Reassuring and Troubling Views on Graph-Based Semi-Supervised Learning

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Outline

1 Graph-Based Semi-Supervised Learning

2 Transduction, Induction, Approximation

3 Curse of Dimensionality

Notations

- Task of **binary classification** with labels $y_i \in \{-1, 1\}$

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- **Transduction** $\Rightarrow \hat{\boldsymbol{Y}}_u = (\hat{y}_{l+1}, \hat{y}_{l+2}, \ldots, \hat{y}_n)^\top$
- **Induction** $\Rightarrow \hat{y} : \boldsymbol{x} \rightarrow \hat{y}(\boldsymbol{x})$

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Trade-off between (1) and (2) $\Rightarrow$ cost function:

$$C(\hat{\boldsymbol{Y}}) = \sum_{i=1}^{l} (\hat{y}_i - y_i)^2 + \frac{\mu}{2} \sum_{i,j=1}^{n} \boldsymbol{W}_{ij} (\hat{y}_i - \hat{y}_j)^2$$

with $\boldsymbol{W}_{ij} = W_X(\boldsymbol{x}_i, \boldsymbol{x}_j)$ a positive weighting function (e.g kernel)

Graph-Based Cost Criterion

Graph Laplacian: $\boldsymbol{L}_{ii} = \sum_{j \neq i} \boldsymbol{W}_{ij}$ and $\boldsymbol{L}_{ij} = -\boldsymbol{W}_{ij}$.

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$C(\hat{\boldsymbol{Y}})$ is minimized when

$$(\boldsymbol{S} + \mu \boldsymbol{L}) \hat{\boldsymbol{Y}} = \boldsymbol{Y}$$

with $\boldsymbol{S}_{ij} = \delta_{i=j} \delta_{i \leq l}$
$\Rightarrow$ **linear system (*n* unknowns and equations)**

From Matrix Inversion to Label Propagation

Linear system rewrites for a labeled point

$$\hat{y}_i = \frac{\sum_j \boldsymbol{W}_{ij}\hat{y}_j + \frac{1}{\mu}y_i}{\sum_j \boldsymbol{W}_{ij} + \frac{1}{\mu}}$$

and for an unlabeled point

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$$\hat{y}_i^{(t+1)} = \frac{\sum_j \boldsymbol{W}_{ij} \hat{y}_j^{(t)} + \frac{1}{\mu} y_i}{\sum_j \boldsymbol{W}_{ij} + \frac{1}{\mu}}$$

and for an unlabeled point

$$\hat{y}_i^{(t+1)} = \frac{\sum_j \boldsymbol{W}_{ij} \hat{y}_j^{(t)}}{\sum_j \boldsymbol{W}_{ij}}.$$

$\Rightarrow$ **Jacobi** or **Gauss-Seidel** iterative algorithms (but there are more refined algorithms for sparse system resolution)

Related Work and Variants

- M. Szummer and T. Jaakkola (2002): *Partially labeled classification with Markov random walks*
- X. Zhu, Z. Ghahramani and J. Lafferty (2003): *Semi-supervised learning using Gaussian fields and harmonic functions*
- D. Zhou, O. Bousquet, T. Navin Lal, J. Weston, B. Schölkopf (2004): *Learning with local and global consistency*
- M. Belkin, I. Matveeva and P. Niyogi (2004): *Regularization and Semi-supervised Learning on Large Graphs*
- . . .

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- **Heat diffusion**, ...

Why Induction?

The previously presented techniques perform **transduction**.

Out-of-sample predictions

What to do with a new test point?

We could retrain, but computationally expensive $O(n^3)$ (or $O((kn)^{3/2})$ if sparse graph with k neighbors).

Trade-off

If we could do induction cheaply, even at the price of losing a bit of the advantage of transduction, it might be useful in practice!

Induction Criterion in a Transductive Framework

Induction as an **approximation to transduction**: force predictor's response to remain fixed on previous training data (labeled and unlabeled), when test point is added.

From Transduction to Induction

Solving the linear system $\Rightarrow$ $\hat{\boldsymbol{Y}}$ (**transduction**).
From a new point $\boldsymbol{x}$ and *already computed* $\hat{\boldsymbol{Y}}$:

$$\min_{\hat{y}(\boldsymbol{x})} C(\hat{y}(\boldsymbol{x})) = C(\hat{\boldsymbol{Y}}) + \frac{\mu}{2} \sum_{i=1}^{n} W_X(\boldsymbol{x}_i, \boldsymbol{x})(\hat{y}_i - \hat{y}(\boldsymbol{x}))^2$$

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$$\Rightarrow \hat{y}(\boldsymbol{x}) = \frac{\sum_{i=1}^{n} W_X(\boldsymbol{x}_i, \boldsymbol{x})\hat{y}_i}{\sum_{i=1}^{n} W_X(\boldsymbol{x}_i, \boldsymbol{x})}$$

Induction like Parzen Windows, but using *estimated* labels $\hat{\boldsymbol{Y}}$

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$$\hat{y}_i \simeq \frac{\sum_{j \in S} \boldsymbol{W}_{ij} \hat{y}_j}{\sum_{j \in S} \boldsymbol{W}_{ij}}$$

i.e. $\hat{\boldsymbol{Y}}_R \simeq \overline{\boldsymbol{W}}_{RS} \hat{\boldsymbol{Y}}_S$.

