Regularization for Nonlinear Dimension Reduction by Subspace Constraint

Billy Chang, Rafal Kustra
Dalla Lana School of Public Health
University of Toronto

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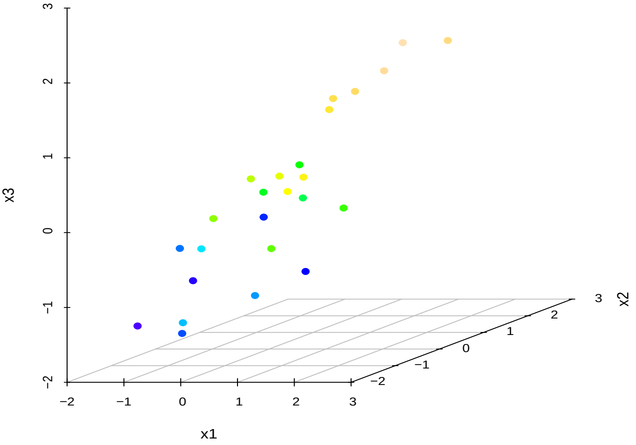
What is Dimension Reduction?



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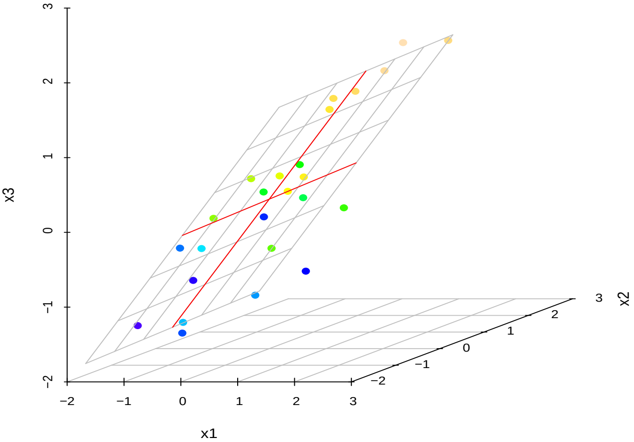
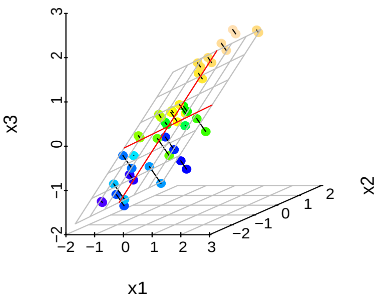
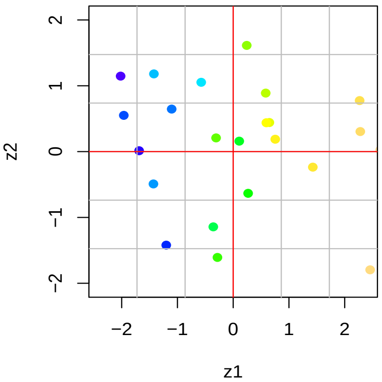


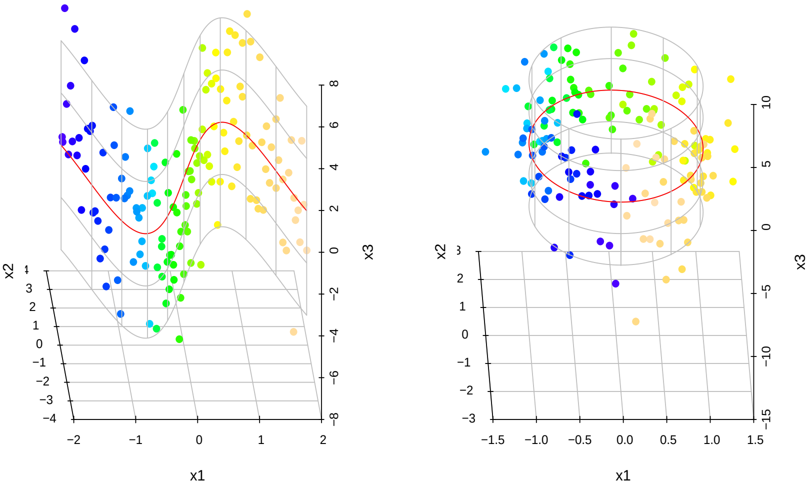
Why Dimension Reduction?



