Computational Data Analysis

Machine Learning

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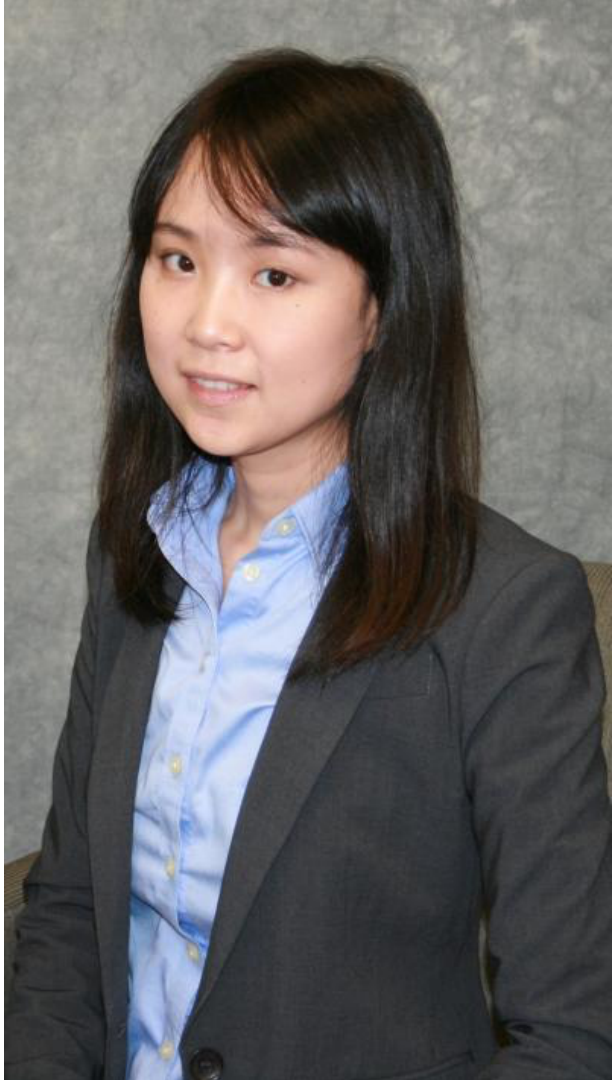
Kernel methods



Revisit nonlinear regression

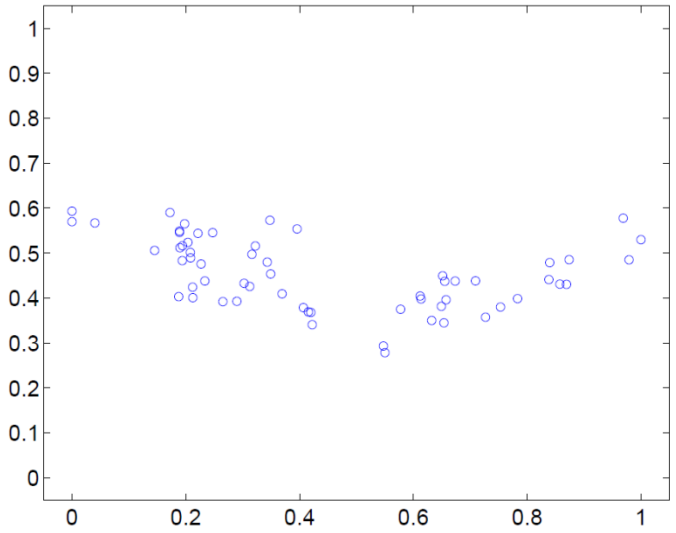
Want to fit a polynomial regression model

$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + \cdots + \theta_n x^d + \epsilon$$

Let $\tilde{x} = \left(1, x, x^2, \ldots, x^d\right)^\top$

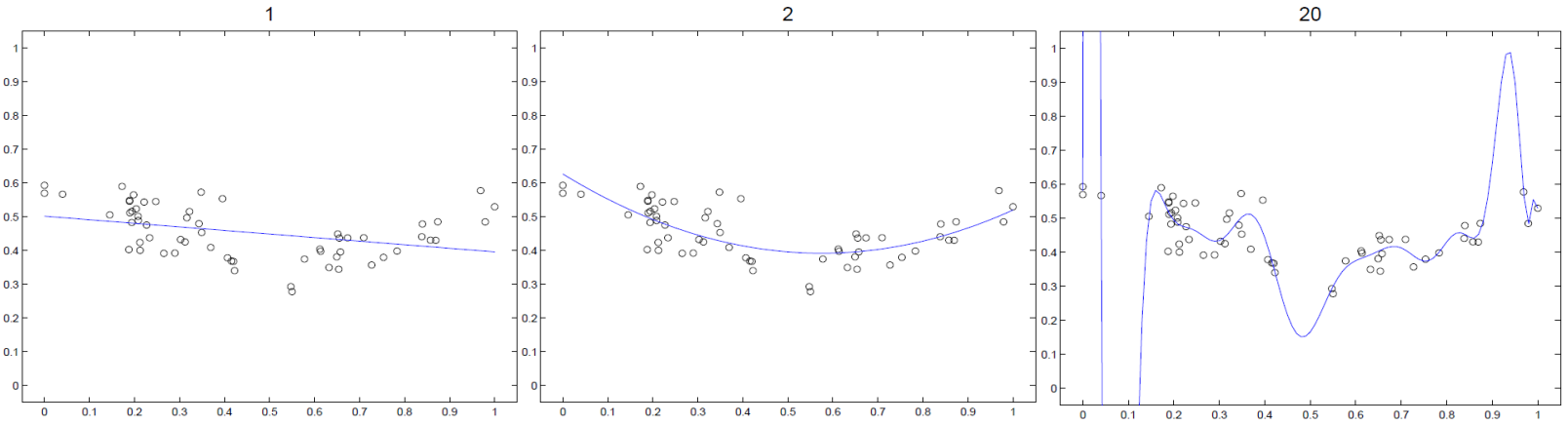
and $\theta = (\theta_0, \theta_1, \theta_2, \ldots, \theta_d)^\top$

