Kernel methods & sparse methods for computer vision

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Machine learning

- Supervised learning
  - Predict $y \in \mathcal{Y}$ from $x \in \mathcal{X}$, given observations (x_i, y_i), $i = 1, \ldots, n$
- Unsupervised learning
  - Find structure in $x \in \mathcal{X}$, given observations x_i, $i = 1, \ldots, n$
- Application to many problems and data types:
  - **Computer vision**
  - Bioinformatics
  - Text processing
  - etc.
- Specifity: exchanges between **theory** / **algorithms** / **applications**

Machine learning for computer vision

- Multiplication of digital media
- Many different tasks to be solved
  - Associated with different machine learning problems
  - Massive data to learn from

Image retrieval

⇒ Classification, ranking, outlier detection

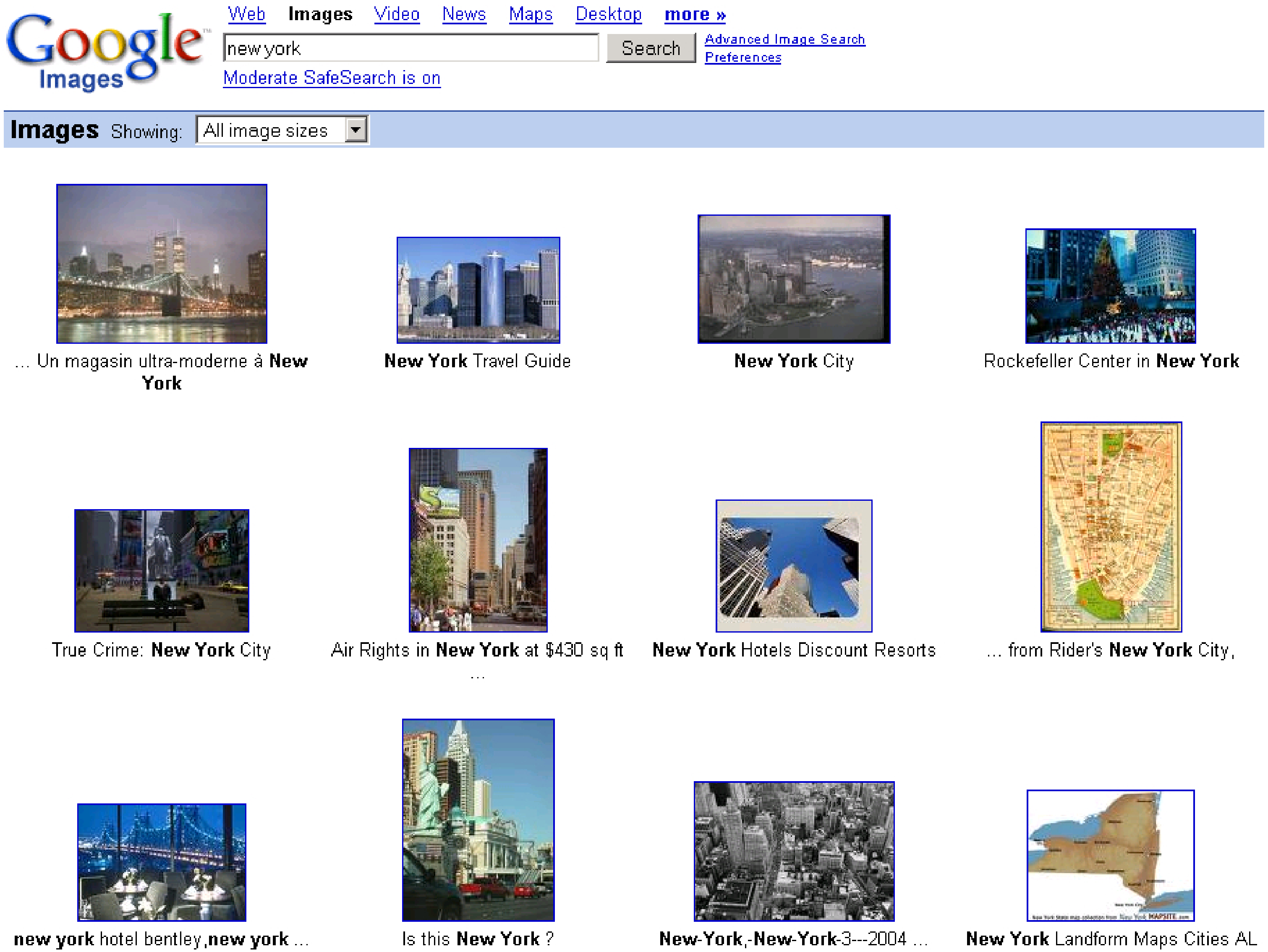

Image retrieval

Classification, ranking, outlier detection

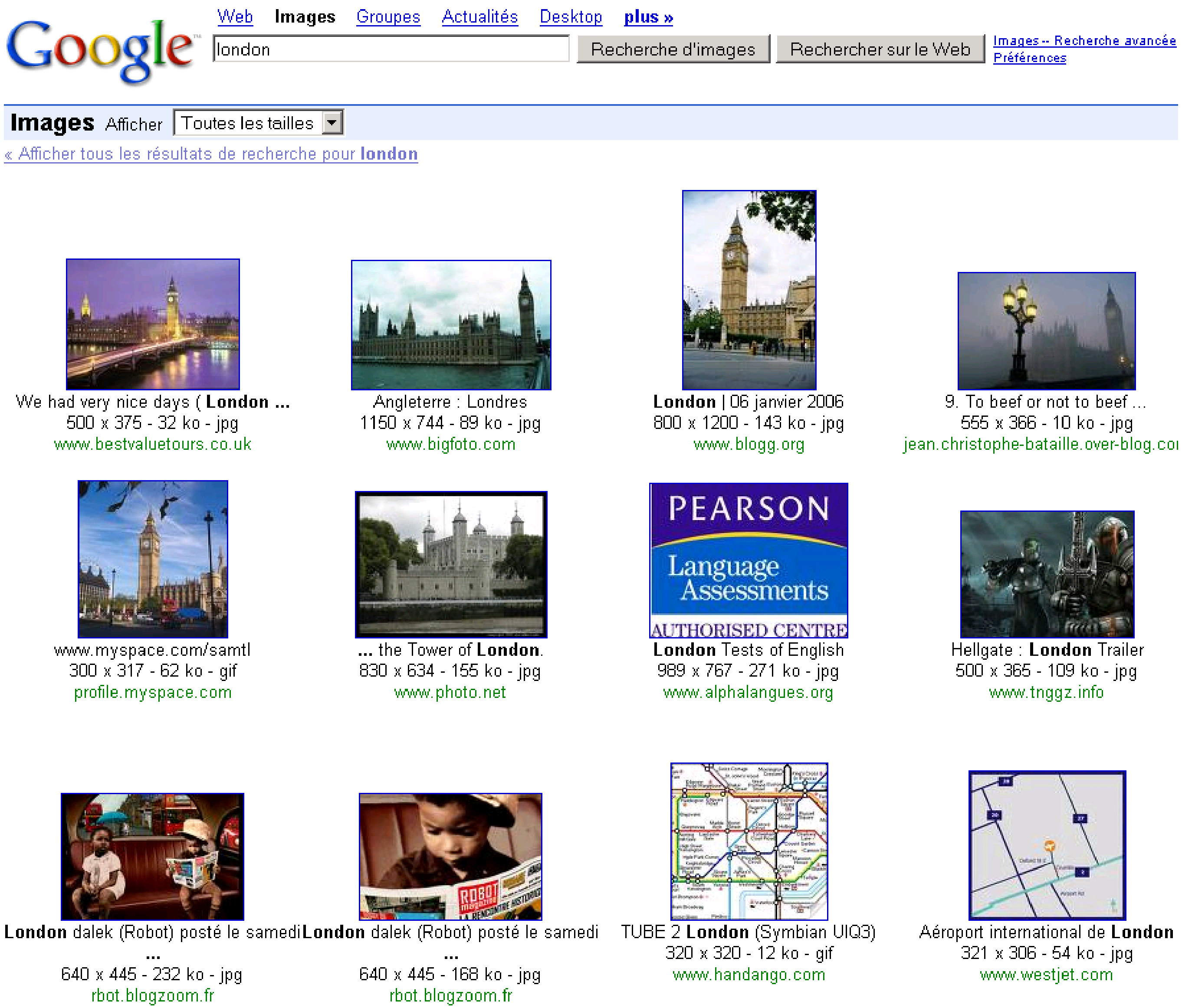

Image retrieval

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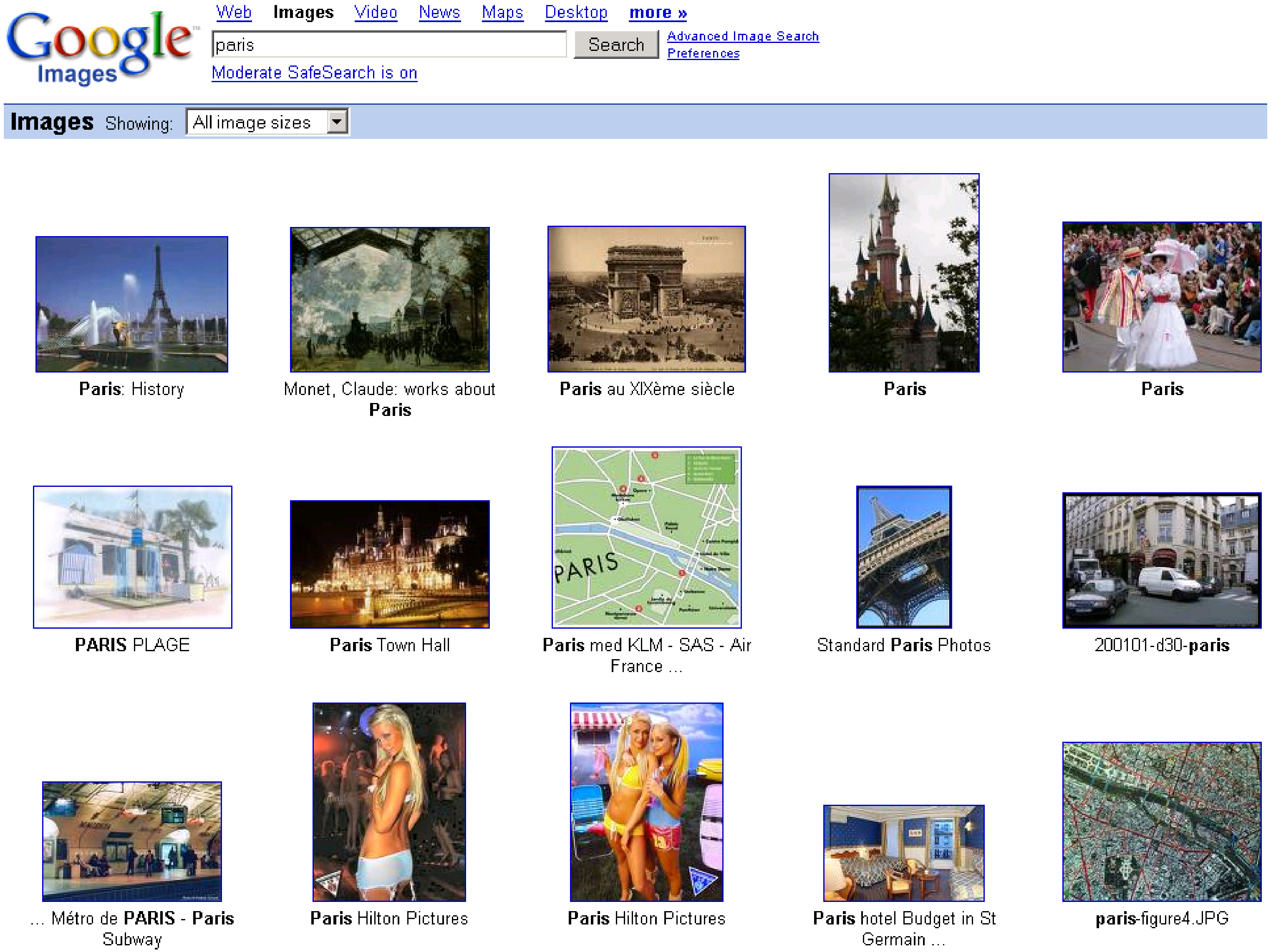


Image annotation
Classification, clustering

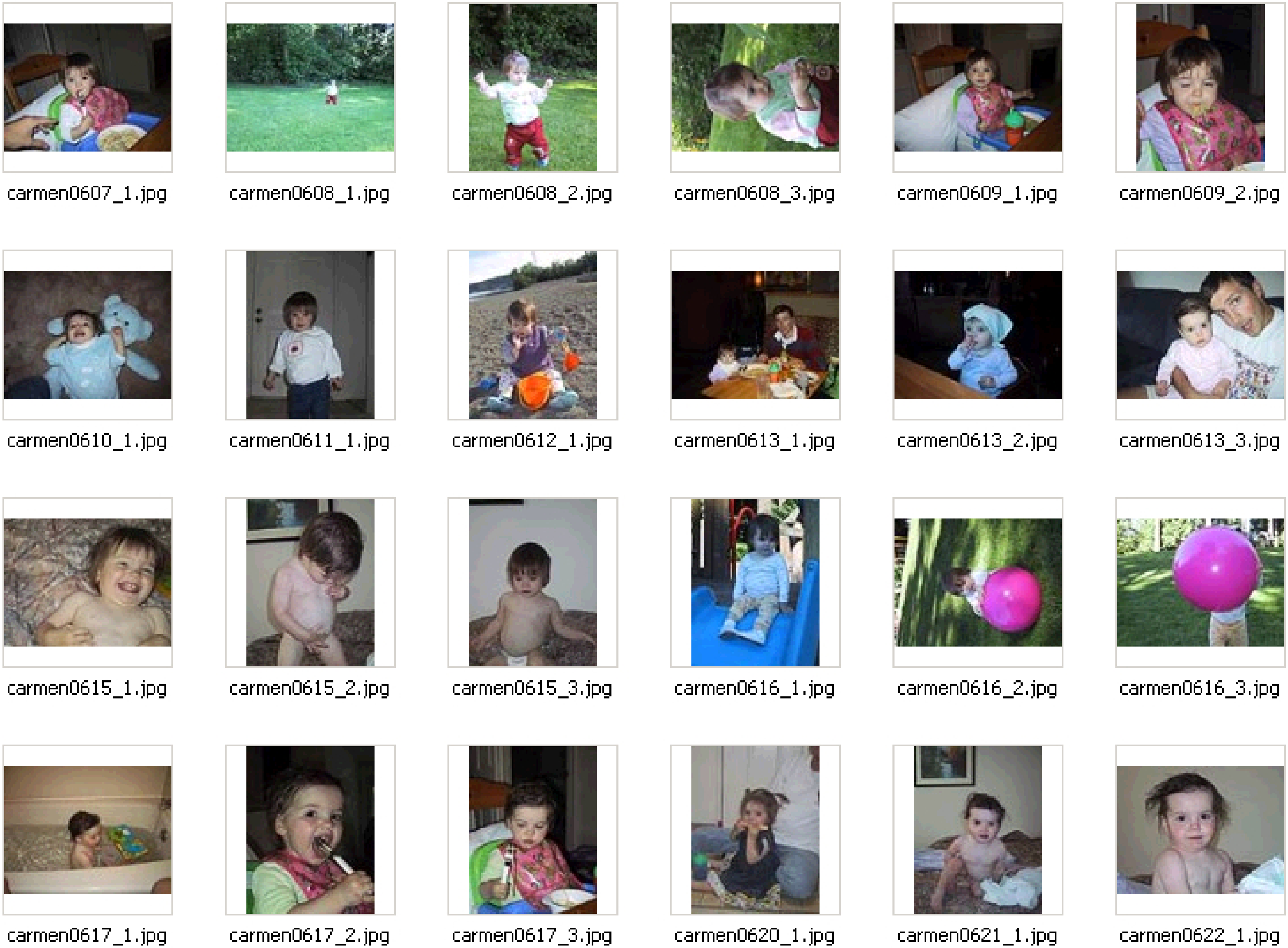





Object recognition ⇒ Multi-label classification

Personal photos

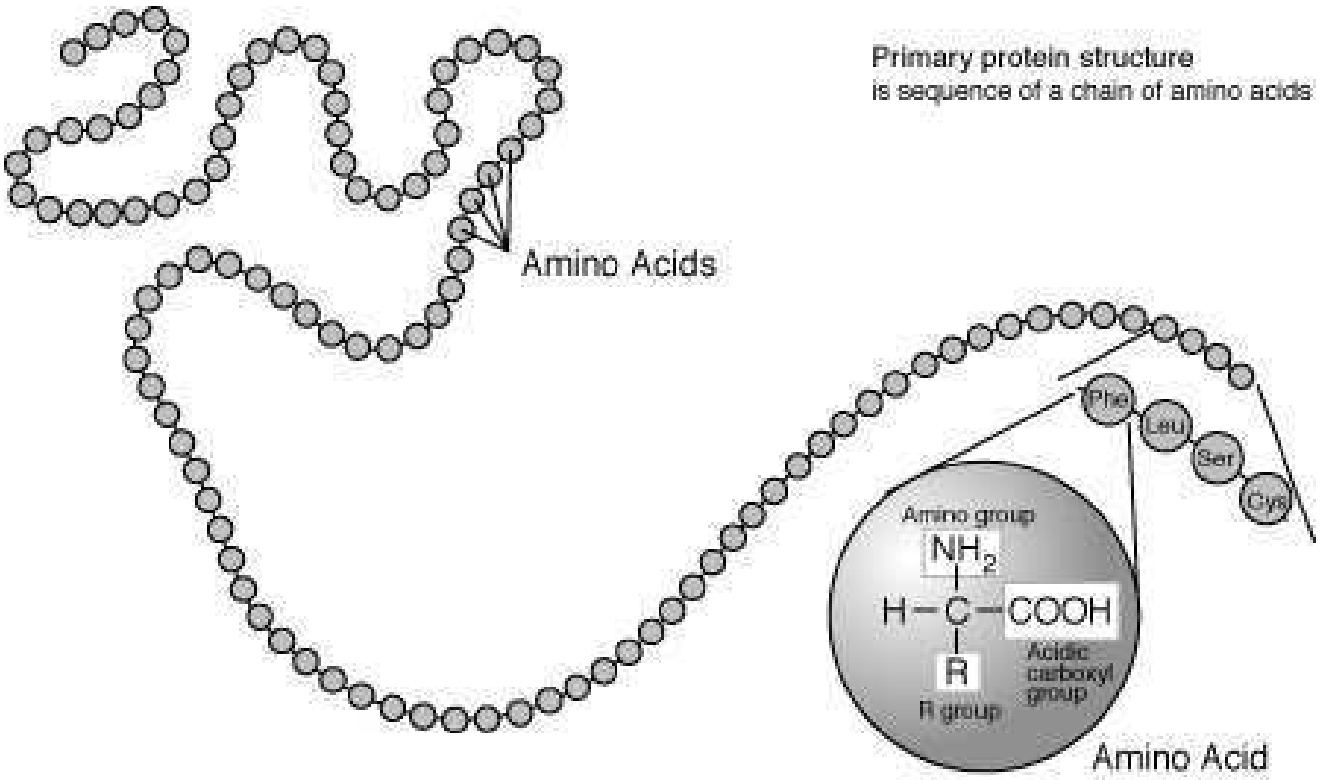
⇒ Classification, clustering, visualization



Machine learning for computer vision

- Multiplication of digital media
- Many different tasks to be solved
  - Associated with different machine learning problems
  - Massive data to learn from
- Similar situations in many fields (e.g., bioinformatics)

Machine learning for bioinformatics (e.g., proteins)



1. Many learning tasks on proteins
   - Classification into functional or structural classes
   - Prediction of cellular localization and interactions

2. Massive data

Machine learning for computer vision

- Multiplication of digital media
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  - Associated with different machine learning problems
  - Massive data to learn from
- Similar situations in many fields (e.g., bioinformatics)

  $\Rightarrow$ **Machine learning for high-dimensional data**

Supervised learning and regularization

- Data: $x_i \in \mathcal{X}$, $y_i \in \mathcal{Y}$, $i = 1, \dots, n$
- Minimize with respect to function $f \in \mathcal{F}$:

$$\sum_{i=1}^{n} \ell(y_i, f(x_i)) \qquad + \qquad \frac{\lambda}{2} \|f\|^2$$

Error on data + Regularization

Loss & function space ? Norm ?