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  i.e. $\hat{\boldsymbol{Y}}_R \simeq \overline{\boldsymbol{W}}_{RS} \hat{\boldsymbol{Y}}_S$.
- Better: minimize **the full cost** over $\hat{\boldsymbol{Y}}_S$ only. $C(\hat{\boldsymbol{Y}}) = C(\hat{\boldsymbol{Y}}_S, \hat{\boldsymbol{Y}}_R) \simeq C(\hat{\boldsymbol{Y}}_S, \overline{\boldsymbol{W}}_{RS} \hat{\boldsymbol{Y}}_S) = C'(\hat{\boldsymbol{Y}}_S)$

$\Rightarrow$ linear system with only $|S|$ unknowns.

More Approximations

$$
\begin{aligned}
C'(\hat{\boldsymbol{Y}}_S) = & \underbrace{\|\hat{\boldsymbol{Y}}_I - \boldsymbol{Y}_I\|^2}_{C_L} && O(l) \\
& + \underbrace{\mu \hat{\boldsymbol{Y}}_S{}^\top \boldsymbol{L}_{SS} \hat{\boldsymbol{Y}}_S}_{C_{SS}} && O(|S|^2) \\
& + \underbrace{2\mu \hat{\boldsymbol{Y}}_R{}^\top \boldsymbol{L}_{RS} \hat{\boldsymbol{Y}}_S}_{C_{RS}} && O(|S||R|) \\
& + \underbrace{\mu \hat{\boldsymbol{Y}}_R{}^\top \boldsymbol{L}_{RR} \hat{\boldsymbol{Y}}_R}_{C_{RR}} && O(|R|^2)
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Cost computation complexity: $O(|R|^2)$ is too much!

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Cost computation complexity: $O(|S||R|)$ is ok!

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- Removing C_{RS} would mean training only on S (too simple)
- Thus we have no choice but to use the proposed cost
- Experiments show it is often better! The approximation

$$\hat{y}_i \simeq \frac{\sum_{k \in S} \boldsymbol{W}_{ik} \hat{y}_k}{\sum_{k \in S} \boldsymbol{W}_{ik}}$$

can be very poor if $\boldsymbol{x}_i \in R$ is far from all samples $\boldsymbol{x}_k \in S$, which can lead to irrelevant terms in C_{RR} *with a significant weight* $\Rightarrow$ overall accuracy is worse

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1. **Random**: fast, easy, crappy.
   Main problem = does not "fill the space" well enough $\Rightarrow$ bad approximation by the induction formula (some points have no near neighbors in the subset)
2. **Heuristic**: greedy construction of subset. Start with the labeled points ($S = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_l\}$) and iteratively add

$$\boldsymbol{x}_i^* = \text{argmax}_{\boldsymbol{x}_i}\ dist(\boldsymbol{x}_i, S) = \text{argmin}_{\boldsymbol{x}_i} \sum_{j \in S} \boldsymbol{W}_{ij}$$

   i.e. choose the point $\boldsymbol{x}_i$ "farthest" from the current subset. (NB: additional tricks to eliminate outliers and sample more points near decision surface)

Experimental Results

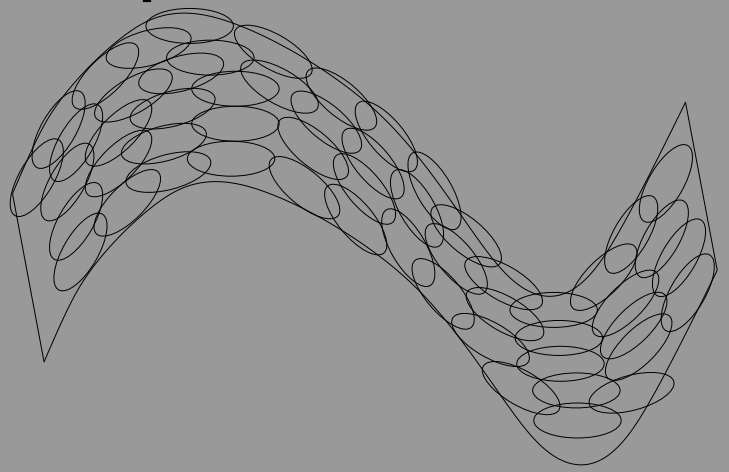
Table: Comparative Classification Error (Induction)

% labeled	LETTERS	MNIST	COVTYPE
1%			
NoSub	56.0	35.8	47.3
$RandSub_{subOnly}$	59.8	29.6	**44.8**
RandSub	57.4	27.7	75.7
SmartSub	**55.8**	**24.4**	45.0
5%			
NoSub	**27.1**	12.8	37.1
$RandSub_{subOnly}$	32.1	14.9	**35.4**
RandSub	29.1	12.6	70.6
SmartSub	28.5	**12.3**	35.8
10%			
NoSub	**18.8**	**9.5**	34.7
$RandSub_{subOnly}$	22.5	11.4	**32.4**
RandSub	20.3	9.7	64.7
SmartSub	19.8	**9.5**	33.4

More comparisons between *RandSub* and *SmartSub* on 8 more UCI datasets $\Rightarrow$ *SmartSub* always performs better.

