Support Vector Machines

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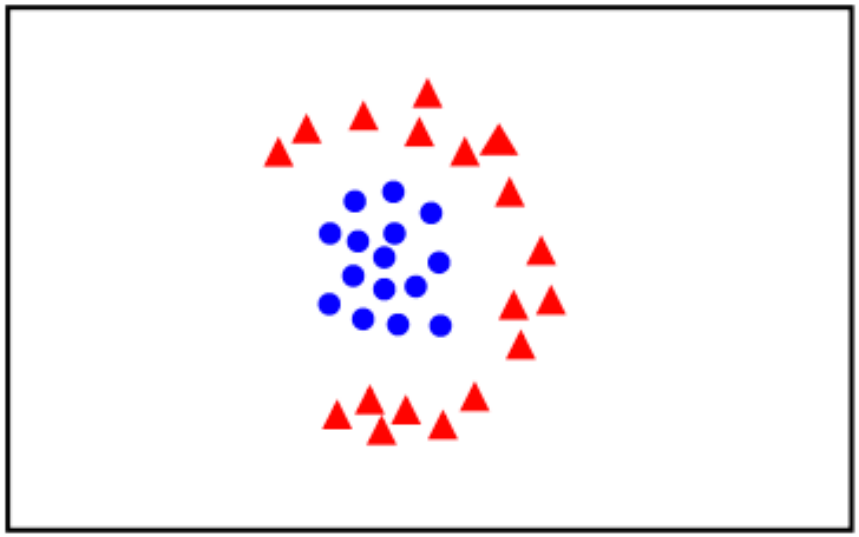
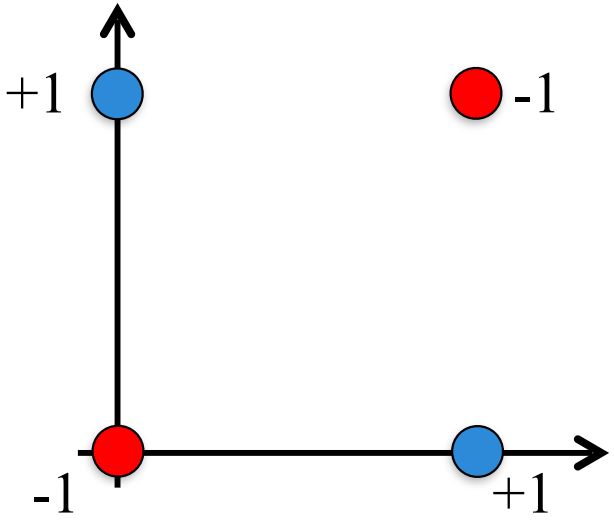
IC-CVLab

Non-Linearly Separable Data



Adaboost can handle this using linear classifiers.

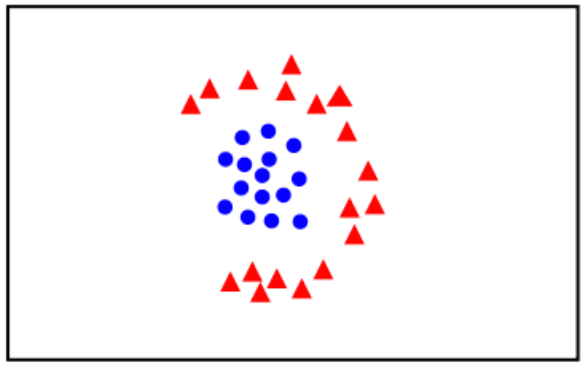


But not this.

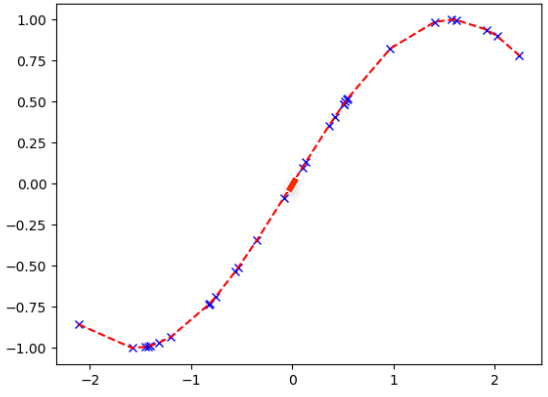
—> Map the data to a higher dimension.

Mapping to a Higher Dimension: Three Examples

1D classification.



2D classification.



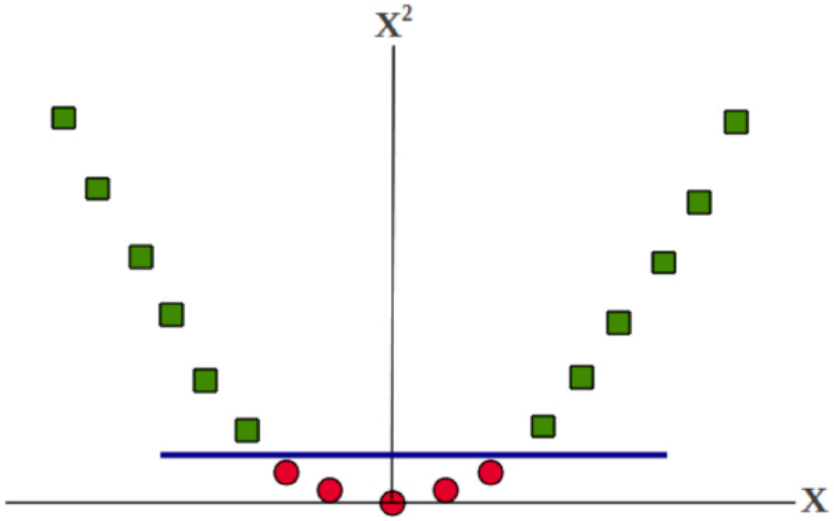
Polynomial approximation.

1D Classification Example

How can we handle this 1D/2-class data?

We can map it to 2D:

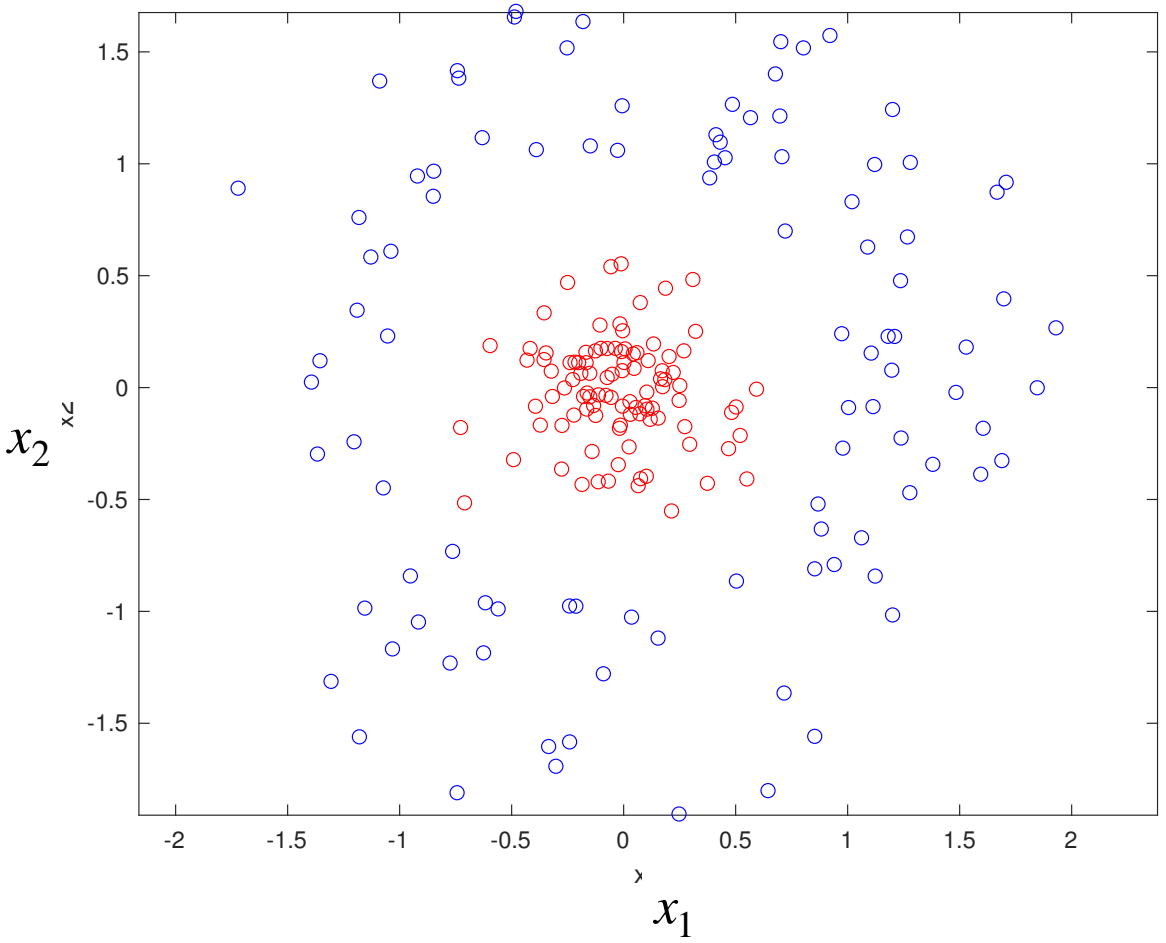
$$x \rightarrow \phi(x) = \begin{bmatrix} x \\ x^2 \end{bmatrix}$$



—> We can now use a linear classifier.

2D Classification Example

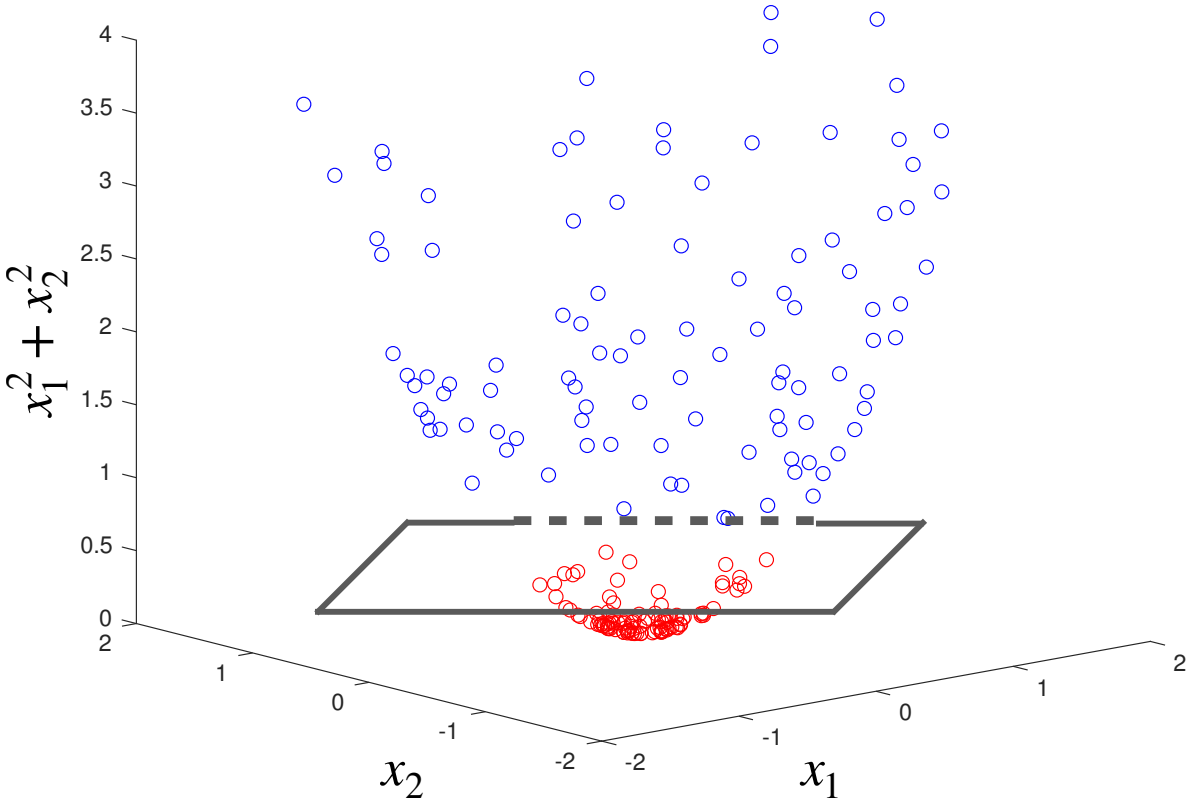
How about this 2D/2-class data?



2D Classification Example

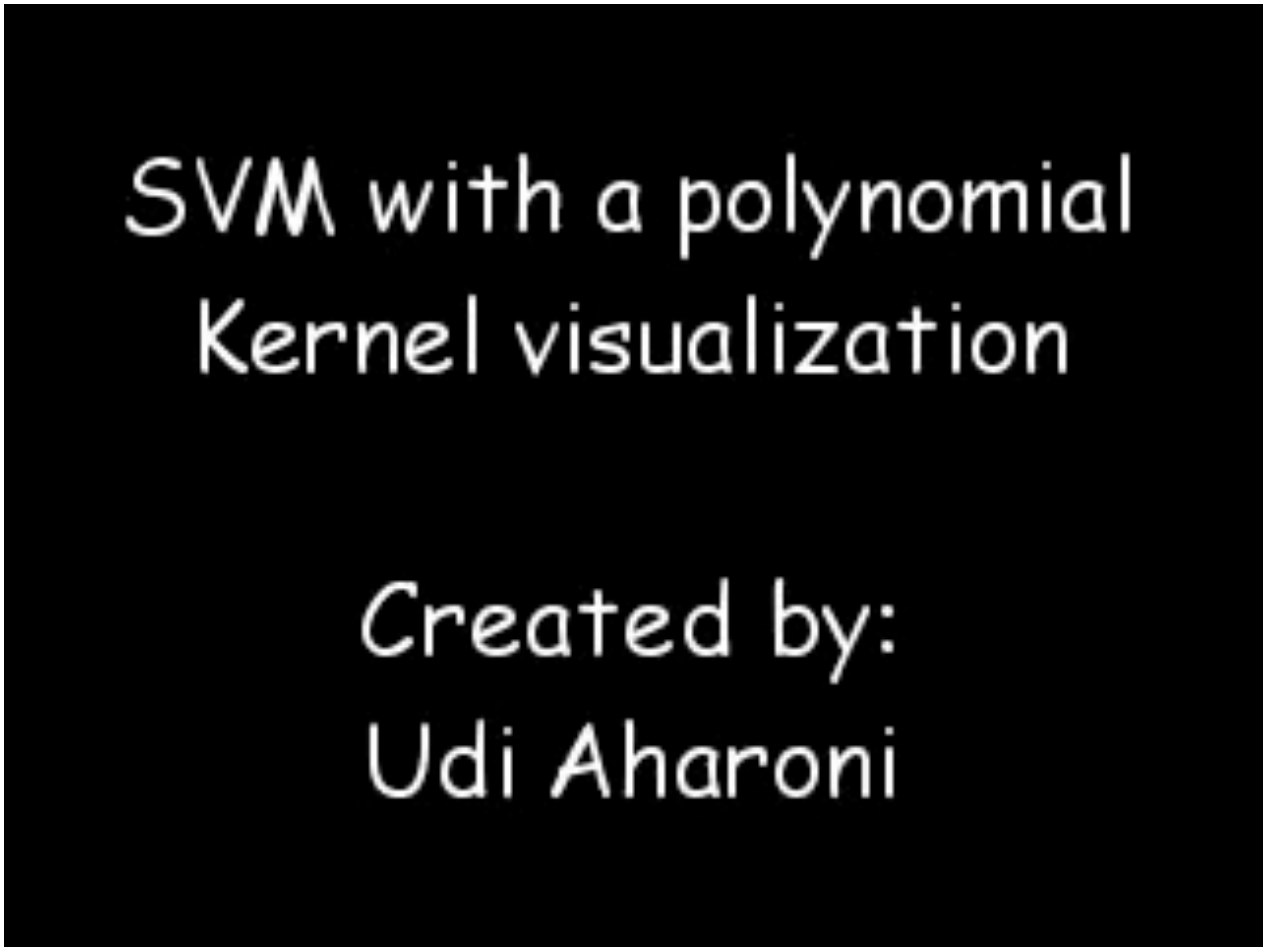
We can map the 2D data to 3D:

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \rightarrow \phi(\mathbf{x}) = \begin{bmatrix} x_1 \\ x_2 \\ x_1^2 + x_2^2 \end{bmatrix}$$

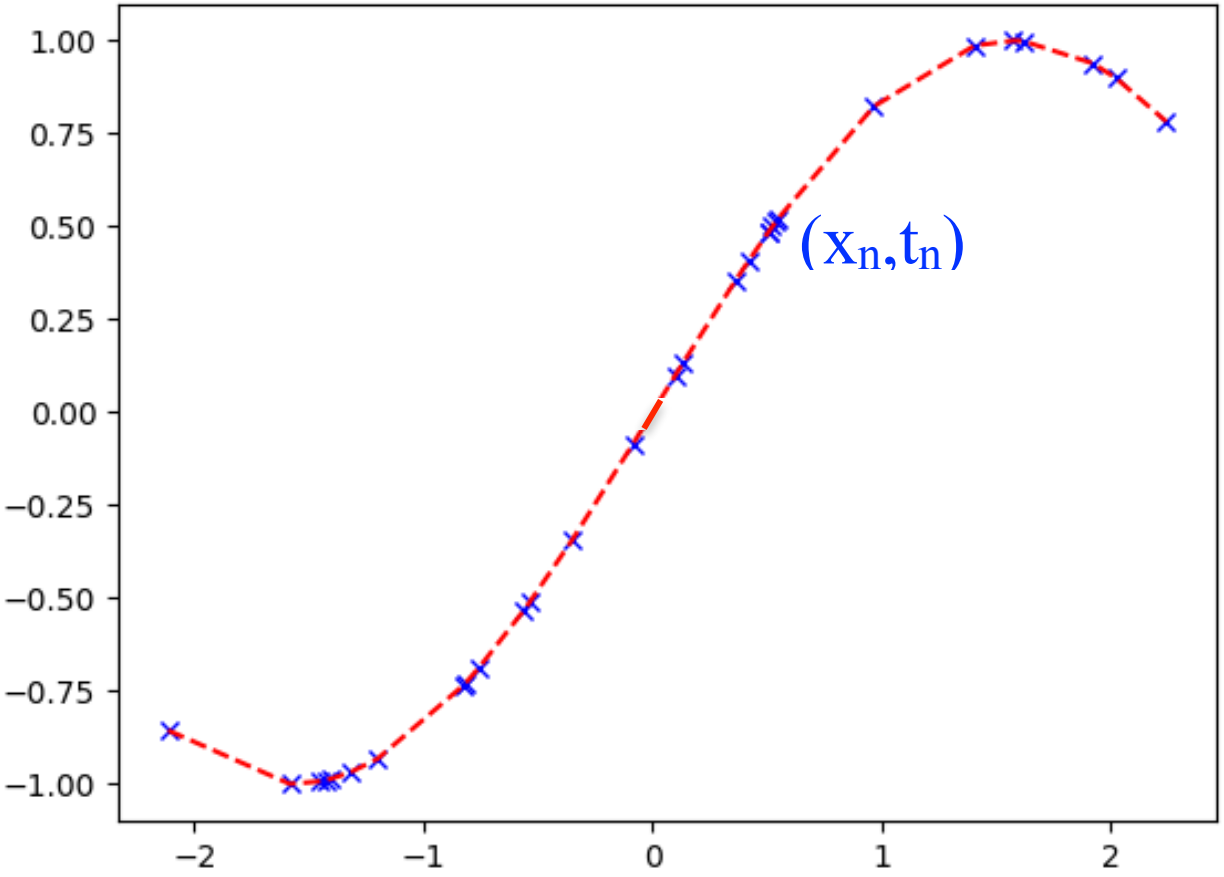


—> We can now use a linear classifier.

Lifting from 2D to 3D



Polynomial Approximation



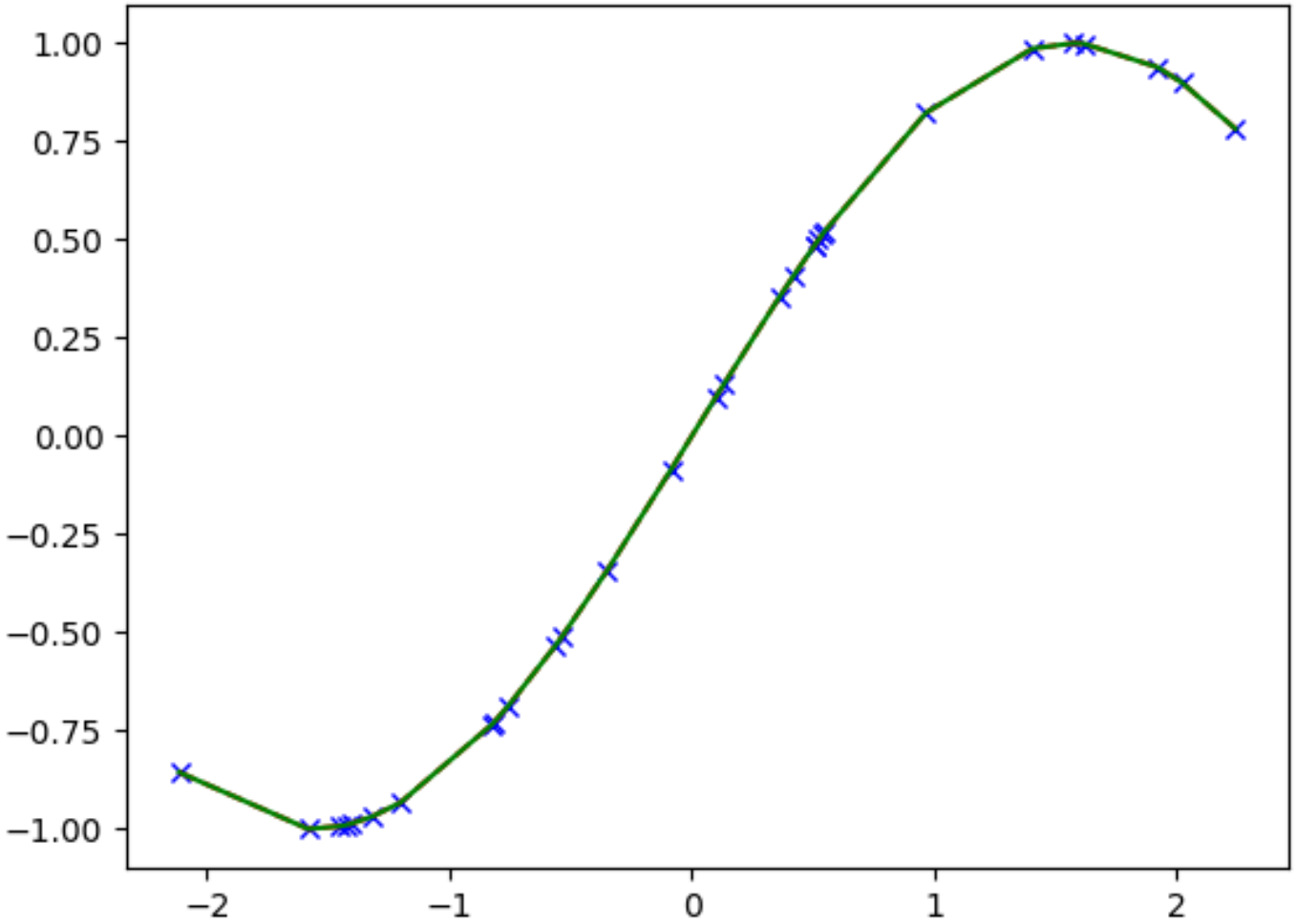
For $1 \leq n \leq N$:

$$t_n = f(x_n) + \varepsilon$$

- The (x_i,t_i) are given.
- f is unknown.

- Find $\mathbf{w} = [w_0, w_1, \ldots, w_M]$ such that: $\forall x, f(x) \approx \sum_{i=0}^{M} w_i x^i$
- Least squares solution: $\mathbf{w}^* = \text{argmin}_{\mathbf{w}} \sum_n (t_n - \sum_{i=0}^{M} w_i x_n^i)^2$
- For M=1, reduces to linear regression.

