Machine Learning: a Basic Toolkit

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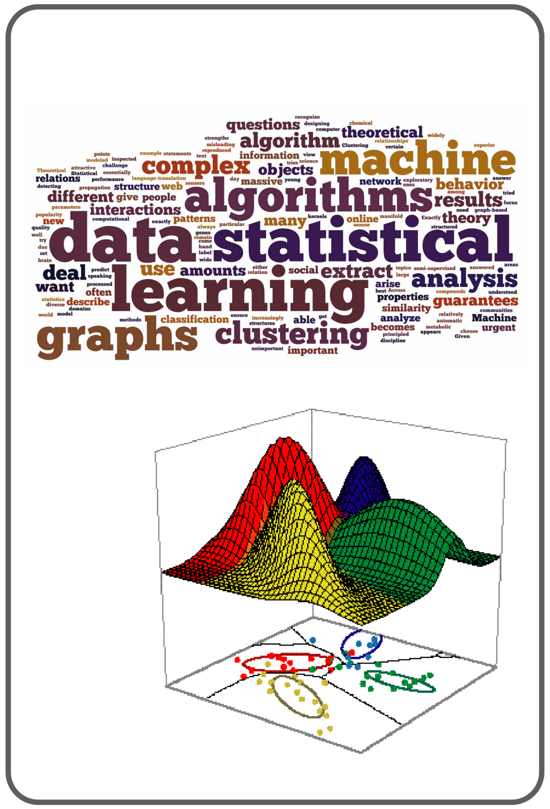
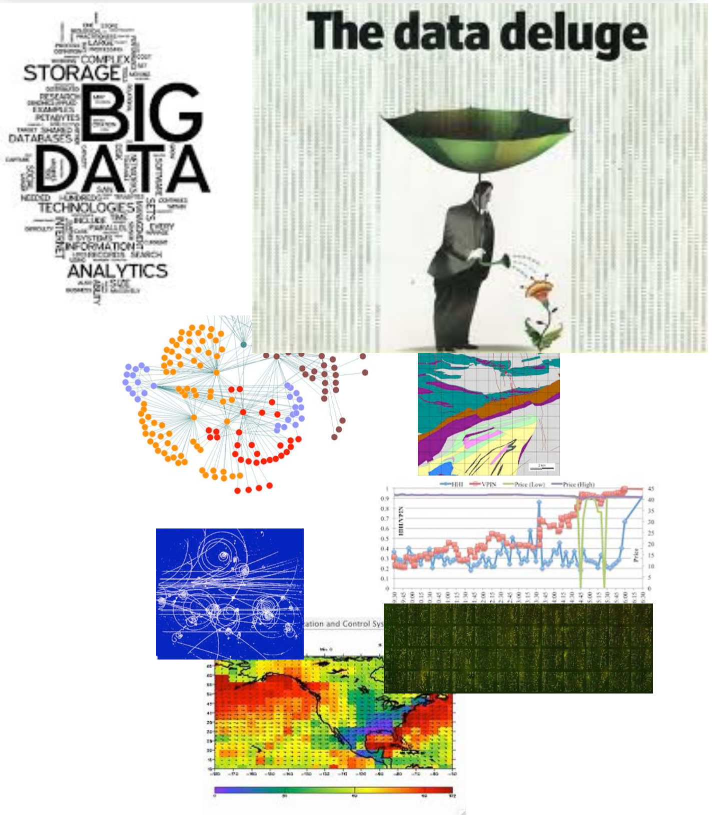
Machine Learning

Intelligent Systems

Data Science





ML Desert Island Compilation

An introduction to ***essential*** Machine Learning:
- Concepts
- Algorithms

PART I

- Local methods
- **Bias-Variance** and Cross Validation

PART II

- **Regularization** I: Linear Least Squares
- Regularization II: Kernel Least Squares

Morning

PART III

- **Variable Selection**: OMP
- Dimensionality Reduction: PCA

PART IV

- Matlab practical session

Afternoon

PART I

- Local methods
- Bias-Variance and Cross Validation

GOAL: Investigate the trade-off between stability and fitting starting from simple machine learning approaches

The goal of supervised learning is to find an underlying input-output relation

$$f(x_{\mathrm{new}}) \sim y,$$

given data.

The data, called *training set*, is a set of n input-output pairs,

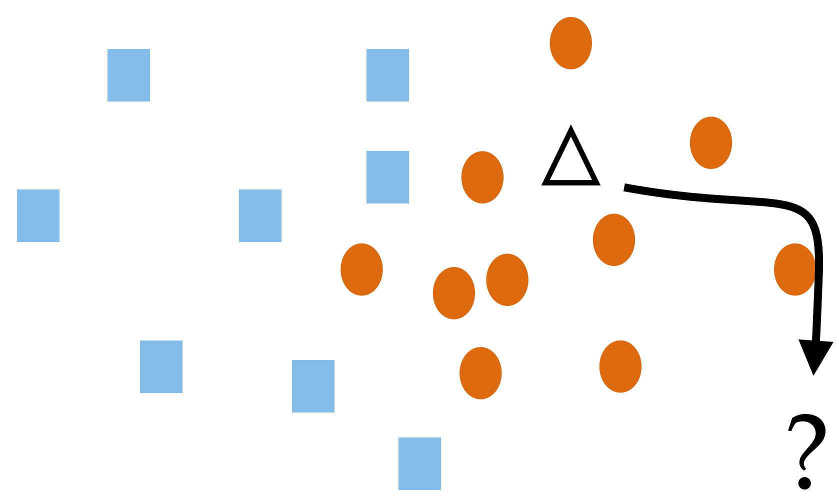
$$S = \{(x_1, y_1), \ldots, (x_n, y_n)\}.$$

170	238	85	255	221	0
68	136	17	170	119	68
221	0	238	136	0	255
119	255	85	170	136	238
238	17	221	68	119	255
85	170	119	221	17	136

$+1$

$$X_n = \begin{pmatrix} x_1^1 & \dots & \dots & \dots & x_1^p \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_n^1 & \dots & \dots & \dots & x_n^p \end{pmatrix} \qquad Y_n = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

-1



Local Methods: Nearby points have similar labels

Nearest Neighbor

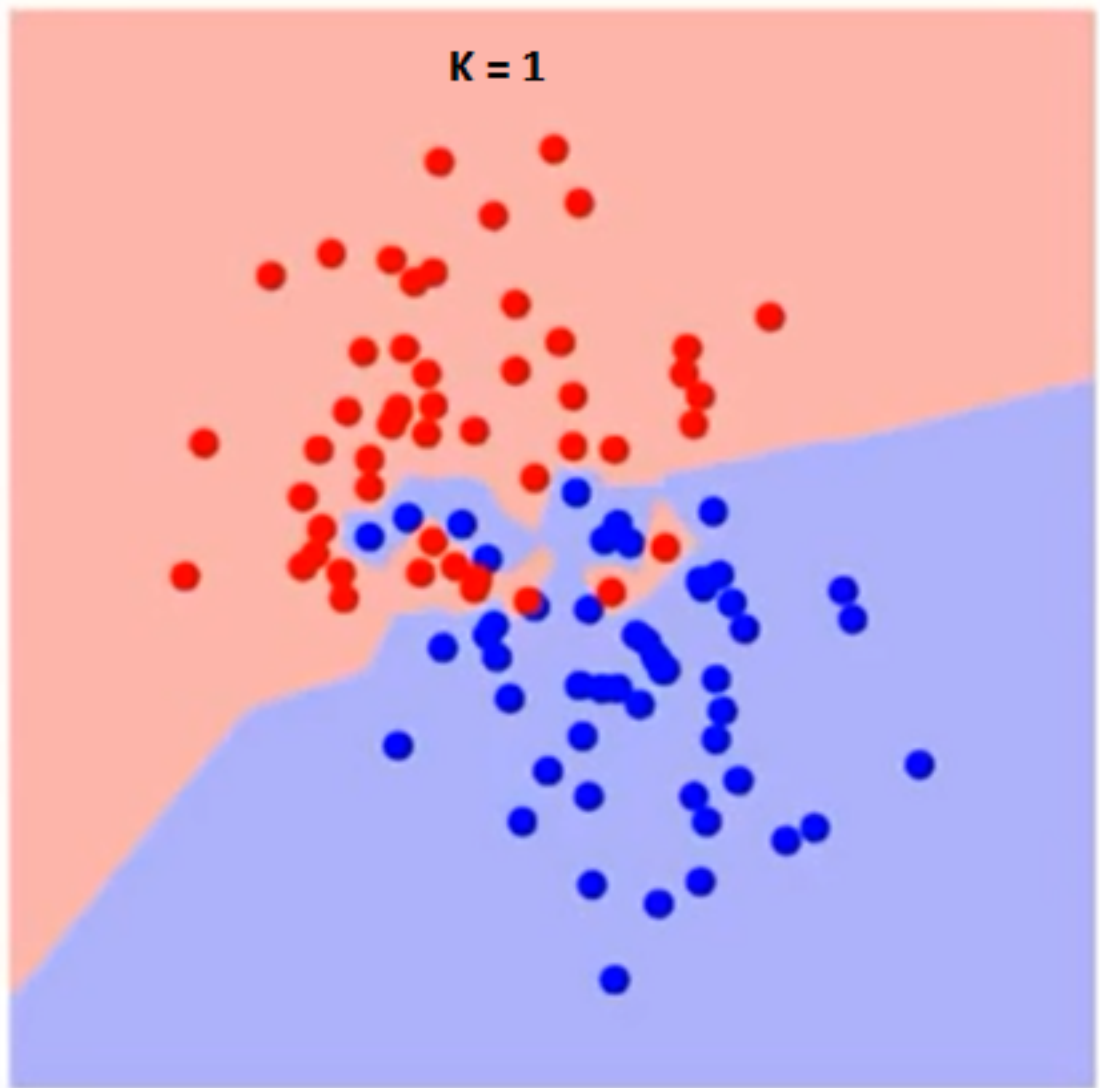
Given an input $\bar{x}$, let

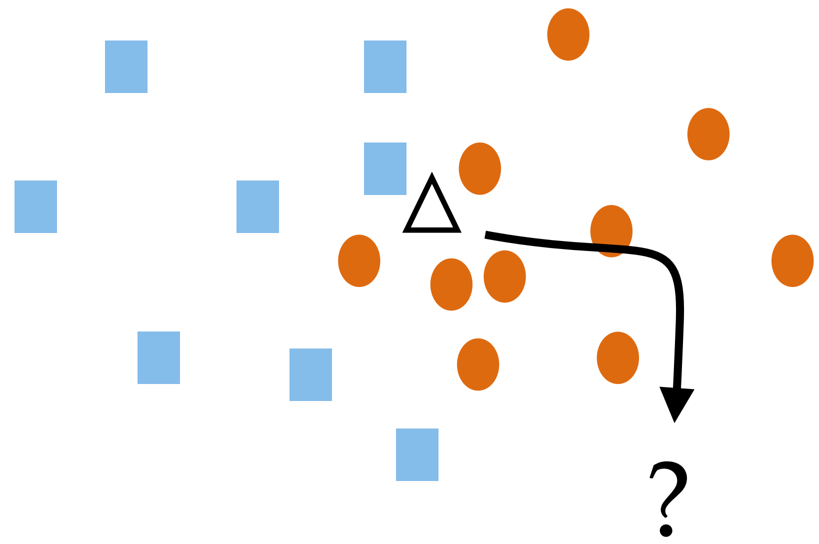
$$i' = \arg\min_{i=1,\ldots,n} \|\bar{x} - x_i\|^2$$

and define the nearest neighbor (NN) estimator as

$$\hat{f}(\bar{x}) = y_{i'}.$$

How does it work?