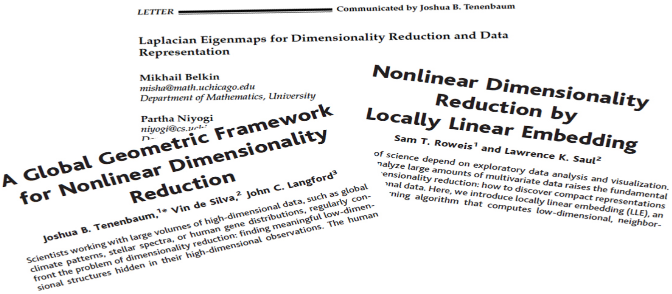


- Visualization, feature extraction for regression.
- Principal Component Analysis, Factor Analysis.
- Measures for model diagnosis: reconstruction error, likelihood.

What is Nonlinear Dimension Reduction?

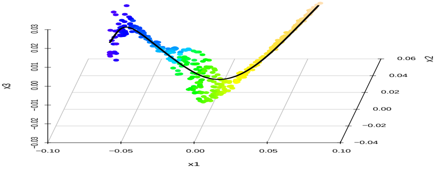


Challenges in Nonlinear Dimension Reduction

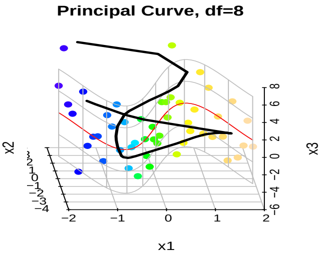


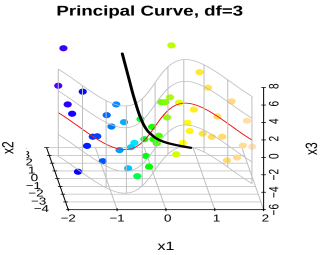
- No explicit mapping from original space to low-dimensional space.
- Model checking and parameter tuning difficult.

Principal Curve (Hastie et. al. 1989)



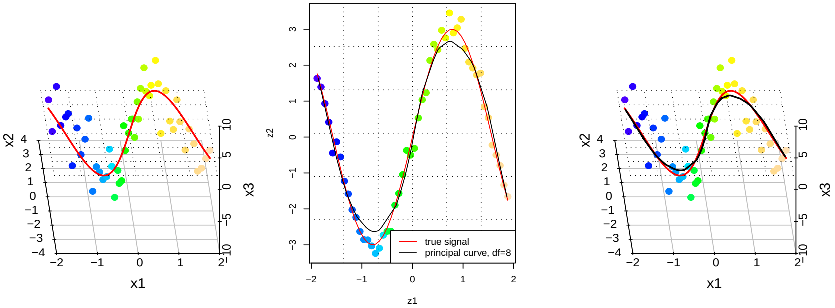
- A curve that passes through the centre of the data.
- Explicit mapping and reconstruction error available.
- Can over-fit, or under-fit.





Subspace Constraint

- Assume the nonlinearity lies on a lower-dimensional subspace.



- Reconstruction: embed the principal curve back into the original space.
- Question: How to find that constraint subspace?

