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# Non-Local Manifold Parzen Windows

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## Summary

**1.** The *curse of dimensionality* in density estimation is due to the **locality** of the estimators: $f(x)$ mostly depends on the neighbors of $x$.

**2.** Previous work on density estimation taking advantage of manifold structure: Manifold Parzen Windows (Vincent & Bengio 2003). Each local Gaussian is flattened in the directions of the manifold. Still **local**.

**3.** Previous work on non-local manifold learning: Manifold Tangent Learning (Bengio and Monperrus, 2005). Learn to predict the tangent vectors of the manifold at $x$ as a function of $x$ and of globally estimated parameters $\theta$. Yields to non-local generalization.

**4.** This work: combine the above two, i.e. predict the *covariance matrix* at $i$-th Gaussian $x_i$ as a function of $x_i$ and of globally estimated parameters $\theta$.

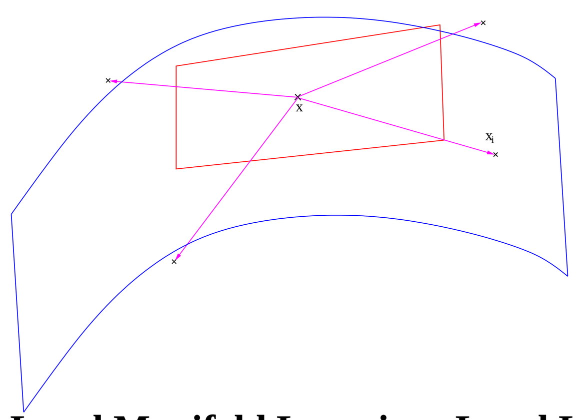
**5.** Results: *better density estimates* than using a local estimator (Parzen Windows or Manifold Parzen Windows or Gaussian Mixtures).


## Curse of Dimensionality for Local Estimators

**Curse of dimensionality for Parzen Windows**

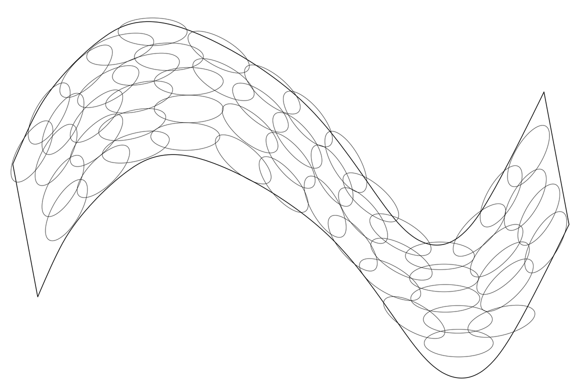
Number of required examples $\propto m^{(4+d)/5}$ where $d$ is the intrinsic dimension of the data and $m$ is the number of examples required to obtain given error level when $d = 1$. See (Silverman, 1986; Hardle et al., 2004).

**Tangent Plane Defined from Neighbhors**



Spectral manifold learning algorithms (LLE, Isomap, etc...) define the local tangent plane at $x$ mainly on the span of the vectors of neighbor differences $x_i - x$.

**Local Manifold Learning: Local Linear Patches**



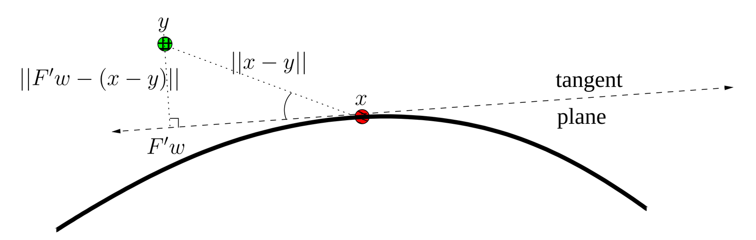
Current manifold learning algorithms cannot handle highly curved manifolds because they are based on locally linear patches estimated locally (possibly aligned globally).