K = 1



K-Nearest Neighbors

Consider

$$d_{\bar{x}} = (\|\bar{x} - x_i\|^2)_{i=1}^n$$

the array of distances of a new point $\bar{x}$ to the input points in the training set. Let

$$s_{\bar{x}}$$

be the above array sorted in increasing order and

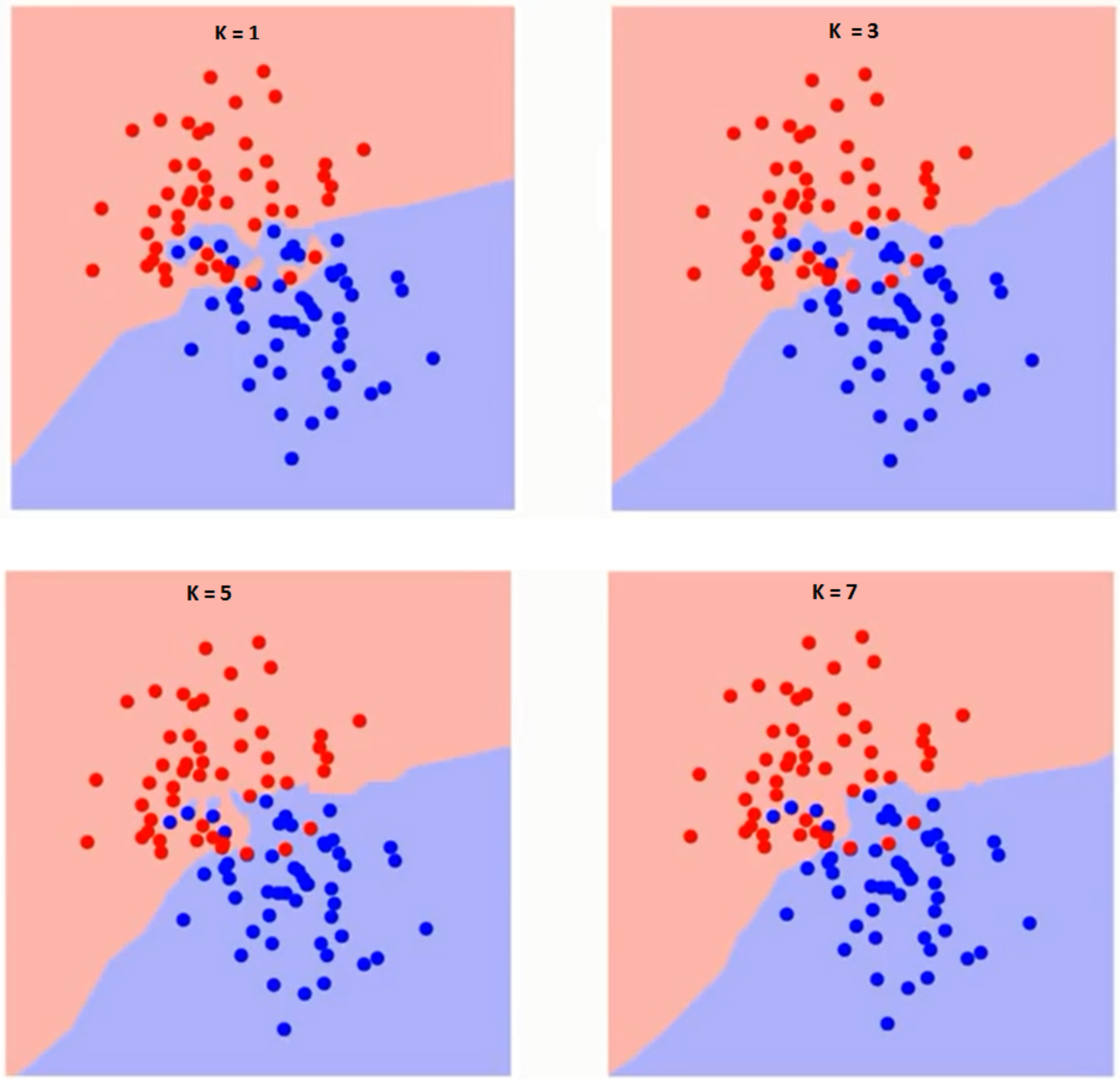
$$I_{\bar{x}}$$

the corresponding vector of indices, and

$$K_{\bar{x}} = \{I_{\bar{x}}^1, \ldots, I_{\bar{x}}^K\}$$

be the array of the first K entries of $I_{\bar{x}}$. The K-nearest neighbor estimator (KNN) is defined as,

$$\hat{f}(\bar{x}) = \sum_{i' \in K_{\bar{x}}} y_{i'},$$


K = 1
K = 3
K = 5
K = 7

Remarks:

Extension I: closer points should count more

$$\hat{f}(\bar{x}) = \frac{\sum_{i=1}^{n} y_i k(\bar{x}, x_i)}{\sum_{i=1}^{n} k(\bar{x}, x_i)}, \qquad \text{Gaussian} \quad k(x', x) = e^{-\|x-x'\|^2/2\sigma^2}.$$

Parzen Windows

Extension II: other metric/similarities

$$X = \{0,1\}^D \qquad d_H(x, \bar{x}) = \frac{1}{D}\sum_{j=1}^{D} \mathbf{1}_{[x^j \neq \bar{x}^j]}$$

There is one parameter controlling fit/stability

How do we choose it?

Is there an optimal value?

Can we compute it?

Is there an optimal value?

Ideally we would like to choose K that minimizes the expected error

$$\mathbf{E}_S \mathbf{E}_{x,y} (y - \hat{f}_K(x))^2.$$

Next: Characterize corresponding minimization problem to uncover one of **the most fundamental aspect of machine learning**.

For the sake of simplicity we consider a regression model

$$y_i = f_*(x_i) + \delta_i, \quad \mathbf{E}\delta_I = 0, \mathbf{E}\delta_i^2 = \sigma^2 \quad i = 1, \dots, n$$

$$\mathbf{E}_S \mathbf{E}_{x,y}(y - \hat{f}_K(x))^2 = \mathbf{E}_x \underbrace{\mathbf{E}_S \mathbf{E}_{y|x}(y - \hat{f}_K(x))^2}_{\varepsilon(K)}.$$

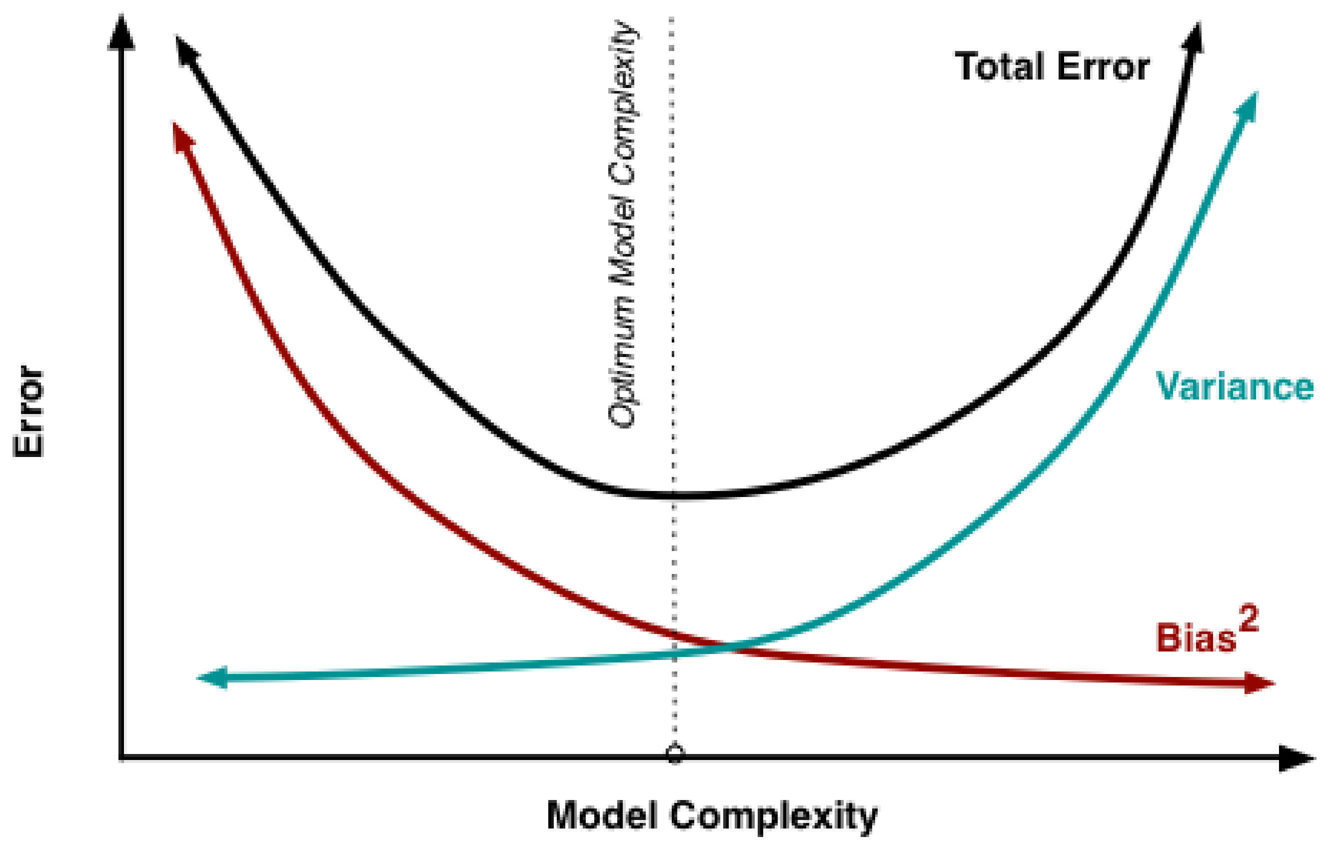
$$\mathbf{E}_{y|x} \hat{f}_K(x) = \frac{1}{K} \sum_{\ell \in K_x} f_*(x_\ell).$$

$$\mathbf{E}_S \mathbf{E}_{y|x}(f_*(x) - \hat{f}_K(x))^2 = \underbrace{(f_*(x) - \mathbf{E}_S \mathbf{E}_{y|x} \hat{f}_K(x))^2}_{Bias} + \underbrace{\mathbf{E}_S \mathbf{E}_{y|x}(\mathbf{E}_{y|x} \hat{f}_K(x) - \hat{f}_K(x))^2}_{Variance}$$

$$(f_*(x) - \frac{1}{K} \sum_{\ell \in K_x} f_*(x_\ell))^2 \qquad \qquad \frac{\sigma^2}{K}$$

Bias Variance Trade-Off

$$\Big(f_*(x) - \frac{1}{K}\sum_{\ell \in K_x} f_*(x_\ell)\Big)^2 + \frac{\sigma^2}{K}$$