Polynomial Approximation



M=0 horizontal line

M=1 linear function

M=2

M=3

M=4

M=6

M=10

For a given M, we plot in green:

$$f_M(x) = \sum_{i=0}^{M} w_i^* x^i$$

Polynomial Feature Expansion

$$x \rightarrow \phi(x) = \begin{bmatrix} 1 \\ x \\ x^2 \\ \vdots \\ x^M \end{bmatrix}$$

The polynomial can be rewritten as:

$$\sum_{i=0}^{M} w_i x^i = \mathbf{w} \cdot \phi(x) = \mathbf{w}^T \phi(x) \text{ with } \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_M \end{bmatrix}$$

The least squares solution becomes:

$$\mathbf{w}^* = \text{argmin}_{\mathbf{w}} \sum_n (t_n - \mathbf{w}^T \phi(x_n))^2$$

Least-Squares Formulation

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \sum_{n=1}^{N} \left(t_n - \mathbf{w}^T \phi(\mathbf{x}_n)\right)^2$$
$$= \arg\min_{\mathbf{w}} \|\Phi\mathbf{w} - \mathbf{t}\|^2$$

with

$$\Phi = \begin{bmatrix} \phi(\mathbf{x}_1)^T \\ \phi(\mathbf{x}_2)^T \\ \vdots \\ \phi(\mathbf{x}_N)^T \end{bmatrix} = \begin{bmatrix} 1 & x_1 & x_1^2 & \dots & x_1^M \\ 1 & x_2 & x_2^2 & \dots & x_2^M \\ \dots & \dots & \dots & \dots & \dots \\ 1 & x_N & x_N^2 & \dots & x_N^M \end{bmatrix}, \quad \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ \dots \\ w_M \end{bmatrix}, \quad \text{and } \mathbf{t} = \begin{bmatrix} t_0 \\ t_1 \\ t_2 \\ \dots \\ t_N \end{bmatrix}.$$

Intuitively: $\Rightarrow \underset{N \times \tilde{M}}{\Phi} \underset{\tilde{M} \times 1}{\mathbf{w}^*} \approx \underset{N \times 1}{\mathbf{t}}$

Formally: $\Rightarrow \underset{\tilde{M} \times \tilde{M}}{(\Phi^T \Phi)} \underset{\tilde{M} \times 1}{\mathbf{w}^*} = \underset{\tilde{M} \times 1}{\Phi^T \mathbf{t}}$

Optional: Proof Sketch

We want to minimize:

$$R = \frac{1}{2}\|\Phi\mathbf{w} - \mathbf{t}\|^2$$
$$= \frac{1}{2}(\Phi\mathbf{w} - \mathbf{t})^T(\Phi\mathbf{w} - \mathbf{t})$$

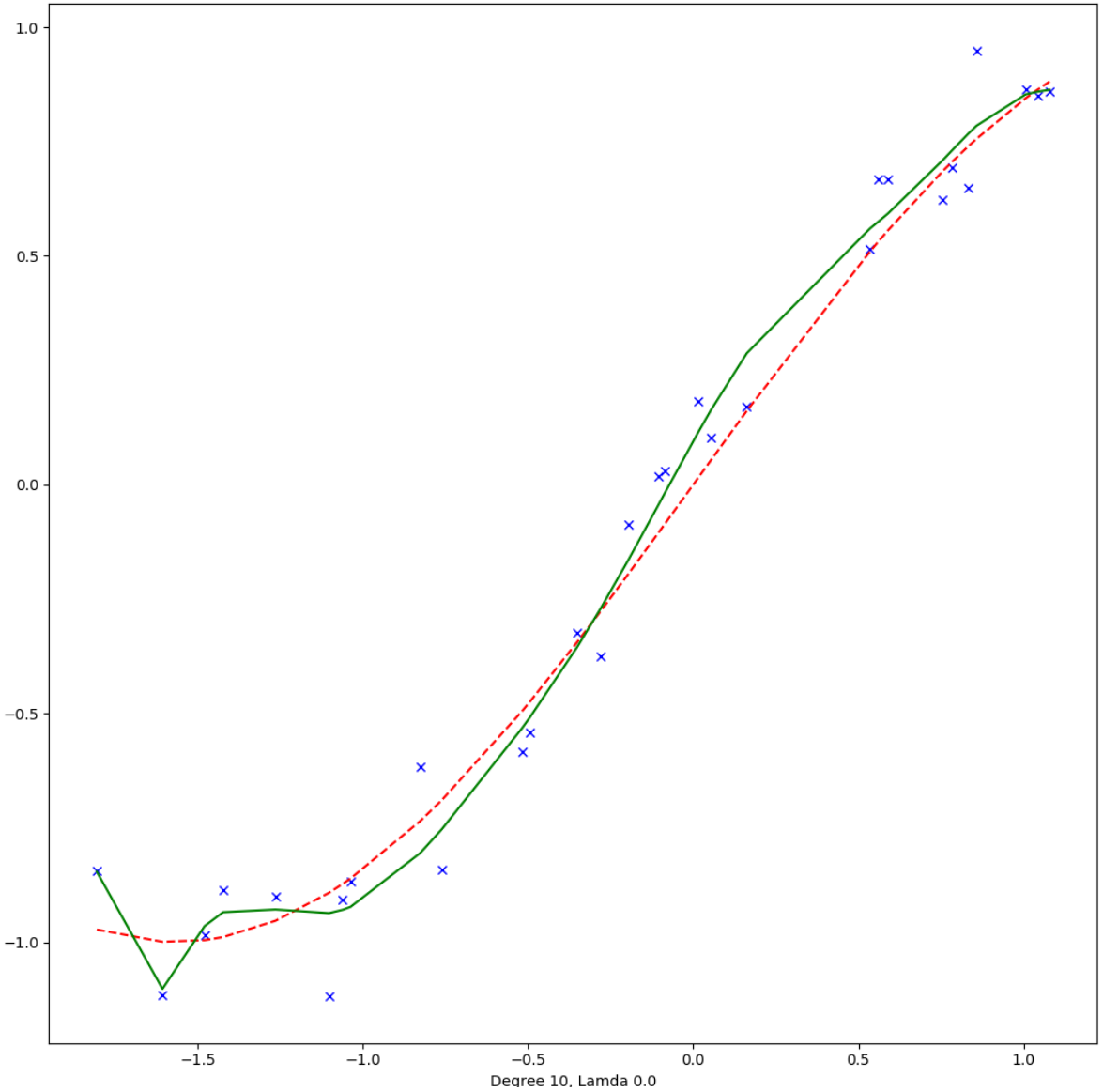
The gradient or R w.r.t $\mathbf{w}$ is:

$$\nabla R = \Phi^T(\Phi\mathbf{w} - \mathbf{t})$$

At the minimum:

$$0 = \nabla R = \Phi^T(\Phi\mathbf{w} - \mathbf{t})$$
$$\Rightarrow \Phi^T\Phi\mathbf{w} = \Phi^T\mathbf{t}$$

Adding Noise



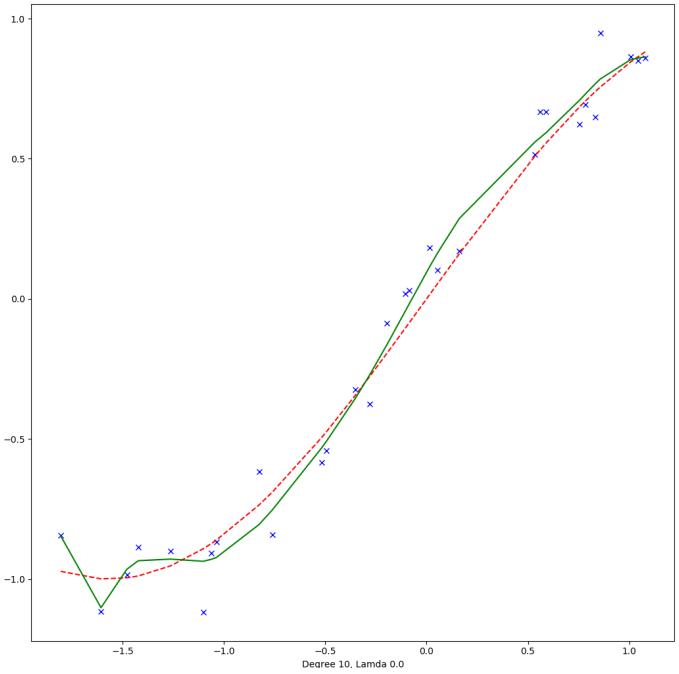
Regularization

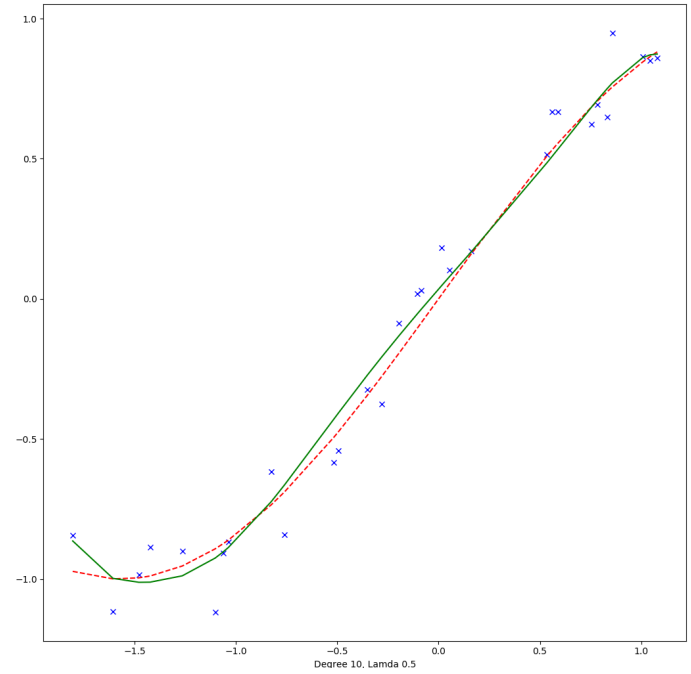
$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \|\Phi\mathbf{w} - \mathbf{t}\|^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

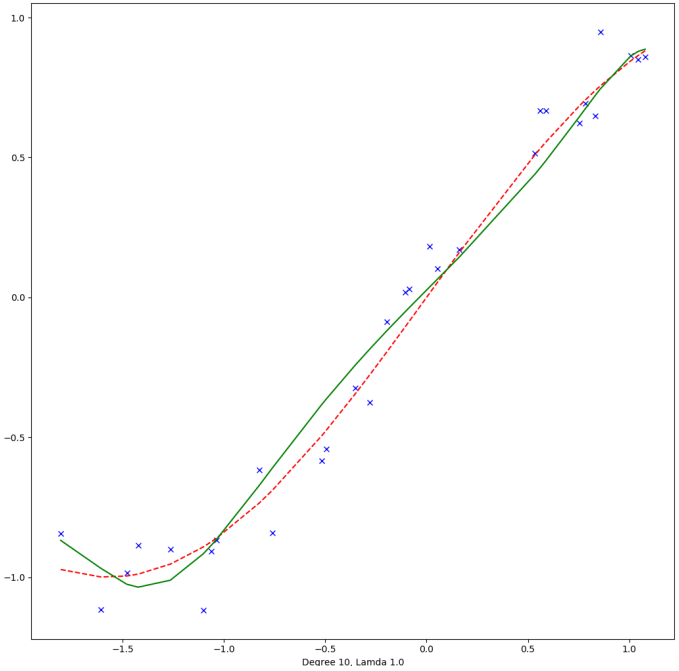
$$\Rightarrow \text{ Solve: } (\Phi^T\Phi + \lambda\mathbf{I})\mathbf{w} = \Phi^T\mathbf{t}$$

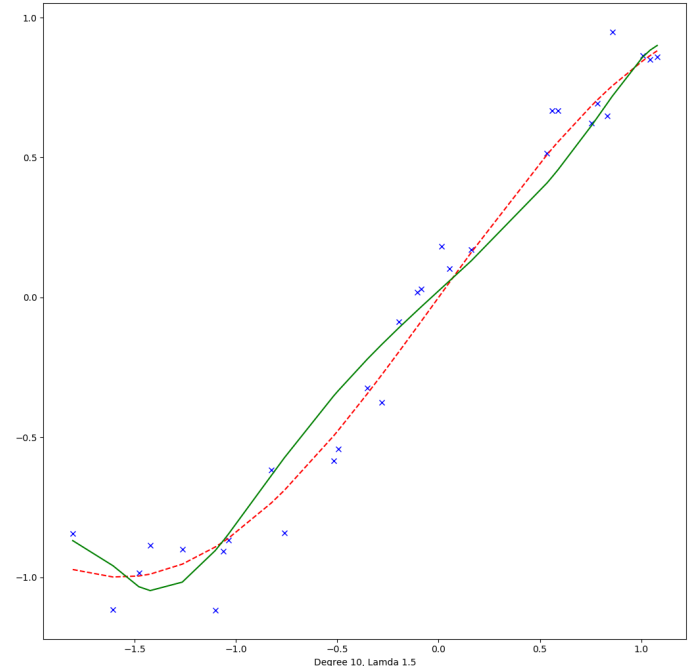
- This is known as weight decay because in iterative algorithms it encourages the weight values to decay to zero, unless supported by the data.
- It discourages large weights and therefore quick variations.

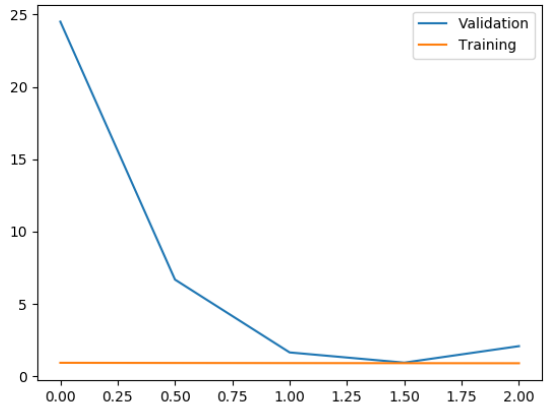
Without and with Regularization





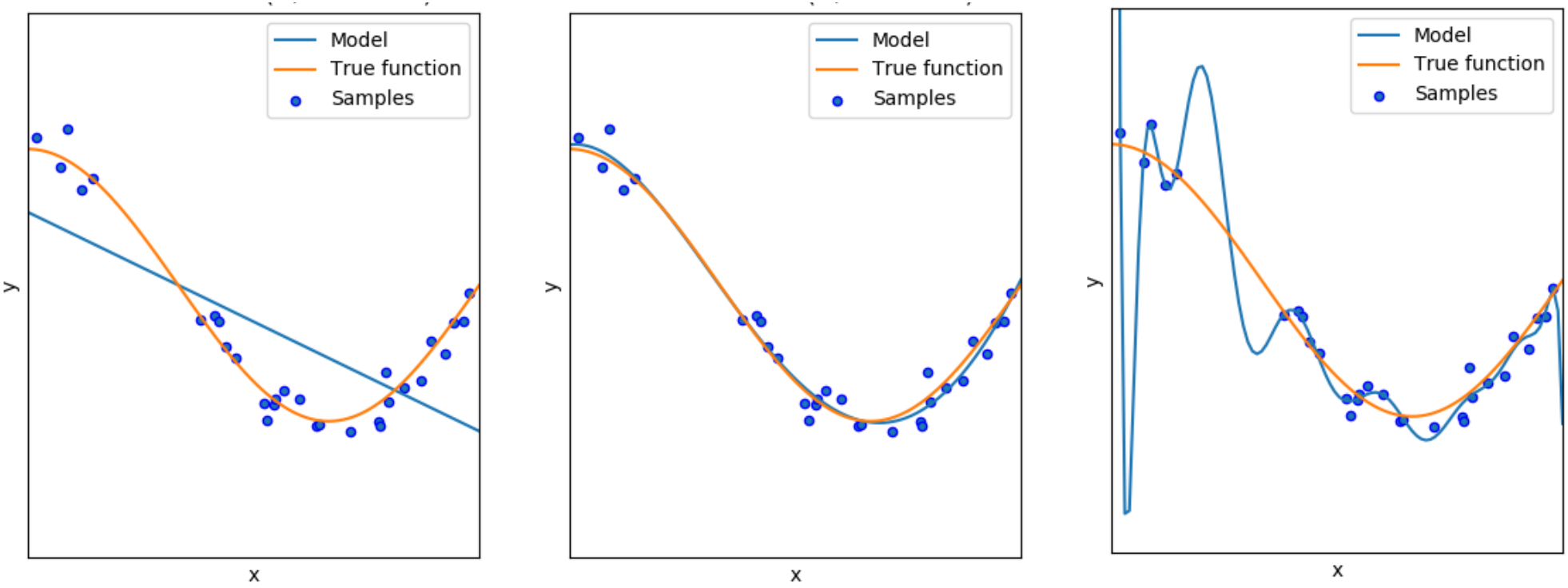






Use cross-validation data to select the value of λ.

Linear and Non-Linear Regression

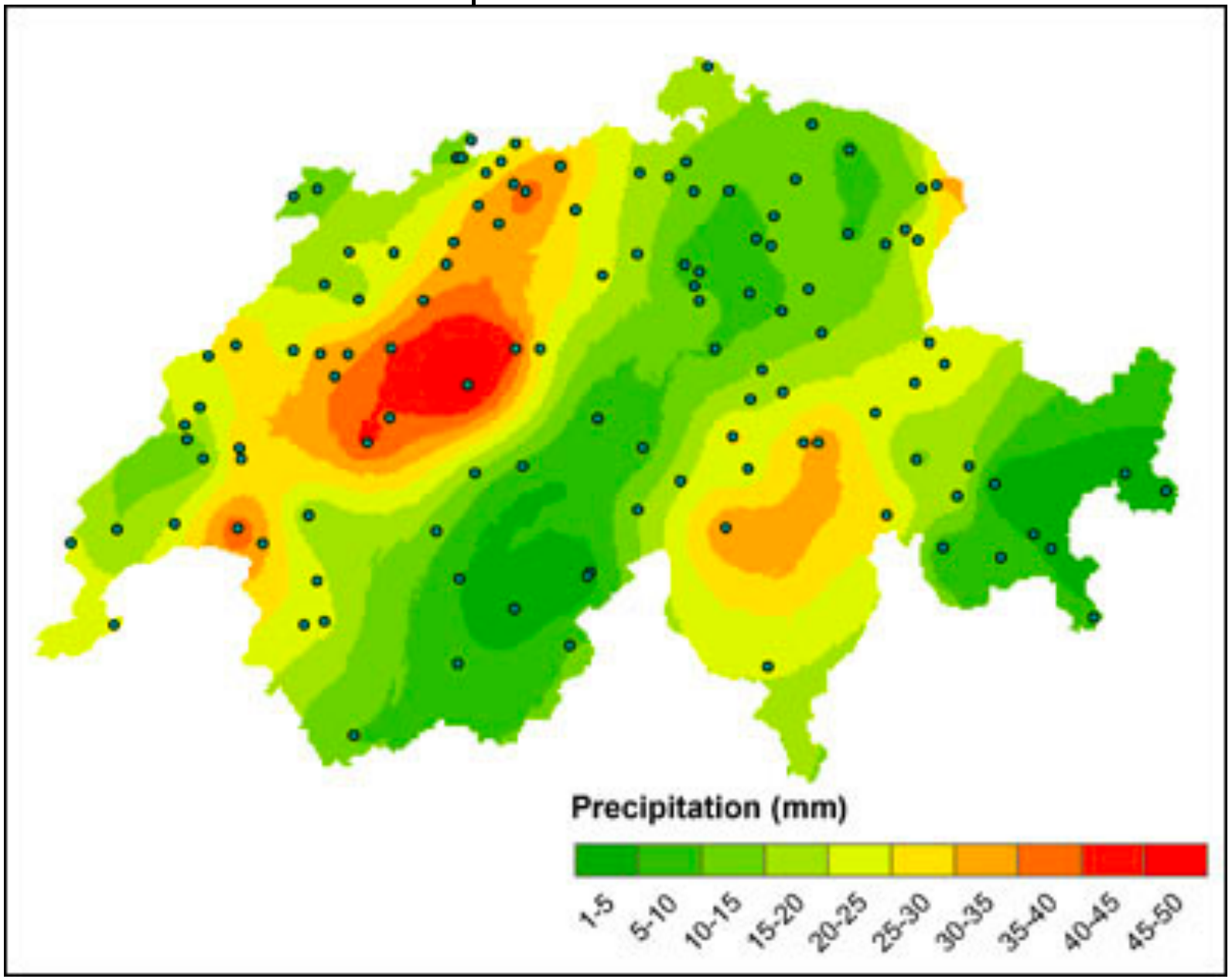


Order 1 Order 4 Order 15

For both kind of regressions, the trick is to find the best compromise between simplicity and goodness of fit.

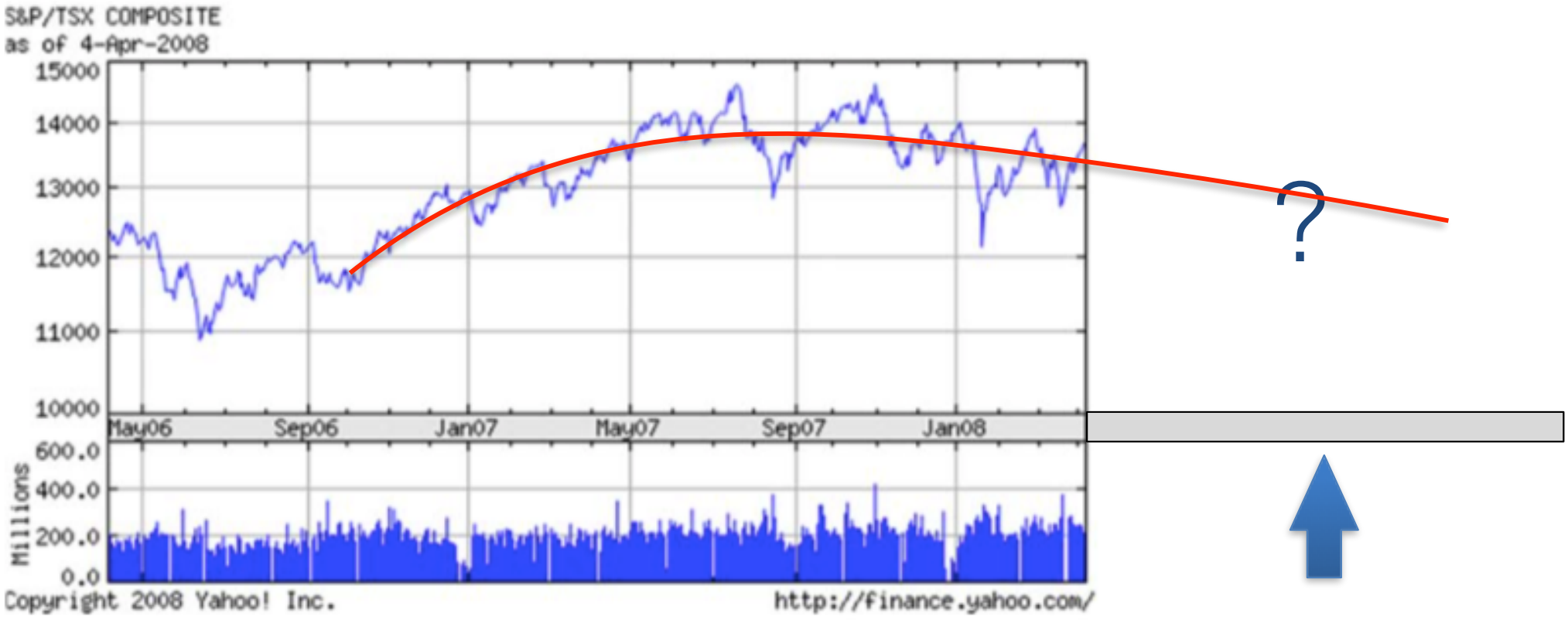
Application: Rainfall in Switzerland

The circles represent actual measurements



—> Extends to Higher Dimensions.

Application: Stock Price Prediction



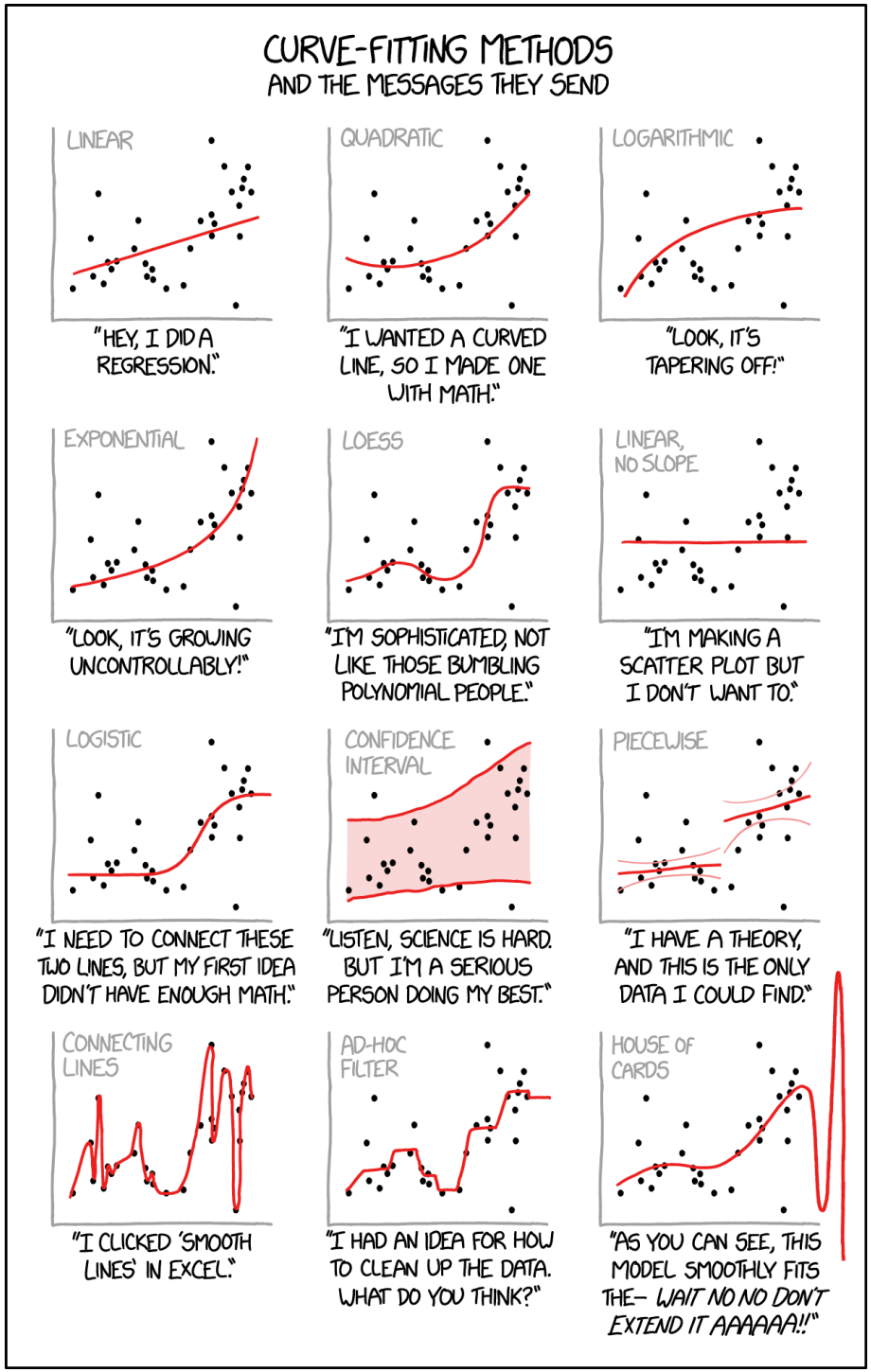
$\mathbf{x}_t$ $x_{t+\Delta t}$

$$\mathbf{x}_t = [x_{t-T+1}, \ldots, x_{t-1}, x_t]$$

$$y(\mathbf{x}_t; \mathbf{w}) = x_{t+\Delta t}$$

—> Regression problem

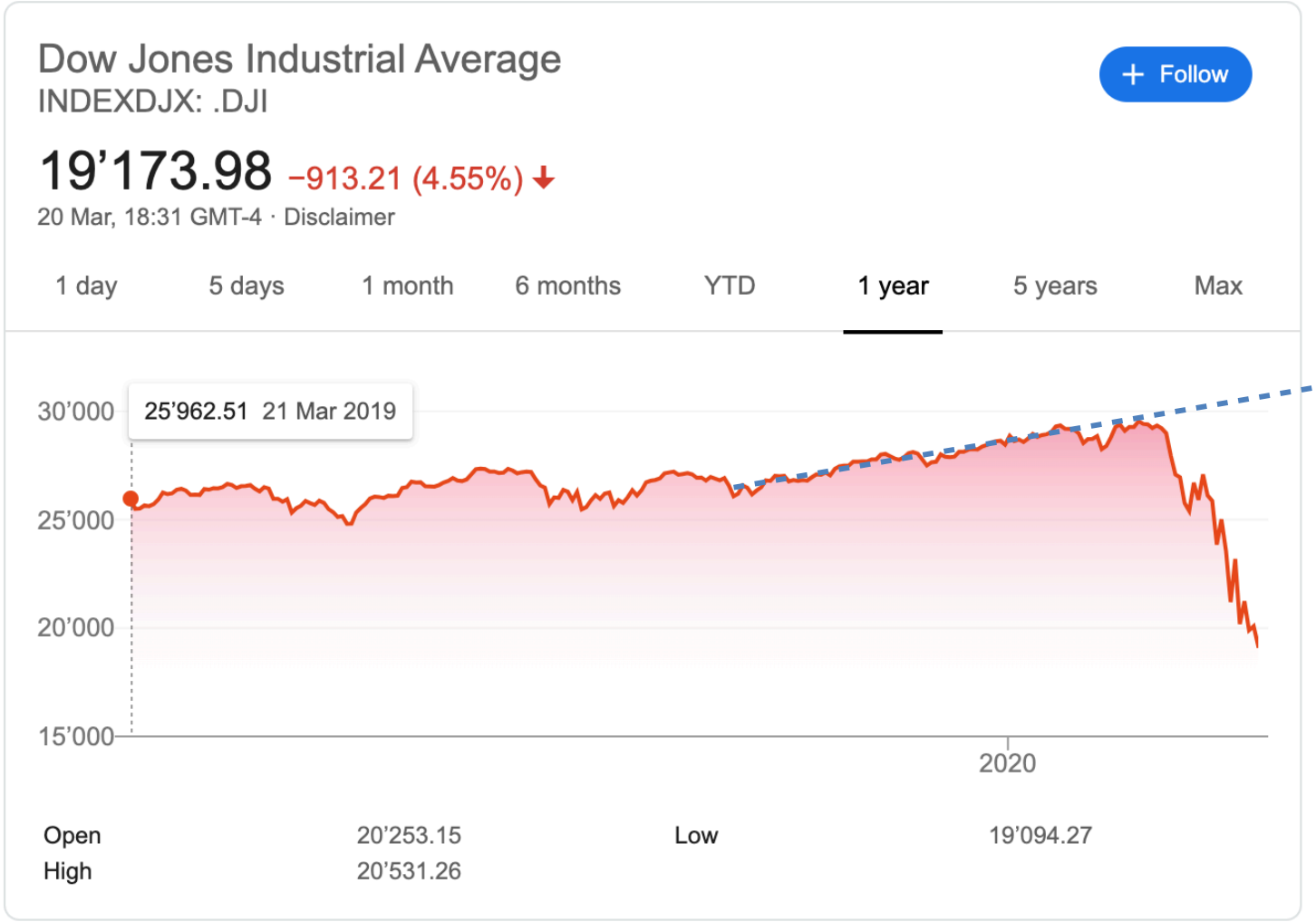
But Be Careful!



