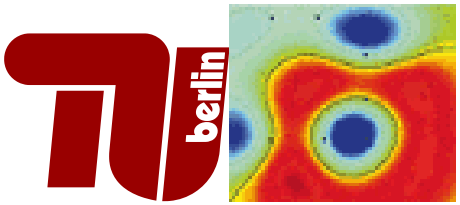

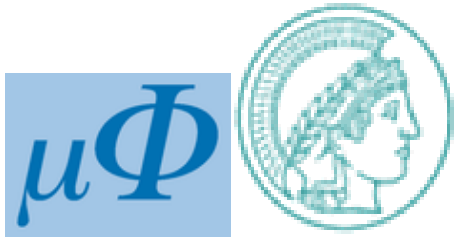

Introduction to Machine Learning

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[1]Technische Universität Berlin
[2]Max Planck Institute of Microstructure Physics

IPAM Tutorial 2013

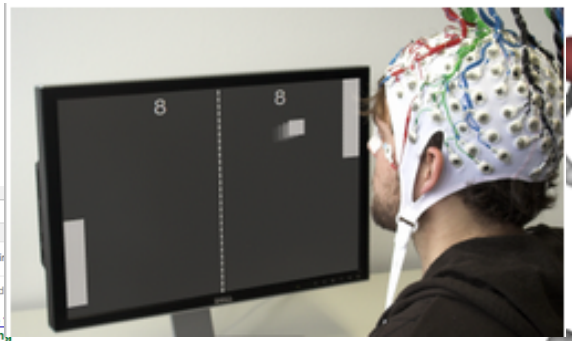
What is Machine Learning?

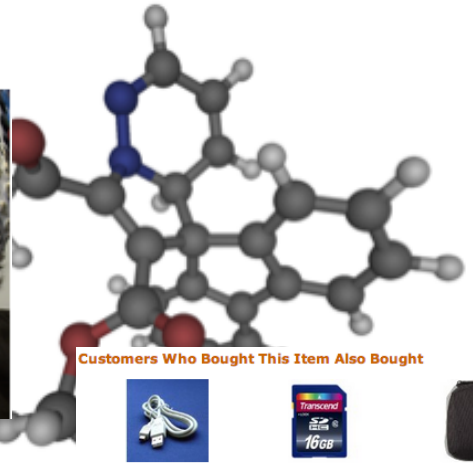
Data with Pattern | Algorithm | ML Model

ML is about learning structure from data

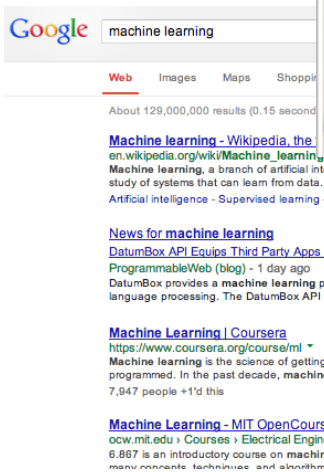
Examples

Drug discovery



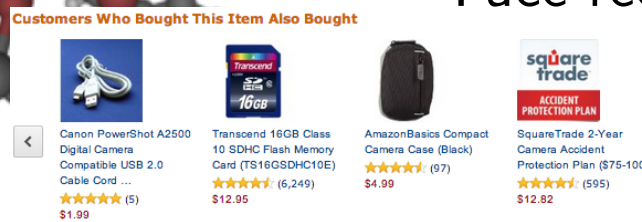


Face recognition

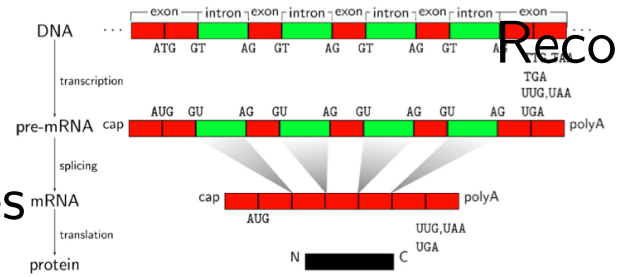


Search engines

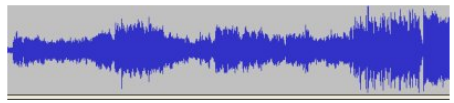
BCI



Recommender systems



DNA splice site detection



Speech recognition

This Talk

Part 1: Learning Theory and Supervised ML

- Basic Ideas of Learning Theory
- Support Vector Machines
- Kernels
- Kernel Ridge Regression

Part 2: Unsupervised ML and Application

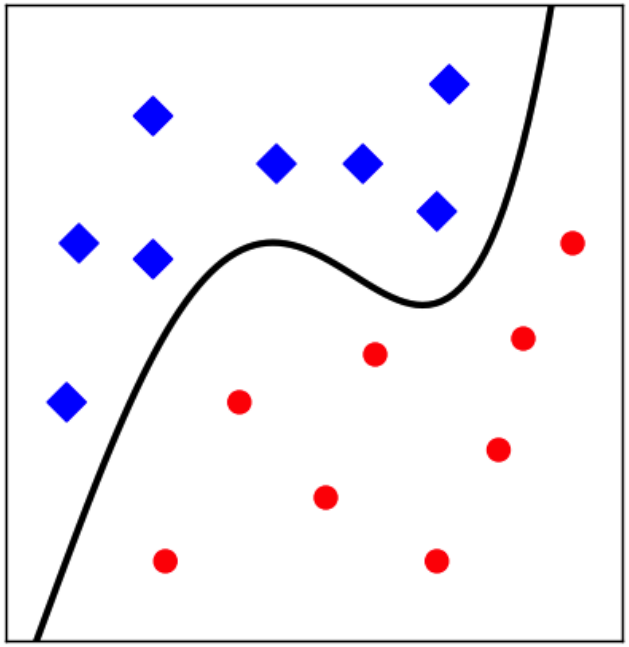
- PCA
- Model Selection
- Feature Representation

Not covered

- Probabilistic Models
- Neural Networks
- Online Learning
- Reinforcement Learning
- Semi-supervised Learning
- etc.

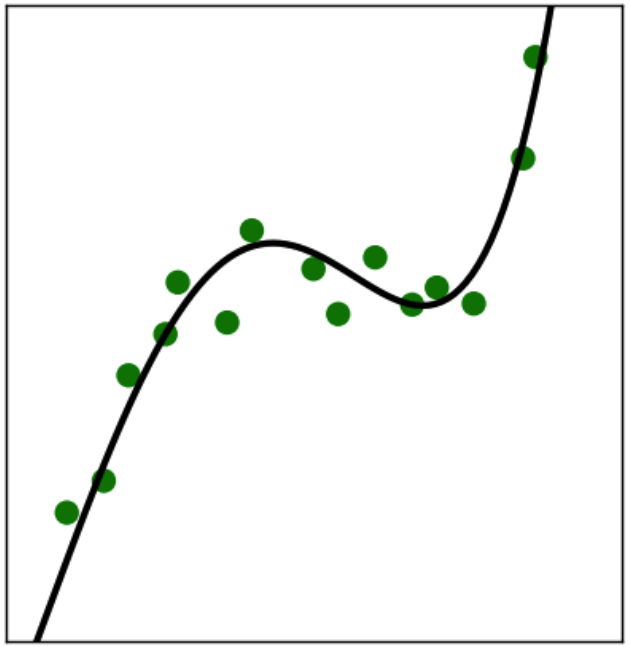
Supervised Learning

Classification



$y_i \in \{-1, +1\}$

Regression



$y_i \in \mathbb{R}$

- Given: *Points* $X = (\mathbf{x}_1, \ldots, \mathbf{x}_N)$ with $\mathbf{x}_i \in \mathbb{R}^d$ and *Labels* $Y = (y_1, \ldots, y_n)$ generated by some joint probability distribution.
- Learn underlying unknown mapping $f(\mathbf{x}) = y$
- Important: Performance on unseen data

Basic Ideas in Learning Theory

Risk minimization (RM)

Learn a model function f from examples

$$(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N) \in \mathbb{R}^d \times \mathbb{R} \text{ or } \{+1, -1\}, \text{ generated from } P(\mathbf{x}, y)$$

such that the expected number of errors on test data (drawn fom $P(\mathbf{x}, y)$),

$$R[f] = \int \frac{1}{2} |f(\mathbf{x}) - y|^2 \mathrm{d}P(\mathbf{x}, y),$$

is minimal.

Problem: Distribution $P(\mathbf{x}, y)$ is unknown

Empirical Risk Minimization (ERM)

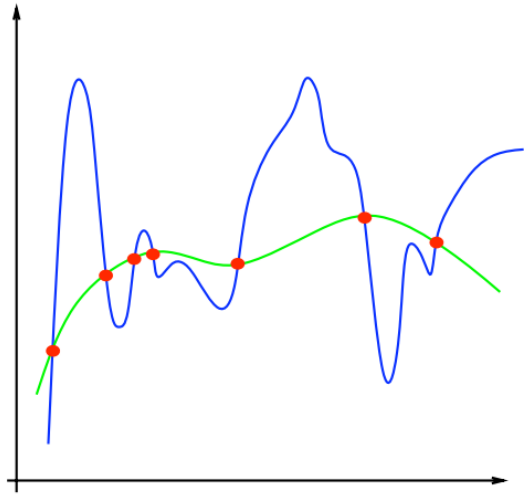
Replace the average over P(x, y) by average of training samples (i.e. *minimize the training error*):

$$R_{\text{emp}}[f] = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{2} |f(\mathbf{x}_i) - y_i|^2$$

Law of large numbers: $R_{\text{emp}}[f] \to R[f]$ as $N \to \infty$.

Question: Does $\min_f R_{\text{emp}}[f]$ give us $\min_f R[f]$ for sufficiently large N?

