Kernel-Based Contrast Functions for Sufficient Dimension Reduction

K. Fukumizu, F. Bach, & M. I. Jordan, (2009).
Annals of Statistics, 37, 1871-1905.

Outline

- Introduction
  – dimension reduction and conditional independence
- Conditional covariance operators on RKHS
- Kernel Dimensionality Reduction for regression
- Manifold KDR
- Summary

Sufficient Dimension Reduction

- Regression setting: observe (X,Y) pairs, where the covariate X is high-dimensional
- Find a (hopefully small) subspace S of the covariate space that retains the information pertinent to the response Y
- *Semiparametric formulation*: treat the conditional distribution $p(Y \mid X)$ nonparametrically, and estimate the parameter S

Perspectives

- Classically the covariate vector *X* has been treated as ancillary in regression
- The sufficient dimension reduction (SDR) literature has aimed at making use of the randomness in *X* (in settings where this is reasonable)
- This has generally been achieved via inverse regression
    - at the cost of introducing strong assumptions on the distribution of the covariate *X*
- We'll make use of the randomness in *X* without employing inverse regression

Dimension Reduction for Regression

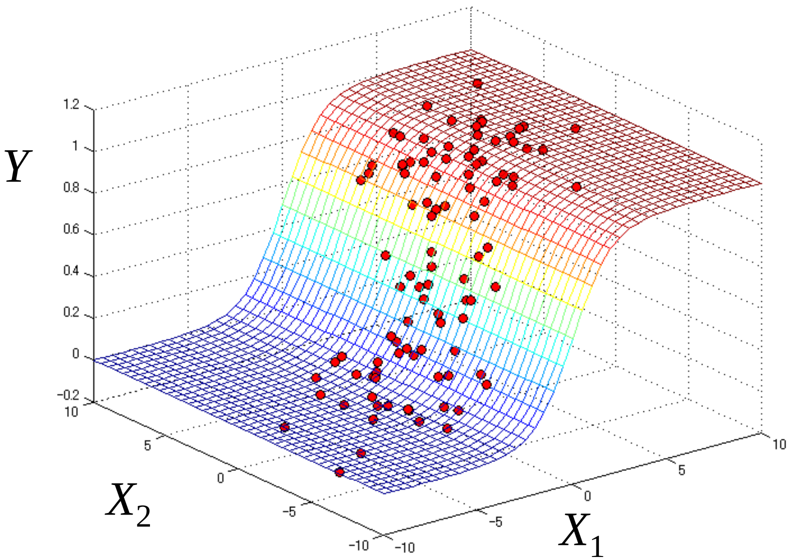
- Regression: $p(Y \mid X)$

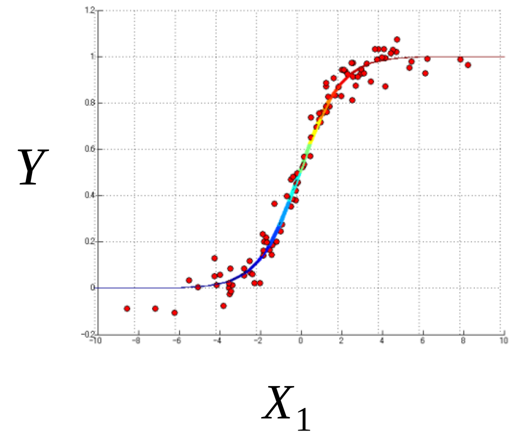
  Y : response variable,

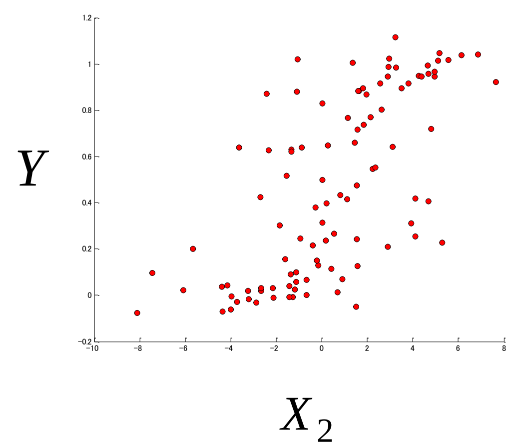
  $X = (X_1,...,X_m)$: m-dimensional covariate