Never trust a statistic you have not faked yourself!

https://xkcd.com/2048/

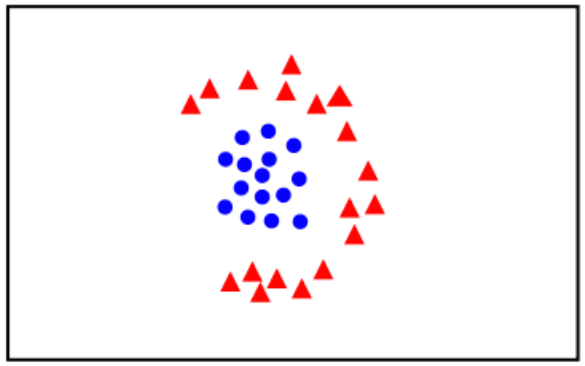
But Be VERY Careful!



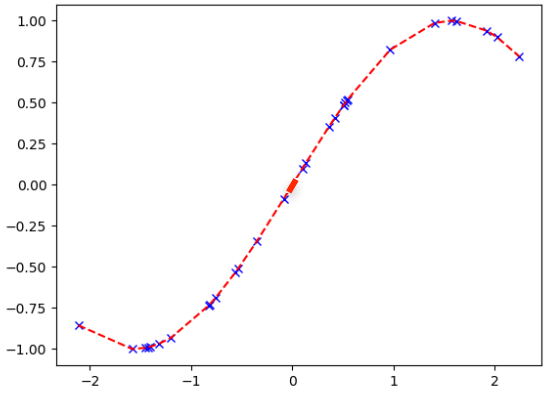
March 2019 to March 2020

Recap: Mapping to a Higher Dimension

1D classification.



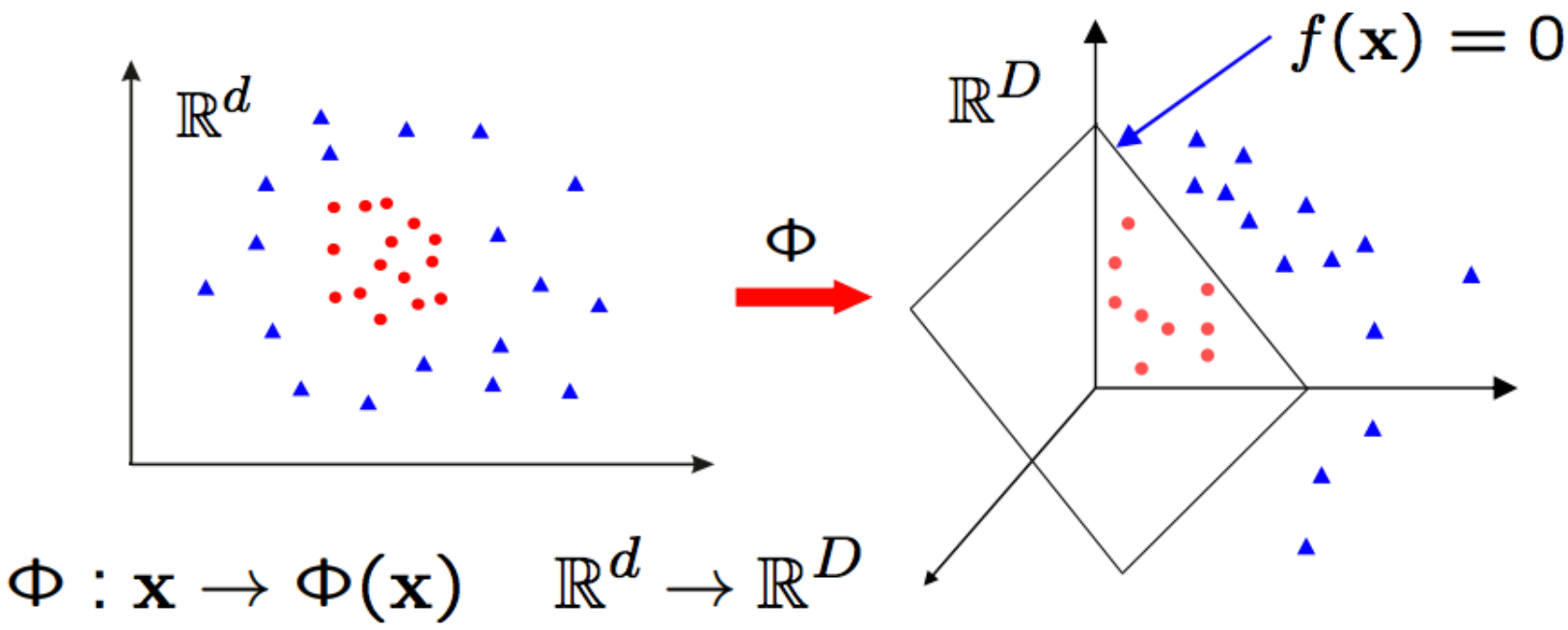
2D classification.



Polynomial approximation.

- We have seen three examples in which mapping to a higher dimension makes the problem linear.
- This idea can be generalized.

Classification in Feature Space



- Map from R^d to R^D
- Learn a linear classifier in R^D

R(D) -> feature space

$$y(\mathbf{x}) = \sigma(\mathbf{w}^T \phi(\mathbf{x}) + w_0)$$

$$\phi : \mathbb{R}^d \rightarrow \mathbb{R}^D$$

Polynomial Feature Expansion

1-Dimensional Input

$$x \rightarrow \phi(x) = \begin{bmatrix} 1 \\ x \\ x^2 \\ \vdots \\ x^M \end{bmatrix}$$

d-Dimensional Input

$$\phi(\mathbf{x}) = \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_d \\ x_1^2 \\ \vdots \\ x_d^2 \\ \vdots \\ x_1^M \\ \vdots \\ x_d^M \\ x_1 x_2 \\ \vdots \\ x_1 x_d \\ \vdots \\ x_{d-1} x_d \\ x_1^2 x_2 \\ \vdots \end{bmatrix}$$

constant

linear

quadratic

M^{th} power

Products of 2 variables

All other possible monomials

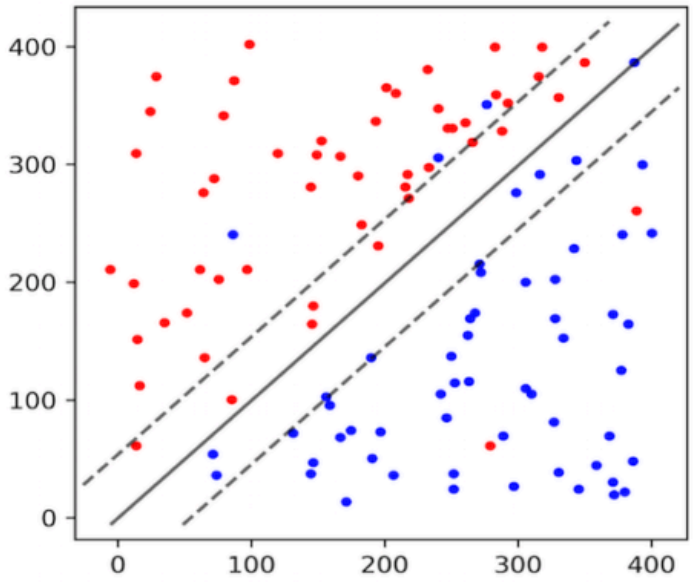
- The dimension of $\phi(\mathbf{x})$ grows quickly with the degree M of the polynomial.
- $\phi(\mathbf{x})$ can be used in any algorithm that we have seen so far.

Reminder: Linear SVM

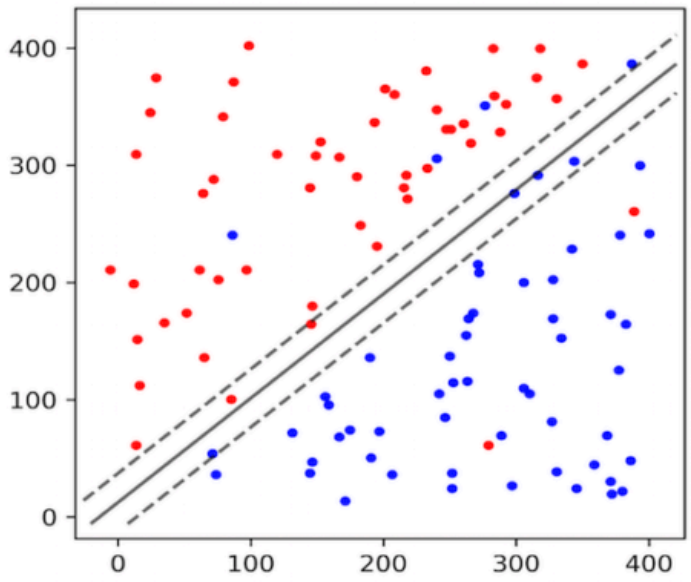
$$\mathbf{w}^* = min_{(\mathbf{w},\{\xi_\mathbf{n}\})} \frac{1}{2} ||\mathbf{w}^2|| + C \sum_{n=1}^{N} \xi_n,$$

$$\text{subject to } \forall n, \quad t_n \cdot (\tilde{\mathbf{w}} \cdot \mathbf{x}_n) \geq 1 - \xi_n \text{ and } \xi_n \geq 0.$$

- C is constant that controls how costly constraint violations are.
- The problem is still convex.



C=1



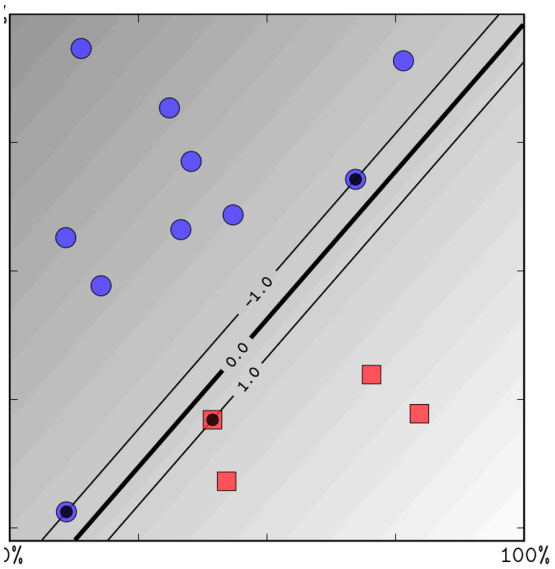
C=100

Polynomial SVM

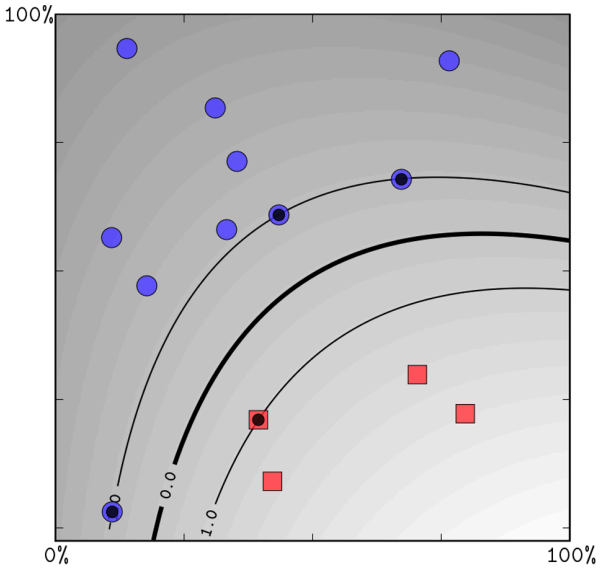
$$\mathbf{w}^* = min_{(\mathbf{w},\{\xi_\mathbf{n}\})} \frac{1}{2} ||\mathbf{w}||^2 + C \sum_{n=1}^{N} \xi_n,$$

$$\text{subject to } \forall n, \quad t_n \cdot (\tilde{\mathbf{w}} \cdot \phi(\mathbf{x}_n)) \geq 1 - \xi_n \text{ and } \xi_n \geq 0.$$

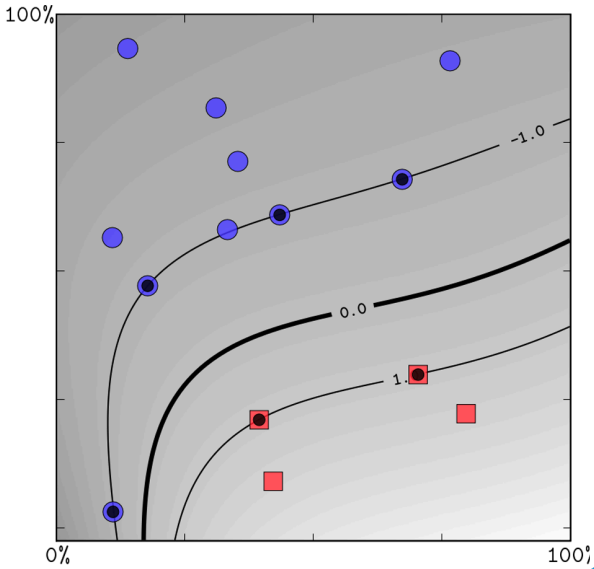
- C is constant that controls how costly constraint violations are.
- The problem is still convex.



M =1

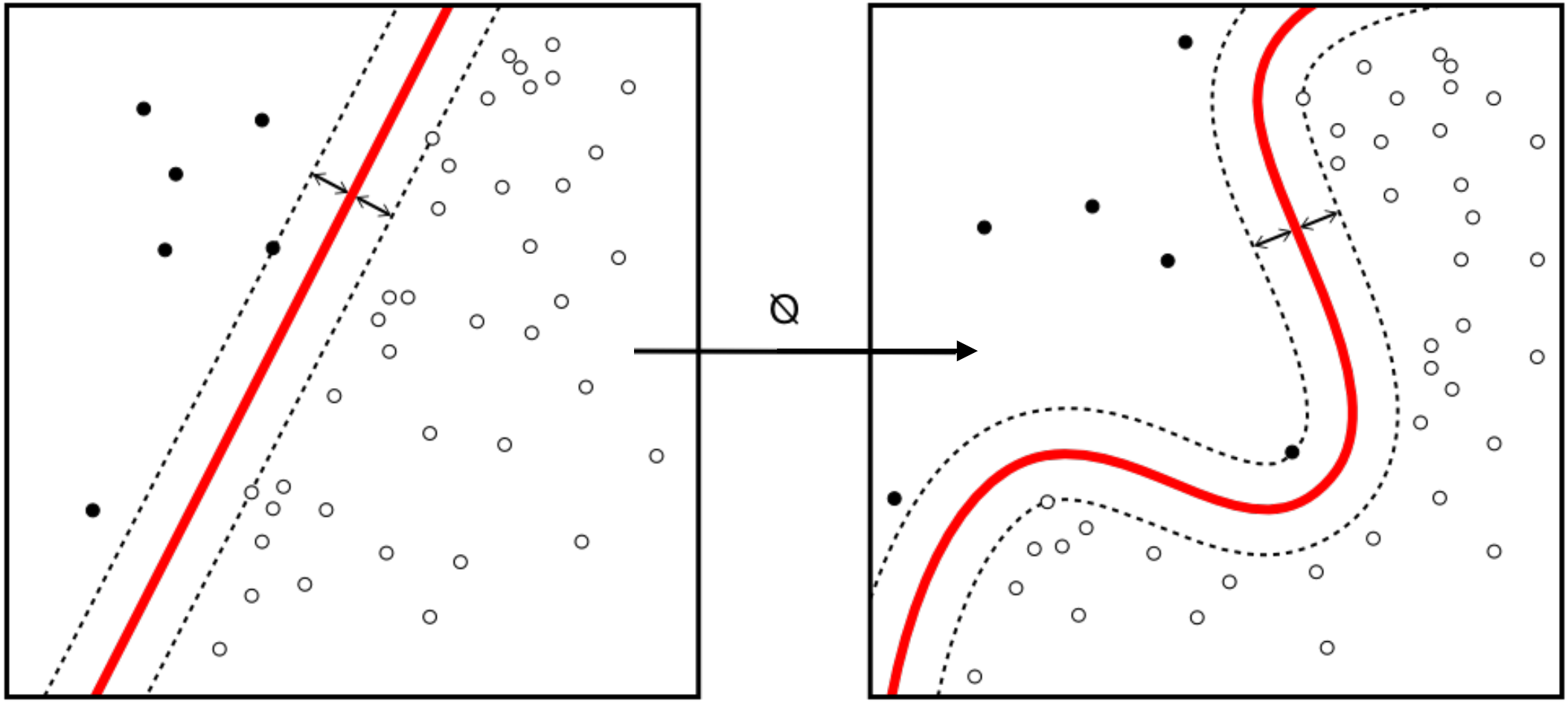


M = 2

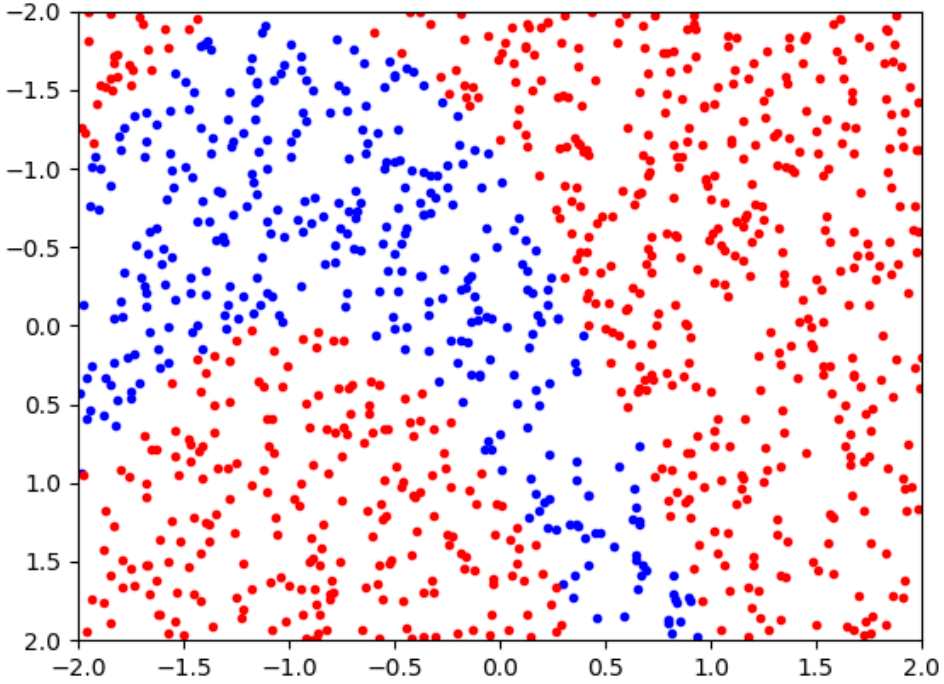


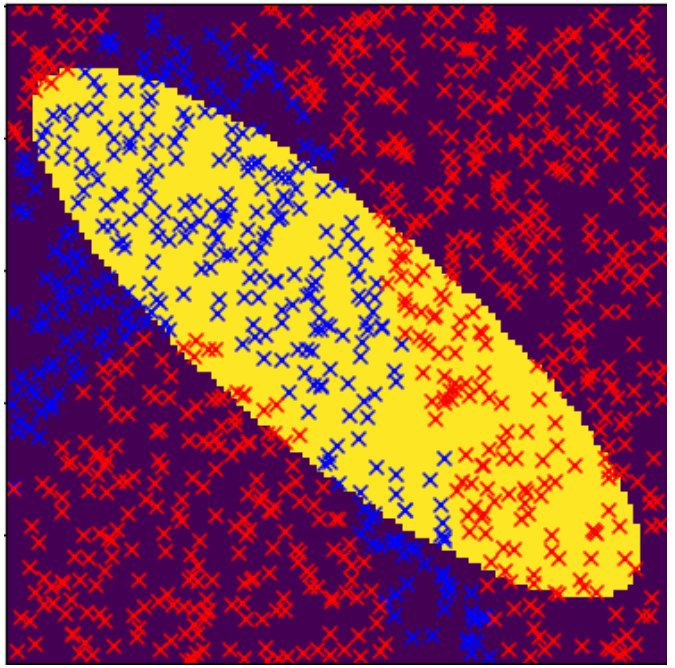
M = 5

Interpretation



The linear decision boundary in a high dimensional space becomes a curvy one in the original low dimensional space.



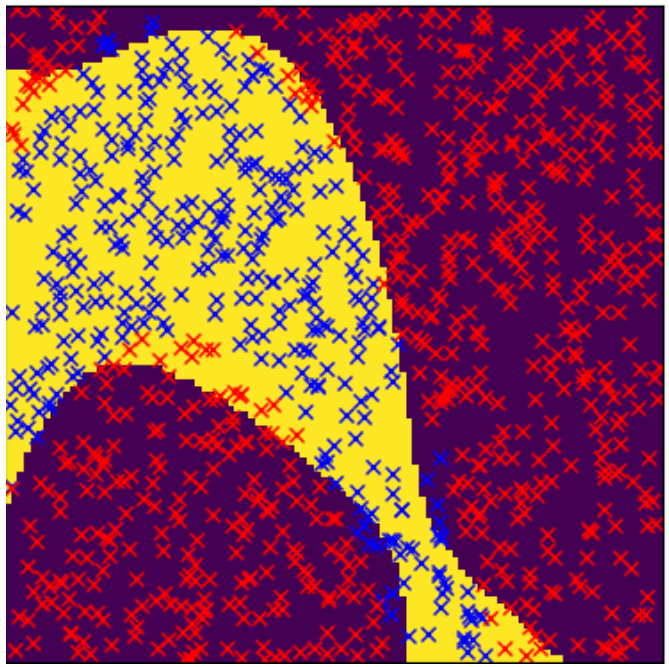


Rosenbrock:

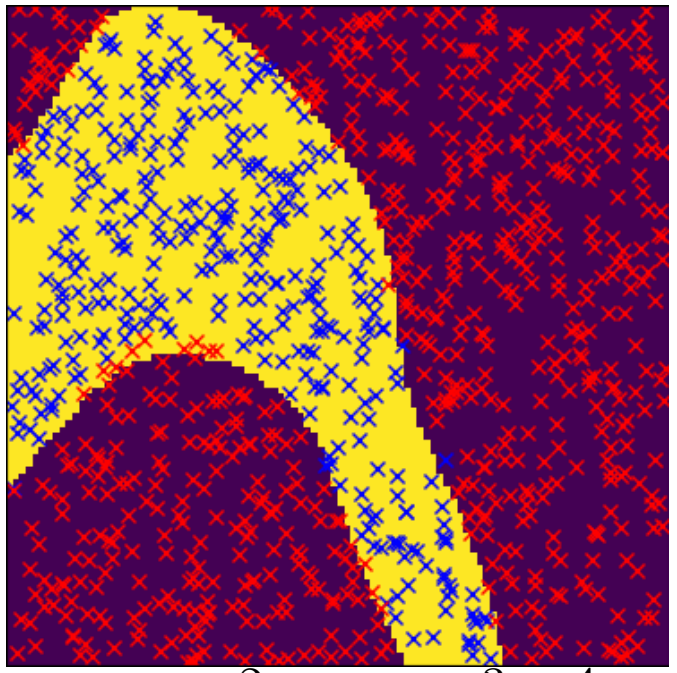
$$r(x,y) = 100 * (y - x^2)^2 + (1 - x)^2$$

$$f(x,y) = \begin{cases} -1 & \text{if } r(x,y) < \mathrm{T} \\ 1 & \text{otherwise} \end{cases}$$

