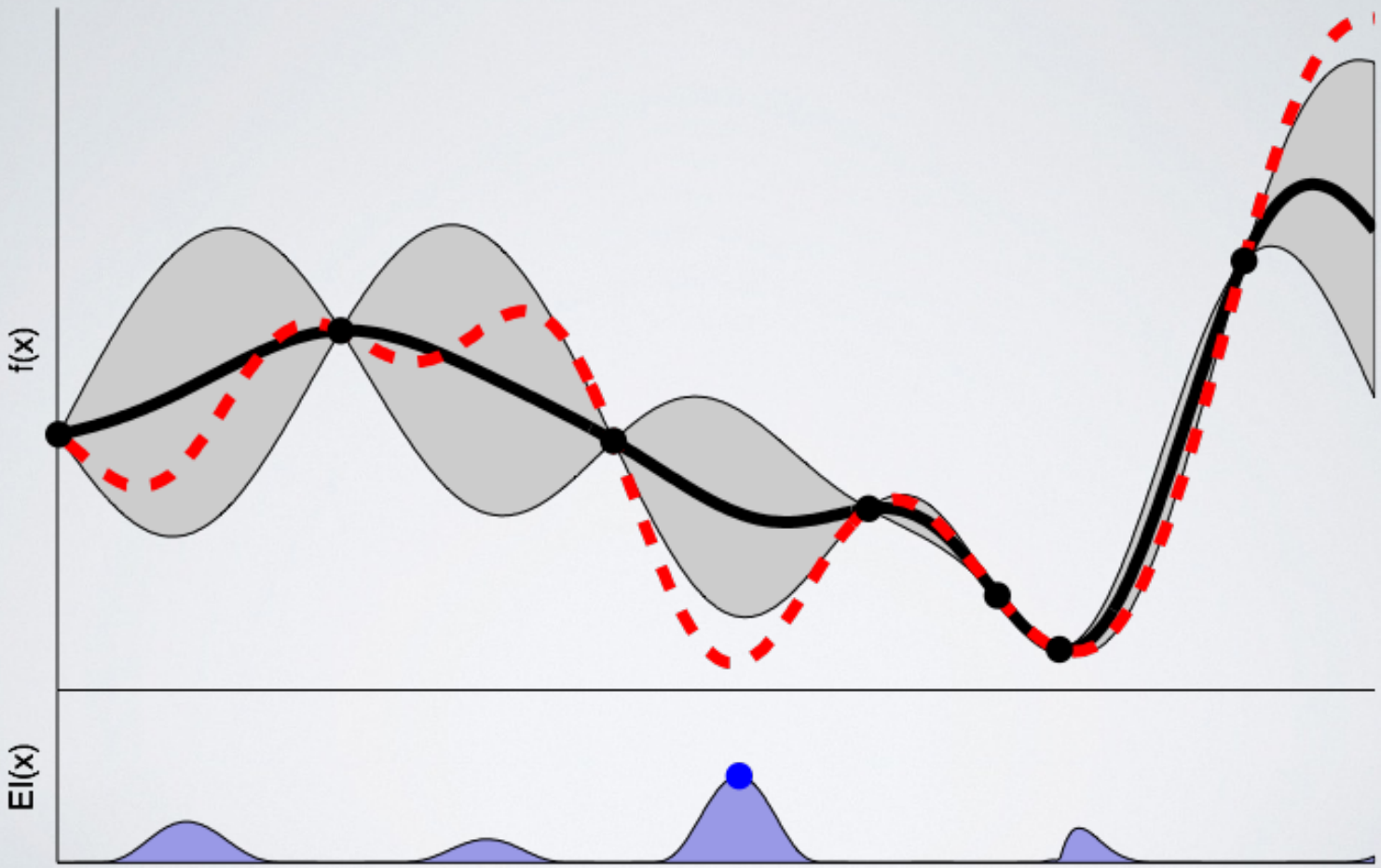

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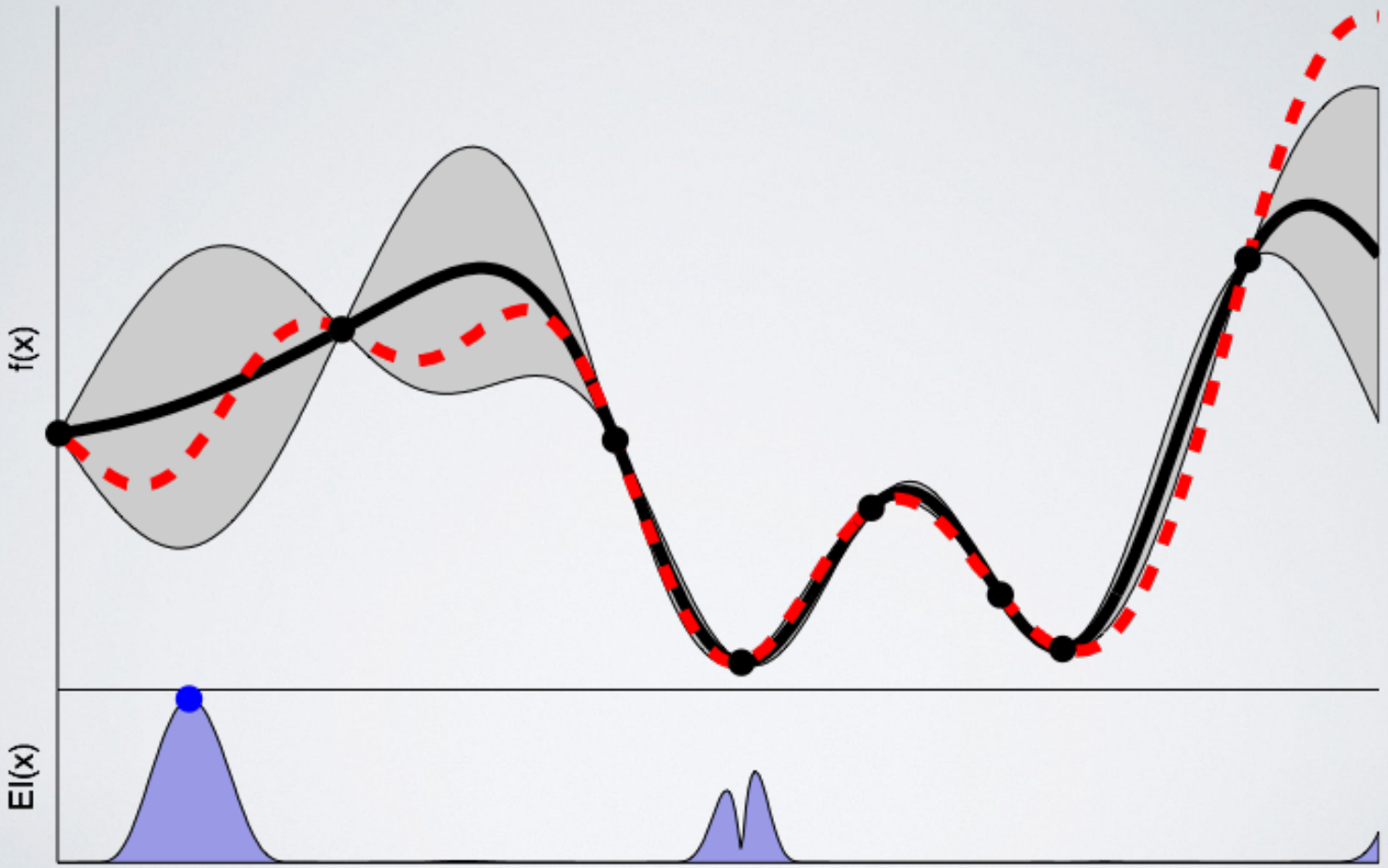

