Geometric perspectives for supervised dimension reduction

A Tale of Two Manifolds

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Information and sufficiency

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$X_1, ..., X_n$ drawn iid form a Gaussian can be reduced to μ, σ^2.

Regression

Assume the model

$$Y = f(X) + \varepsilon, \quad \mathbb{E}\varepsilon = 0,$$

with $X \in \mathcal{X} \subset \mathbb{R}^p$ and $Y \in \mathbb{R}$.

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Data – $D = \{(x_i, y_i)\}_{i=1}^n \overset{iid}{\sim} \rho(X, Y)$.

Dimension reduction

If the data lives in a p-dimensional space $X \in \mathbb{R}^p$ replace X with $\Theta(X) \in \mathbb{R}^d$, $p \gg d$.

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My belief: physical, biological and social systems are inherently low dimensional and variation of interest in these systems can be captured by a low-dimensional submanifold.

Supervised dimension reduction (SDR)

Given response variables $Y_1, ..., Y_n \in \mathbb{R}$ and explanatory variables or covariates $X_1, ..., X_n \in \mathcal{X} \subset \mathbb{R}^p$

$$Y_i = f(X_i) + \varepsilon_i, \quad \varepsilon_i \overset{iid}{\sim} \text{No}(0, \sigma^2).$$

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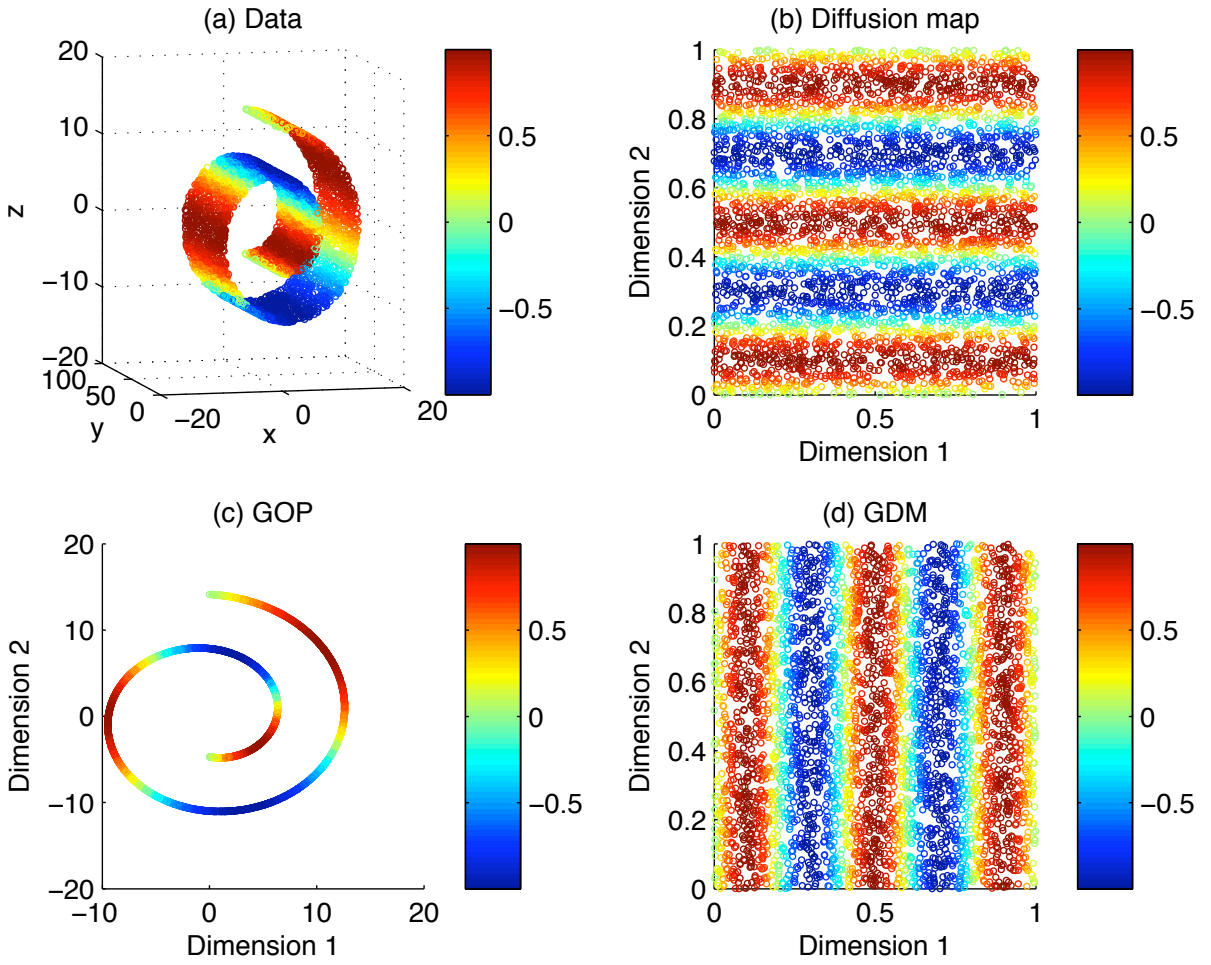
Is there a submanifold $\mathcal{S} \equiv \mathcal{S}_{Y|X}$ such that $Y \perp\!\!\!\perp X \mid P_{\mathcal{S}}(X)$?