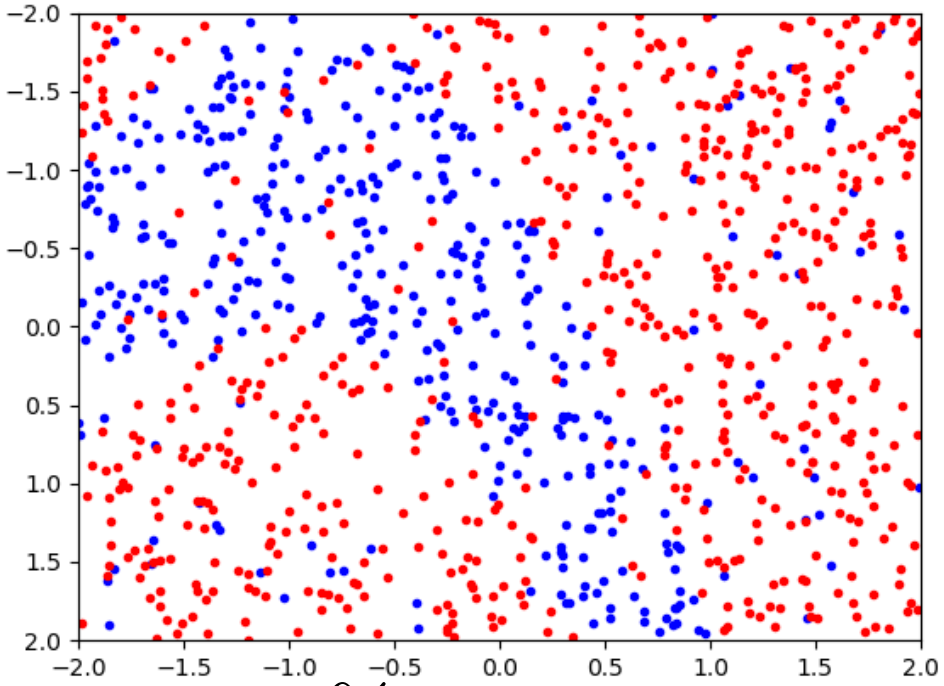
$[x, y, xy]$



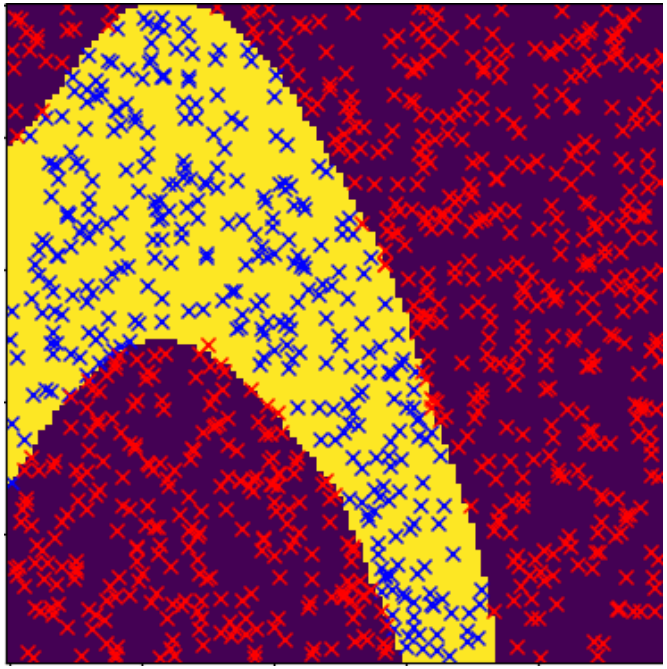
$[x, y, x^2, \ldots, xy^2, y^3]$



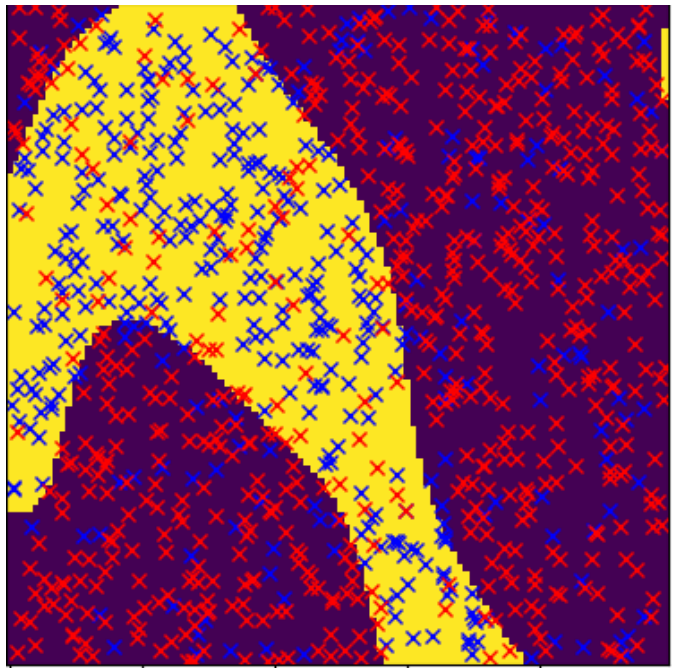
$[x, y, x^2, \ldots, xy^3, y^4]$



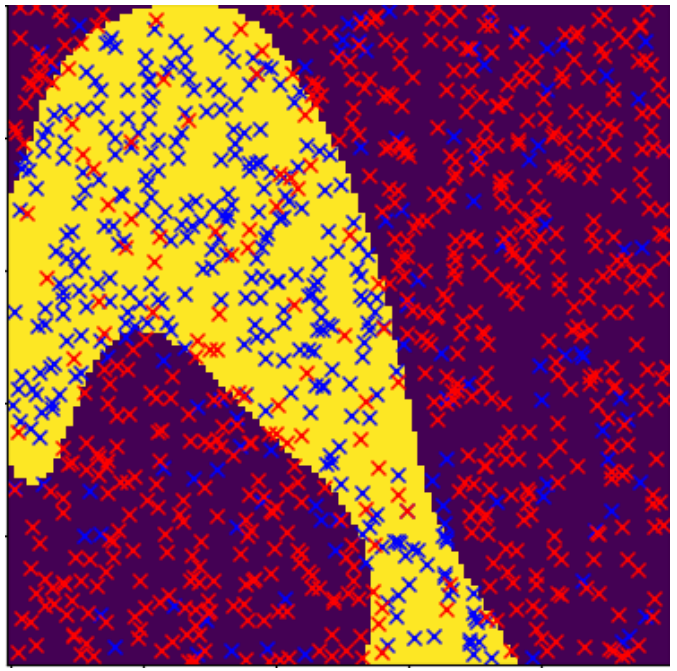
$10\%noise$



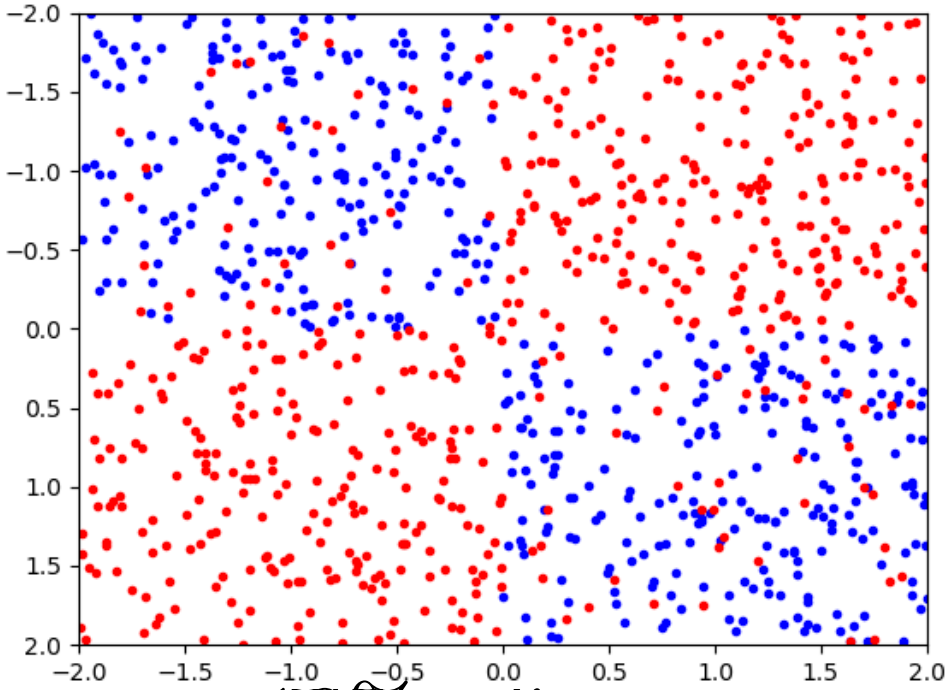
$[x, y, x^2, \ldots, xy^7, y^8]$



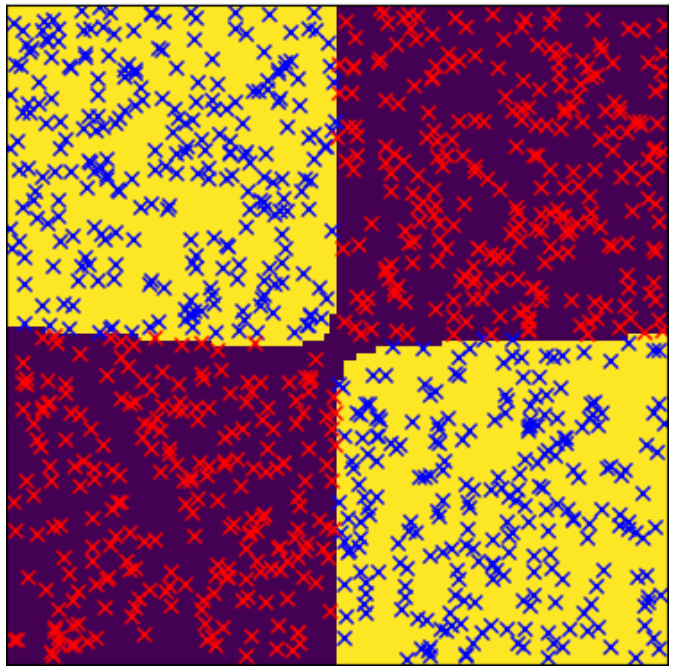
$5\%noise$



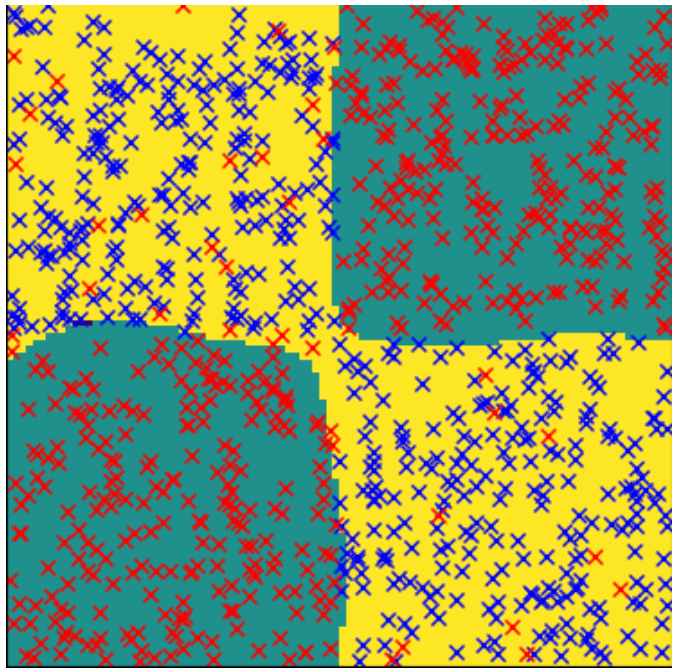
$10\%noise$



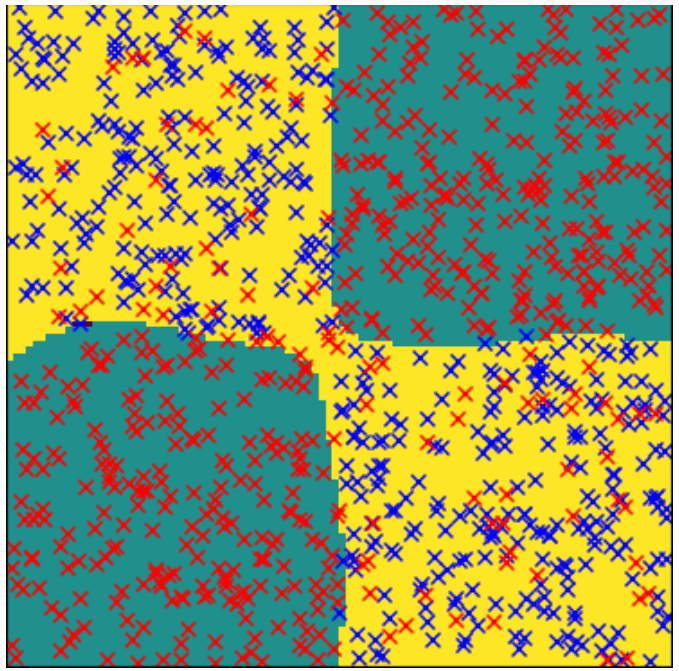
15%noise



$[x, y, x^2, \ldots, xy^7, y^8]$



5%noise



10%noise

Polynomial SVM

- A higher-degree polynomial expansion yields a more flexible boundary.
- It also increases the dimensionality of the problem.
- The computational complexity of training SVMs grows like the cube of the dimension.

—> Inherent limitation of polynomial SVMs.

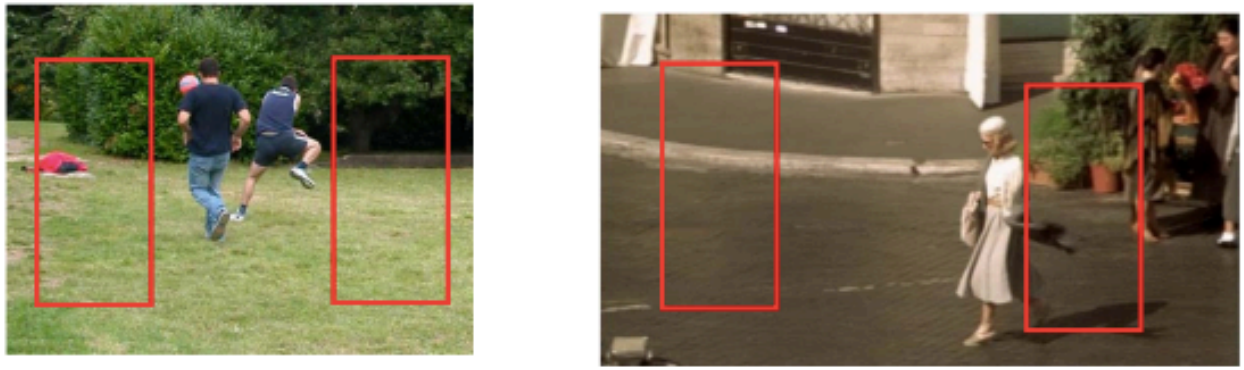
Another Way to Map to a Higher Dimension

People Detection in Images

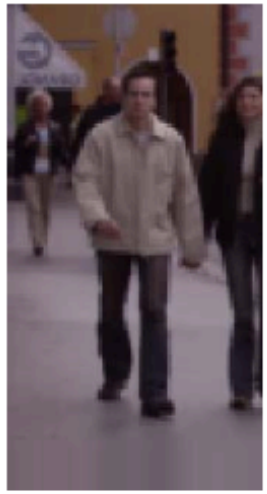
Training Data

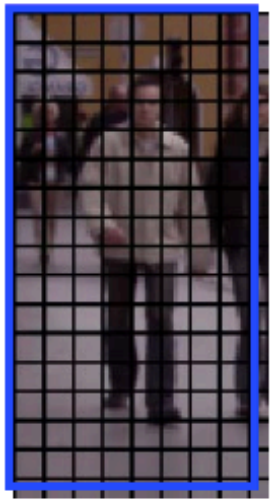
- Positive data – 1208 positive window examples

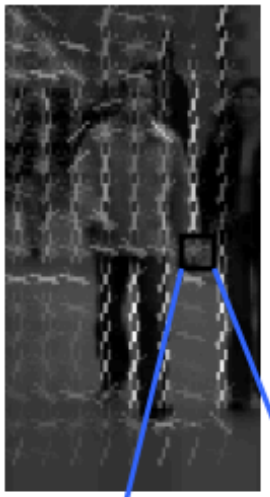
- Negative data – 1218 negative window examples (initially)



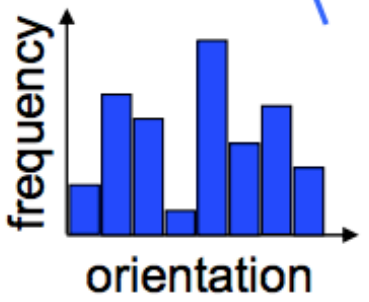
Histogram of Oriented Gradients







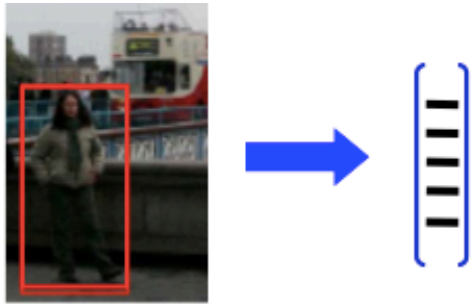
- tile window into 8 x 8 pixel cells
- each cell represented by HOG



Feature vector dimension = 16 x 8 (for tiling) x 8 (orientations) = 1024

Training:

- Represent each example window by a HOG classifier.



$$\mathbf{x}_i \in \mathbb{R}^d, \text{ with } d = 1024$$

- Train a linear classifier.

Testing:

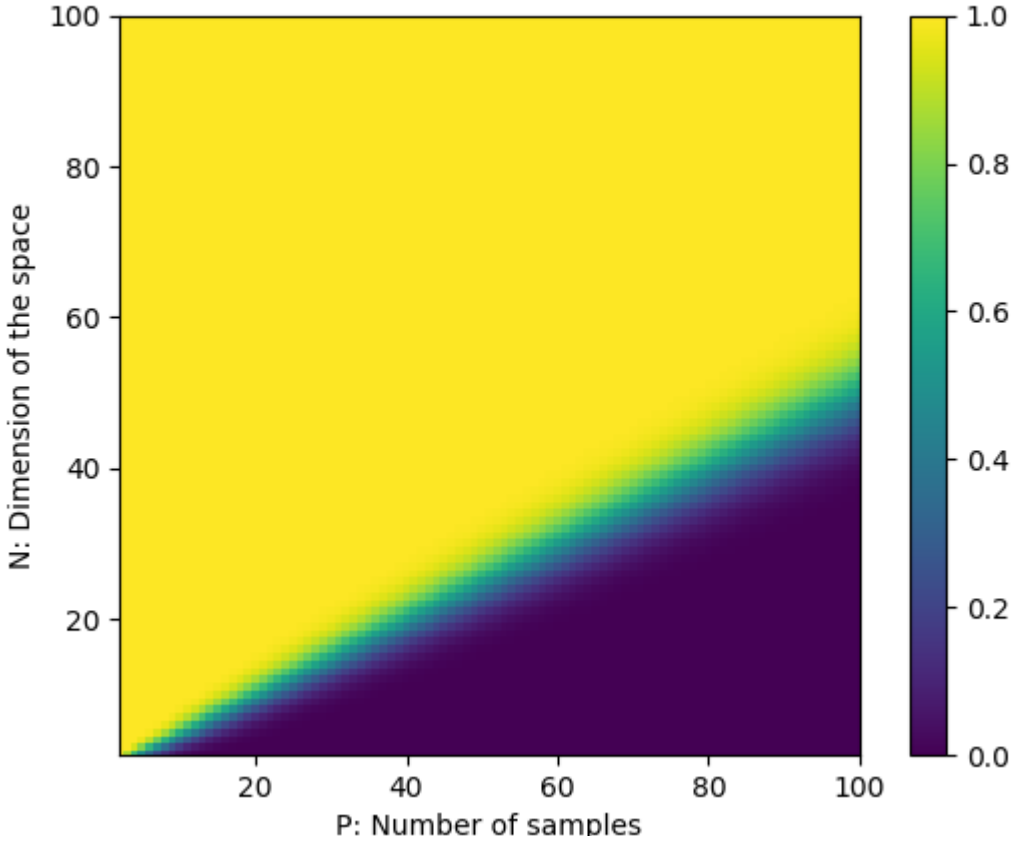
- Sliding window classifier.

$$y(\mathbf{x}; \mathbf{w}, w_0) = \sigma(\mathbf{w}^T \mathbf{x} + w_0)$$

Cover's Theorem

A complex pattern-classification problem, cast in a high-dimensional space nonlinearly, is more likely to be linearly separable than in a low-dimensional space, provided that the space is not densely populated.

Geometrical and Statistical properties of systems of linear inequalities with applications,1965



N : Dimension of space

p : Number of samples

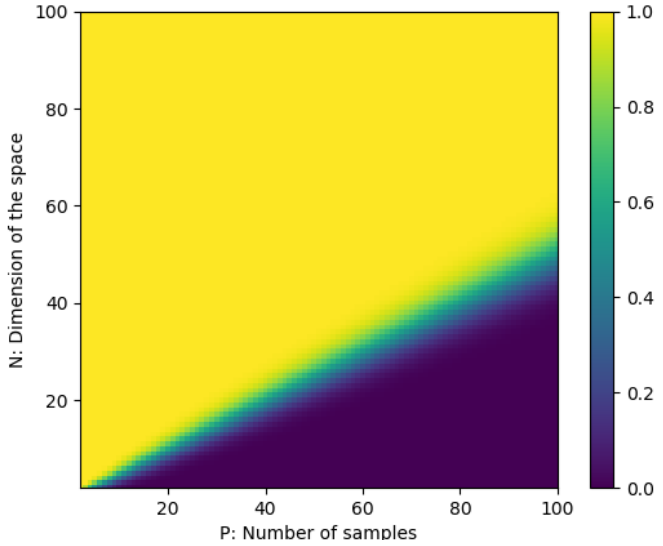
$\frac{C(p,N)}{2^p}$: Percentage of separable partitions

Optional: Recursive Computation

p\n	N=1	N=2	N=3
p=1	2	2	2
p=2	3	4	4
p=3	4	7	8
p=4	5	11	15

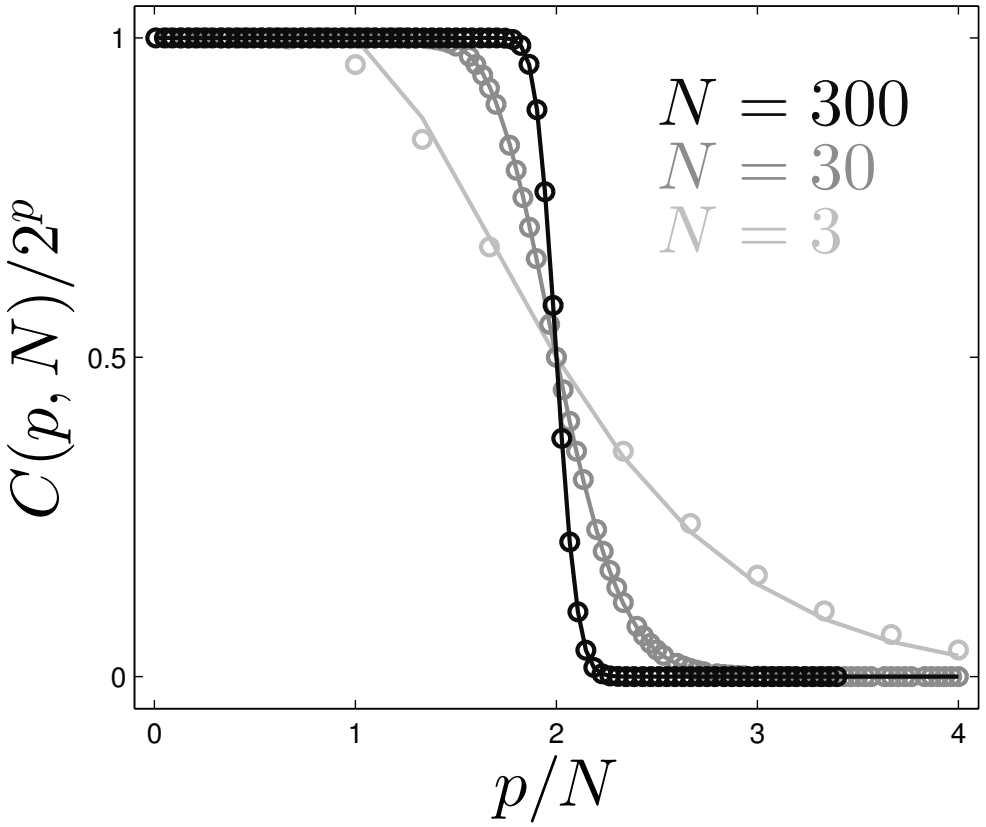
$$\forall n \ , \ C(1, n) = 2$$
$$\forall p \ , \ C(p, 1) = p + 1$$

$$C(p, N) = C(p - 1, N) + C(p - 1, N - 1)$$



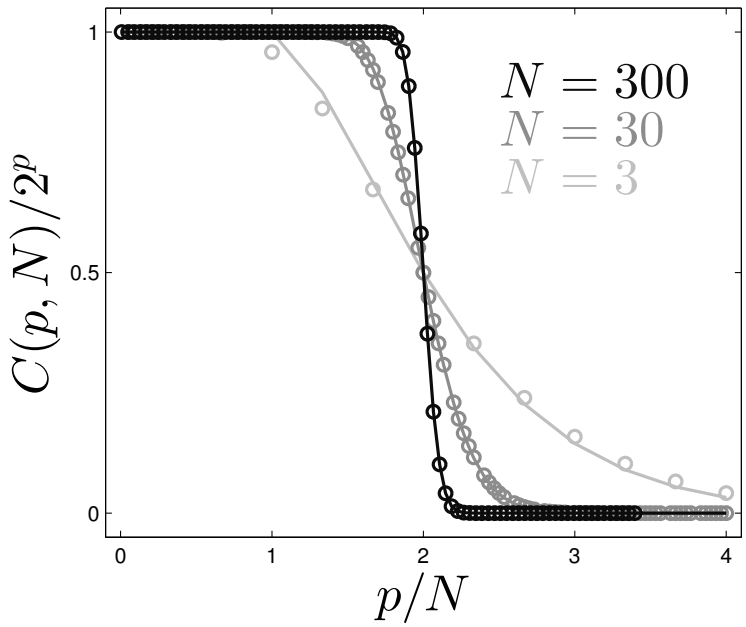
http://www.cns.nyu.edu/~eorhan/notes/covers-theorem.pdf

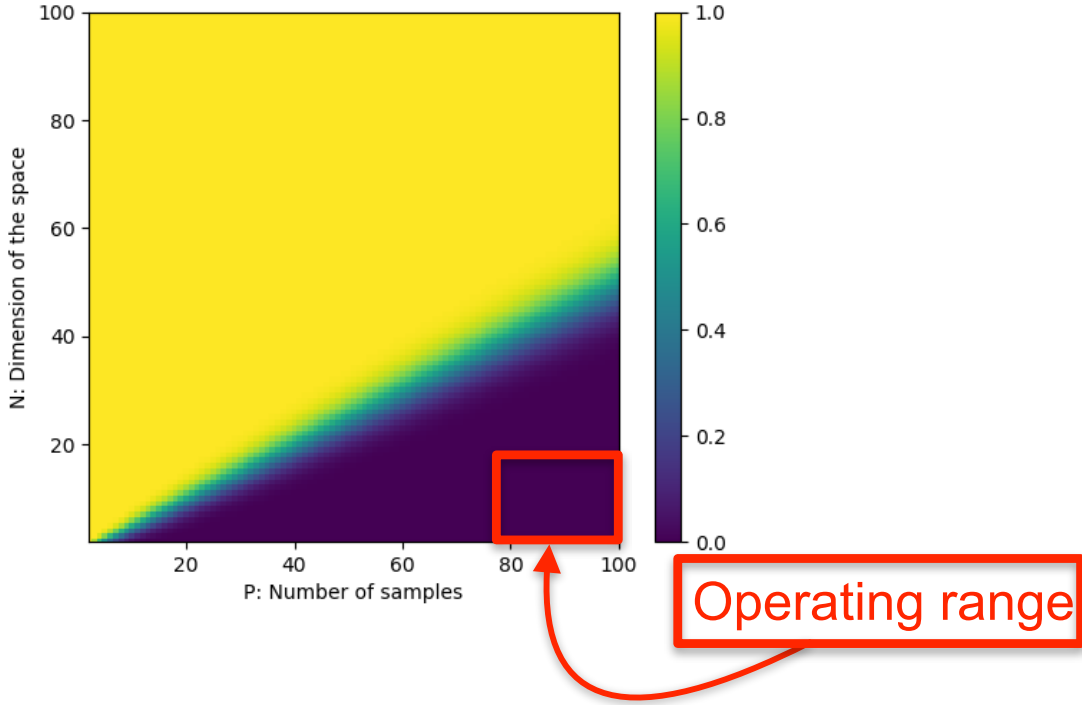
High Dimension is Good



When N is large, almost all partitions are separable if the number p of samples is less than 2N.