Curse of Dimensionality: Geometric Intuition

If we have to tile the space or manifold where bulk of the distribution is concentrated, then will need **exponential number of "patches"**:



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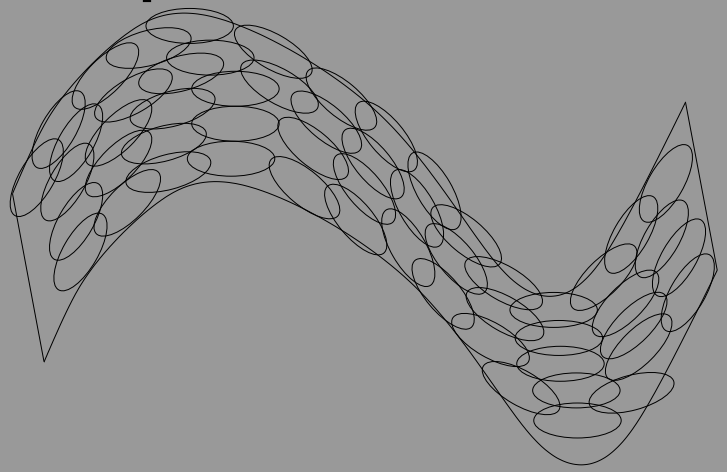

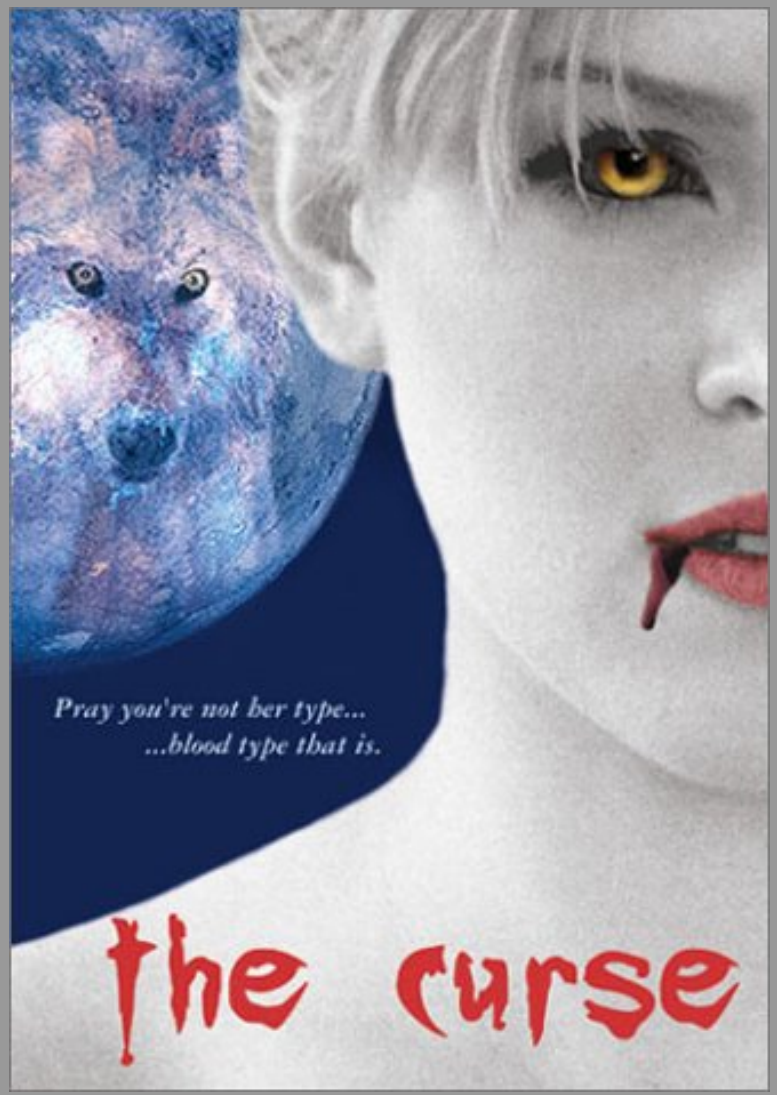

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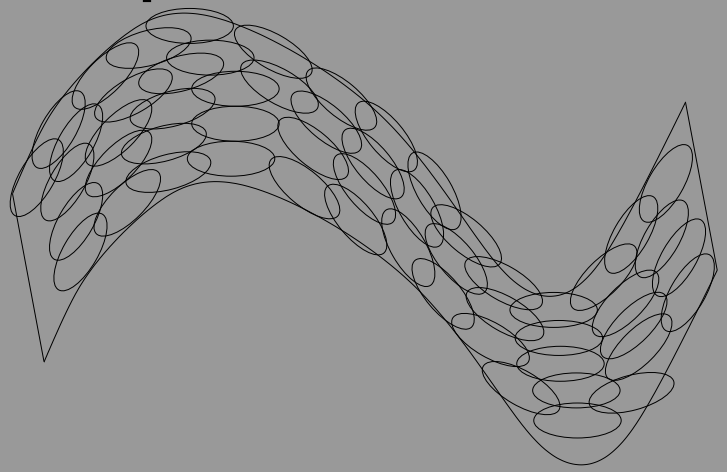