Visualization of SDR



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Semiparametric model

$$Y_i = f(X_i) + \varepsilon_i = g(b_1^T X_i, \ldots, b_d^T X_i) + \varepsilon_i,$$

span B is the dimension reduction (d.r.) subspace.

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span B is the dimension reduction (d.r.) subspace.

Assume marginal distribution ρ_X is concentrated on a manifold $\mathcal{M} \subset \mathbb{R}^p$ of dimension $d \ll p$.

Gradients and outer products

Given a smooth function f the gradient is

$$\nabla f(x) = \left(\frac{\partial f(x)}{\partial x_1}, \ldots, \frac{\partial f(x)}{\partial x_p} \right)^T.$$

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Define the gradient outer product matrix Γ

$$\begin{aligned} \Gamma_{ij} &= \int_{\mathcal{X}} \frac{\partial f}{\partial x_i}(x) \frac{\partial f}{\partial x_j}(x) d\rho_X(x), \\ \Gamma &= \mathbb{E}[(\nabla f) \otimes (\nabla f)]. \end{aligned}$$

GOP captures the d.r. space

Suppose

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$$\lambda_i b_i = \Gamma b_i.$$

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Note that for $B = (b_1, ..., b_d)$

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For $i = 1, .., d$

$$\frac{\partial f(x)}{\partial v_i} = v_i^T \left(\nabla f(x)\right) \neq 0 \Rightarrow b_i^T \Gamma b_i \neq 0.$$

If $w \perp b_i$ for all i then $w^T \Gamma w = 0$.

Statistical interpretation

Linear case

$$y = \beta^T x + \varepsilon, \qquad \varepsilon \overset{iid}{\sim} \mathrm{No}(0, \sigma^2).$$

$\Omega = \mathrm{cov}\left(\mathbb{E}[X|Y]\right)$, $\Sigma_X = \mathrm{cov}\left(X\right)$, $\sigma_Y^2 = \mathrm{var}\left(Y\right)$.

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$$\Gamma = \sigma_Y^2 \left(1 - \frac{\sigma^2}{\sigma_Y^2}\right)^2 \Sigma_X^{-1} \Omega \Sigma_X^{-1} \approx \sigma_Y^2 \, \Sigma_X^{-1} \Omega \Sigma_X^{-1}.$$

Statistical interpretation

For smooth $f(x)$

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$\Omega = \mathrm{cov}\left(\mathbb{E}[X|Y]\right)$ not so clear.

Nonlinear case

Partition into sections and compute local quantities

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$$\Gamma \approx \sum_{i=1}^{\mathcal{I}} m_i \, \sigma_i^2 \, \Sigma_i^{-1} \, \Omega_i \, \Sigma_i^{-1}.$$

Estimating the gradient

Taylor expansion

$$\begin{aligned} y_i \approx f(x_i) &\approx f(x_j) + \langle \nabla f(x_j), x_j - x_i \rangle \\ &\approx y_j + \langle \nabla f(x_j), x_j - x_i \rangle \quad \text{if } x_i \approx x_j. \end{aligned}$$

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Let $\vec{f} \approx \nabla f$ the following should be small

$$\sum_{i,j} w_{ij} (y_i - y_j - \langle \vec{f}(x_j), x_j - x_i \rangle)^2,$$

$w_{ij} = \frac{1}{s^{p+2}} \exp(-\|x_i - x_j\|^2 / 2s^2)$ enforces $x_i \approx x_j$.

Estimating the gradient

The gradient estimate

$$\vec{f}_D = \arg\min_{\vec{f} \in \mathcal{H}^p} \left[\frac{1}{n^2} \sum_{i,j=1}^{n} w_{ij} \left(y_i - y_j - (\vec{f}(x_j))^T (x_j - x_i) \right)^2 + \lambda \|\vec{f}\|_K^2 \right]$$

where $\|\vec{f}\|_K$ is a smoothness penalty, reproducing kernel Hilbert space norm.

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Goto board.

Computational efficiency

The computation requires fewer than n^2 parameters and is $O(n^6)$ time and $O(pn)$ memory

$$\vec{f}_D(x) = \sum_{i=1}^{n} c_{i,D} K(x_i, x)$$

$c_D = (c_{1,D}, \ldots, c_{n,D})^T \in \mathbb{R}^{np}$.