No: uniform convergence needed



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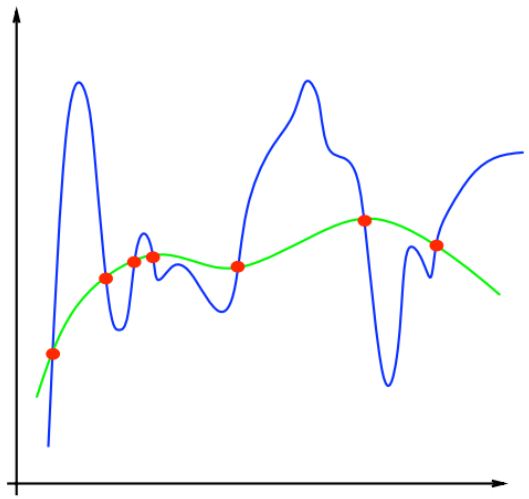


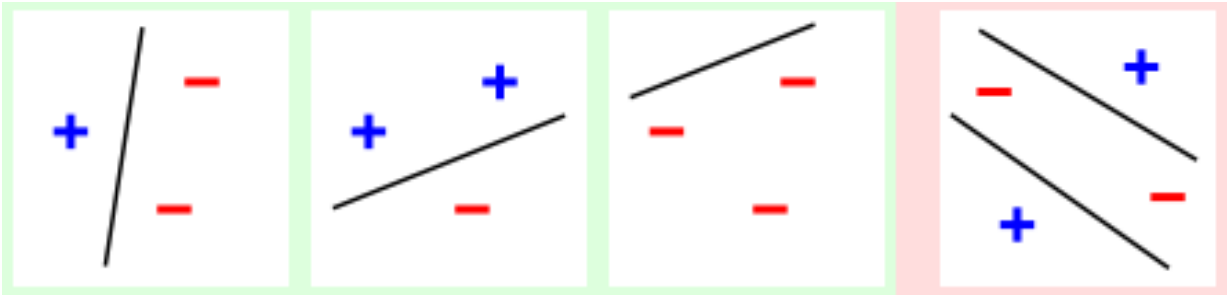
Error bound for classification

With probablity of at least $1 - \eta$:

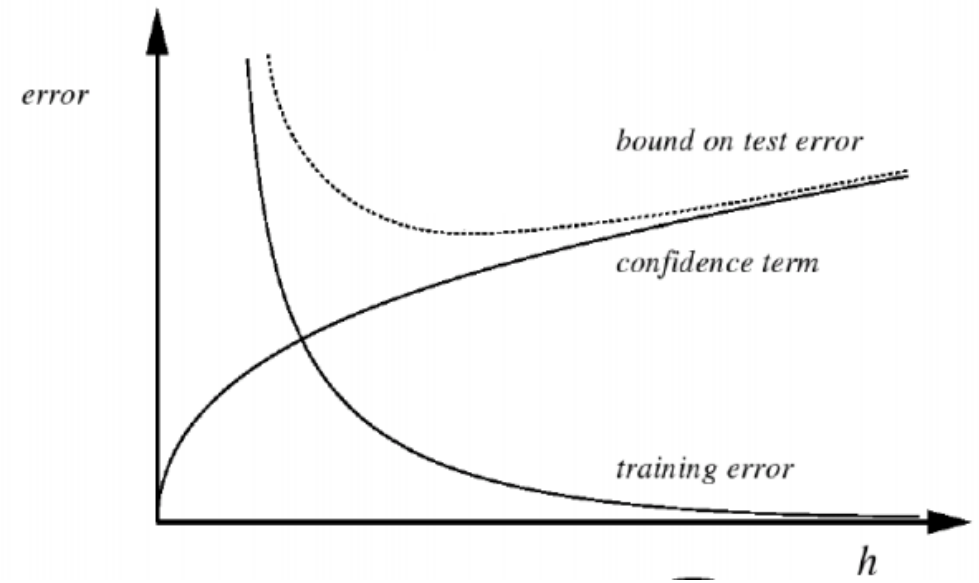
$$R[f] \leq R_{\text{emp}}[f] + \sqrt{\frac{D(\log \frac{2N}{D} + 1) - \log(\frac{\eta}{4})}{N}}$$

where D is the VC dimension (Vapnik and Chervonenkis (1971)).

Introduce structure on set of possible functions and use Structural Risk Minimization (SRM).