Subspace Search: Kernel PCA and Maximum Eigenvalue Maximization

- Kernel PCA (Schölkopf et. al. 1998) solves:

$$\max_{g \in \mathcal{H}_K : \|g\|_{\mathcal{H}_K}=1} \hat{var}(g(\mathbf{x})), \tag{1}$$

  where $\mathcal{H}_K$ is the Hilbert Space of functions induced by the kernel K (Hastie et. al. 2009).
- Assuming the objective (1) is a measure of nonlinearity, we search for a projection matrix $\mathbf{H}$ such that:

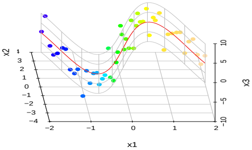
$$\max_{\mathbf{H}:\mathbf{H}^T\mathbf{H}=\mathbf{I}} \left\{ \max_{g \in \mathcal{H}_K : \|g\|_{\mathcal{H}_K}=1} \hat{var}(g(\mathbf{H}^{\mathbf{T}}\mathbf{x})) \right\}$$

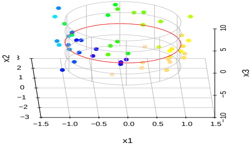
- The term inside {} is proportional to the largest eigenvalue of the Gaussian kernel matrix $\mathbf{K}^{\mathbf{H}}$ for the projected data:

$$\mathbf{K}^{\mathbf{H}}_{ij} = e^{-\frac{\|\mathbf{H}^T(\mathbf{x}_i - \mathbf{x}_j)\|^2}{\sigma}}$$

- Further dimension reduction can be performed on $(\mathbf{I} - \mathbf{H}\mathbf{H}^T)\mathbf{x}$.

Simulation

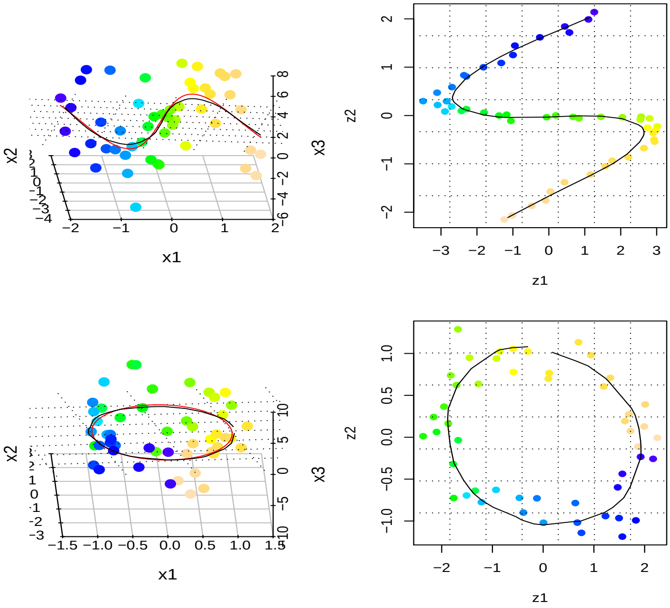




Sinusoidal	Circular
$x_1 = (-0.6\pi ... 0.6\pi)$	$\theta = (-\pi ... \pi)$
$x_2 = 3sin(2x_1) + \epsilon$	$x_1 = sin(\theta) + \epsilon_1$
$x_3 \sim N(0, \sigma = 3)$	$x_2 = 2cos(\theta) + \epsilon_2$
	$x_3 \sim N(0, \sigma = 3)$

- 50 training samples, 500 validation samples.
- d.f. for principal curve and σ for Gaussian Kernel chosen by reconstruction error on the validation set.

Results (—- True Curve, —- Fitted Principal Curve)



Conclusion

- Regularization for nonlinear dimension reduction: roughness-penalty is not enough.
- Subspace constraint regularizes by controlling the direction principal curve can move.
- Future work: a better measure of nonlinearity.

Reference

- Schölkopf, B, Smola, A. & Muller, K.R. (1998) Nonlinear Component Analysis as a Kernel Eigenvalue Problem. Neural Computation 10, 1299-1319.
- Hastie, T. & Stuetzle, W. (1989) Principal Curves. JASA. 84(406):502-516.
- Hastie, T, Tibshirani, R. & Friedman, J. (2009) The Elements of Statistical Learning, 2nd Ed. Springer.