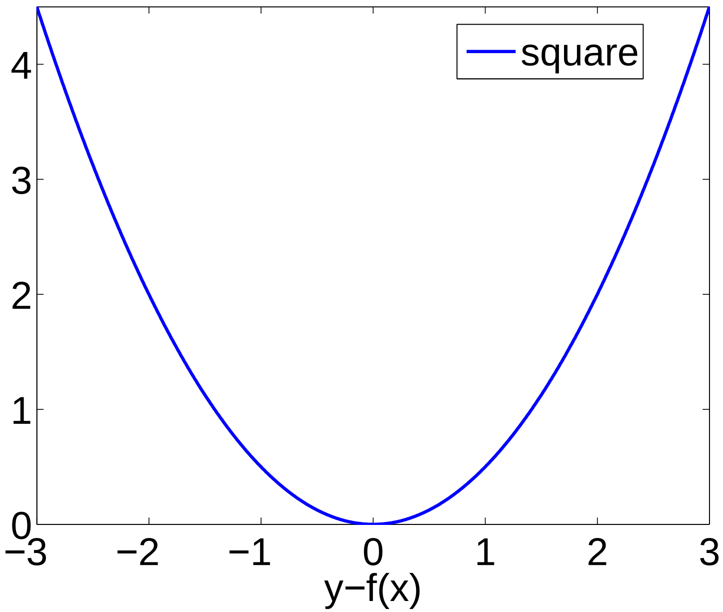
- Two theoretical/algorithmic issues:
  - Loss
  - Function space / norm

Course outline

1. **Losses for particular machine learning tasks**
   - Classification, regression, etc...
2. **Regularization by Hilbert norms (kernel methods)**
   - Kernels and representer theorem
   - Convex duality, optimization and algorithms
   - Kernel methods
   - Kernel design
3. **Regularization by sparsity-inducing norms**
   - ℓ_1-norm regularization
   - Multiple kernel learning
   - Theoretical results
   - Learning on matrices

Losses for regression (Shawe-Taylor and Cristianini, 2004)

- **Response**: $y \in \mathbb{R}$, prediction $\hat{y} = f(x)$,
  - quadratic (square) loss $\ell(y, f(x)) = \frac{1}{2}(y - f(x))^2$
  - Not many reasons to go beyond square loss!



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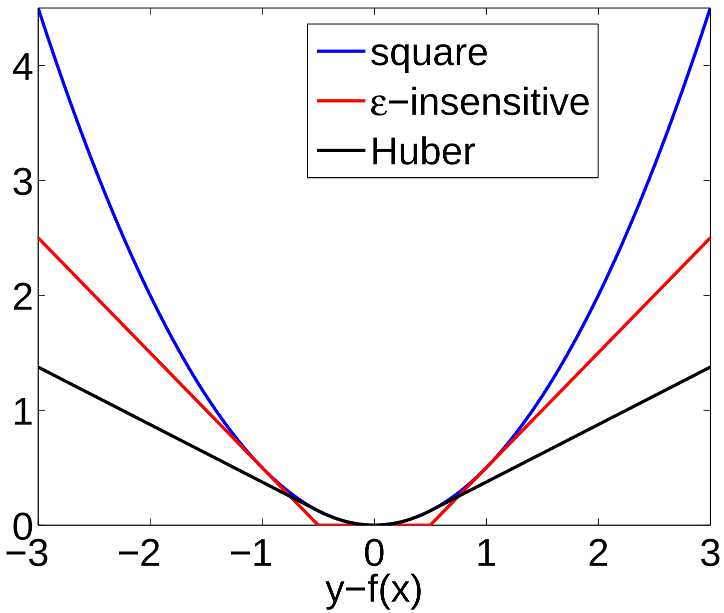
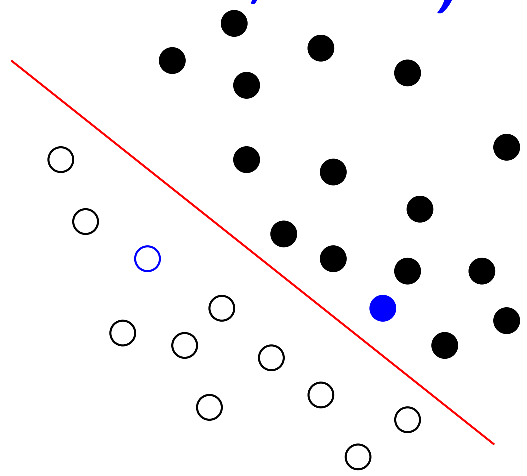
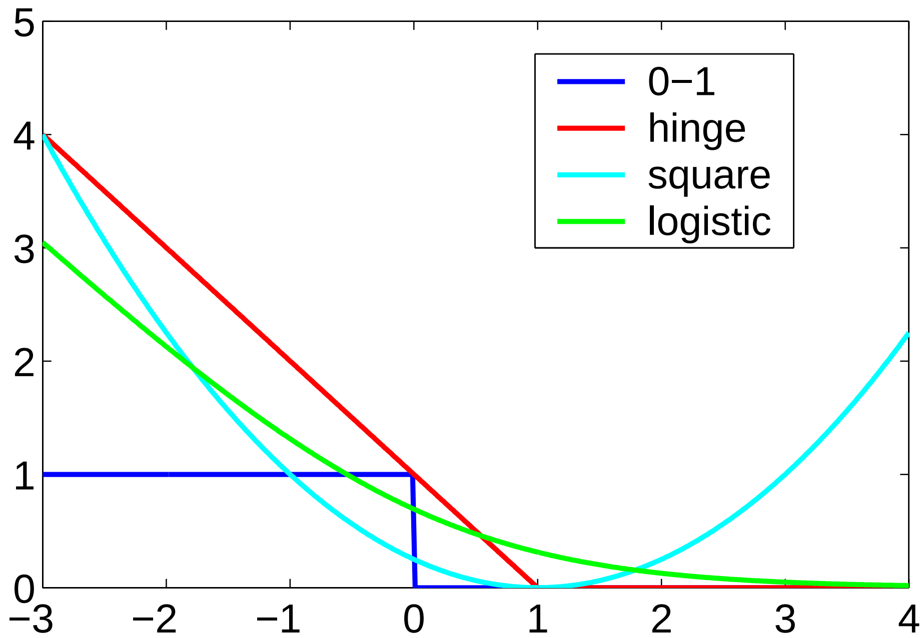
- Other convex losses "with added benefits"
  - ε-insensitive loss $\ell(y, f(x)) = (|y - f(x)| - \varepsilon)_+$
  - Hüber loss (mixed quadratic/linear): robustness to outliers



Losses for classification (Shawe-Taylor and Cristianini, 2004)



- **Label** : $y \in \{-1, 1\}$, prediction $\hat{y} = \text{sign}(f(x))$
  - loss of the form $\ell(y, f(x)) = \ell(yf(x))$
  - "True" cost: $\ell(yf(x)) = 1_{yf(x)<0}$
  - Usual convex costs:



- **Differences between hinge and logistic loss: differentiability/sparsity**

Image annotation $\Rightarrow$ multi-class classification





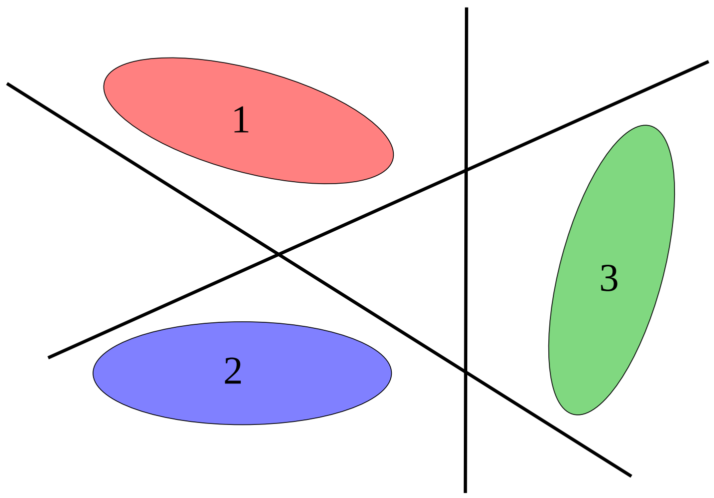

Losses for multi-label classification (Schölkopf and Smola, 2001; Shawe-Taylor and Cristianini, 2004)

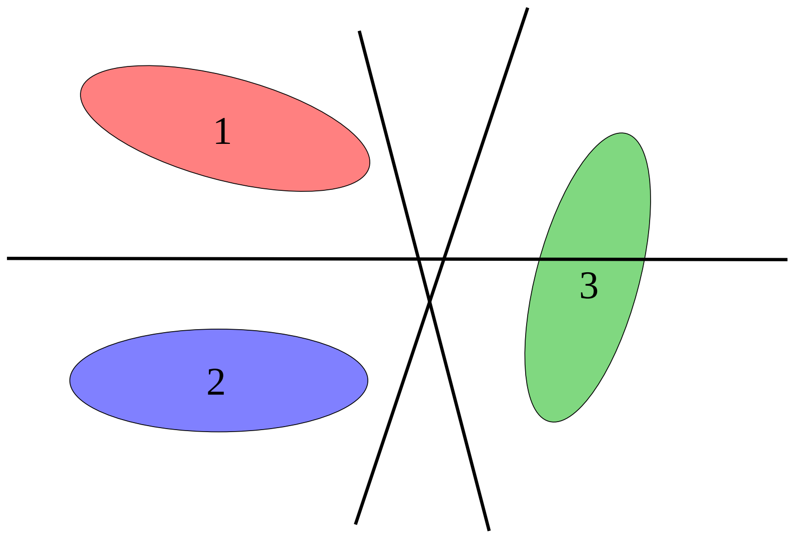
- **Two main strategies** for k classes (with unclear winners)

1. Using existing binary classifiers (efficient code!) $+$ voting schemes
   - "one-vs-rest" : learn k classifiers on the entire data
   - "one-vs-one" : learn $k(k-1)/2$ classifiers on portions of the data

Losses for multi-label classification - Linear predictors

- Using binary classifiers (left: “one-vs-rest”, right: “one-vs-one”)





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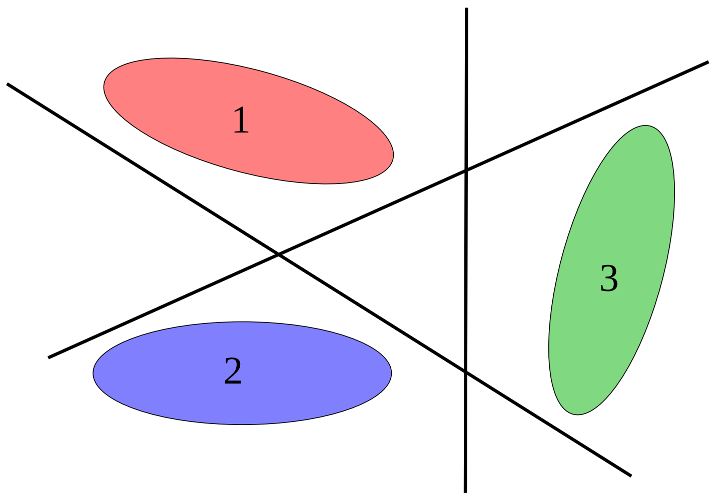
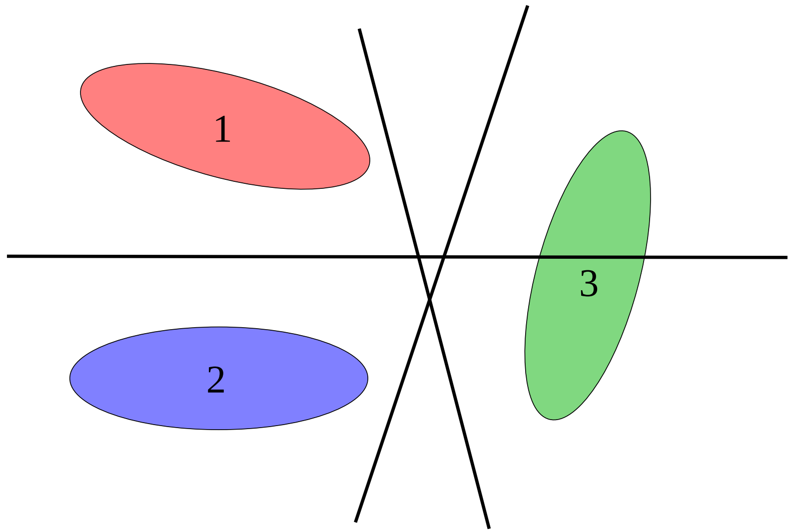
   - "one-vs-rest" : learn k classifiers on the entire data
   - "one-vs-one" : learn $k(k-1)/2$ classifiers on portions of the data
2. Dedicated loss functions for prediction using $\arg\max_{i \in \{1,\dots,k\}} f_i(x)$
   - Softmax regression: loss $= -\log(e^{f_y(x)} / \sum_{i=1}^k e^{f_i(x)})$
   - Multi-class SVM - 1: loss $= \sum_{i=1}^k (1 + f_i(x) - f_y(x))_+$
   - Multi-class SVM - 2: loss $= \max_{i \in \{1,\dots,k\}} (1 + f_i(x) - f_y(x))_+$

- Strategies do not consider same predicting functions

Losses for multi-label classification - Linear predictors

- Using binary classifiers (left: "one-vs-rest", right: "one-vs-one")