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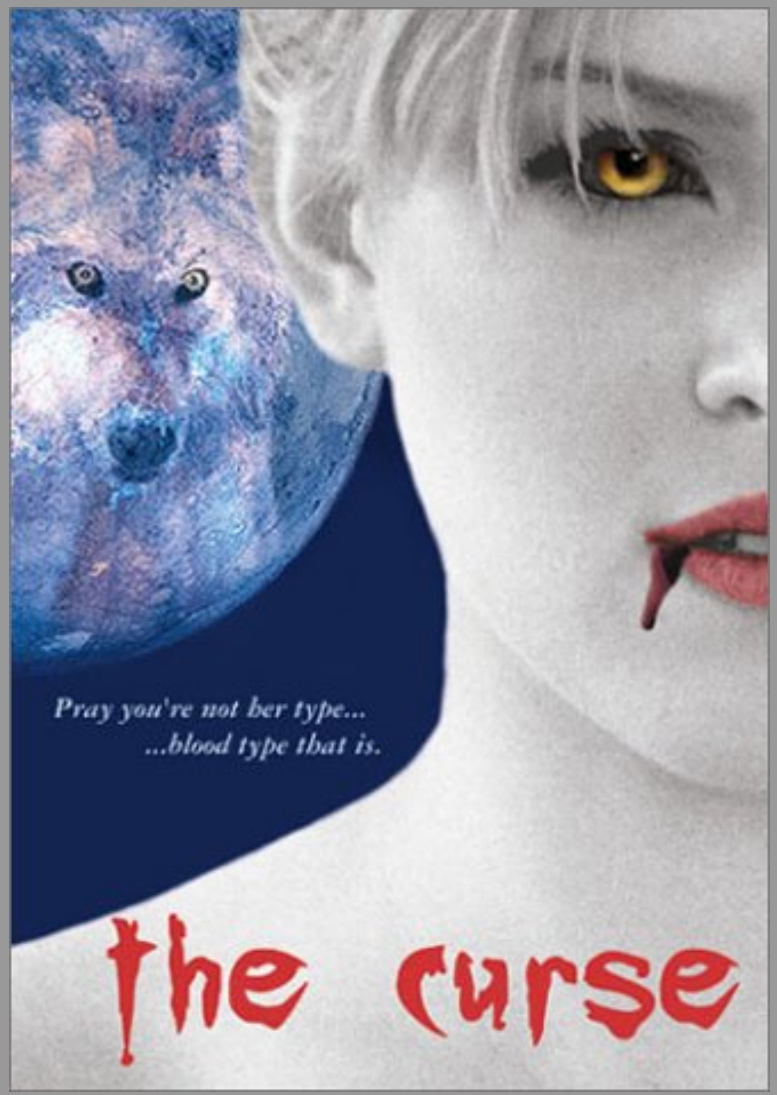

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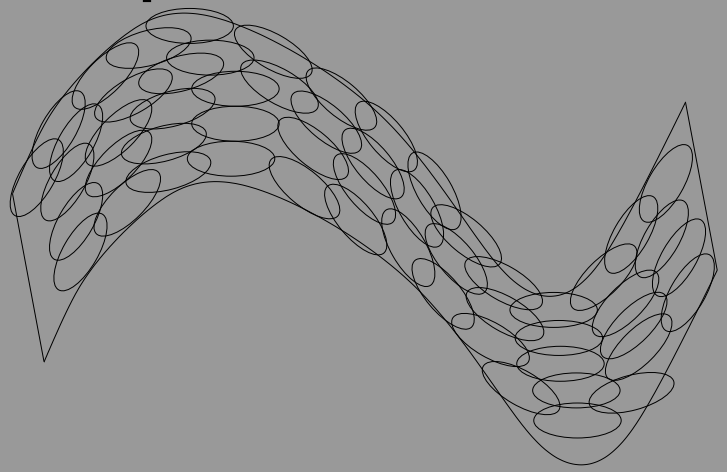