Problem Solved?





- Facebook or Google deal with BILLIONS of images.
- p and therefore N should be of that magnitude.
- Dealing with matrices of dimension NxN is impractical.

Neither Solved nor Hopeless

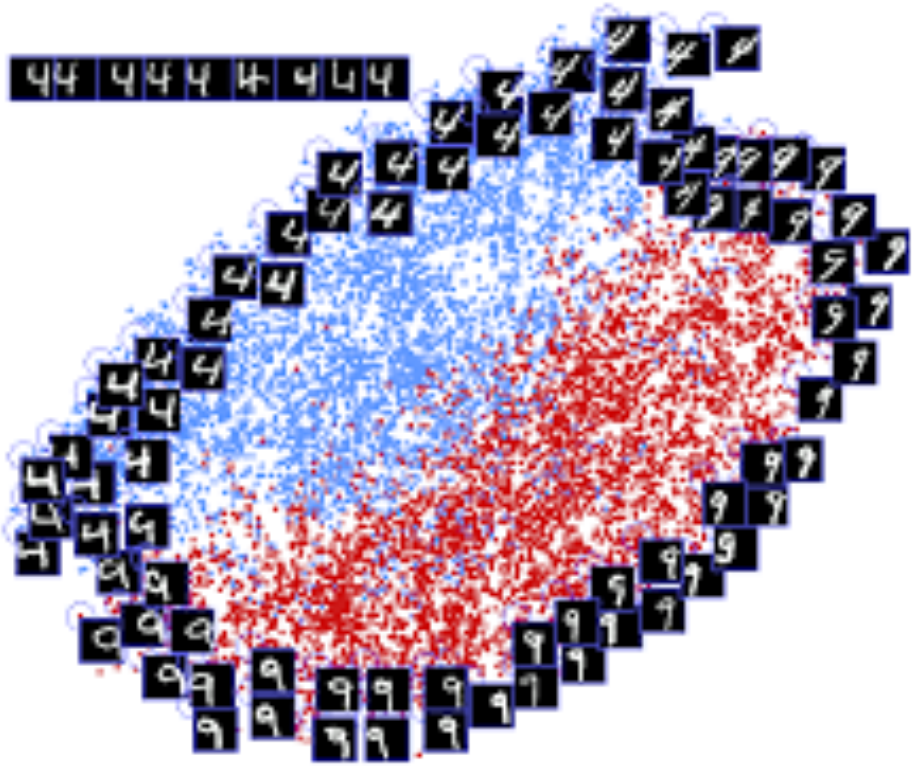
Bad news:

- The ratio of the number of points to the dimension must be less than 2.
- The dimension must be huge for large databases.
- As the dimension increases, the boundaries become increasingly irregular and sensitive to noise.

Good news:

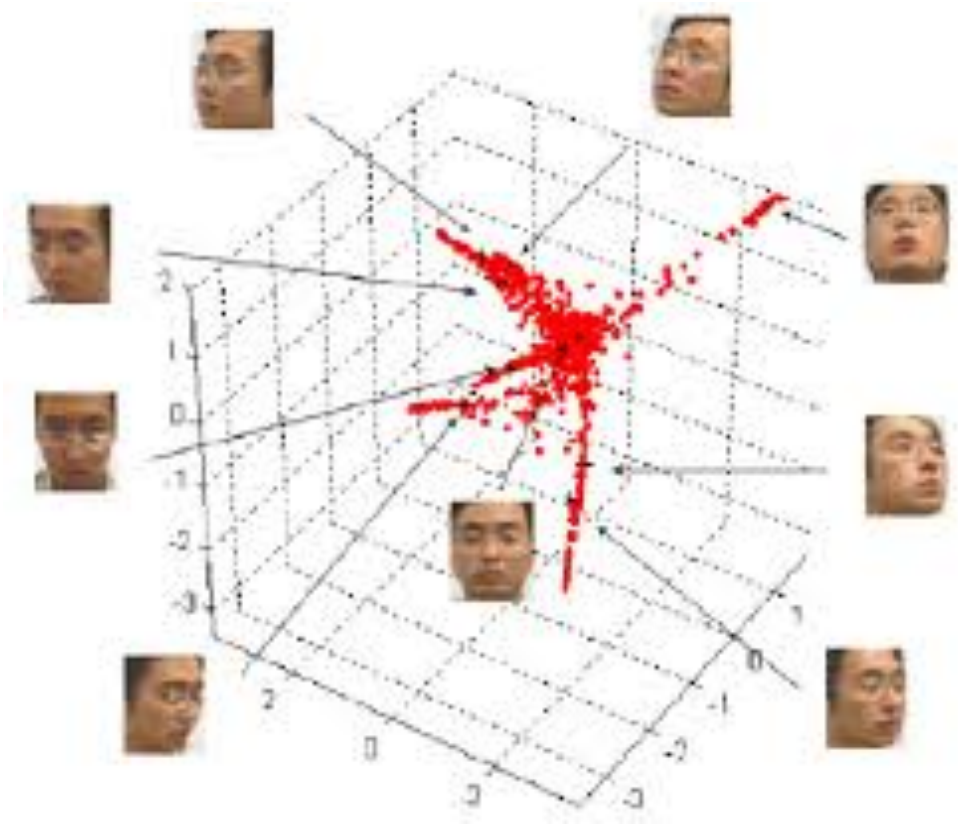
- The world is structured and the points we want to classify are NOT randomly distributed.
- We can compute feature vectors that are “close” for objects that belong to the same class.

Dimensionality Reduction



- The MNIST images are 28x28 arrays.
- They are **not** uniformly distributed in R^{784}.
- In fact they exist on a low dimensional manifold.

Face Images



- The same can be said about face images.
- And of many other things.

—> Non linear classification is a practical proposition.

Increasing the Dimension Further

Can we increase the dimension massively:

- in a principled way,
- while keeping the computational burden down?

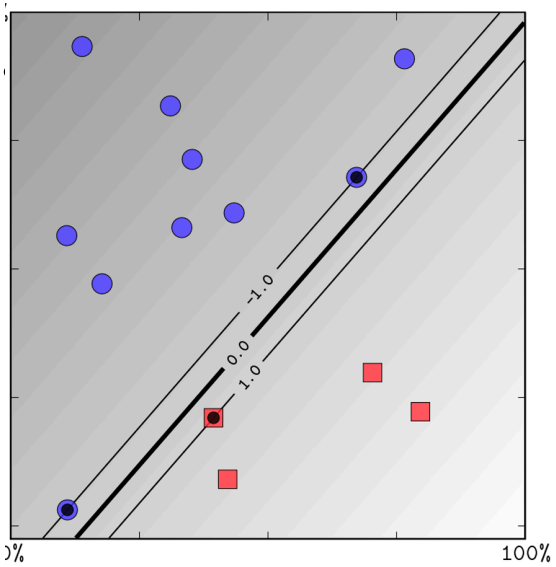
—> Non-linear support vector machines that use the so-called kernel trick.

Reminder: Polynomial SVM

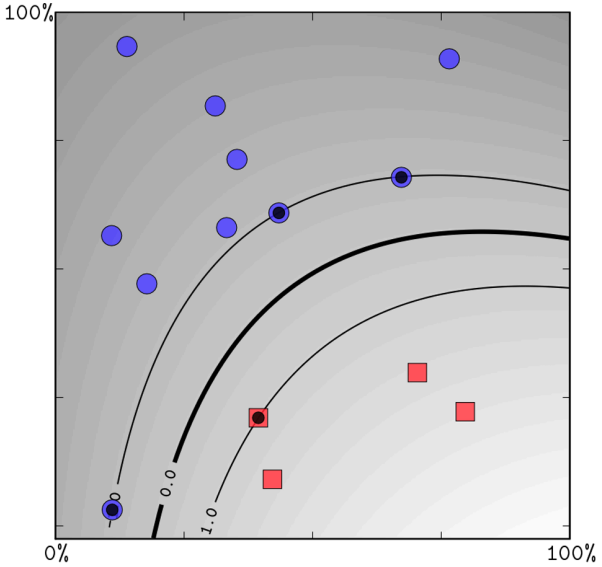
$$\mathbf{w}^* = min_{(\mathbf{w},\{\xi_\mathbf{n}\})} \frac{1}{2} ||\mathbf{w}||^2 + C \sum_{n=1}^{N} \xi_n,$$

$$\text{subject to } \forall n, \quad t_n \cdot (\tilde{\mathbf{w}} \cdot \phi(\mathbf{x})_n) \geq 1 - \xi_n \text{ and } \xi_n \geq 0.$$

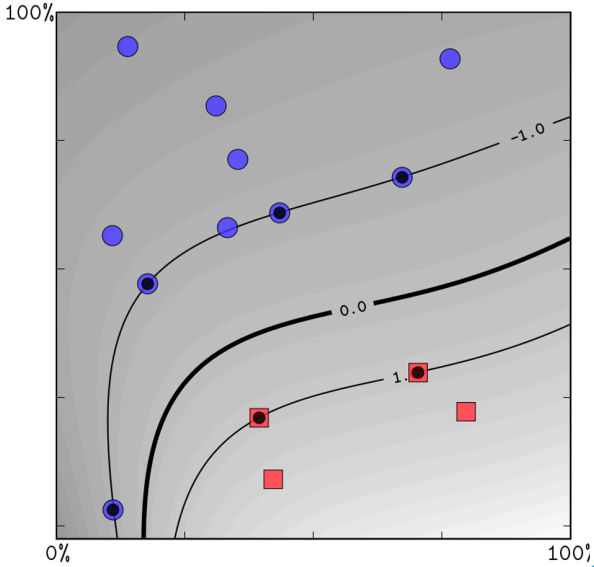
- C is constant that controls how costly constraint violations are.



M =1



M = 2



M = 5

Polynomial SVM w/o Slack Variables

- For simplicity

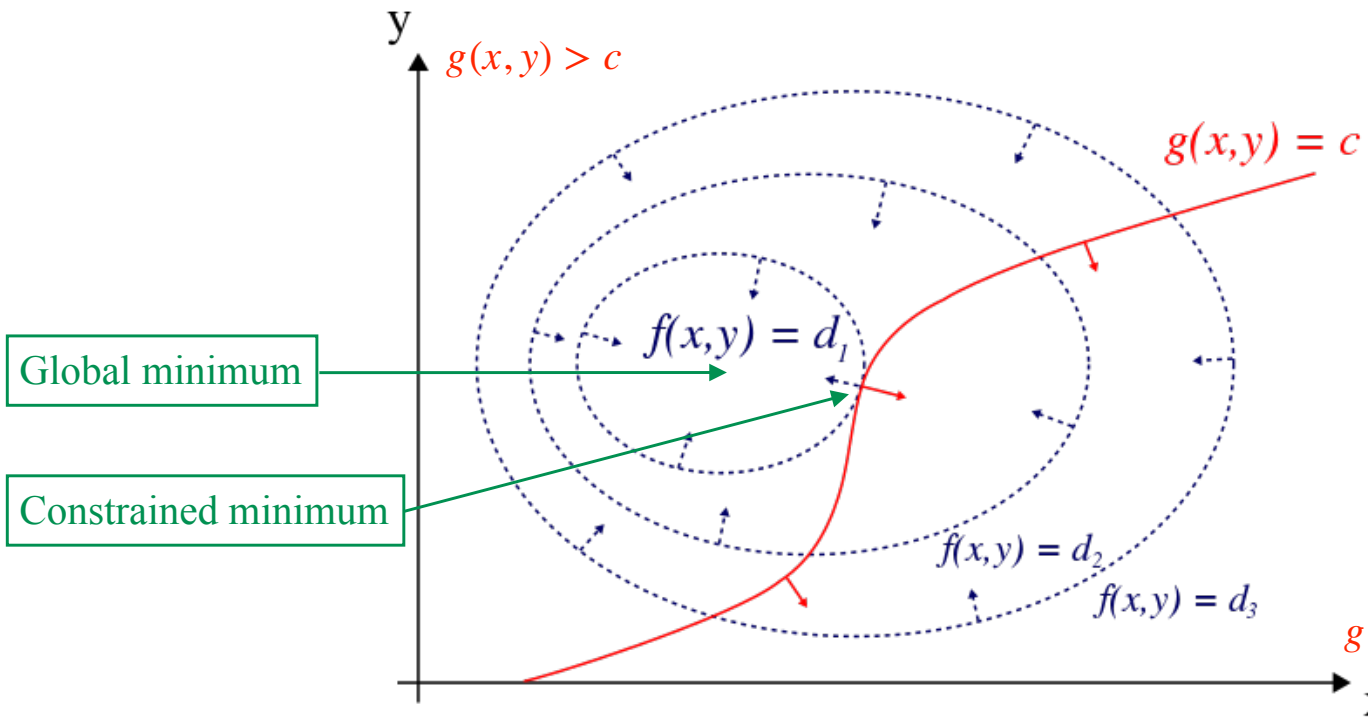
$$\mathbf{w}^* = min_{\mathbf{w}} \frac{1}{2} ||\mathbf{w}^2||,$$

$$\text{subject to } \forall n, \quad t_n \cdot (\tilde{\mathbf{w}} \cdot \phi(\mathbf{x})_n) \geq 1.$$

- We will re-introduce the slack variables later.

—> Constrained optimization.

Reminder: Constrained Optimization



- Blue dotted lines are "level" lines.
- In this example, $d_1 < d_2 < d_3$.
- The blue arrows represent ∇f.
- The red arrows represent ∇g.

- Minimize $f(x, y)$subject to $g(x, y) \leq c$.
- At the constrained minimum

$$\exists \lambda \in R, \nabla f = \lambda \nabla g$$

- λ is known as a Lagrange multiplier.

Reminder: Lagrangian Formulation

Lagrangian:

$$L(\mathbf{w}, \Lambda) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{n=1}^{N} \lambda_n (t_n \tilde{\mathbf{w}} \cdot \phi(\mathbf{x}_n) - 1)$$

$$\Lambda = [\lambda_1, \ldots, \lambda_n]$$

Lagrange multipliers.
One per constraint.

Theorem:

A solution of the constrained minimization problem must be such that L is minimized with respect to the components of vector $\mathbf{w}$ and maximized with respect to the Lagrange multipliers, which must remain greater or equal to zero.

Optional: Minimizing the Lagrangian

$$L(\mathbf{w}, \Lambda) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{n=1}^{N} \lambda_n (t_n \tilde{\mathbf{w}} \cdot \phi(\mathbf{x}_n) - 1)$$

$$\mathbf{w} = \sum_n \lambda_n t_n \phi(\mathbf{x}_n)$$

Setting the derivatives of $L(\mathbf{w}, \Lambda)$ to zero with respects to the elements of $\mathbf{w}$ and b yieds

$$\begin{aligned} \mathbf{w} &= \sum_{n=1}^{N} \lambda_n t_n \phi(\mathbf{x}_n) \ , \\ 0 &= \sum_{n=1}^{N} \lambda_n t_n \ . \end{aligned}$$

Optional: Dual Problem

Therefore, we minimize

$$\tilde{L}(\Lambda) = L(\mathbf{w}, \Lambda) = \sum_{n=1}^{N} \lambda_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \lambda_n \lambda_m t_n t_m k(\mathbf{x}_n, \mathbf{x}_m)$$

subject to

$$\lambda_n \geq 0 \; \forall n \; ,$$

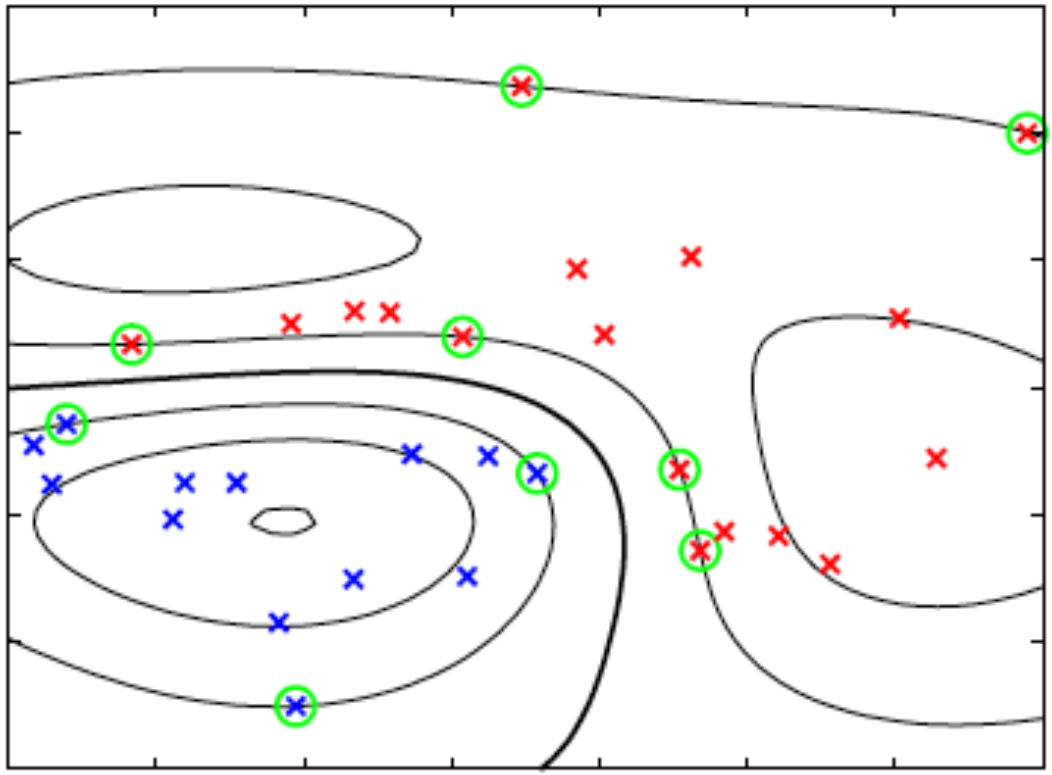
$$\sum_{n=1}^{N} \lambda_n t_n = 0$$

and with

$$k(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x})^T \phi(\mathbf{x}') \; .$$

—> Quadratic programming problem with N variables.
—> Complexity in $O(N^3)$ instead of $O(D^3)$.

Support Vectors



$$\mathbf{w} = \sum_{n=1}^{N} \lambda_n t_n \phi(\mathbf{x}_n) \ .$$

$$y(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) + b \ ,$$

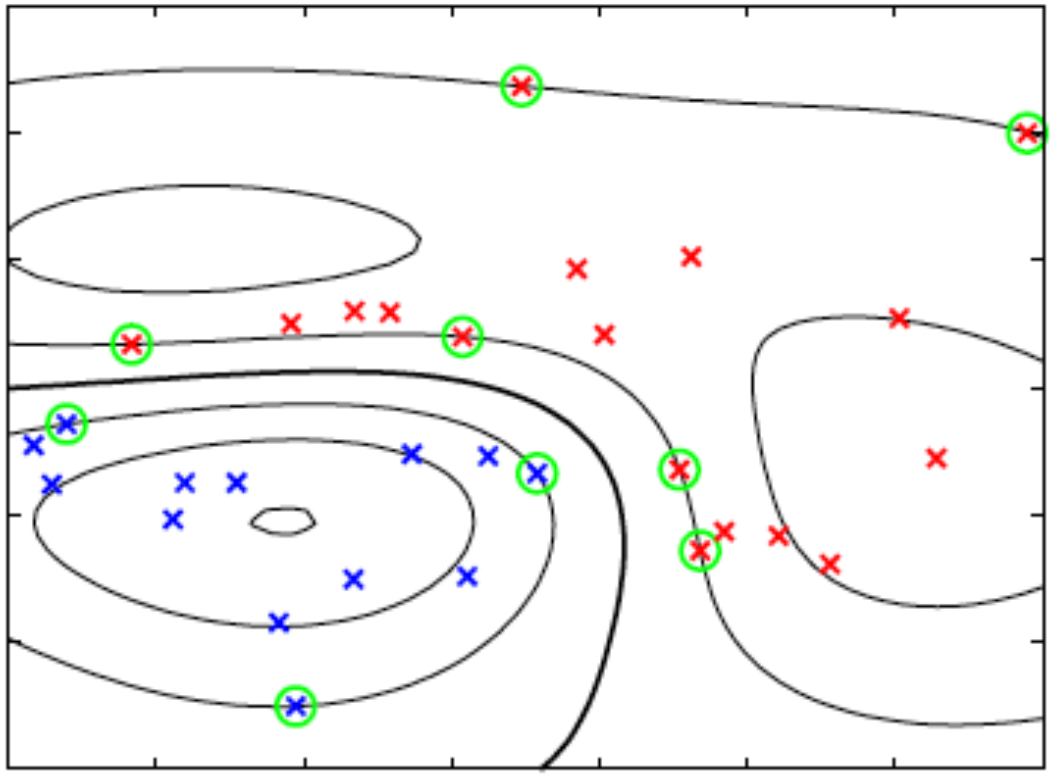
$$= \sum_{n=1}^{N} \lambda_n t_n k(\mathbf{x}, \mathbf{x}_n) + b \ ,$$

$$\text{with } k(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x})^T \phi(\mathbf{x}') \ .$$

- Only for a subset of the data points is λ_n is non zero.
- The are denoted by green circles.
- The corresponding x_n are the support vectors and satisfy $t_n y(\mathbf{x}_n)=1$.
- They are the only ones that need to be considered as test time.

—> That is what makes SVMs practical!

At Inference Time



$$y(\mathbf{x}) = \sum_{n=1}^{N} \lambda_n t_n k(\mathbf{x}, \mathbf{x}_n) + b$$
$$= \sum_{n \in \mathcal{S}} \lambda_n t_n k(\mathbf{x}, \mathbf{x}_n) + b$$

- Only for a subset of the data points is a_n is non zero.
- The feature vector $\phi(\mathbf{x})$ does **not** appear explicitly anymore.
- The kernel function k(.,.) can be understood as a similarity measure.

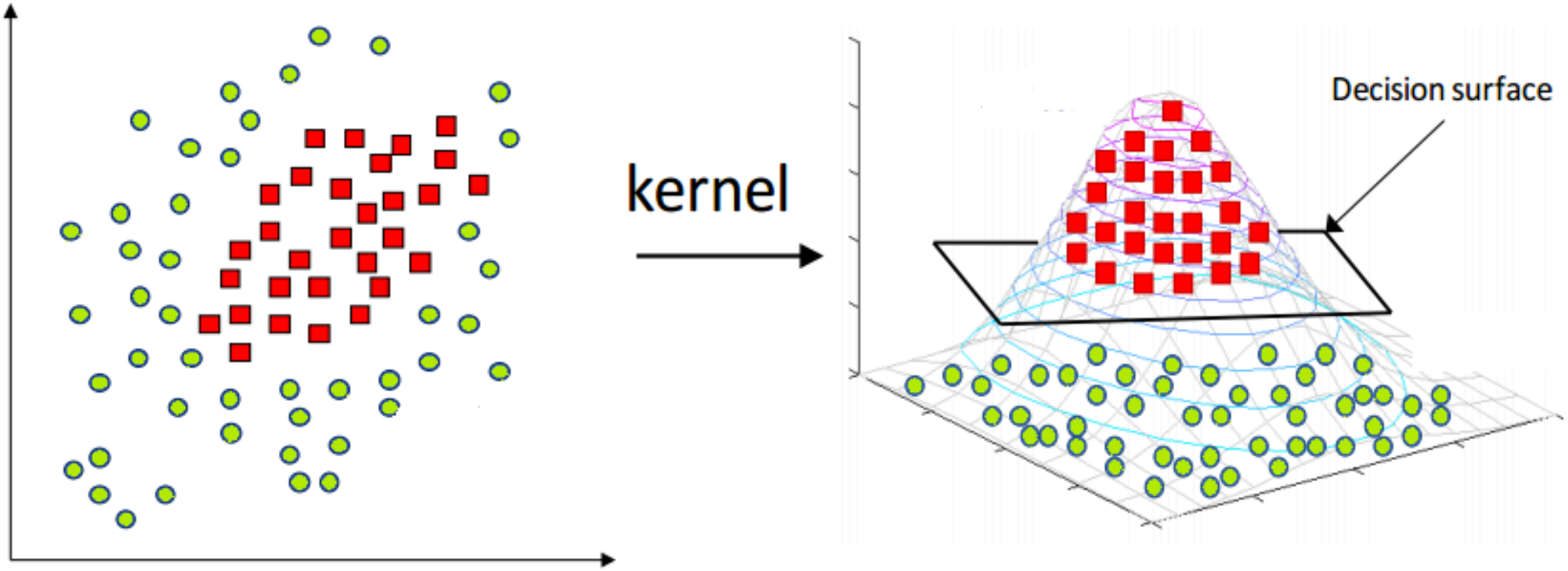
The Kernel Trick

$$y(\mathbf{x}) = \sum_{n \in \mathcal{S}} \lambda_n t_n k(\mathbf{x}, \mathbf{x}_n) + b$$

$$k(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x})^T \phi(\mathbf{x}')$$

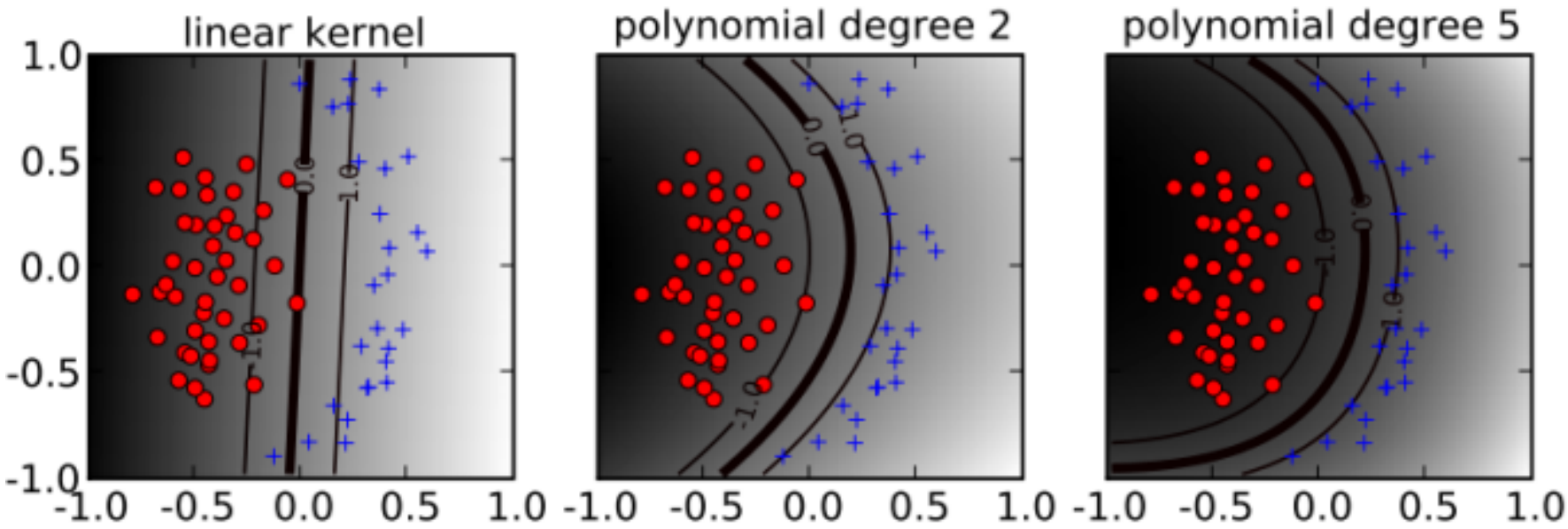
- ϕ is implicit: In practice, we never compute it.
- We only need to compute k.
- This is known as the kernel trick and is used in many different algorithms besides SVMs.