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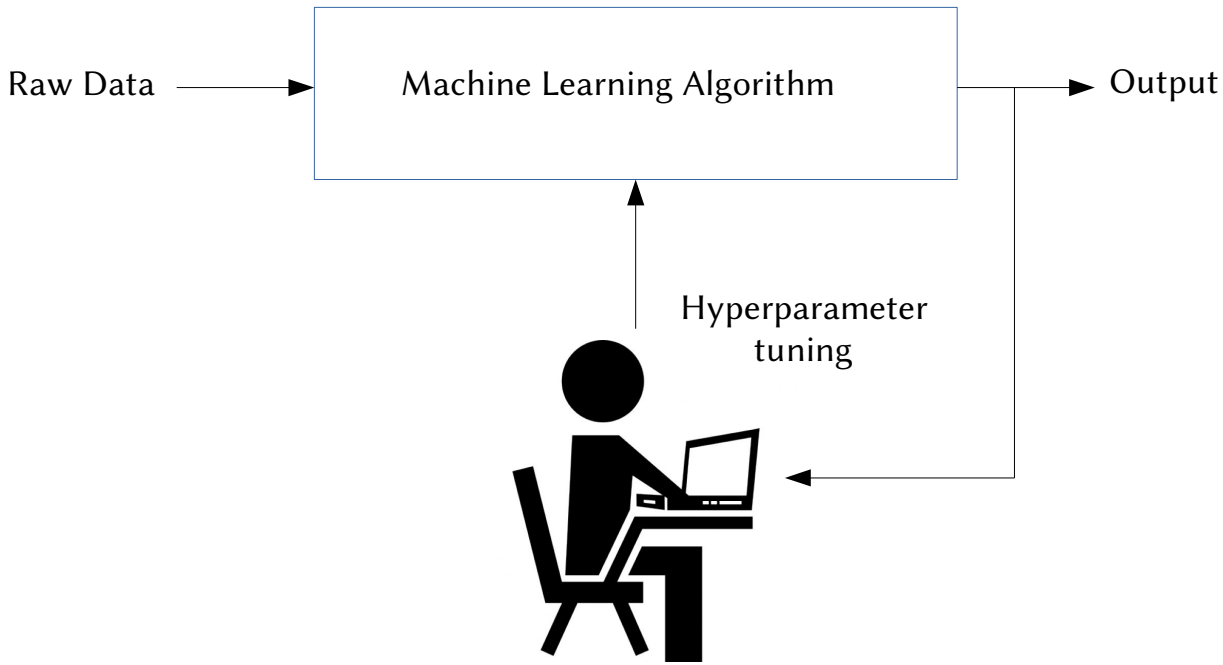
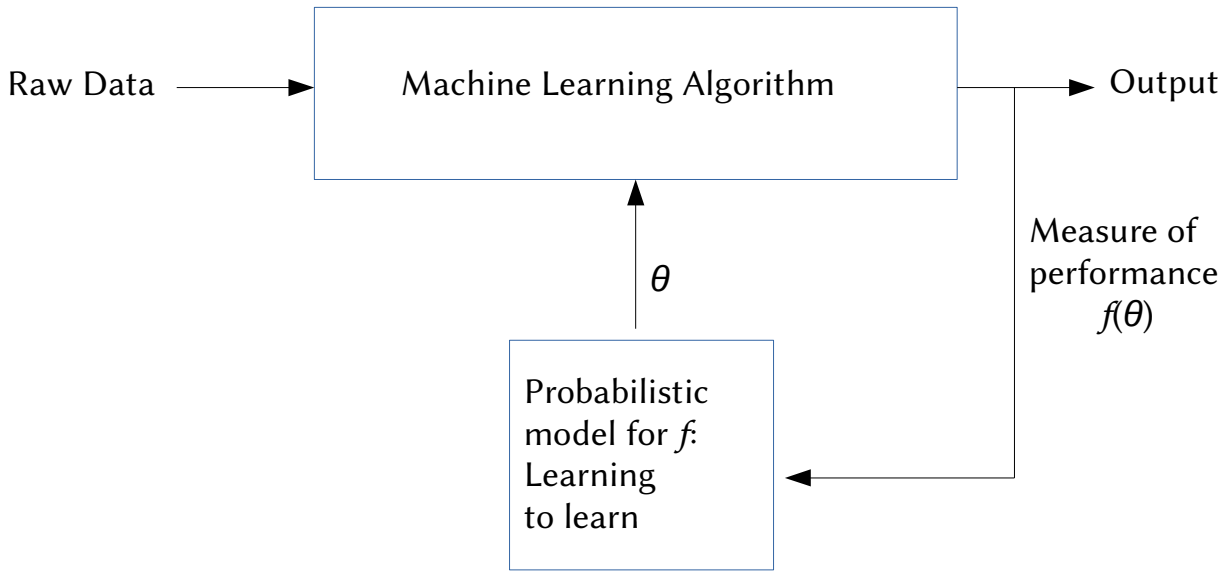
Towards End-to-End Learning

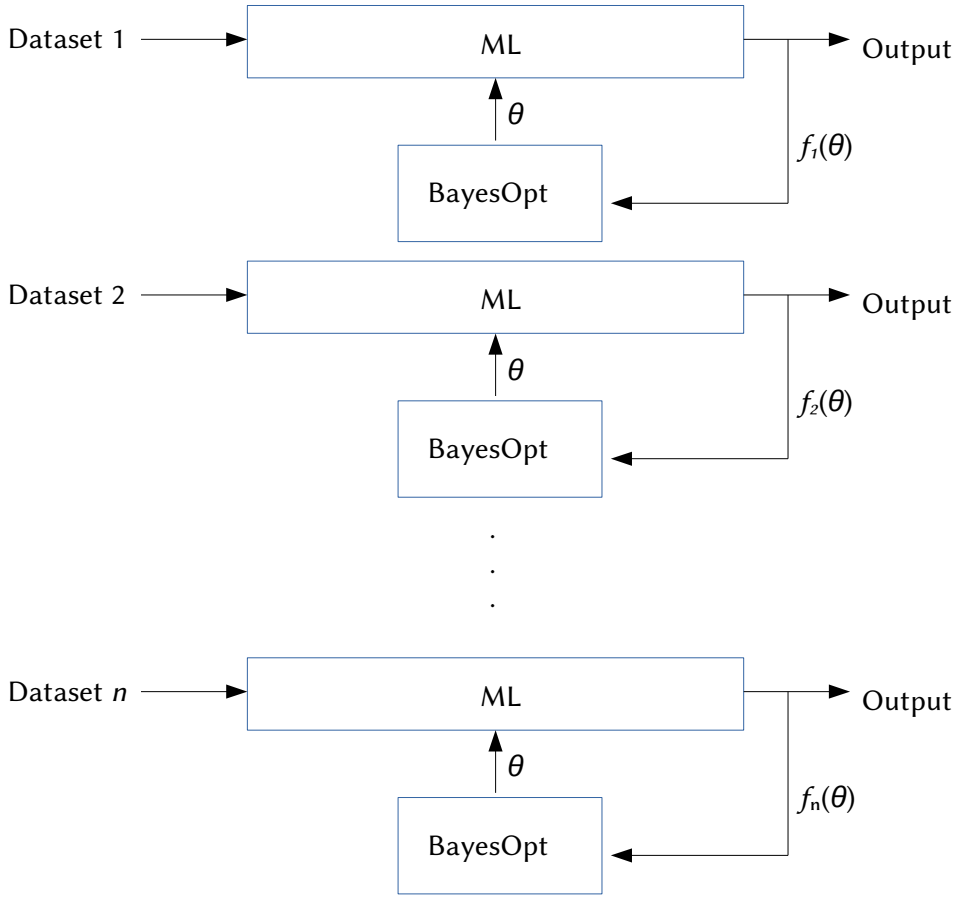


Towards End-to-End Learning



Transfer Hyperparameter Learning

- Multiple hyperparameter learning tasks which share the same model: variability in f across tasks is due to changing datasets.
- Is performance measure f really a black-box function of hyperparameters? Highly structured problem corresponding to training a specific model on a specific dataset.



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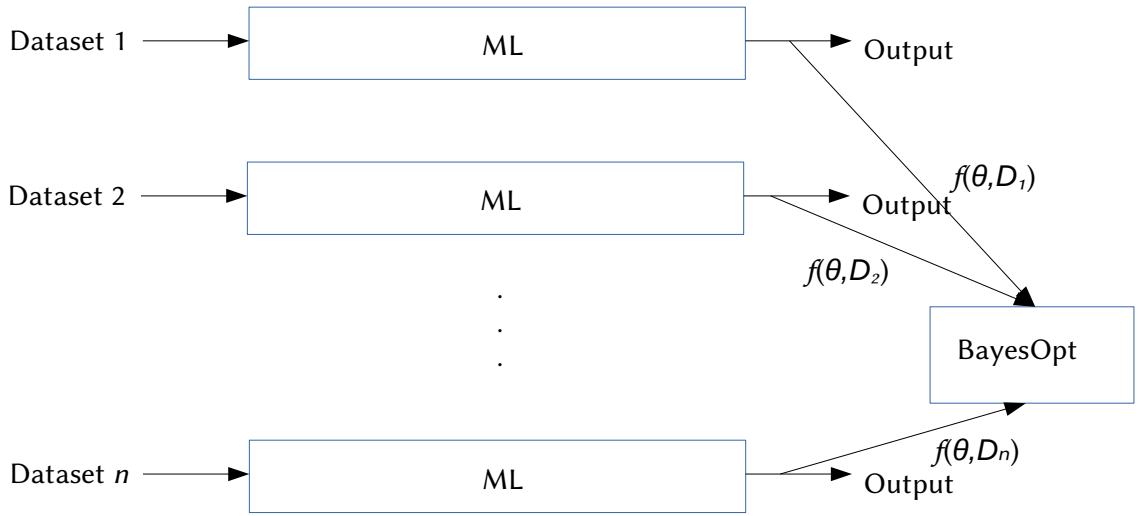