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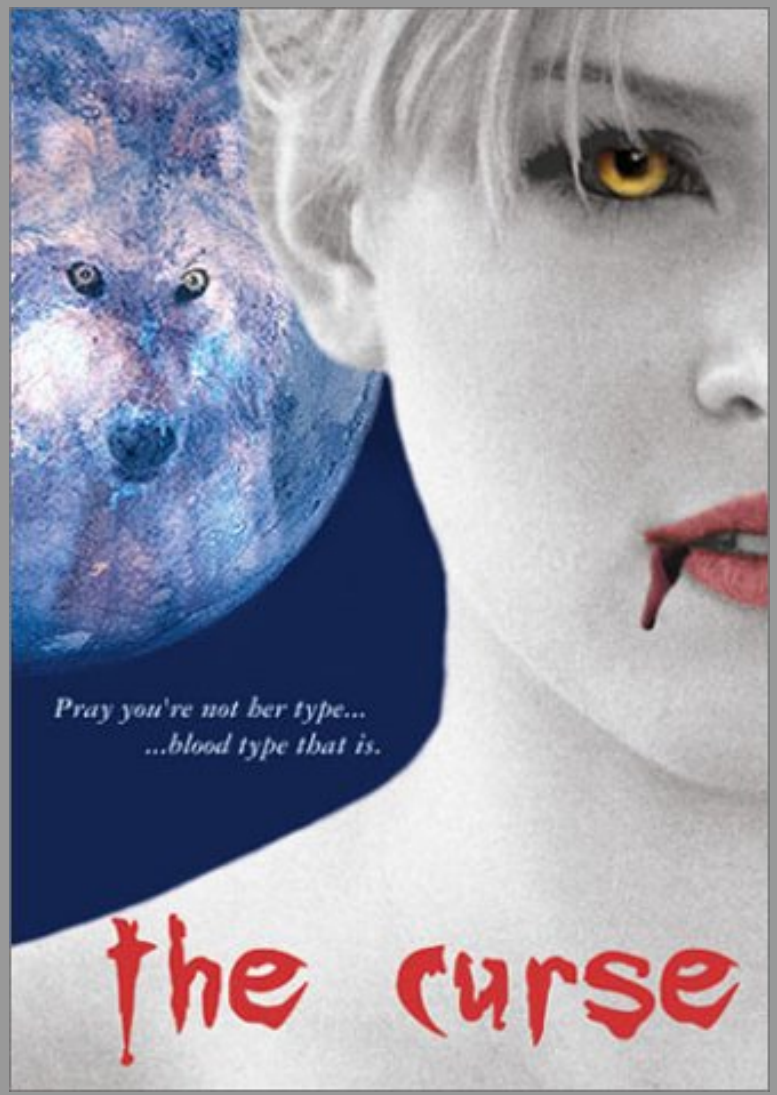
May require $O(\text{const}^d)$ examples!



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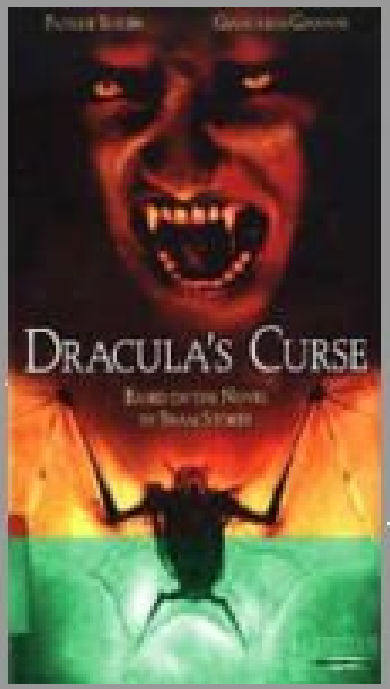
2. in order to approximate the (true) decision surface correctly, $\mathcal{N}(\boldsymbol{x})$ must be small enough, as P is only valid locally (e.g. the true normal vector may vary a lot)
3. for $\mathcal{N}(\boldsymbol{x})$ to be small, one needs many training samples (possibly a number exponential in the dimension)

Curse of Dimensionality (2)



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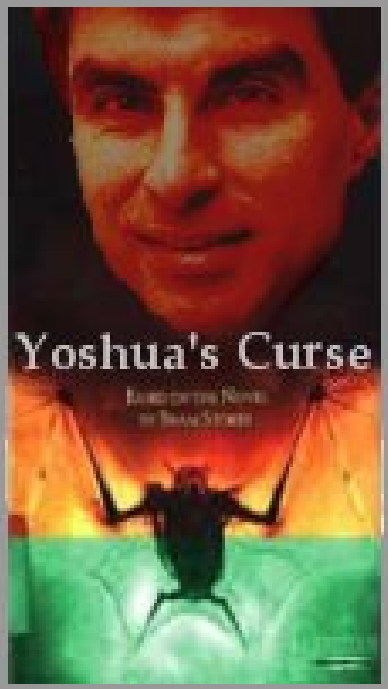

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Curse #2 The number of labeled samples must be higher than the number of regions with constant label

$\Rightarrow$ may need lots of **labeled** data if there are many such regions (possibly exponential in the dimension)

Highly Varying: Parity Function

parity:

$$(b_1, \ldots, b_d) \in \{0,1\}^d \mapsto \begin{cases} 1 \text{ if even } \sum_{i=1}^{d} b_i \\ -1 \text{ otherwise} \end{cases}$$