**Fundamental Problem with Local Manifold Learning:** curse of dimensionality. Can't generalize "far" from training examples. $O((1/r)^d)$ patches needed, $> O(d)$ data/patch ($\propto$ noise).

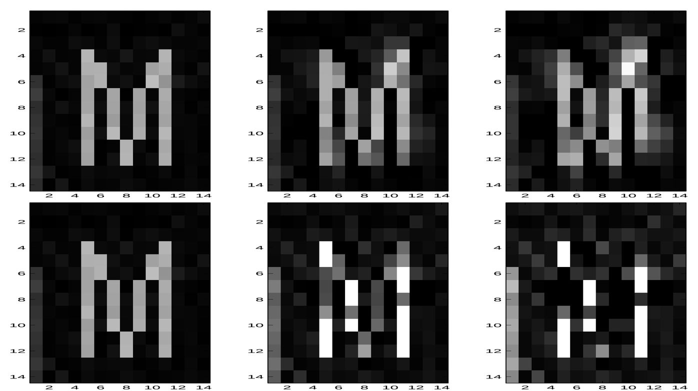
## Non-Local Tangent Plane Predictors

Tangent plane basis vectors = learned function of $x$ and global parameters $\theta$, with flexibly parametrized matrix-valued $d \times n$ function $F(x)$.

Train $d \times n$ function $F(x)$ to approximately span the differences between $x$ and its neighbors $y$.




Train on rotated DIGITS and generalize on LETTERS! Learn rotation manifold.



Top: using neural network DOES rotate. Bottom: using local predictor DOES NOT rotate.

## Manifold Parzen Windows

Regularized Gaussian mixture, Gaussians centered near each training example $x_i$, covariance matrices flat in "principal directions":

$$p(y) = \frac{1}{n}\sum_{i=1}^{n} \mathrm{Normal}(y; x_i + \mu(x_i), S(x_i))$$

where $x_i + \mu(x_i)$ = Gaussian center and $S(x_i)$ = covariance of $i$-th component, with

$$S(x_i) = \sigma^2_{noise}(x_i) I + \sum_{j=1}^{k} s_j(x_i) v_j(x_i) v_j(x_i)'$$

where $s_j(x_i)$ and $\sigma^2_{noise}(x_i)$ are scalars, and $v_j(x_i)$ denotes a "principal" direction with variance $s_j(x_i) + \sigma^2_{noise}(x_i)$, while $\sigma^2_{noise}(x_i)$ is the noise variance (the variance in all the other directions).

In (Vincent and Bengio, 2003), $\mu(x_i) = 0$, and $\sigma^2_{noise}(x_i) = \sigma^2$ is a global hyper-parameter, while $(\lambda_j(x_i), v_j(x_i)) = (s_j(x_i) + \sigma^2_{noise}(x_i), v_j(x_i))$ are leading (eigenvalue,eigenvector) of local empirical covariance.