- Dedicated loss function

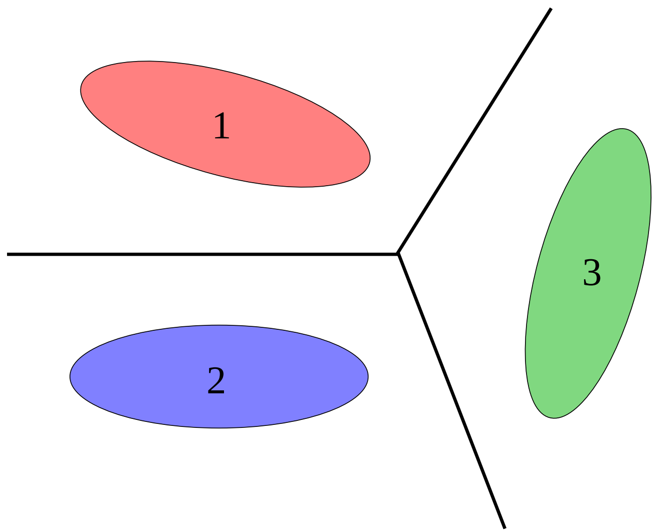


Image retrieval ⇒ ranking

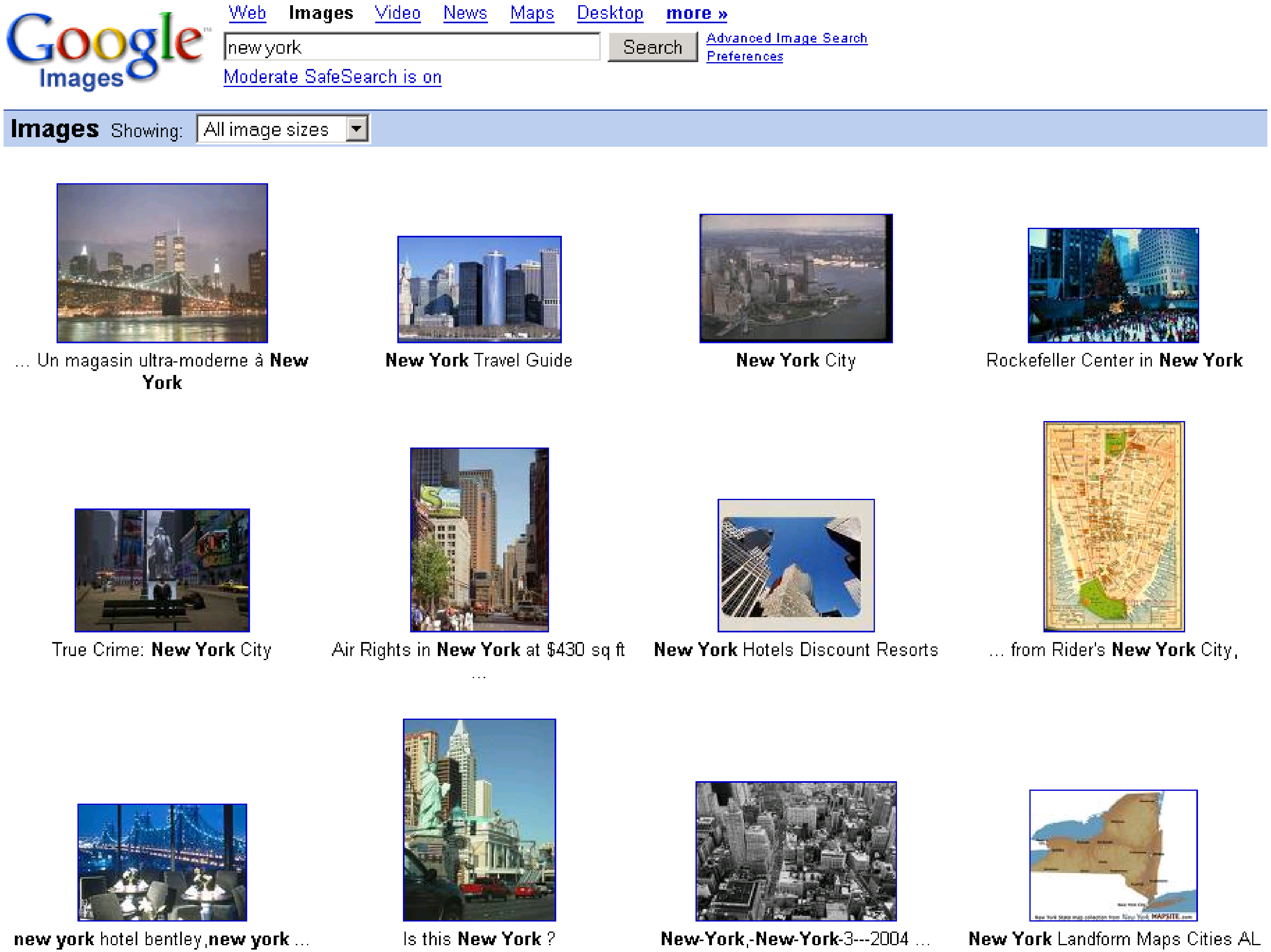
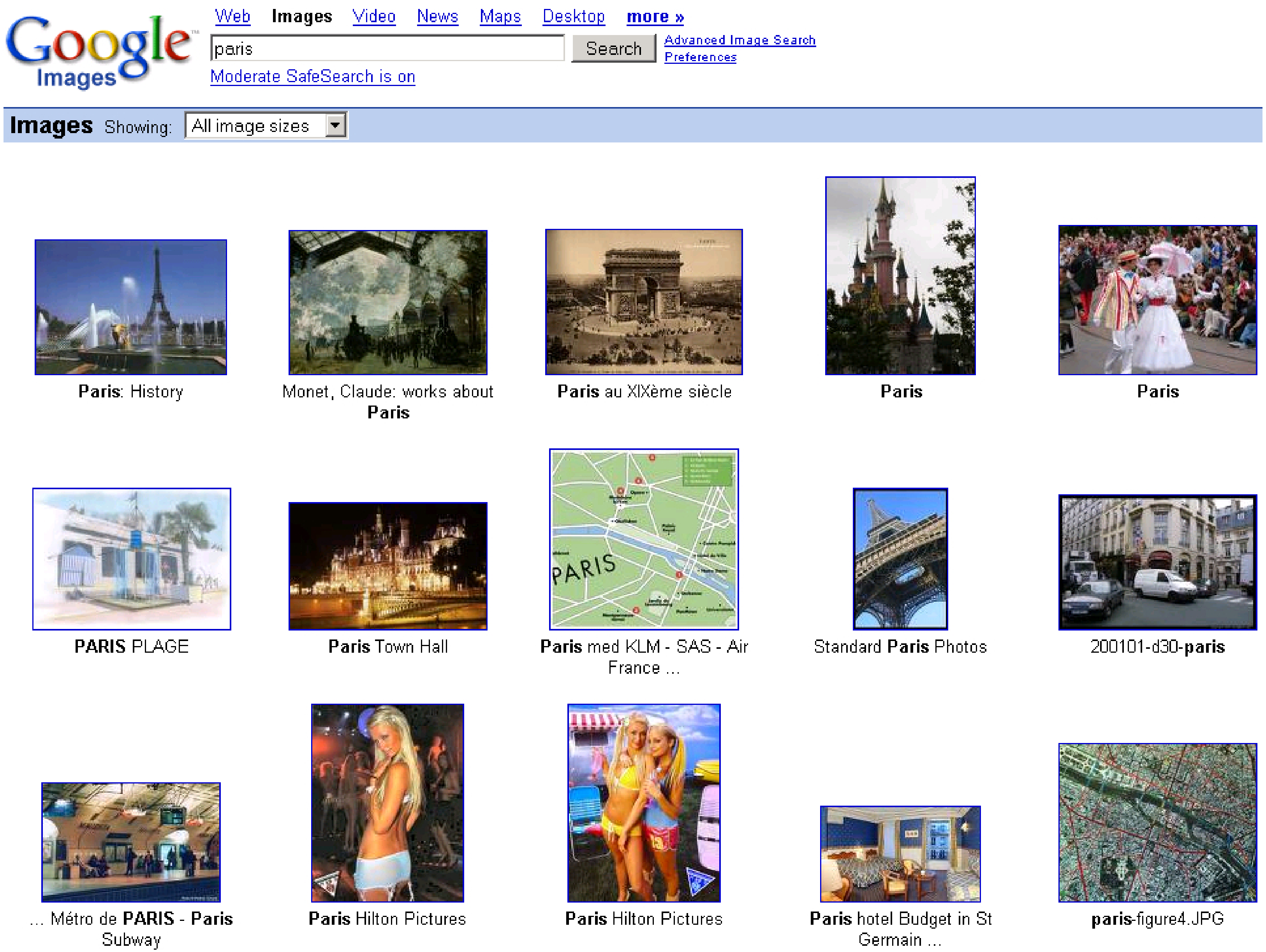


Image retrieval ⇒ outlier/novelty detection



Losses for ther tasks

- Outlier detection (Schölkopf et al., 2001; Vert and Vert, 2006)
  - one-class SVM: learn only with positive examples
- Ranking
  - simple trick: transform into learning on pairs (Herbrich et al., 2000), i.e., predict $\{x > y\}$ or $\{x \leqslant y\}$
  - More general "structured output methods" (Joachims, 2002)
- General structured outputs
  - Very active topic in machine learning and computer vision
  - see, e.g., Taskar (2005)

Dealing with asymmetric cost or unbalanced data in binary classification

- Two cases with similar issues:
  - Asymmetric cost (e.g., spam filterting, detection)
  - Unbalanced data, e.g., lots of positive examples (example: detection)

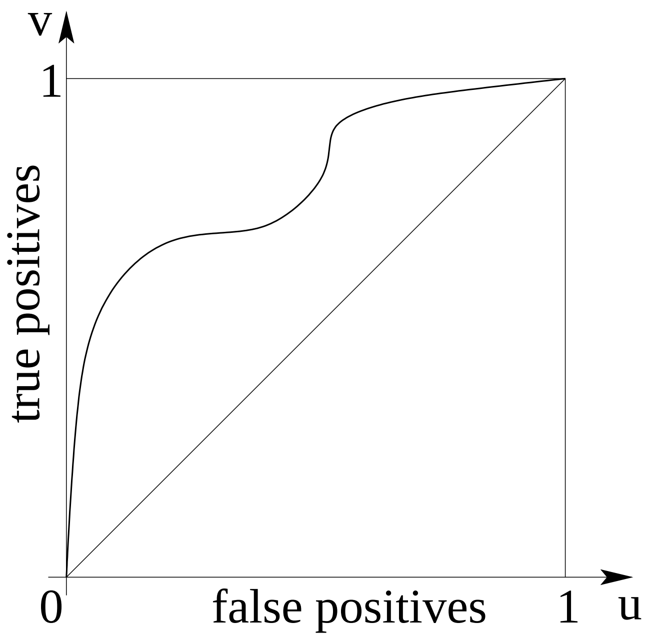
- **One number is not enough to characterize the asymmetric properties**
  - ROC curves (Flach, 2003) – cf. precision-recall curves

- Training using asymmetric losses (Bach et al., 2006)

$$\min_{f \in \mathcal{F}} \quad C_+ \sum_{i, y_i = 1} \ell(y_i f(x_i)) + C_- \sum_{i, y_i = -1} \ell(y_i f(x_i)) + \|f\|^2$$

ROC curves

- ROC plane (u, v)
- $u =$ proportion of false positives $= P(f(x) = 1|y = -1)$
- $v =$ proportion of true positives $= P(f(x) = 1|y = 1)$
- Plot a set of classifiers $f_\gamma(x)$ for $\gamma \in \mathbb{R}$



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Regularizations

- Main goal: avoid overfitting (see course by Jean-Yves Audibert)

- Two main lines of work:

  1. Use Hilbertian (RKHS) norms
     - Non parametric supervised learning and kernel methods
     - Well developped theory (Schölkopf and Smola, 2001; Shawe-Taylor and Cristianini, 2004; Wahba, 1990)
  2. Use "sparsity inducing" norms
     - main example: ℓ_1-norm $\|w\|_1 = \sum_{i=1}^p |w_i|$
     - Perform model selection as well as regularization
     - Theory "in the making"

- **Goal of (this part of) the course: Understand how and when to use these different norms**

Kernel methods for machine learning

- **Definition**: given a set of objects $\mathcal{X}$, a positive definite kernel is a symmetric function $k(x, x')$ such that for all finite sequences of points $x_i \in \mathcal{X}$ and $\alpha_i \in \mathbb{R}$,

$$\sum_{i,j} \alpha_i \alpha_j k(x_i, x_j) \geqslant 0$$

  (i.e., the matrix $(k(x_i, x_j))$ is symmetric positive semi-definite)

- Main example: $k(x, x') = \langle \Phi(x), \Phi(x') \rangle$

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(i.e., the matrix $(k(x_i,x_j))$ is symmetric positive semi-definite)

- **Aronszajn theorem** (Aronszajn, 1950): k is a positive definite kernel if and only if there exists a Hilbert space $\mathcal{F}$ and a mapping $\Phi : \mathcal{X} \mapsto \mathcal{F}$ such that

$$\forall (x,x') \in \mathcal{X}^2, \; k(x,x') = \langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}}$$

- $\mathcal{X}$ = "input space", $\mathcal{F}$ = "feature space", Φ = "feature map"

- Functional view: reproducing kernel Hilbert spaces

Classical kernels: kernels on vectors $x \in \mathbb{R}^d$

- Linear kernel $k(x, y) = x^\top y$
  - $\Phi(x) = x$
- Polynomial kernel $k(x, y) = (1 + x^\top y)^d$
  - $\Phi(x) =$ monomials
- Gaussian kernel $k(x, y) = \exp(-\alpha \|x - y\|^2)$
  - $\Phi(x) = ??$
- PROOF

Reproducing kernel Hilbert spaces

- Assume k is a positive definite kernel on $\mathcal{X} \times \mathcal{X}$
- **Aronszajn theorem** (1950): there exists a Hilbert space $\mathcal{F}$ and a mapping $\Phi : \mathcal{X} \mapsto \mathcal{F}$ such that

$$\forall (x, x') \in \mathcal{X}^2, \ \ k(x, x') = \langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}}$$

- $\mathcal{X}$ = "input space", $\mathcal{F}$ = "feature space", Φ = "feature map"
- RKHS: particular instantiation of $\mathcal{F}$ as a function space
  - $\Phi(x) = k(\cdot, x)$
  - function evaluation $\boxed{f(x) = \langle f, \Phi(x) \rangle}$
  - reproducing property: $k(x, y) = \langle k(\cdot, x), k(\cdot, y) \rangle$
- Notations : $f(x) = \langle f, \Phi(x) \rangle = f^\top \Phi(x)$, $\|f\|^2 = \langle f, f \rangle$

Classical kernels: kernels on vectors $x \in \mathbb{R}^d$

- Linear kernel $k(x,y) = x^\top y$
  - Linear functions
- Polynomial kernel $k(x,y) = (1 + x^\top y)^d$
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- Gaussian kernel $k(x,y) = \exp(-\alpha \|x-y\|^2)$
  - Smooth functions

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- Gaussian kernel $k(x, y) = \exp(-\alpha \|x - y\|^2)$
  - Smooth functions
- **Parameter selection? Structured domain?**

Regularization and representer theorem

- Data: $x_i \in \mathcal{X}$, $y_i \in \mathcal{Y}$, $i = 1, \dots, n$, kernel k (with RKHS $\mathcal{F}$)

- Minimize with respect to f: $\boxed{\min_{f \in \mathcal{F}} \sum_{i=1}^n \ell(y_i, f^\top \Phi(x_i)) + \frac{\lambda}{2} \|f\|^2}$

- No assumptions on cost ℓ or n

- **Representer theorem** (Kimeldorf and Wahba, 1971): optimum is reached for weights of the form
$$f = \sum_{j=1}^n \alpha_j \Phi(x_j) = \sum_{j=1}^n \alpha_j k(\cdot, x_j)$$

- PROOF

Regularization and representer theorem

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$$f = \sum_{j=1}^n \alpha_j \Phi(x_j) = \sum_{j=1}^n \alpha_j k(\cdot, x_j)$$
- $\alpha \in \mathbb{R}^n$ dual parameters, $K \in \mathbb{R}^{n \times n}$ kernel matrix:
$$K_{ij} = \Phi(x_i)^\top \Phi(x_j) = k(x_i, x_j)$$
- Equivalent problem: $\boxed{\min_{\alpha \in \mathbb{R}^n} \sum_{i=1}^n \ell(y_i, (K\alpha)_i) + \frac{\lambda}{2} \alpha^\top K \alpha}$

Kernel trick and modularity

- Kernel trick: any algorithm for finite-dimensional vectors that only uses pairwise dot-products can be applied in the feature space.
  - Replacing dot-products by kernel functions
  - Implicit use of (very) large feature spaces
  - Linear to non-linear learning methods

Kernel trick and modularity

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- Modularity of kernel methods
  1. Work on new algorithms and theoretical analysis
  2. Work on new kernels for specific data types

Representer theorem and convex duality

- The parameters $\alpha \in \mathbb{R}^n$ may also be interpreted as Lagrange multipliers

- Assumption: cost function is convex, $\varphi_i(u_i) = \ell(y_i, u_i)$

- Primal problem: $\boxed{\min_{f \in \mathcal{F}} \sum_{i=1}^n \varphi_i(f^\top \Phi(x_i)) + \frac{\lambda}{2}\|f\|^2}$

- What about the constant term b? replace $\Phi(x)$ by $(\Phi(x), c)$, c large

	$\varphi_i(u_i)$
LS regression	$\frac{1}{2}(y_i - u_i)^2$
Logistic regression	$\log(1 + \exp(-y_i u_i))$
SVM	$(1 - y_i u_i)_+$

Representer theorem and convex duality
Proof

- Primal problem: $\boxed{\min_{f \in \mathcal{F}} \sum_{i=1}^n \varphi_i(f^\top \Phi(x_i)) + \frac{\lambda}{2}\|f\|^2}$

- Define $\psi_i(v_i) = \max_{u_i \in \mathbb{R}} v_i u_i - \varphi_i(u_i)$ as the *Fenchel conjugate* of φ_i

- Main trick: introduce constraint $u_i = f^\top \Phi(x_i)$ and associated Lagrange multipliers α_i

- Lagrangian $\mathcal{L}(\alpha, f) = \displaystyle\sum_{i=1}^n \varphi_i(u_i) + \frac{\lambda}{2}\|f\|^2 + \lambda \sum_{i=1}^n \alpha_i(u_i - f^\top \Phi(x_i))$

  – Maximize with respect to $u_i \Rightarrow$ term of the form $-\psi_i(-\lambda \alpha_i)$
  – Maximize with respect to $f \Rightarrow f = \sum_{i=1}^n \alpha_i \Phi(x_i)$

Representer theorem and convex duality

- Assumption: cost function is convex $\varphi_i(u_i) = \ell(y_i, u_i)$
- Primal problem: $\boxed{\min_{f \in \mathcal{F}} \sum_{i=1}^n \varphi_i(f^\top \Phi(x_i)) + \frac{\lambda}{2} \|f\|^2}$
- Dual problem: $\boxed{\max_{\alpha \in \mathbb{R}^n} - \sum_{i=1}^n \psi_i(-\lambda \alpha_i) - \frac{\lambda}{2} \alpha^\top K \alpha}$

  where $\psi_i(v_i) = \max_{u_i \in \mathbb{R}} v_i u_i - \varphi_i(u_i)$ is the Fenchel conjugate of φ_i
- Strong duality
- Relationship between primal and dual variables (at optimum):
$$f = \sum_{i=1}^n \alpha_i \Phi(x_i)$$
- NB: adding constant term $b \Leftrightarrow$ add constraints $\sum_{i=1}^n \alpha_i = 0$

“Classical” kernel learning (2-norm regularization)

Primal problem	$\min_{f \in \mathcal{F}} \left(\sum_i \varphi_i(f^\top \Phi(x_i)) + \frac{\lambda}{2} \|\|f\|\|^2 \right)$
Dual problem	$\max_{\alpha \in \mathbb{R}^n} \left(-\sum_i \psi_i(\lambda \alpha_i) - \frac{\lambda}{2} \alpha^\top K \alpha \right)$
Optimality conditions	$f = \sum_{i=1}^n \alpha_i \Phi(x_i)$

- Assumptions on loss φ_i:
  - $\varphi_i(u)$ convex
  - $\psi_i(v)$ Fenchel conjugate of $\varphi_i(u)$, i.e., $\psi_i(v) = \max_{u \in \mathbb{R}} (vu - \varphi_i(u))$

	$\varphi_i(u_i)$	$\psi_i(v)$
LS regression	$\frac{1}{2}(y_i - u_i)^2$	$\frac{1}{2}v^2 + vy_i$
Logistic regression	$\log(1 + \exp(-y_i u_i))$	$(1+vy_i)\log(1+vy_i) - vy_i \log(-vy_i)$
SVM	$(1 - y_i u_i)_+$	$vy_i \times 1_{-vy_i \in [0,1]}$

Particular case of the support vector machine

- Primal problem: $\boxed{\min_{f \in \mathcal{F}} \sum_{i=1}^n (1 - y_i f^\top \Phi(x_i))_+ + \frac{\lambda}{2} \|f\|^2}$

- Dual problem: $\boxed{\max_{\alpha \in \mathbb{R}^n} \left(- \sum_i \lambda \alpha_i y_i \times 1_{-\lambda \alpha_i y_i \in [0,1]} - \frac{\lambda}{2} \alpha^\top K \alpha \right)}$

- Dual problem (by change of variable $\alpha \leftarrow -\operatorname{Diag}(y)\alpha$ and $C = 1/\lambda$):

$$\boxed{\max_{\alpha \in \mathbb{R}^n,\ 0 \leqslant \alpha \leqslant C} \sum_{i=1}^n \alpha_i - \frac{1}{2} \alpha^\top \operatorname{Diag}(y) K \operatorname{Diag}(y) \alpha}$$

Particular case of the support vector machine

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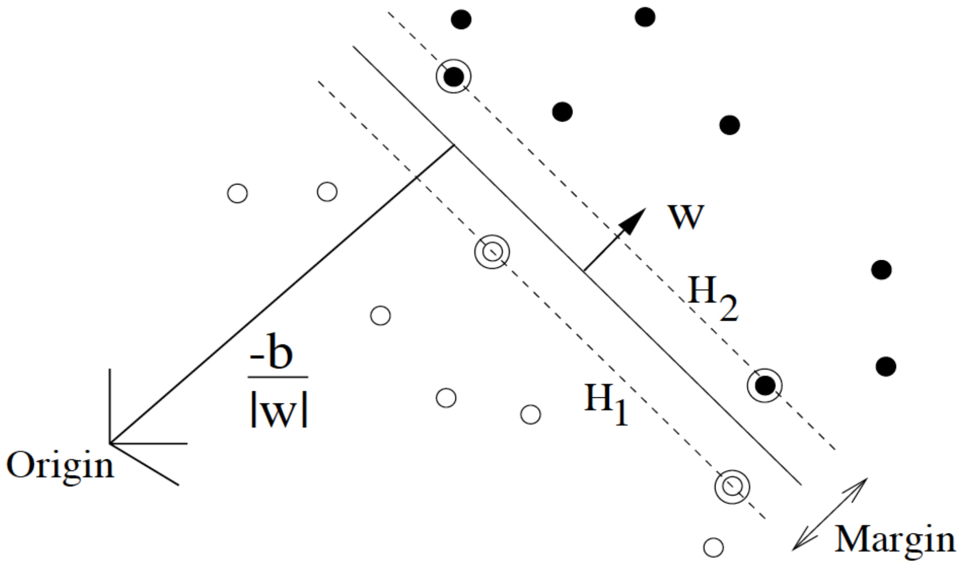
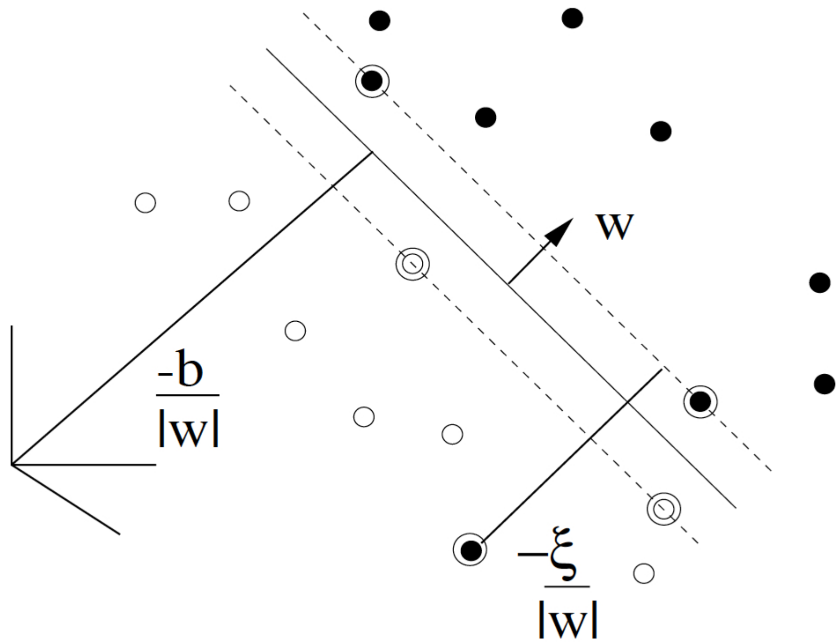
- What about the traditional picture?