$$\mathrm{y} = \theta^\top \tilde{x} + \epsilon$$



Overfitting / Underfitting by different polynomial degrees

- Blue points: training data points, Red points: test data points
- Choose the correct polynomial degree is not easy (needs cross-validation)



Under-fitting

Over-fitting

Problem of explicitly constructing features

- Explicitly construct feature map $\phi(x): R^n \mapsto F$, feature space can grow really large and really quickly.

- The if consider all polynomial feature of degree d
  - E.g. x_1^d, $x_1 x_2 \dots x_d$, $x_1^2 x_2 \dots x_{d-1}$
  - Total number of such feature is

$$\binom{d+n-1}{d} = \frac{(d+n-1)!}{d!\,(n-1)!}$$

  - $d = 6, n = 100$, there are 1.6 billion terms

Can we avoid expanding features: kernel trick

- Rather than consider features explicitly, let's consider their inner product

- Can we merge two steps using a clever function $k(x_i, x_j)$

  E.g. Polynomial $d = 2$

  - $\phi(x)^\top \phi(y) = \begin{pmatrix} x_1^2 \\ x_1 x_2 \\ x_2^2 \\ x_2 x_1 \end{pmatrix}^\top \begin{pmatrix} y_1^2 \\ y_1 y_2 \\ y_2^2 \\ y_2 y_1 \end{pmatrix} = x_1^2 y_1^2 + 2x_1 x_2 y_1 y_2 + x_2^2 y_2^2$
  - $= (x_1 y_1 + x_2 y_2)^2 = (x^\top y)^2$

$O(n)$ *computation*!

- Polynomial kernel degreee d, $k(x, y) = (x^\top y)^d = \phi(x)^\top \phi(y)$

Feature space is not unique

Eg. Polynomial $d = 2$

$$\phi(x)^\top \phi(y) = \begin{pmatrix} x_1^2 \\ x_1 x_2 \\ x_2^2 \\ x_2 x_1 \end{pmatrix}^\top \begin{pmatrix} y_1^2 \\ y_1 y_2 \\ y_2^2 \\ y_2 y_1 \end{pmatrix} = x_1^2 y_1^2 + 2x_1 x_2 y_1 y_2 + x_2^2 y_2^2$$
$$= (x_1 y_1 + x_2 y_2)^2 = (x^\top y)^2$$

$$\phi(x)^\top \phi(y) = \begin{pmatrix} x_1^2 \\ \sqrt{2} x_1 x_2 \\ x_2^2 \end{pmatrix}^\top \begin{pmatrix} y_1^2 \\ \sqrt{2} y_1 y_2 \\ y_2^2 \end{pmatrix} = x_1^2 y_1^2 + 2x_1 x_2 y_1 y_2 + x_2^2 y_2^2$$
$$= (x_1 y_1 + x_2 y_2)^2 = (x^\top y)^2$$

What $k(x, y)$ can be called a kernel function?

- $k(x, y)$ equivalent to compute inner product of features

$$k(x, y) = \phi(x)^{\top}\phi(y)$$

- Given a dataset $D = \{x^1, \ldots x^m\}$, compute pairwise kernel function $k\left(x^i, x^j\right)$ and form a $m \times m$ kernel matrix (Gram matrix)

$$K = \begin{pmatrix} k(x^1, x^1) & \ldots & k(x^1, x^m) \\ \vdots & \ddots & \vdots \\ k(x^m, x^1) & \ldots & k(x^m, x^m) \end{pmatrix}$$

- $k(x, y)$ is a kernel function, if and only if the Gram matrix K is positive semi-definite

$$\forall v \in R^m, v^{\top}Kv \geq 0$$

Typical kernel for vector data

- Polynomial of degree d
  - $k(x, y) = (x^\top y)^d$
- Polynomial of degree up to d
  - $k(x, y) = (x^\top y + c)^d$
- Exponential kernel (infinite degree polynomials)
  - $k(x, y) = \exp(s \cdot x^\top y)$
- Gaussian RBF kernel
  - $k(x, y) = \exp\left(-\frac{\|x-y\|^2}{2\sigma^2}\right)$
- Laplace Kernel
  - $k(x, y) = \exp\left(-\frac{\|x-y\|}{2\sigma^2}\right)$
- Exponentiated distance
  - $k(x, y) = \exp\left(-\frac{d(x,y)^2}{s^2}\right)$

