Probabilistic Dimensionality Reduction

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Probabilistic Scientific Computing at Brown

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Outline

Dimensionality Reduction

Conclusions

Motivation for Non-Linear Dimensionality Reduction

USPS Data Set Handwritten Digit

- 3648 Dimensions
  - 64 rows by 57 columns

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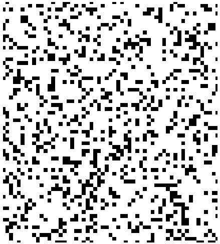

Motivation for Non-Linear Dimensionality Reduction

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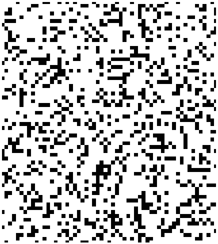

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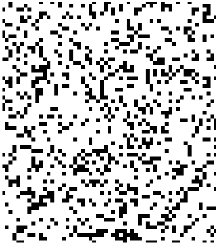

Simple Model of Digit

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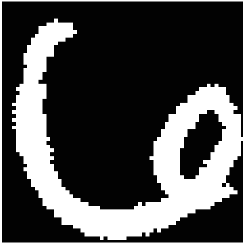

MATLAB Demo

```
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```

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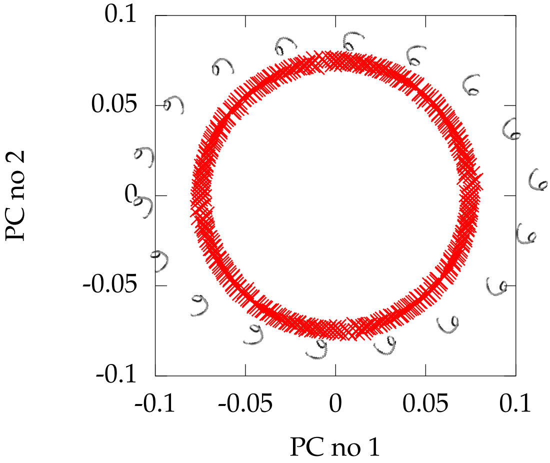
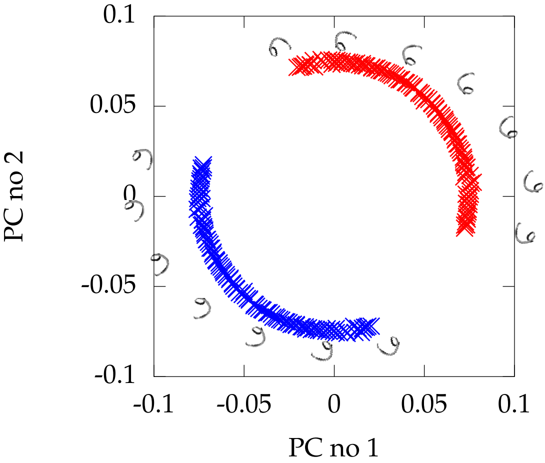


MATLAB Demo