Transfer Hyperparameter Learning

- Consider a standard supervised learning setting: $f(\theta, D)$ is a performance measure of a trained ML model with hyperparameters θ and data $D = \{\mathbf{x}_l, y_l\}_{l=1}^{s}$, $\mathbf{x}_l \in \mathcal{X}$ covariates and $y_l \in \mathcal{Y}$ labels. Assume the same domains $\mathcal{X}$ and $\mathcal{Y}$ for all tasks.
- Assume that we have already solved n source tasks by computing N_i evaluations of the objective, i.e. we have $\{\theta_r^i, f(\theta_r^i, D_i)\}_{r=1}^{N_i}$, with source datasets

$$D_i = \{\mathbf{x}_l^i, y_l^i\}_{l=1}^{s_i}, i = 1, \ldots, n.$$

- The goal is to utilise information from source tasks to help us model $f^{\text{target}}(\theta) = f(\theta, D_{\text{target}})$ and speed up BayesOpt on an unseen target dataset

$$D_{\text{target}} = \{\mathbf{x}_l^{\text{target}}, y_l^{\text{target}}\}_{l=1}^{s_{\text{target}}},$$

i.e.

$$\theta_*^{\text{target}} = \text{argmin}_{\theta \in \Theta} f^{\text{target}}(\theta)$$

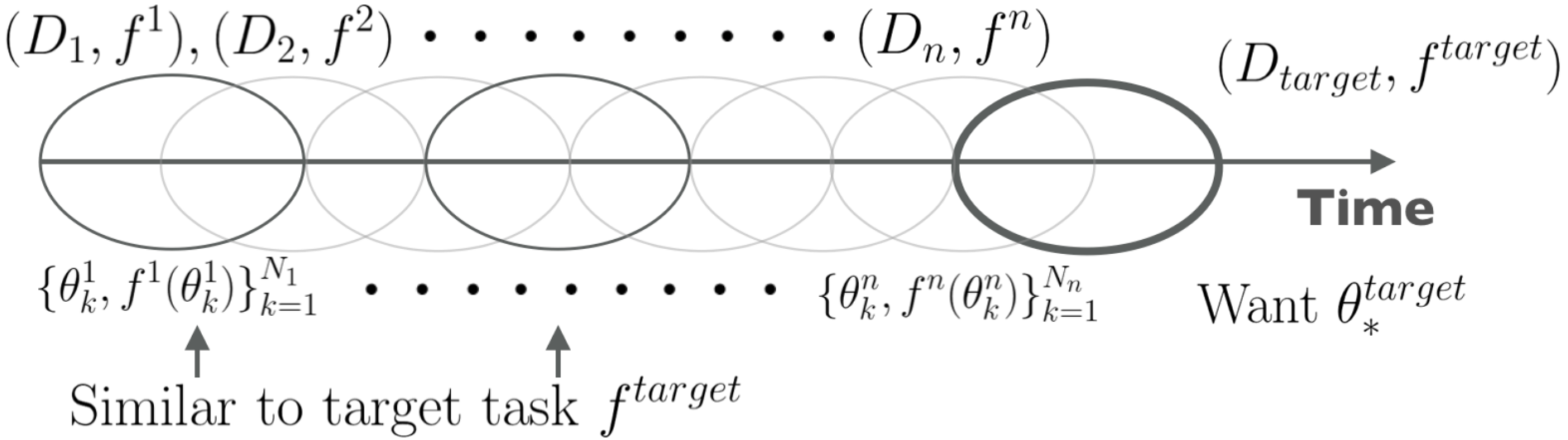
Motivating Example

Example from [Poloczek et al, 2016] to motivate warm-starting Bayesian optimization.

- Model that assigns drivers to passengers (e.g. Uber or Lyft)
- Have to tune hyperparameters θ, with objective f
- Live stream of data arriving in time

Problem:

- Re-train model every 12 hours, on the last 24 hours of data, and deploy asap.
- Optimal hyperparameters θ shift as data distribution changes e.g. weekend vs weekday or holiday vs no holiday
- Not all previous tasks are equally useful.



Dataset representation for hyperparameter learning

Assume $D = \{\mathbf{x}_l, y_l\}_{l=1}^{s} \overset{i.i.d.}{\sim} P_{XY}$ and that f is the empirical risk, i.e.

$$f(\theta, D) = \frac{1}{s} \sum_{\ell=1}^{s} L\left(h_\theta(\mathbf{x}_\ell), y_\ell\right),$$

where L is the loss function and h_θ is the model's predictor.

For a fixed ML model, there are three sources of variability to the performance measure f:

- Hyperparameters θ
- Joint (empirical) measure $\mathcal{P}_{XY}$ of the dataset
- Sample size s

Thus we will model $f(\theta, \mathcal{P}_{XY}, s)$, assuming that f varies smoothly not only as a function of θ, but also as a function of $\mathcal{P}_{XY}$ and s ([Klein et al, 2016] considers f varying in s to speed up BayesOpt on a single large dataset).

Dataset representation for hyperparameter learning

To model a joint GP in $(\theta, \mathcal{P}_{XY}, s)$, we construct a product covariance function:

$$K(\{\theta_1, \mathcal{P}^1_{XY}, s_1\}, \{\theta_2, \mathcal{P}^2_{XY}, s_2\}) = k_\theta(\theta_1, \theta_2) k_p(\psi(\mathcal{P}^1_{XY}), \psi(\mathcal{P}^2_{XY})) k_s(s_1, s_2)$$

Common choices might include k_θ are k_p as Matérn-$3/2$, and k_s as the sample size kernel from [Klein et al, 2016]

Need to learn representation $\psi(\mathcal{P}_{XY})$ useful for hyperparameter learning, i.e. the one which can yield representations invariant to variations in the training data irrelevant for hyperparameter choice.

AutoML: representing datasets using metafeatures

No joint GP model, but warmstart target hyperparameters to the optimal values from source datasets with closest metafeatures.

[Michie et al, 1994; Pfahringer et al, 2000; Bardenet et al, 2013; Feurer et al, 2014; Hutter et al, 2019]

- General:
  - *Skewness, kurtosis of each input dimension*: extract the minimum, maximum, mean and standard deviation across the dimensions.
  - *Correlation, covariance of each pair of input dimensions*: extract the minimum, maximum, mean and standard deviation across the pairs.
  - *PCA skewness, kurtosis*: run PCA, project onto the first principal component and compute skewness and kurtosis.
  - *Intrinsic dimensionality*: number of principal components to explain 95% of variance.
- Classification specific:
  - *Label summaries*: empirical class distribution and its entropy.
  - *Classification landmarkers*: accuracy on a held out dataset of 1-nn classifier, linear discriminant analysis, naive Bayes and decision tree classifier.
- Regression specific:
  - *Label summaries*: Mean, stdev, skewness, kurtosis of the labels $\{y_\ell^i\}_{\ell=1}^{s_i}$.
  - *Regression landmarkers*: accuracy on a held out dataset of 1-nn, linear and decision tree regression.

Learning kernel embeddings

Need to learn a representation of empirical joint distributions for comparison across tasks.

- Start with parametrized feature maps (e.g. neural networks) $\phi_x(\mathbf{x})$, $\phi_y(y)$ and $\phi_{xy}([\mathbf{x}, y])$ which we will learn (treated as GP kernel parameters).
- Marginal Distribution $\mathcal{P}_X$: $\hat{\mu}_{P_X} = \frac{1}{s}\sum_{\ell=1}^{s} \phi_x(\mathbf{x}_\ell)$ (*e.g. noisier covariates require less complex models*).
- Conditional Distribution $\mathcal{P}_{Y|X}$:

$$\hat{\mathcal{C}}_{Y|X} = \Phi_y^\top (\Phi_x \Phi_x^\top + \lambda I)^{-1} \Phi_x$$

  where $\Phi_x = [\phi_x(\mathbf{x}_1), \ldots, \phi_x(\mathbf{x}_s)]^T$, $\Phi_y = [\phi_y(y_1), \ldots, \phi_y(y_s)]^T$ and λ is a parameter that we learn. (*e.g. captures smoothess of the regression functions*).
- Joint Distribution $\mathcal{P}_{XY}$:

$$\hat{\mathcal{C}}_{XY} = \frac{1}{s}\sum_{\ell=1}^{s} \phi_x(\mathbf{x}_\ell) \otimes \phi_y(y_\ell) = \frac{1}{s}\Phi_x^\top \Phi_y$$

  Alternatively, learn a joint feature map ϕ_{xy} and compute $\hat{\mu}_{P_{XY}} = \frac{1}{s}\sum_{\ell=1}^{s} \phi_{xy}([\mathbf{x}_\ell, y_\ell])$.