Kernel are used to develop nonlinear methods

- Strategy: We do not directly construct feature map, but choose a kernel function (represent inner product of data features)
- Replacing inner product with kernels
- Examples
    - Kernel SVM
    - Kernel Ridge regression
    - Kernel PCA
    - Kernel method for comparing distributions (two-sample test)

Example: SVM dual problem and kernelize

- Dual problem for SVM

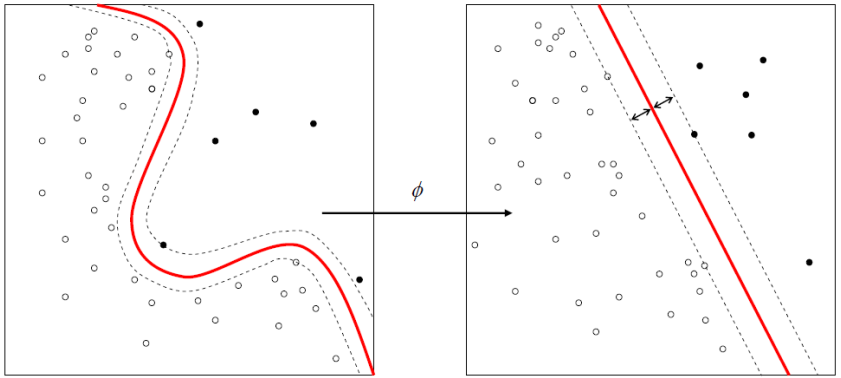
$$\text{Max}_\alpha \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y^i y^j x^{i\top} x^j$$

$$s.t. \sum_i \alpha_i y^i = 0$$

$$0 \le \alpha_i \le C$$

Replace by $k(x^i, x^j)$

- Equivalent to finding a non-linear decision boundary
  - implicitly map data to a new nonlinear feature space
  - find linear decision boundary in the new space



Developing kernel ridge regression

- Matrix inversion lemma ($B \in R^{n \times m}$):

$$(BB^\top + \lambda I)^{-1} B = B(B^\top B + \lambda I)^{-1}$$

- Note that $X = (x^1, x^2, \ldots x^m)$

- Evaluate ridge regression solution: $\theta^r = (XX^\top + \lambda I)^{-1} Xy$ on a new test point x

$$\begin{aligned} x^\top \theta^r &= x^\top (XX^\top + \lambda I)^{-1} \, Xy \\ &= x^\top X (X^\top X + \lambda I)^{-1} \, y \end{aligned}$$

Kernel ridge regression

- Prediction

$$x^\top \theta^r = \theta^{rT} x = y^\top (X^\top X + \lambda I_n)^{-1} X^\top x$$

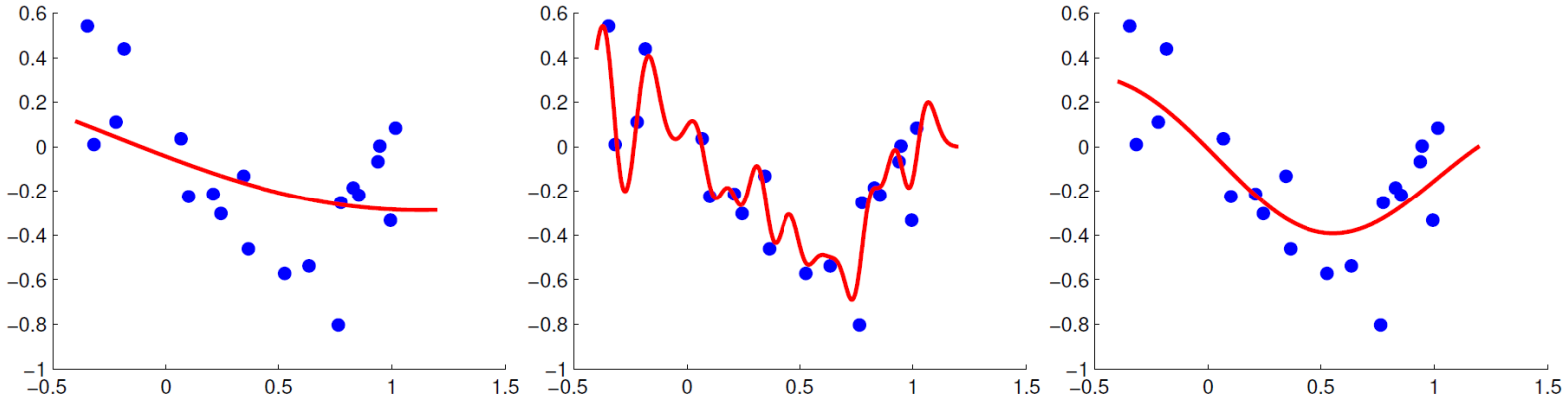
only depends on inner products!