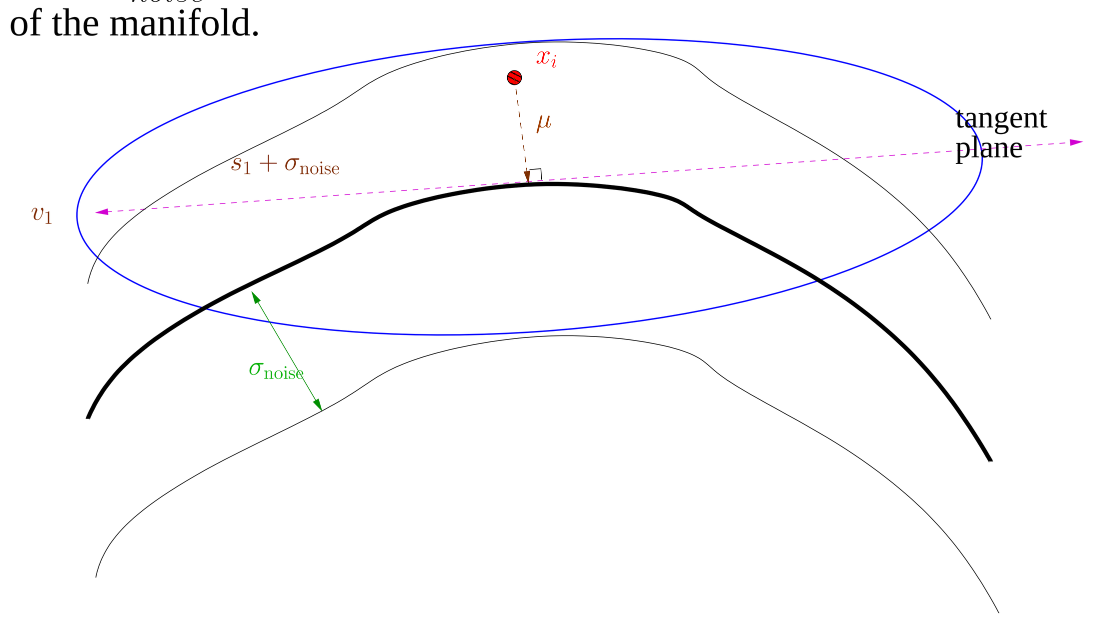
Hyper-parameters: $k$ and $\sigma^2_{noise}$.

## Non-Local Manifold Parzen Windows

Consider $\mu(x_i)$ and $S(x_i)$ as **functions** of $x_i$ with *global parameters*: **share information about the density across different regions of space**.

Neural network with $x_i$ in input to predict $\mu(x_i)$, $\sigma^2_{noise}(x_i)$, and the $s_j(x_i)$ and $v_j(x_i)$. The $v_j(x_i)$ do not need to be orthonormal.

- The Gaussian near $x_i$ tells how neighbors of $x_i$ are expected to differ from $x_i$.
- Its "principal" vectors $v_j(x_i)$ span the tangent of the manifold near $x_i$.
- $\mu(x_i)$ tells how $x_i$ is located with respect to its projection on the manifold.
- $\sigma^2_{noise}(x_i)$ tells us how far from the manifold to expect neighbors.
- $s_j(x_i) + \sigma^2_{noise}(x_i)$ tell us how far to expect neighbors on the different local axes of the manifold.

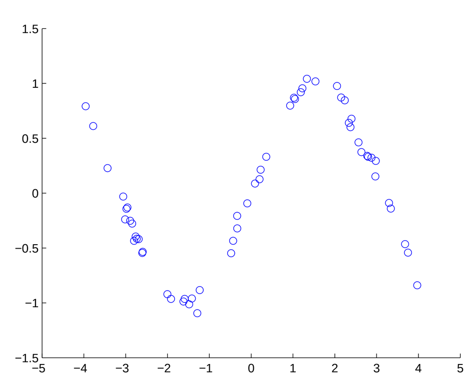



## Semi-Spherical Variant

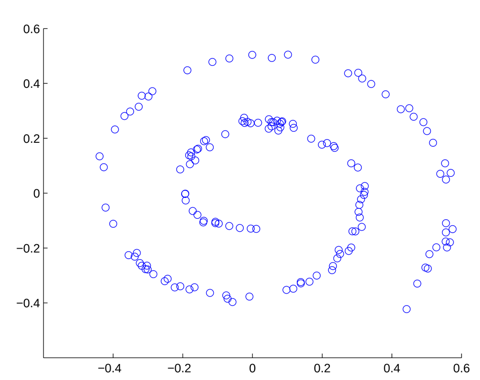
A simplified version of the above model has been implemented for the experiments described here. The simplification is that the *same variance is assumed for all the principal eigenvectors*, i.e. $s_j(x) = s_1(x)$.

In addition to the matrix $F(x_i)$ with rows $v_j(x_i)$, the outputs of the neural networks are the 'noise variance' $\sigma^2_{noise}(x_i)$, the excess 'on-manifold variance' $s_1(x_i)$, and the Gaussian mean displacement $\mu(x_i)$.