Is there an optimal value? YES! **Can we compute it?**

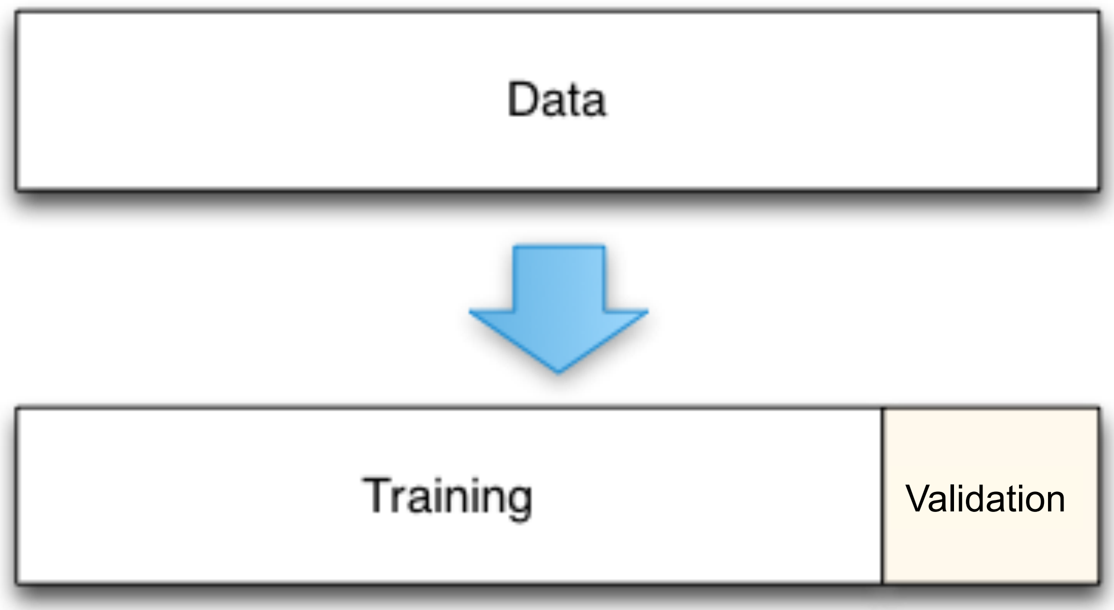
Not quite…

$$\left(f_*(x) - \frac{1}{K}\sum_{\ell \in K_x} f_*(x_\ell)\right)^2 + \frac{\sigma^2}{K}$$

…enter Cross Validation

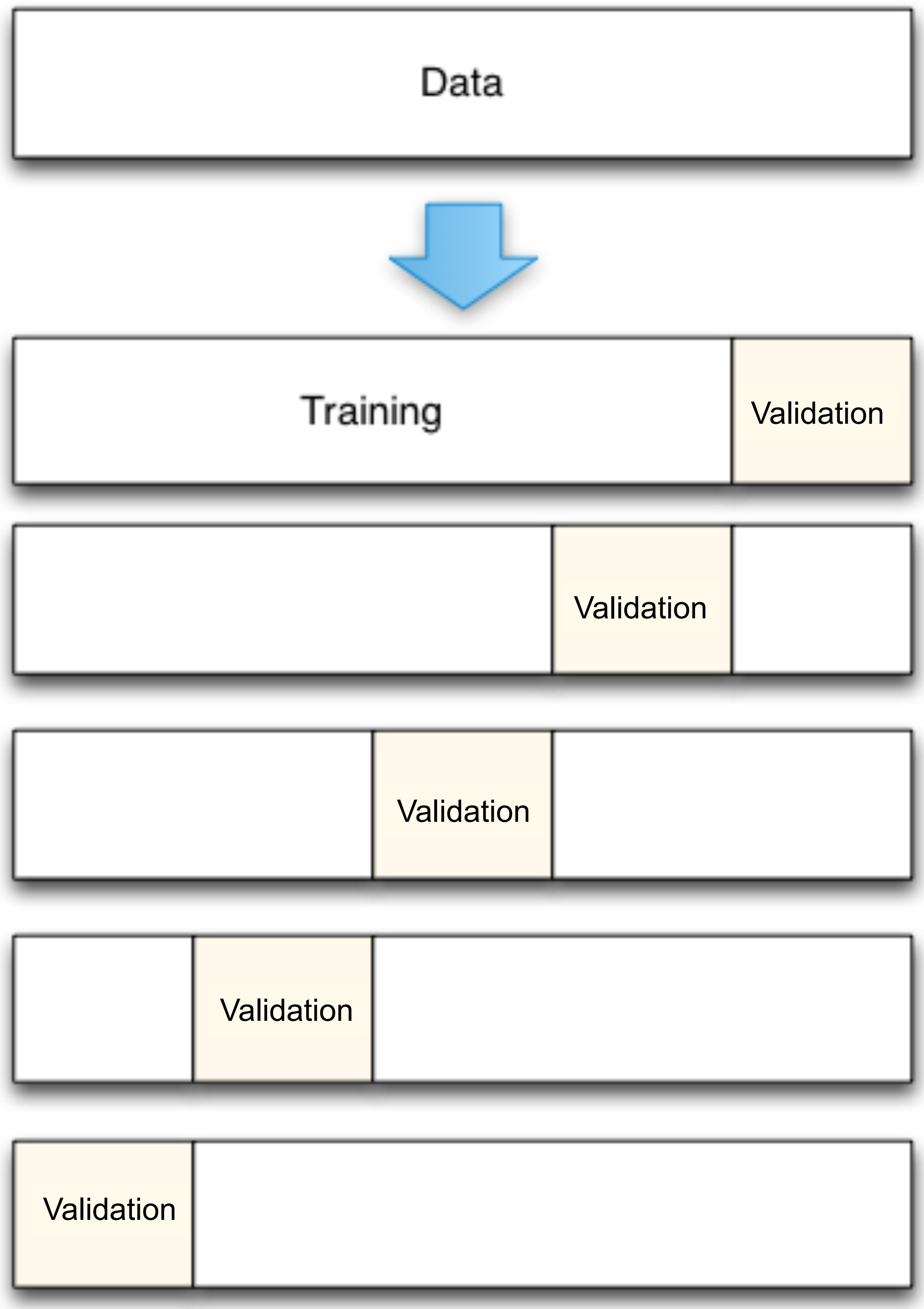
Split data: train on some, tune on some other

Cross Validation Flavors



Hold-Out

Cross Validation Flavors



V-Fold, (V=n is Leave-One-Out)

End of PART I

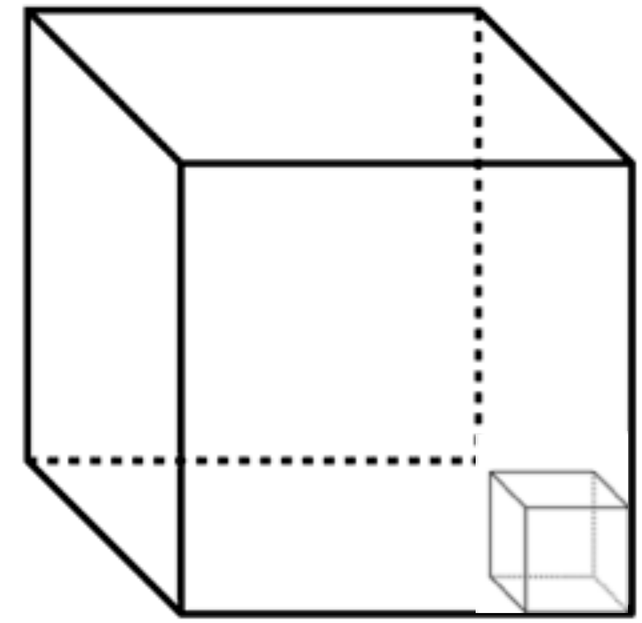
- Local methods
- Bias-Variance and Cross Validation

Stability - Overfitting - Bias/Variance - Cross-Validation

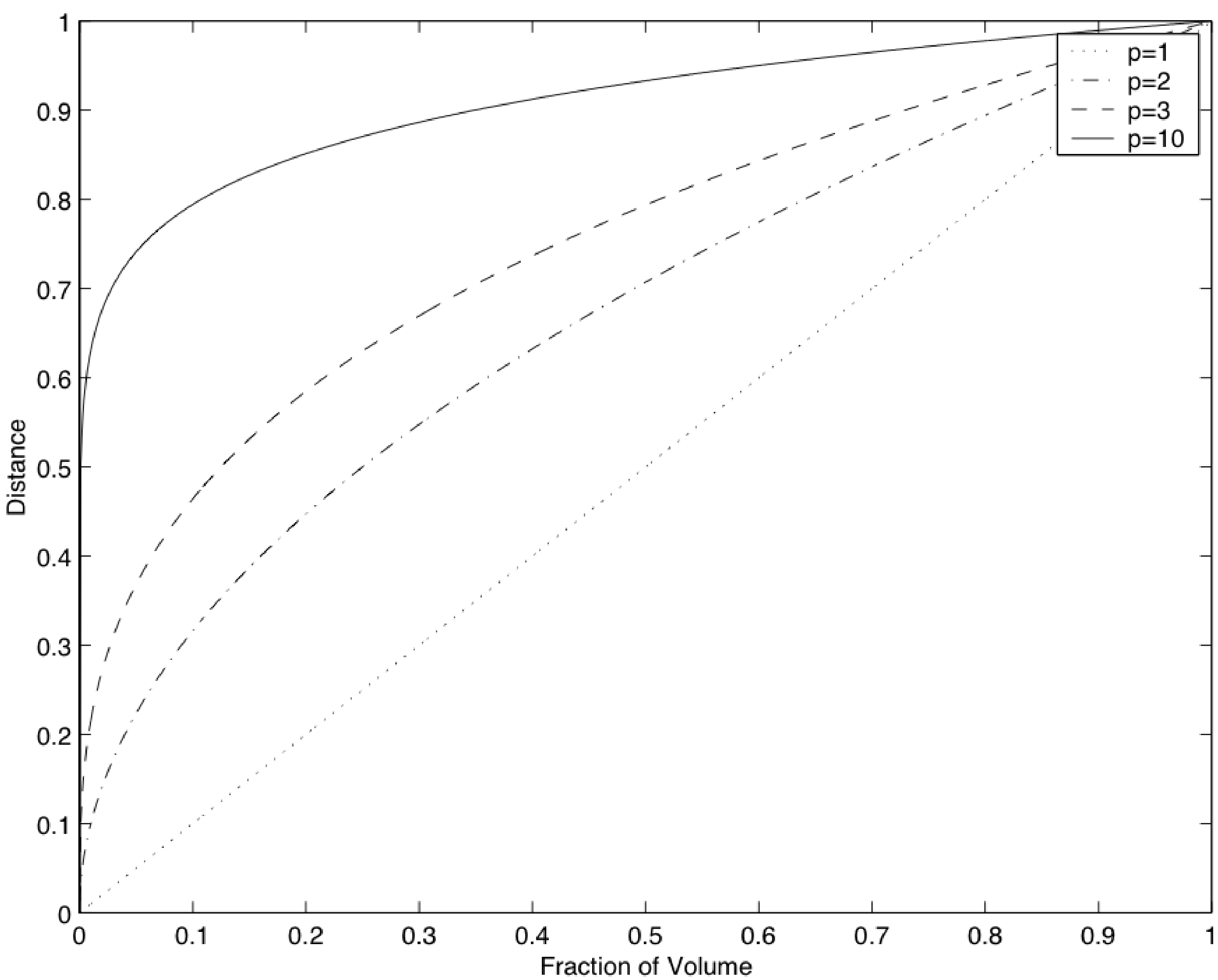
End of the Story?

<u>High Dimensions</u> and Neighborhood

tell me the length of the edge of a cube containing 1% of the volume of a cube with edge 1



Cubes and Dth-roots



Curse of dimensionality!