- Kernel ridge regression: replace inner product by a kernel function
  - $X^\top X \to K = \left(k\left(x^i, x^j\right)\right)_{m \times m}$
  - $X^\top x \to k_x = \left(k\left(x^i, x\right)\right)_{m \times 1}$
  - Prediction $f(x) = y^\top (K + \lambda I_n)^{-1} k_x$

Kernel ridge regression

Use Gaussian rbf kernel

$$k(x, y) = \exp\left(-\frac{\|x-y\|^2}{2\sigma^2}\right)$$



$large\ \sigma, large\ \lambda$ | $small\ \sigma, small\ \lambda$ | $small\ \sigma, large\ \lambda$

Use cross-validation to choose parameters

Principal component analysis (PCA)

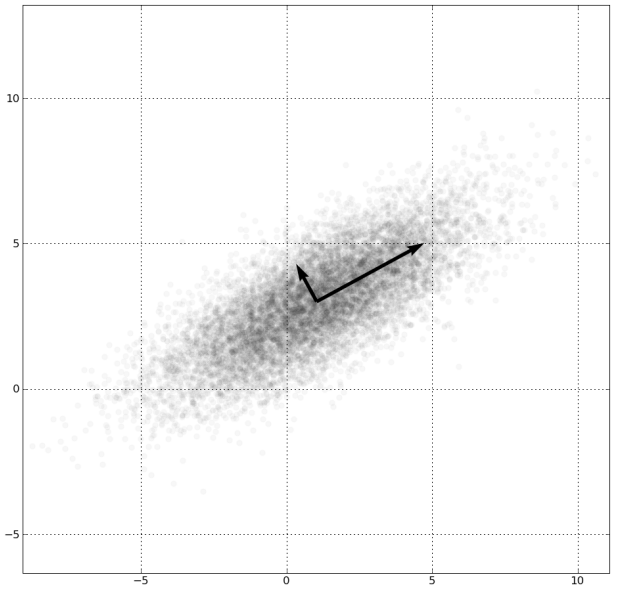
- Given a set of m centered observations $x^i \in R^d$, PCA finds the direction that maximizes the variance

$$w^* = argmax_{\|w\|\leq 1} \frac{1}{m} \sum_i \left(w^\top x^i\right)^2$$

$$= argmax_{\|w\|\leq 1} \frac{1}{m} w^\top X X^\top w$$

- $X = (x^1, x^2, \ldots, x^m)$
- $C = \frac{1}{m} X X^\top$
- w^* can be found by solving the following eigenvalue problem

$$Cw = \lambda w$$



Alternative expression for PCA

- We can show the principal component lies in the span of the data

$$w = \sum_{i=1}^{m} \alpha_i x^i = X\alpha$$

- Plug this in we have
  - $Cw = \frac{1}{m} XX^\top X\alpha = \lambda\, X\alpha = \lambda w$

- Furthermore, for each data point x^i, the following relation holds
  - ${x^i}^\top Cw = \frac{1}{m} {x^i}^\top XX^\top X\alpha = \lambda {x^i}^\top X\alpha, \forall i$
  - In matrix form, $\frac{1}{m} X^\top XX^\top X\alpha = \lambda X^\top X\alpha$

Only depends on inner product matrix

Kernel PCA

- Key Idea: Replace inner product matrix by kernel matrix
  - PCA: $\frac{1}{M} X^\top X X^\top X \alpha = \lambda X^\top X \alpha$
- Kernel PCA:
  - $\frac{1}{m} K K \alpha = \lambda K \alpha$, equivalent to

$$\frac{1}{m} K \alpha = \lambda \alpha$$

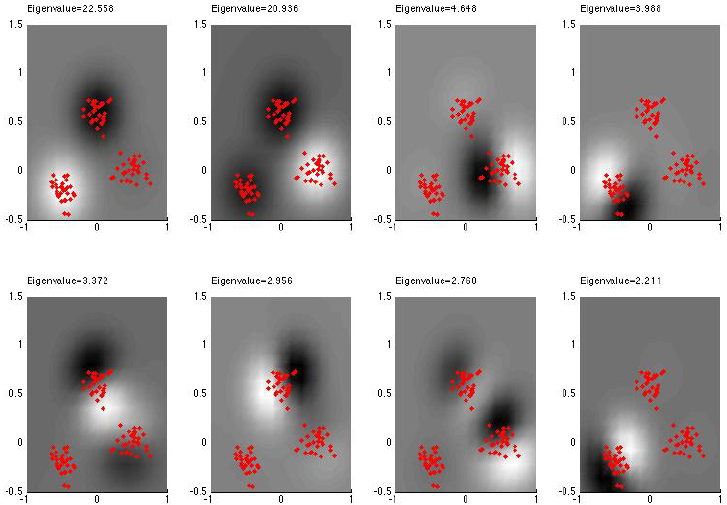
assuming Gram matrix is invertible

form an $m \times m$ kernel matrix K, and then perform eigen-decomposition on K

Kernel PCA

- Gaussian RBF kernel $\exp\left(-\frac{\|x-x'\|^2}{2\sigma^2}\right)$ over 2-dimensional space
- Eigenvector evaluated at a test point x is a function