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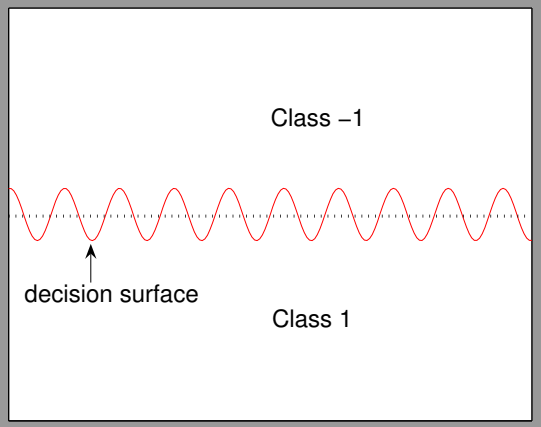
Theorem

A Gaussian kernel classifier needs at least 2^{d-1} Gaussians (i.e. support vectors) to learn the parity function (when Gaussians have fixed width and are centered on training points).

Simple but Highly Variable Functions: Difficult to Learn



This “complex” sinusoidal decision surface requires many Gaussians to learn, but in “C” language, it has a high prior.
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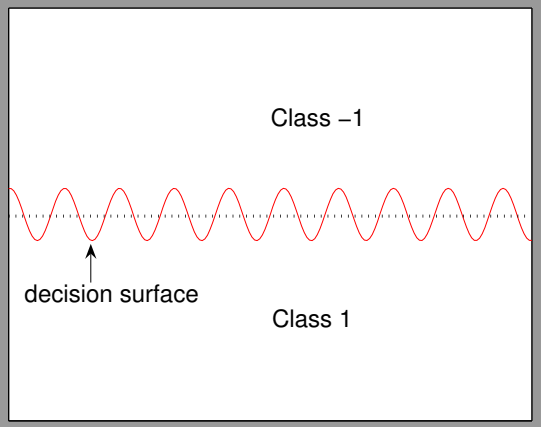

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Corollary of (Schmitt 2002)

If $\exists$ a line in $\boldsymbol{R}^d$ that intersects m times with the decision surface S (and is not included in S), then one needs at least $\lceil \frac{m}{2} \rceil$ Gaussians (of same width) to learn S with a Gaussian kernel classifier.

Local-Derivative Kernels

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Local-derivative kernel: when $\partial f / \partial x$ is (approximately) contained in **the span of the vectors** $(x - x_j)$ **with** x_j **a neighbor of** x:

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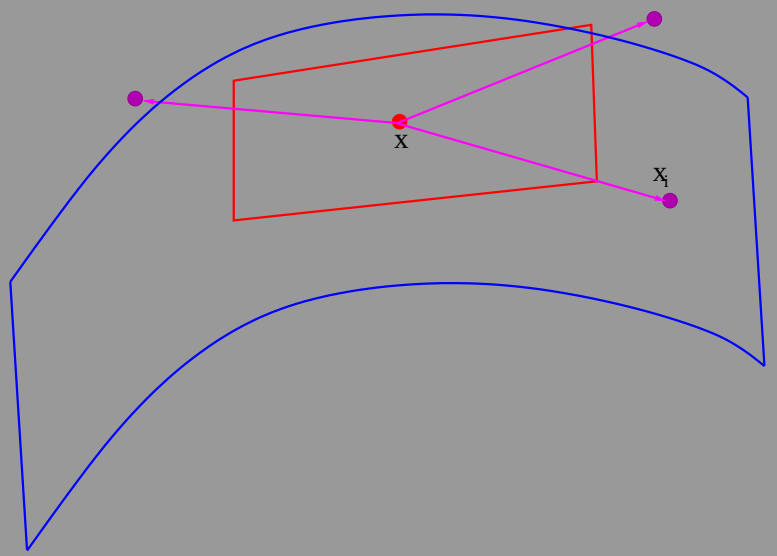