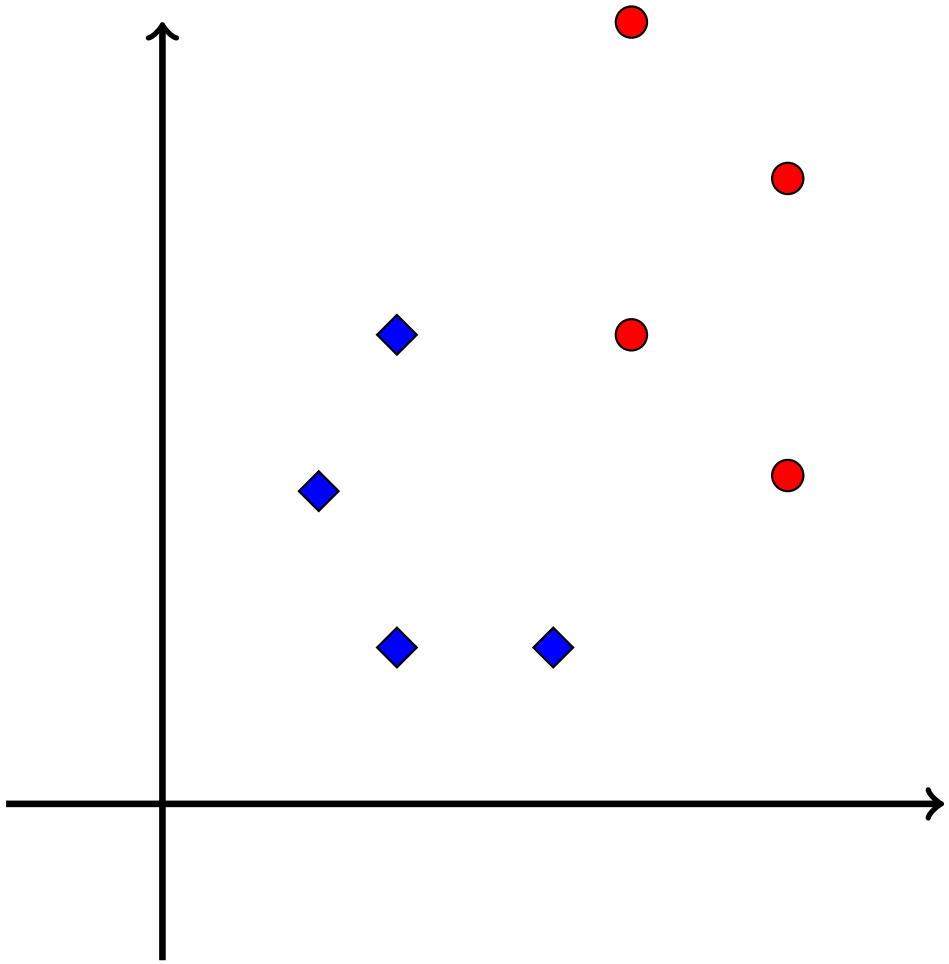


The linear function class has VC-dimension $D = 3$

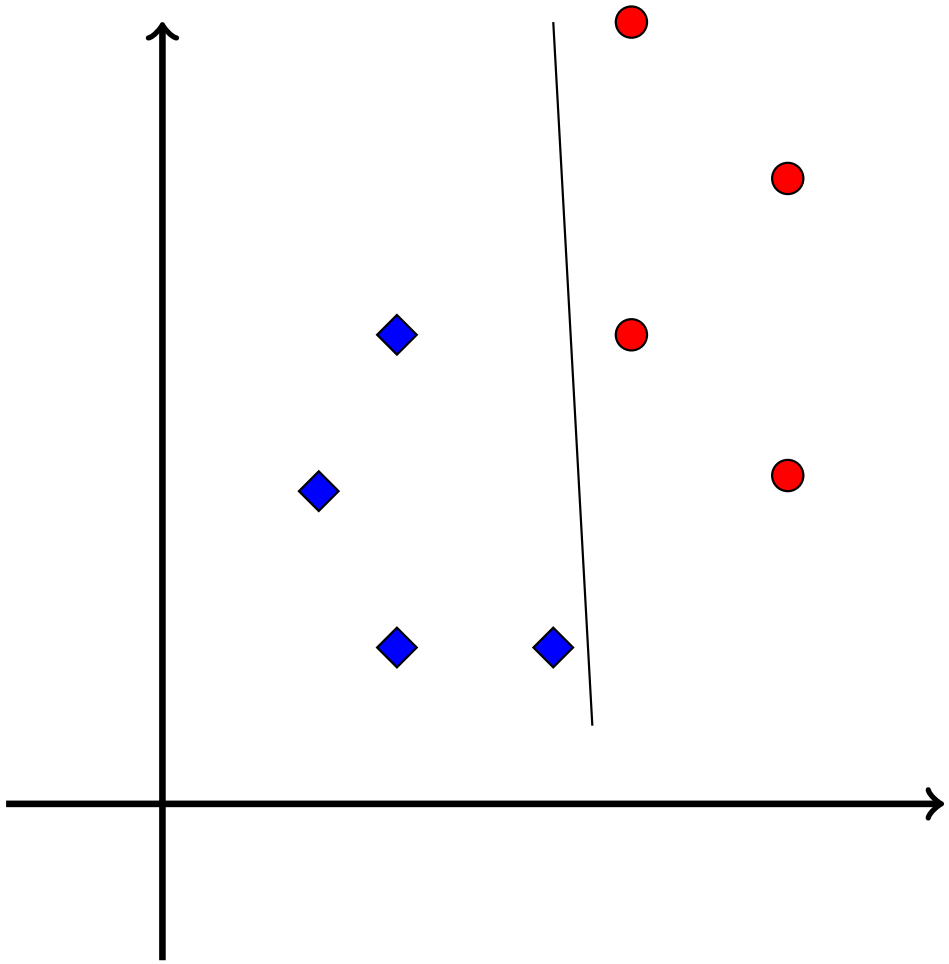


$$\min_f \quad R_{\text{emp}}[f] + \text{Complexity}[f]$$

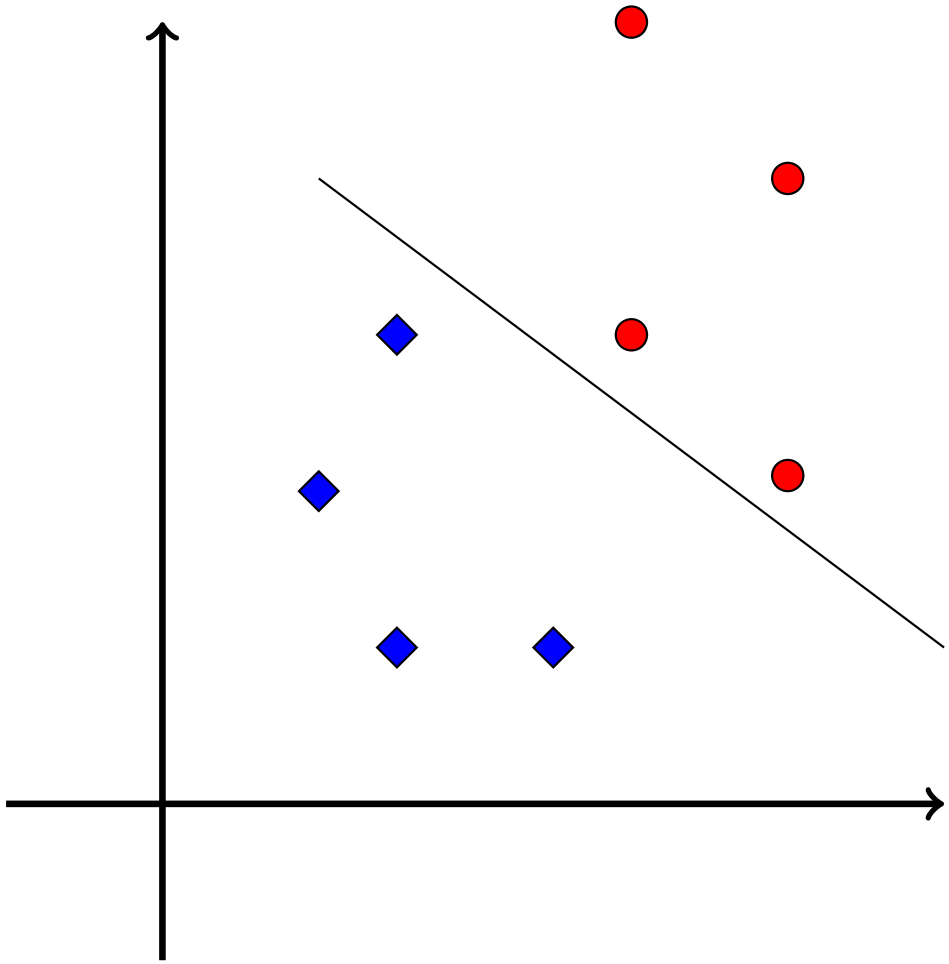
Support Vector Machines (SVM)



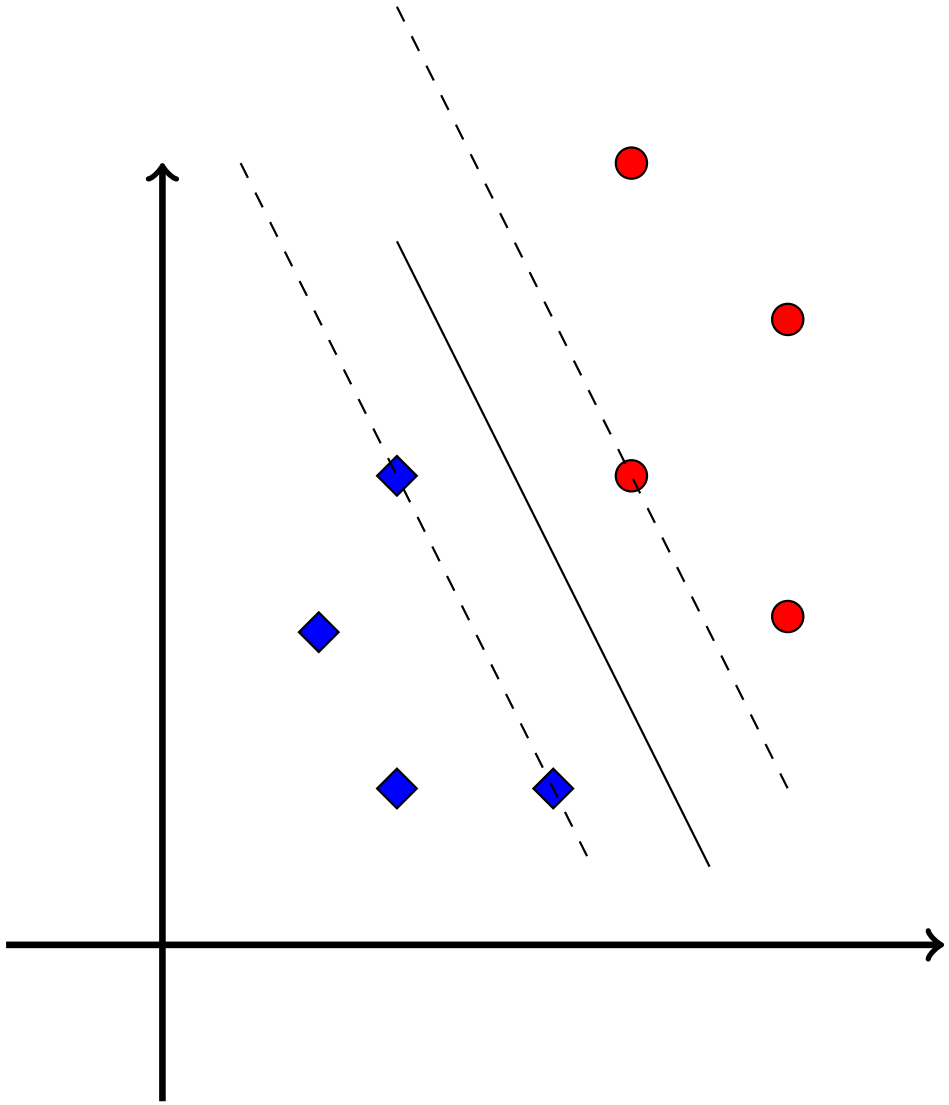
Support Vector Machines (SVM)



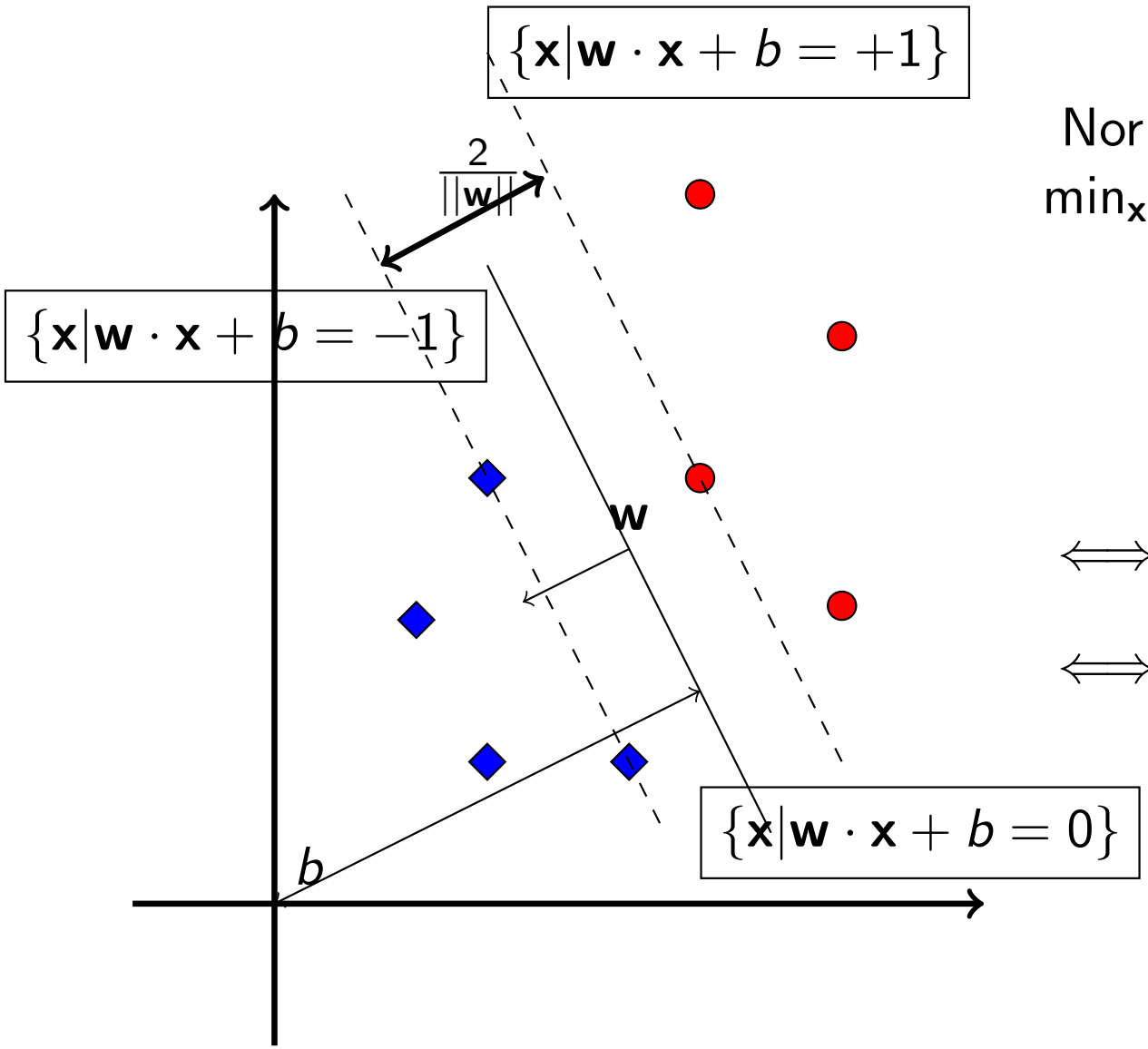
Support Vector Machines (SVM)



Support Vector Machines (SVM)



Support Vector Machines (SVM)



Normalize $\mathbf{w}$ so that $\min_{\mathbf{x}_i} \mathbf{w}\cdot\mathbf{x}_i + b = 1$.

$$\begin{aligned}
&\mathbf{w}\cdot\mathbf{x}_1 + b = +1 \\
&\mathbf{w}\cdot\mathbf{x}_2 + b = -1 \\
\iff &\mathbf{w}\cdot(\mathbf{x}_1 - \mathbf{x}_2) = 2 \\
\iff &\frac{\mathbf{w}}{||\mathbf{w}||}\cdot(\mathbf{x}_1 - \mathbf{x}_2) = \frac{2}{||\mathbf{w}||}
\end{aligned}$$

VC Dimension of Hyperplane Classifiers

Theorem (Cortes and Vapnik (1995))

Hyperplanes in canonical form have VC Dimension

$$D \leq \min\{R^2||\mathbf{w}||^2 + 1,\ N + 1\}$$

where R the radius of the smallest sphere containing the data.