DistBO Algorithm

With a joint GP model on inputs $(\theta, \mathcal{P}_{XY}, s)$, we can now

1. Fit the GP on all performance evaluations so far:

$$\mathcal{E} = \{\{(\theta_r^i, \mathcal{P}_{XY}^i, s_i), f^i(\theta_r^i)\}_{r=1}^{N_i}\}_{i=1}^n,$$

   fitting any GP kernel parameters (e.g. those of feature maps ϕ_x, ϕ_y) by maximising the marginal likelihood of the GP.
2. Let $f^{target}(\theta) = f(\theta, \mathcal{P}_{XY}^{target}, s_{target})$. Maximise the acquisition function at the target $\alpha(\theta; f^{target})$ to select next θ_{new}
3. Evaluate $f^{target}(\theta_{new})$, add $\{(\theta_{new}, \mathcal{P}_{XY}^{target}, s_{target}), f^{target}(\theta_{new})\}$ to $\mathcal{E}$ and go to 1.

Adaptive Bayesian Linear Regression: DistBLR

- Joint GP modelling comes at a high computational cost: $O(N^3)$ time and $O(N^2)$ storage, where N is the total number of observations: $N = \sum_{i=1}^{n} N_i$
- GP cost can outweigh the cost of computing f in the first place.
- Since we are learning dataset representation inside the kernel anyway – can instead simply adopt Bayesian linear regression ($O(N)$ time and storage)

$$z|\beta \sim \mathcal{N}(\Upsilon\beta, \sigma^2 I) \qquad \beta \sim \mathcal{N}(0, \alpha I)$$

$$\Upsilon = [\upsilon([\theta_1^1, \Psi_1]), \ldots, \upsilon([\theta_{N_1}^1, \Psi_1]), \ldots, \upsilon([\theta_1^n, \Psi_n]), \ldots, \upsilon([\theta_{N_n}^n, \Psi_n])]^\top \in \mathbb{R}^{N \times d}$$

where $\alpha > 0$ denotes the prior regularisation. Here υ denotes a feature map of dimension d on concatenated hyperparameters θ, data embedding $\psi(D)$ and sample size s.

Conceptually similar setting to [Perrone et al, 2018] who fit a single BLR per task.

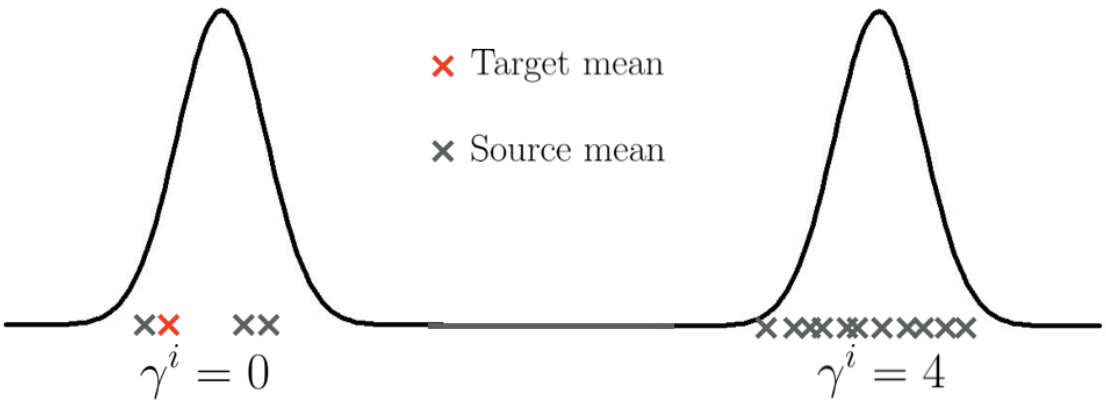
Experiments

We will compare **DistBO** with the following baselines:

- **manualBO**: joint GP with $\psi(D)$ as the selection of 13 AutoML meta-features,
- **multiBO**: i.e. multiGP [Swersky et al, 2013] and multiBLR [Perrone et al, 2018] which uses no meta-information, i.e. each task is encoded by its index, but the representation of hyperparameters is shared across tasks,
- **initBO**: plain BayesOpt warm-started with the top 3 hyperparameters from the three most similar source tasks in terms of AutoML meta-features,
- **noneBO**: plain BayesOpt,
- **RS**: random search.

Implementation in *TensorFlow*, with GP/BLR marginal likelihood optimized using ADAM. To obtain source task evaluations, we use standard BayesOpt.

Toy Example



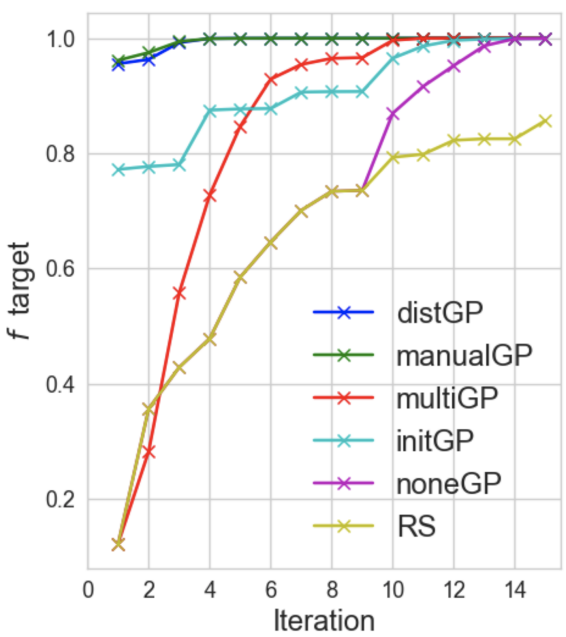
D_i is obtained for some fixed γ^i as $\mu^i \sim \mathcal{N}(\gamma^i, 1)$, $\quad \{x_\ell^i\}_{\ell=1}^{s_i} | \mu^i \overset{i.i.d.}{\sim} \mathcal{N}(\mu^i, 1)$ and the objective to maximize is

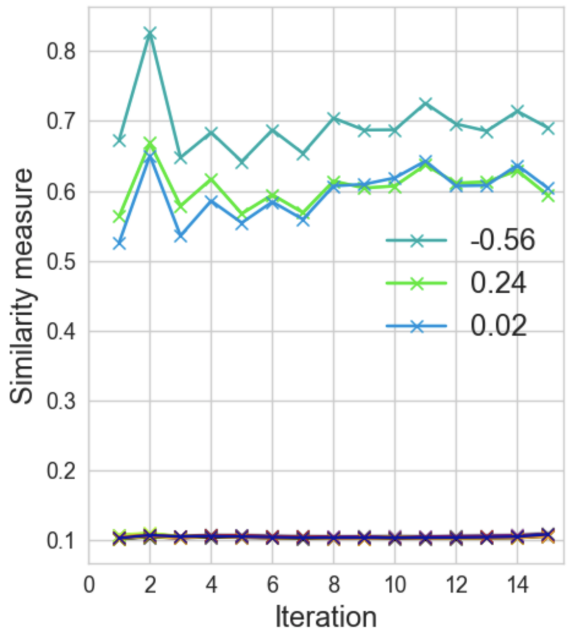
$$f(\theta; D_i) = \exp\left(-\frac{(\theta - \frac{1}{s_i}\sum_{\ell=1}^{s_i} x_\ell^i)^2}{2} \right),$$

where θ plays the role of a "hyperparameter".

15 source tasks, 3 with $\gamma_i = 0$ and 12 with $\gamma_i = 4$. Target has $\gamma_i = 0$.