- Goal: Find the central subspace, which is defined via:

$$p(Y \mid X) = \tilde{p}(Y \mid b_1^T X, ..., b_d^T X) \quad \left(= \tilde{p}(Y \mid B^T X) \right)$$







$$Y = \frac{1}{1+\exp(-X_1)} + N(0; 0.1^2)$$

central subspace = X_1 axis

Some Existing Methods

- Sliced Inverse Regression (SIR, Li 1991)
  - PCA of $\mathrm{E}[X|Y]$ → use slice of Y
  - Elliptic assumption on the distribution of X
- Principal Hessian Directions (pHd, Li 1992)
  - Average Hessian $\Sigma_{yxx} \equiv E[(Y-\bar{Y})(X-\bar{X})(X-\bar{X})^T]$ is used
  - If X is Gaussian, eigenvectors gives the central subspace
  - Gaussian assumption on X. Y must be one-dimensional
- Projection pursuit approach (e.g., Friedman et al. 1981)
  - Additive model $E[Y|X] = g_1(b_1^T X) + \ldots + g_d(b_d^T X)$ is used
- Canonical Correlation Analysis (CCA) / Partial Least Squares (PLS)
  - Linear assumption on the regression
- Contour Regression (Li, Zha & Chiaromonte, 2004)
  - Elliptic assumption on the distribution of X

Dimension Reduction and Conditional Independence

- $(U, V)=(B^T X, C^T X)$

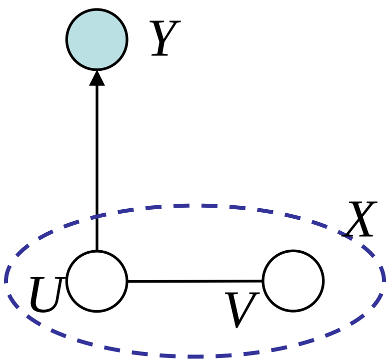
  where C: m x $(m\text{-}d)$ with columns orthogonal to B

- B gives the projector onto the central subspace

  $\Leftrightarrow \quad p_{Y|X}(y \mid x) = p_{Y|U}(y \mid B^T x)$

  $\Leftrightarrow \quad p_{Y|U,V}(y \mid u,v) = p_{Y|U}(y \mid u)$ for all y,u,v

  $\Leftrightarrow$ Conditional independence $Y \perp\!\!\!\perp V \mid U$



- Our approach: *Characterize conditional independence*

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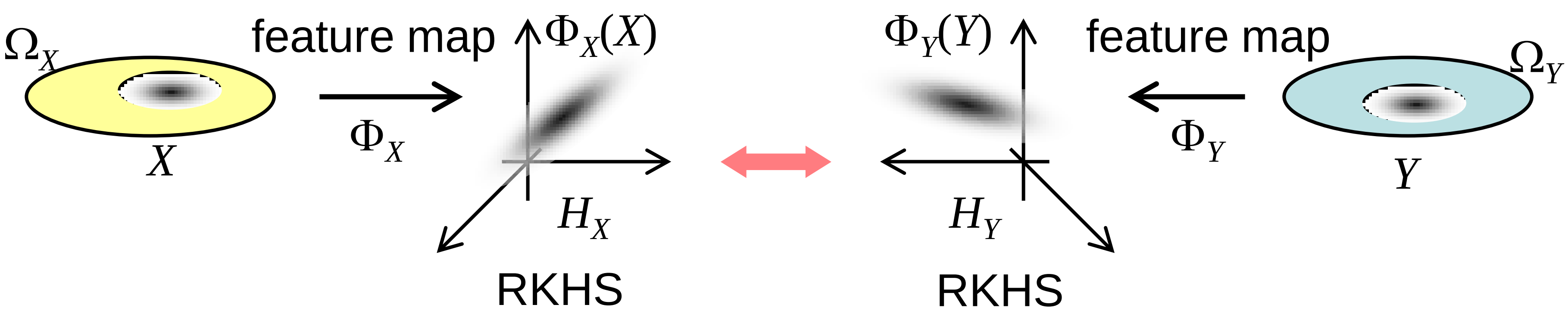
Reproducing Kernel Hilbert Spaces

- "Kernel methods"
  - RKHS's have generally been used to provide basis expansions for regression and classification (*e.g.*, support vector machine)
  - *Kernelization*: map data into the RKHS and apply linear or second-order methods in the RKHS
  - But RKHS's can also be used to characterize independence and conditional independence



Positive Definite Kernels and RKHS

- Positive definite kernel (p.d. kernel)

  $k : \Omega \times \Omega \to \mathbf{R}$

  k is positive definite if $k(x,y) = k(y,x)$ and for any $n \in \mathbf{N}$, $x_1, \ldots x_n \in \Omega$ the matrix $\left(k(x_i, x_j)\right)_{i,j}$ (Gram matrix) is positive semidefinite.