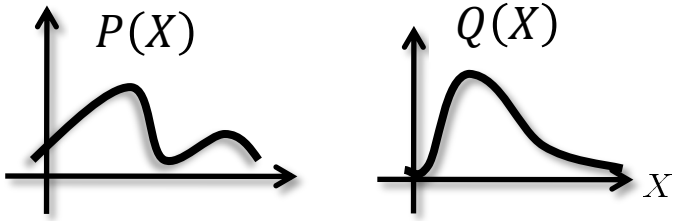
$$w^\top \phi(x) = \sum_i \alpha_i \langle \phi(x^i), \phi(x) \rangle = \sum_i \alpha_i k(x^i, x)$$



Comparing two distributions (two-sample test)

- Two-sample test for general distributions,
  - $H_0: P(x) = Q(x)?$
- We can use KL-divergence

$$KL(P||Q) = \int P(x) \log \frac{P(x)}{Q(x)} dx$$



- Given a set of samples

$$(x^1, \dots, x^m) \sim P(X), \left(\tilde{x}^1, \dots, \tilde{x}^{m'}\right) \sim Q(X)$$

$$\int P(x) \log \frac{P(x)}{Q(x)} dx \approx \int \hat{P}(x) \log \frac{\hat{P}(x)}{\hat{Q}(x)} dx$$

Need to estimate the density function first, and they can be noisy

Embedding distributions into feature space

- Summary statistics for distributions

$E_{X\sim P}[X]$ Mean

$E_{X\sim P}[XX^T]$ Covariance

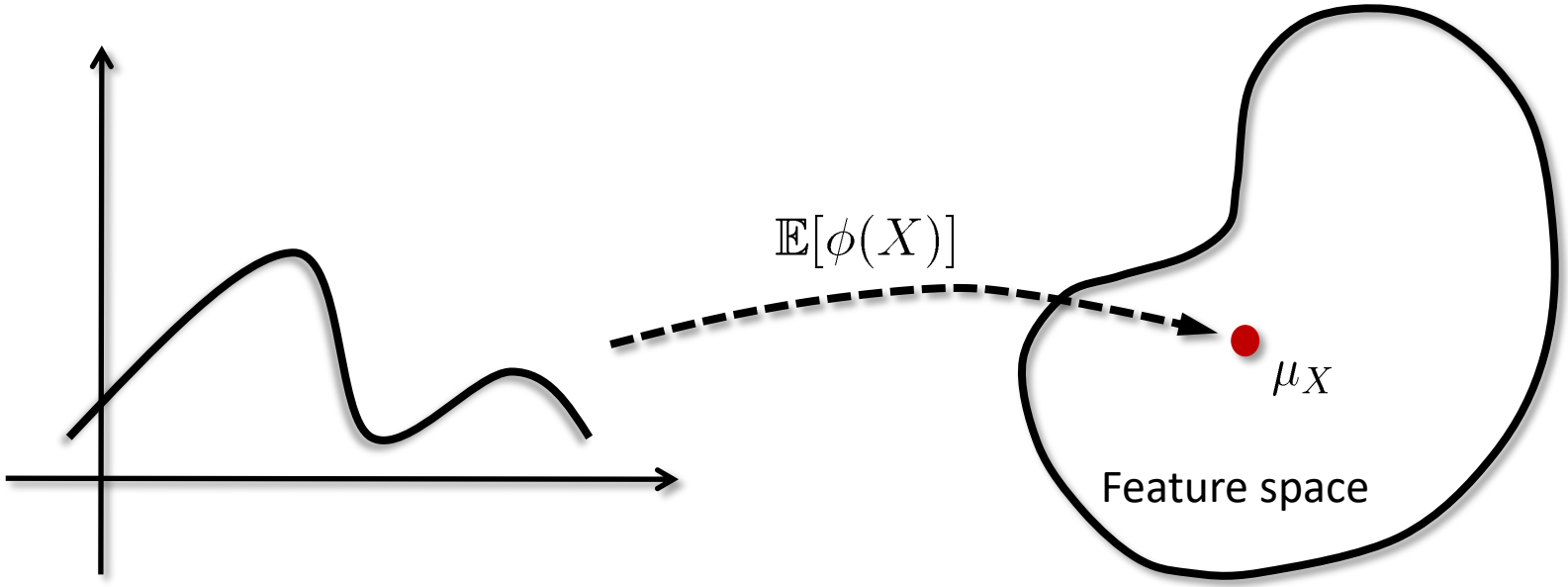
$E_{X\sim P}[\phi(X)]$ expected features