```
demDigitsManifold([1 2], 'sixnine')
```



Low Dimensional Manifolds

Pure Rotation is too Simple

- In practice the data may undergo several distortions.
  - *e.g.* digits undergo 'thinning', translation and rotation.
- For data with 'structure':
  - we expect fewer distortions than dimensions;
  - we therefore expect the data to live on a lower dimensional manifold.
- Conclusion: deal with high dimensional data by looking for lower dimensional non-linear embedding.

Existing Methods

Spectral Approaches

- Classical Multidimensional Scaling (MDS) (Mardia et al., 1979).
  - Uses eigenvectors of similarity matrix.
    - Isomap (Tenenbaum et al., 2000) is MDS with a particular proximity measure.
  - Kernel PCA (Schölkopf et al., 1998)
    - Provides a representation and a mapping — dimensional expansion.
    - Mapping is implied throught he use of a kernel function as a similarity matrix.
  - Locally Linear Embedding (Roweis and Saul, 2000).
    - Looks to preserve locally linear relationships in a low dimensional space.

Existing Methods II

Iterative Methods

- Multidimensional Scaling (MDS)
  - Iterative optimisation of a stress function (Kruskal, 1964).
  - Sammon Mappings (Sammon, 1969).
    - Strictly speaking not a mapping — similar to iterative MDS.
- NeuroScale (Lowe and Tipping, 1997)
  - Augmentation of iterative MDS methods with a mapping.

Existing Methods III

Probabilistic Approaches

- Probabilistic PCA (Tipping and Bishop, 1999; Roweis, 1998)
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- Probabilistic PCA (Tipping and Bishop, 1999; Roweis, 1998)
  - A linear method.
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- Generative Topographic Mapping (GTM) (Bishop et al., 1998)
  - Uses a grid based sample and an RBF network.

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- Probabilistic PCA (Tipping and Bishop, 1999; Roweis, 1998)
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Difficulty for Probabilistic Approaches

- Propagate a probability distribution through a non-linear mapping.

The New Model

A Probabilistic Non-linear PCA

- PCA has a probabilistic interpretation (Tipping and Bishop, 1999; Roweis, 1998).
- It is difficult to 'non-linearise'.

Dual Probabilistic PCA

- We present a new probabilistic interpretation of PCA (Lawrence, 2005).