Role of the Kernel



Polynomial kernels: From small to high dimension.
Gaussian kernels: From small to infinite dimension.

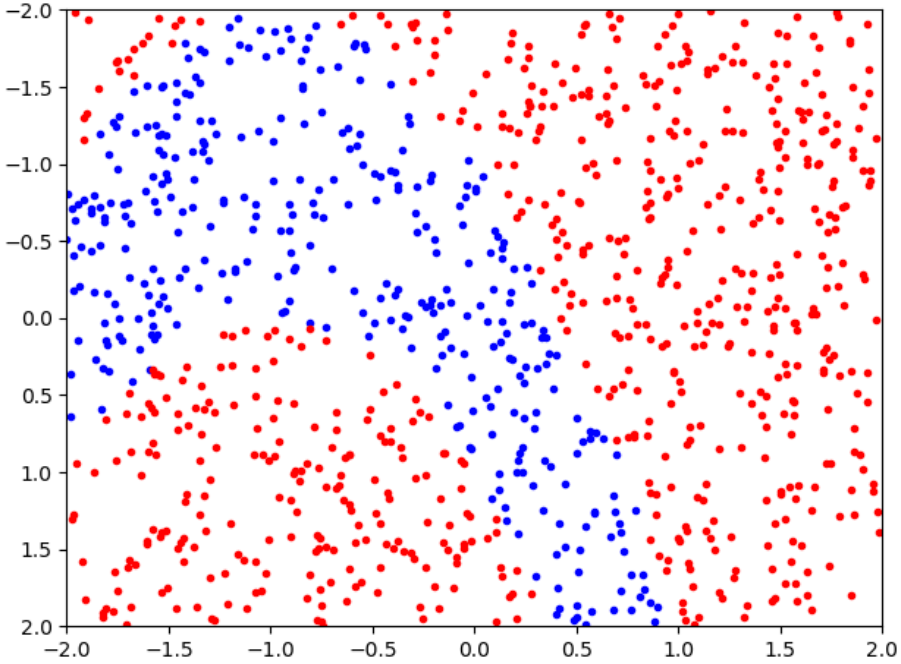
Influence of the Kernel

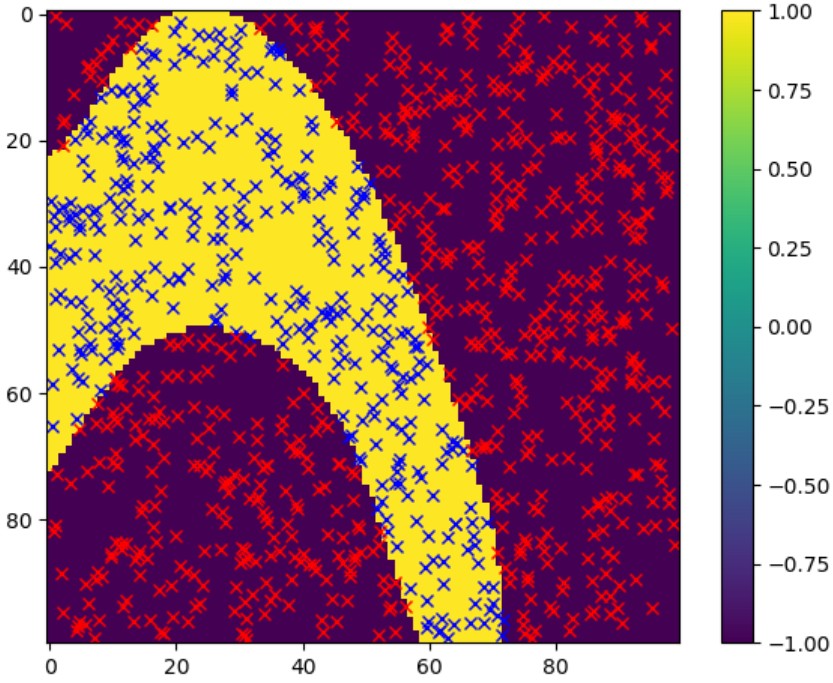


$$y(\mathbf{x}) = \sum_{n=1}^{N} \lambda_n t_n k(\mathbf{x}, \mathbf{x}_n) + b \ ,$$

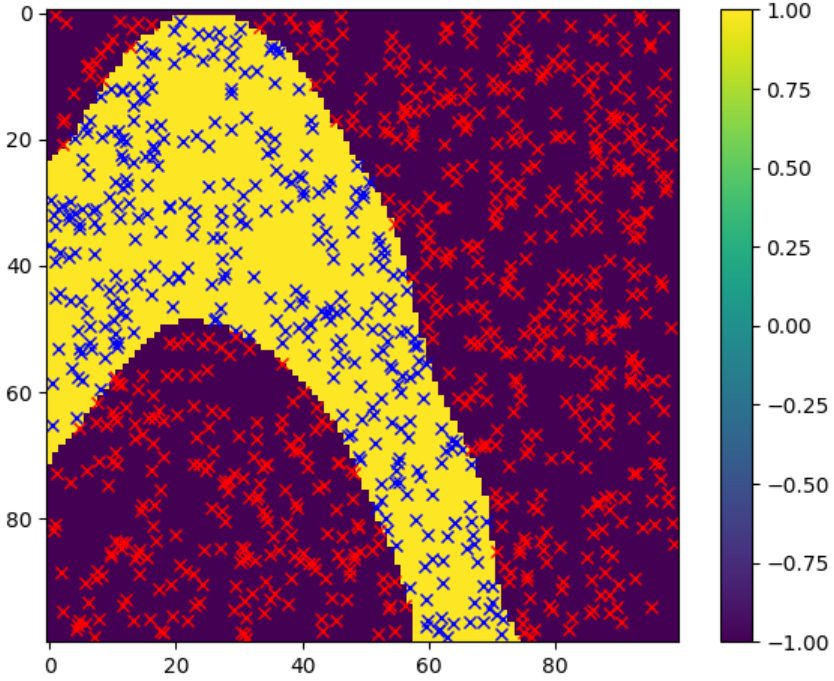
$$k(\mathbf{x}, \mathbf{x}') = 1 + (\mathbf{x}^T \mathbf{x}')^d \qquad \text{(Polynomial terms up to degree } d\text{)}.$$

$$k(\mathbf{x}, \mathbf{x}') = \exp(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{\sigma^2}) \text{ (Gaussian, feature space of infinite dimension)}.$$

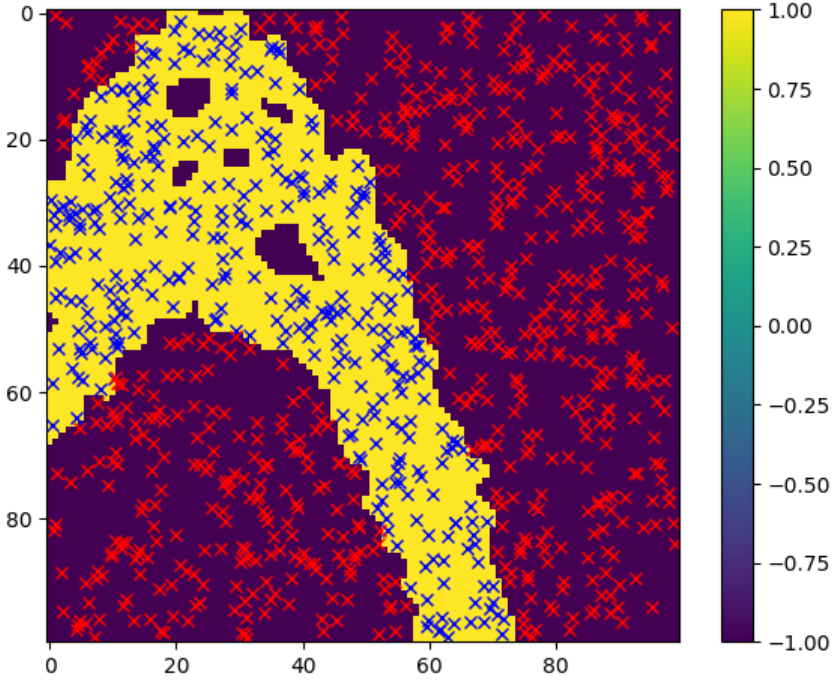




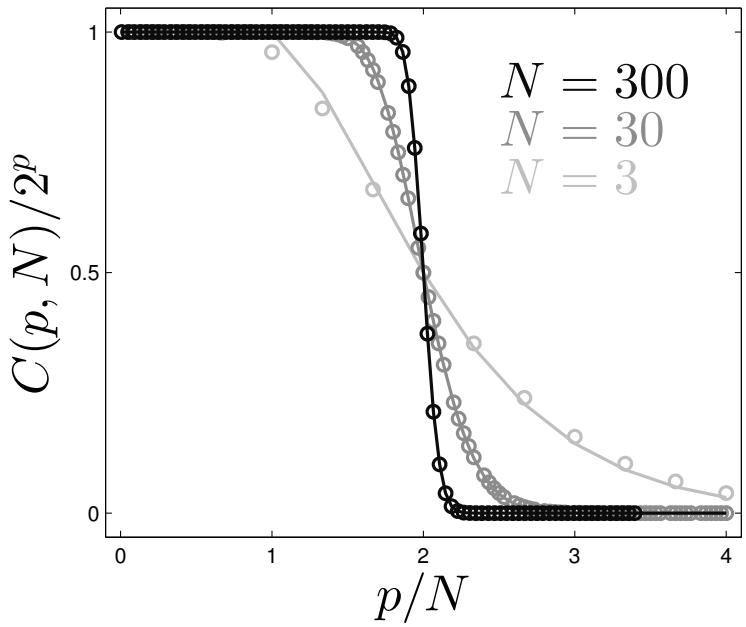
Rbf, $\sigma = 1.0$

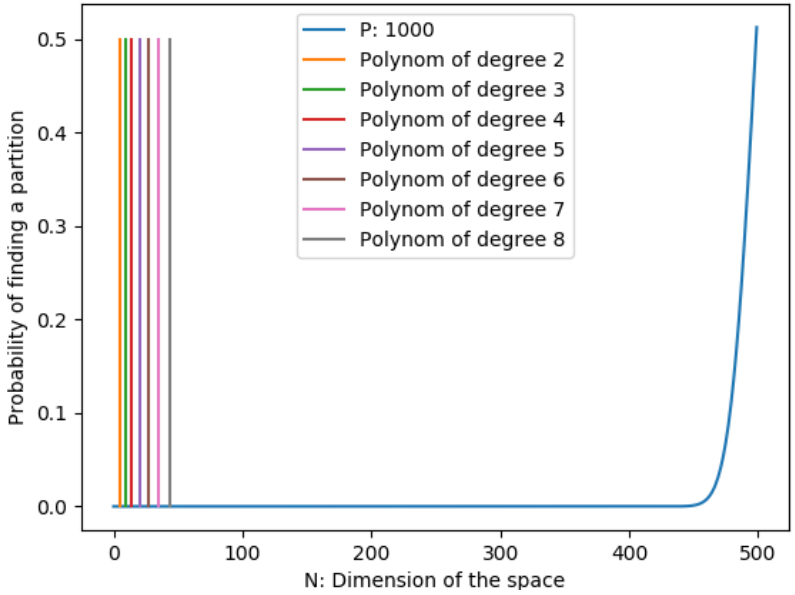


Rbf, $\sigma = 0.01$



Back to Cover's Theorem

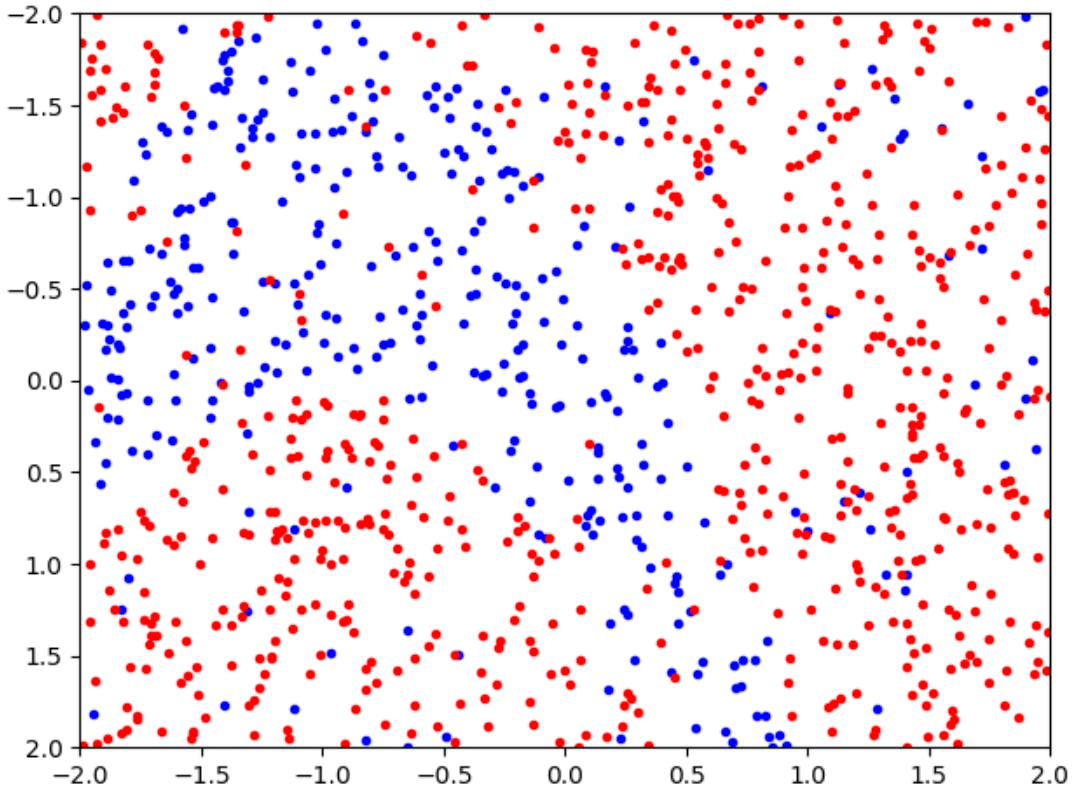




- Good news: Working with a Gaussian kernel virtually makes the dimension as large as the number of samples.

- Bad news: It is still not ideal for very large values of the number of points N due to the $O(N^3)$ computational complexity.

Overlapping Class Distributions



Some blues among the reds and some reds among the blues.

- Some training examples must be allowed to be misclassified.
- Cannot satisfy all the hard constraints.
- For linear SVMs, we used slack variables to achieve this.
- For kernel SVMs, we can do so by bounding the Lagrange multipliers.

Optional: Dual Problem with Slack Variables

We now minimize

$$\tilde{L}(\Lambda) = L(\mathbf{w}, \Lambda) = \sum_{n=1}^{N} \lambda_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \lambda_n \lambda_m t_n t_m k(\mathbf{x}_n, \mathbf{x}_m)$$

subject to

$$\forall n, \quad 0 \leq \lambda_n \leq C \,,$$

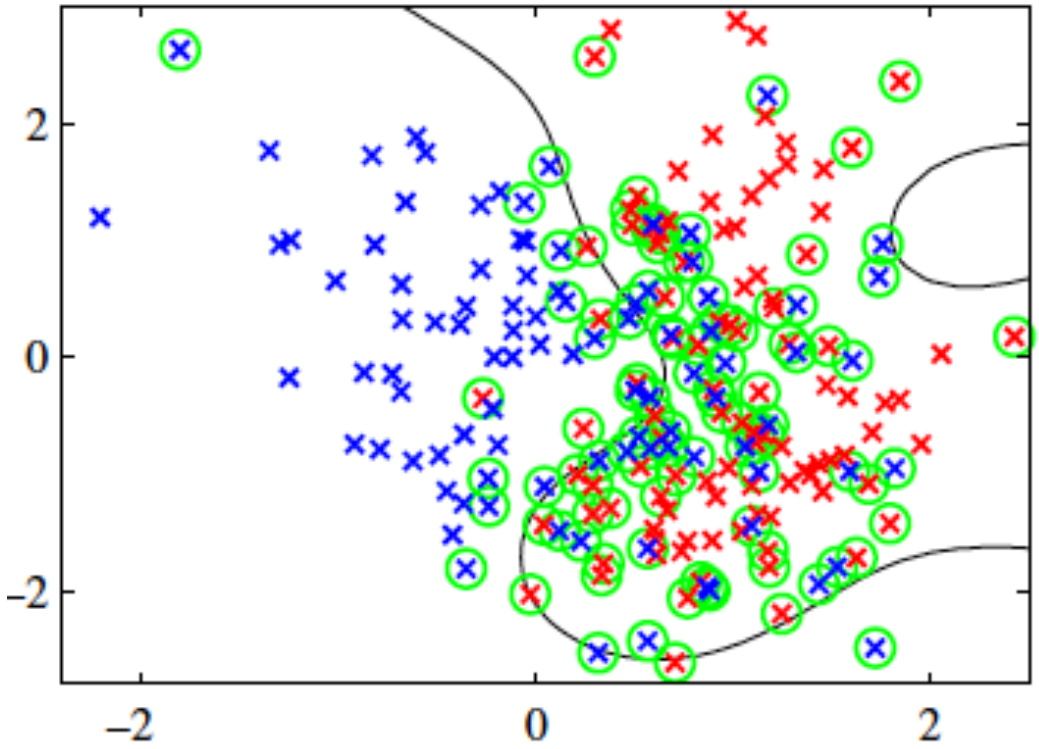
λ_n cannot become infinite and therefore some of the constraints can be violated.

$$\sum_{n=1}^{N} \lambda_n t_n = 0$$

and with

$$k(\mathbf{x}, \mathbf{x}') = \phi(\mathbf{x})^T \phi(\mathbf{x}') \,.$$

Finally a Simple Usable Formula

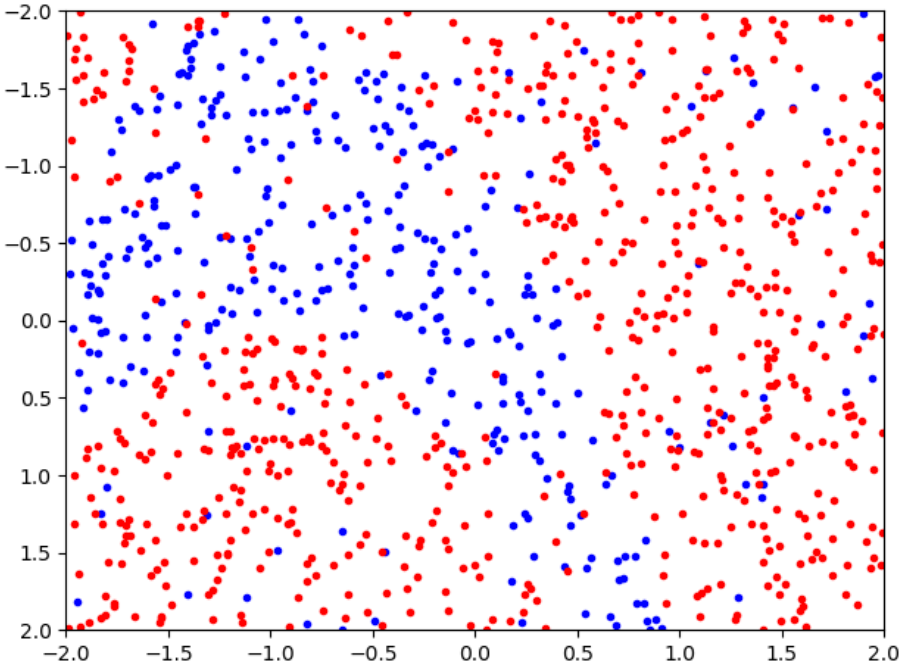


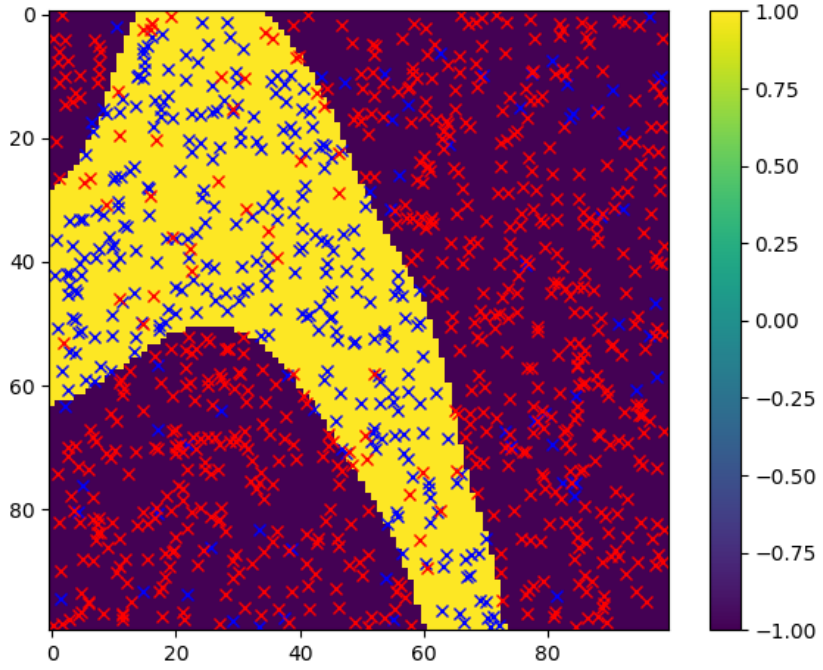
The green circles denote the support vectors.

$$y(\mathbf{x}) = \sum_{n \in \mathcal{S}} \lambda_n t_n k(\mathbf{x}, \mathbf{x}_n) + b$$

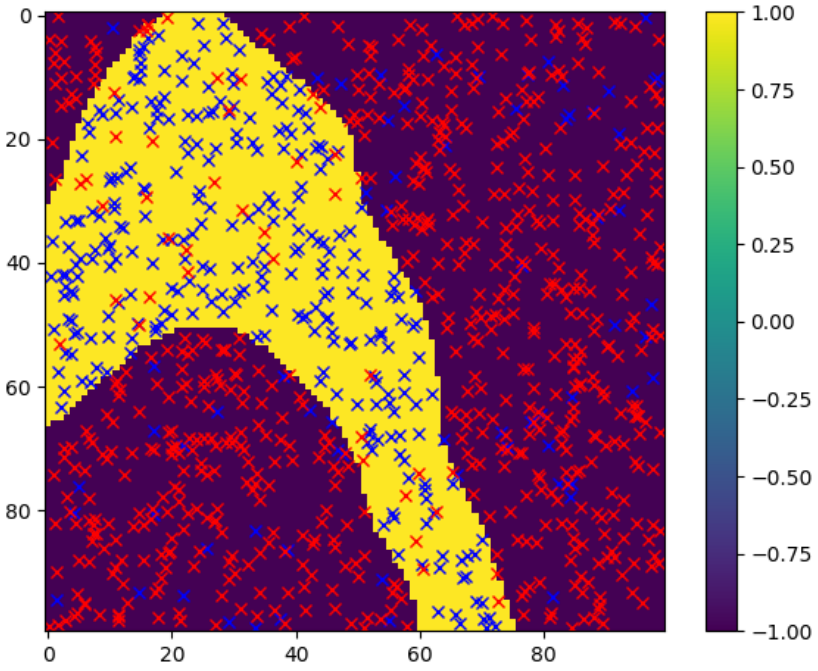
where S is the set of support vectors.

- $\lambda_n < C$: x_n lies on the margin.
- $\lambda_n = C$: x_n lies inside the margin.