PART II

- Regularization I: Linear Least Squares
- Regularization II: Kernel Least Squares

GOAL: Introduce the basic (global) regularization methods with parametric and non parametric models

Going Global + Impose Smoothness

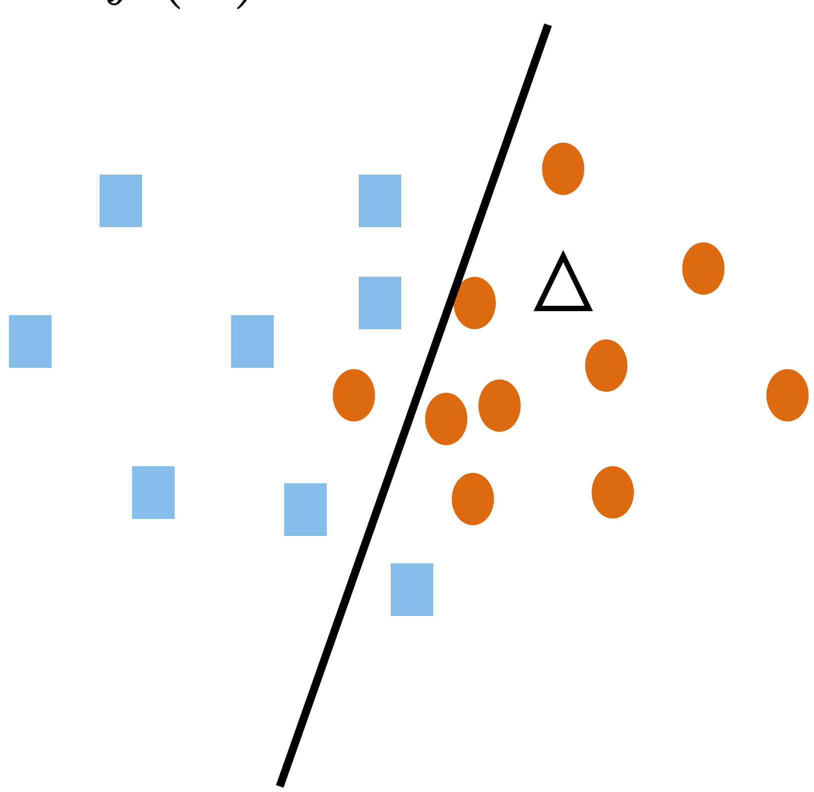
Of all the principles which can be proposed for that purpose, I think there is none more general, more exact, and more easy of application, that of which we made use in the preceding researches, and which consists of rendering the ***sum of squares of the errors*** *a minimum.*

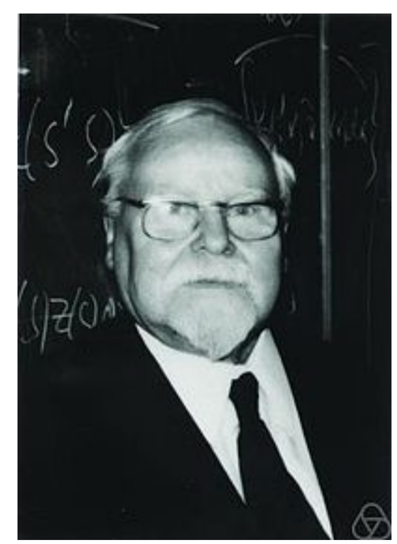
(Legendre 1805)

We consider the following algorithm

$$\min_{w \in \mathbb{R}^D} \frac{1}{n} \sum_{i=1}^{n} (y_i - w^\top x_i)^2 + \lambda w^\top w, \quad \lambda \geq 0$$

$$f(x) = w^T x = 0$$





?

?

Tikhonov '62 Phillips '62 Hoerl et al. '62

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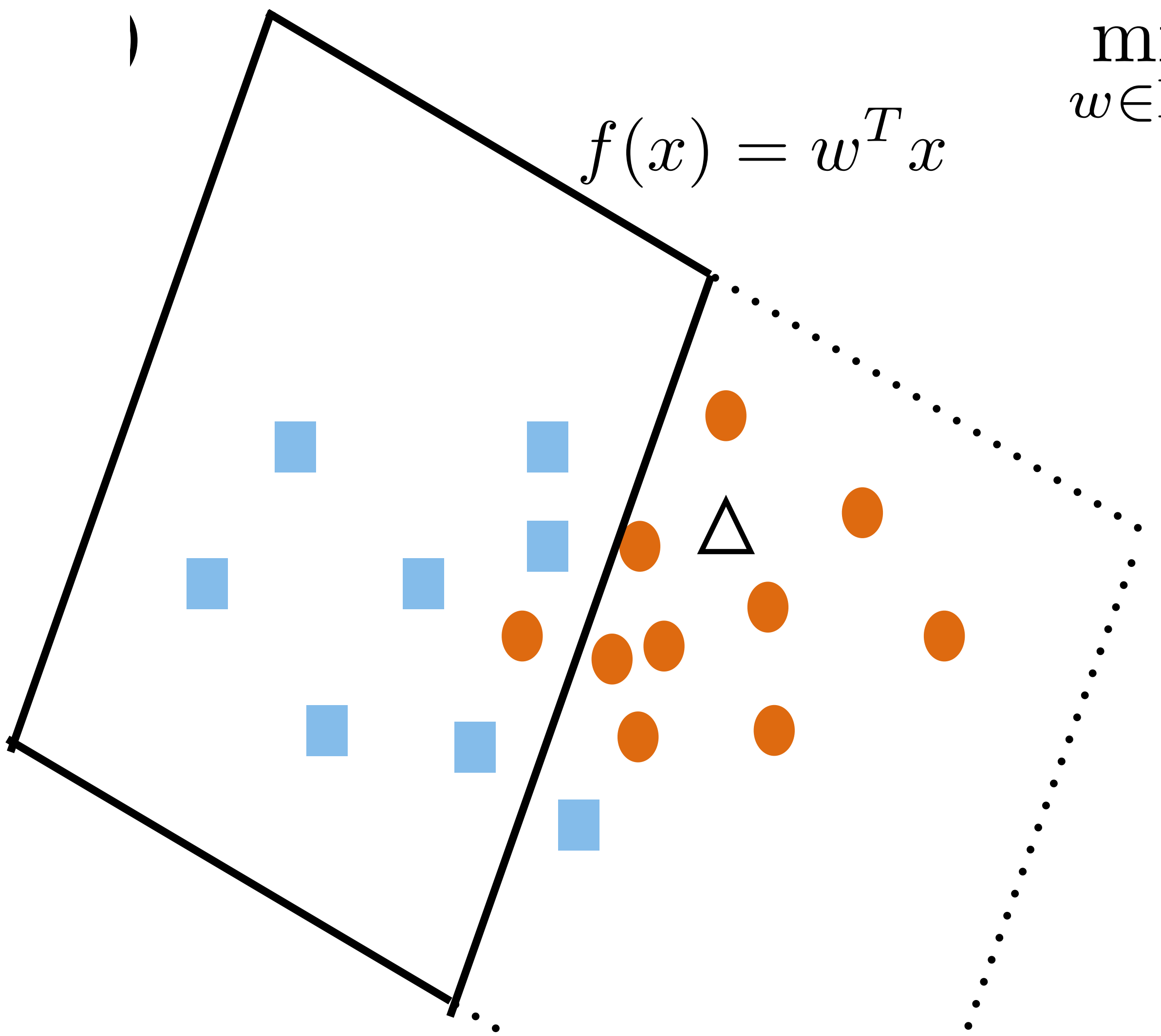
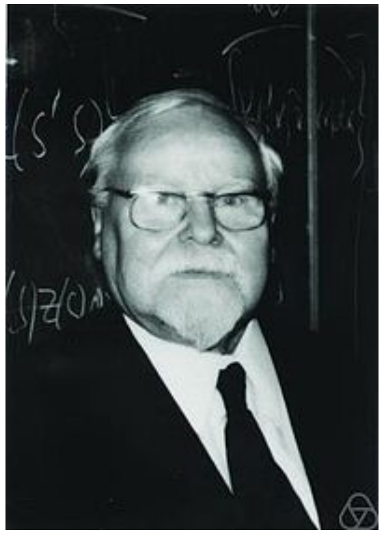
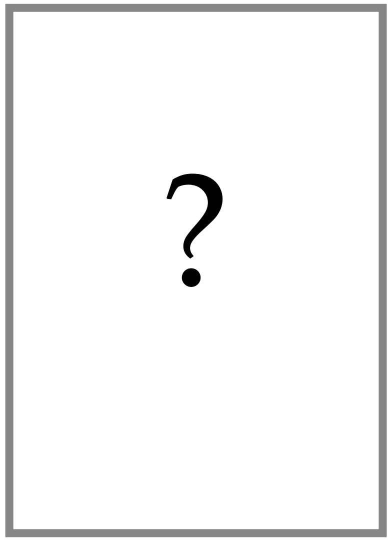
$$\min_{w \in \mathbb{R}^D} \frac{1}{n} \sum_{i=1}^{n} (y_i - w^\top x_i)^2 + \lambda w^\top w, \quad \lambda \geq 0$$

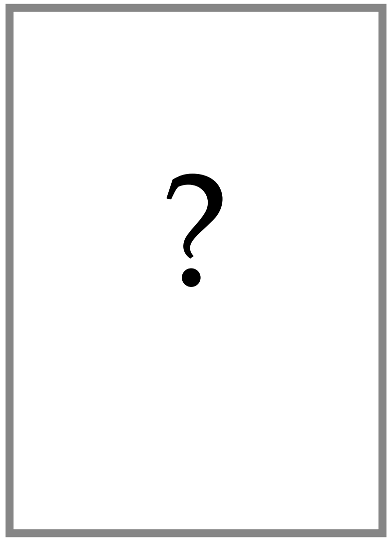




Tikhonov '62



Phillips '62



Hoerl et al. '62

$$\min_{w \in \mathbb{R}^D} \frac{1}{n} \sum_{i=1}^{n} (y_i - w^\top x_i)^2 + \lambda w^\top w, \quad \lambda \geq 0$$

Computations? **Statistics?**

$$\min_{w\in\mathbb{R}^D} \frac{1}{n}\sum_{i=1}^{n}(y_i - w^\top x_i)^2 + \lambda w^\top w, \quad \lambda \geq 0$$

Computations?

Notation $\quad \frac{1}{n}\sum_{i=1}^{n}(y_i - w^T x_i))^2 = \frac{1}{n}\|Y_n - X_n w\|^2$

$$-\frac{2}{n}X_n^T(Y_n - X_n w), \quad \text{and,} \quad 2w$$

Setting gradients…

…to zero $\quad (X_n^T X_n + \lambda n I)w = X_n^T Y_n$

OK, but what is this doing?