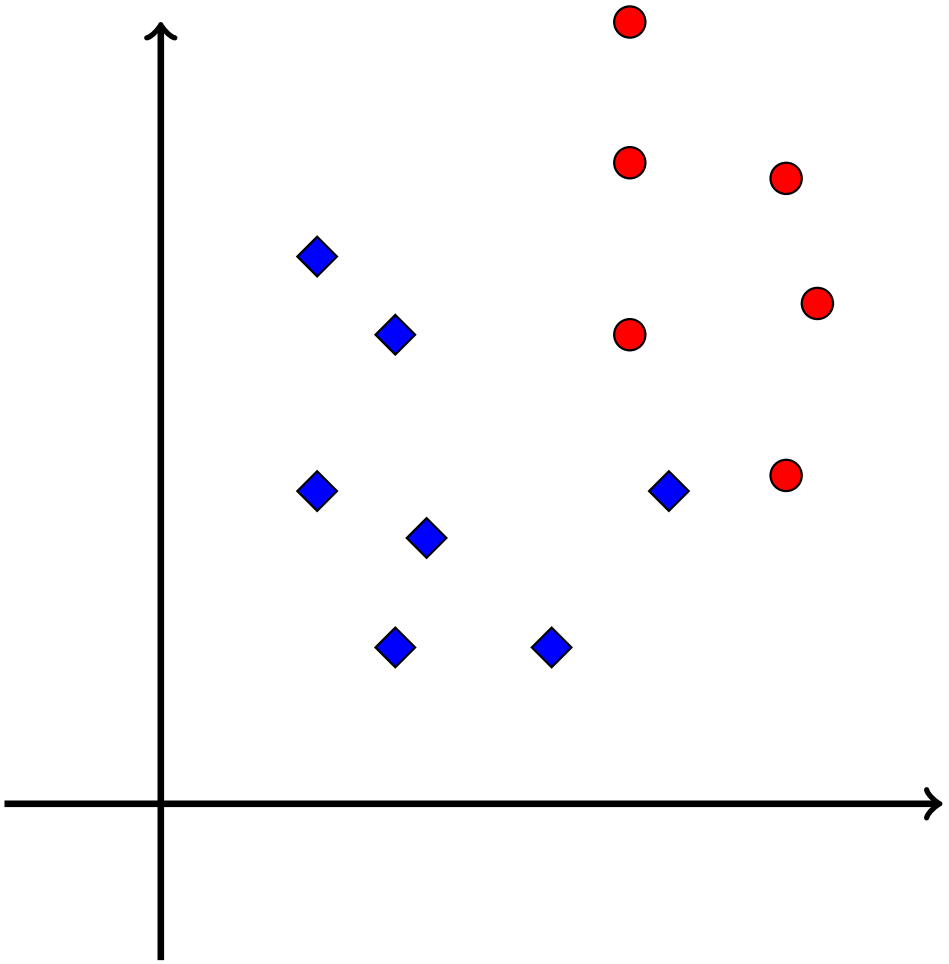
SRM Bound:

$$R[f] \leq R_{\text{emp}}[f] + \sqrt{\frac{D(\log \frac{2N}{D} + 1) - \log(\frac{\eta}{4})}{N}}$$

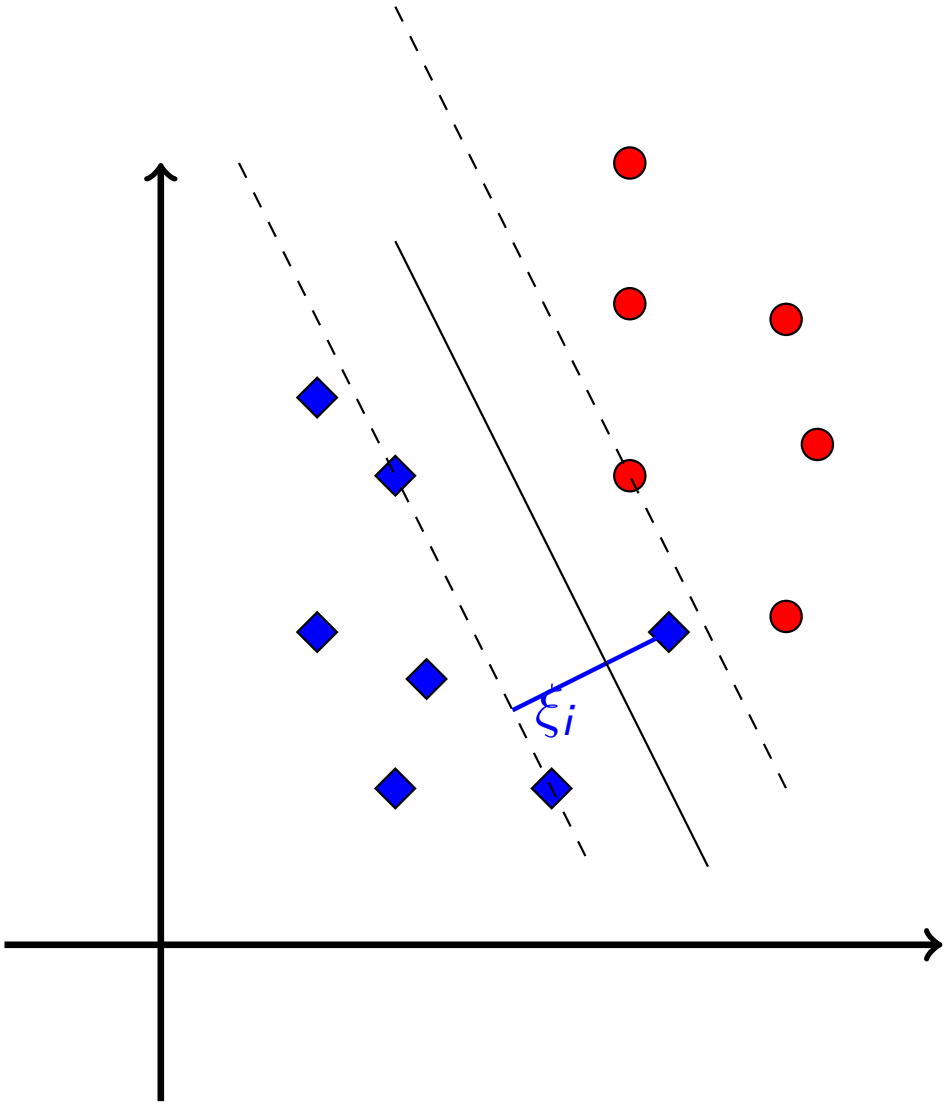
maximal margin = minimum $||\mathbf{w}||^2 \rightarrow$ good generalization, i.e. low risk:

$$\begin{aligned} \min_{\mathbf{w},b} \quad & ||\mathbf{w}||^2 \\ \text{subject to} \quad & y_i(\mathbf{w} \cdot \mathbf{x_i} + b) \geq 1 \quad \text{for } i = 1 \ldots N \end{aligned}$$

Slack variables



Slack variables



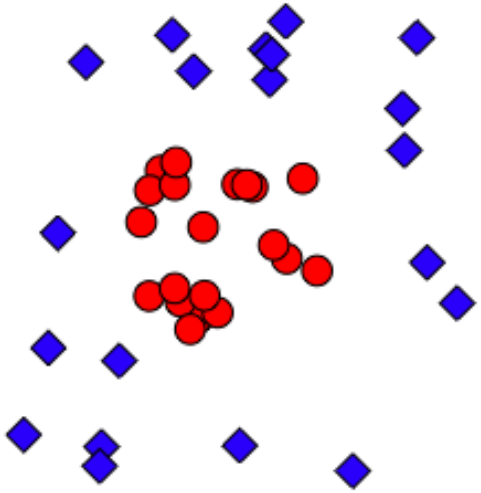
Introduce slack variables ξ_i:

$$\min_{\mathbf{w},b,\xi_i} \quad ||\mathbf{w}||^2 + C\sum_{i=1}^{N}\xi_i$$

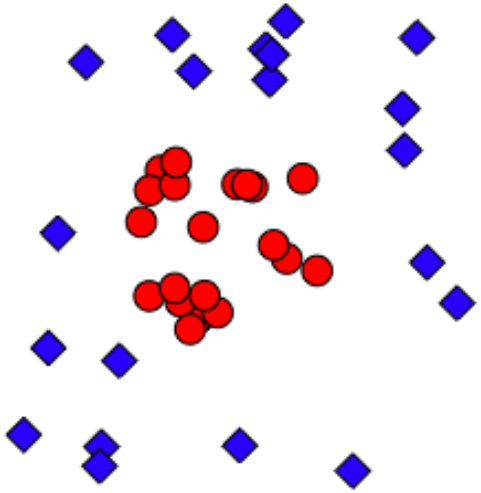
$$\text{subject to} \quad y_i(\mathbf{w}\cdot\mathbf{x_i}+b) \geq 1-\xi_i$$

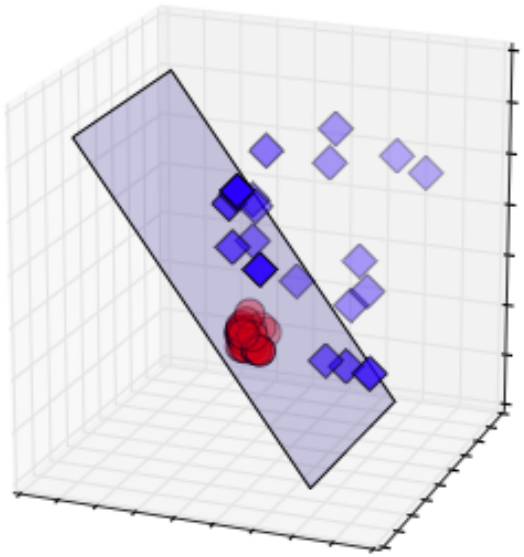
$$\xi_i \geq 0$$

Non-linear hyperplanes



Non-linear hyperplanes





Map into a higher dimensional feature space:

$$\Phi: \quad \mathbb{R}^2 \quad \rightarrow \quad \mathbb{R}^3$$

$$(x_1, x_2) \quad \mapsto \quad (x_1^2, \sqrt{2}x_1x_2, x_2^2)$$

Dual SVM

Primal

$$\min_{\mathbf{w},b,\xi_i} \quad ||\mathbf{w}||^2 + C\sum_{i=1}^{N}\xi_i$$

$$\text{subject to} \quad y_i(\mathbf{w}\cdot\Phi(\mathbf{x_i}) + b) \geq 1 - \xi_i \;\text{ and }\; \xi_i \geq 0 \quad \text{for } i = 1\ldots N$$

Dual

$$\max_{\alpha} \quad \sum_{i=1}^{N}\alpha_i - \frac{1}{2}\sum_{i,j=1}^{N}\alpha_i\alpha_j y_i y_j \left(\Phi(\mathbf{x_i})\cdot\Phi(\mathbf{x_j})\right)$$

$$\text{subject to} \quad \sum_{i=1}^{N}\alpha_i y_i = 0 \;\text{ and }\; C \geq \alpha_i \geq 0 \quad \text{for } i = 1\ldots N$$

Data points x_i only appear in scalar products $(\Phi(\mathbf{x_i})\cdot\Phi(\mathbf{x_j}))$.