Toy Example





- feature representation learned to place high similarity on the three source datasets sharing the same γ^i and hence having similar values of μ^i, while placing low similarity on the other source datasets
- manualBO also few-shots the optimum as it encodes the mean feature
- initBO and multiBO converge more slowly without any meta-information

D_i is obtained for some fixed γ^i as $\mu^i \sim \mathcal{N}(\gamma^i, 1)$, $\quad \{x_\ell^i\}_{\ell=1}^{s_i} | \mu^i \overset{i.i.d.}{\sim} \mathcal{N}(\mu^i, 1)$ and the objective to maximize is

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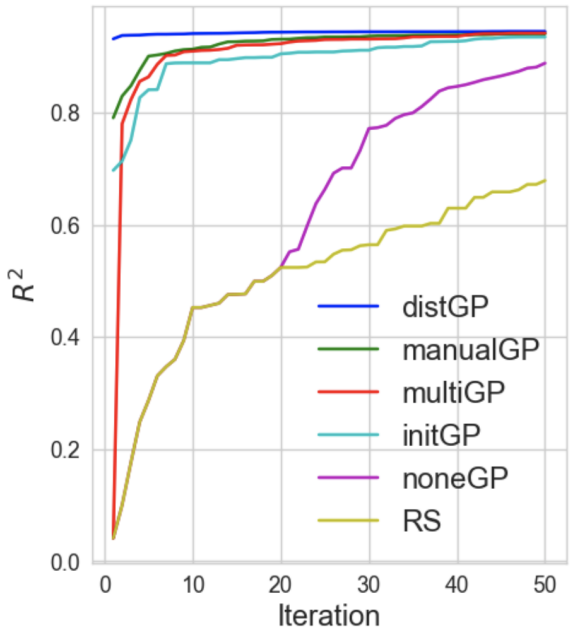
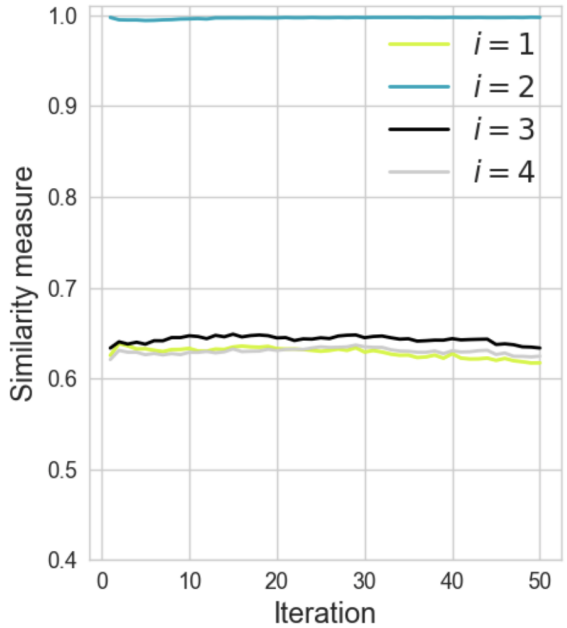
Switching feature relevance





- handcrafted meta-features do not capture any information about the optimal hyperparameters
- three-variable interaction: the difference between tasks is invisible by considering marginal distributions of covariates and their pairwise relationships.

Dataset i with $\mathbf{x}_\ell^i \in \mathbb{R}^6$ and $y_\ell^i \in \mathbb{R}$:

$$\begin{aligned} \left[\mathbf{x}_\ell^i\right]_j &\overset{i.i.d.}{\sim} \mathcal{N}(0, 2^2), \quad j = 1, \ldots, 6, \\ \left[\mathbf{x}_\ell^i\right]_{i+2} &= \text{sign}([\mathbf{x}_\ell^i]_1 [\mathbf{x}_\ell^i]_2) \left|[\mathbf{x}_\ell^i]_{i+2}\right|, \\ y_\ell^i &= \log\left(1 + \left(\prod_{j \in \{1,2,i+2\}} [\mathbf{x}_\ell^i]_j\right)^3\right) + \mathcal{N}(0, 0.5^2). \end{aligned}$$

i, ℓ, j denote task, sample and dimension, respectively; sample size is $s_i = 5000$.

Protein data classification

- Datasets on 7 proteins extracted from ChEMBL database [Gaulton et al, 2016]. Each protein corresponds to a task, containing $1037 - 4434$ molecules with binary features $\mathbf{x}_\ell^i \in \mathbb{R}^{166}$ computed using chemical fingerprinting. The binary label per molecule is whether it can bind to the protein target.
- Two classifiers: Jaccard kernel C-SVM (hyperparameter C), and random forest (hyperparameters `n_trees`, `max_depth`, `min_samples_split`, `min_samples_leaf`).
- Designate each protein as the target task, while using remaining 6 as source tasks. Results reported obtained by averaging over target tasks (20 runs per task).

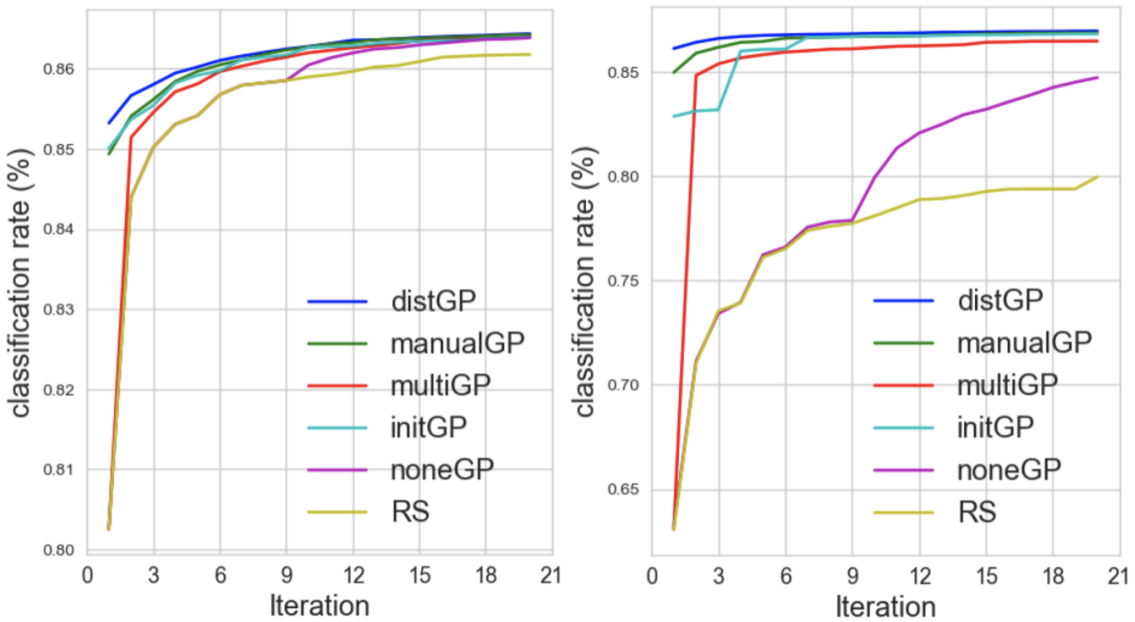


Figure: **Left:** Jaccard kernel C-SVM. **Right:** Random forest

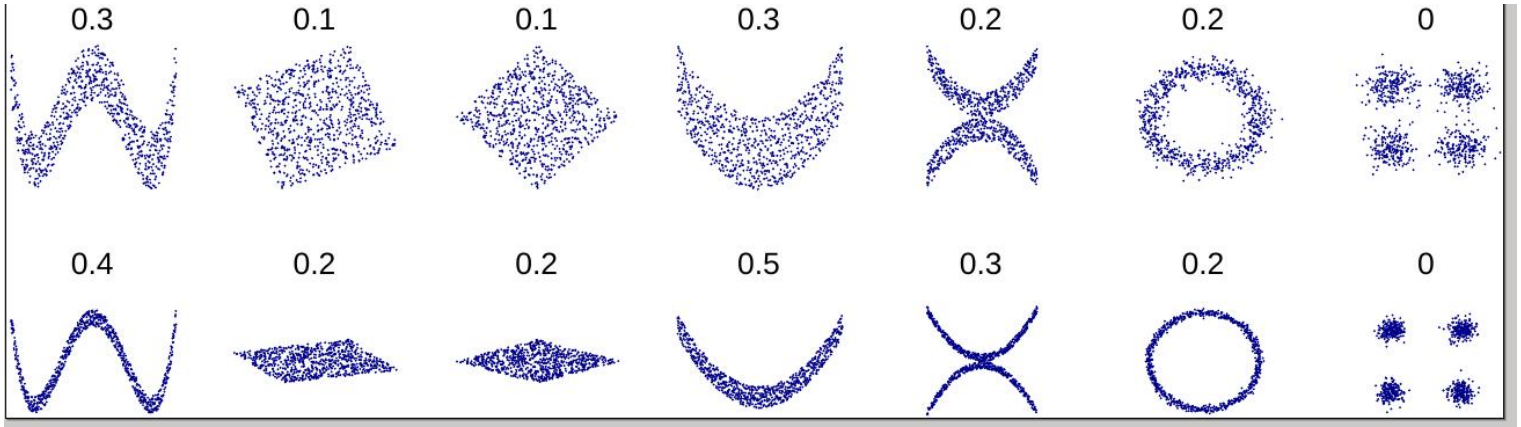
Conclusion

- Method to borrow strength between multiple hyperparameter learning tasks by making use of the similarity between training datasets.
- Allows few-shot hyperparameter learning especially if similar prior tasks are present.
- Towards opening the black box function of hyperparameter learning: consider model performance as a function of all its sources of variability.
- Future work: straightforward to consider the setting where we solve multiple tasks jointly, due to the presence of the joint GP model. Acquisition function?