Interlude: Linear Systems

$$Ma = b,$$

- If M is a diagonal $M = diag(\sigma_1, \dots, \sigma_D)$ where $\sigma_i \in (0, \infty)$ for all $i = 1, \dots, D$, then
$$M^{-1} = diag(1/\sigma_1, \dots, 1/\sigma_D), \quad (M + \lambda I)^{-1} = diag(1/(\sigma_1 + \lambda), \dots, 1/(\sigma_D + \lambda))$$

- If M is symmetric and positive definite, then considering the eigendecomposition
$$M = V\Sigma V^\top, \quad \Sigma = diag(\sigma_1, \dots, \sigma_D),\ VV^\top = I,$$
then
$$M^{-1} = V\Sigma^{-1}V^\top, \quad \Sigma^{-1} = diag(1/\sigma_1, \dots, 1/\sigma_D),$$
and
$$(M + \lambda I)^{-1} = V\Sigma_\lambda V^\top, \quad \Sigma_\lambda = diag(1/(\sigma_1 + \lambda), \dots, 1/(\sigma_D + \lambda))$$

$$\min_{w \in \mathbb{R}^D} \frac{1}{n} \sum_{i=1}^{n} (y_i - w^\top x_i)^2 + \lambda w^\top w, \quad \lambda \geq 0$$

Statistics?

$$(X_n^T X_n + \lambda n I) w = X_n^T Y_n$$

another story that shall be told another time

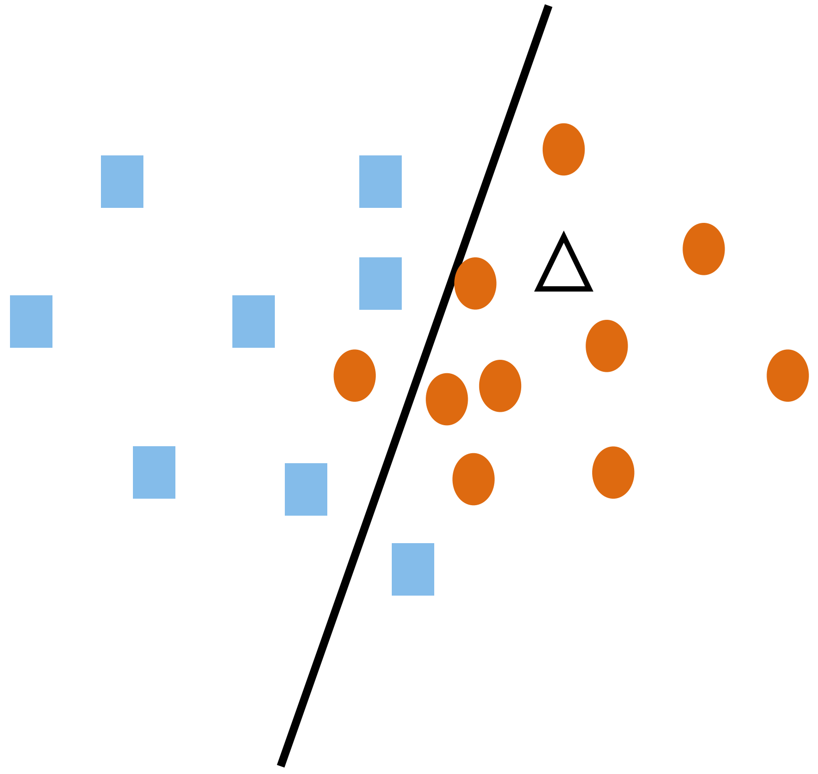
(Stein ’56, James and Stein ’61)

$$\min_{w \in \mathbb{R}^D} \frac{1}{n} \sum_{i=1}^{n} (y_i - w^T x_i))^2 + \lambda w^T w, \quad \lambda \geq 0.$$

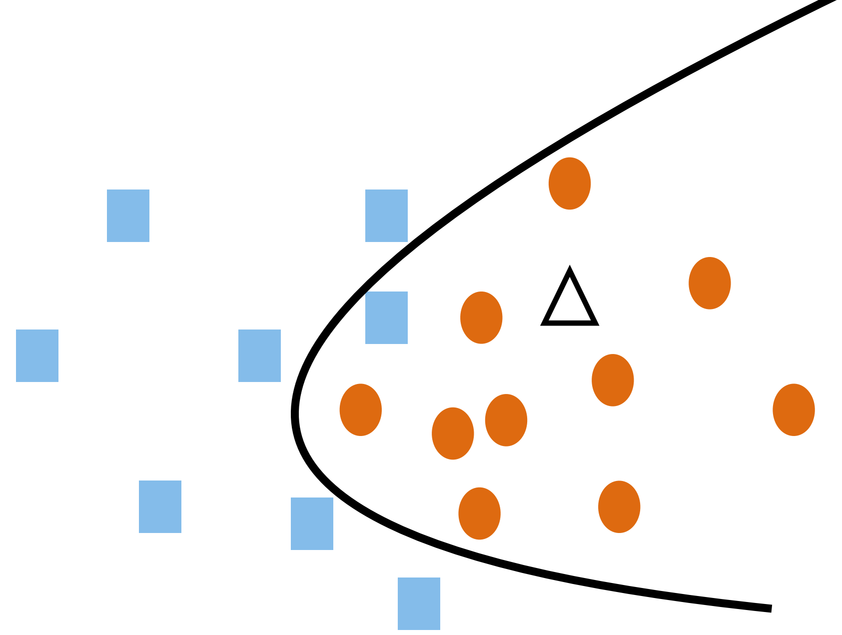
$$f_w(x) = w^T x = \sum_{i=1}^{v} w^j x^j$$

$$\sum_{j=1}^{D} (w^j)^2$$

Shrinkage - Stein Effect- Admissible Estimator



Why a linear decision rule?



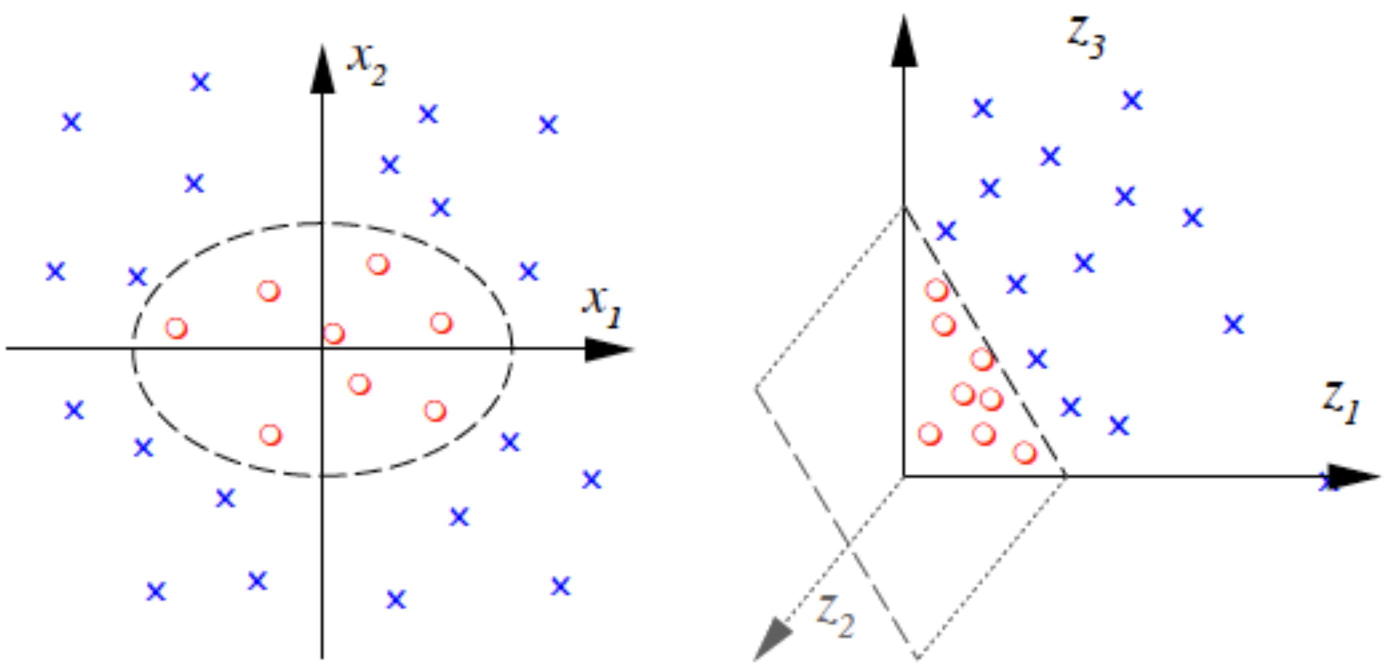
Dictionaries

$$x \mapsto \tilde{x} = (\phi_1(x), \ldots, \phi_p(x)) \in \mathbb{R}^p$$

$$f(x) = w^T \tilde{x} = \sum_{j=1}^{p} \phi_j(x) w^j$$

$$\Phi : R^2 \to R^3$$

$$(x_1, x_2) \mapsto (z_1, z_2, z_3) := (x_1^2, \sqrt{2} x_1 x_2, x_2^2)$$



$$(X_n^T X_n + \lambda n I)w = X_n^T Y_n \qquad \mapsto \qquad (\tilde{X}_n^T \tilde{X}_n + \lambda n Y)w = \tilde{X}_n^T Y_n$$

What About Computational Complexity?

Complexity Vademecum

M n by p matrix and v, v' p dimensional vectors

- $v^T v' \mapsto O(p)$
- $Mv' \mapsto O(np)$
- $MM^T \mapsto O(n^2 p)$
- $(MM^T)^{-1} \mapsto O(n^3)$

$$(X_n^T X_n + \lambda n I) w = X_n^T Y_n \qquad \mapsto \qquad (\tilde{X}_n^T \tilde{X}_n + \lambda n I) w = \tilde{X}_n^T Y_n$$

What About Computational Complexity?

$$O(p^3) + O(p^2 n)$$

What if *p* is much larger than *n*?

$$(X_n^T X_n + \lambda n I)^{-1} X_n^T = X_n^T (X_n X_n^T + \lambda n I)^{-1}$$

$$w = X_n^T \underbrace{(X_n X_n^T + \lambda n I)^{-1} Y_n}_{c} = \sum_{i=1}^{n} x_i^T c_i$$

$$(X_n^T X_n + \lambda n I)^{-1} X_n^T = X_n^T (X_n X_n^T + \lambda n I)^{-1}$$

$$w = X_n^T \underbrace{(X_n X_n^T + \lambda n I)^{-1} Y_n}_{c} = \sum_{i=1}^{n} x_i^T c_i$$

Computational Complexity: $O(p^3) + O(p^2 n)$

$O(n^3) + O(pn^2)$

$$(X_n^T X_n + \lambda n I)^{-1} X_n^T = X_n^T (X_n X_n^T + \lambda n I)^{-1}$$

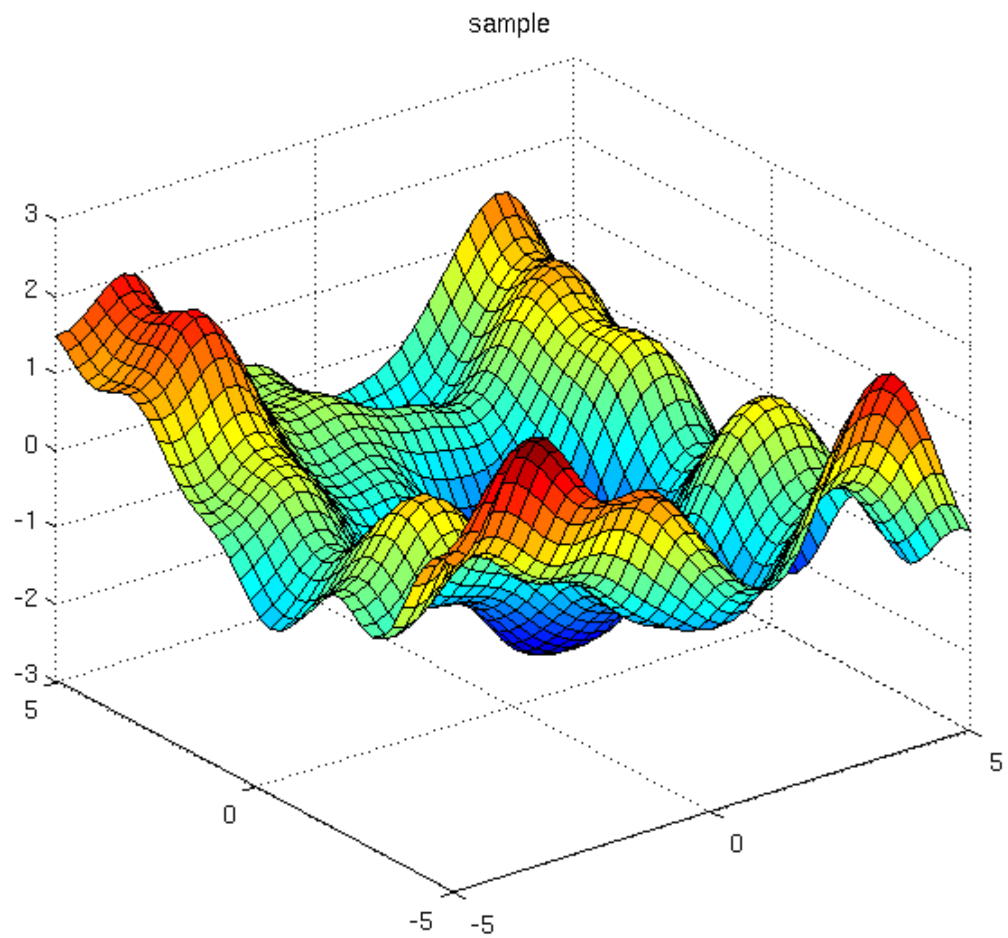
$$w = X_n^T \underbrace{(X_n X_n^T + \lambda n I)^{-1} Y_n}_{c} = \sum_{i=1}^{n} x_i^T c_i$$