  – Example: Gaussian RBF kernel $k(x,y) = \exp\left(-\|x-y\|^2/\sigma^2\right)$

- Reproducing kernel Hilbert space (RKHS)

  k: p.d. kernel on Ω

  $\Rightarrow$ $\exists H$: reproducing kernel Hilbert space (RKHS)

  1) $k(\cdot, x) \in H$ for all $x \in \Omega$.

  2) $\mathrm{Span}\{k(\cdot, x) \mid x \in \Omega\}$ is dense in H.

  3) $\langle k(\cdot, x), f \rangle_H = f(x)$ (reproducing property)

Functional data

$$\Phi : \Omega \to H, \quad x \mapsto k(\cdot, x) \qquad i.e. \quad \Phi(x) = k(\cdot, x)$$

Data: $X_1, \ldots, X_N$ → $\Phi_X(X_1), \ldots, \Phi_X(X_N)$: functional data

Why RKHS?

- By the reproducing property, computing the inner product on RKHS is easy:

$$\langle \Phi(x), \Phi(y) \rangle = k(x, y)$$

$$f = \sum_{i=1}^{N} a_i \Phi(x_i) = \sum_i a_i k(\cdot, x_i), \qquad g = \sum_{j=1}^{N} b_j \Phi(x_j) = \sum_j b_j k(\cdot, x_j)$$

$$\Rightarrow \quad \langle f, g \rangle = \sum_{i,j} a_i b_j k(x_i, x_j)$$

- The computational cost essentially depends on the sample size. Advantageous for high-dimensional data of small sample size.

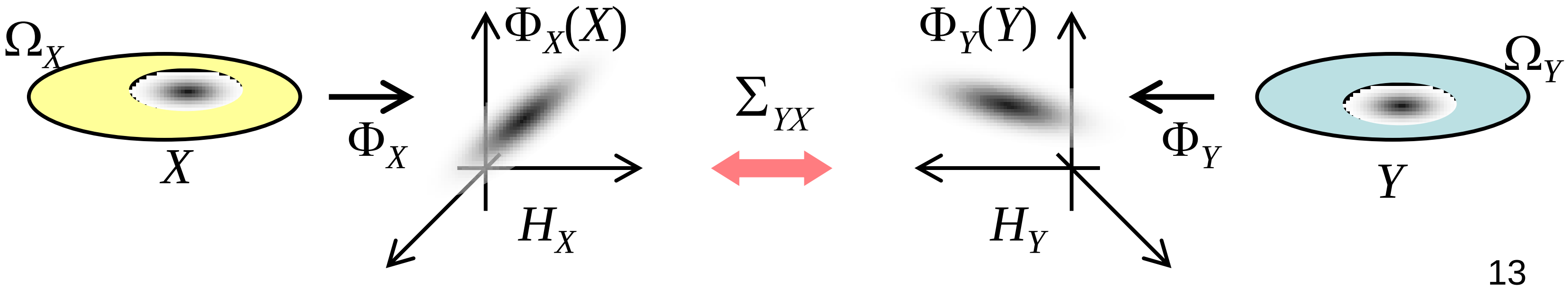
Covariance Operators on RKHS

- X , Y : random variables on Ω_X and Ω_Y , resp.
- Prepare RKHS (H_X, k_X) and (H_Y, k_Y) defined on Ω_X and Ω_Y, resp.
- Define random variables on the RKHS H_X and H_Y by

$$\Phi_X(X) = k_X(\cdot, X) \qquad \Phi_Y(Y) = k_Y(\cdot, Y)$$

- Define the covariance operator Σ_{YX}

$$\Sigma_{YX} = E[\Phi_Y(Y)\langle \Phi_X(X), \cdot \rangle] - E[\Phi_Y(Y)]E[\langle \Phi_X(X), \cdot \rangle]$$