- This interpretation can be made non-linear.
- The result is non-linear probabilistic PCA.

Notation

q— dimension of latent/embedded space
p— dimension of data space
n— number of data points

centred data, $\mathbf{Y} = [\mathbf{y}_{1,:}, \dots, \mathbf{y}_{n,:}]^\top = \left[\mathbf{y}_{:,1}, \dots, \mathbf{y}_{:,p}\right] \in \Re^{n\times p}$
latent variables, $\mathbf{X} = [\mathbf{x}_{1,:}, \dots, \mathbf{x}_{n,:}]^\top = \left[\mathbf{x}_{:,1}, \dots, \mathbf{x}_{:,q}\right] \in \Re^{n\times q}$
mapping matrix, $\mathbf{W} \in \Re^{p\times q}$

$\mathbf{a}_{i,:}$ is a vector from the ith row of a given matrix $\mathbf{A}$
$\mathbf{a}_{:,j}$ is a vector from the jth row of a given matrix $\mathbf{A}$

Reading Notation

$\mathbf{X}$ and $\mathbf{Y}$ are *design matrices*

- Covariance given by $n^{-1}\mathbf{Y}^\top\mathbf{Y}$.
- Inner product matrix given by $\mathbf{Y}\mathbf{Y}^\top$.

Linear Dimensionality Reduction

Linear Latent Variable Model

- Represent data, $\mathbf{Y}$, with a lower dimensional set of latent variables $\mathbf{X}$.
- Assume a linear relationship of the form

$$\mathbf{y}_{i,:} = \mathbf{W}\mathbf{x}_{i,:} + \boldsymbol{\epsilon}_{i,:},$$

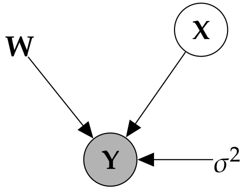
where

$$\boldsymbol{\epsilon}_{i,:} \sim \mathcal{N}\left(\mathbf{0}, \sigma^2\mathbf{I}\right).$$

Linear Latent Variable Model

Probabilistic PCA

- Define *linear-Gaussian relationship* between latent variables and data.



$$p\left(\mathbf{Y}|\mathbf{X},\mathbf{W}\right)=\prod_{i=1}^{n}\mathcal{N}\left(\mathbf{y}_{i,:}|\mathbf{W}\mathbf{x}_{i,:},\sigma^{2}\mathbf{I}\right)$$

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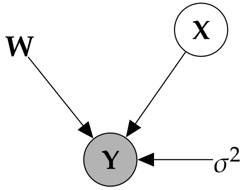

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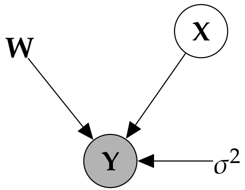

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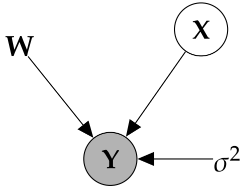

Probabilistic PCA

- Define *linear-Gaussian relationship* between latent variables and data.
- **Standard** Latent variable approach:
  - Define Gaussian prior over *latent space*, **X**.
  - Integrate out *latent variables*.

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$$p(\mathbf{X}) = \prod_{i=1}^{n} \mathcal{N}\left(\mathbf{x}_{i,:}|\mathbf{0}, \mathbf{I}\right)$$