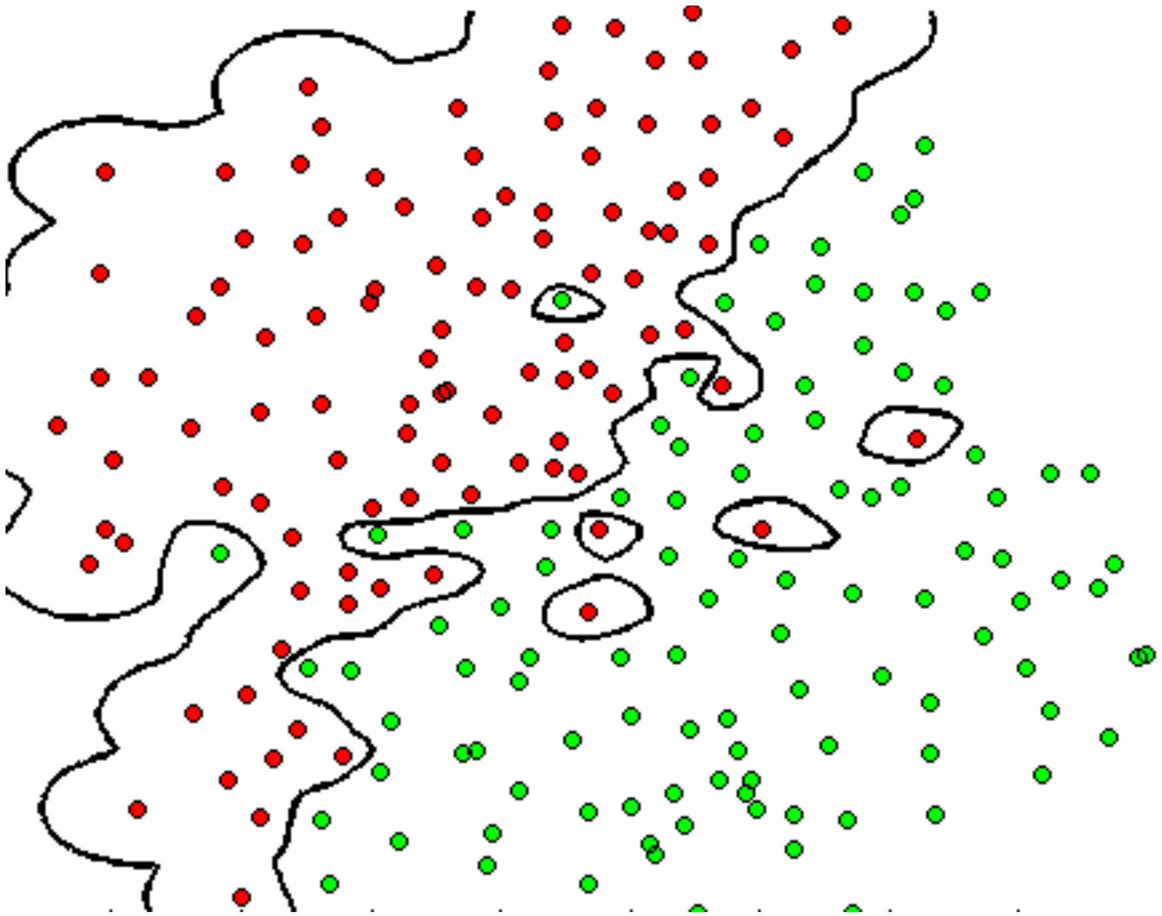
Kernels $$w = \sum_{j=1}^{n} x_i c_i \Rightarrow f(x) = x^T w = \sum_{j=1}^{n} \underbrace{x^T x_i}_{K(x, x_i)} c_i$$

$$(K_n + \lambda n I)^{-1} c = Y_n, \quad (K_n)_{i,j} = K(x_i, x_j)$$

- the linear kernel $K(x, x') = x^T x'$,
- the polynomial kernel $K(x, x') = (x^T x' + 1)^d$,
- the Gaussian kernel $K(x, x') = e^{-\frac{\|x - x'\|^2}{2\sigma^2}}$,

Learning with the Gaussian kernel





$$\hat{f}(x) = \sum_{i=1}^{n} K(x_i, x) c_i.$$

things I won't tell you about

- Reproducing Kernel Hilbert Spaces
- Gaussian Processes
- Integral Equations
- Sampling Theory / Inverse Problems

- Loss functions- SVM, Logistic…
- Multi - task, labels, outputs, classes

End of PART II

- Regularization I: Linear Least Squares
- Regularization II: Kernel Least Squares

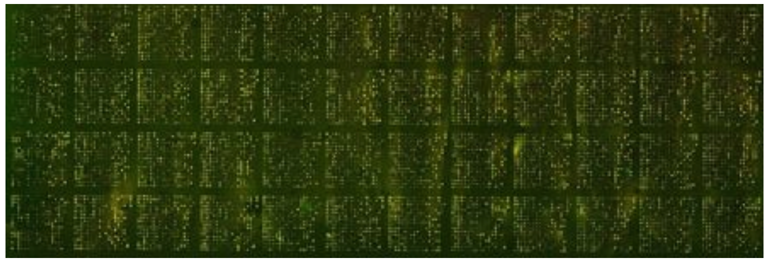
Regularized Least Squares - Dictionaries - Kernels

PART III

- **a) Variable Selection: OMP**
- b) Dimensionality Reduction: PCA

GOAL: To introduce methods that allow to learn *interpretable* models from data

n patients p gene expression measurements



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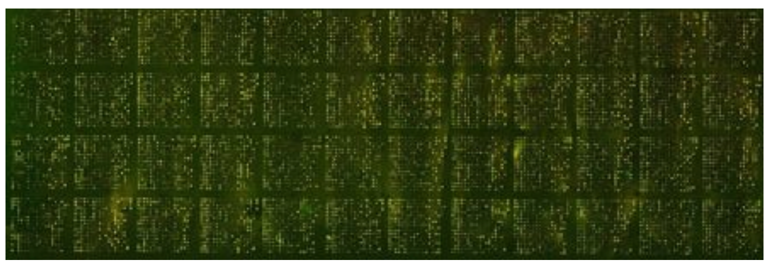

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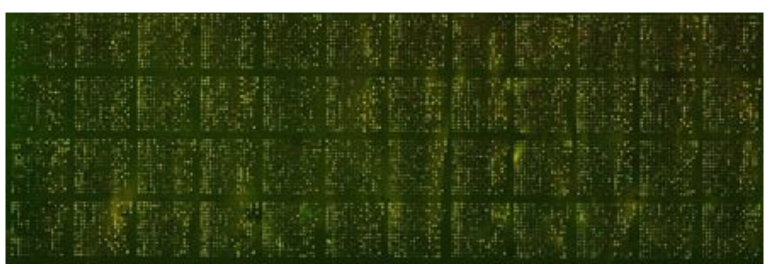

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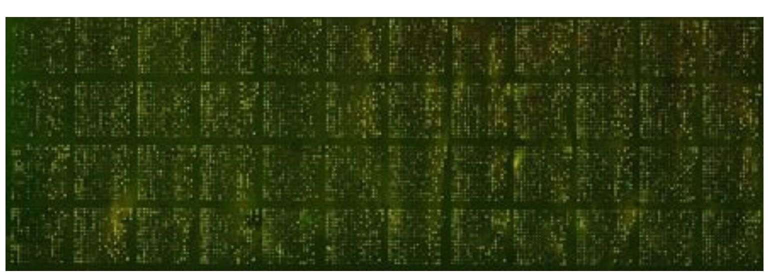


$$X_n = \begin{pmatrix} x_1^1 & \dots & \dots & \dots & x_1^p \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_n^1 & \dots & \dots & \dots & x_n^p \end{pmatrix}; Y_n = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

$$f_w(x) = w^T x = \sum_{j=1}^{D} x^j w^j$$

Which variables are important for prediction?

or

Torture the data until they confess

Sparsity: only some of the coefficients are non zero

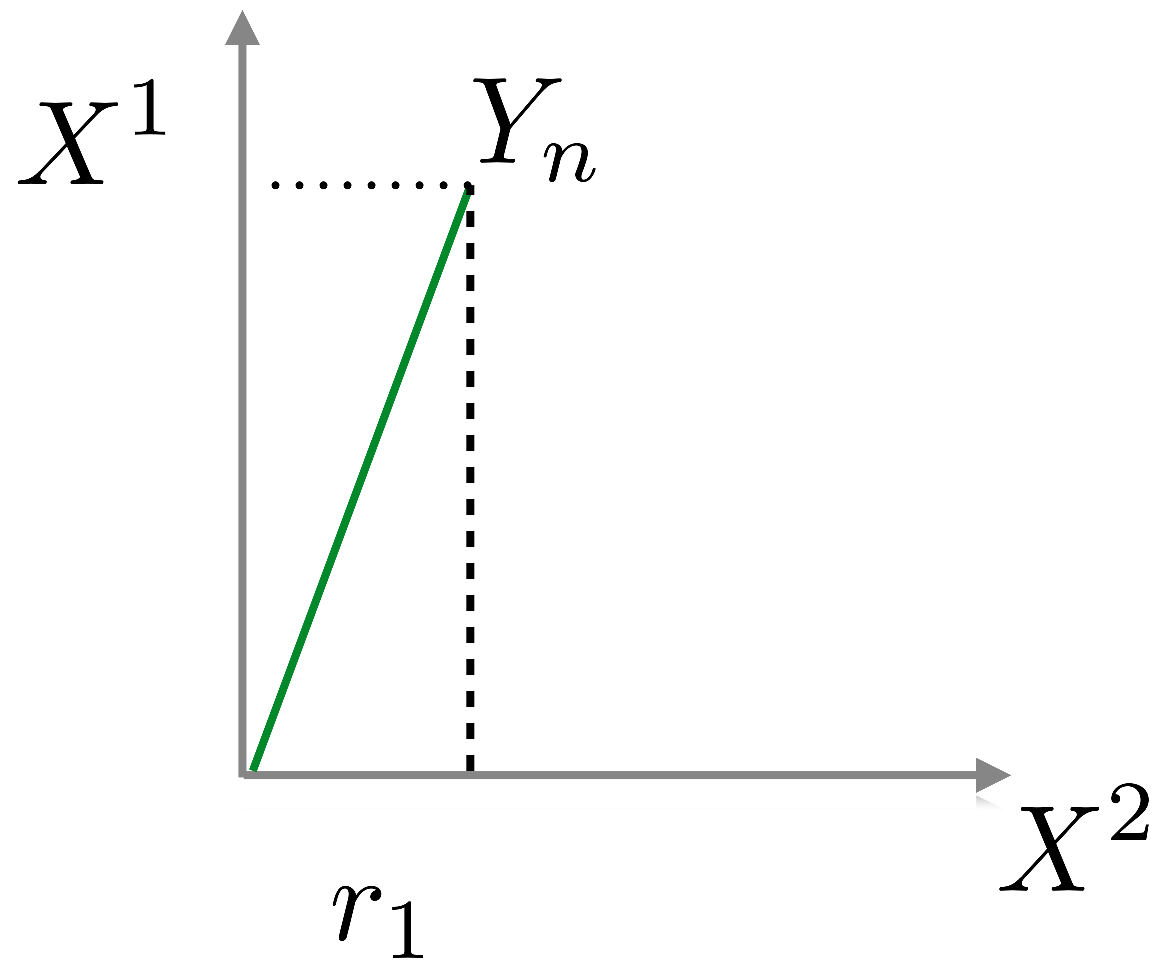
Brute Force Approach

check all individual variables, then all couple, triplets…..