Covariance Operators on RKHS

- Definition

$$\Sigma_{YX} = E[\Phi_Y(Y)\langle \Phi_X(X), \cdot \rangle] - E[\Phi_Y(Y)]E[\langle \Phi_X(X), \cdot \rangle]$$

Σ_{YX} is an operator from H_X to H_Y such that

$$\langle g, \Sigma_{YX} f \rangle = E[g(Y) f(X)] - E[g(Y)]E[f(X)] \quad (= \mathrm{Cov}[f(X), g(Y)])$$

for all $f \in H_X, g \in H_Y$

- *cf.* Euclidean case

$V_{YX} = \mathrm{E}[YX^T] - \mathrm{E}[Y]\mathrm{E}[X]^T$: covariance matrix

$$(b, V_{YX} a) = Cov[(b, Y), (a, X)]$$

Characterization of Independence

- Independence and cross-covariance operators

If the RKHS's are "rich enough":

$$X \perp\!\!\!\perp Y \quad \Leftrightarrow \quad \Sigma_{XY} = O$$

$$\Updownarrow$$

$\mathrm{Cov}[f(X), g(Y)] = 0$

or

$E[g(Y)f(X)] = E[g(Y)]E[f(X)]$

for all $f \in H_X, g \in H_Y$

$\Rightarrow$ is always true

$\Leftarrow$ requires an assumption on the kernel (universality)

e.g., Gaussian RBF kernels are universal

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

– *cf*. for Gaussian variables,

X and Y are independent $\Leftrightarrow$ $V_{XY} = O$ i.e. uncorrelated

- Independence and characteristic functions

  Random variables X and Y are independent

$$\Leftrightarrow \; E_{XY}\left[e^{i\omega^T X} e^{i\eta^T Y}\right] = E_X\left[e^{i\omega^T X}\right] E_Y\left[e^{i\eta^T Y}\right] \qquad \text{for all } \omega \text{ and } \eta$$

  I.e., $e^{i\omega^T x}$ and $e^{i\eta^T y}$ work as test functions

- RKHS characterization

  Random variables $X \in \Omega_X$ and $Y \in \Omega_Y$ are independent

$$\Leftrightarrow \quad E_{XY}\left[f(X)g(Y)\right] = E_X\left[f(X)\right] E_Y\left[g(Y)\right] \qquad \text{for all } f \in \mathcal{H}_X, \; g \in \mathcal{H}_Y$$

  – RKHS approach is a generalization of the characteristic-function approach

RKHS and Conditional Independence

- Conditional covariance operator

  X and Y are random vectors. $\mathcal{H}_X$, $\mathcal{H}_Y$: RKHS with kernel k_X, k_Y, resp.

  Def. $\Sigma_{YY|X} \equiv \Sigma_{YY} - \Sigma_{YX}\Sigma_{XX}^{-1}\Sigma_{XY}$: conditional covariance operator

  – Under a universality assumption on the kernel

$$\langle g, \Sigma_{YY|X} g \rangle = E\left[\mathrm{Var}[g(Y) \mid X]\right]$$

  cf. For Gaussian $\mathrm{Var}_{Y|X}[a^T Y \mid X = x] = a^T \left(V_{YY} - V_{YX} V_{XX}^{-1} V_{XY}\right) a$

  – Monotonicity of conditional covariance operators

  $X = (U, V)$: random vectors

$$\boxed{\Sigma_{YY|U} \geq \Sigma_{YY|X}}$$

$\geq$: in the sense of self-adjoint operators

- Conditional independence

Theorem

$X = (U,V)$ and Y are random vectors.

$\mathcal{H}_X$, $\mathcal{H}_U$, $\mathcal{H}_Y$: RKHS with Gaussian kernel k_X, k_U, k_Y, resp.

$$\Rightarrow \qquad Y \perp\!\!\!\perp V \mid U \quad \Leftrightarrow \quad \Sigma_{YY|U} = \Sigma_{YY|X}$$

This theorem provides a new methodology for solving the sufficient dimension reduction problem

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Kernel Dimension Reduction

- Use a universal kernel for $B^T X$ and Y

$$\Sigma_{YY|B^T X} \geq \Sigma_{YY|X}$$

($\geq$: the partial order of self-adjoint operators)

$$\Sigma_{YY|B^T X} = \Sigma_{YY|X} \quad \Leftrightarrow \quad X \perp\!\!\!\perp Y \mid B^T X$$