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Define gram matrix K where $K_{ij} = K(x_i, x_j)$

$$\hat{\Gamma} = c_D K c_D^T.$$

Estimates on manifolds

Mrginal distribution ρ_X is concentrated on a compact Riemannian manifold $\mathcal{M} \in \mathbb{R}^d$ with isometric embedding $\varphi : \mathcal{M} \to \mathbb{R}^p$ and metric $d_{\mathcal{M}}$ and $\mathrm{d}\mu$ is the uniform measure on $\mathcal{M}$.
Assume regular distribution

(i) The density $\nu(x) = \frac{\mathrm{d}\rho_X(x)}{\mathrm{d}\mu}$ exists and is Hölder continuous ($c_1 > 0$ and $0 < \theta \leq 1$)

$$|\nu(x) - \nu(u)| \leq c_1 \, d^{\theta}_{\mathcal{M}}(x, u) \quad \forall x, u \in \mathcal{M}.$$

(ii) The measure along the boundary is small: ($c_2 > 0$)

$$\rho_{\mathcal{M}}\left(\{x \in \mathcal{M} : d_{\mathcal{M}}(x, \partial\mathcal{M}) \leq t\} \right) \leq c_2 \, t \qquad \forall t > 0.$$

Convergence to gradient on manifold

Theorem

Under above regularity conditions on ρ_X *and* $f \in C^2(\mathcal{M})$, *with probability* $1 - \delta$

$$\|(\mathrm{d}\varphi)^* \vec{f}_D - \nabla_{\mathcal{M}} f\|^2_{L^2_{\rho_{\mathcal{M}}}} \leq C \log\left(\frac{1}{\delta}\right)\left(n^{-\frac{1}{d}}\right).$$

where $(d\varphi)^*$ *(projection onto tangent space) is the dual of the map* $d\varphi$.

Multi-task learning

Definition

Single Task Notation n_t *samples* (x_i, y_i)
$x_i \in \mathbb{R}^d$
$y_i \in \{-1, 1\}$ *for classification*
Assume to be working in $d \gg n_t$ *paradigm.*

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Definition

Multi-task Learning (MTL) Formulation Given T *tasks with* $t \in \{1, \ldots, T\}$

$$F_t(x) = f_0(x) + f_t(x) + \varepsilon, \ \varepsilon \overset{iid}{\backsim} No(0, \sigma^2).$$

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Estimate not just the functions

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This provides us with $T + 1$ matrices

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1. $\hat{\Gamma}^0$ is the GOP estimate across all the tasks
2. $\hat{\Gamma}^1, \ldots, \hat{\Gamma}^T$ are the task specific GOP estimates.

Principal components analysis (PCA)

Algorithmic view of PCA:

1. Given $X = (X_1, ..., X_n)$ a $p \times n$ matrix construct

$$\hat{\Sigma} = (X - \bar{X})(X - \bar{X})^T$$

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2. Eigen-decomposition of $\hat{\Sigma}$

$$\lambda_i v_i = \hat{\Sigma} v_i.$$

Probabilistic PCA

$X \in \mathbb{R}^p$ is charterized by a multivariate normal

$$X \sim \mathrm{No}(\mu + A\nu, \Delta),$$
$$\nu \sim \mathrm{No}(0, \mathbf{I}_d)$$

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ν is a latent variable

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Principal fitted components (PFC)

Define $X_y \equiv (X \mid Y = y)$ and specify multivariate normal distribution

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Captures global linear predictive structure. Does not generalize to manifolds.

Mixture models and localization

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A driving idea in probabilistic modeling is that mixture models are flexible and can capture "nonparametric" distributions.

Mixture models can capture local nonlinear predictive manifold structure.

Model specification

$$X_y \sim \mathrm{No}(\mu_{yx}, \Delta)$$
$$\mu_{yx} = \mu + A\nu_{yx}$$
$$\nu_{yx} \sim G_y$$

G_y: density indexed by y having multiple clusters
$\mu \in \mathbb{R}^p$
$\varepsilon \sim N(0, \Delta)$ with $\Delta \in \mathbb{R}^{p \times p}$
$A \in \mathbb{R}^{p \times d}$
$\nu_{xy} \in \mathbb{R}^d$.

Dimension reduction space

Proposition

For this model the d.r. space is the span of $B = \Delta^{-1}A$

$$Y \mid X \stackrel{d}{=} Y \mid (\Delta^{-1}A)^T X.$$

Sampling distribution

Define $\nu_i \equiv \nu_{y_i x_i}$. Sampling distribution for data

$$x_i \mid (y_i, \mu, \nu_i, A, \Delta) \sim N(\mu + A\nu_i, \Delta)$$
$$\nu_i \sim G_{y_i}.$$

Categorical response: modeling G_y

$Y = \{1, ..., C\}$, so each category has a distribution

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Likelihood

$$\text{Lik}(\text{data} \mid \theta) \equiv \text{Lik}(\text{data} \mid A, \Delta, \nu_1, ..., \nu_n, \mu)$$

$$\text{Lik}(\text{data} \mid \theta) \quad \propto \quad \det(\Delta^{-1})^{\frac{n}{2}} \times \exp\left[-\frac{1}{2}\sum_{i=1}^{n}(x_i - \mu - A\nu_i)^T \Delta^{-1}(x_i - \mu - A\nu_i)\right].$$

Posterior inference

Given data

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3. Sample from $\mathcal{P}_\theta$?