Outline

1. Preliminaries on Kernel Embeddings
2. Hyperparameter Learning for Distributional Transfer
3. Meta Learning for Conditional Density Estimation

Beyond Functional Relationships

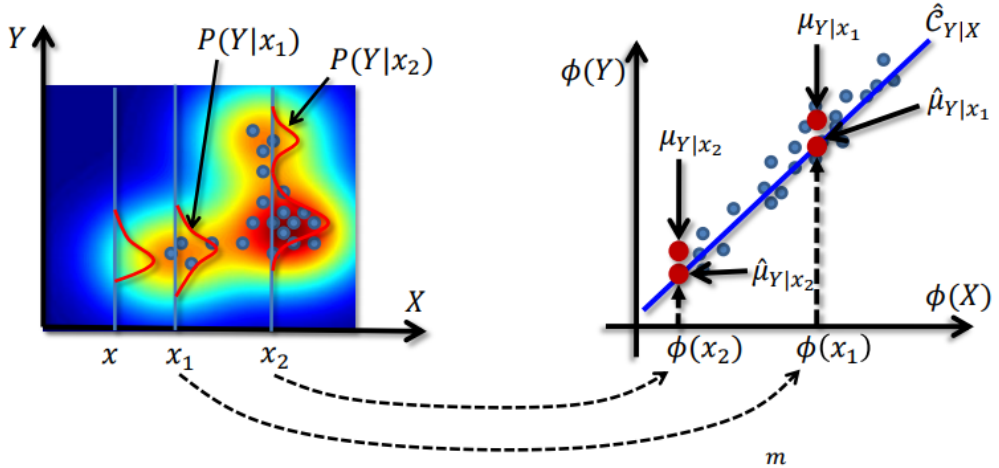


- In supervised learning, we often focus on functional relationships, e.g. conditional expectations $\mathbb{E}[y|x]$ in regression.
- More expressive representation may be needed due to e.g. multimodality or heteroscedasticity: y cannot be meaningfully represented using a single function $f(x)$ of the features x, such as $\mathbb{E}[y|x]$.
- Example: $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$ sampled uniformly from an annulus $r^2 \leq x^2 + y^2 \leq R^2$ – any regression model would fail to capture the dependence between y and x because clearly $\mathbb{E}[y|x] = 0$.
- Goal: conditional density estimation $p(y|x)$ based on paired samples $\{(x_i, y_i)\}_{i=1}^n$.
- Use a flexible **nonparametric model** of the full conditional density in the **meta learning setting**.

Conditional Embeddings

- "Augment" the representation of y by using a feature map $\phi_y(y)$ –e.g. $\phi_y(y) = [y,\ y^2]$ renders relationship trivial in the annulus example.
- In general, we require an expressive feature map ϕ_y so that CME $\mathbb{E}[\phi_y(y)|x]$ captures the relevant information about the relationship between y and x.
- However, CMEs do not give a way to estimate *conditional densities*.

$$\widehat{\mathcal{C}}_{Y|X} = \Phi_y(K_{xx} + \lambda I)^{-1}\Phi_x^T, \quad \hat{\mu}_{Y|X=x} = \hat{\mathbb{E}}[\phi_y(y)|x] = \widehat{\mathcal{C}}_{Y|X}\phi_x(x).$$



$$\hat{\mu}_{Y|x} = \hat{\mathcal{C}}_{Y|X}\phi(x) = \hat{\mathcal{C}}_{YX}\left(\hat{\mathcal{C}}_{XX} + \lambda I\right)^{-1}\phi(x) = \sum_i^m \beta_i(x)\phi(y_i)$$

Conditional Embeddings

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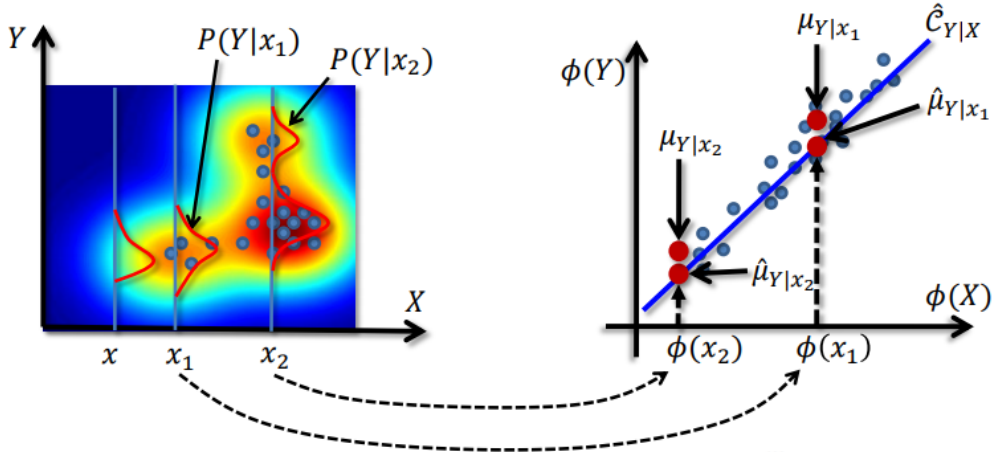
- In general, we require an expressive feature map ϕ_y so that CME $\mathbb{E}[\phi_y(y)|x]$ captures the relevant information about the relationship between y and x.
- However, CMEs do not give a way to estimate *conditional densities*.
- Idea: use the conditional mean embedding operator as a task embedding of a given conditional density estimation task.

$$\widehat{\mathcal{C}}_{Y|X} = \Phi_y(K_{xx} + \lambda I)^{-1}\Phi_x^T, \quad \hat{\mu}_{Y|X=x} = \hat{\mathbb{E}}[\phi_y(y)|x] = \widehat{\mathcal{C}}_{Y|X}\phi_x(x).$$



Noise Contrastive Estimation

Noise contrastive estimation [Gutmann and Hyvärinen, 2010] is an approach to the model parameter estimation based on classifiers discriminating between true and artificial (fake) samples. In our case, $y_i|x_i \sim p_\theta(y|x)$, and those from $\{y^f_{i,j}\}_{j=1}^{\kappa} \sim p_f(y)$, for a given $p_f(y)$. Giving weights proportional to $(1, \kappa)$, probability that the sample came from the true model is:

$$P_\theta(\text{True}|y, x) = \frac{p_\theta(y|x)}{p_\theta(y|x) + \kappa p_f(y)}.$$

Assuming that the learned classifier is Bayes optimal:

$$p_\theta(y|x) = \frac{\kappa p_f(y) P_\theta(\text{True}|y, x)}{1 - P_\theta(\text{True}|y, x)}.$$

Density model

Consider the density model given by

$$p_\theta(y|x) = \frac{\exp(s_\theta(x,y))}{\int \exp(s_\theta(x,y'))dy'} = \exp(s_\theta(x,y) + b_\theta(x))$$

for some scoring function $s_\theta : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ and $b_\theta(x)$ models the normalizing constant. Hence

$$\begin{aligned} P_\theta(\text{True}|y,x) &= \frac{\exp(s_\theta(x,y) + b_\theta(x))}{\exp(s_\theta(x,y) + b_\theta(x)) + \kappa p_f(y)} \\ &= \sigma\left(s_\theta(x,y) + b_\theta(x) - \log(\kappa p_f(y))\right). \end{aligned}$$

where $\sigma(t) = 1/(1+e^{-t})$ is the logistic function.

Defining s_θ

- Map x_i and y_i using feature maps (neural networks) $\phi_x : \mathcal{X} \to \mathcal{H}_X$ and $\phi_y : \mathcal{Y} \to \mathcal{H}_Y$ with all parameters collated into θ
- Estimate the conditional mean embedding operator $\widehat{\mathcal{C}}_{Y|X} = \Phi_y (K_{xx} + \lambda I)^{-1} \Phi_x^T$
- Given $\widehat{\mathcal{C}}_{Y|X}$, we can estimate the conditional mean embedding for any new x' using

$$\hat{\mu}_{Y|X=x'} = \widehat{\mathcal{C}}_{Y|X} \phi_x(x')$$

- We can then evaluate the conditional mean embedding at any new y' using

$$\hat{\mu}_{Y|X=x'}(y') = \langle \hat{\mu}_{Y|X=x'}, \phi_y(y') \rangle_{\mathcal{H}_Y} = \langle \widehat{\mathcal{C}}_{Y|X} \phi_x(x'), \phi_y(y') \rangle_{\mathcal{H}_Y}$$

Scoring function:

$$s_\theta(x', y') = \hat{\mu}_{Y|X=x'}(y')$$

Defining s_θ

- Scoring function:

$$s_\theta(x', y') = \hat{\mu}_{Y|X=x'}(y')$$

- We expect this value to be high when y' is drawn from the true conditional distribution $Y|X = x'$ and low in cases where y' falls in a region where the true conditional density $p(y|x')$ is low:

$$\mu_{Y|X=x'}(y') = \mathbb{E}\left[k_y(y', Y)|X = x'\right] = \int k_y(y', y)p(y|x')dy,$$

where $k_y(y, y') := \langle \phi_y(y), \phi_y(y') \rangle_{\mathcal{H}_y}$.