Local-Derivative Kernels

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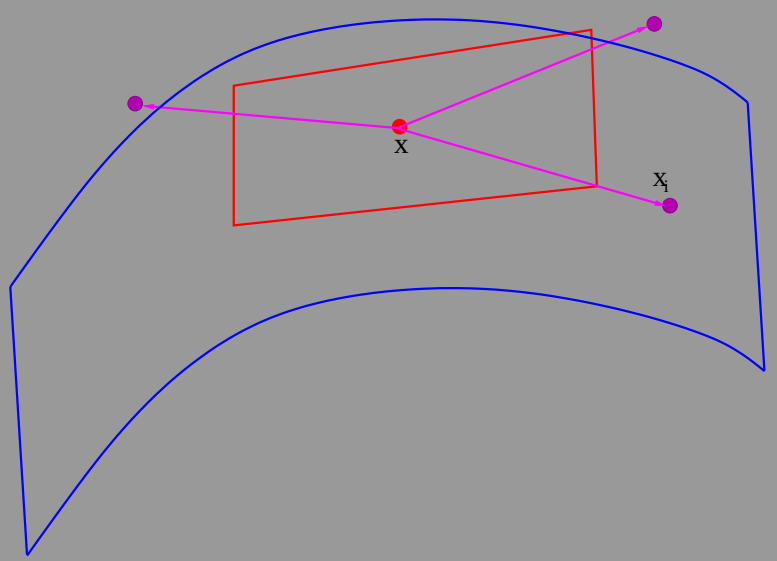
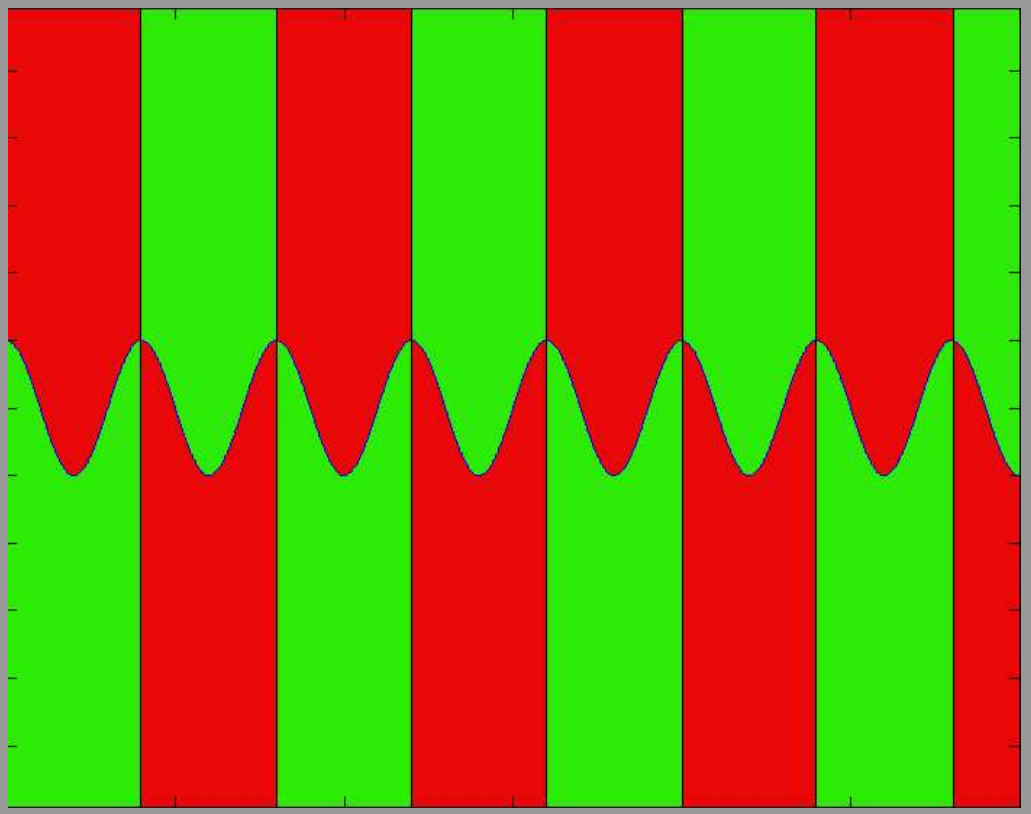


Bad News!

Shape of manifold (tangent vector at x) mostly determined by neighbors of x in the graph.

Semi-Supervised Need of Examples



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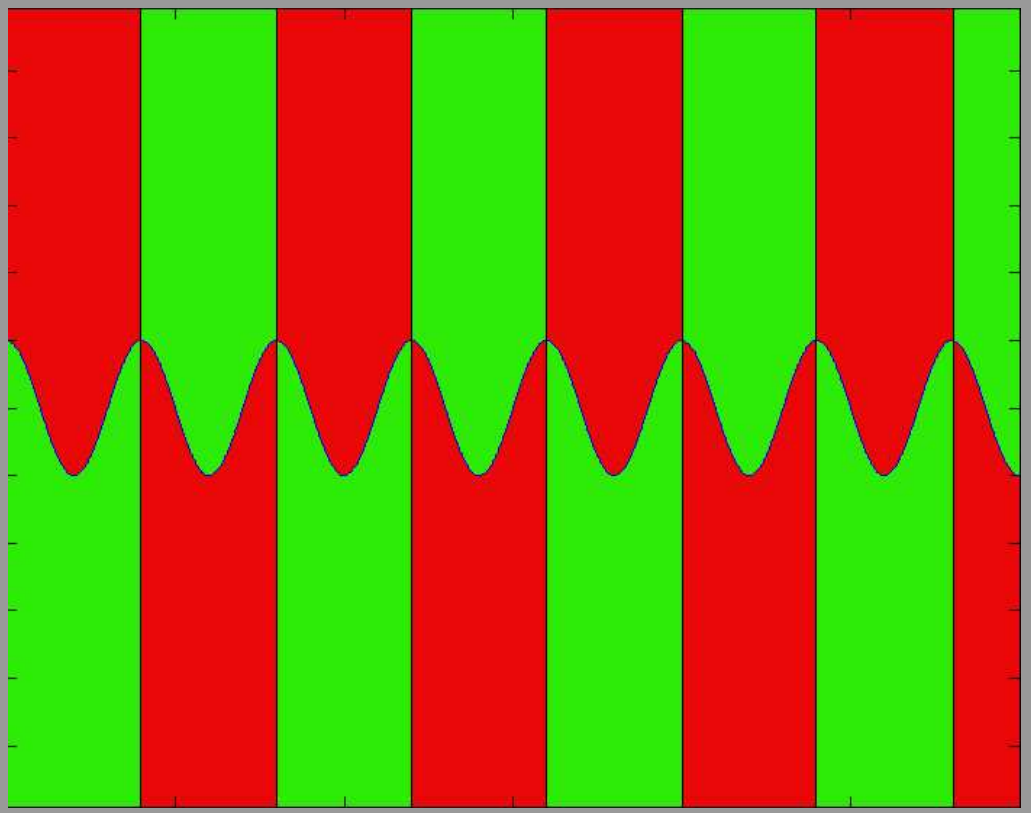