- Pick a kernel, and generate a different summary statistic

$$k(x, x') = \langle \phi(x), \phi(x') \rangle$$

Illustration: embedding of distribution

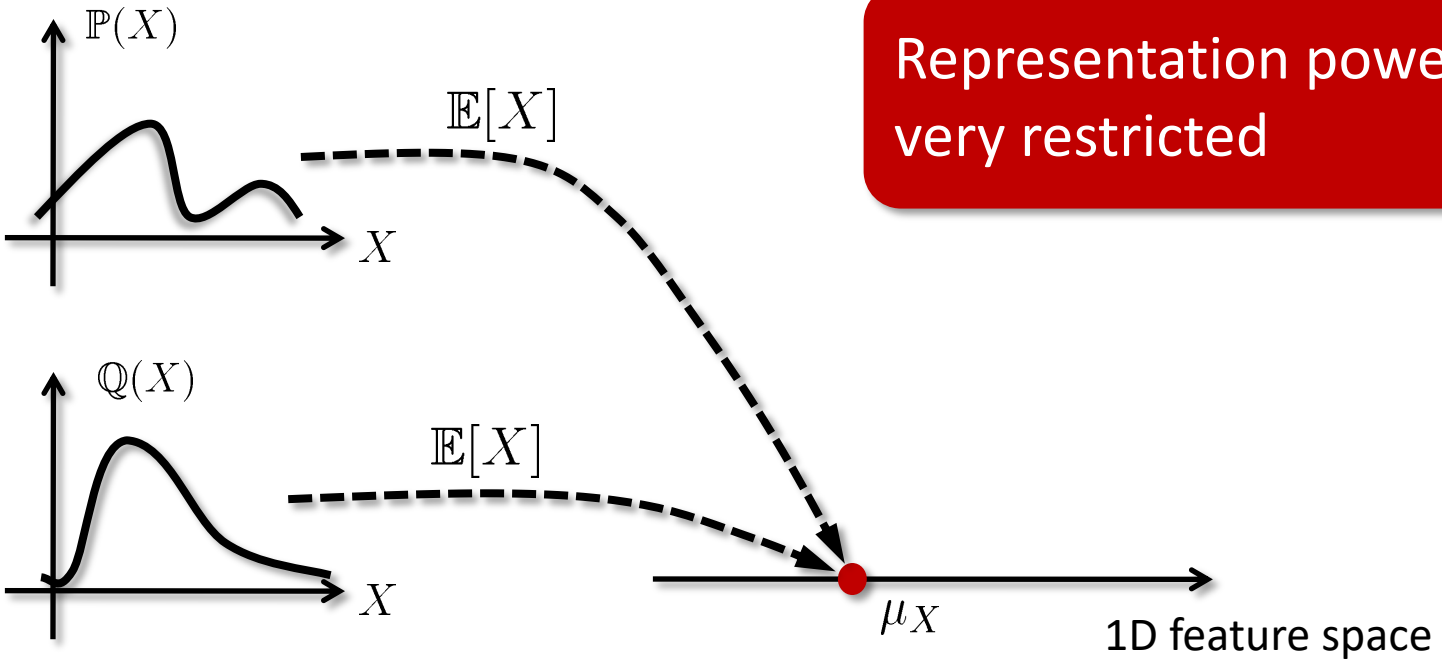
Transform the ***entire*** distribution to expected features



Feature map: $\phi(X)$

Embedding distributions: Mean

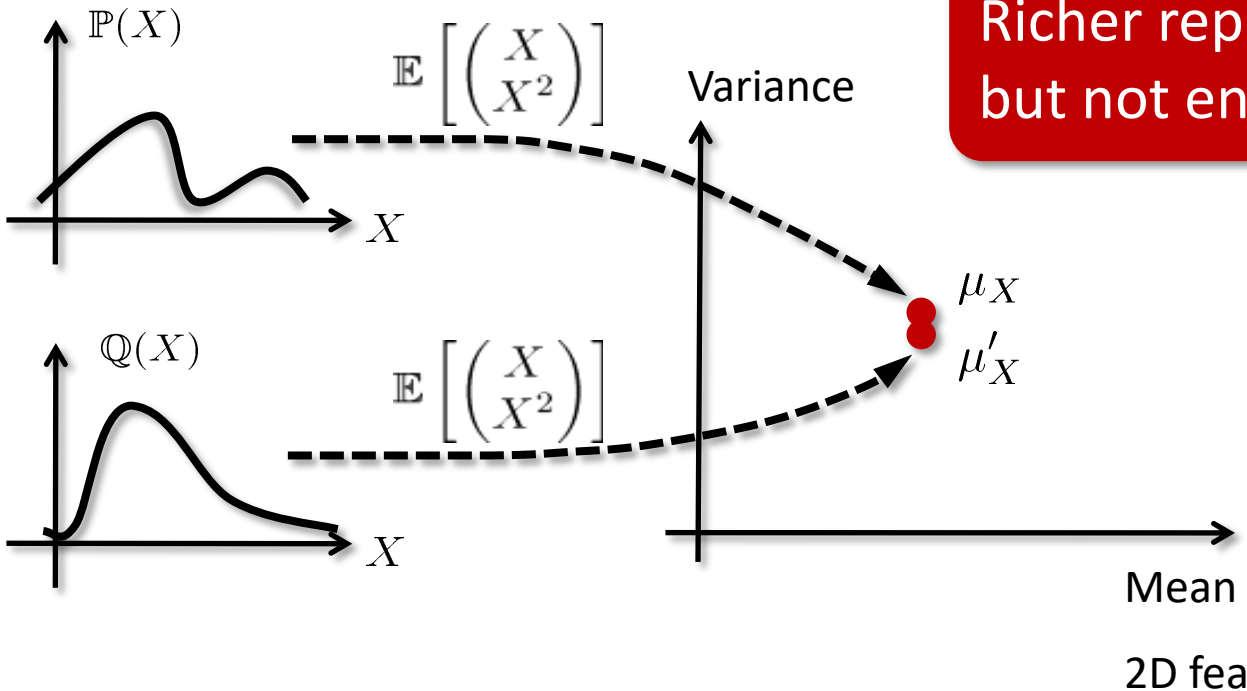
Mean reduces the ***entire*** distribution to a single number



