Supervised Dimension Reduction:
A Tale of Two Manifolds

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Information and sufficiency

A fundamental idea in statistical thought is to reduce data to relevant information. This was the paradigm of R.A. Fisher (beloved Bayesian) and goes back to at least Adcock 1878 and Edgeworth 1884.
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$X_1, ..., X_n$ drawn iid form a Gaussian can be reduced to $\mu, \sigma^2$. 
Regression

Assume the model

\[ Y = f(X) + \varepsilon, \quad \mathbf{E}\varepsilon = 0, \]

with \( X \in \mathcal{X} \subset \mathbb{R}^p \) and \( Y \in \mathbb{R} \).
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Data \(-\) \( D = \{(x_i, y_i)\}_{i=1}^n \overset{iid}{\sim} \rho(X, Y) \).
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.
Given response variables $Y_1, \ldots, Y_n \in \mathbb{R}$ and explanatory variables or covariates $X_1, \ldots, X_n \in \mathcal{X} \subset \mathbb{R}^p$

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

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Is there a submanifold $S \equiv S_{Y|X}$ such that $Y \perp X \mid P_S(X)$?
Visualization of SDR

(a) Data

(b) Diffusion map

(c) GOP

(d) GDM
Supervised Dimension Reduction:

Supervised dimension reduction

Linear projections capture nonlinear manifolds

In this talk $P_S(X) = B^T X$ where $B = (b_1, ..., b_d)$. 
Linear projections capture nonlinear manifolds

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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.
Supervised Dimension Reduction: Learning gradients

**SDR model**

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Assume marginal distribution \( \rho_X \) 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

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

Given a smooth function $f$ the gradient is
\[ \nabla f(x) = \left( \frac{\partial f(x)}{\partial x_1}, \ldots, \frac{\partial f(x)}{\partial x_p} \right)^T. \]

Define the gradient outer product matrix $\Gamma$
\[ \Gamma_{ij} = \int_{\mathcal{X}} \frac{\partial f}{\partial x_i}(x) \frac{\partial f}{\partial x_j}(x) d\rho_x(x), \]
\[ \Gamma = \mathbb{E}[(\nabla f) \otimes (\nabla f)]. \]
GOP captures the d.r. space

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For \( i = 1, \ldots, d \)

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

If \( w \perp b_i \) for all \( i \) then \( w^T \Gamma w = 0. \)
Statistical interpretation

Linear case

\[ y = \beta^T x + \varepsilon, \quad \varepsilon \overset{iid}{\sim} \text{No}(0, \sigma^2). \]

\[ \Omega = \text{cov} (\mathbb{E}[X|Y]), \quad \Sigma_X = \text{cov} (X), \quad \sigma_Y^2 = \text{var} (Y). \]
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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 $f(x)$

$$y = f(x) + \varepsilon, \quad \varepsilon \sim \text{No}(0, \sigma^2).$$

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

Partition into sections and compute local quantities

$$\mathcal{X} = \bigcup_{i=1}^{I} \chi_i$$
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\[ m_i = \rho_{X} (\chi_i). \]
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\[ \Gamma \approx \sum_{i=1}^{I} m_i \sigma_i^2 \Sigma_i^{-1} \Omega_i \Sigma_i^{-1}. \]
Estimating the gradient

Taylor expansion

\[ y_i \approx f(x_i) \approx f(x_j) + \langle \nabla f(x_j), x_j - x_i \rangle \]
\[ \approx y_j + \langle \nabla f(x_j), x_j - x_i \rangle \text{ if } x_i \approx x_j. \]
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Let \( \hat{\vec{f}} \approx \nabla f \) the following should be small

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

\[ w_{ij} = \frac{1}{s^{p+2}} \exp\left(-\|x_i - x_j\|^2/2s^2\right) \text{ enforces } x_i \approx x_j. \]
Supervised Dimension Reduction:

Learning gradients

Estimating the gradient

The gradient estimate

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

where \( \| \tilde{f} \|_K \) is a smoothness penalty, reproducing kernel Hilbert space norm.
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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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$c_D = (c_{1,D}, \ldots, c_{n,D})^T \in \mathbb{R}^{np}$.

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

$$\hat{\Gamma} = c_D K c_D^T.$$
Marginal distribution $\rho_X$ 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 $d\mu$ is the uniform measure on $\mathcal{M}$.