$$p(\mathbf{Y}|\mathbf{W}) = \prod_{i=1}^{n} \mathcal{N}\left(\mathbf{y}_{i,:}|\mathbf{0}, \mathbf{W}\mathbf{W}^\top + \sigma^2\mathbf{I}\right)$$

Computation of the Marginal Likelihood

$$\mathbf{y}_{i,:} = \mathbf{W}\mathbf{x}_{i,:} + \boldsymbol{\epsilon}_{i,:}, \quad \mathbf{x}_{i,:} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), \quad \boldsymbol{\epsilon}_{i,:} \sim \mathcal{N}\left(\mathbf{0}, \sigma^2\mathbf{I}\right)$$

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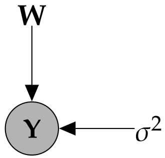

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$$\mathbf{W} = \mathbf{U}_q\mathbf{L}\mathbf{R}^{\top}, \quad \mathbf{L} = \left(\mathbf{\Lambda}_q - \sigma^2\mathbf{I}\right)^{\frac{1}{2}}$$

where $\mathbf{R}$ is an arbitrary rotation matrix.

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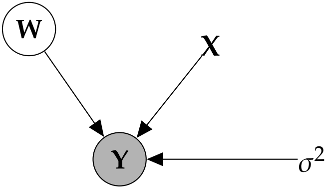
Dual Probabilistic PCA

- Define *linear-Gaussian relationship* between latent variables and data.



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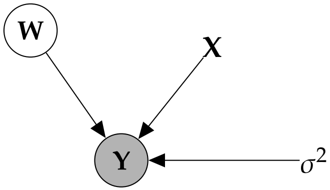

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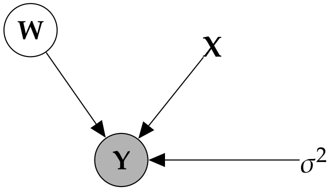

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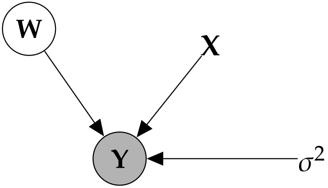

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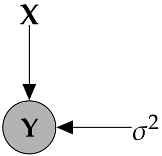
Dual Probabilistic PCA Max. Likelihood Soln (Lawrence, 2004, 2005)



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where $\mathbf{R}$ is an arbitrary rotation matrix.

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PPCA Max. Likelihood Soln (Tipping and Bishop, 1999)

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Equivalence of Formulations

The Eigenvalue Problems are equivalent

- Solution for Probabilistic PCA (solves for the mapping)

$$\mathbf{Y}^\top \mathbf{Y} \mathbf{U}_q = \mathbf{U}_q \boldsymbol{\Lambda}_q \qquad \mathbf{W} = \mathbf{U}_q \mathbf{L} \mathbf{R}^\top$$

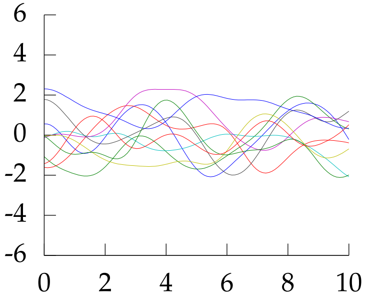
- Solution for Dual Probabilistic PCA (solves for the latent positions)

$$\mathbf{Y} \mathbf{Y}^\top \mathbf{U}_q' = \mathbf{U}_q' \boldsymbol{\Lambda}_q \qquad \mathbf{X} = \mathbf{U}_q' \mathbf{L} \mathbf{R}^\top$$

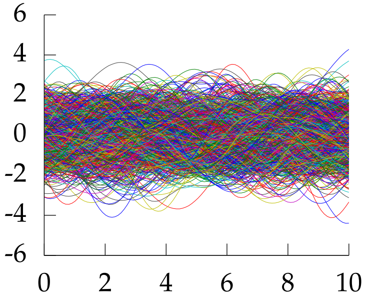
- Equivalence is from

$$\mathbf{U}_q = \mathbf{Y}^\top \mathbf{U}_q' \boldsymbol{\Lambda}_q^{-\frac{1}{2}}$$