Representation power very restricted

Embedding distributions: Mean + Variance

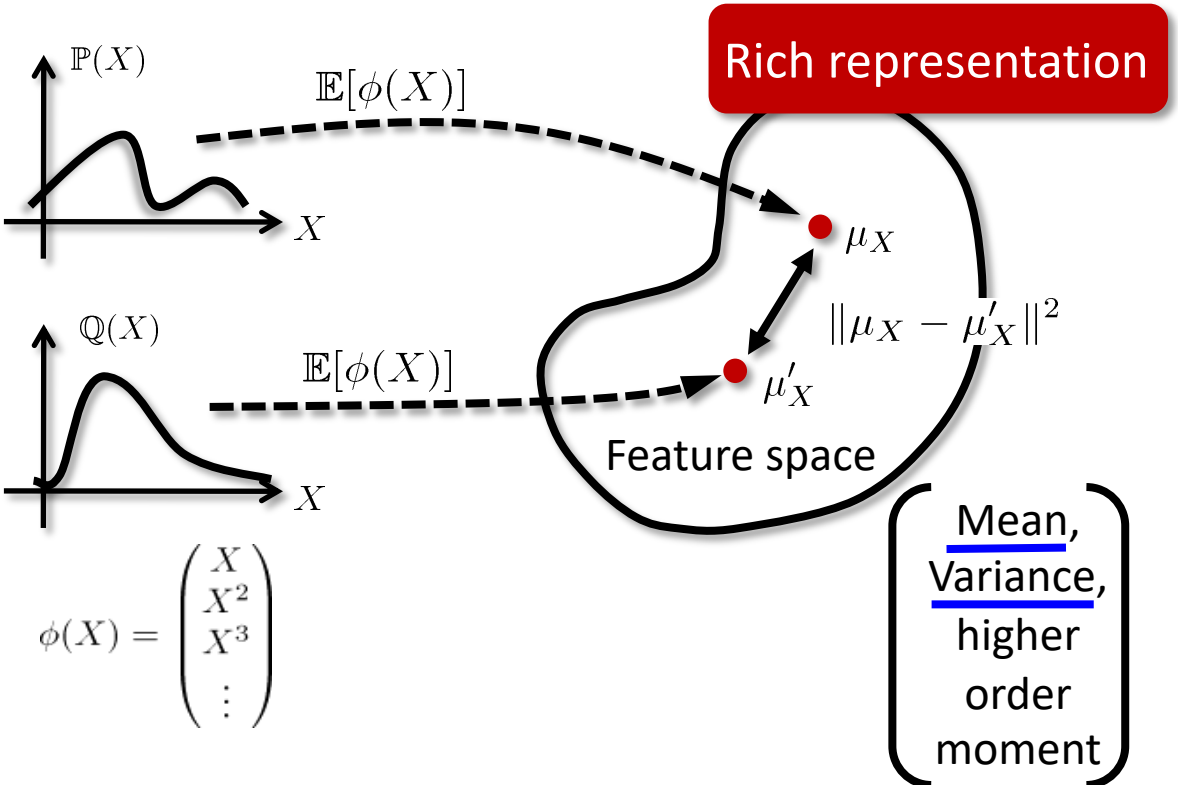
Mean and variance reduces the ***entire*** distribution to two numbers