- KDR objective function:

$$\boxed{\min_{B:\, B^T B = I_d} \mathrm{Tr}\left[\Sigma_{YY|B^T X} \right]}$$

which is an optimization over the Stiefel manifold

Estimator

- Empirical cross-covariance operator

$$\hat{\Sigma}_{YX}^{(N)} = \frac{1}{N}\sum_{i=1}^{N}\left\{k_Y(\cdot, Y_i) - \hat{m}_Y\right\} \otimes \left\{k_X(\cdot, X_i) - \hat{m}_X\right\}$$

$$\hat{m}_X = \frac{1}{N}\sum_{i=1}^{N} k_X(\cdot, X_i) \qquad \hat{m}_Y = \frac{1}{N}\sum_{i=1}^{N} k_Y(\cdot, Y_i)$$

$\hat{\Sigma}_{YX}^{(N)}$ gives the empirical covariance:

$$\left\langle g, \hat{\Sigma}_{YX}^{(N)} f \right\rangle = \tfrac{1}{N}\sum_{i=1}^{N} f(X_i) g(Y_i) - \tfrac{1}{N}\sum_{i=1}^{N} f(X_i)\,\tfrac{1}{N}\sum_{i=1}^{N} g(Y_i)$$

- Empirical conditional covariance operator

$$\hat{\Sigma}_{YY|X}^{(N)} = \hat{\Sigma}_{YY}^{(N)} - \hat{\Sigma}_{YX}^{(N)}\left(\hat{\Sigma}_{XX}^{(N)} + \varepsilon_N I\right)^{-1}\hat{\Sigma}_{XY}^{(N)}$$

ε_N: regularization coefficient

- Estimating function for KDR:

$$\mathrm{Tr}\left[\hat{\Sigma}_{YY|U}^{(N)}\right] = \mathrm{Tr}\left[\hat{\Sigma}_{YY}^{(N)} - \hat{\Sigma}_{YU}^{(N)}\left(\hat{\Sigma}_{UU}^{(N)} + \varepsilon_N I\right)^{-1}\hat{\Sigma}_{UY}^{(N)}\right] \qquad U = B^T X$$

$$= \mathrm{Tr}\left[G_Y - G_Y G_U\left(G_U + N\varepsilon_N I_N\right)^{-1}\right]$$

where

$$G_U = \left(I_N - \tfrac{1}{N}\mathbf{1}_N\mathbf{1}_N^T\right)K_U\left(I_N - \tfrac{1}{N}\mathbf{1}_N\mathbf{1}_N^T\right)$$: centered Gram matrix

$$K_U = k(B^T X_i, B^T X_j)$$

- Optimization problem:

$$\boxed{\min_{B:B^T B = I_d} \mathrm{Tr}\left[G_Y\left(G_{B^T X} + N\varepsilon_N I_N\right)^{-1}\right]}$$