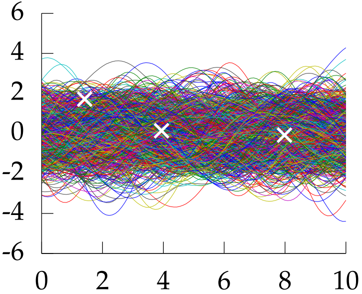
Gaussian Processes: Extremely Short Overview



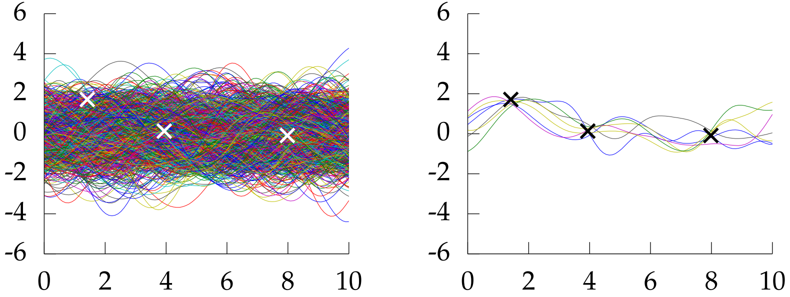
Gaussian Processes: Extremely Short Overview



Gaussian Processes: Extremely Short Overview



Gaussian Processes: Extremely Short Overview



GPSS: Gaussian Process Summer School

- http://gpss.cc
- Next one is in Sheffield in September 2017.
- Talks and tutorials on line.
- Jupyter based lab classes.
- GPy and GPyOpt software available from github.

Non-Linear Matrix Factorization

- The marginal likelihood of DPPCA is that of a Bayesian linear regression

$$p\left(\mathbf{Y}|\mathbf{X},\sigma^2,\alpha_x\right)=\prod_{j=1}^{D}\mathcal{N}\left(\mathbf{y}_{:,j}|\mathbf{0},\alpha_w^{-1}\mathbf{X}\mathbf{X}^\top+\sigma^2\mathbf{I}\right).$$

Non-Linear Matrix Factorization

- The marginal likelihood of DPPCA is that of a Bayesian linear regression

$$p\left(\mathbf{Y}|\mathbf{X},\sigma^2,\alpha_x\right)=\prod_{j=1}^{D}\mathcal{N}\left(\mathbf{y}_{:,j}|\mathbf{0},\alpha_w^{-1}\mathbf{K}+\sigma^2\mathbf{I}\right).$$

- Replace inner product matrix with covariance function for non-linear model.

Missing values

- For the product of GPs marginalizing missing values is straightforward.
- Let $\mathbf{y}_\mathbf{i}$ be the observed subset of $\mathbf{y}$.

$$\mathbf{y}_\mathbf{i} \sim \mathcal{N}\left(\boldsymbol{\mu}_\mathbf{i}, \boldsymbol{\Sigma}_{\mathbf{i},\mathbf{i}}\right),$$

- For sparse data

$$p\left(\mathbf{Y}|\mathbf{X}, \sigma^2, \alpha_x\right) = \prod_{j=1}^{D} \mathcal{N}\left(\mathbf{y}_{\mathbf{i}_j,j}|\mathbf{0}, \mathbf{K}_{\mathbf{i}_j,\mathbf{i}_j}\right).$$

Example: Latent Doodle Space

(Baxter and Anjyo, 2006)

Example: Latent Doodle Space

(Baxter and Anjyo, 2006)

Generalization with much less Data than Dimensions

- Powerful uncertainly handling of GPs leads to surprising properties.
- Non-linear models can be used where there are fewer data points than dimensions *without overfitting*.

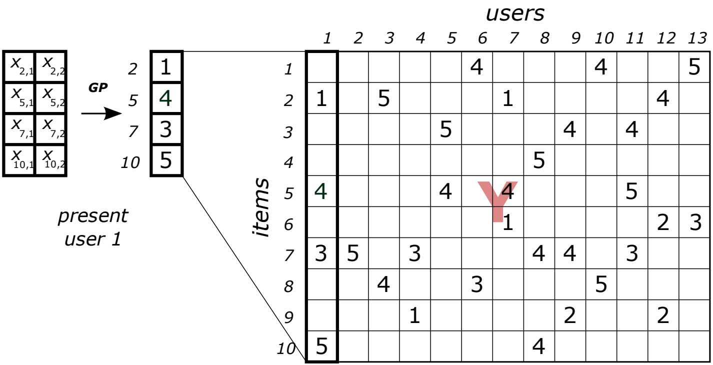
Stochastic Gradient Descent

$\mathbf{Y}$

items \ users	1	2	3	4	5	6	7	8	9	10	11	12	13
1						4				4			5
2	1		5				1					4	
3					5				4		4		
4								5					
5	4				4		4				5		
6							1					2	3
7	3	5		3				4	4		3		
8			4			3				5			
9				1					2			2	
10	5							4					