Markov chain Monte Carlo

No closed form for $\mathcal{P}_\theta$.

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   with stationary distribution $\mathcal{P}_\theta$.

2. Run the Markov chain to obtain $\theta_1, ..., \theta_T$.

Sampling from the posterior

Inference consists of drawing samples $\theta_{(t)} = (\mu_{(t)}, A_{(t)}, \Delta_{(t)}^{-1}, \nu_{(t)})$ from the posterior.

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Define

$$\begin{aligned}
\theta^{/\mu}_{(t)} &\equiv (A_{(t)}, \Delta^{-1}_{(t)}, \nu_{(t)}) \\
\theta^{/A}_{(t)} &\equiv (\mu_{(t)}, \Delta^{-1}_{(t)}, \nu_{(t)}) \\
\theta^{/\Delta^{-1}}_{(t)} &\equiv (\mu_{(t)}, A_{(t)}, \nu_{(t)}) \\
\theta^{/\nu}_{(t)} &\equiv (\mu_{(t)}, A_{(t)}, \Delta^{-1}_{(t)}).
\end{aligned}$$

Gibbs sampling

Conditional probabilities can be used to sample μ, Δ^{-1}, A

$$\mu_{(t+1)} \mid \left(\text{data}, \theta^{/\mu}_{(t)}\right) \quad \sim \quad \text{No}\left(\text{data}, \theta^{/\mu}_{(t)}\right),$$

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\end{aligned}$$

Sampling $\nu_{(t)}$ is more involved.

Posterior draws from the Grassmann manifold

Given samples $(\Delta_{(t)}^{-1}, A_{(t)})_{t=1}^{m}$ compute $\mathcal{B}_{(t)} = \Delta_{(t)}^{-1} A_{(t)}$.

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Each $\mathcal{B}_{(t)}$ is a subspace which is a point in the Grassmann manifold $\mathcal{G}_{(d,p)}$. There is a Riemannian metric on this manifold. This has two implications.

Posterior mean and variance

Given draws $(\mathcal{B}_{(t)})_{t=1}^{m}$ the posterior mean and variance should be computed with respect to the Riemannian metric.

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Given two subspaces $\mathcal{W}$ and $\mathcal{U}$ spanned by orthonormal bases W and V the Karcher mean is

$$\begin{aligned} (I - X(X^T X)^{-1} X^T) Y (X^T Y)^{-1} &= U \Sigma V^T \\ \Theta &= \operatorname{atan}(\Sigma) \\ \operatorname{dist}(\mathcal{W}, \mathcal{V}) &= \sqrt{\operatorname{Tr}(\Theta^2)}. \end{aligned}$$

Posterior mean and variance

The posterior mean subspace

$$\mathcal{B}_{\text{Bayes}} = \arg \min_{\mathcal{B} \in \mathcal{G}_{(d,p)}} \sum_{i=1}^{m} \text{dist}(\mathcal{B}_i, \mathcal{B}).$$

Posterior mean and variance

The posterior mean subspace

$$\mathcal{B}_{\text{Bayes}} = \arg \min_{\mathcal{B} \in \mathcal{G}_{(d,p)}} \sum_{i=1}^{m} \text{dist}(\mathcal{B}_i, \mathcal{B}).$$

Uncertainty

$$\text{var}(\{\mathcal{B}_1, \cdots, \mathcal{B}_m\}) = \frac{1}{m} \sum_{i=1}^{m} \text{dist}(\mathcal{B}_i, \mathcal{B}_{\text{Bayes}}).$$

Distribution theory on Grassmann manifolds

If B is a linear space of d central normal vectors in $\mathbb{R}^p$ with covariance matrix Σ the density of Grassmannian distribution $\mathscr{G}_\Sigma$ w.r.t. reference measure $\mathscr{G}_\mathbf{I}$ is

$$\frac{d\mathscr{G}_\Sigma}{d\mathscr{G}_\mathbf{I}}(\langle X\rangle) = \left(\frac{\det(X^T X)}{\det(X^T\Sigma^{-1}X)}\right)^{d/2},$$

where $\langle X\rangle \equiv \text{span}(X)$ where $X = (x_1, \ldots x_d)$.