## Toy Data



Samples used for training



Samples used for training


## References

Bengio, Y. and Monperrus, M. (2005). Non-local manifold tangent learning. In Saul, L., Weiss, Y., and Bottou, L., editors, *Advances in Neural Information Processing Systems 17*. MIT Press.

Hardle, W., Muller, M., Sperlich, S., and Werwatz, A. (2004). *Nonparametric and Semiparametric Models*. Springer, http://www.xplore-stat.de/ebooks/ebooks.html.

Silverman, B. W. (1986). *Density Estimation for Statistics and Data Analysis*. Chapman and Hall, London.

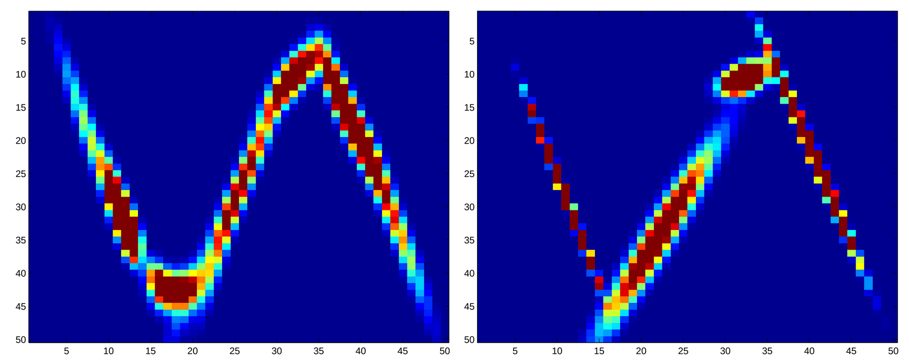
Vincent, P. and Bengio, Y. (2003). Manifold parzen windows. In Becker, S., Thrun, S., and Obermayer, K., editors, *Advances in Neural Information Processing Systems 15*, Cambridge, MA. MIT Press.


## Experimental Results

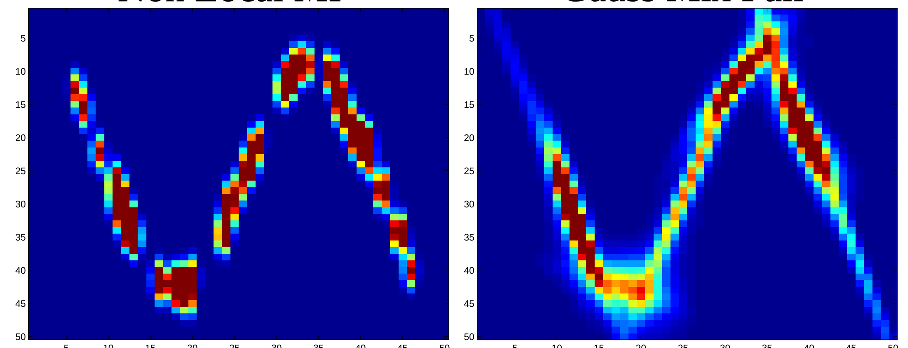
Hyper-parameters chosen by cross-validation
Out-of-sample Negative Log-Likelihood (NLL):

| **Algorithm** | **NLL on sinus** | **NLL on spiral** |
|---|---|---|
| Non Local MP | 1.409768 | -1.35885 |
| Gauss Mix Full | 1.56653 | -0.5747403 |
| Gauss Mix Diag | 2.593532 | -0.6400698 |
| Gauss Mix Spher | 2.672263 | -0.1716301 |
| Manifold Parzen | 1.697273 | -0.6077337 |
| Parzen Window | 1.841497 | -0.513347 |