$$\min_{w \in \mathbb{R}^D} \frac{1}{n} \sum_{i=1}^{n} (y_i - f_w(x_i))^2 + \lambda \|w\|_0,$$

$$\|w\|_0 = |\{j \mid w^j \neq 0\}|$$

Greedy approaches/Matching Pursuit



(1) initialize the residual, the coefficient vector, and the index set,
(2) find the variable most correlated with the residual,
(3) update the index set to include the index of such variable,
(4) update/compute coefficient vector,
(5) update residual.

Matching Pursuit

(Mallat Zhang '93)

$$r_0 = Y_n, \quad , w_0 = 0, \quad I_0 = \emptyset.$$

for $i = 1, \dots, T-1$

$$k = \arg \max_{j=1,\dots,D} a_j, \quad a_j = \frac{(r_{i-1}^T X^j)^2}{\|X^j\|^2}, \circledast$$

$$I_i = I_{i-1} \cup \{k\}$$

$$w_i = w_{i-1} + w_k, \quad w_k = v_k e_k$$

$$r_i = r_{i-1} - X w^k.$$

end

$$\circledast \; v^j = \frac{r_{i-1}^T X^j}{\|X^j\|^2} = \arg\min_{v \in \mathbb{R}} \|r_{i-1} - X^j v\|^2, \quad \|r_{i-1} - X^j v^j\|^2 = \|r_{i-1}\|^2 - a_j$$

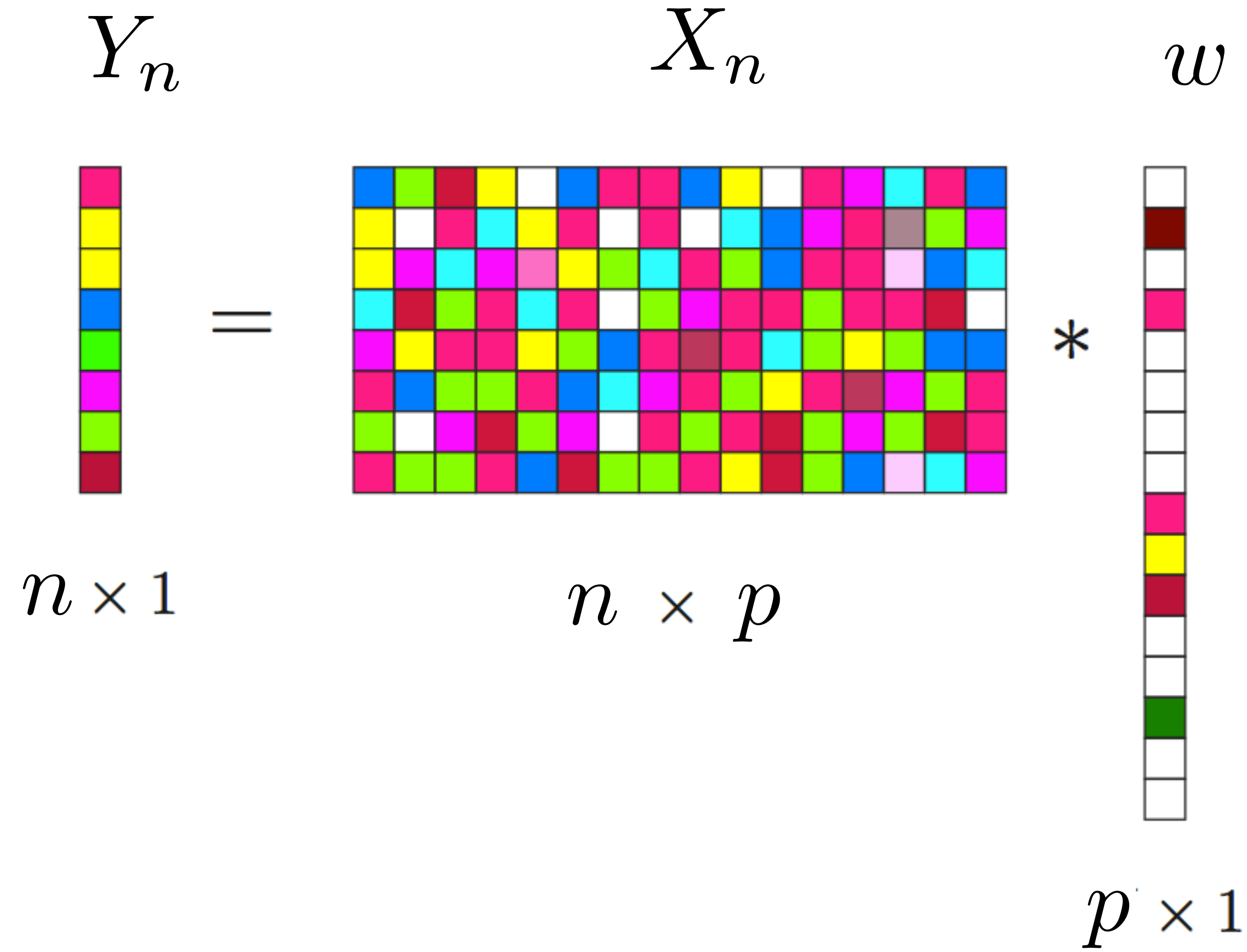
Basis Pursuit/Lasso

(Chen Donoho Saunders ~95, Tibshirani ‘96)

$$\|w\|_1 = \sum_{j=1}^{D} |w^j|$$

$$\min_{w \in \mathbb{R}^D} \frac{1}{n} \sum_{i=1}^{n} (y_i - f_w(x_i))^2 + \lambda \cancel{\|w\|_0},$$

Problem is now **convex** and can be solved using convex optimization, in particular so called *proximal methods*



things I won't tell you about

- Solving underdetermined systems
- Sampling theory
- Compressed Sensing
- Structured Sparsity
- From vector to matrices- from sparsity to low rank

End of PART III a)

- **a) Variable Selection: OMP**
- b) Dimensionality Reduction: PCA

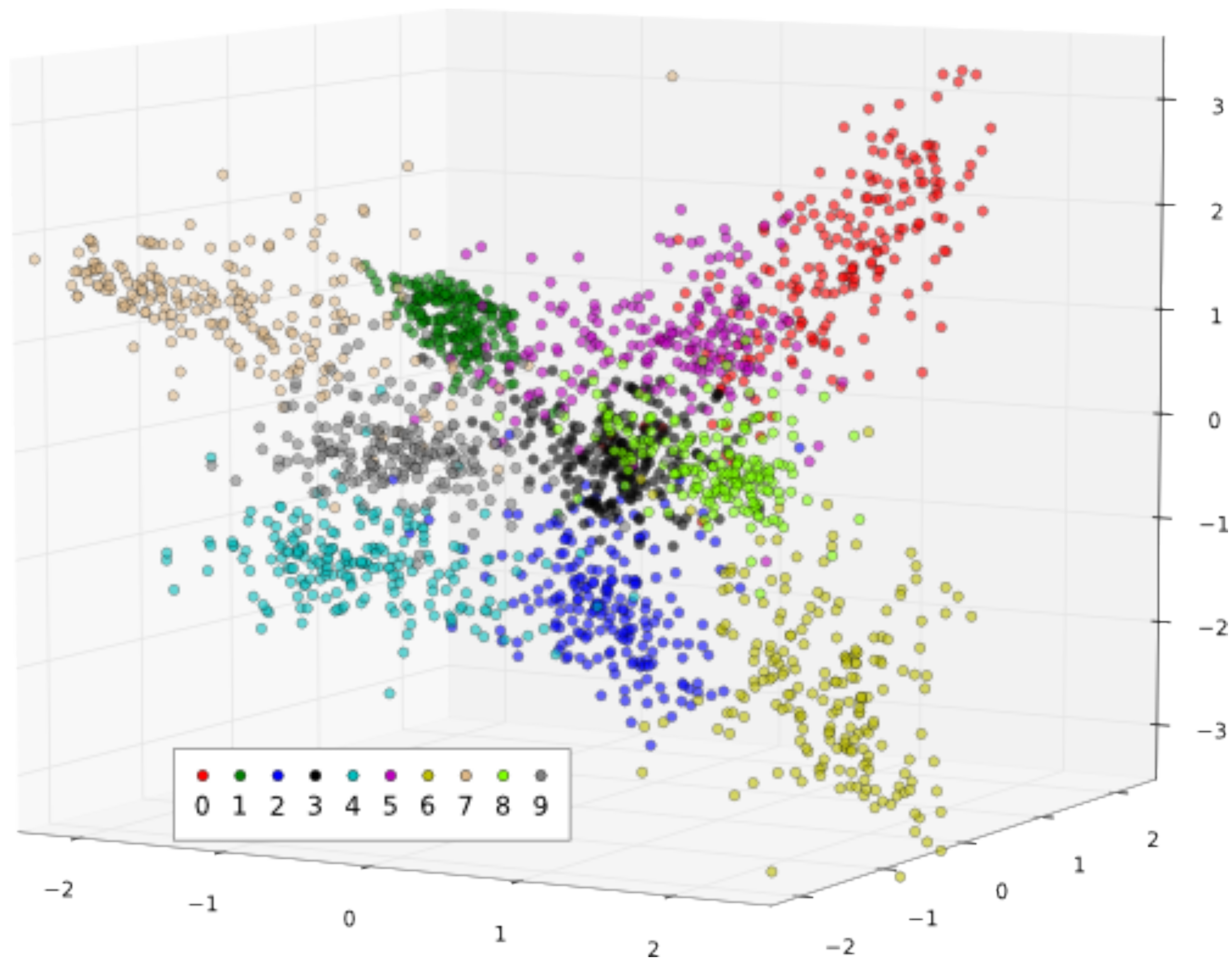
Interpretability - Sparsity - Greedy & Convex Relaxation Approaches

PART III b)

- a) Variable Selection: OMP
- **b) Dimensionality Reduction: PCA**

GOAL: To introduce methods that allow to reduce data dimensionality in absence of labels, namely **unsupervised learning**

Dimensionality Reduction for Data Visualization



Dimensionality Reduction

$$M : X = \mathbb{R}^D \to \mathbb{R}^k, \quad k \ll D,$$

Dimensionality Reduction

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Consider first $k = 1$

Dimensionality Reduction

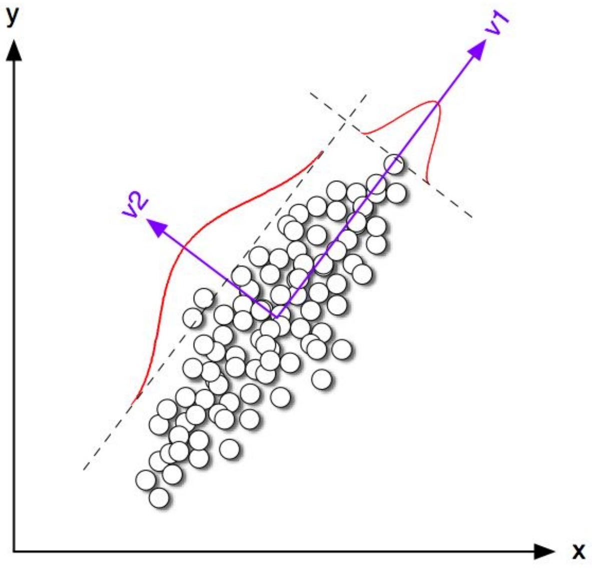
$$M : X = \mathbb{R}^D \to \mathbb{R}^k, \quad k \ll D,$$

Consider first $k = 1$

PCA

$$\min_{w \in \mathbb{S}^{D-1}} \frac{1}{n} \sum_{i=1}^{n} \|x_i - (w^T x_i) w\|^2,$$

$w^T w = 1$



Computations?