- Recall that

$$P_\theta(\text{True}|y, x) = \sigma\left(s_\theta(x, y) + b_\theta(x) - \log(\kappa p_f(y))\right).$$

MetaCDE

- Three neural networks $\phi_x(x)$, $\phi_y(y)$, $b_\theta(x)$ (all parameters collated into θ).
- Let $\mathcal{T} = \{T_1, \ldots, T_L\}$ be the set of L conditional density estimation tasks with each T_l divided into context data $\mathcal{D}_c^l = \{(x_i^{l,c}, y_i^{l,c})\}$ and target data $\mathcal{D}_t^l = \{(x_i^{l,t}, y_i^{l,t})\}$
- For every target input $x_i^{l,t}$, we generate κ fake responses $y_{i,j}^{l,f}$ from $p_f(y)$.
- Now train the True/Fake classifier by maximizing conditional log-likelihood of the True/Fake labels, i.e. minimizing the logistic loss across all tasks jointly (SGD):

$$\min_\theta \sum_l \sum_i \left\{ \log\left(1 + \frac{\kappa p_f(y_i^{l,t})}{\exp(s_\theta^l(x_i^{l,t}, y_i^{l,t}) + b_\theta(x_i^{l,t}))}\right) + \sum_{j=1}^{\kappa} \log\left(1 + \frac{\exp(s_\theta^l(x_i^{l,t}, y_{i,j}^{l,f}) + b_\theta(x_i^{l,t}))}{\kappa p_f(y_{i,j}^{l,f})}\right) \right\}$$

with

$$s_\theta(x, y) = \langle \widehat{\mathcal{C}}_{Y|X}^l \phi_x(x), \phi_y(y) \rangle_{\mathcal{H}_Y},$$

and $\widehat{\mathcal{C}}_{Y|X}^l$ computed on the context set $\mathcal{D}_c^l$.

Synthetic data experiment

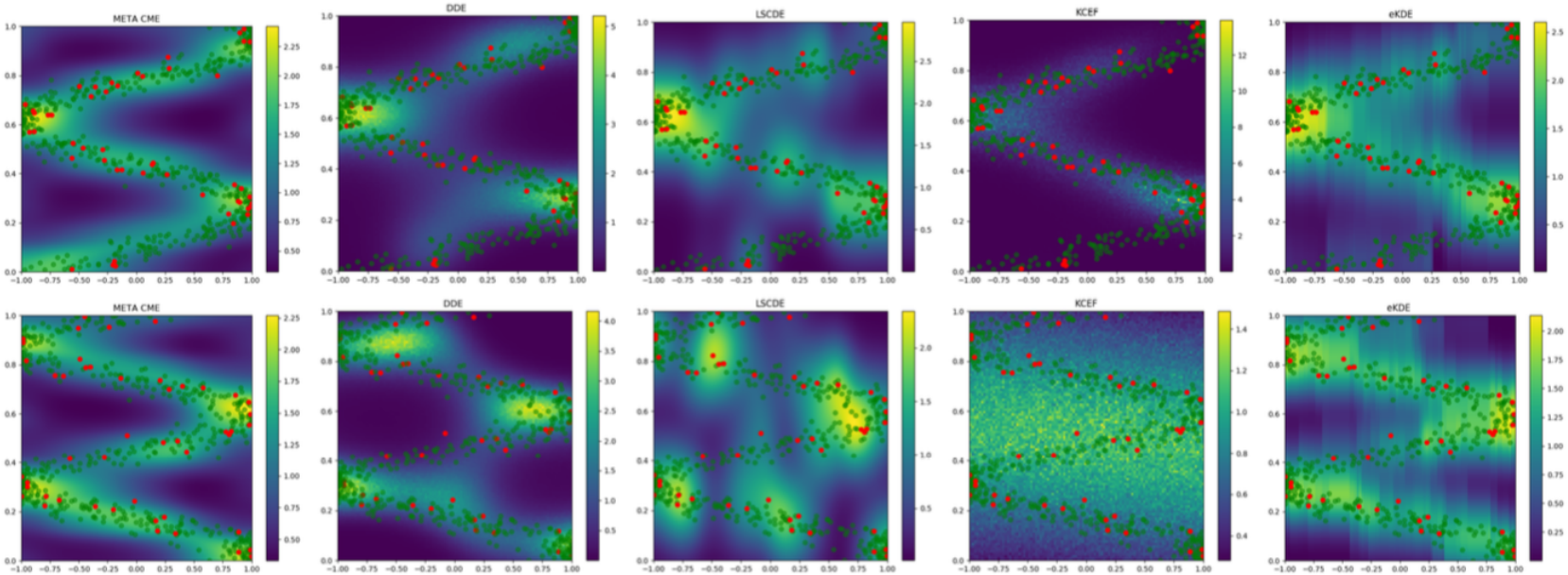


Figure: Left to right: MetaCDE (ours), DDE, LSCDE, KCEF, ϵ-KDE. The red dots are the context/training points and the green dots are points from the true density.

- $y_i \sim \mathrm{U}(0,1)$, $x_i|y_i = \cos(ay_i + b) + \mathcal{N}(0, \sigma^2)$, where a, b, σ^2 vary between tasks.
- Note that in this case x can be written as a simple function of y with added noise, but not vice versa, leading to the multimodality of $p(y|x)$.

Synthetic data experiment

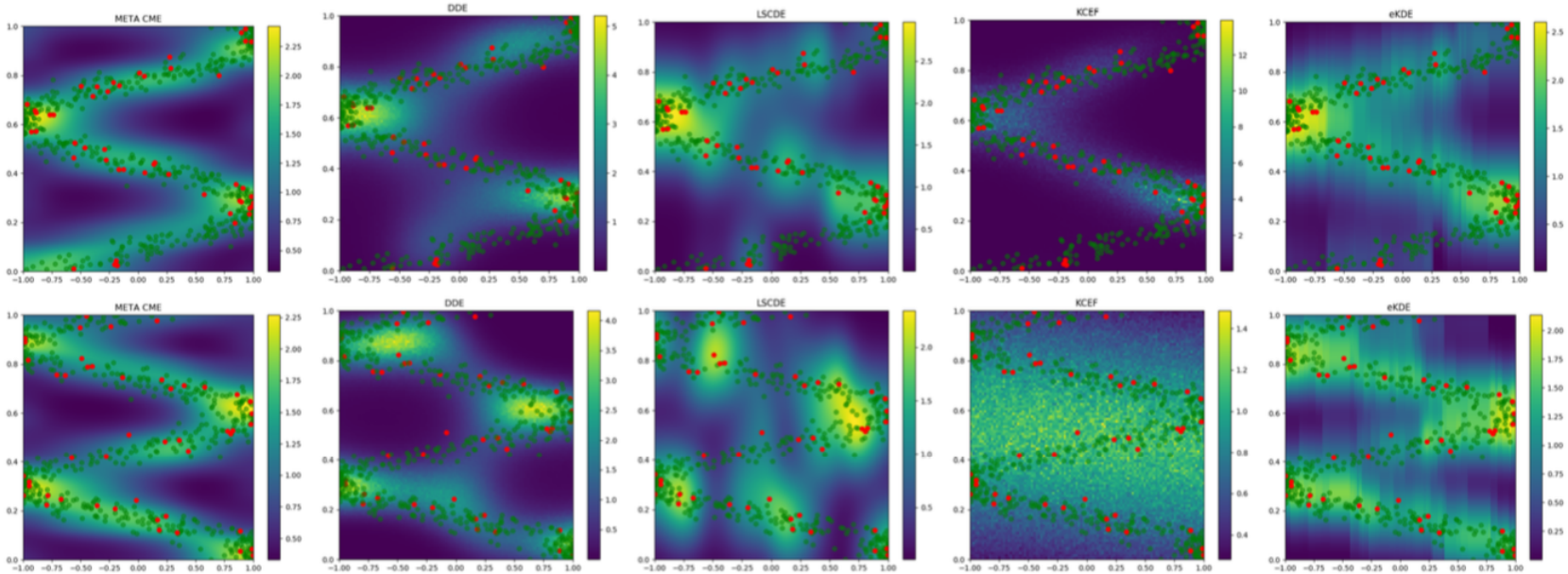


Figure: Left to right: MetaCDE (ours), DDE, LSCDE, KCEF, ϵ-KDE. The red dots are the context/training points and the green dots are points from the true density.