Assume regular distribution

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

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

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

$$\rho_\mathcal{M}( \{ x \in \mathcal{M} : d_\mathcal{M}(x, \partial \mathcal{M}) \leq t \} ) \leq c_2 \ t \quad \forall t > 0.$$
Convergence to gradient on manifold

Theorem
Under above regularity conditions on $\rho_X$ and $f \in C^2(M)$, with probability $1 - \delta$

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

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

Algorithmic view of PCA:

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

$$\hat{\Sigma} = (X - \bar{X})(X - \bar{X})^T$$
Principal components analysis (PCA)

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\[
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\]

2. Eigen-decomposition of \( \hat{\Sigma} \)

\[
\lambda_i v_i = \hat{\Sigma} v_i.
\]
Probabilistic PCA

\( X \in \mathbb{R}^p \) is characterized by a multivariate normal

\[
X \sim \text{No}(\mu + A\nu, \Delta), \\
\nu \sim \text{No}(0, I_d)
\]

\( \mu \in \mathbb{R}^p \)
\( A \in \mathbb{R}^{p \times d} \)
\( \Delta \in \mathbb{R}^{p \times p} \)
\( \nu \in \mathbb{R}^d \).
Probabilistic PCA

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\( \nu \) is a latent variable.
Supervised Dimension Reduction: 
Baysian Mixture of Inverses

SDR model

Semiparametric model

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span \( B \) is the dimension reduction (d.r.) subspace.
Principal fitted components (PFC)

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

$$X_y \sim \text{No}(\mu_y, \Delta),$$
$$\mu_y = \mu + A\nu_y$$

$\mu \in \mathbb{R}^p$
$A \in \mathbb{R}^{p \times d}$
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$B = \Delta^{-1}A$. 
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Captures global linear predictive structure. Does not generalize to manifolds.
Mixture models and localization

A driving idea in manifold learning is that manifolds are locally Euclidean.
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A driving idea in probabilistic modeling is that mixture models are flexible and can capture "nonparametric" distributions.
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A driving idea in manifold learning is that manifolds are locally Euclidean.

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.
Supervised Dimension Reduction: Bayesian Mixture of Inverses

Model specification

\[ X_y \sim \text{No}(\mu_{yx}, \Delta) \]
\[ \mu_{yx} = \mu + A\nu_{yx} \]
\[ \nu_{yx} \sim G_y \]

\( G_y \): density indexed by \( y \) having multiple clusters

\( \mu \in \mathbb{R}^p \)
\( \varepsilon \sim \mathcal{N}(0, \Delta) \) with \( \Delta \in \mathbb{R}^{p \times p} \)
\( A \in \mathbb{R}^{p \times d} \)
\( \nu_{xy} \in \mathbb{R}^d \).
Proposition

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

\[ Y \mid X \overset{d}{=} Y \mid (\Delta^{-1}A)^T X. \]
Define $\nu_i \equiv \nu_{y_i \mid x_i}$. 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 $G_y$

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

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$\nu_i$ modeled as a mixture of $C$ distributions $G_1, ..., G_C$ with a Dirichlet process model for each distribution

$$G_c \sim DP(\alpha_0, G_0).$$
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Goto board.
Likelihood

\[ \text{Lik}(\text{data} \mid \theta) \equiv \text{Lik}(\text{data} \mid A, \Delta, \nu_1, \ldots, \nu_n, \mu) \]

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

Given data

\[ P_\theta \equiv \text{Post}(\theta \mid \text{data}) \propto \text{Lik}(\theta \mid \text{data}) \times \pi(\theta). \]
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1. \( P_\theta \) provides estimate of (un)certainty on \( \theta \)
2. Requires prior on \( \theta \)
3. Sample from \( P_\theta \)
Markov chain Monte Carlo

No closed form for $P_\theta$. 

Supervised Dimension Reduction:

Bayesian Mixture of Inverses
Markov chain Monte Carlo

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

1. Specify Markov transition kernel

$$K(\theta_t, \theta_{t+1})$$

with stationary distribution $\mathcal{P}_\theta$. 
Markov chain Monte Carlo

No closed form for $P_\theta$.

1. Specify Markov transition kernel

$$K(\theta_t, \theta_{t+1})$$

with stationary distribution $P_\theta$.

2. Run the Markov chain to obtain $\theta_1, \ldots, \theta_T$. 
Sampling from the posterior

Inference consists of drawing samples $\theta(t) = (\mu(t), A(t), \Delta^{-1}(t), \nu(t))$ from the posterior.
Sampling from the posterior

Inference consists of drawing samples $\theta(t) = (\mu(t), A(t), \Delta_{(t)}^{-1}, \nu(t))$ from the posterior.