The Kernel Trick

Replace scalar products with kernel function (Müller et al. (2001)):

$$k(x, y) = \Phi(x) \cdot \Phi(y)$$

- Compute kernel matrix $K_{ij} = k(x_i, x_j)$, i.e. never use Φ directly
- Underlying mapping Φ can be unknown
- Kernels can be adopted to specific task, e.g. using prior knowledge (kernels for graphs, trees, strings, ...)

Common kernels

Gaussian Kernel:	$k(x, y)$	$=$	$\exp\left(-\frac{\|\|x-y\|\|^2}{2\sigma^2}\right)$
Linear Kernel:	$k(x, y)$	$=$	$x \cdot y$
Polynomial Kernel:	$k(x, y)$	$=$	$(x \cdot y + c)^d$

The Support Vectors in SVM

$$\max_{\alpha} \quad \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} \alpha_i \alpha_j y_i y_j \left(\Phi(\mathbf{x_i}) \cdot \Phi(\mathbf{x_j})\right)$$

$$\text{subject to} \quad \sum_{i=1}^{N} \alpha_i y_i = 0 \;\text{ and }\; C \geq \alpha_i \geq 0 \quad \text{for } i = 1 \ldots N$$

KKT conditions

$$y_i \left[\mathbf{w}\Phi(\mathbf{x_i})) + b\right] > 1 \Longrightarrow \qquad a_i = 0 \longrightarrow \qquad x_i \text{ irrelevant}$$

$$y_i \left[\mathbf{w}\Phi(\mathbf{x_i})) + b\right] = 1 \Longrightarrow \quad \text{on/in margin} \longrightarrow \quad x_i \text{ Support Vector}$$

Old model $f(x) = w \cdot \Phi(x_i) + b$ becomes via $w = \sum_{i=1}^{N} \alpha_i y_i \Phi(x_i)$:

$$f(x) = \sum_{i=1}^{N} \alpha_i y_i k(x_i, x) + b \quad \longrightarrow \quad f(x) = \sum_{x_i \in SV} \alpha_i y_i k(x_i, x) + b$$

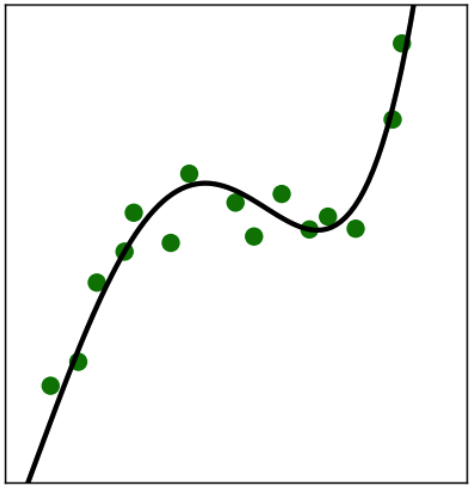
Kernel Ridge Regression (KRR)

Ridge Regression

$$\min_w \sum_{i=1}^{N} ||y_i - w \cdot \mathbf{x_i}||^2 + \lambda ||w||^2$$

Setting derivative to zero gives

$$w = \left(\lambda I + \sum_{i=1}^{N} x_i x_i^T \right)^{-1} \sum_{i=1}^{N} y_i x_i$$



Linear Model: $f(x) = w \cdot x$

Kernelizing Ridge Regression

Setting $X = (x_1, \ldots, x_N) \in \mathbb{R}^{d \times N}$ and $Y = (y_1, \ldots, y_n)^\intercal \in \mathbb{R}^N$:

$$w = (\lambda I + XX^\intercal)^{-1} XY$$

Apply Woodbury Matrix identity:

$$w = X (X^\intercal X + \lambda I)^{-1} Y$$

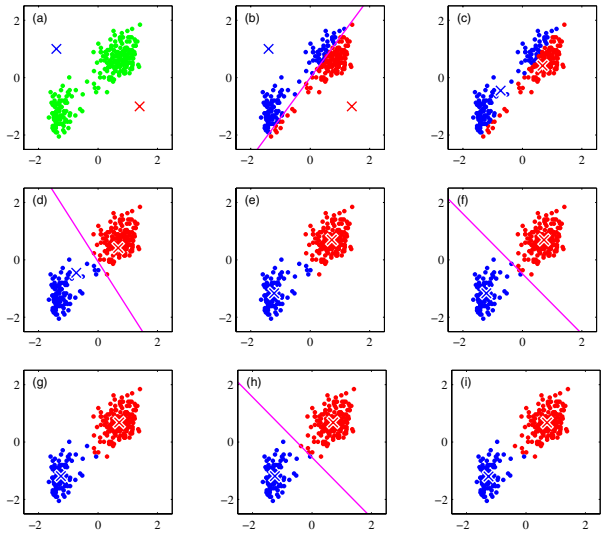
Introduce α:

$$\alpha = (K + \lambda I)^{-1} Y \quad \text{and} \quad w = \sum_{i=1}^{N} \Phi(\mathbf{x_i}) \alpha_i$$

Kernel Model: $f(x) = w \cdot \Phi(x) = \sum_{i=1}^{N} \alpha_i k(\mathbf{x}_i, \mathbf{x})$

Unsupervised Learning

- Learn structure from unlabeled data
- Fit an assumed model / distribution to the data
- Examples
  - clustering
  - blind source separation
  - outlier detection
  - dimensionality reduction



Principal Component Analysis (PCA)

Given centered data matrix $X = (x_1, \ldots, x_N)^\intercal \in \mathbb{R}^{N \times D}$

- best linear approximation

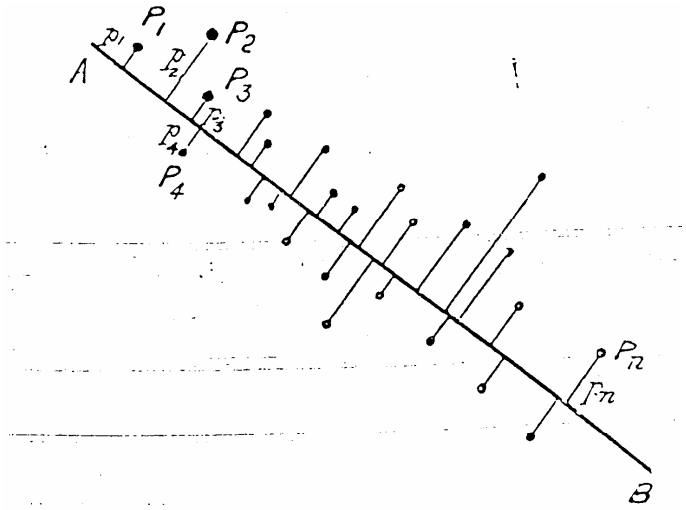
$$w_1 = \arg \min_{\|w\|=1} \left\{ \|X - X w w^\intercal\|^2 \right\}$$

- direction of largest variance

$$w_1 = \arg \max_{\|w\|=1} \left\{ \|X w\|^2 \right\}$$

- matrix reduction for further components

$$X_{k+1} = X_k - X_k w w^\intercal$$



Pearson (1901)

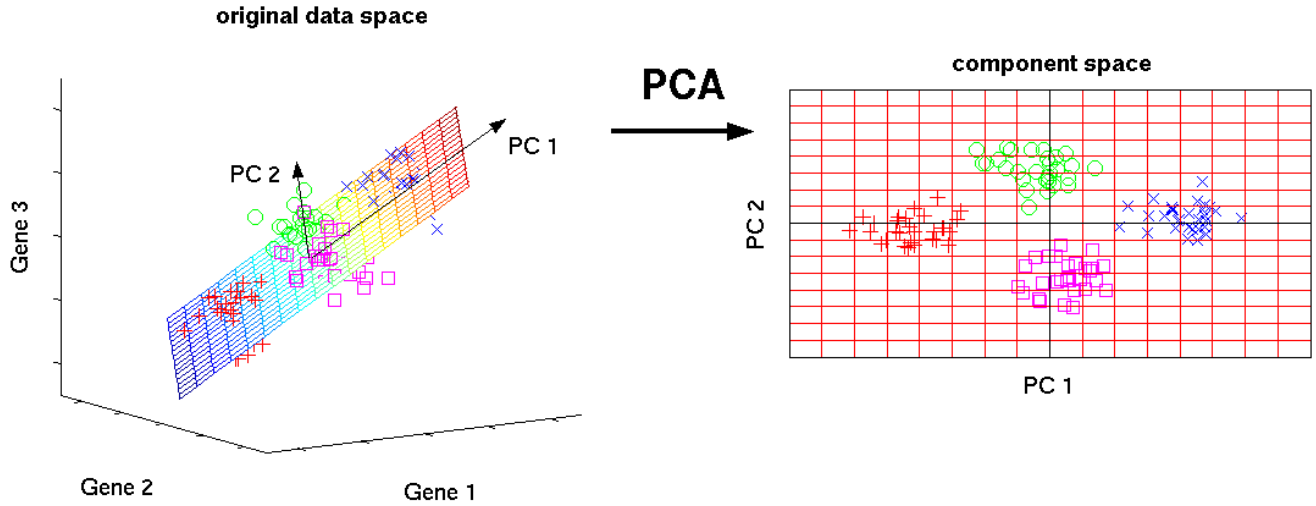
Principal Component Analysis (PCA)

Given centered data matrix $X \in \mathbb{R}^{N \times D}$, decompose correlated data matrix into uncorrelated, orthogonal *PCs*

- diagonalize covariance matrix $\Sigma = \frac{1}{N} X^\intercal X$

$$\Sigma \mathbf{w}_k = \sigma_k^2 \mathbf{w}_k$$

- order principal components $\mathbf{w}_k$ by variance σ_k^2
- project data to first n principal components