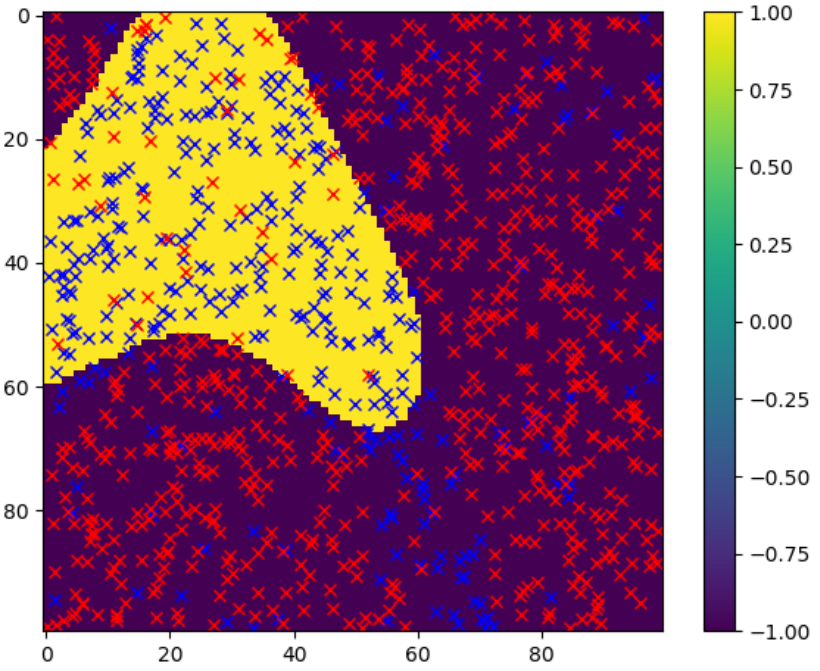




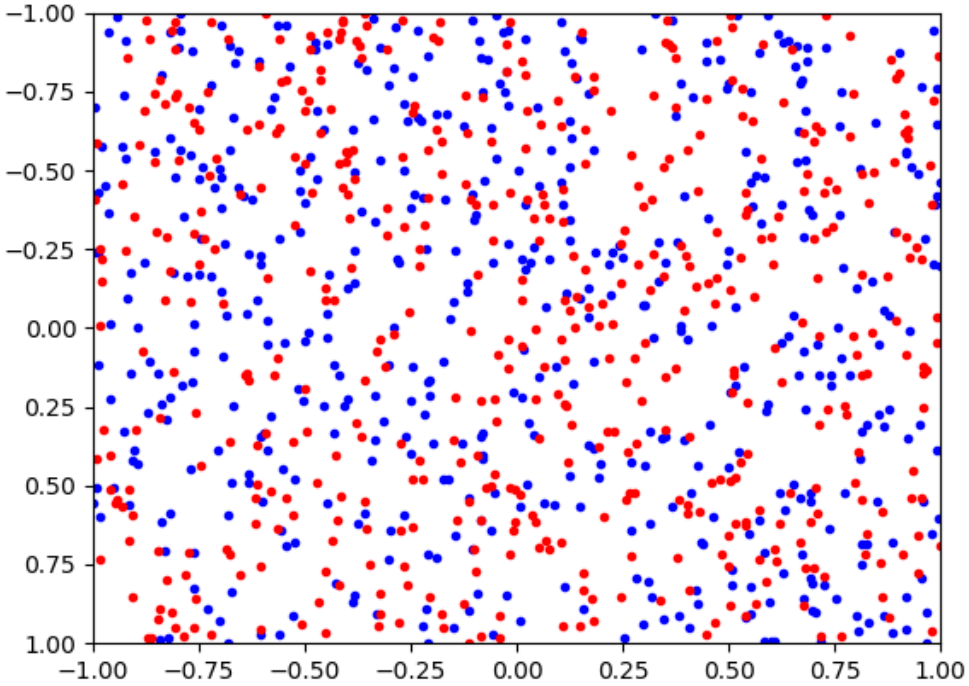
Rbf, σ = 1.0, C=1.0

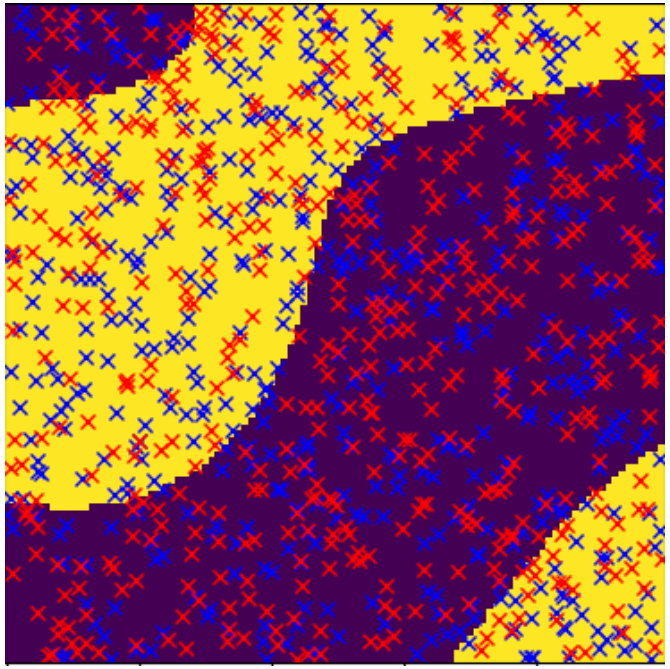


Rbf, σ = 1.0, C= 100.0

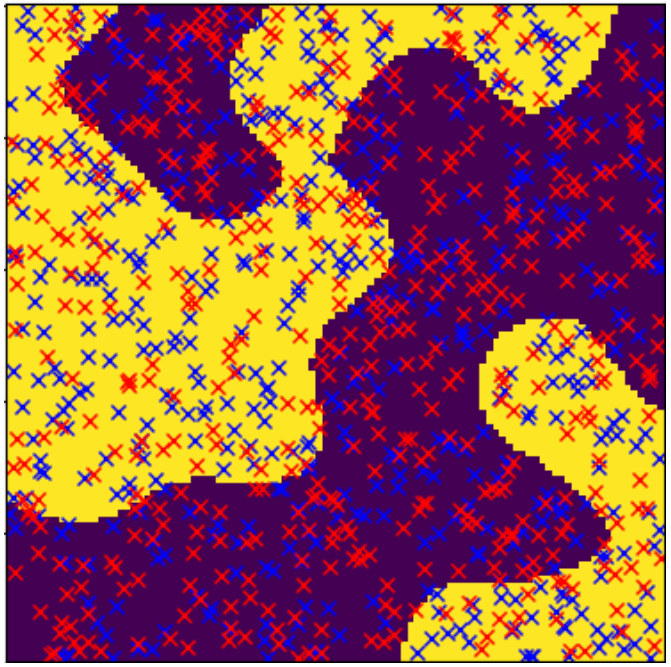


Rbf, σ = 1.0, C= 0.1

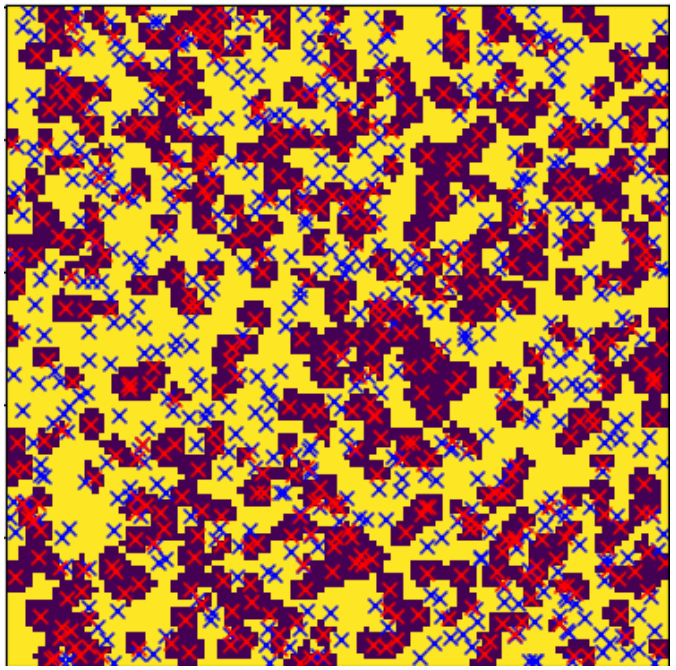




Rbf, σ = 1.0, C = 1.0

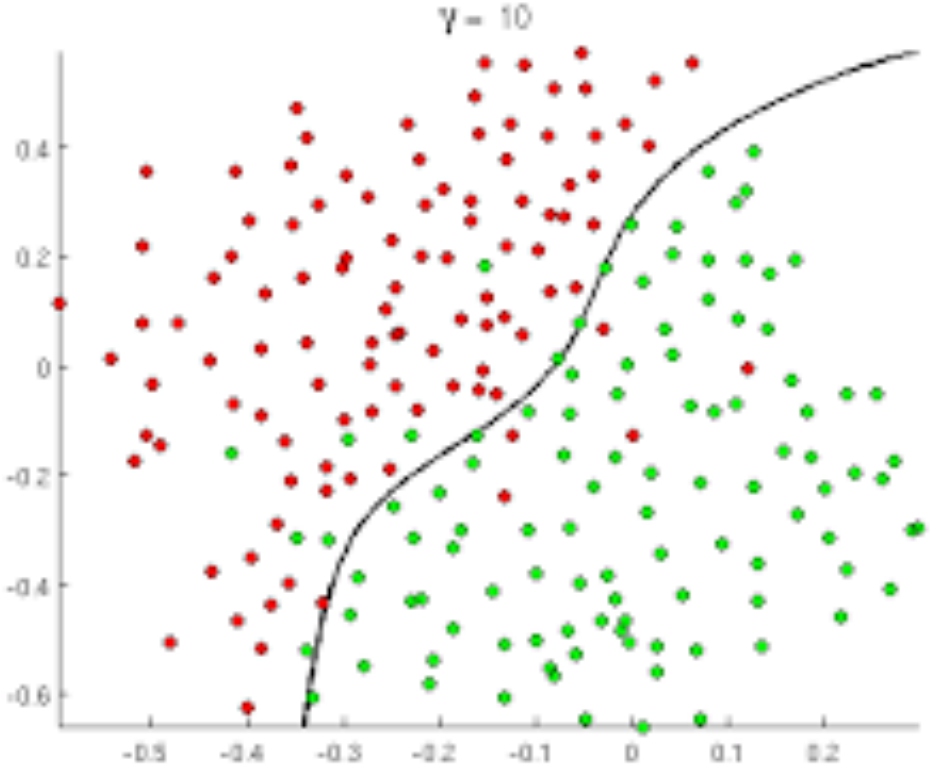


Rbf, σ = 0.1, C = 1.0



Rbf, σ = 0.05, C = 1.0

Non-Separable Distributions



The slack variables allow some training points to be misclassified.

- A large σ sigma tends to smooth the decision boundary.
- A large C tends to minimize the number of misclassified training points.

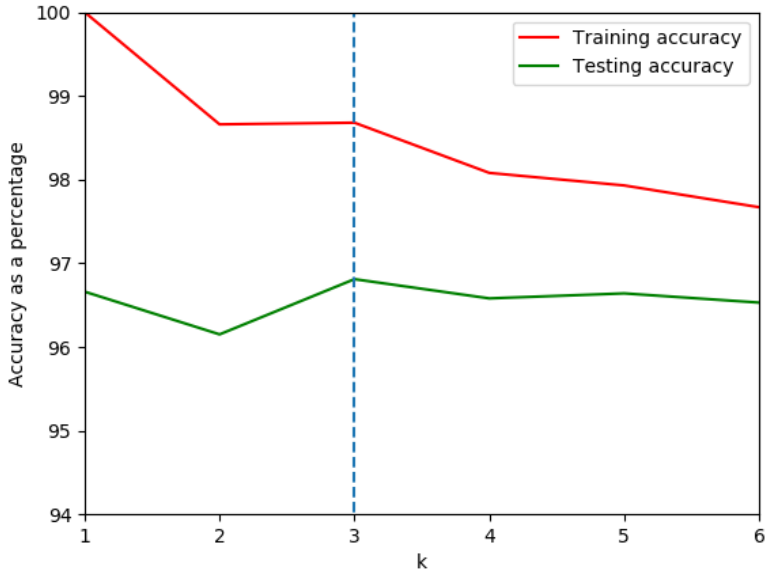
—> Validation data is required to choose them properly.

Recognizing Hand-Written Digits

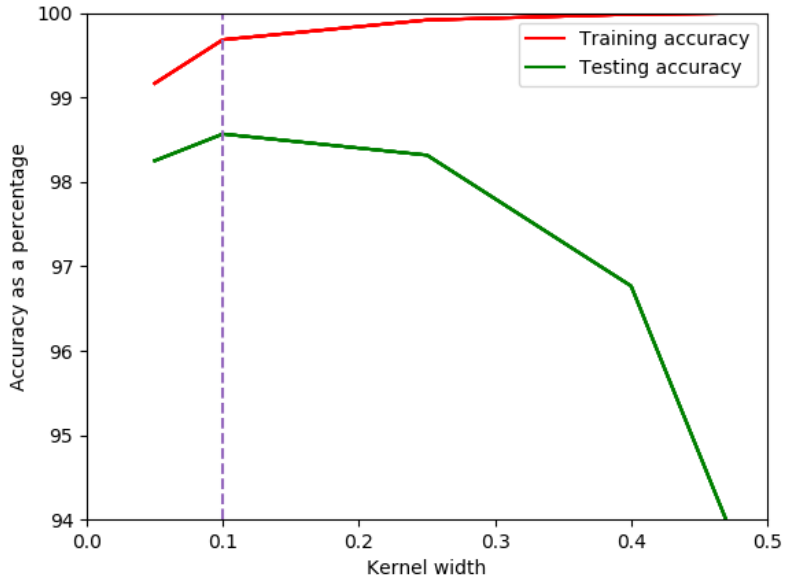
Test sample

Nearest neighbors

k-Nearest Neighbors vs SVM on MNIST



Knn: 96.8%



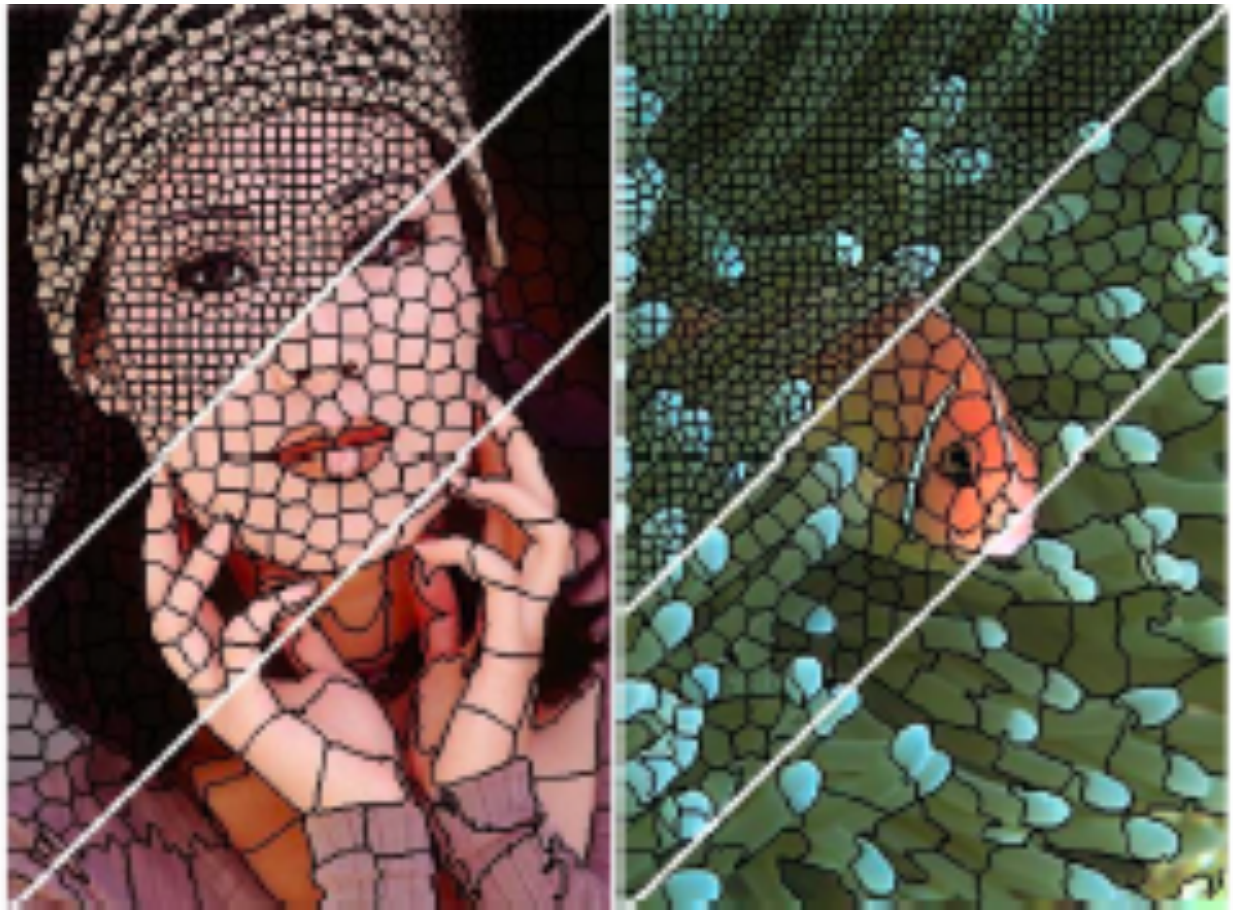
Rbf-SVM: 98.6%

- Better accuracy.
- But the kernel and its parameters must be well chosen.

SVMs in Short

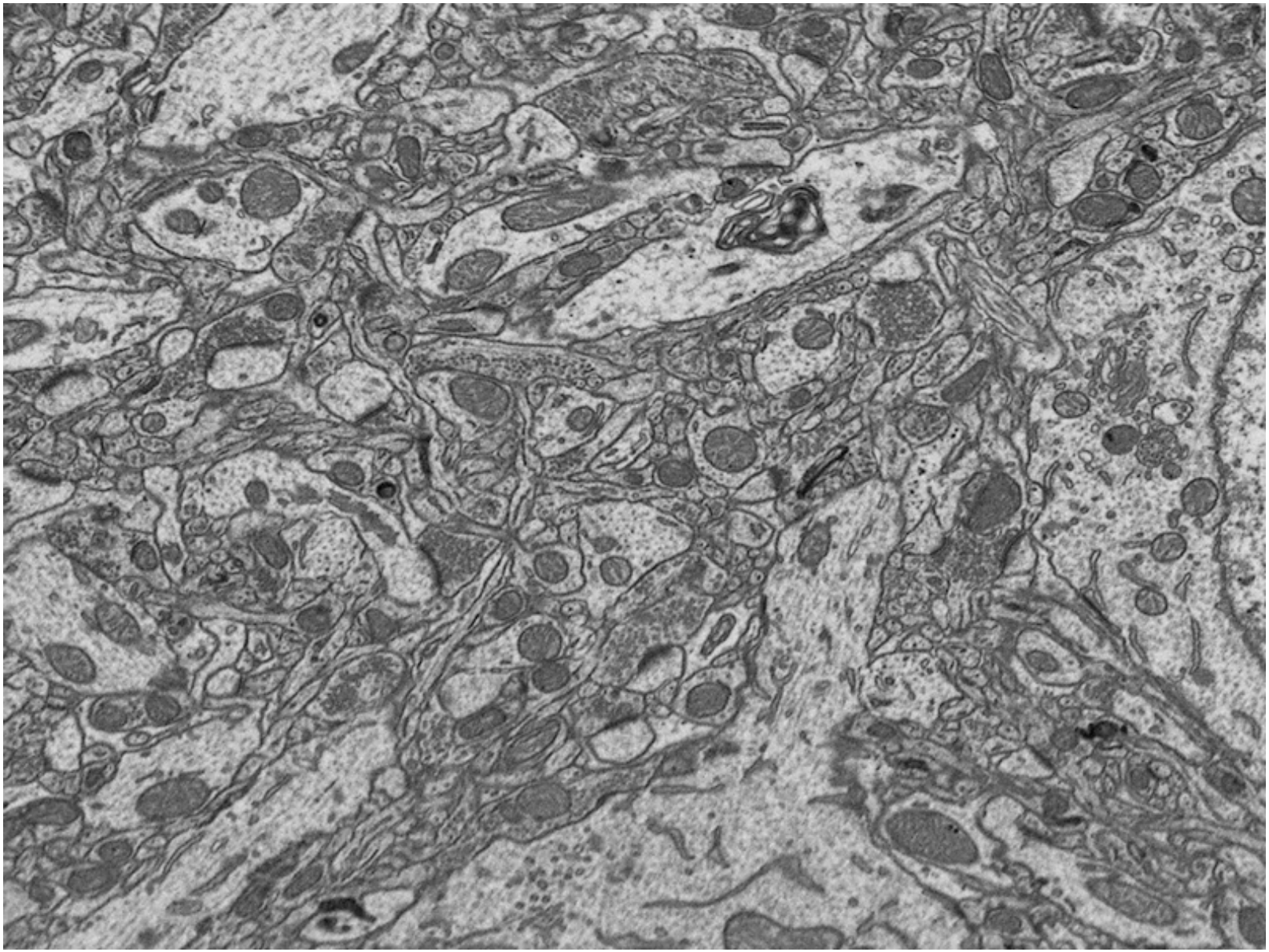
- The data can be separable in a high-dimensional feature space without being separable in the input space.
- Classifiers can be learned in the feature space without having to actually perform the mapping.
- However the $O(D^3)$ or $O(N^3)$ complexity at training time makes it hard to exploit large training sets.

Reminder: SLIC Superpixels



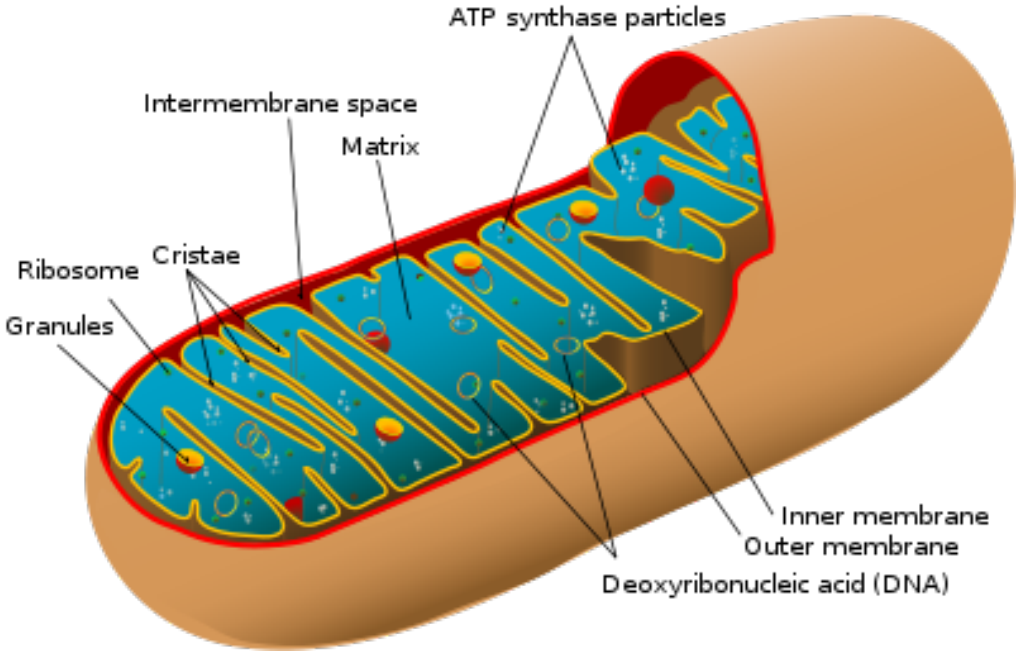
- Superpixel segmentations with centers on a 64x64, 256x256, and 1024x1024 grid.
- Can be used to describe the image in terms of a set of small regions.

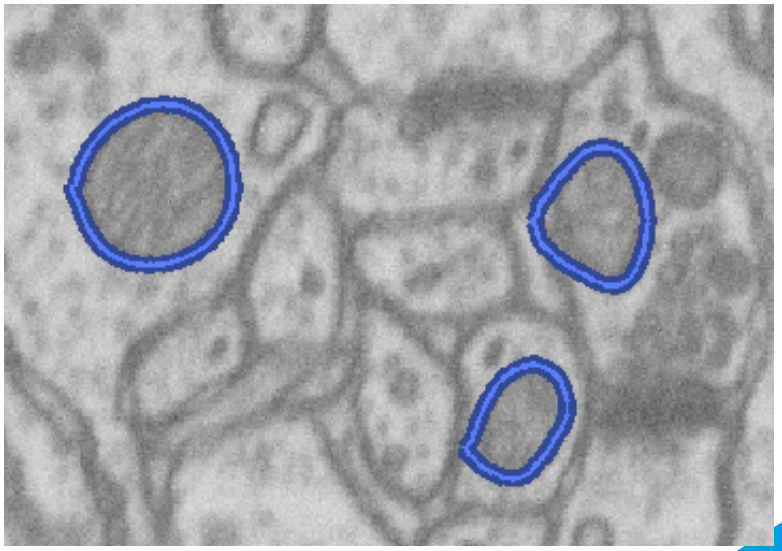
Optional: Electron Microscopy



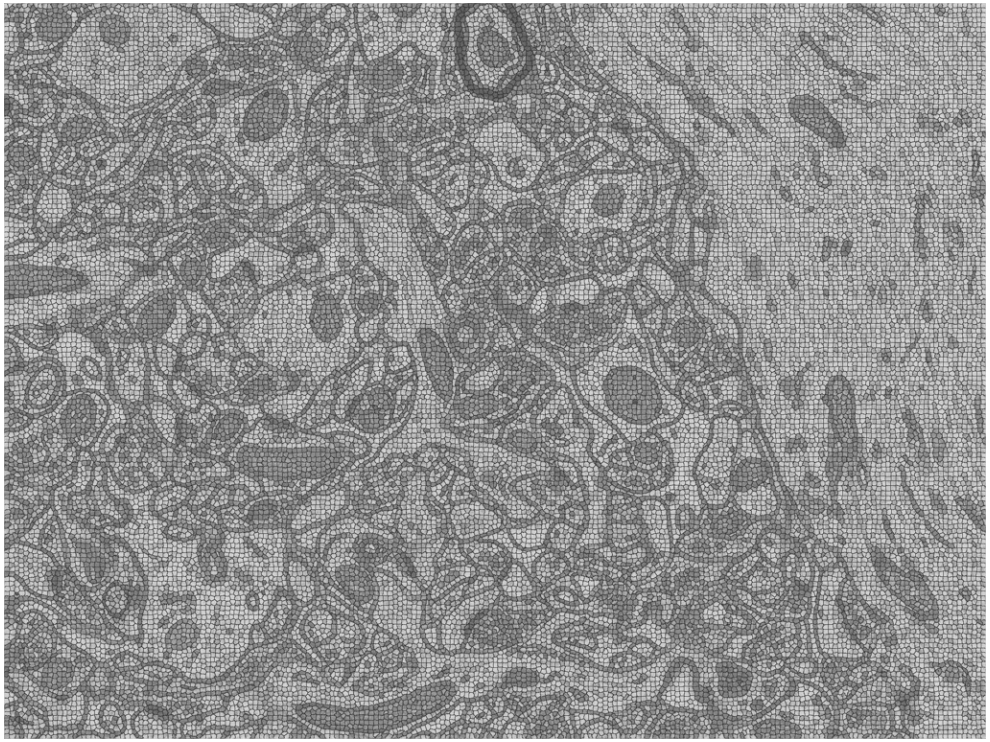
Let us SVMs to model structures of interest!