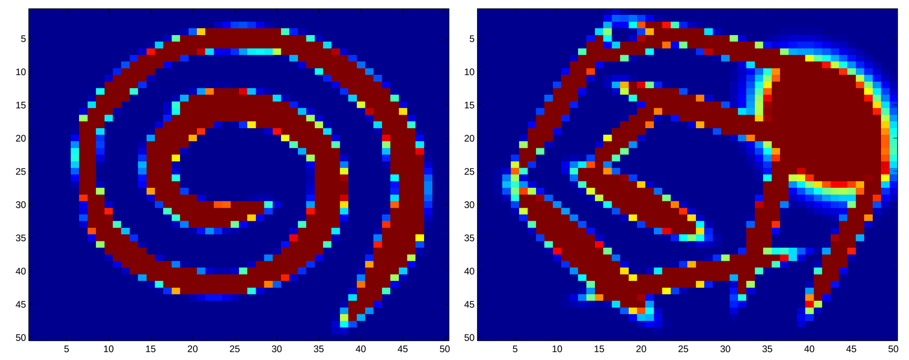
And the obtained distributions are:



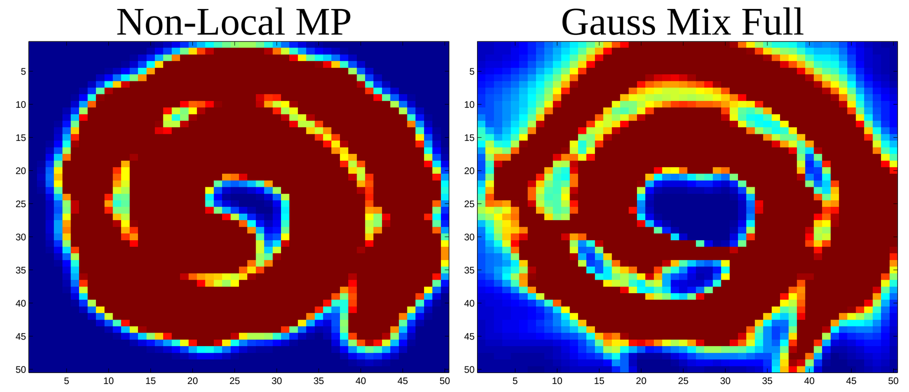
Non Local MP — Gauss Mix Full



Parzen Window — Manifold Parzen

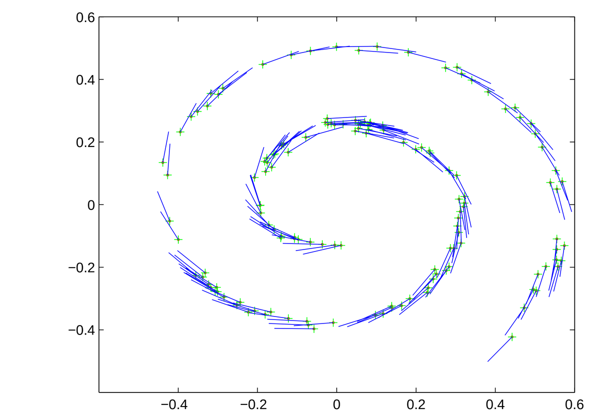


Non-Local MP — Gauss Mix Full

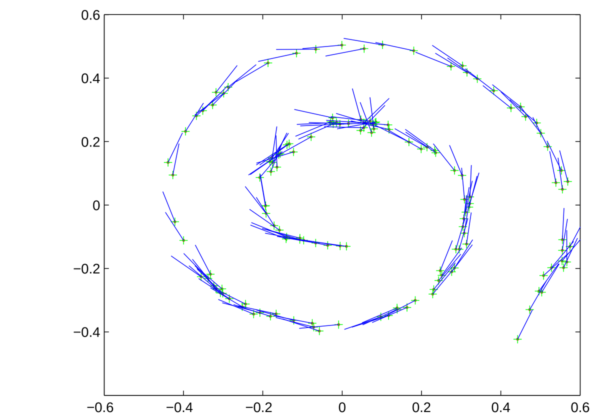


Parzen Window — Manifold Parzen

The use of global parameters helps to find principal directions that are smoother and more consistent with the global structure of the data:



Principal directions learned with Non-Local Manifold Parzen



Principal directions learned with Manifold Parzen