Richer representation, but not enough

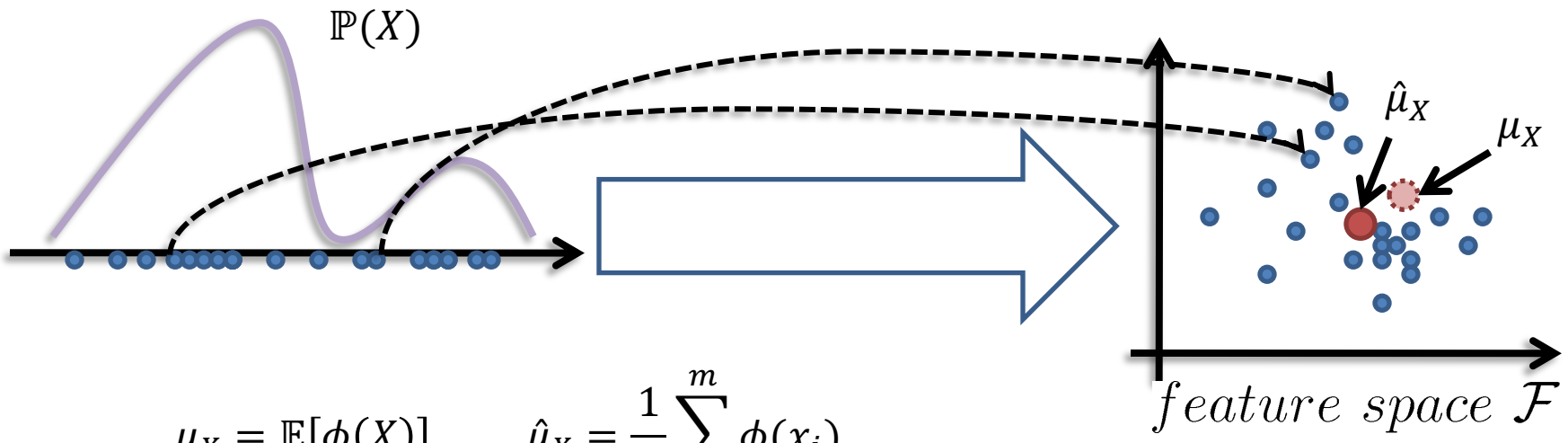
Embedding with kernel features

Transform distribution to infinite dimensional vector



Empirical estimation using data

- One-to-one mapping from $\mathbb{P}(X)$ to $\mu(X)$ for given kernels
- Sample average converges to true mean at $O_p(m^{-1/2})$



$$\mu_X = \mathbb{E}[\phi(X)], \qquad \hat{\mu}_X = \frac{1}{m}\sum_{i=1}^{m}\phi(x_i)$$

Estimating embedding distances

- Given samples $(x^1, \ldots, x^m) \sim P(X), \left(\tilde{x}^1, \ldots, \tilde{x}^{m'}\right) \sim Q(X)$
- Distance between distributions can be represented as inner products

$$||\mu_X - \mu'_X||^2 = \langle \mu_X, \mu_X \rangle - 2\langle \mu_X, \mu'_X \rangle + \langle \mu'_X, \mu'_X \rangle$$

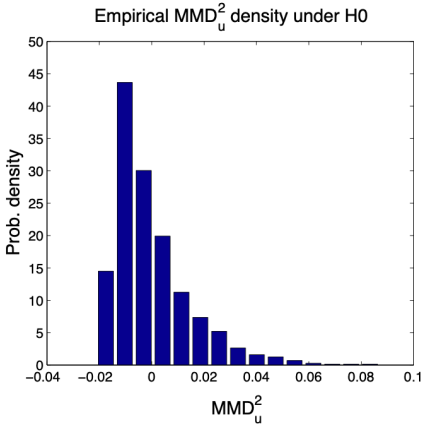
$$\begin{aligned} \langle \mu_X, \mu'_X \rangle &= \left\langle \mathbb{E}_{X \sim P}[\phi(X)], \mathbb{E}_{X' \sim Q}[\phi(X')] \right\rangle \\ &= \mathbb{E}_{X \sim P, X' \sim Q}[\underbrace{\langle \phi(X), \phi(X') \rangle}_{k(X, X')}] \end{aligned}$$

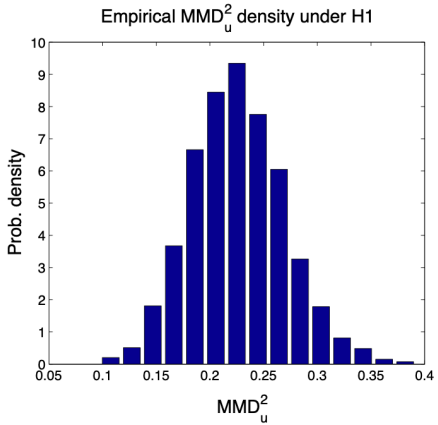
$$\approx \frac{1}{mm'} \sum_{i=1}^{m} \sum_{j=1}^{m'} k\left(x^i, \tilde{x}^j\right)$$

Empirical estimates

Kernel two-sample test

- Given two sets of samples $(x^1, \ldots, x^m) \sim P(X), \left(\tilde{x}^1, \ldots, \tilde{x}^{m'}\right) \sim Q(X)$
- Decide the distributions of the two sets of samples are different when the empirical estimate of $||\mu_X - \mu'_X||^2$ is greater than a threshold
- Application: anomaly detection, clinical trial - deciding whether or not a drug is effective, etc.





Gretton, Arthur, Karsten M. Borgwardt, Malte J. Rasch, Bernhard Schölkopf, and Alexander Smola. "A kernel two-sample test." *The Journal of Machine Learning Research* 13, no. 1 (2012): 723-773.


SUMMARY