Experiments with KDR

■ Wine data

Data

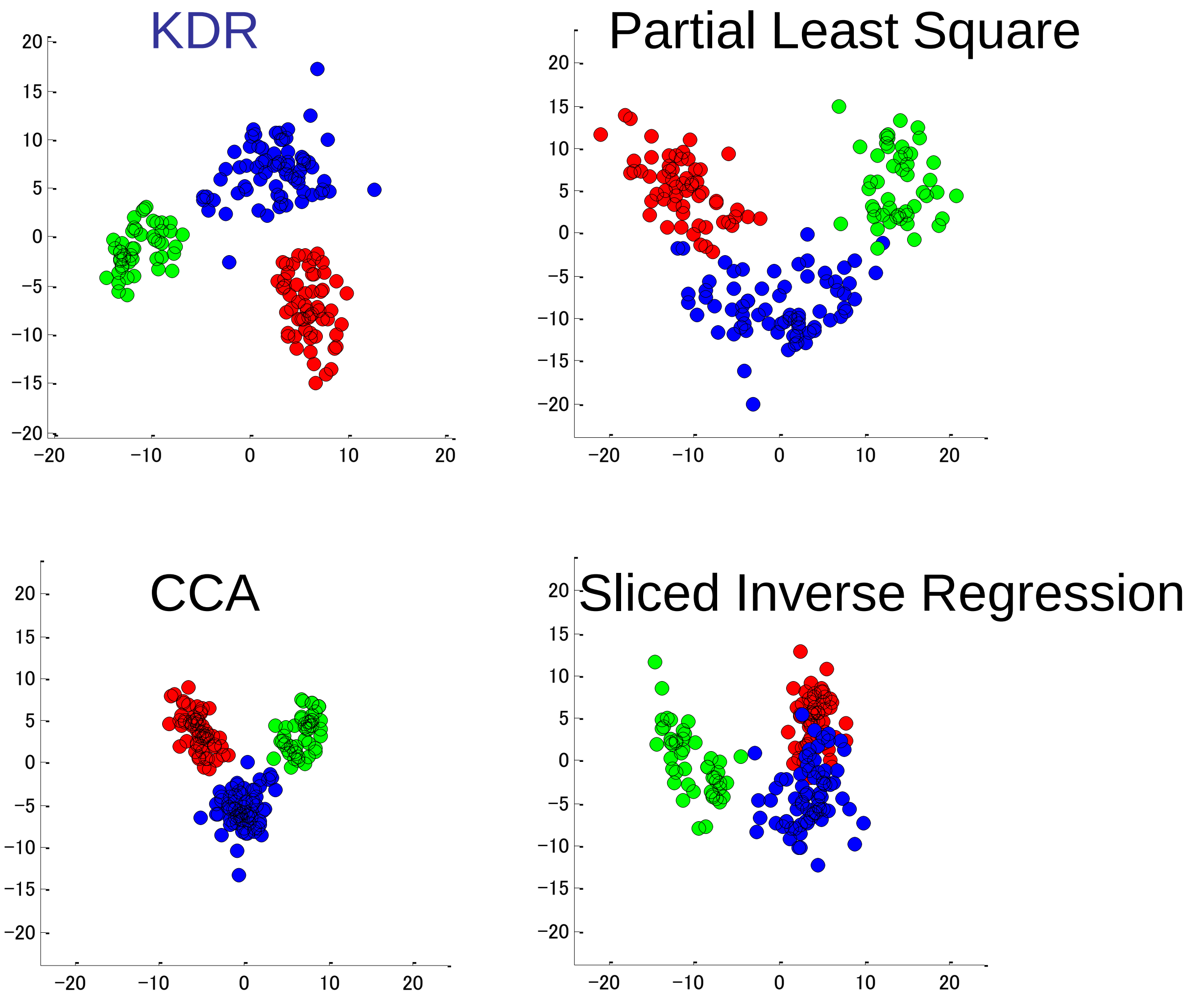
13 dim. 178 data

3 classes

2 dim. projection

$$k(z_1, z_2) = \exp\left(-\|z_1 - z_2\|^2 / \sigma^2\right)$$

$$\sigma = 30$$



Consistency of KDR

<u>Theorem</u>

Suppose k_d is bounded and continuous, and

$$\varepsilon_N \to 0,\ \ N^{1/2}\varepsilon_N \to \infty \ \ (N \to \infty).$$

Let S_0 be the set of optimal parameters:

$$S_0 = \left\{ B \mid B^T B = I_d,\ \mathrm{Tr}\left[\Sigma_{YY|X}^{B} \right] = \min_{B'} \mathrm{Tr}\left[\Sigma_{YY|X}^{B'} \right] \right\}$$

Then, under some conditions, for any open set $U \supset S_0$

$$\Pr\left(\hat{B}^{(N)} \in U \right) \to 1 \quad (N \to \infty).$$

Lemma

Suppose k_d is bounded and continuous, and

$$\varepsilon_N \to 0, \ \ N^{1/2}\varepsilon_N \to \infty \ \ (N \to \infty).$$

Then, under some conditions,

$$\sup_{B:B^T B = I_d} \left| \mathrm{Tr}\left[\hat{\Sigma}_{YY|X}^{B(N)} \right] - \mathrm{Tr}\left[\Sigma_{YY|X}^{B} \right] \right| \to 0 \ \ (N \to \infty)$$

in probability.

Conclusions

- Are you a Bayesian or a frequentist?
- My own answer is “both,” but there are days where I'm much more clearly one than the other
  - and it is an ongoing intellectual challenge to try to understand the ramifications of this distinction
- I view them as complementary perspectives, but there is a wave/particle uncomfortableness at times
- A main conclusion: machine learning is a part of statistics; don't just read the machine learning literature---read, ponder and contribute to the broad statistical literature