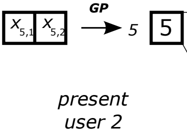
Present data a column at a time.

Stochastic Gradient Descent



Each step updates $\mathbf{X}_{\mathbf{i}_j,:}$.

Stochastic Gradient Descent

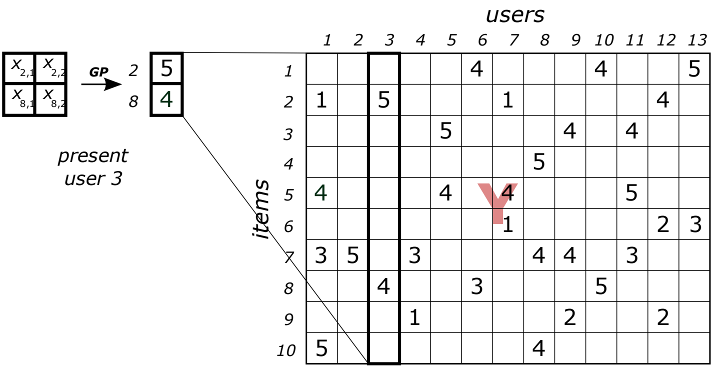


users / items — $\mathbf{Y}$

items \ users	1	2	3	4	5	6	7	8	9	10	11	12	13
1						4				4			5
2	1		5				1					4	
3					5				4		4		
4								5					
5	4				4		4				5		
6							1					2	3
7	3	5		3				4	4		3		
8			4			3				5			
9				1					2			2	
10	5							4					

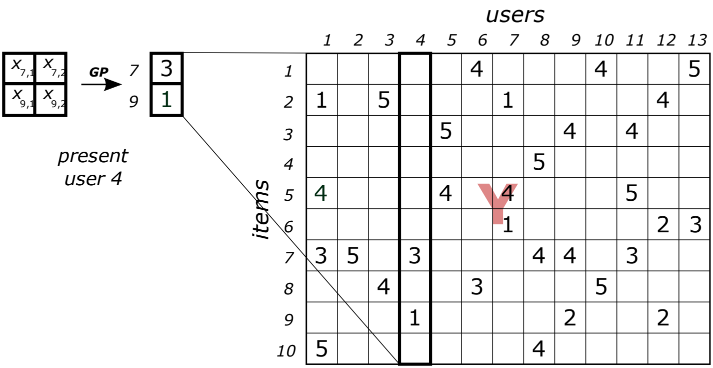
Complexity of GP cubic in N_j not N.

Stochastic Gradient Descent



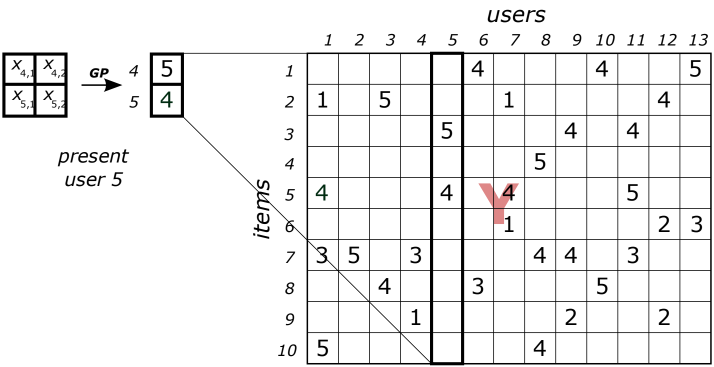
No Sparse GP approximations required.

Stochastic Gradient Descent



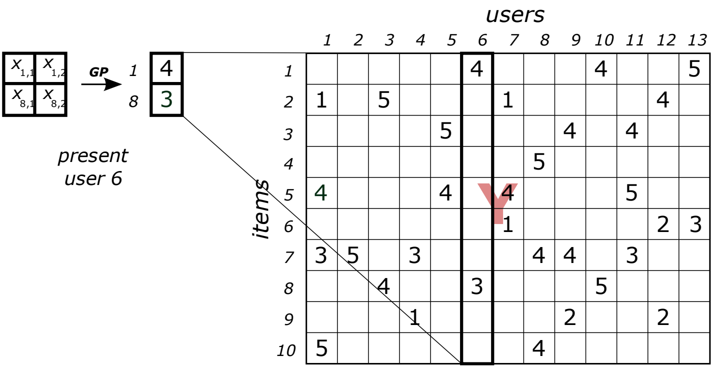
No Sparse GP approximations required.

Stochastic Gradient Descent



No Sparse GP approximations required.

Stochastic Gradient Descent



No Sparse GP approximations required.

Probabilistic Matrix Factorization for Automated Machine Learning

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Abstract

In order to achieve state-of-the-art performance, modern machine learning techniques require careful data pre-processing and hyperparameter tuning. Moreover,

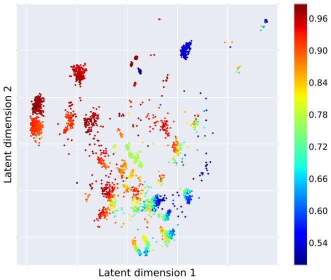
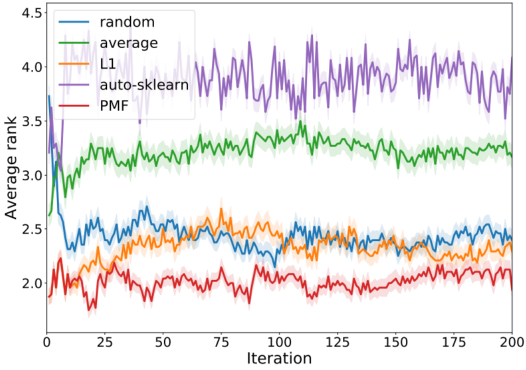
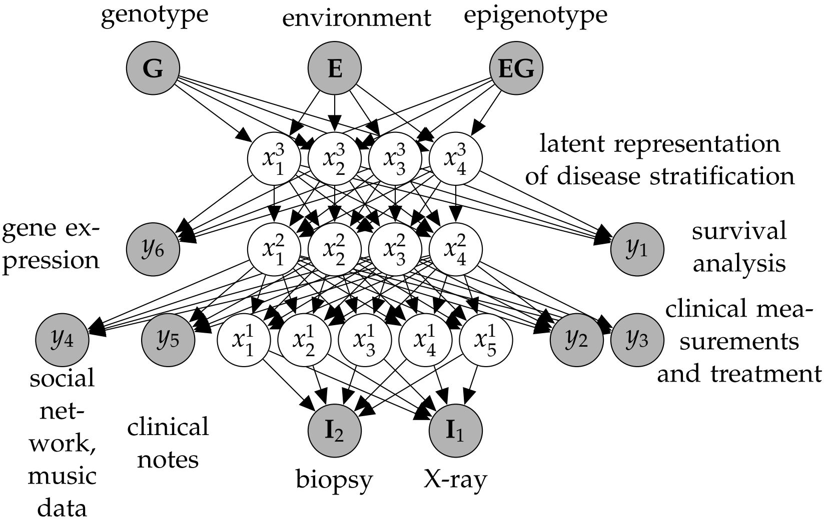


Figure 1: Two-dimensional embedding of 5,000 ML pipelines across 576 OpenML datasets. Each point corresponds to a pipeline and is colored by the AUROC obtained by that pipeline in one of the OpenML datasets (OpenML dataset id 943).



random
average
L1
auto-sklearn
PMF
Average rank
Iteration
4.5
4.0
3.5
3.0
2.5
2.0
0
25
50
75
100
125
150
175
200

Deep Health


genotype
environment
epigenotype
G
E
EG
latent representation of disease stratification
gene expression
survival analysis
clinical measurements and treatment
social network, music data
clinical notes
biopsy
X-ray
x_1^3 x_2^3 x_3^3 x_4^3
y_6 x_1^2 x_2^2 x_3^2 x_4^2 y_1
y_4 y_5 x_1^1 x_2^1 x_3^1 x_4^1 x_5^1 y_2 y_3
$\mathbf{I}_2$ $\mathbf{I}_1$

Summary

- Many data is usefully summarized with low dimensions.
- Classically pushing probability through non linear functions leads to intractability.
- GP-LVM presents a way around this.
- Recent use case in Automatic Machine Learning

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