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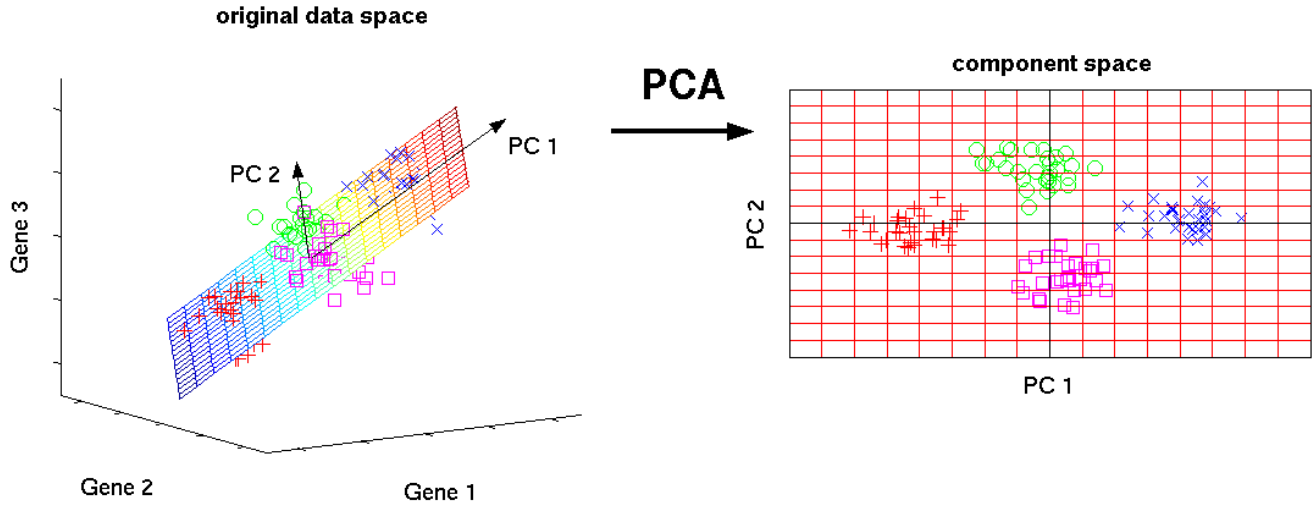

What about nonlinear correlations?

Kernel Principal Component Analysis (kPCA)

Transformation to feature space $X \mapsto X_f$:

$$\Sigma_f = \frac{1}{N} X_f^\intercal X_f,\ K = X_f X_f^\intercal, K_{ij} = k(x_i, x_j)$$

$$\Sigma_f \mathbf{w}_k = \sigma_k^2 \mathbf{w}_k$$

Kernel Principal Component Analysis (kPCA)

Transformation to feature space $X \mapsto X_f$:

$$\Sigma_f = \frac{1}{N} X_f^\intercal X_f,\ K = X_f X_f^\intercal, K_{ij} = k(x_i, x_j)$$

$$X_f^\intercal X_f \mathbf{w}_k = N\sigma_k^2 \mathbf{w}_k$$

Kernel Principal Component Analysis (kPCA)

Transformation to feature space $X \mapsto X_f$:

$$\Sigma_f = \frac{1}{N} X_f^\intercal X_f,\ K = X_f X_f^\intercal, K_{ij} = k(x_i, x_j)$$

$$\begin{aligned} X_f^\intercal X_f \mathbf{w}_k &= N\sigma_k^2 \mathbf{w}_k \\ \Downarrow \mathbf{w}_k &= X_f^\intercal \boldsymbol{\alpha}_k \\ X_f^\intercal X_f X_f^\intercal \boldsymbol{\alpha}_k &= N\sigma_k^2 X_f^\intercal \boldsymbol{\alpha}_k \end{aligned}$$

Kernel Principal Component Analysis (kPCA)

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Kernel Principal Component Analysis (kPCA)

Transformation to feature space $X \mapsto X_f$:

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Kernel Principal Component Analysis (kPCA)

Transformation to feature space $X \mapsto X_f$:

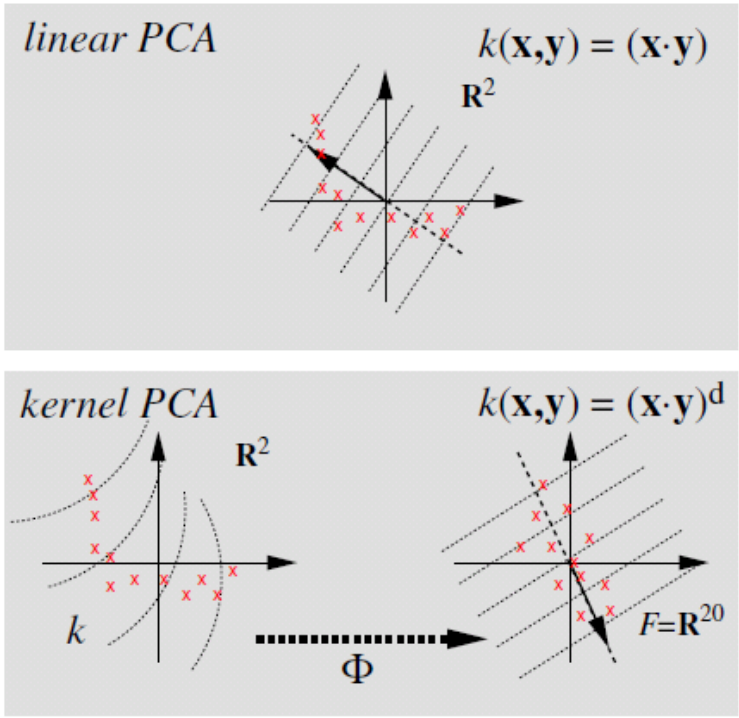
$$\Sigma_f = \frac{1}{N} X_f^\intercal X_f,\ K = X_f X_f^\intercal, K_{ij} = k(x_i, x_j)$$

$$\begin{aligned}
X_f^\intercal X_f \mathbf{w}_k &= N\sigma_k^2 \mathbf{w}_k \\
&\Downarrow \mathbf{w}_k = X_f^\intercal \boldsymbol{\alpha}_k \\
X_f^\intercal X_f X_f^\intercal \boldsymbol{\alpha}_k &= N\sigma_k^2 X_f^\intercal \boldsymbol{\alpha}_k \\
&\Downarrow X_f \cdot \\
K^2 \boldsymbol{\alpha}_k &= N\sigma_k^2 K \boldsymbol{\alpha}_k \\
&\Downarrow K^{-1} \cdot \\
K \boldsymbol{\alpha}_k &= N\sigma_k^2 \boldsymbol{\alpha}_k
\end{aligned}$$

Kernel Principal Component Analysis (kPCA)

Projection:

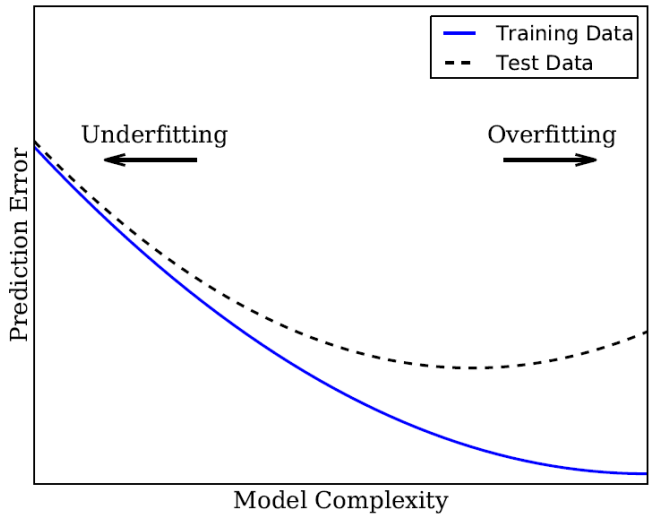
$$x_f^\mathsf{T} w_k = x_f^\mathsf{T} X_f^\mathsf{T} \boldsymbol{\alpha}_k$$
$$= \sum_{i=1}^{N} \alpha_{k,i} k(x, x_i)$$



Schölkopf et al. (1997)

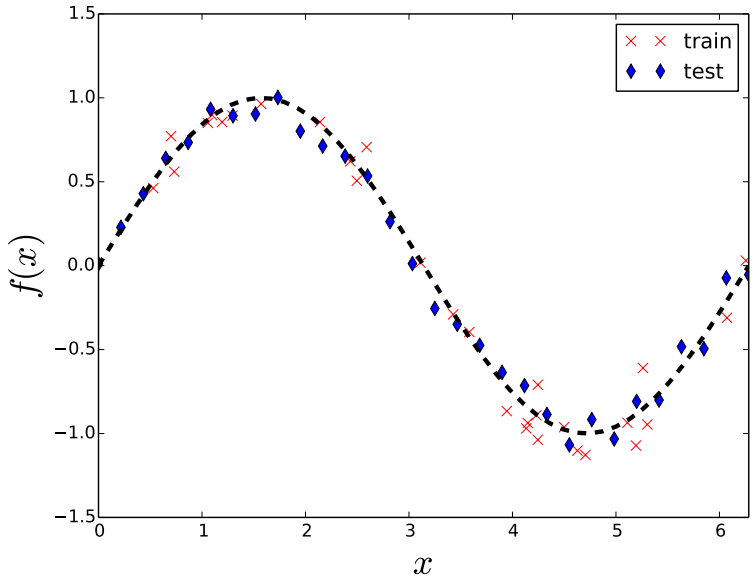
Model Selection

- Find the model that best fits the data distribution
- We can only estimate this distribution
- Consider
  - noise ratio / distribution
  - data correlation



Hyperparameters

- adjust model complexity
  - regularization, kernel parameters, etc.
- have to be tuned using examples **not** used for training
- standard solution: exhaustive search over parameter grid