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Kernel ridge regression (a.k.a spline smoothing) - I

- Data $x_1, \dots, x_n \in \mathcal{X}$, p.d. kernl k, $y_1, \dots, y_n \in \mathbb{R}$

- Least-squares

$$\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2 + \lambda \|f\|_{\mathcal{F}}^2$$

- View 1: representer theorem $\Rightarrow f = \sum_{i=1}^{n} \alpha_i k(\cdot, x_i)$
  - equivalent to

$$\min_{\alpha \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^{n} (y_i - (K\alpha)_i)^2 + \lambda \alpha^\top K \alpha$$

  - Solution equal to $\alpha = (K + n\lambda I)^{-1} y + \varepsilon$ with $K\varepsilon = 0$
  - Unique solution f

Kernel ridge regression (a.k.a spline smoothing) - II

- Links with spline smoothing

- Other view: $\mathcal{F} \in \mathbb{R}^d$, $\Phi \in \mathbb{R}^{n \times d}$

$$\min_{w \in \mathbb{R}^d} \frac{1}{n} \|y - \Phi w\|^2 + \lambda \|w\|^2$$

- Solution equal to $w = (\Phi^\top \Phi + n\lambda I)^{-1} \Phi^\top y$

- Note that $w = \Phi^\top (\Phi \Phi^\top + n\lambda I)^{-1} y$

- Φw equal to $K\alpha$

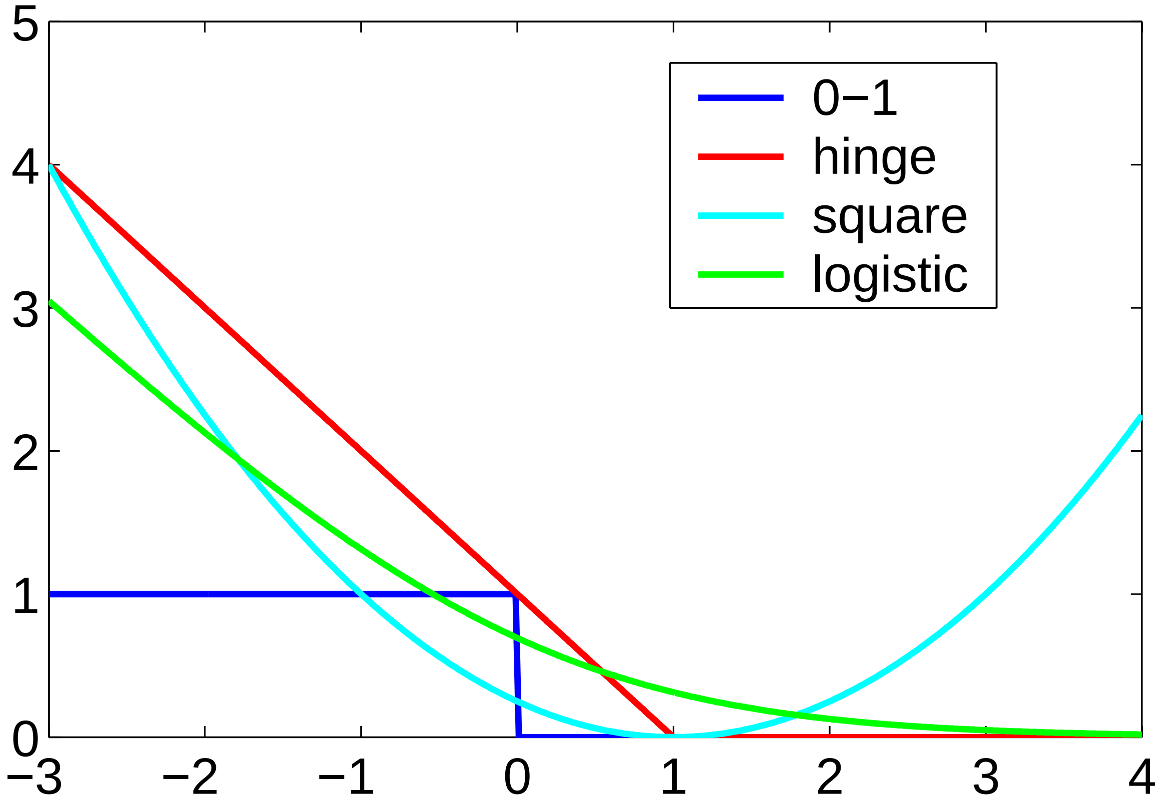
Kernel ridge regression (a.k.a spline smoothing) - III

- Dual view:
  - dual problem: $\max_{\alpha \in \mathbb{R}^n} -\frac{n\lambda}{2}\|\alpha\|^2 - \alpha^\top y - \frac{1}{2}\alpha^\top K \alpha$
  - solution: $\alpha = (K + \lambda I)^{-1} y$

- Warning: same solution obtained from different point of views

Losses for classification

- Usual convex costs:



- **Differences between hinge and logistic loss: differentiability/sparsity**

Support vector machine or logistic regression?

- Predictive performance is similar
- Only true difference is numerical
  - SVM: sparsity in α
  - Logistic: differentiable loss function
- Which one to use?
  - Linear kernel $\Rightarrow$ Logistic $+$ Newton/Gradient descent
  - Nonlinear kernel $\Rightarrow$ SVM $+$ dual methods or simpleSVM

Algorithms for supervised kernel methods

- Four formulations
  1. Dual: $\max_{\alpha \in \mathbb{R}^n} - \sum_i \psi_i(\lambda \alpha_i) - \frac{\lambda}{2} \alpha^\top K \alpha$
  2. Primal: $\min_{f \in \mathcal{F}} \sum_i \varphi_i(f^\top \Phi(x_i)) + \frac{\lambda}{2} ||f||^2$
  3. Primal + Representer: $\min_{\alpha \in \mathbb{R}^n} \sum_i \varphi_i((K\alpha)_i) + \frac{\lambda}{2} \alpha^\top K \alpha$
  4. Convex programming

- **Best strategy depends on loss (differentiable or not) and kernel (linear or not)**

Dual methods

- Dual problem: $\max_{\alpha \in \mathbb{R}^n} - \sum_i \psi_i(\lambda \alpha_i) - \frac{\lambda}{2} \alpha^\top K \alpha$

- Main method: coordinate descent (a.k.a. sequential minimal optimization - SMO) (Platt, 1998; Bottou and Lin, 2007; Joachims, 1998)
  - Efficient when loss is piecewise quadratic (i.e., hinge = SVM)
  - Sparsity may be used in the case of the SVM

- Computational complexity: between quadratic and cubic in n

- **Works for all kernels**

Primal methods

- Primal problem: $\min_{f \in \mathcal{F}} \sum_i \varphi_i(f^\top \Phi(x_i)) + \frac{\lambda}{2} ||f||^2$

- Only works directly if $\Phi(x)$ may be built explicitly and has small dimension
  - Example: linear kernel in small dimensions

- Differentiable loss: gradient descent or Newton's method are very efficient in small dimensions

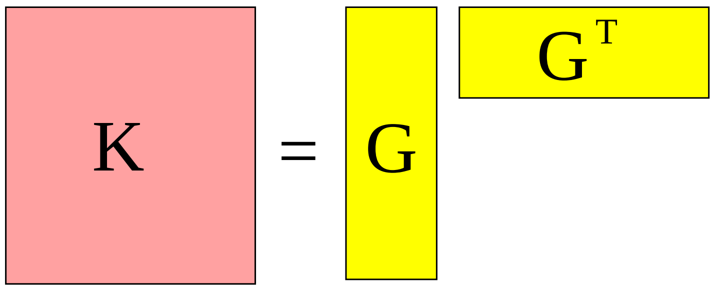
- Larger scale: stochastic gradient descent (Shalev-Shwartz et al., 2007; Bottou and Bousquet, 2008)

Primal methods with representer theorems

- Primal problem in α: $\min_{\alpha \in \mathbb{R}^n} \sum_i \varphi_i((K\alpha)_i) + \frac{\lambda}{2} \alpha^\top K \alpha$

- Direct optimization in α poorly conditioned (K has low-rank) unless Newton method is used (Chapelle, 2007)

- General kernels: use incomplete Cholesky decomposition (Fine and Scheinberg, 2001; Bach and Jordan, 2002) to obtain a square root $K = GG^\top$



G of size $n \times m$,
where $m \ll n$

  - "Empirical input space" of size m obtained using rows of G
  - Running time to compute G: $O(m^2 n)$

Direct convex programming

- **Convex programming toolboxes $\Rightarrow$ very inefficient!**
- May use special structure of the problem
  - e.g., SVM and sparsity in α
- Active set method for the SVM: **SimpleSVM** (Vishwanathan et al., 2003; Loosli et al., 2005)
  - Cubic complexity in the number of support vectors
- Full regularization path for the SVM (Hastie et al., 2005; Bach et al., 2006)
  - Cubic complexity in the number of support vectors
  - May be extended to other settings (Rosset and Zhu, 2007)

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   - Theoretical results
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Kernel methods - I

- Distances in the "feature space"

$$d_k(x,y)^2 = \|\Phi(x) - \Phi(y)\|_{\mathcal{F}}^2 = k(x,x) + k(y,y) - 2k(x,y)$$

- Nearest-neighbor classification/regression

Kernel methods - II
Simple discrimination algorithm

- Data $x_1, \ldots, x_n \in \mathcal{X}$, classes $y_1, \ldots, y_n \in \{-1, 1\}$
- Compare distances to mean of each class
- Equivalent to classifying x using the sign of

$$\frac{1}{\#\{i, y_i = 1\}} \sum_{i, y_i = 1} k(x, x_i) - \frac{1}{\#\{i, y_i = -1\}} \sum_{i, y_i = -1} k(x, x_i)$$

- Proof...
- Geometric interpretation of Parzen windows

Kernel methods - III
Data centering

- n points $x_1, \ldots, x_n \in \mathcal{X}$
- kernel matrix $K \in \mathbb{R}^n$, $K_{ij} = k(x_i, x_j) = \langle \Phi(x_i), \Phi(x_j) \rangle$
- Kernel matrix of centered data $\tilde{K}_{ij} = \langle \Phi(x_i) - \mu, \Phi(x_j) - \mu \rangle$ where $\mu = \frac{1}{n} \sum_{i=1}^n \Phi(x_i)$
- Formula: $\tilde{K} = \Pi_n K \Pi_n$ with $\Pi_n = I_n - \frac{E}{n}$, and E constant matrix equal to 1.
- Proof...
- NB: μ is not of the form $\Phi(z)$, $z \in \mathcal{X}$ (cf. preimage problem)

Kernel PCA

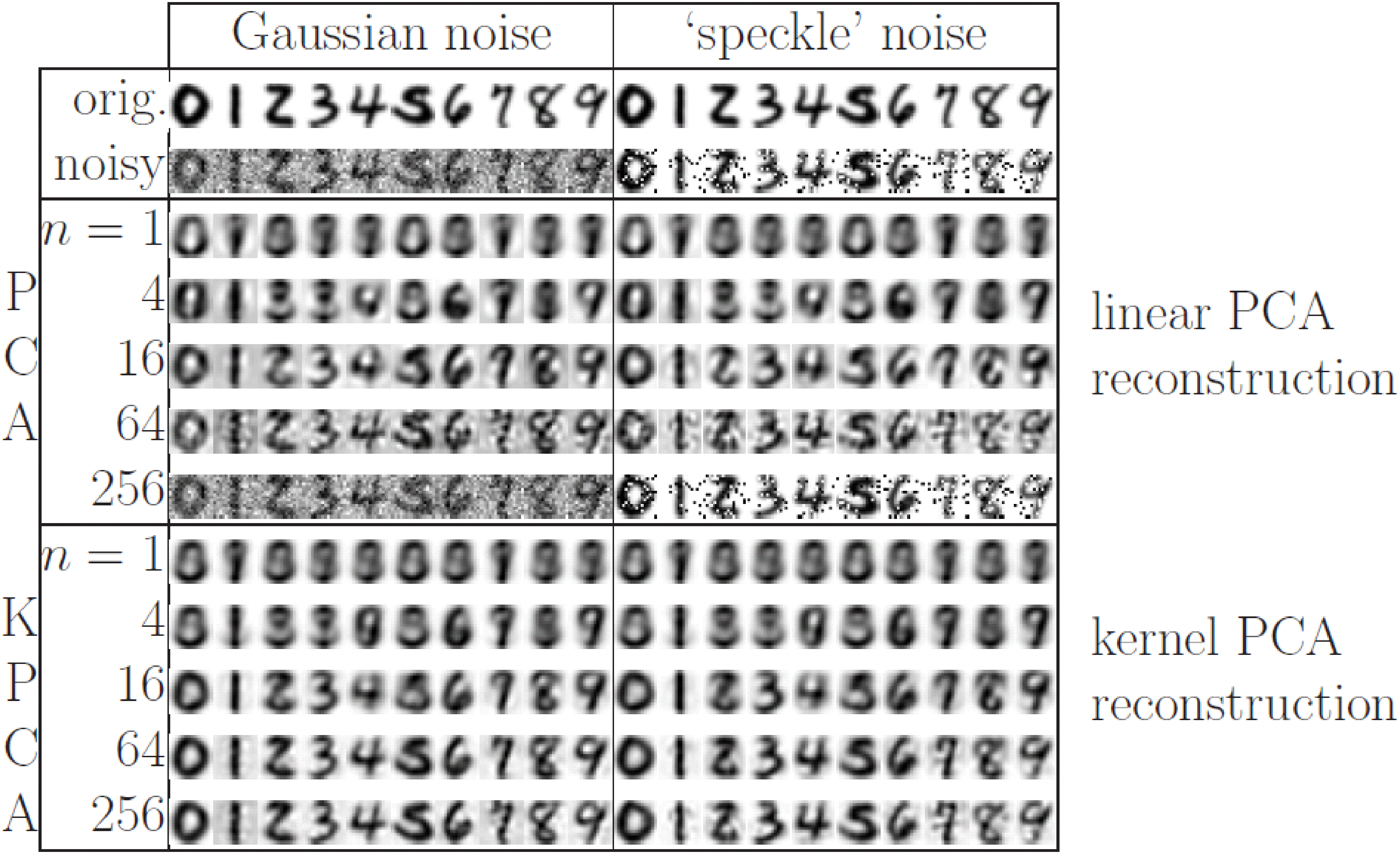
- Linear principal component analysis
  - data $x_1, \dots, x_n \in \mathbb{R}^p$,

$$\max_{w \in \mathbb{R}^p} \frac{w^\top \hat{\Sigma} w}{w^\top w} = \max_{w \in \mathbb{R}^p} \frac{\operatorname{var}(w^\top X)}{w^\top w}$$

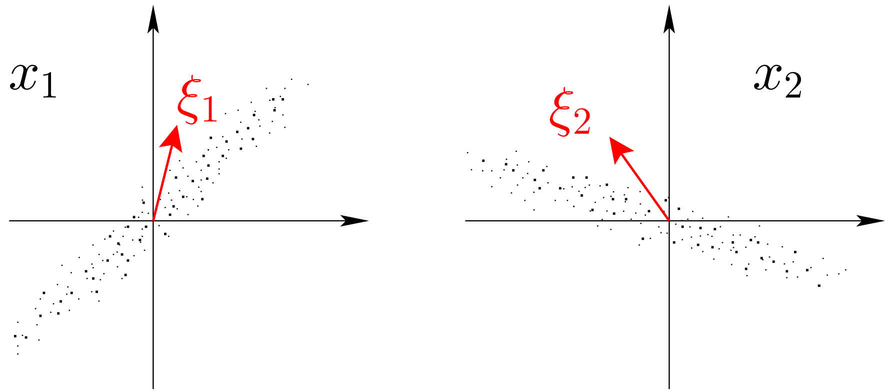
  - w is largest eigenvector of $\hat{\Sigma}$
  - Denoising, data representation

- Kernel PCA: data $x_1, \dots, x_n \in \mathcal{X}$, p.d. kernel k
  - View 1: $\max_{w \in \mathcal{F}} \frac{\operatorname{var}(\langle \Phi(X), w \rangle)}{w^\top w}$ View 2: $\max_{f \in \mathcal{F}} \frac{\operatorname{var}(f(X))}{\|f\|_{\mathcal{F}}^2}$
  - Solution: $f, w = \sum_{i=1}^n \alpha_i k(\cdot, x_i)$ and α first eigenvector of $\tilde{K} = \Pi_n K \Pi_n$
  - Interpretation in terms of covariance operators

Denoising with kernel PCA (From Schölkopf, 2005)