Statistics?

$$\min_{w \in \mathbb{S}^{D-1}} \frac{1}{n} \sum_{i=1}^{n} \|x_i - (w^T x_i) w\|^2,$$

Statistics?

$$\min_{w \in \mathbb{S}^{D-1}} \frac{1}{n} \sum_{i=1}^{n} \|x_i - (w^T x_i) w\|^2,$$

Statistics?

$$\|x_i - (w^T x_i) w\|^2 = \|x_i\| - (w^T x_i)^2,$$

$$\min_{w \in \mathbb{S}^{D-1}} \frac{1}{n} \sum_{i=1}^{n} \|x_i - (w^T x_i) w\|^2,$$

Statistics?

$$\|x_i - (w^T x_i) w\|^2 = \|x_i\|^2 - (w^T x_i)^2$$

$$\implies \max_{w \in \mathbb{S}^{D-1}} \frac{1}{n} \sum_{i=1}^{n} (w^T x_i)^2.$$

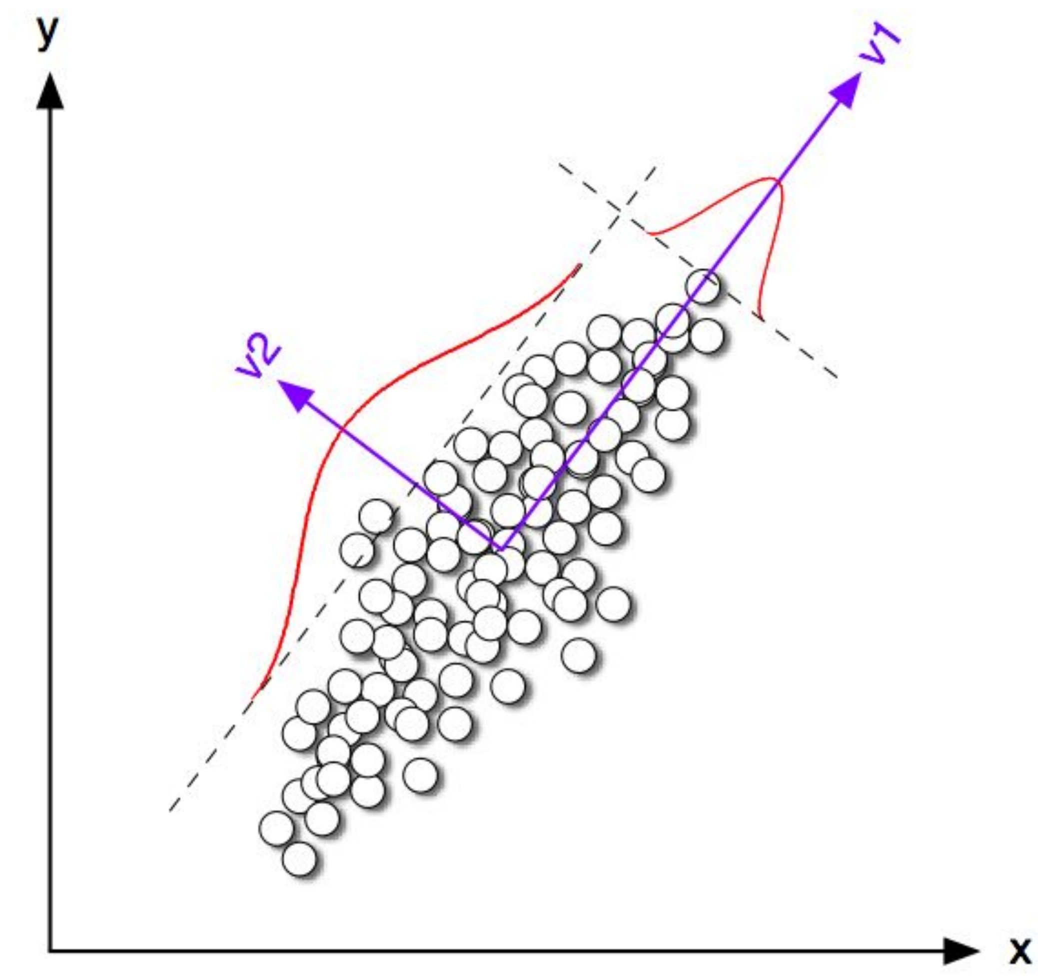
$$\min_{w \in \mathbb{S}^{D-1}} \frac{1}{n} \sum_{i=1}^{n} \|x_i - (w^T x_i) w\|^2,$$

Statistics?

$$\|x_i - (w^T x_i) w\|^2 = \|x_i\|^2 - (w^T x_i)^2$$

$$\implies \quad \max_{w \in \mathbb{S}^{D-1}} \frac{1}{n} \sum_{i=1}^{n} (w^T x_i)^2.$$

$$\implies \quad \max_{w \in \mathbb{S}^{D-1}} \frac{1}{n} \sum_{i=1}^{n} (w^T (x_i - \bar{x}))^2,$$



$$\min_{w \in \mathbb{S}^{D-1}} \frac{1}{n} \sum_{i=1}^{n} \|x_i - (w^T x_i) w\|^2,$$

Computations?

$$\min_{w\in\mathbb{S}^{D-1}} \frac{1}{n}\sum_{i=1}^{n} \|x_i - (w^T x_i)w\|^2,$$

Computations?

w_1 max eigenvector of C_n

$$\max_{w\in\mathbb{S}^{D-1}} \frac{1}{n}\sum_{i=1}^{n}(w^T x_i)^2. \quad \Leftrightarrow \quad \max_{w\in\mathbb{S}^{D-1}} w^T C_n w, \quad C_n = \frac{1}{n}\sum_{i=1}^{n} x_i x_i^T$$

$$\frac{1}{n}\sum_{i=1}^{n}(w^T x_i)^2 = \frac{1}{n}\sum_{i=1}^{n} w^T x_i w^T x_i = \frac{1}{n}\sum_{i=1}^{n} w^T x_i x_i^T w = w^T(\frac{1}{n}\sum_{i=1}^{n} x_i x_i^T)w$$

Dimensionality Reduction

$$M : X = \mathbb{R}^D \to \mathbb{R}^k, \quad k \ll D,$$

What about $k = 2$?

$$\dots$$

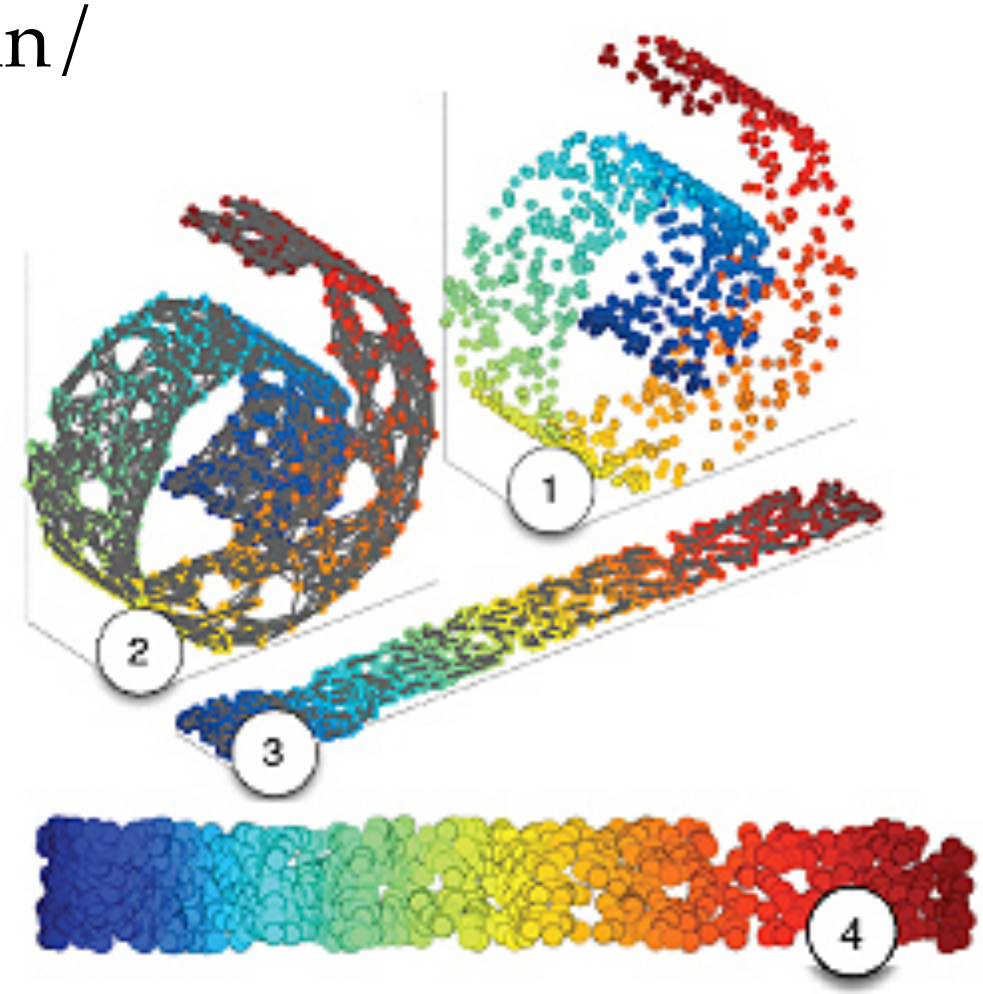
w_2 second eigenvector of C_n

$$\max_{\substack{w \in \mathbb{S}^{D-1} \\ w \perp w_1}} w^T C_n w, \quad C_n = \frac{1}{n} \sum_{i=1}^{n} x_i x_i^T.$$

$$M : X = \mathbb{R}^D \to \mathbb{R}^k, \quad k \ll D,$$

things I won't tell you about

- **Random** Maps: Johnson-Linderstrauss Lemma
- **Non Linear** Maps: Kernel PCA, Laplacian/ Diffusion maps



End of PART III b)

- a) Variable Selection: OMP
- **b) Dimensionality Reduction: PCA**

Interpretability - Sparsity - Greedy & Convex Relaxation Approaches

The End

PART IV

- Matlab practical session

Afternoon