Define

$$\theta_{\mu}(t) \equiv (A(t), \Delta_{(t)}^{-1}, \nu(t))$$

$$\theta_{A}(t) \equiv (\mu(t), \Delta_{(t)}^{-1}, \nu(t))$$

$$\theta_{\Delta^{-1}}(t) \equiv (\mu(t), A(t), \nu(t))$$

$$\theta_{\nu}(t) \equiv (\mu(t), A(t), \Delta_{(t)}^{-1})$$.
Gibbs sampling

Conditional probabilities can be used to sample $\mu, \Delta^{-1}, A$

$$\mu_{(t+1)} \mid \left(\text{data}, \theta^{/\mu}_{(t)}\right) \sim \text{No} \left(\text{data}, \theta^{/\mu}_{(t)}\right),$$
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Conditional probabilities can be used to sample $\mu, \Delta^{-1}, A$

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

\[
\Delta^{-1}(t+1) \mid \left(\text{data, } \theta^{/\Delta^{-1}}_{(t)}\right) \sim \text{InvWishart} \left(\text{data, } \theta^{/\Delta^{-1}}_{(t)}\right)
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Gibbs sampling

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$$A^{(t+1)} \mid \left( \text{data, } \theta^{/A} \right) \sim \text{No} \left( \text{data}, \theta^{/A} \right).$$

Sampling $\nu^{(t)}$ is more involved.
Posterior draws from the Grassmann manifold

Given samples $(\Delta_{(t)}, A(t))_{t=1}^{m}$ compute $B(t) = \Delta_{(t)}^{-1}A(t)$. 
Supervised Dimension Reduction:
Baysian Mixture of Inverses

Posterior draws from the Grassmann manifold

Given samples \((\Delta^{-1}_t, A(t))_{t=1}^m\) compute \(B(t) = \Delta^{-1}_t A(t)\).

Each \(B(t)\) is a subspace which is a point in the Grassmann manifold \(G_{(d,p)}\). There is a Riemannian metric on this manifold. This has two implications.
Posterior mean and variance

Given draws \((B_t(t))_{t=1}^{m}\) 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 \(\mathcal{W}\) and \(\mathcal{V}\) the Karcher mean is

\[
(I - X(X^T X)^{-1}X^T) Y(X^T Y)^{-1} = U\Sigma V^T
\]

\[
\Theta = \text{atan}(\Sigma)
\]

\[
\text{dist}(\mathcal{W}, \mathcal{V}) = \sqrt{\text{Tr}(\Theta^2)}.
\]
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 $\Sigma$ the density of Grassmannian distribution $G_\Sigma$ w.r.t. reference measure $G_I$ is

$$
\frac{dG_\Sigma}{dG_I}(\langle X \rangle) = \left( \frac{\det(X^T X)}{\det(X^T \Sigma^{-1} X)} \right)^{d/2},
$$

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

Results on data

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

\[ Y = \sin(5\pi\theta) + h^2 + \varepsilon, \quad \varepsilon \sim \text{No}(0, 0.01). \]
Supervised Dimension Reduction:
  Results on data
  Swiss roll

Pictures
Supervised Dimension Reduction:
Results on data
Swiss roll

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

Boxplot for the Distances
Error as a function of $d$
Supervised Dimension Reduction:

Results on data

Digits

![Images of digit representations generated by supervised dimension reduction.](image-url)
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.
Supervised Dimension Reduction:
- Results on data
- Digits

**BMI**
### All ten digits

<table>
<thead>
<tr>
<th>digit</th>
<th>Nonlinear</th>
<th>Linear</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.04(± 0.01)</td>
<td>0.05 (± 0.01)</td>
</tr>
<tr>
<td>1</td>
<td>0.01(± 0.003)</td>
<td>0.03 (± 0.01)</td>
</tr>
<tr>
<td>2</td>
<td>0.14(± 0.02)</td>
<td>0.19 (± 0.02)</td>
</tr>
<tr>
<td>3</td>
<td>0.11(± 0.01)</td>
<td>0.17 (± 0.03)</td>
</tr>
<tr>
<td>4</td>
<td>0.13(± 0.02)</td>
<td>0.13 (± 0.03)</td>
</tr>
<tr>
<td>5</td>
<td>0.12(± 0.02)</td>
<td>0.21 (± 0.03)</td>
</tr>
<tr>
<td>6</td>
<td>0.04(± 0.01)</td>
<td>0.0816 (± 0.02)</td>
</tr>
<tr>
<td>7</td>
<td>0.11(± 0.01)</td>
<td>0.14 (± 0.02)</td>
</tr>
<tr>
<td>8</td>
<td>0.14(± 0.02)</td>
<td>0.20 (± 0.03)</td>
</tr>
<tr>
<td>9</td>
<td>0.11(± 0.02)</td>
<td>0.15 (± 0.02)</td>
</tr>
<tr>
<td>average</td>
<td>0.09</td>
<td>0.14</td>
</tr>
</tbody>
</table>

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

\[ n = 38 \text{ samples with expression levels for } p = 7129 \text{ genes or ests} \]

19 samples are Acute Myeloid Leukemia (AML)
19 are Acute Lymphoblastic Leukemia, these fall into two subclusters – B-cell and T-cell.
Substructure captured
Supervised Dimension Reduction:

The end

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