Canonical correlation analysis



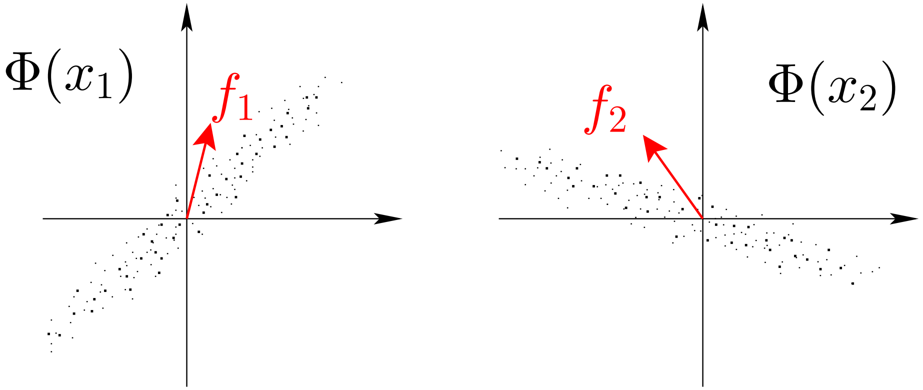
- Given two multivariate random variables x_1 and x_2, finds the pair of directions ξ_1, ξ_2 with maximum correlation:

$$\rho(x_1, x_2) = \max_{\xi_1, \xi_2} \operatorname{corr}(\xi_1^T x_1, \xi_2^T x_2) = \max_{\xi_1, \xi_2} \frac{\xi_1^T C_{12} \xi_2}{\left(\xi_1^T C_{11} \xi_1\right)^{1/2} \left(\xi_2^T C_{22} \xi_2\right)^{1/2}}$$

- Generalized eigenvalue problem:

$$\begin{pmatrix} 0 & C_{12} \\ C_{21} & 0 \end{pmatrix} \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix} = \rho \begin{pmatrix} C_{11} & 0 \\ 0 & C_{22} \end{pmatrix} \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}.$$

Canonical correlation analysis in feature space



- Given two random variables x_1 and x_2 and two RKHS $\mathcal{F}_1$ and $\mathcal{F}_2$, finds the pair of functions f_1, f_2 with maximum regularized correlation:

$$\max_{f_1, f_2 \in \mathcal{F}} \frac{\operatorname{cov}(f_1(X_1), f_2(X_2))}{(\operatorname{var}(f_1(X_1)) + \lambda_n \|f_1\|^2_{\mathcal{F}_1})^{1/2} (\operatorname{var}(f_2(X_2)) + \lambda_n \|f_2\|^2_{\mathcal{F}_2})^{1/2}}$$

- Criteria for independence (NB: independence $\neq$ uncorrelation)

Kernel Canonical Correlation Analysis

- Analogous derivation as Kernel PCA

- K_1, K_2 Gram matrices of $\{x_1^i\}$ and $\{x_2^i\}$

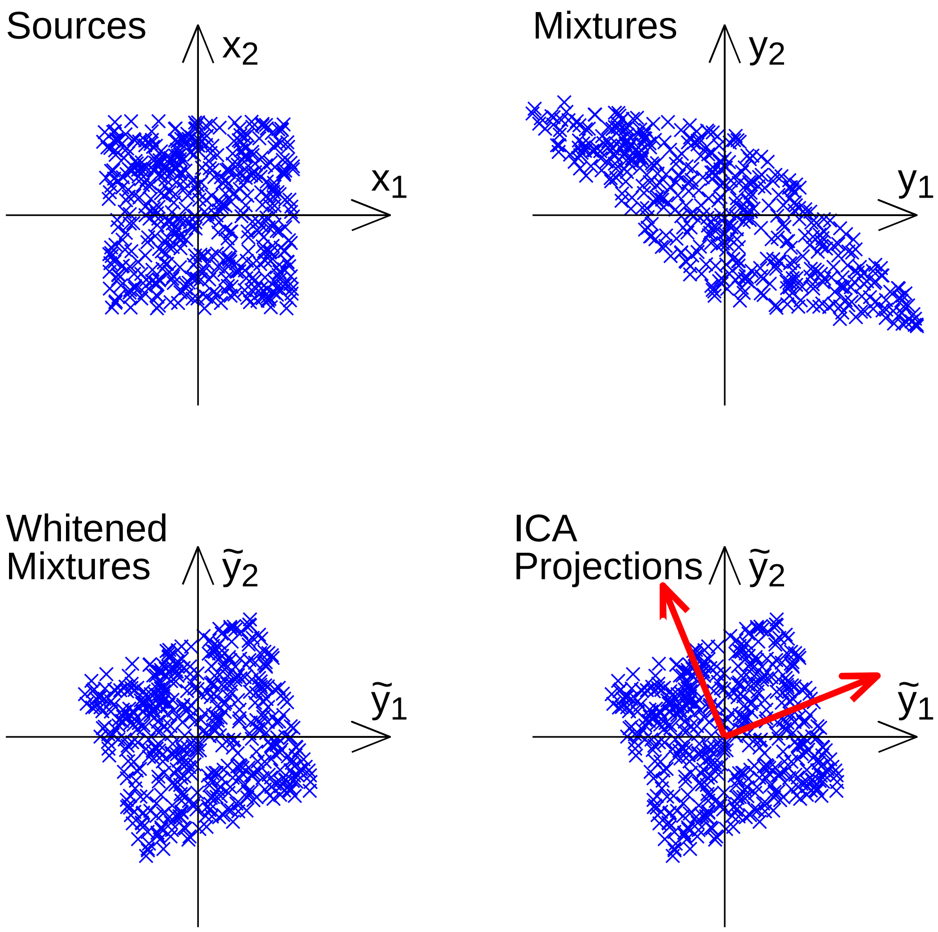
$$\max_{\alpha_1,\ \alpha_2 \in \Re^N} \frac{\alpha_1^T K_1 K_2 \alpha_2}{(\alpha_1^T (K_1^2 + \lambda K_1)\alpha_1)^{1/2} (\alpha_2^T (K_2^2 + \lambda K_2)\alpha_2)^{1/2}}$$

- Maximal generalized eigenvalue of

$$\begin{pmatrix} 0 & K_1 K_2 \\ K_2 K_1 & 0 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \rho \begin{pmatrix} K_1^2 + \lambda K_1 & 0 \\ 0 & K_2^2 + \lambda K_2 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}$$

Kernel CCA
Application to ICA (Bach & Jordan, 2002)

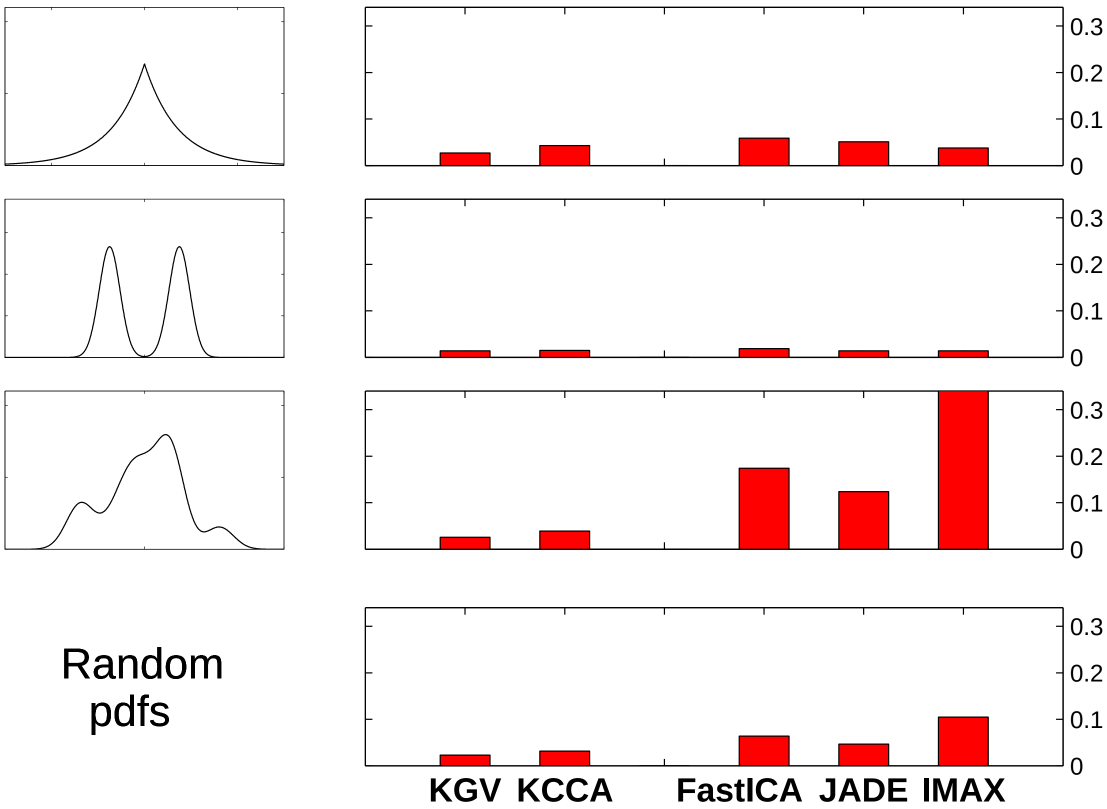
- Independent component analysis: linearly transform data such to get independent variables



Empirical results - Kernel ICA

- Comparison with other algorithms: FastICA (Hyvarinen,1999), Jade (Cardoso, 1998), Extended Infomax (Lee, 1999)

- Amari error : standard ICA distance from true sources



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Kernel design

- Principle: **kernel on $\mathcal{X}$ = space of functions on $\mathcal{X}$ + norm**

- Two main design principles

  1. Constructing kernels from kernels by algebraic operations
  2. Using usual algebraic/numerical tricks to perform efficient kernel computation with very high-dimensional feature spaces

- Operations: $k_1(x,y) = \langle \Phi_1(x), \Phi_1(y) \rangle$, $k_2(x,y) = \langle \Phi_2(x), \Phi_2(y) \rangle$

  – **Sum = concatenation of feature spaces**:

$$k_1(x,y) + k_2(x,y) = \left\langle \binom{\Phi_1(x)}{\Phi_2(x)}, \binom{\Phi_1(y)}{\Phi_2(y)} \right\rangle$$

  – **Product = tensor product of feature spaces**:

$$k_1(x,y)k_2(x,y) = \left\langle \Phi_1(x)\Phi_2(x)^\top, \Phi_1(y)\Phi_2(y)^\top \right\rangle$$

Classical kernels: kernels on vectors $x \in \mathbb{R}^d$

- Linear kernel $k(x, y) = x^\top y$
  – Linear functions
- Polynomial kernel $k(x, y) = (1 + x^\top y)^d$
  – Polynomial functions
- Gaussian kernel $k(x, y) = \exp(-\alpha \|x - y\|^2)$
  – Smooth functions
- Data are not always vectors!

Efficient ways of computing large sums

- Goal: $\Phi(x) \in \mathbb{R}^p$ high-dimensional, compute $\sum_{i=1}^{p} \Phi_i(x)\Phi_i(y)$ **in** $o(p)$

- **Sparsity**: many $\Phi_i(x)$ equal to zero (example: pyramid match kernel)

- **Factorization and recursivity**: replace sums of many products by product of few sums (example: polynomial kernel, graph kernel)

$$(1 + x^\top y)^d = \sum_{\alpha_1+\cdots+\alpha_k \leqslant d} \binom{d}{\alpha_1, \ldots, \alpha_k} (x_1 y_1)^{\alpha_1} \cdots (x_k y_k)^{\alpha_k}$$

Kernels over (labelled) sets of points

- Common situation in computer vision (e.g., interest points)
- Simple approach: compute averages/histograms of certain features
  - valid kernels over histograms h and h' (Hein and Bousquet, 2004)
  - **intersection**: $\sum_i \min(h_i, h'_i)$, **chi-square**: $\exp\left(-\alpha \sum_i \frac{(h_i - h'_i)^2}{h_i + h'_i}\right)$

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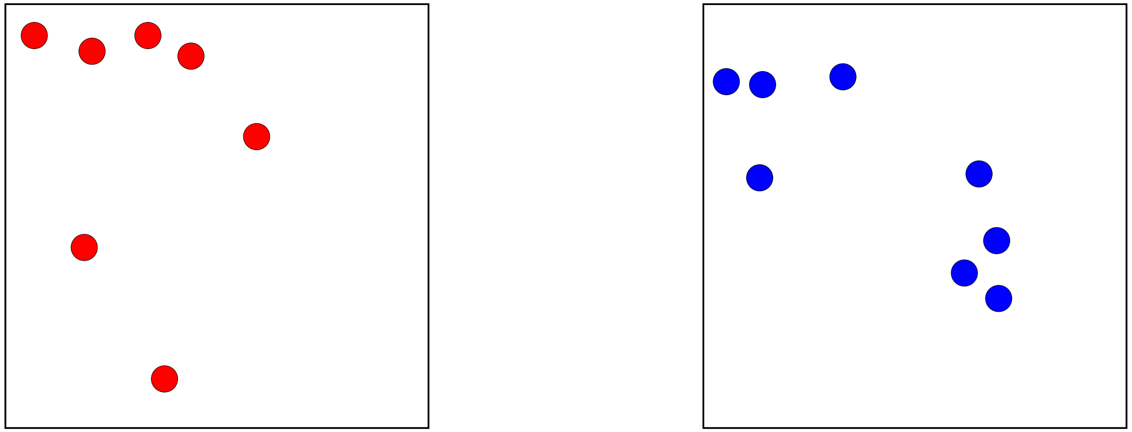
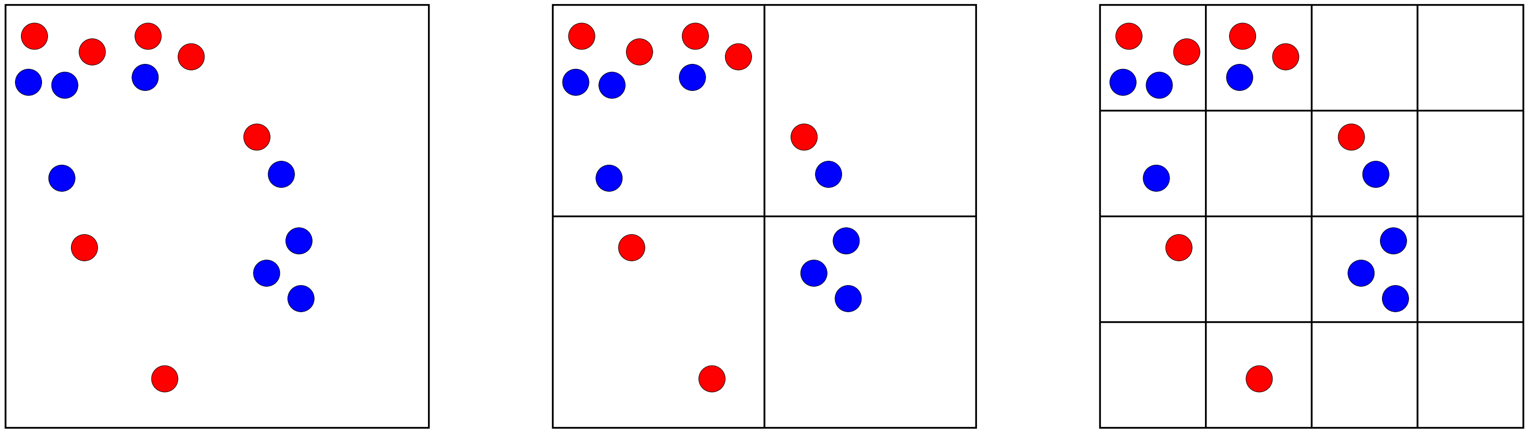
- Pyramid match (Grauman and Darrell, 2007): efficiently introducing localization
  - Form a regular pyramid on top of the image
  - Count the number of common elements in each bin
  - Give a weight to each bin
  - Many bins but most of them are empty
    $\Rightarrow$ use sparsity to compute kernel efficiently

Pyramid match kernel
(Grauman and Darrell, 2007; Lazebnik et al., 2006)

- Two sets of points



- Counting matches at several scales: 7, 5, 4



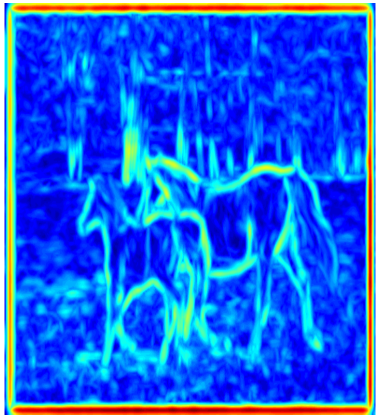
Kernels from segmentation graphs

- Goal of segmentation: extract objects of interest
- Many methods available, ...
  - ... but, rarely find the object of interest entirely
- Segmentation graphs
  - Allows to work on "more reliable" over-segmentation
  - Going to a large square grid (millions of pixels) to a small graph (dozens or hundreds of regions)
- How to build a kernel over segmenation graphs?
  - NB: more generally, kernelizing existing representations?