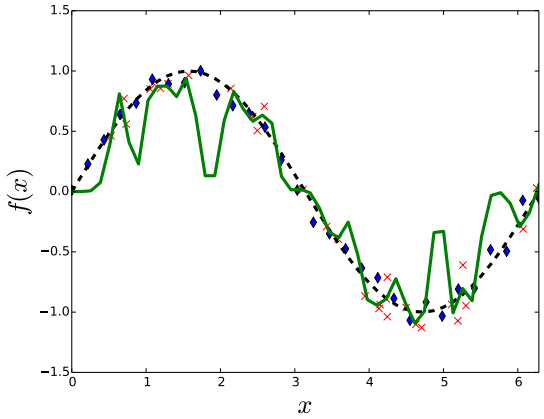


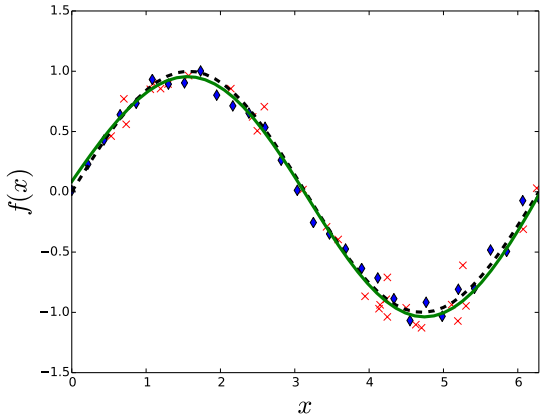
$$f(x) = \sin(x)$$

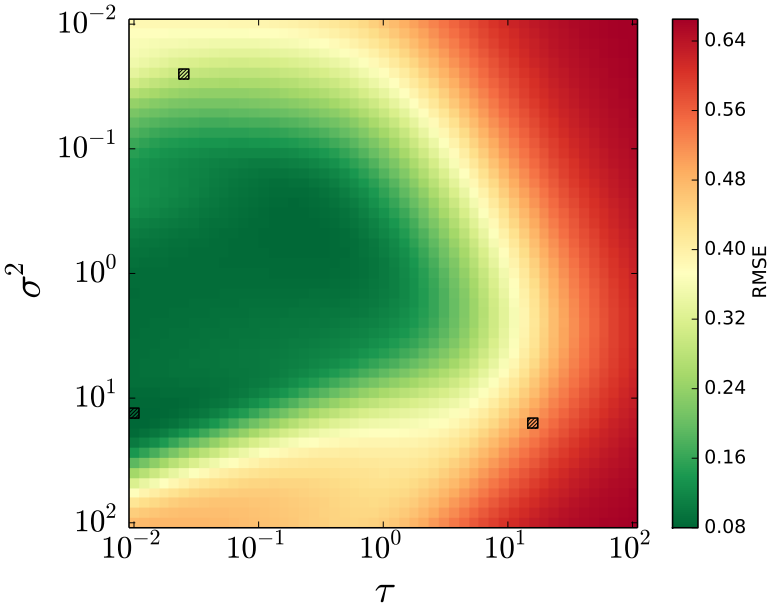
$$\bar{f}(x) = \sum_i \alpha_i \exp\left(\frac{\|x - x_i\|^2}{\sigma^2}\right)$$

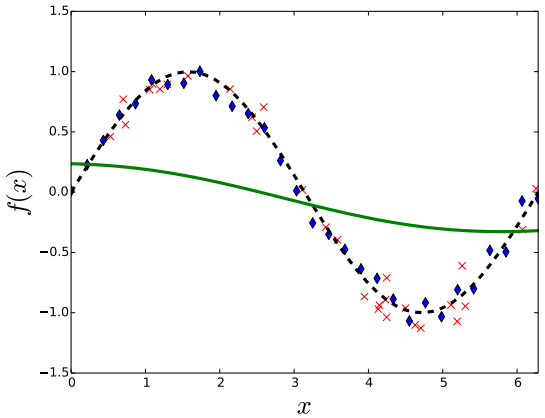
$$\boldsymbol{\alpha} = (K + \tau I)^{-1} y$$

Grid Search

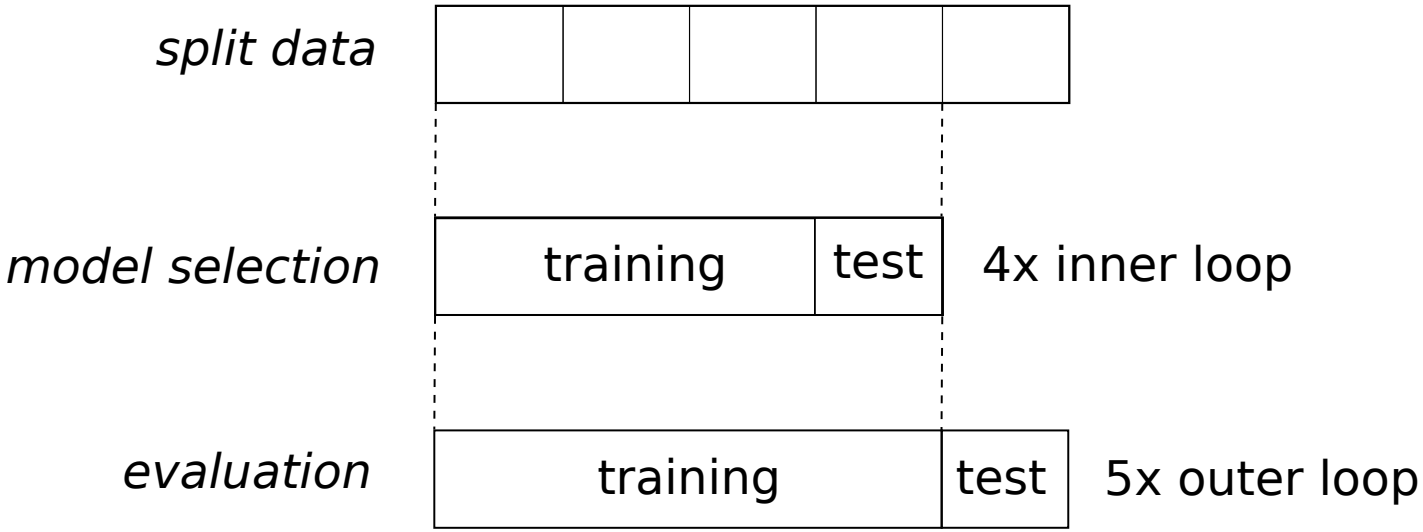








k-fold cross-validation



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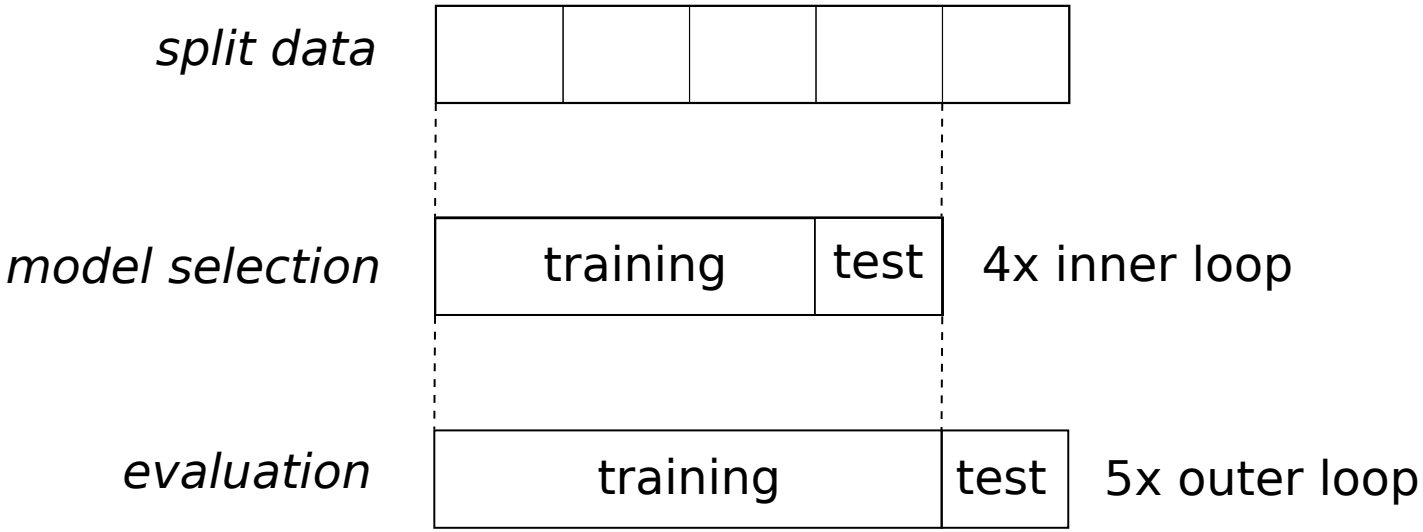


Don't even think about looking at the test set!

From objects to vectors

How to represent complex objects for kernel methods?

- explicit map to vector space: $\phi : M \to \mathbb{R}^n$
  - use standard kernel (e.g., linear, polynomial, gaussian) $k : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ on mapped features
- direct use of kernel function: $k : M \times M \to \mathbb{R}$

Feature Representation

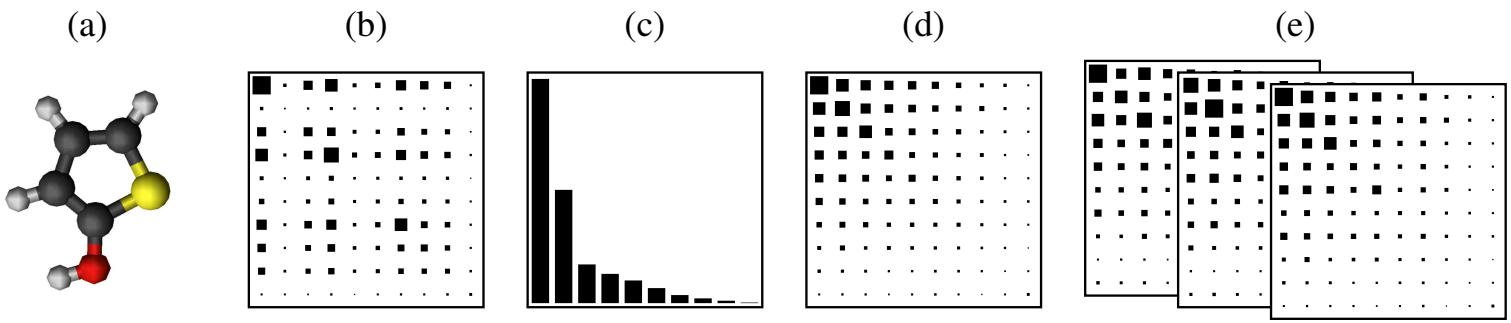
Given a physical object (molecule, crystal, etc.) and a property of interest, what is a good ML representation?