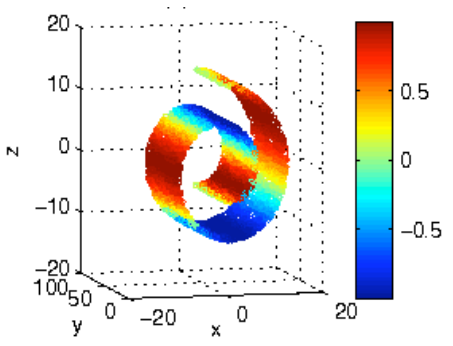
Swiss roll

$$X_1 = t\cos(t), \quad X_2 = h, \quad X_3 = t\sin(t), \quad X_{4,\ldots,10} \overset{iid}{\sim} \text{No}(0,1)$$

where $t = \frac{3\pi}{2}(1+2\theta)$, $\theta \sim \text{Unif}(0,1)$, $h \sim \text{Unif}(0,1)$ and

$$Y = \sin(5\pi\theta) + h^2 + \varepsilon, \quad \varepsilon \sim \text{No}(0, 0.01).$$

Pictures

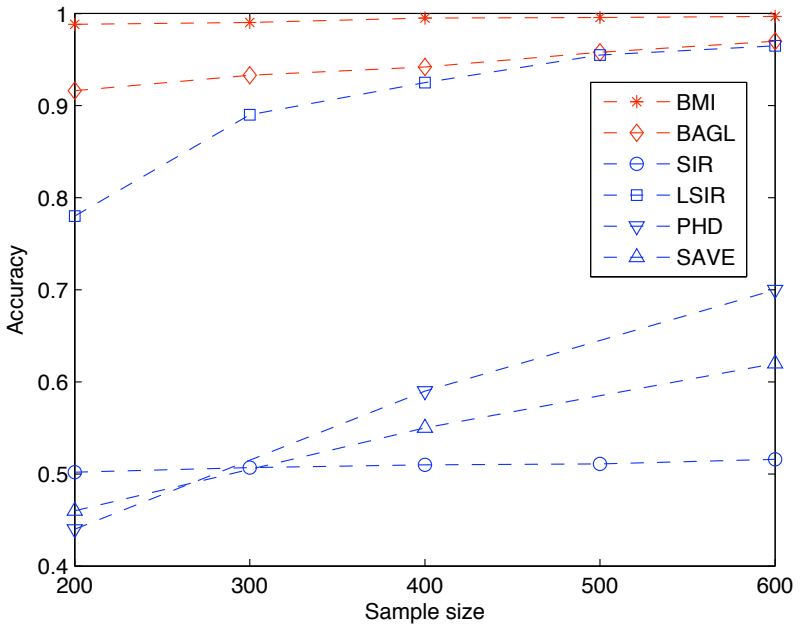


Metric

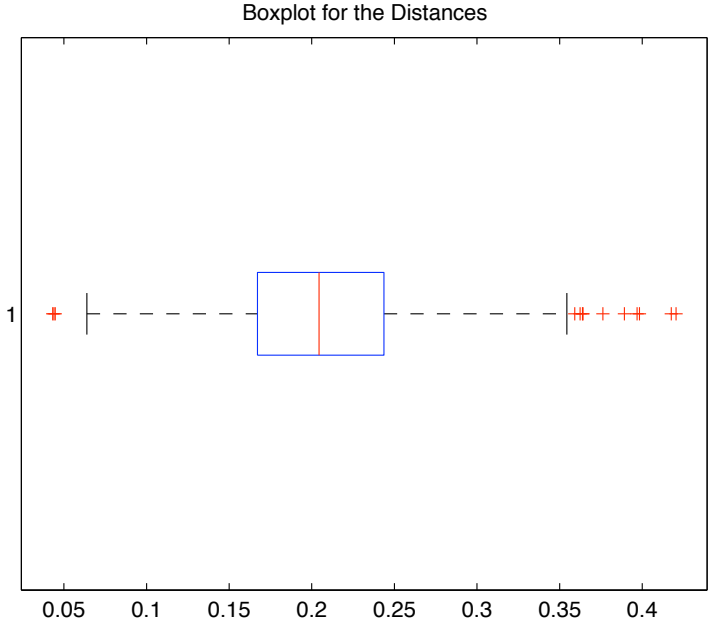
Projection of the estimated d.r. space $\hat{B} = (\hat{b}_1, \cdots, \hat{b}_d)$ onto B

$$\frac{1}{d}\sum_{i=1}^{d} ||P_B \hat{b}_i||^2 = \frac{1}{d}\sum_{i=1}^{d} ||(BB^T)\hat{b}_i||^2$$