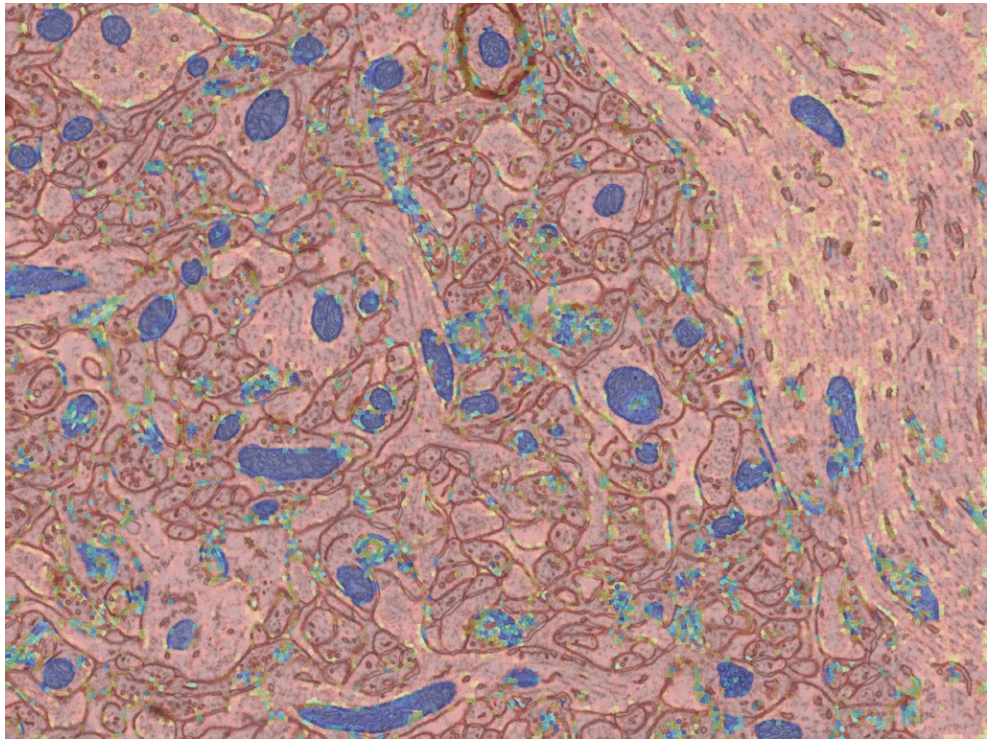
Optional: Mitochondria Segmentation





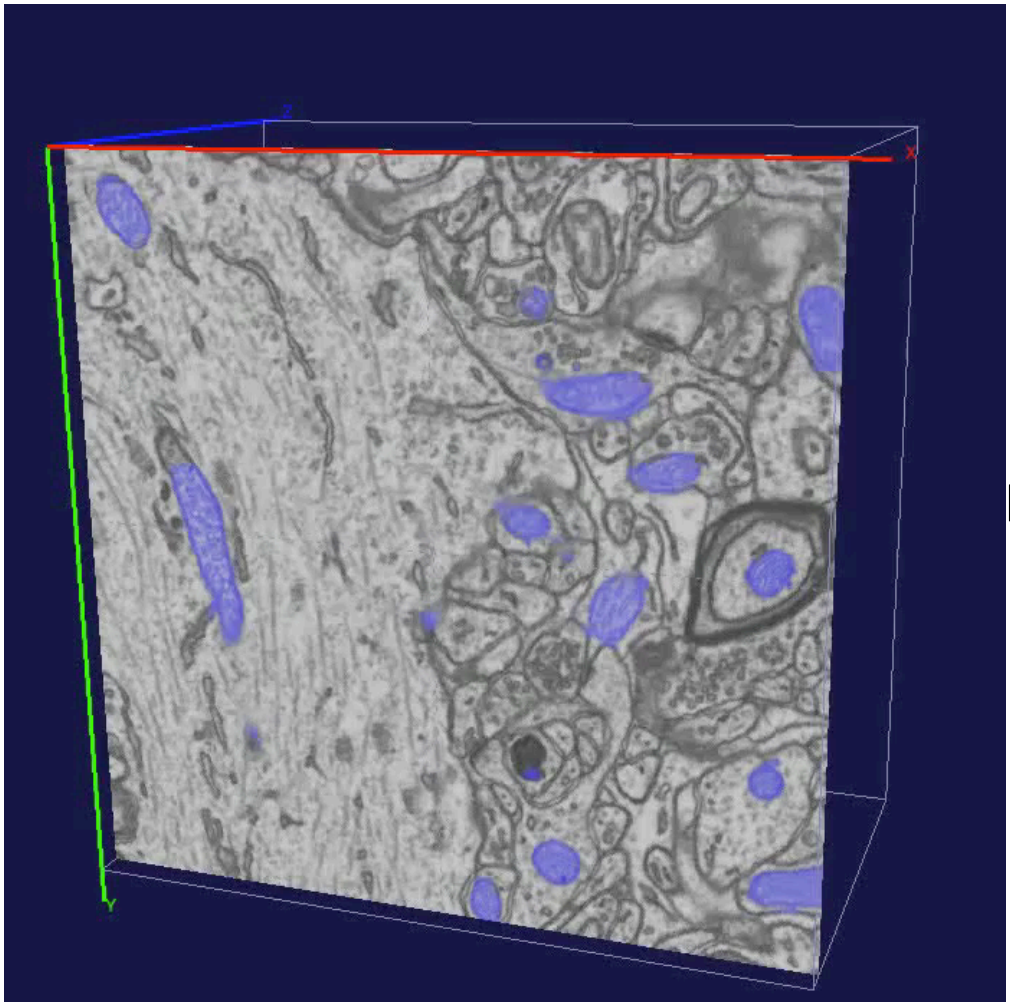
Optional: Assigning Probabilities

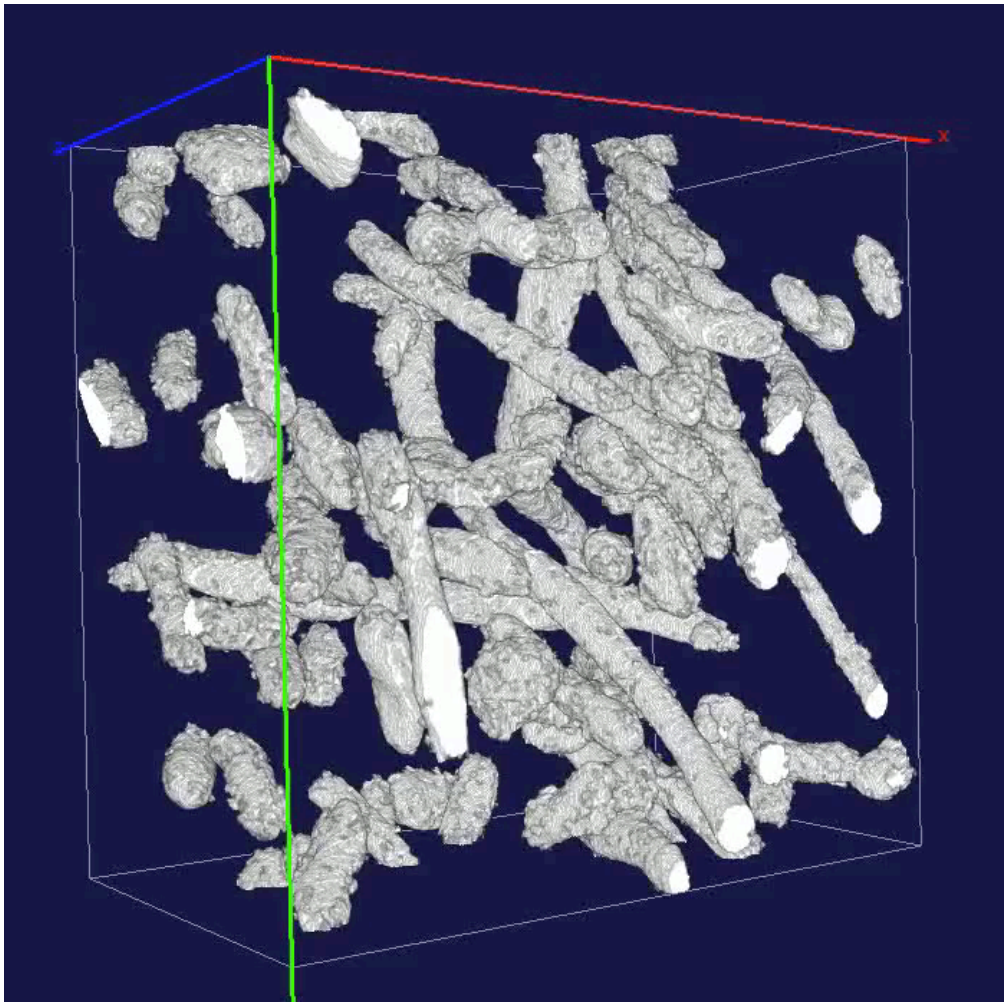




- Compute image features for each superpixel.
- Train an SVM classifier to assign a probability to be within a mitochondria.
- Can be used to produce segmentations using graph-based techniques.

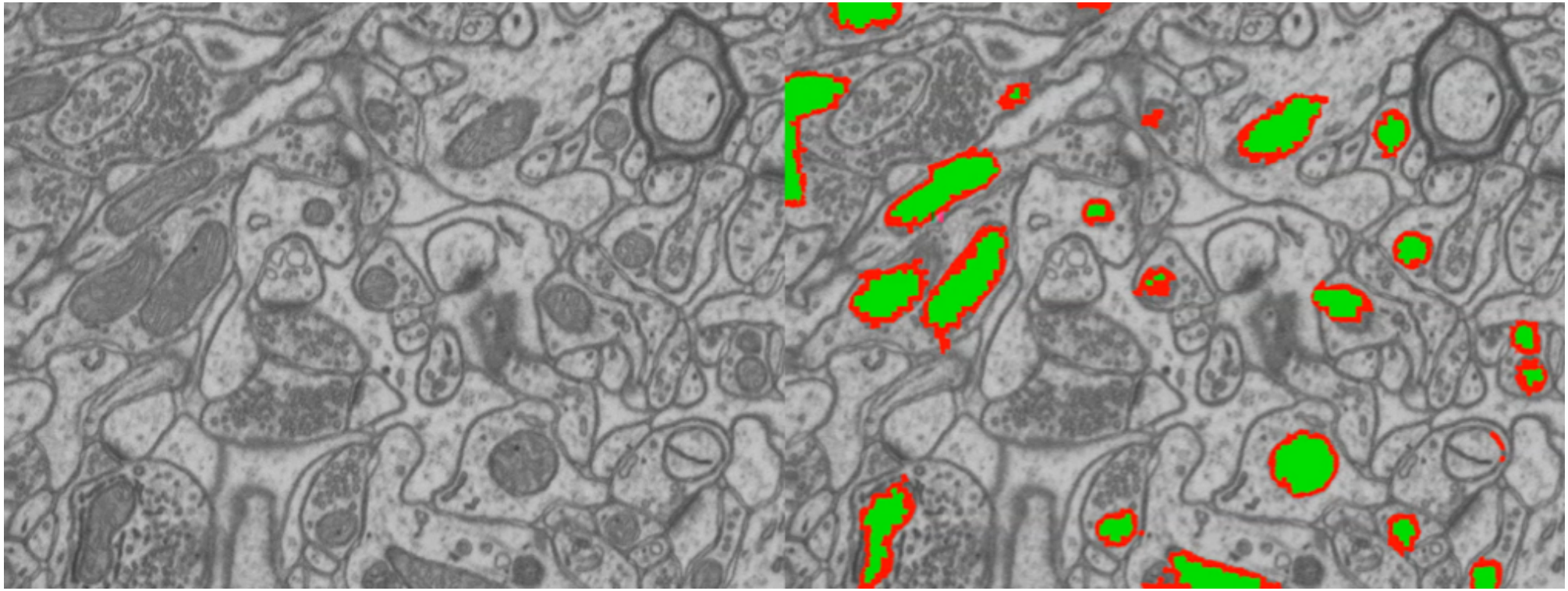
Optional: 3D Mitochondria





Lucchi et al. TMI'11

Optional: Modeling Membranes



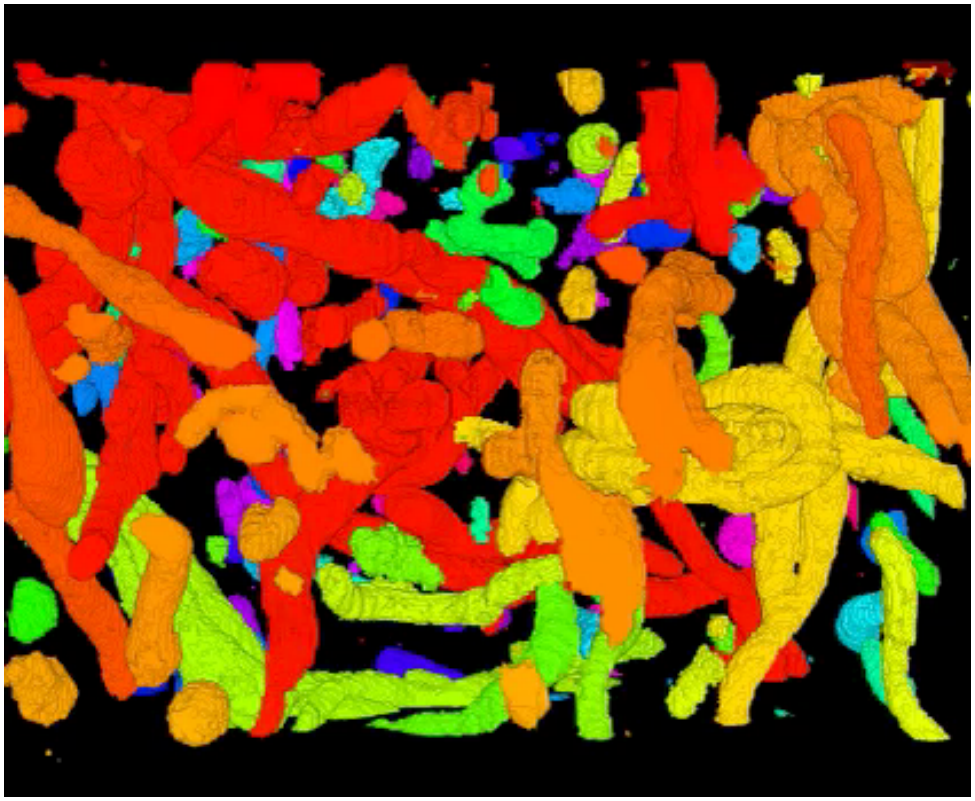
Here we use three classes instead of two:

- Inside
- Membrane
- Everything else

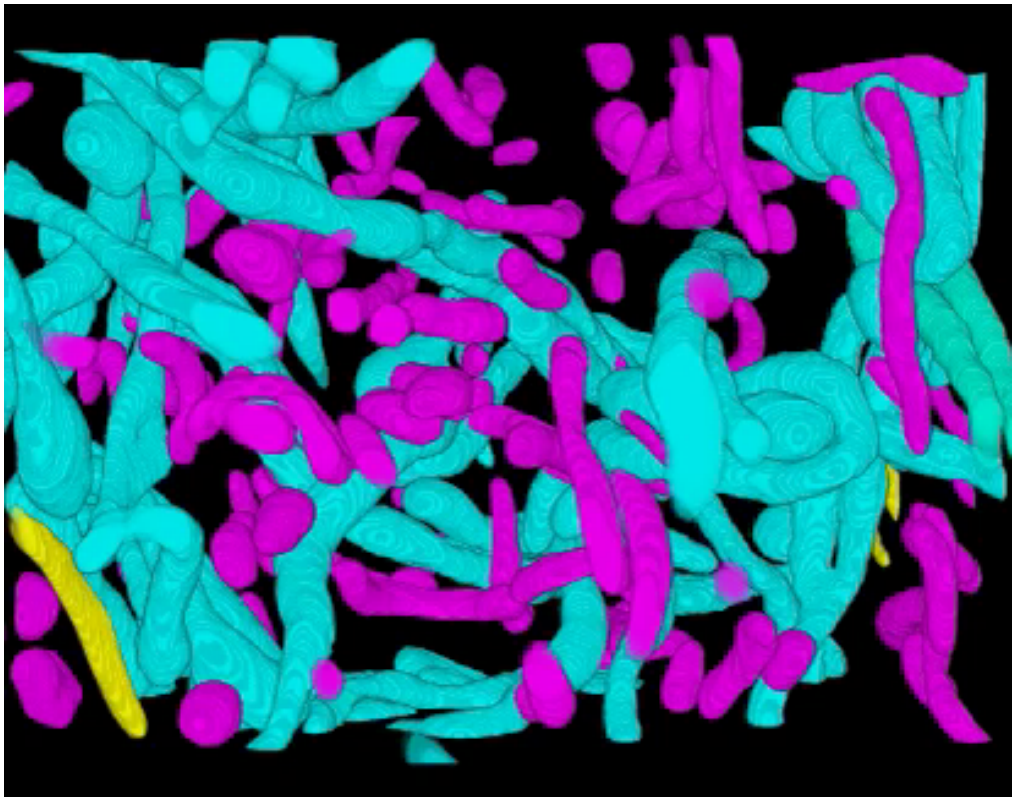
—>Because the inside is fully enclosed by the membranes, we can still find a global optimum.

Optional: Speeding up the Analysis

3.21 µm × 3.21 µm × 1.08 µm: 53 mitochondria



Automated result

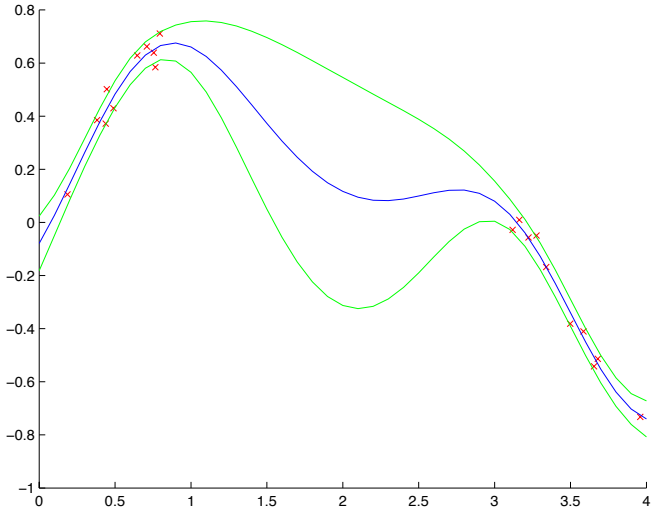


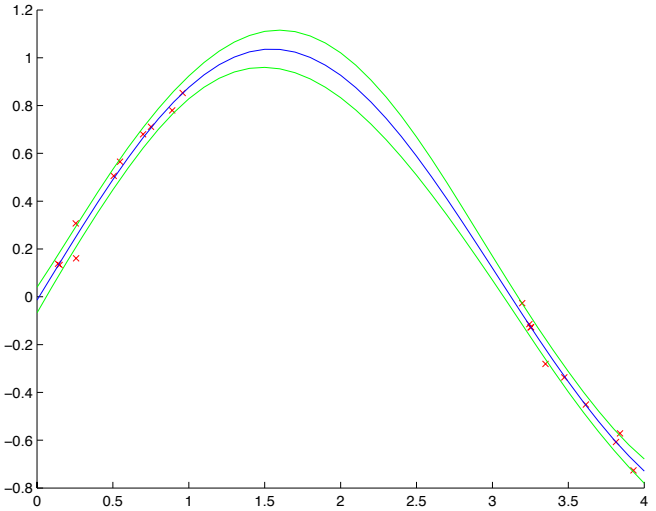
Interactively cleaned-up result

- By hand: 6 hours.
- Semi-automatically: 1.5 hours

—> Substantial time saving for the neuroscientists.

Optional: Non-Linear Regression





- Let $(\mathbf{x}_n, \mathbf{t}_n)_{1 \leq n \leq N}$ be N training pairs where the $\mathbf{x}_n$ are d dimensional and the $\mathbf{t}_n$ D dimensional.
- Let y be the function defined as $y(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x})$, where $\mathbf{w}$ is a $M \times D$ matrix, and ϕ denotes a function from $R^{\mathbf{d}}$ to $R^{\mathbf{M}}$.

Our goal is to minimize

$$J(\mathbf{w}) = \frac{1}{2} \Sigma_{n=1}^{N} ||\mathbf{w}^T \phi(\mathbf{x}_n) - \mathbf{t}_n||^2 + \frac{\lambda}{2} ||\mathbf{w}||^2 \quad ,$$

with respect to $\mathbf{w}$.

Data term

Regularization term

Optional: Kernel Trick Again

Let $\mathbf{a}_n = \frac{1}{\lambda}\{\mathbf{w}^T\phi(x_n) - \mathbf{t}_n\}$. It can be shown that the minimum is achieved for

$$\begin{bmatrix} \mathbf{a}_1^T \\ \dots \\ \mathbf{a}_N^T \end{bmatrix} = (\mathbf{K} + \lambda\mathbf{I})^{-1} \begin{bmatrix} \mathbf{t}_1^T \\ \dots \\ \mathbf{t}_N^T \end{bmatrix} ,$$

where $\mathbf{K}$ is the $N \times N$ symmetric Gram matrix with elements

$$\mathbf{K}_{n,m} = \phi(\mathbf{x}_n)^T\phi(\mathbf{x}_m) = k(\mathbf{x}_n, \mathbf{x}_m) .$$

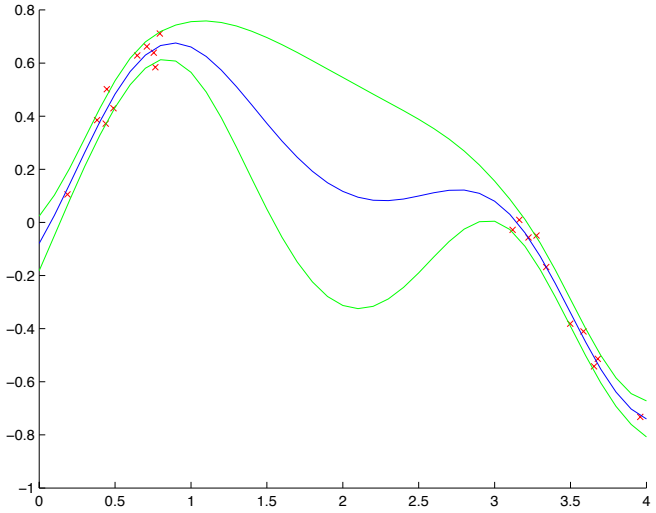
Therefore

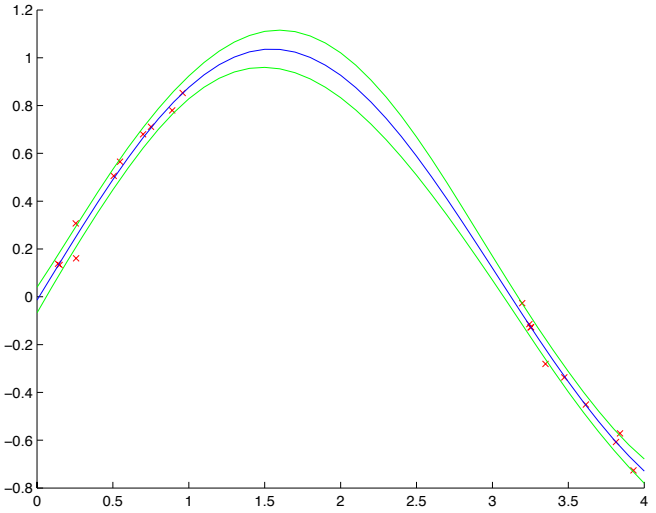
$$y(\mathbf{x}) = \mathbf{w}^T\phi(\mathbf{x}) = \mathbf{k}(\mathbf{x})(\mathbf{K} + \lambda\mathbf{I})^{-1} \begin{bmatrix} \mathbf{t}_1^T \\ \dots \\ \mathbf{t}_N^T \end{bmatrix} ,$$

where $\mathbf{k}(\mathbf{x}) = [k(\mathbf{x}, \mathbf{x}_1), ..., k(\mathbf{x}, \mathbf{x}_N)]^T$.

ϕ does not appear explicitly anymore!

Optional: Gaussian Processes





$$y(\mathbf{x}) = \mathbf{k}(\mathbf{x})(\mathbf{K} + \lambda\mathbf{I})^{-1} \begin{bmatrix} \mathbf{t}_1^T \\ ... \\ \mathbf{t}_N^T \end{bmatrix} ,$$

$$\mathbf{K}_{n,m} = k(\mathbf{x}_n, \mathbf{x}_m) ,$$

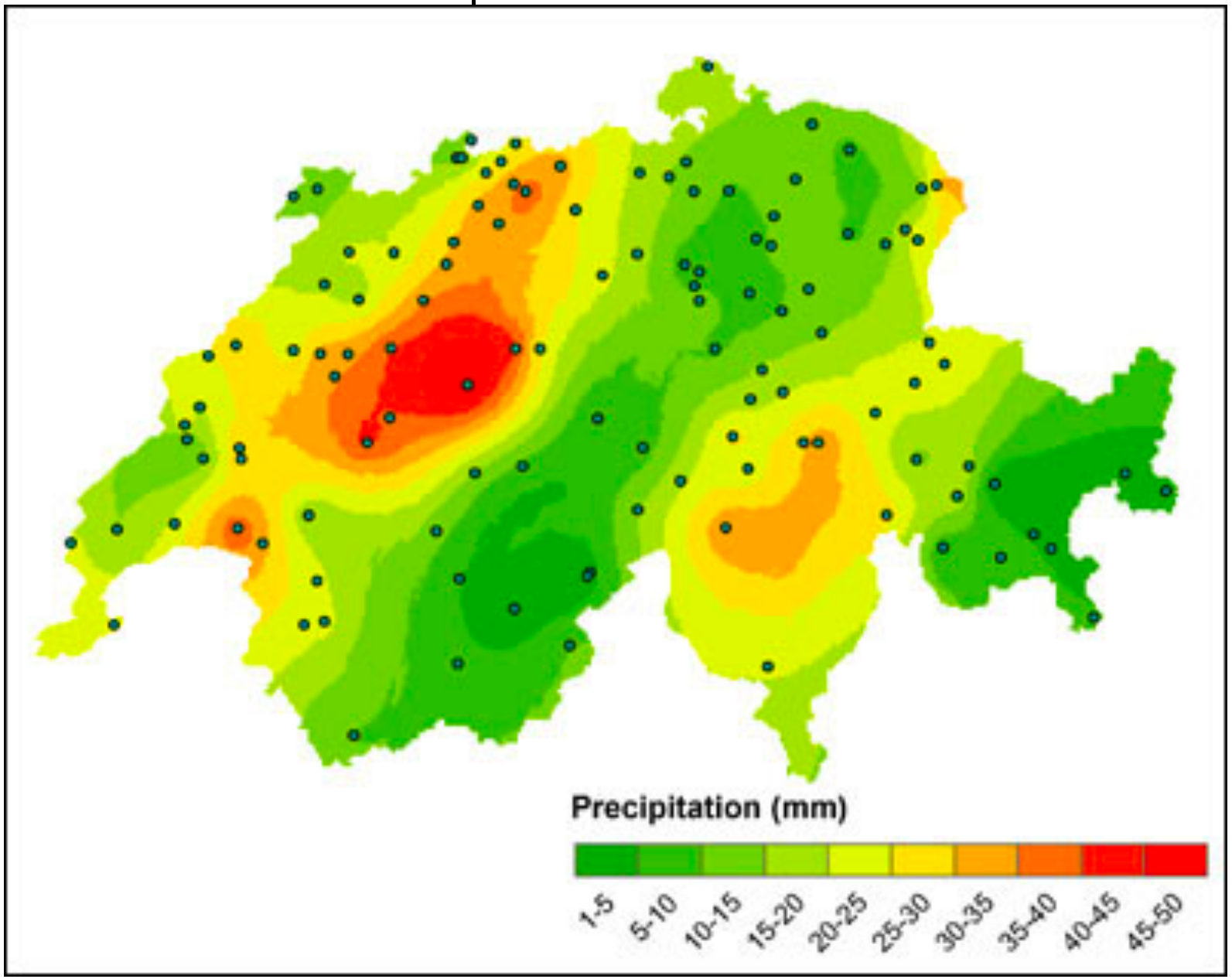
$$\mathbf{k}(\mathbf{x}) = [k(\mathbf{x}, \mathbf{x}_1), ..., k(\mathbf{x}, \mathbf{x}_N)]^T ,$$

$$k(\mathbf{x}, \mathbf{x}') = \theta_0(\exp(-(\frac{\theta_1}{2}||\mathbf{x} - \mathbf{x}'||^2) + \theta_2 + \theta_3 \mathbf{x}^T \mathbf{x}') .$$

$\Theta = [\theta_0, \theta_1, \theta_2, \theta_3]$ is the vector of hyper-parameters.

Application: Rainfall in Switzerland

The circles represent actual measurements



This is how the rainfall map was generated.