Segmentation by watershed transform (Meyer, 2001)

image

gradient



watershed

287 segments

64 segments

10 segments

Segmentation by watershed transform (Meyer, 2001)

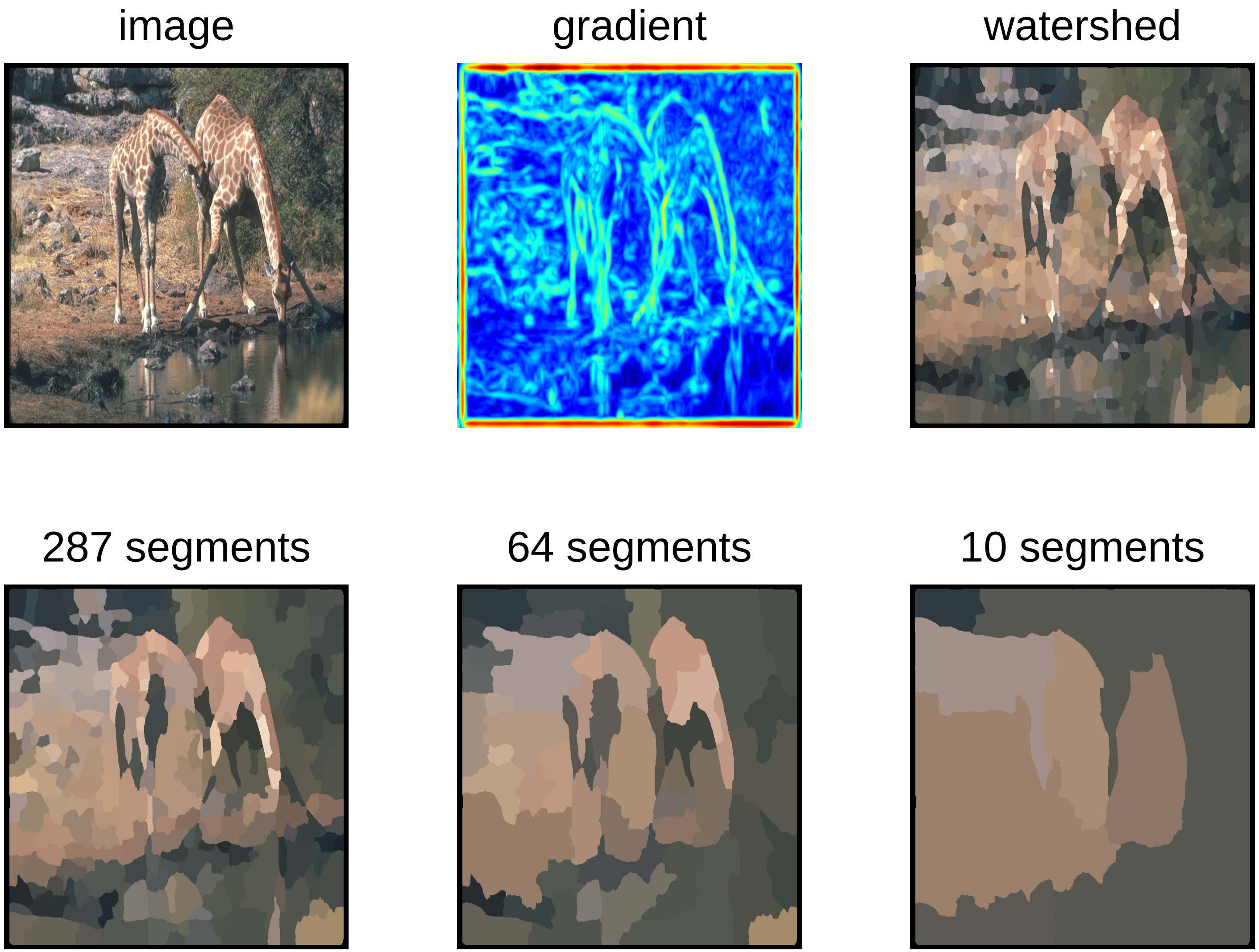


Image as a segmentation graph

- Labelled undirected graph
  - Vertices: connected segmented regions
  - Edges: between spatially neighboring regions
  - Labels: region pixels

$\Rightarrow$

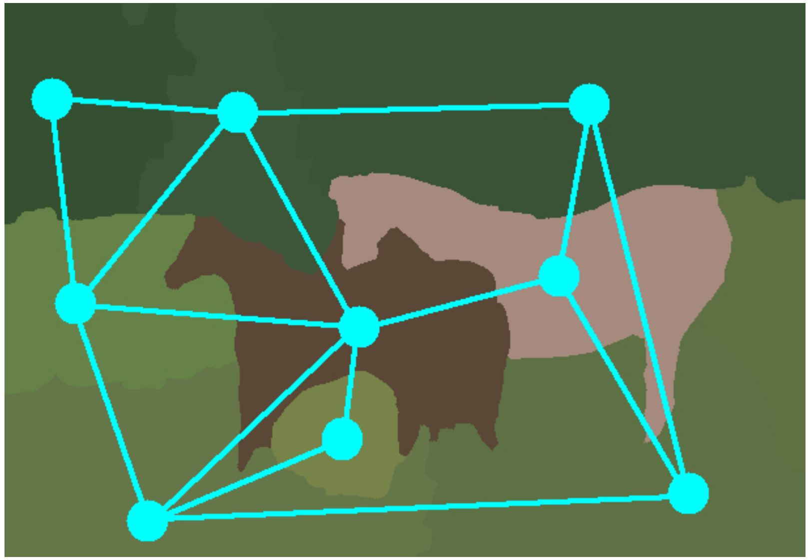


Image as a segmentation graph

- Labelled undirected graph
  - Vertices: connected segmented regions
  - Edges: between spatially neighboring regions
  - Labels: region pixels

- Difficulties
  - Extremely high-dimensional labels
  - Planar undirected graph
  - Inexact matching

- **Graph kernels** (Gärtner et al., 2003; Kashima et al., 2004; Harchaoui and Bach, 2007) provide an elegant and efficient solution

Kernels between structured objects

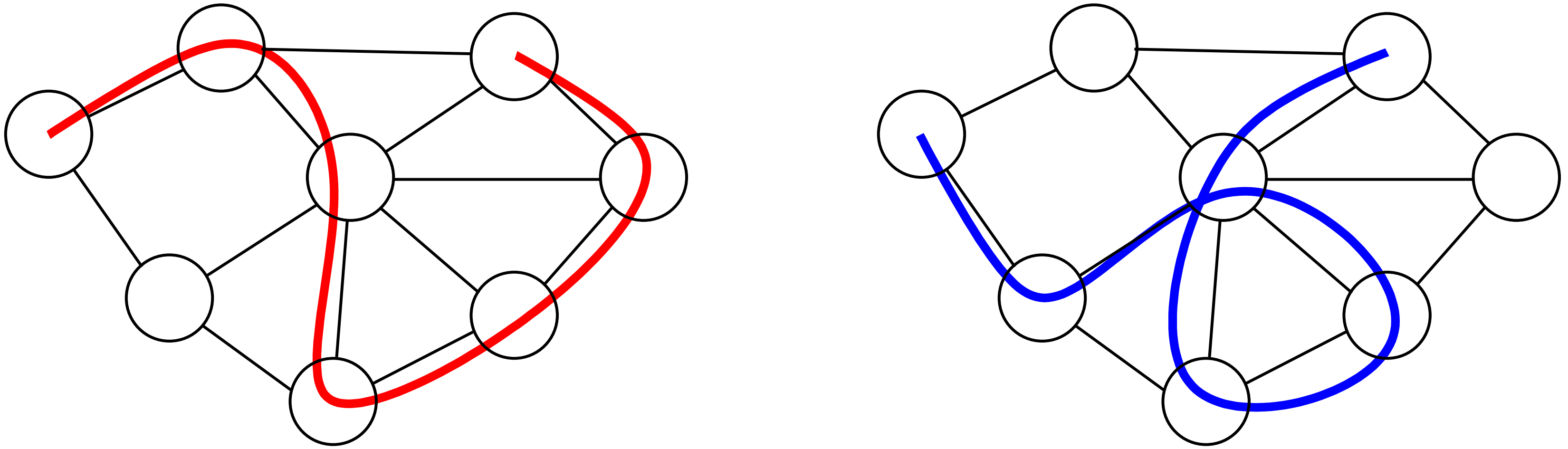
Strings, graphs, etc... (Shawe-Taylor and Cristianini, 2004)

- Numerous applications (text, bio-informatics, speech, vision)
- Common design principle: **enumeration of subparts** (Haussler, 1999; Watkins, 1999)
  - Efficient for strings
  - Possibility of gaps, partial matches, very efficient algorithms
- Most approaches fails for general graphs (even for undirected trees!)
  - NP-Hardness results (Ramon and Gärtner, 2003)
  - Need specific set of subparts

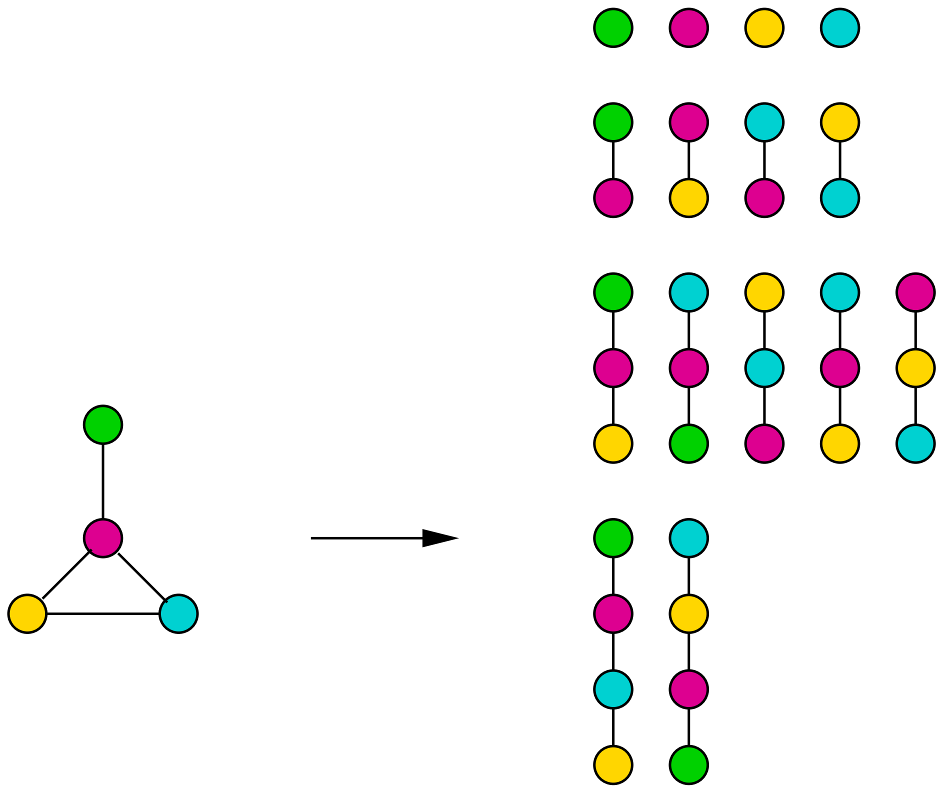
Paths and walks

- Given a graph G,
  - A path is a sequence of distinct neighboring vertices
  - A walk is a sequence of neighboring vertices

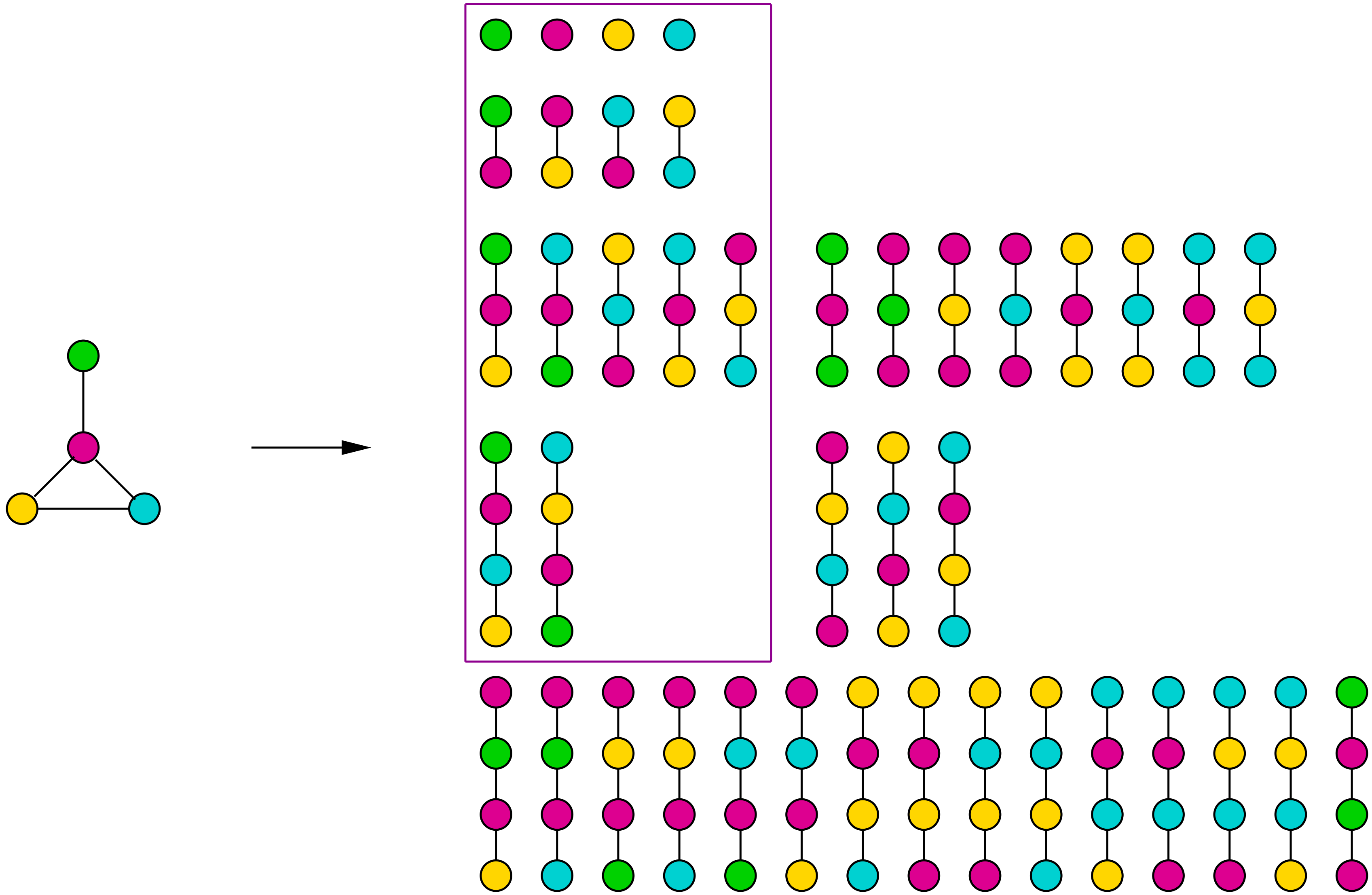
- Apparently similar notions



Paths



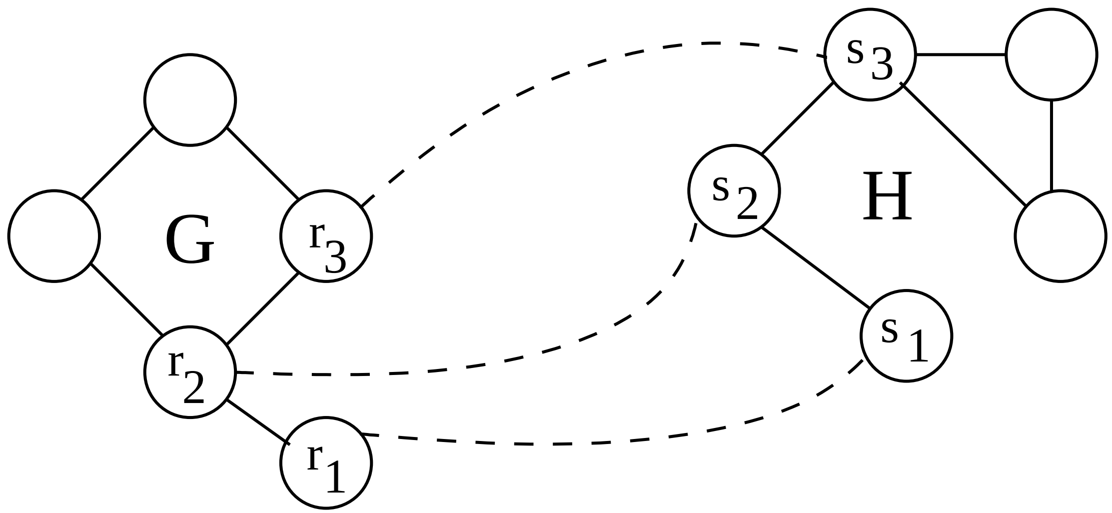
Walks



Walk kernel (Kashima et al., 2004; Borgwardt et al., 2005)

- $\mathcal{W}^p_{\mathbf{G}}$ (resp. $\mathcal{W}^p_{\mathbf{H}}$) denotes the set of walks of length p in $\mathbf{G}$ (resp. $\mathbf{H}$)
- Given *basis kernel* on labels $k(\ell, \ell')$
- p-th order walk kernel:

$$k^p_{\mathcal{W}}(\mathbf{G}, \mathbf{H}) = \sum_{\substack{(r_1, \ldots, r_p) \in \mathcal{W}^p_{\mathbf{G}} \\ (s_1, \ldots, s_p) \in \mathcal{W}^p_{\mathbf{H}}}} \prod_{i=1}^{p} k(\ell_{\mathbf{G}}(r_i), \ell_{\mathbf{H}}(s_i)).$$



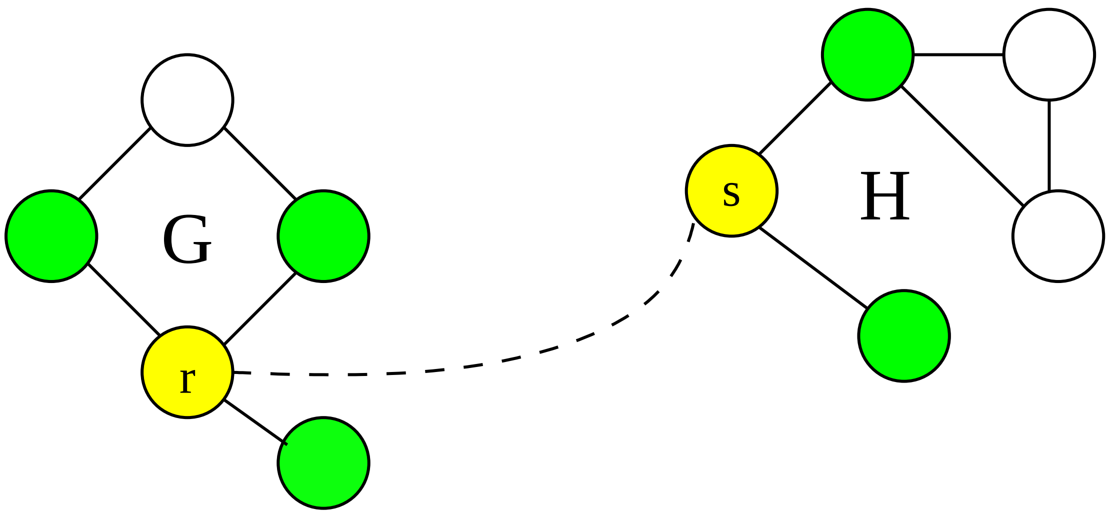
Dynamic programming for the walk kernel

- Dynamic programming in $O(pd_{\mathbf{G}}d_{\mathbf{H}}n_{\mathbf{G}}n_{\mathbf{H}})$

- $k^p_{\mathcal{W}}(\mathbf{G},\mathbf{H},r,s)$ = sum restricted to walks starting at r and s

- recursion between $p-1$-th walk and p-th walk kernel

$$k^p_{\mathcal{W}}(\mathbf{G},\mathbf{H},r,s)=k(\ell_{\mathbf{G}}(r),\ell_{\mathbf{H}}(s))\sum_{\substack{r'\in\mathcal{N}_{\mathbf{G}}(r)\\ s'\in\mathcal{N}_{\mathbf{H}}(s)}} k^{p-1}_{\mathcal{W}}(\mathbf{G},\mathbf{H},r',s').$$



Dynamic programming for the walk kernel

- Dynamic programming in $O(pd_{\mathbf{G}}d_{\mathbf{H}}n_{\mathbf{G}}n_{\mathbf{H}})$

- $k_{\mathcal{W}}^{p}(\mathbf{G},\mathbf{H},r,s)$ = sum restricted to walks starting at r and s

- recursion between $p-1$-th walk and p-th walk kernel

$$k_{\mathcal{W}}^{p}(\mathbf{G},\mathbf{H},r,s) = k(\ell_{\mathbf{G}}(r),\ell_{\mathbf{H}}(s)) \sum_{\substack{r' \in \mathcal{N}_{\mathbf{G}}(r) \\ s' \in \mathcal{N}_{\mathbf{H}}(s)}} k_{\mathcal{W}}^{p-1}(\mathbf{G},\mathbf{H},r',s')$$

- Kernel obtained as $k_{\mathcal{T}}^{p,\alpha}(\mathbf{G},\mathbf{H}) = \sum_{r \in \mathcal{V}_{\mathbf{G}}, s \in \mathcal{V}_{\mathbf{H}}} k_{\mathcal{T}}^{p,\alpha}(\mathbf{G},\mathbf{H},r,s)$

Extensions of graph kernels

- Main principle: **compare all possible subparts of the graphs**
- Going from paths to subtrees
  - Extension of the concept of walks $\Rightarrow$ tree-walks (Ramon and Gärtner, 2003)
- Similar dynamic programming recursions (Harchaoui and Bach, 2007)
- Need to play around with subparts to obtain efficient recursions
  - Do we actually need positive definiteness?