	MetaCDE	DDE	LSCDE	KCEF	ϵ-KDE
Mean over 100 log-likelihoods	**197.36 ± 25.26**	162.98 ± 68.67	44.95 ± 74.36	-388.30 ± 699.65	116.31 ± 235.80
P-value for Wilcoxon test	NA	9.681e-06	<2.2e-16	< 2.2e-16	1.92e-07

Table: Average held out log-likelihood on 100 different synthetic $\cos$ tasks. Also reporting the p-values for the one sided signed Wilcoxon test wrt to MetaCDE.

Dihedral angles in molecules

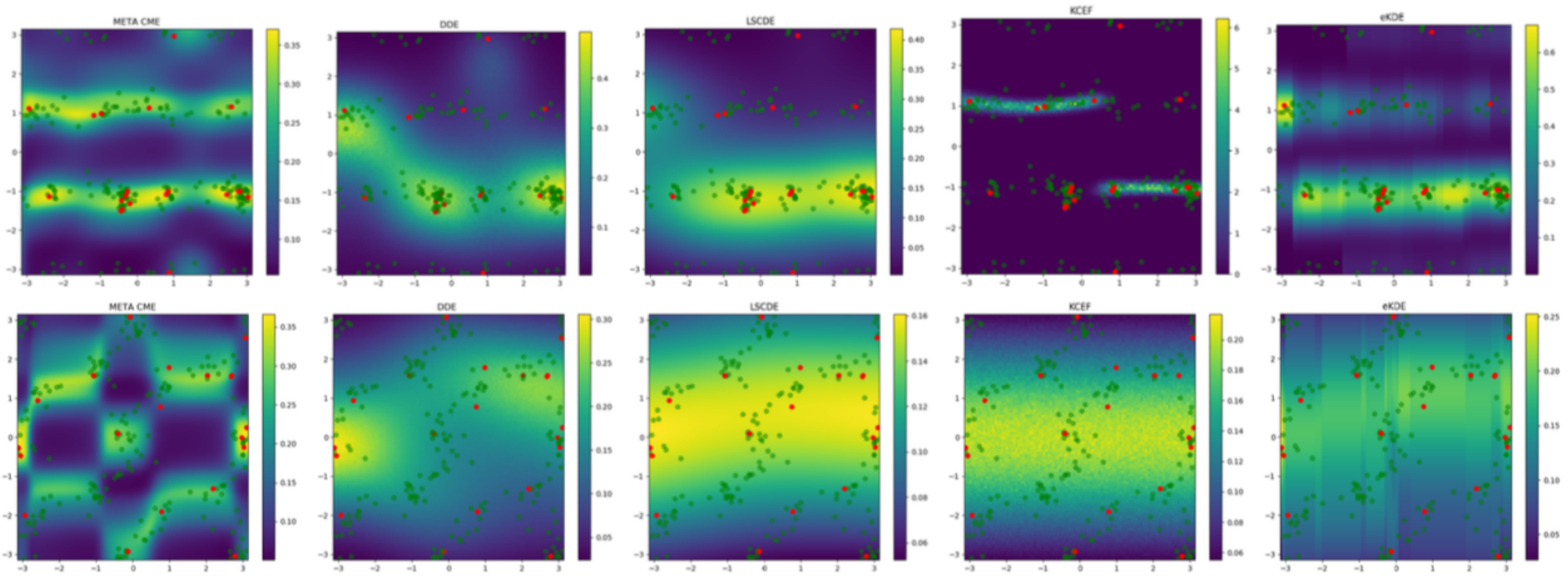


Figure: Left to right: MetaCDE (ours), DDE, LSCDE, KCEF, ϵ-KDE. The red dots are the context/training points and the green dots are points from the true density.

- Interested in understanding possible conformations of molecular structures, i.e. energetically allowed regions of dihedral angles in bonds. The data extracted from crystallography database COD [Gražulis et al, 2011].
- The multimodality of the dataset arises from the molecular symmetries such as reflection and rotational symmetry.

Dihedral angles in molecules

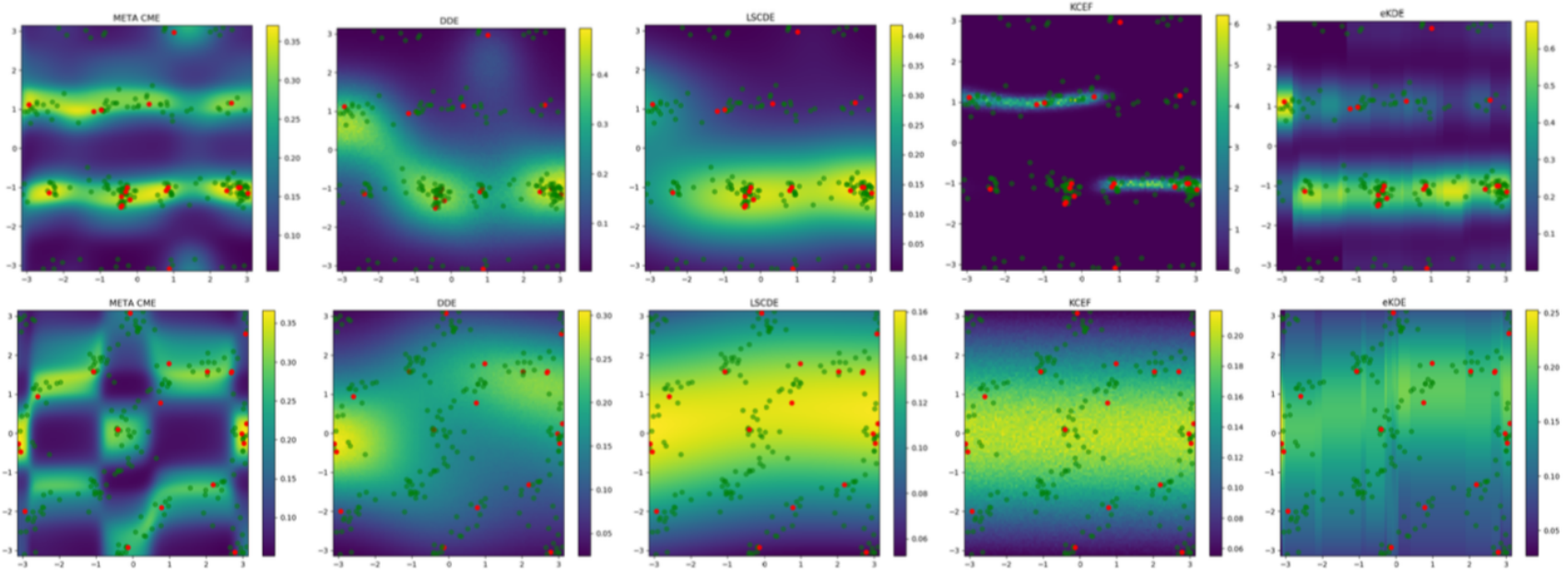


Figure: Left to right: MetaCDE (ours), DDE, LSCDE, KCEF, ϵ-KDE. The red dots are the context/training points and the green dots are points from the true density.

	MetaCDE	DDE	LSCDE	KCEF	ϵ-KDE
Mean over 100 Log-likelihoods	**-297.58 ± 67.63**	-315.49 ± 204.82	-335.85 ± 192.09	-596.95 ± 871.97	-422.99± 346.46
P-value for Wilcoxon test	NA	4.932e-05	2.692e-05	1.397e-05	9.49e-07

Table: Average held out log-likelihood on 100 different molecules. Also reporting the p-values for the one sided signed Wilcoxon test wrt to MetaCDE.

Conclusions

- Learn a data representation informative for the conditional density estimation tasks, by borrowing strength across tasks.
- Reminiscent to neural processes [Garnelo et al, 2018]: MetaCDE learns a task embedding, but the task embedding based on context set, but this embedding takes a specific form of the conditonal embedding operator and it is the feature maps that are learned.
- Future work: choices of fake distributions, including those depending on the conditioning variable.

Summary

- Statistical modelling can be brought to bear in tandem with performant machine learning models.
- Increasing confluence between statistics and ML: making use of the well engineered ML infrastructure, with bespoke statistical models for the problem at hand.
- Flexibility of the RKHS framework as a common ground between machine learning and statistical inference.

References

- Ho Chung Leon Law, Peilin Zhao, Lucian Chan, Junzhou Huang, and DS. **Hyperparameter Learning via Distributional Transfer**. *ArXiv e-prints:1810.06305*, 2018.
- Jean-Francois Ton, Lucian Chan, Yee Whye Teh, and DS. **Noise Contrastive Meta Learning for Conditional Density Estimation using Kernel Mean Embeddings**. *ArXiv e-prints:1906.02236*, 2019.