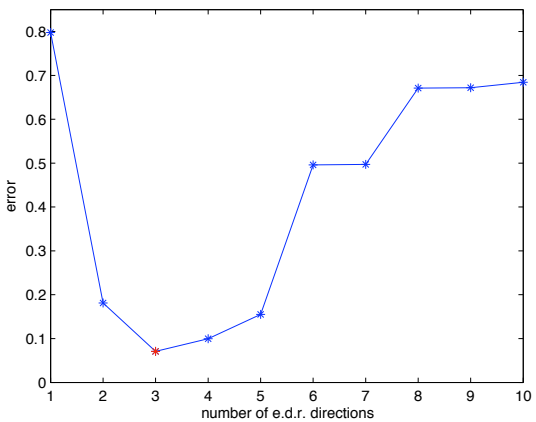
Comparison of algorithms

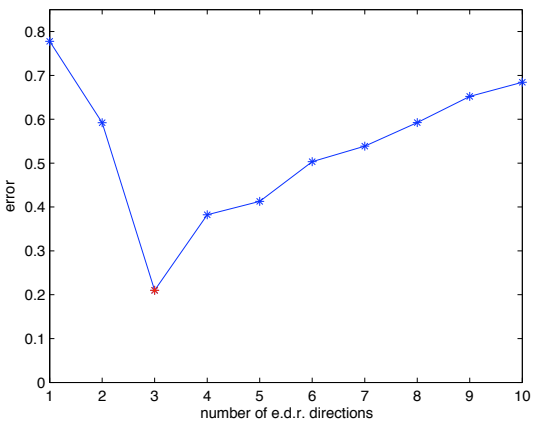


Posterior variance

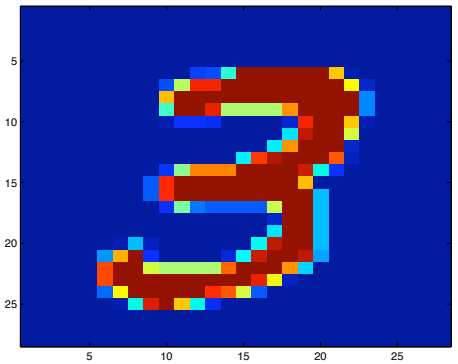


Error as a function of d





Digits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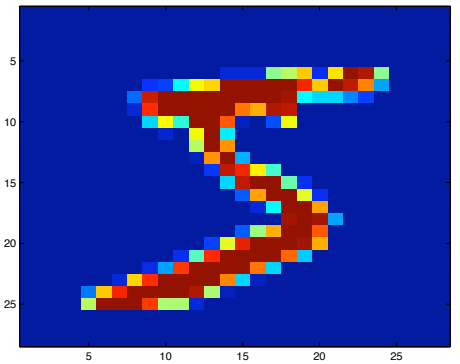
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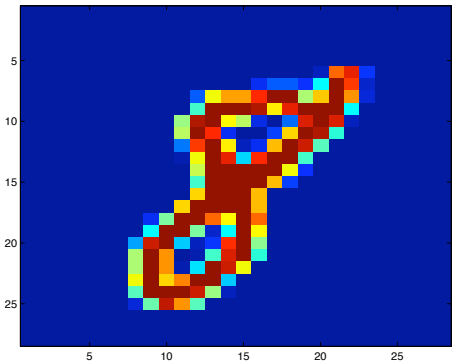
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Two classification problems

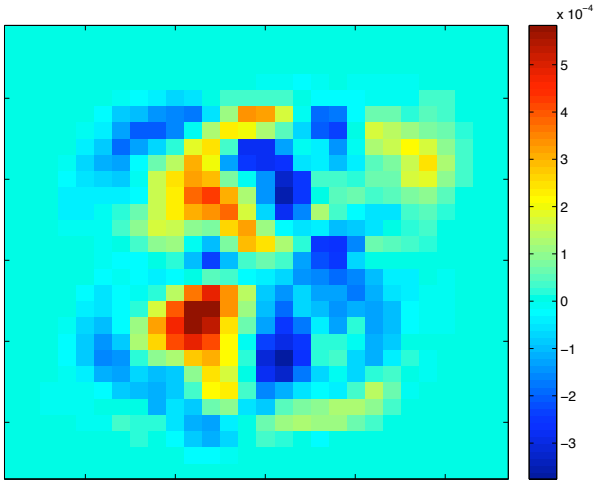
3 vs. 8 and 5 vs. 8.

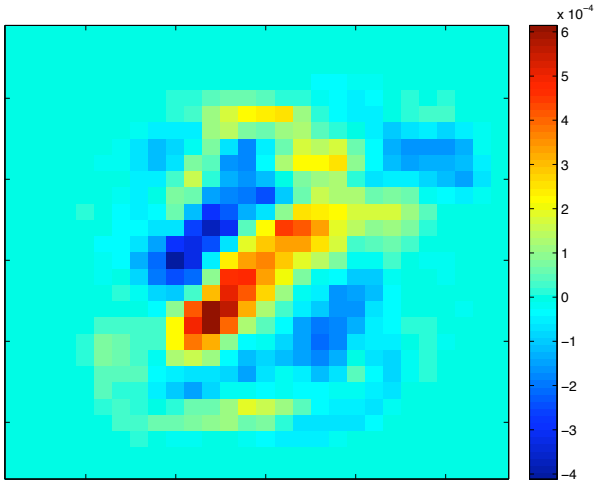
Two classification problems

3 vs. 8 and 5 vs. 8.

100 training samples from each class.