- no loss of valuable information
- support generalization
  - remove invariances
  - decompose problem
- incorporation of domain knowledge
- depends on data set, target function and learning method

Feature Representation - Molecules

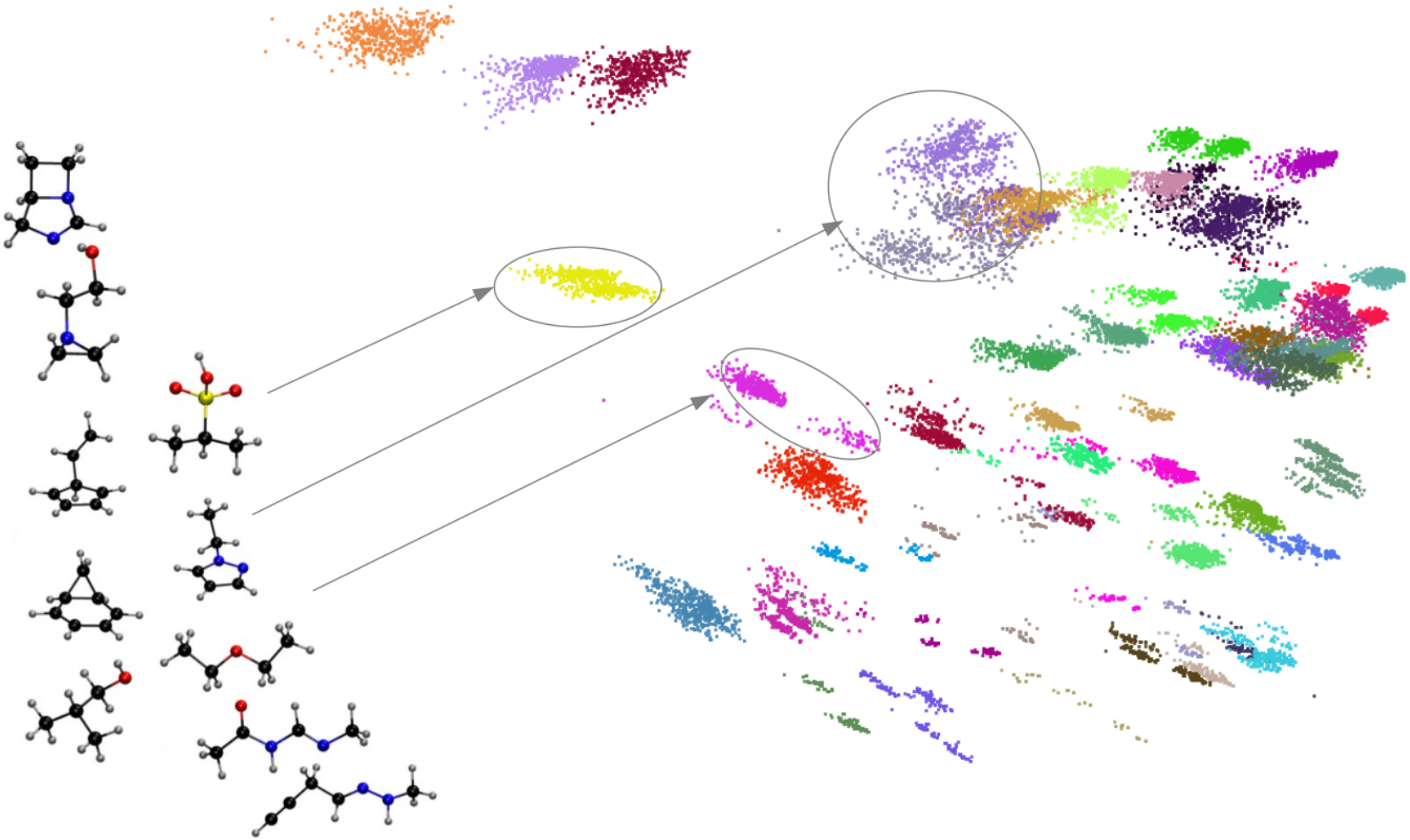
Coulomb matrix:

$$C_{ij} = \begin{cases} 0.5 Z_i^{2.4} & \text{if } i = j \\ \dfrac{Z_i Z_j}{\|r_i - r_j\|} & \text{if } i \neq j \end{cases}$$



(Rupp et al., 2012; Montavon et al., 2012)

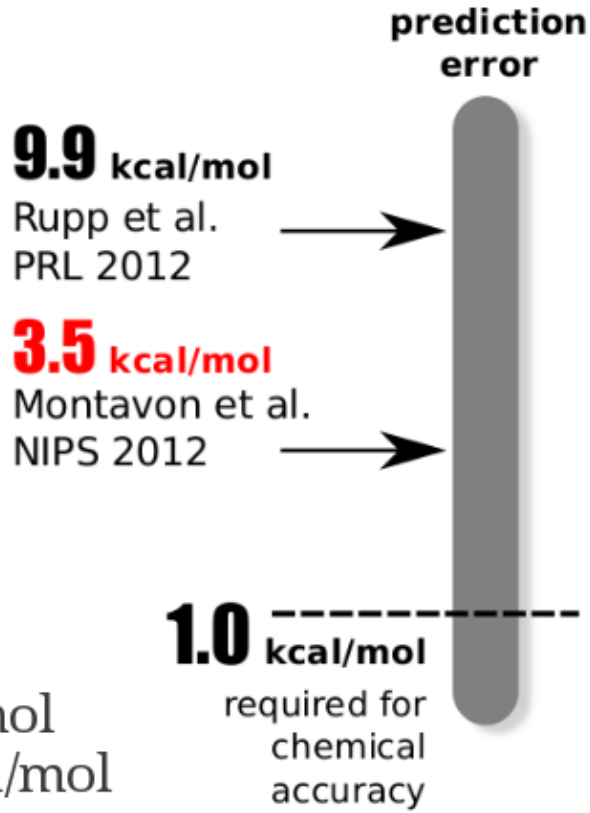
Feature Representation - Molecules



PCA of Coulomb matrices with atom permutations Montavon et al. (2013)

Results - Molecules

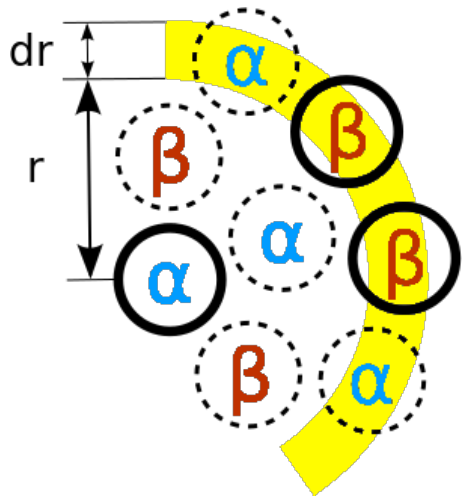
Results:
Mean predictor: **179** kcal/mol
K-nearest neighbors: **70** kcal/mol
Linear regression: **20.7** kcal/mol
Deep net, backprop: **11.8** kcal/mol
Gaussian kernel ridge regression: **8.7** kcal/mol
Deep net, backprop + permutations: **3.5** kcal/mol



G. Montavon, K. Hansen, S. Fazli, M. Rupp, F. Biegler, A. Ziehe, A. Tkatchenko, O. A. von Lilienfeld, K.-R. Müller, Learning Invariant Representations of Molecules for Atomization Energy Prediction, Advances in Neural Information Processing Systems (NIPS), 2012

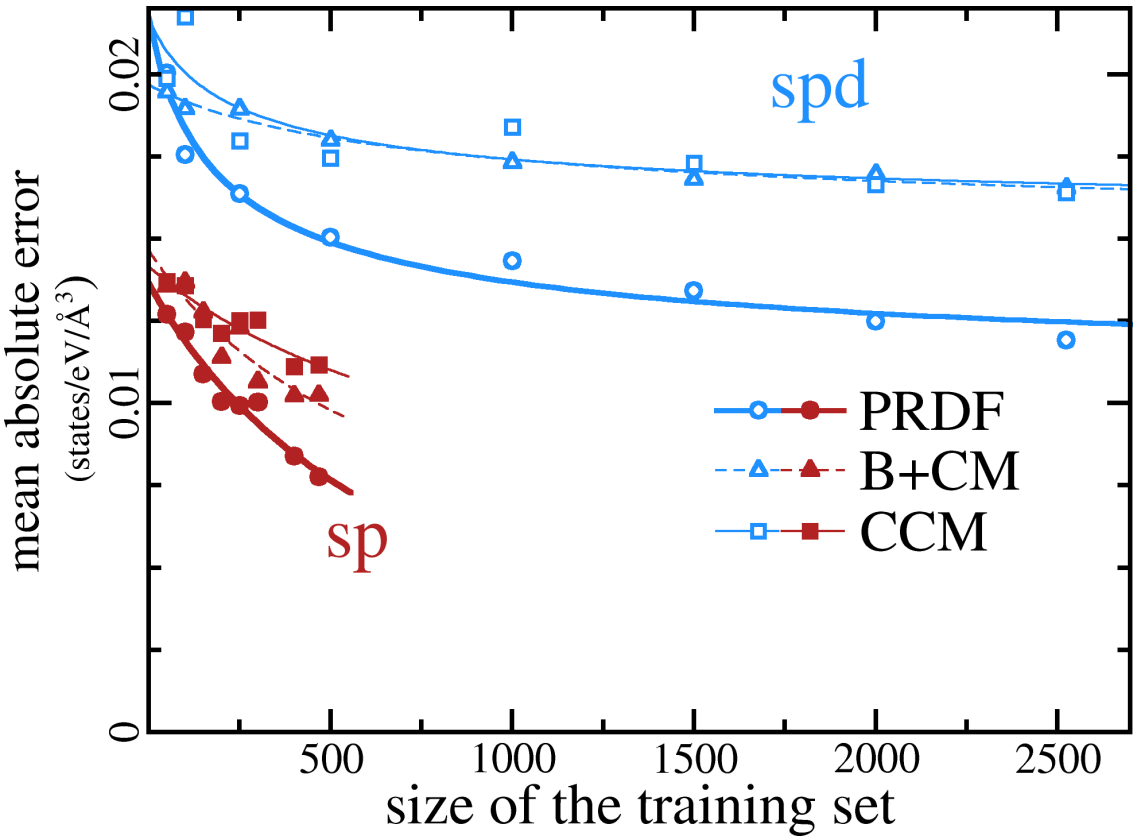
Feature Representation - Crystals

element pair	r_1	$\cdots$	r_n
$\alpha\ \alpha$	$g_{\alpha\alpha}(r_1)$	$\cdots$	$g_{\alpha\alpha}(r_n)$
$\alpha\ \beta$	$g_{\alpha\beta}(r_1)$	$\cdots$	$g_{\alpha\beta}(r_n)$
$\beta\ \alpha$	$g_{\beta\alpha}(r_1)$	$\cdots$	$g_{\beta\alpha}(r_n)$
$\beta\ \beta$	$g_{\beta\beta}(r_1)$	$\cdots$	$g_{\beta\beta}(r_n)$



Results - Crystals

Learning curve of DOS_{fermi} predictions



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Feature representation is key!

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