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Number of labeled and unlabeled examples to learn such decision surface may grow **exponentially** with dimension.

Theorem

After running a label propagation algorithm minimizing quadratic cost, number of regions with constant estimated label $\leq$ number of labeled examples.

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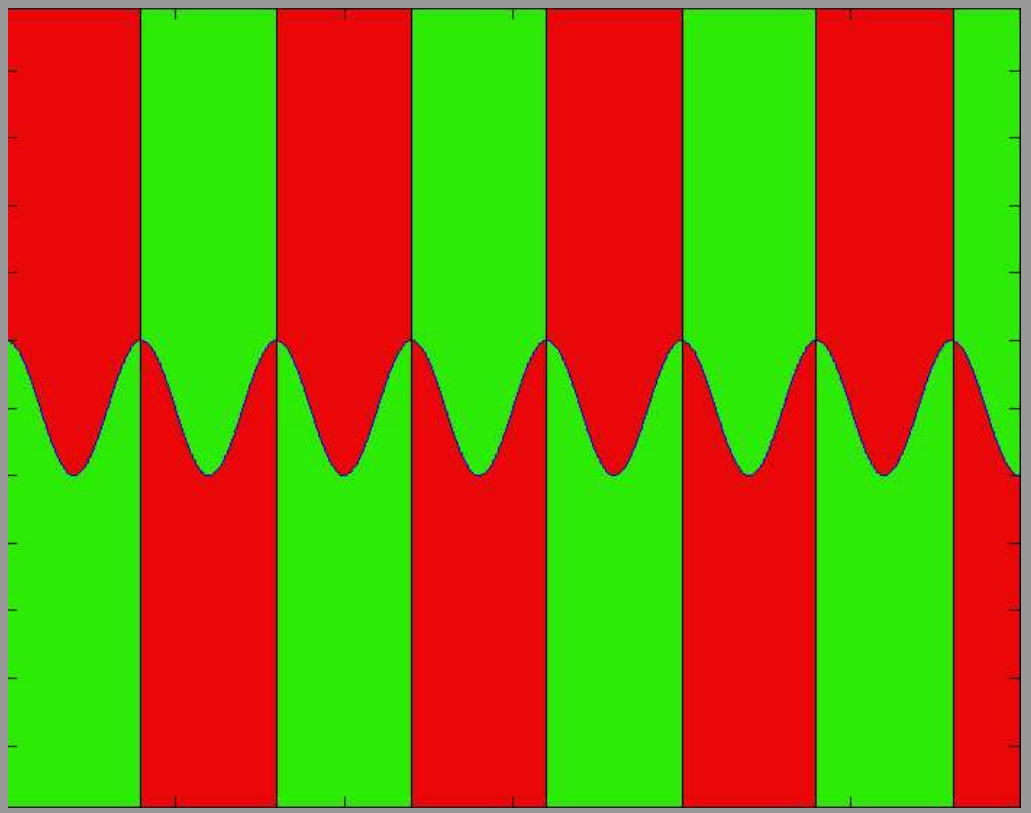

Need unlabeled examples along *sinus* decision surface + labeled ones in each class region.
Number of labeled and unlabeled examples to learn such decision surface may grow **exponentially** with dimension.
This could be **easily** learned with a non-local learning algorithm.

Theorem

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Philosophical Question

Most common non-parametric approaches based on smoothness prior, which leads to “local” learning algorithms, e.g. most kernel-based ones, yielding to **curse of dimensionality** = difficulty to learn structured but highly variable functions.

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Is there hope? Humans seem to learn highly-varying yet structured functions! There might be loose enough priors on general classes of functions that allow non-local learning algorithms to learn them.

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- Limitations of local weights: curse of dimensionality
- Is there hope to discover **non-local** semi-supervised learning? yes!

References

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