Performance on Corel14 (Harchaoui and Bach, 2007)

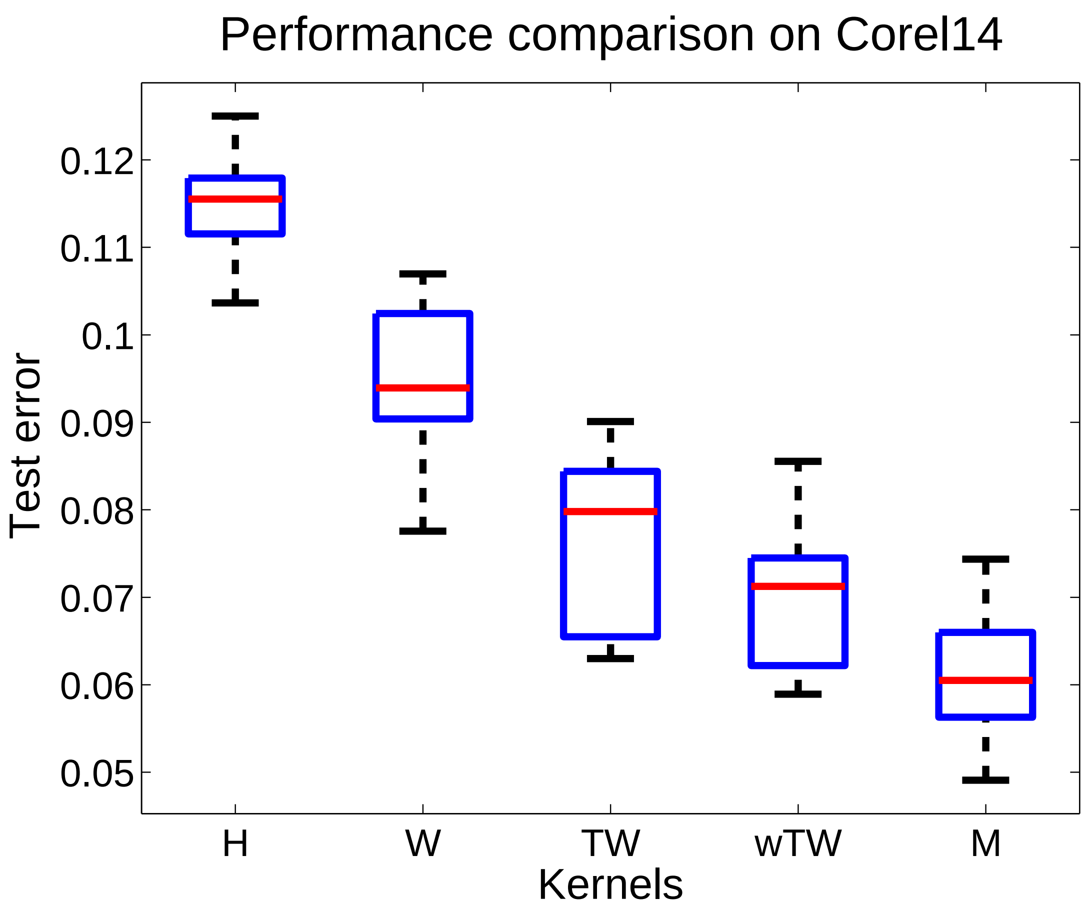
- `Corel14`: 1400 natural images with 14 classes

Performance on Corel14 (Harchaoui & Bach, 2007)
Error rates

- Histogram kernels (**H**)
- Walk kernels (**W**)
- Tree-walk kernels (**TW**)
- Weighted tree-walks (**wTW**)
- MKL (**M**)



Kernel methods - Summary

- Kernels and representer theorems
  - Clear distinction between representation/algorithms
- Algorithms
  - Two formulations (primal/dual)
  - Logistic or SVM?
- Kernel design
  - Very large feature spaces with efficient kernel evaluations

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Supervised learning and regularization

- Data: $x_i \in \mathcal{X}$, $y_i \in \mathcal{Y}$, $i = 1, \dots, n$
- Minimize with respect to function $f : \mathcal{X} \to \mathcal{Y}$:

$$\sum_{i=1}^{n} \ell(y_i, f(x_i)) \qquad + \qquad \frac{\lambda}{2} \|f\|^2$$

Error on data + Regularization

Loss & function space ? Norm ?

- Two theoretical/algorithmic issues:

1. Loss
2. **Function space / norm**

Regularizations

- **Main goal: avoid overfitting**

- **Two main lines of work**:

  1. Euclidean and Hilbertian norms (i.e., ℓ_2-norms)
     - Possibility of non linear predictors
     - Non parametric supervised learning and kernel methods
     - Well developped theory and algorithms (see, e.g., Wahba, 1990; Schölkopf and Smola, 2001; Shawe-Taylor and Cristianini, 2004)

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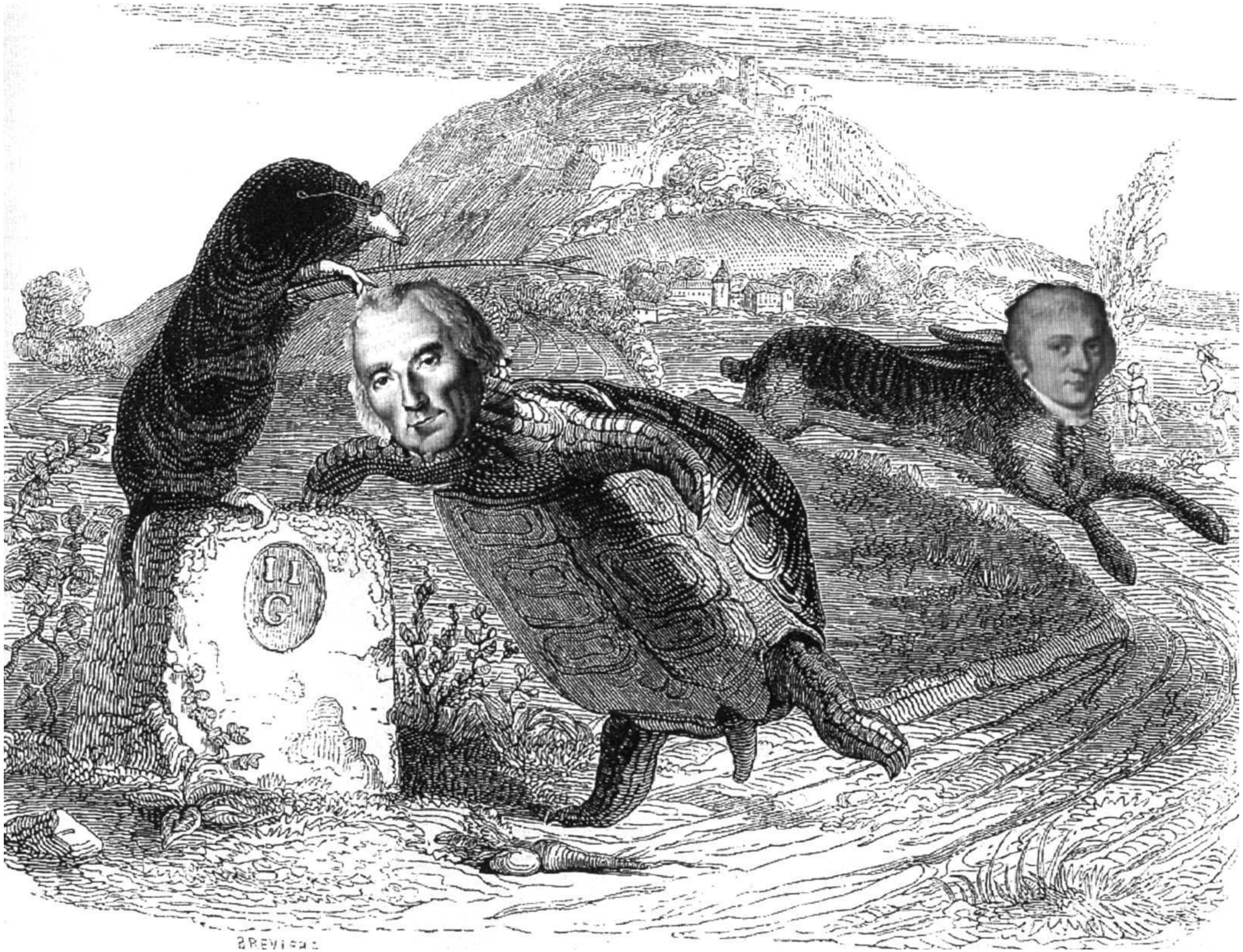
     - Well developped theory and algorithms (see, e.g., Wahba, 1990; Schölkopf and Smola, 2001; Shawe-Taylor and Cristianini, 2004)
  2. Sparsity-inducing norms
     - Usually restricted to linear predictors on vectors $f(x) = w^\top x$
     - Main example: ℓ_1-norm $\|w\|_1 = \sum_{i=1}^p |w_i|$
     - Perform model selection as well as regularization
     - **Theory and algorithms "in the making"**

ℓ_2-norm vs. ℓ_1-norm

- ℓ_1-norms lead to interpretable models
- ℓ_2-norms can be run implicitly with very large feature spaces
- **Algorithms**:
  - Smooth convex optimization vs. nonsmooth convex optimization
- **Theory**:
  - better predictive performance?

ℓ_2 vs. ℓ_1 - Gaussian hare vs. Laplacian tortoise



- First-order methods (Fu, 1998; Wu and Lange, 2008)
- Homotopy methods (Markowitz, 1956; Efron et al., 2004)

Lasso - Two main recent theoretical results

1. **Support recovery condition** (Zhao and Yu, 2006; Wainwright, 2006; Zou, 2006; Yuan and Lin, 2007): the Lasso is sign-consistent if and only if

$$\|\mathbf{Q}_{\mathbf{J}^c\mathbf{J}}\mathbf{Q}_{\mathbf{J}\mathbf{J}}^{-1}\text{sign}(\mathbf{w}_\mathbf{J})\|_\infty \leqslant 1,$$

where $\mathbf{Q} = \lim_{n\to+\infty}\frac{1}{n}\sum_{i=1}^n x_i x_i^\top \in \mathbb{R}^{p\times p}$ and $\mathbf{J} = \text{Supp}(\mathbf{w})$

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2. **Exponentially many irrelevant variables** (Zhao and Yu, 2006; Wainwright, 2006; Bickel et al., 2009; Lounici, 2008; Meinshausen and Yu, 2008): under appropriate assumptions, consistency is possible as long as
$$\log p = O(n)$$

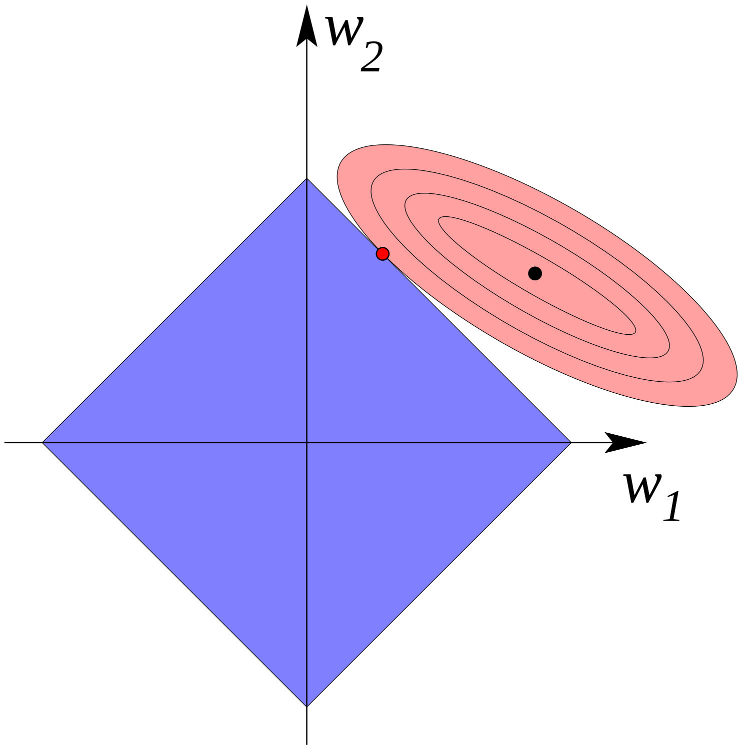
Going beyond the Lasso

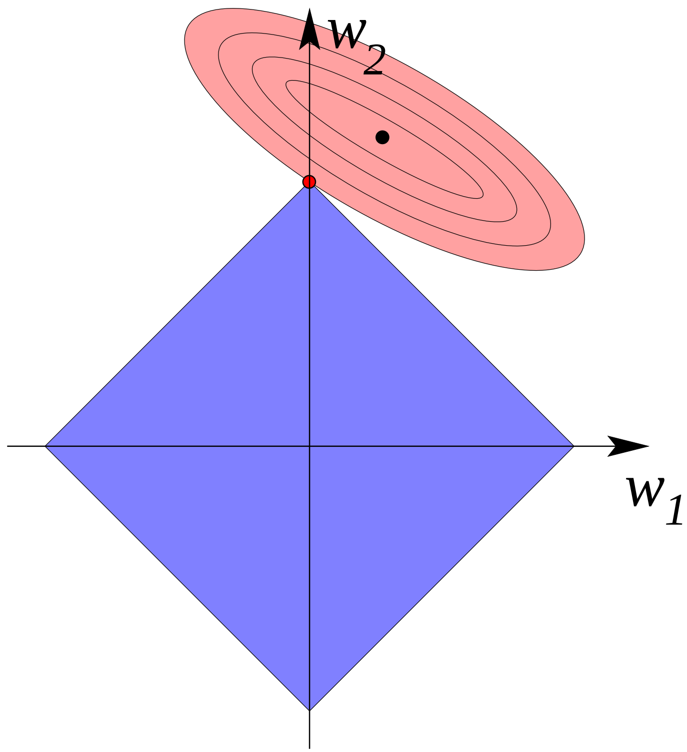
- ℓ_1-norm for **linear** feature selection in **high dimensions**
  - Lasso usually not applicable directly
- **Non-linearities**
- **Dealing with exponentially many features**
- **Sparse learning on matrices**

Why ℓ_1-norm constraints leads to sparsity?

- Example: minimize quadratic function $Q(w)$ subject to $\|w\|_1 \leqslant T$.
  - coupled soft thresholding

- Geometric interpretation
  - NB : penalizing is "equivalent" to constraining





ℓ_1-norm regularization (linear setting)

- Data: covariates $x_i \in \mathbb{R}^p$, responses $y_i \in \mathcal{Y}$, $i = 1, \ldots, n$

- Minimize with respect to loadings/weights $w \in \mathbb{R}^p$:

$$J(w) = \underbrace{\sum_{i=1}^{n} \ell(y_i, w^\top x_i)}_{\text{Error on data}} \quad + \quad \underbrace{\lambda \|w\|_1}_{\text{Regularization}}$$

- Including a constant term b? Penalizing or constraining?

- square loss $\Rightarrow$ basis pursuit in signal processing (Chen et al., 2001), Lasso in statistics/machine learning (Tibshirani, 1996)

First order methods for convex optimization on $\mathbb{R}^p$

Smooth optimization

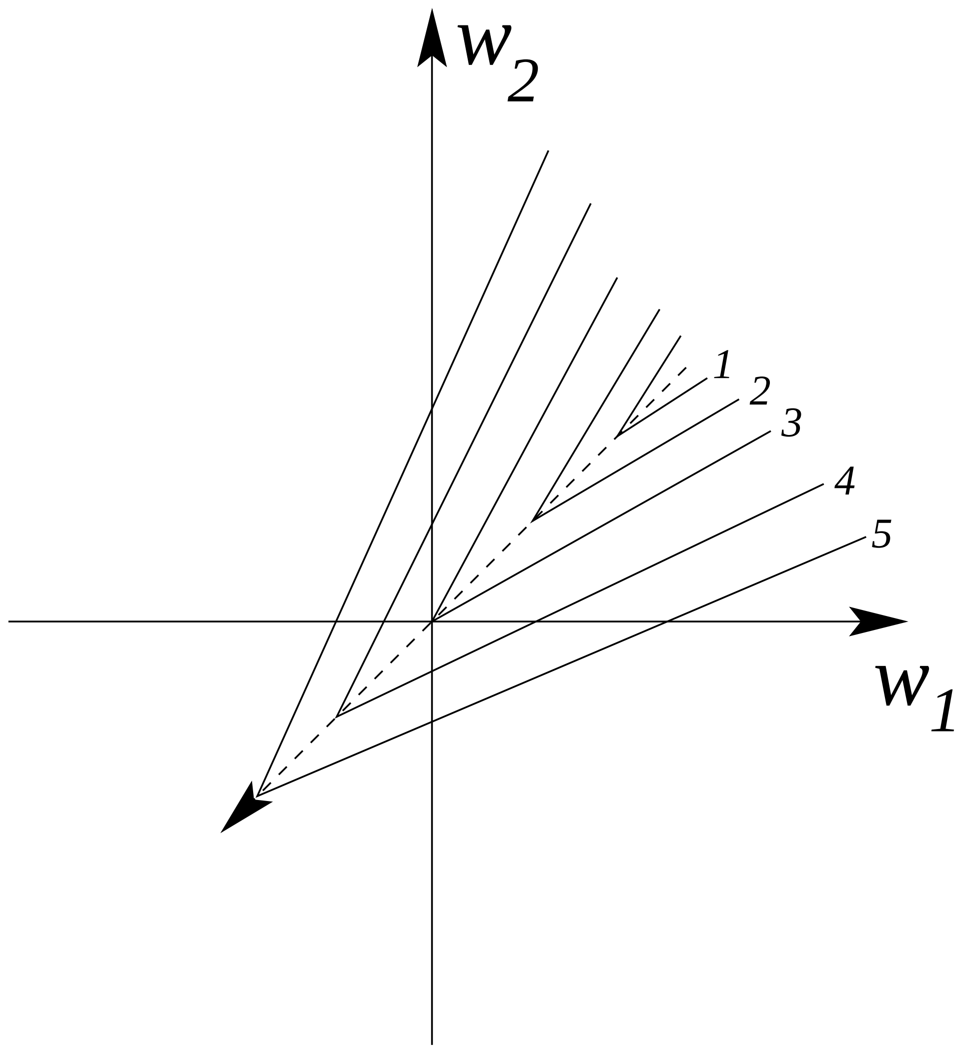
- **Gradient descent**: $w_{t+1} = w_t - \alpha_t \nabla J(w_t)$
  - with line search: search for a decent (not necessarily best) α_t
  - fixed diminishing step size, e.g., $\alpha_t = a(t+b)^{-1}$
- Convergence of $f(w_t)$ to $f^* = \min_{w \in \mathbb{R}^p} f(w)$ (Nesterov, 2003)
  - f convex and M-Lipschitz: $f(w_t) - f^* = O\big(M/\sqrt{t}\big)$
  - and, differentiable with L-Lipschitz gradient: $f(w_t) - f^* = O\big(L/t\big)$
  - and, f μ-strongly convex: $f(w_t) - f^* = O\big(L \exp(-4t\frac{\mu}{L})\big)$
- $\frac{\mu}{L}$ = condition number of the optimization problem
- Coordinate descent: similar properties
- NB: "optimal scheme" $f(w_t) - f^* = O\big(L \min\{\exp(-4t\sqrt{\mu/L}), t^{-2}\}\big)$