BMI





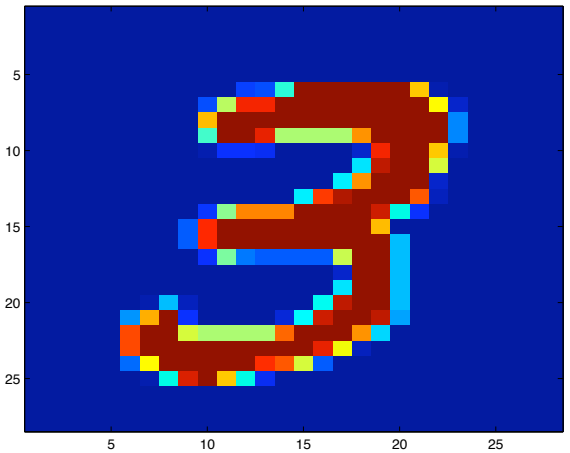
3, 5, 8 Classification Problem

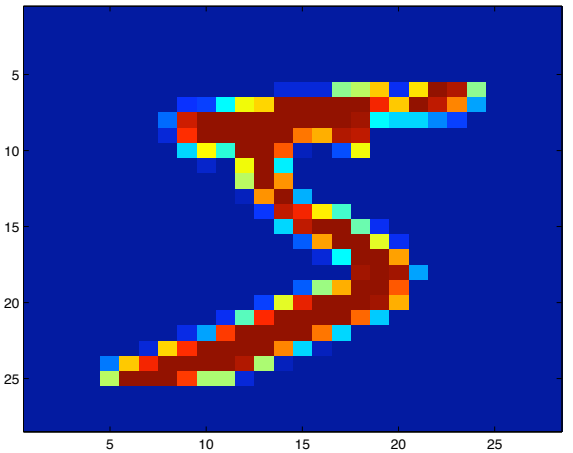
Goal

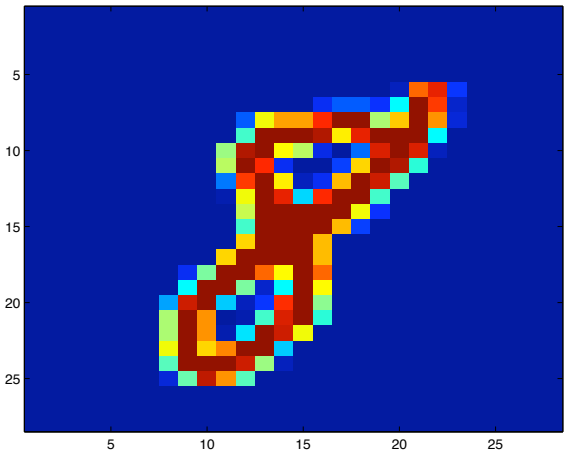
Learn features for predictive model:

- 3 vs 8
- 5 vs 8
- 3 **and** 5 vs 8

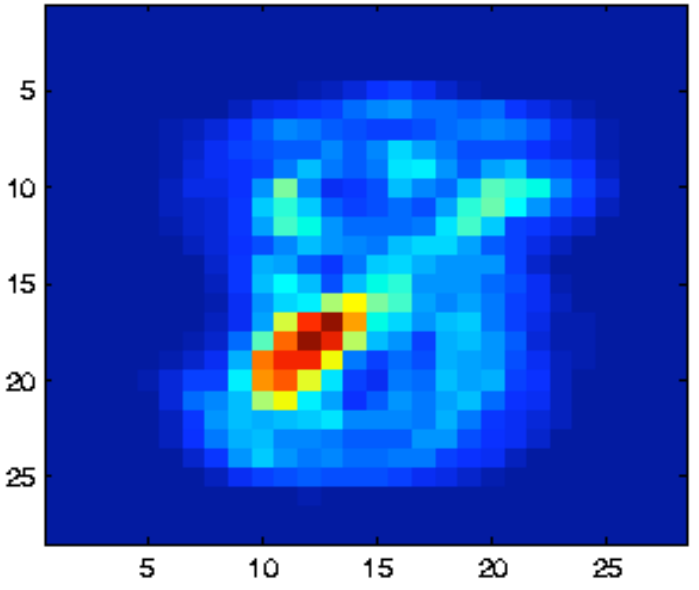
3, 5, 8 Classification problem



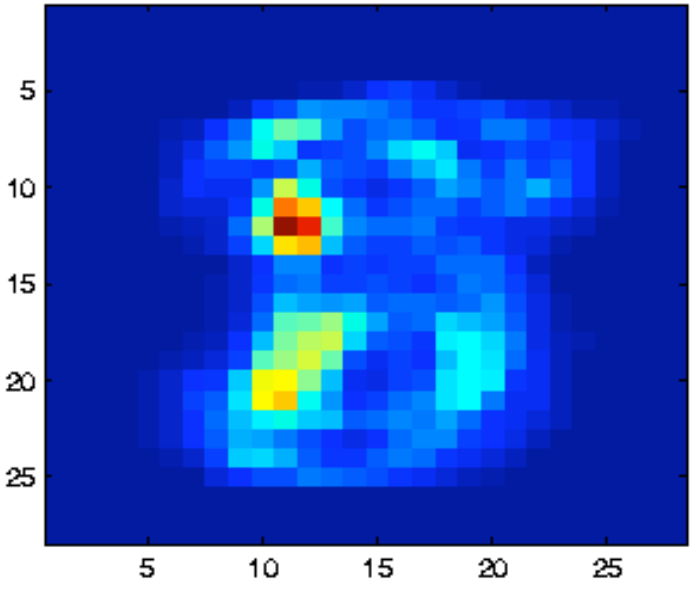




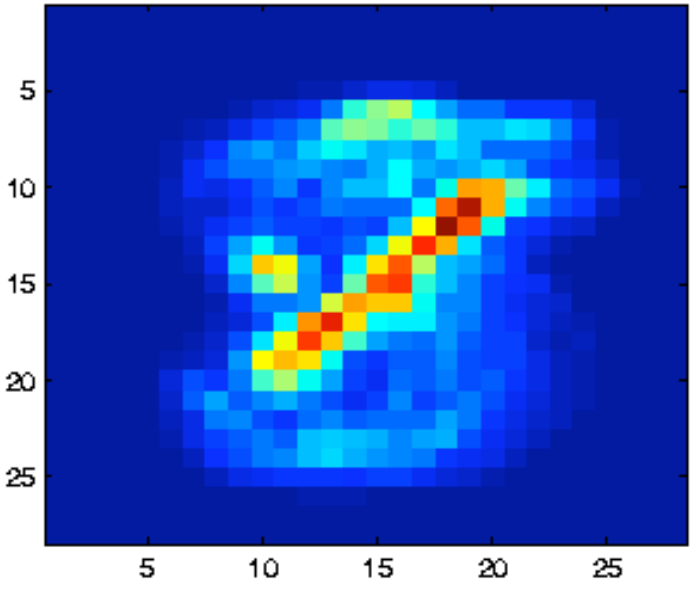
Top features: 3 and 5 vs 8



Top features: 3 vs 8



Top features: 5 vs 8



All ten digits

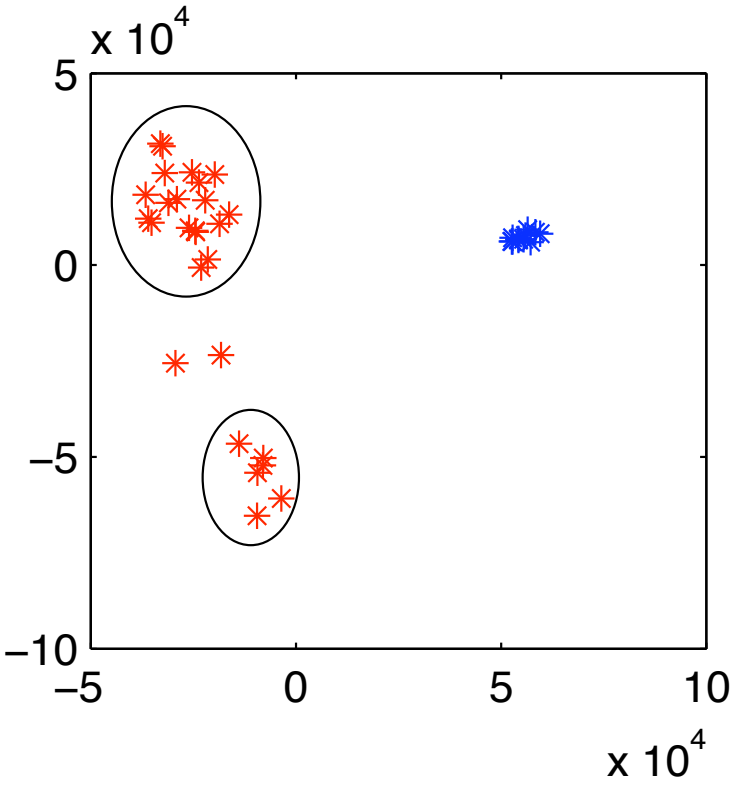
digit	Nonlinear	Linear
0	0.04($\pm$ 0.01)	0.05 ($\pm$ 0.01)
1	0.01($\pm$ 0.003)	0.03 ($\pm$ 0.01)
2	0.14($\pm$ 0.02)	0.19 ($\pm$ 0.02)
3	0.11($\pm$ 0.01)	0.17 ($\pm$ 0.03)
4	0.13($\pm$ 0.02)	0.13 ($\pm$ 0.03)
5	0.12($\pm$ 0.02)	0.21 ($\pm$ 0.03)
6	0.04($\pm$ 0.01)	0.0816 ($\pm$ 0.02)
7	0.11($\pm$ 0.01)	0.14 ($\pm$ 0.02)
8	0.14($\pm$ 0.02)	0.20 ($\pm$ 0.03)
9	0.11($\pm$ 0.02)	0.15 ($\pm$ 0.02)
average	0.09	0.14

Table: Average classification error rate and standard deviation on the digits data.

Cancer classification

$n = 38$ samples with expression levels for $p = 7129$ genes or ests
19 samples are Acute Myeloid Leukemia (AML)
19 are Acute Lymphoblastic Leukemia, these fall into two subclusters – B-cell and T-cell.

Substructure captured



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