First-order methods for convex optimization on $\mathbb{R}^p$
Non smooth optimization

- First-order methods for non differentiable objective
  - Subgradient descent: $w_{t+1} = w_t - \alpha_t g_t$, with $g_t \in \partial J(w_t)$, i.e., such that $\forall \Delta, g_t^\top \Delta \leqslant \nabla J(w_t, \Delta)$
    - with exact line search: not always convergent (see counter-example)
    - diminishing step size, e.g., $\alpha_t = a(t+b)^{-1}$: convergent
  - Coordinate descent: not always convergent (show counter-example)

- Convergence rates (f convex and M-Lipschitz): $f(w_t) - f^* = O\big(\frac{M}{\sqrt{t}}\big)$

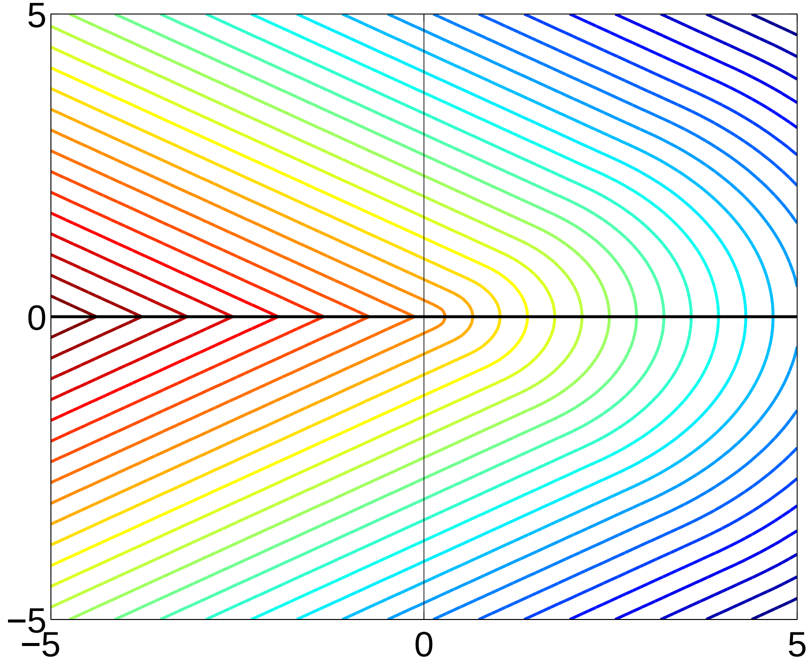
Counter-example
Coordinate descent for nonsmooth objectives



Counter-example (Bertsekas, 1995)
Steepest descent for nonsmooth objectives

- $q(x_1, x_2) = \begin{cases} -5(9x_1^2 + 16x_2^2)^{1/2} & \text{if } x_1 > |x_2| \\ -(9x_1 + 16|x_2|)^{1/2} & \text{if } x_1 \leqslant |x_2| \end{cases}$

- Steepest descent starting from any x such that $x_1 > |x_2| > (9/16)^2 |x_1|$



Regularized problems - Proximal methods

- Gradient descent as a proximal method (differentiable functions)
  - $w_{t+1} = \arg\min_{w \in \mathbb{R}^p} J(w_t) + (w - w_t)^\top \nabla J(w_t) + \frac{L}{2}\|w - w_t\|_2^2$
  - $w_{t+1} = w_t - \frac{1}{L}\nabla J(w_t)$

- Problems of the form: $\boxed{\min_{w \in \mathbb{R}^p} L(w) + \lambda\Omega(w)}$
  - $w_{t+1} = \arg\min_{w \in \mathbb{R}^p} L(w_t) + (w - w_t)^\top \nabla L(w_t) + \lambda\Omega(w) + \frac{L}{2}\|w - w_t\|_2^2$
  - Thresholded gradient descent

- Similar convergence rates than smooth optimization
  - Acceleration methods (Nesterov, 2007; Beck and Teboulle, 2009)
  - **depends on the condition number of the loss**

Second order methods

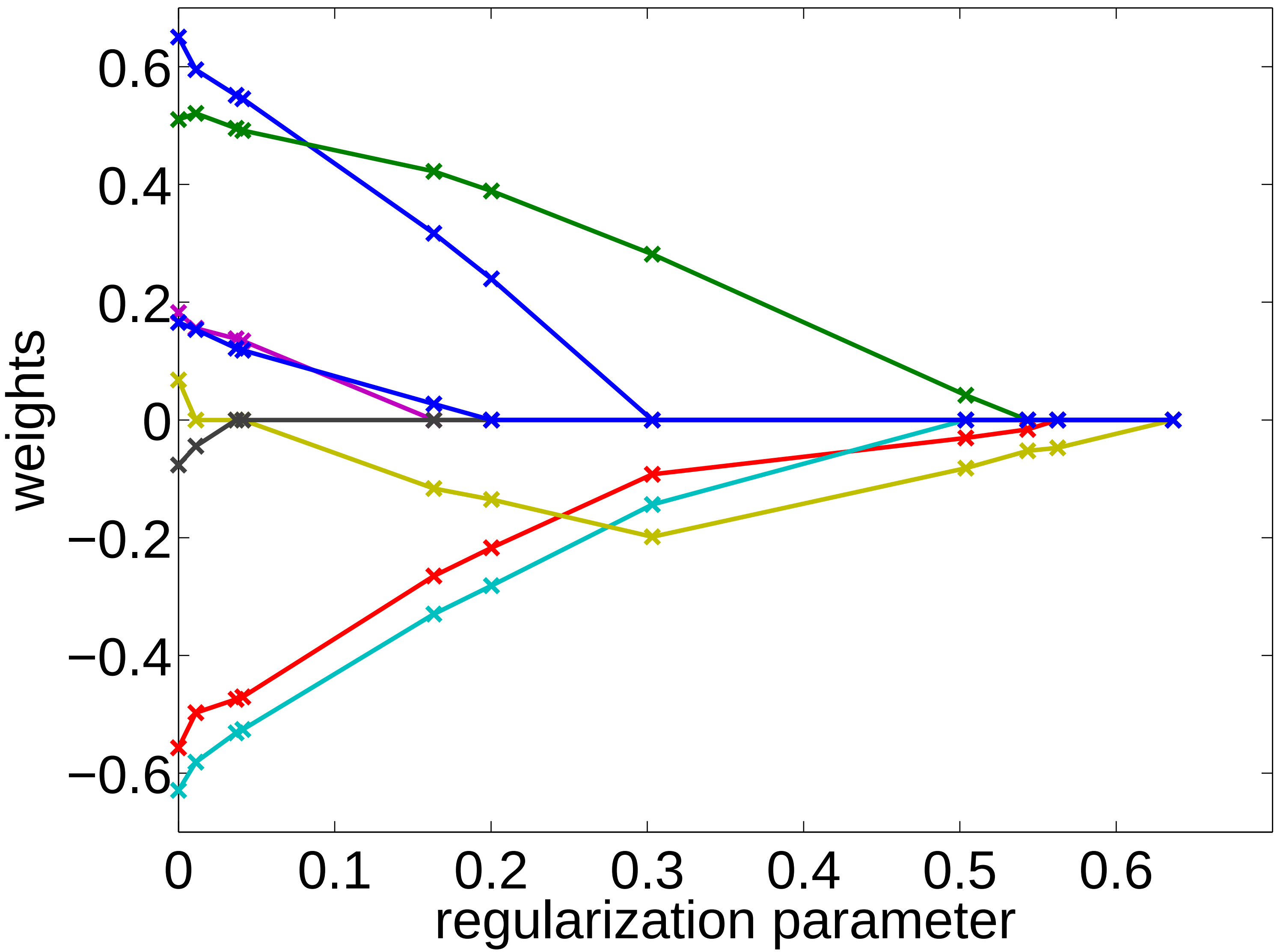
- Differentiable case
  - Newton: $w_{t+1} = w_t - \alpha_t H_t^{-1} g_t$
    * Traditional: $\alpha_t = 1$, but non globally convergent
    * globally convergent with line search for α_t (see Boyd, 2003)
    * $O(\log\log(1/\varepsilon))$ (slower) iterations
  - Quasi-newton methods (see Bonnans et al., 2003)

- Non differentiable case (interior point methods)
  - Smoothing of problem + second order methods
    * See example later and (Boyd, 2003)
    * Theoretically $O(\sqrt{p})$ Newton steps, usually $O(1)$ Newton steps

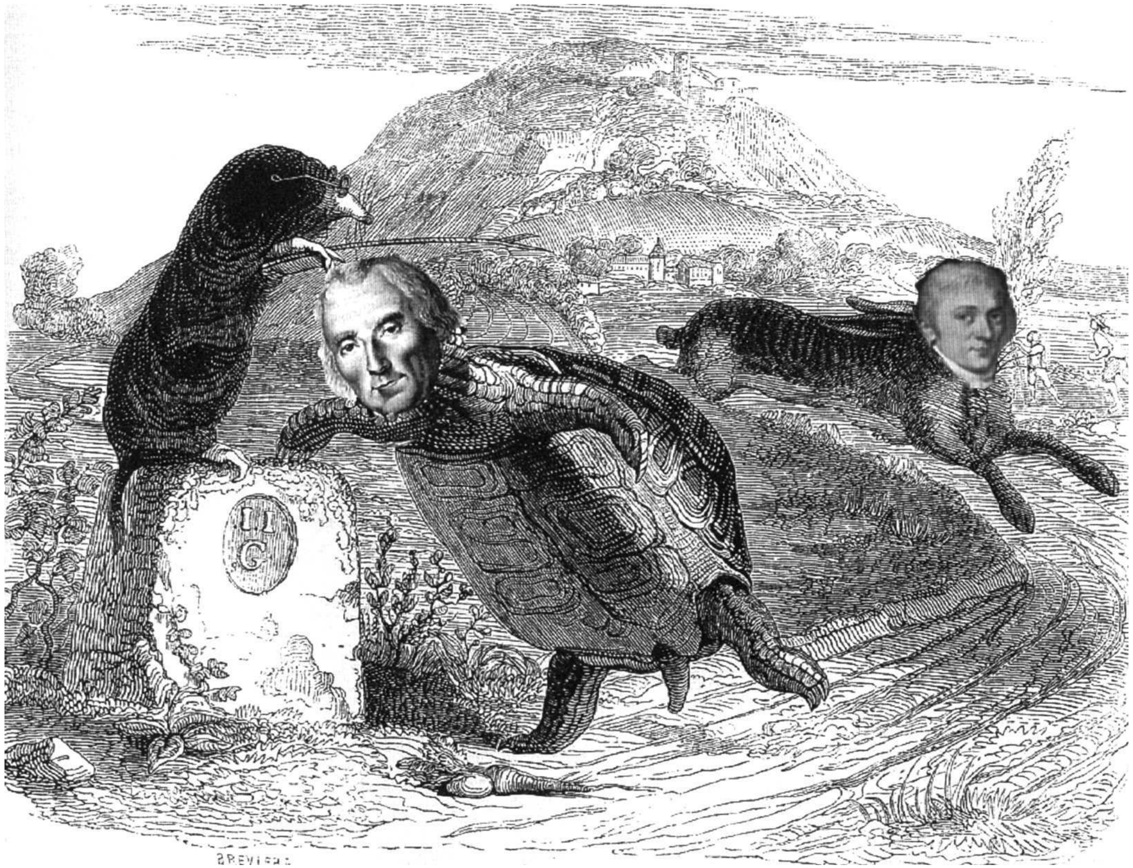
First order or second order methods for machine learning?

- objecive defined as average (i.e., up to $n^{-1/2}$): no need to optimize up to 10^{-16}!
  - Second-order: slower but worryless
  - First-order: faster but care must be taken regarding convergence
- Rule of thumb
  - Small scale $\Rightarrow$ second order
  - Large scale $\Rightarrow$ first order
  - Unless dedicated algorithm using structure (like for the Lasso)
- See Bottou and Bousquet (2008) for further details

Piecewise linear paths



Algorithms for ℓ_1-norms (square loss): Gaussian hare vs. Laplacian tortoise



- Coordinate descent: $O(pn)$ per iterations for ℓ_1 and ℓ_2
- "Exact" algorithms: $O(kpn)$ for ℓ_1 **vs.** $O(p^2n)$ for ℓ_2

Additional methods - Softwares

- Many contributions in signal processing, optimization, machine learning
  - Extensions to stochastic setting (Bottou and Bousquet, 2008)
- Extensions to other sparsity-inducing norms
  - Computing proximal operator
- **Softwares**
  - Many available codes
  - SPAMS (SPArse Modeling Software)
    `http://www.di.ens.fr/willow/SPAMS/`

Course outline

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    - Kernels and representer theorem
    - Convex duality, optimization and algorithms
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    - Kernel design
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    - Multiple kernel learning
    - Theoretical results
    - Learning on matrices

Theoretical results - Square loss

- Main assumption: data generated from a certain sparse $\mathbf{w}$

- Three main problems:

  1. **Regular consistency**: convergence of estimator $\hat{w}$ to $\mathbf{w}$, i.e., $\|\hat{w} - \mathbf{w}\|$ tends to zero when n tends to ∞
  2. **Model selection consistency**: convergence of the sparsity pattern of $\hat{w}$ to the pattern $\mathbf{w}$
  3. **Efficiency**: convergence of predictions with $\hat{w}$ to the predictions with $\mathbf{w}$, i.e., $\frac{1}{n}\|X\hat{w} - X\mathbf{w}\|_2^2$ tends to zero

- Main results:

  – **Condition for model consistency (support recovery)**
  – **High-dimensional inference**

Model selection consistency (Lasso)

- Assume $\mathbf{w}$ sparse and denote $\mathbf{J} = \{j, \mathbf{w}_j \neq 0\}$ the nonzero pattern
- **Support recovery condition** (Zhao and Yu, 2006; Wainwright, 2006; Zou, 2006; Yuan and Lin, 2007): the Lasso is sign-consistent if and only if

$$\boxed{\|\mathbf{Q}_{\mathbf{J}^c\mathbf{J}}\mathbf{Q}_{\mathbf{J}\mathbf{J}}^{-1}\mathrm{sign}(\mathbf{w}_\mathbf{J})\|_\infty \leqslant 1}$$

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where $\mathbf{Q} = \lim_{n\to+\infty} \frac{1}{n}\sum_{i=1}^n x_i x_i^\top \in \mathbb{R}^{p\times p}$ and $\mathbf{J} = \mathrm{Supp}(\mathbf{w})$
- Condition depends on $\mathbf{w}$ and $\mathbf{J}$ (may be relaxed)
  - may be relaxed by maximizing out $\mathrm{sign}(\mathbf{w})$ or $\mathbf{J}$
- Valid in low and high-dimensional settings
- Requires lower-bound on magnitude of nonzero $\mathbf{w}_j$

Model selection consistency (Lasso)

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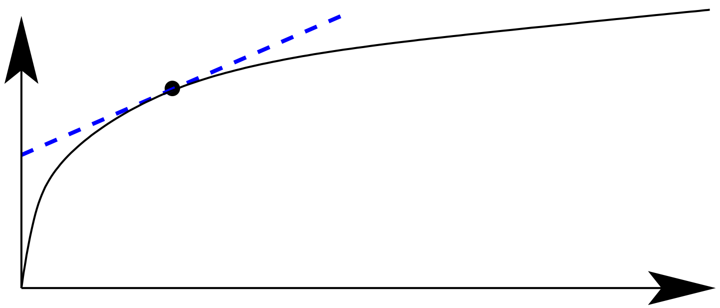
- **The Lasso is usually not model-consistent**
  - Selects more variables than necessary (see, e.g., Lv and Fan, 2009)
  - **Fixing the Lasso**: adaptive Lasso (Zou, 2006), relaxed Lasso (Meinshausen, 2008), thresholding (Lounici, 2008), Bolasso (Bach, 2008a), stability selection (Meinshausen and Bühlmann, 2008), Wasserman and Roeder (2009)

Adaptive Lasso and concave penalization

- **Adaptive Lasso** (Zou, 2006; Huang et al., 2008)
  - Weighted ℓ_1-norm: $\displaystyle \min_{w \in \mathbb{R}^p} L(w) + \lambda \sum_{j=1}^{p} \frac{|w_j|}{|\hat{w}_j|^\alpha}$
  - $\hat{w}$ estimator obtained from ℓ_2 or ℓ_1 regularization

- **Reformulation in terms of concave penalization**

$$\min_{w \in \mathbb{R}^p} L(w) + \sum_{j=1}^{p} g(|w_j|)$$



  - Example: $g(|w_j|) = |w_j|^{1/2}$ or $\log |w_j|$. Closer to the ℓ_0 penalty
  - Concave-convex procedure: replace $g(|w_j|)$ by affine upper bound
  - Better sparsity-inducing properties (Fan and Li, 2001; Zou and Li, 2008; Zhang, 2008b)

High-dimensional inference (Lasso)

- **Main result**: we only need $k \log p = O(n)$
  - if $\mathbf{w}$ is sufficiently sparse
  - **and** input variables are not too correlated

- Precise conditions on covariance matrix $\mathbf{Q} = \frac{1}{n}X^\top X$.
  - **Mutual incoherence** (Lounici, 2008)
  - **Restricted eigenvalue conditions** (Bickel et al., 2009)
  - Sparse eigenvalues (Meinshausen and Yu, 2008)
  - Null space property (Donoho and Tanner, 2005)

- Links with signal processing and compressed sensing (Candès and Wakin, 2008)

- Assume that $\mathbf{Q}$ has unit diagonal

Mutual incoherence (uniform low correlations)

- **Theorem** (Lounici, 2008):
  - $y_i = \mathbf{w}^\top x_i + \varepsilon_i$, ε i.i.d. normal with mean zero and variance σ^2
  - $\mathbf{Q} = X^\top X/n$ with unit diagonal and cross-terms less than $\dfrac{1}{14k}$
  - if $\|\mathbf{w}\|_0 \leqslant k$, and $A^2 > 8$, then, with $\lambda = A\sigma\sqrt{n \log p}$

$$\mathbb{P}\left(\|\hat{w} - \mathbf{w}\|_\infty \leqslant 5A\sigma \left(\frac{\log p}{n} \right)^{1/2} \right) \geqslant 1 - p^{1-A^2/8}$$

- Model consistency by thresholding if $\displaystyle\min_{j, \mathbf{w}_j \neq 0} |\mathbf{w}_j| > C\sigma\sqrt{\frac{\log p}{n}}$

- Mutual incoherence condition depends *strongly* on k

- Improved result by averaging over sparsity patterns (Candès and Plan, 2009)

Alternative sparse methods
Greedy methods

- Forward selection
- Forward-backward selection
- Non-convex method
  - Harder to analyze
  - Simpler to implement
  - Problems of stability
- Positive theoretical results (Zhang, 2009, 2008a)
  - Similar sufficient conditions than for the Lasso

Comparing Lasso and other strategies for linear regression

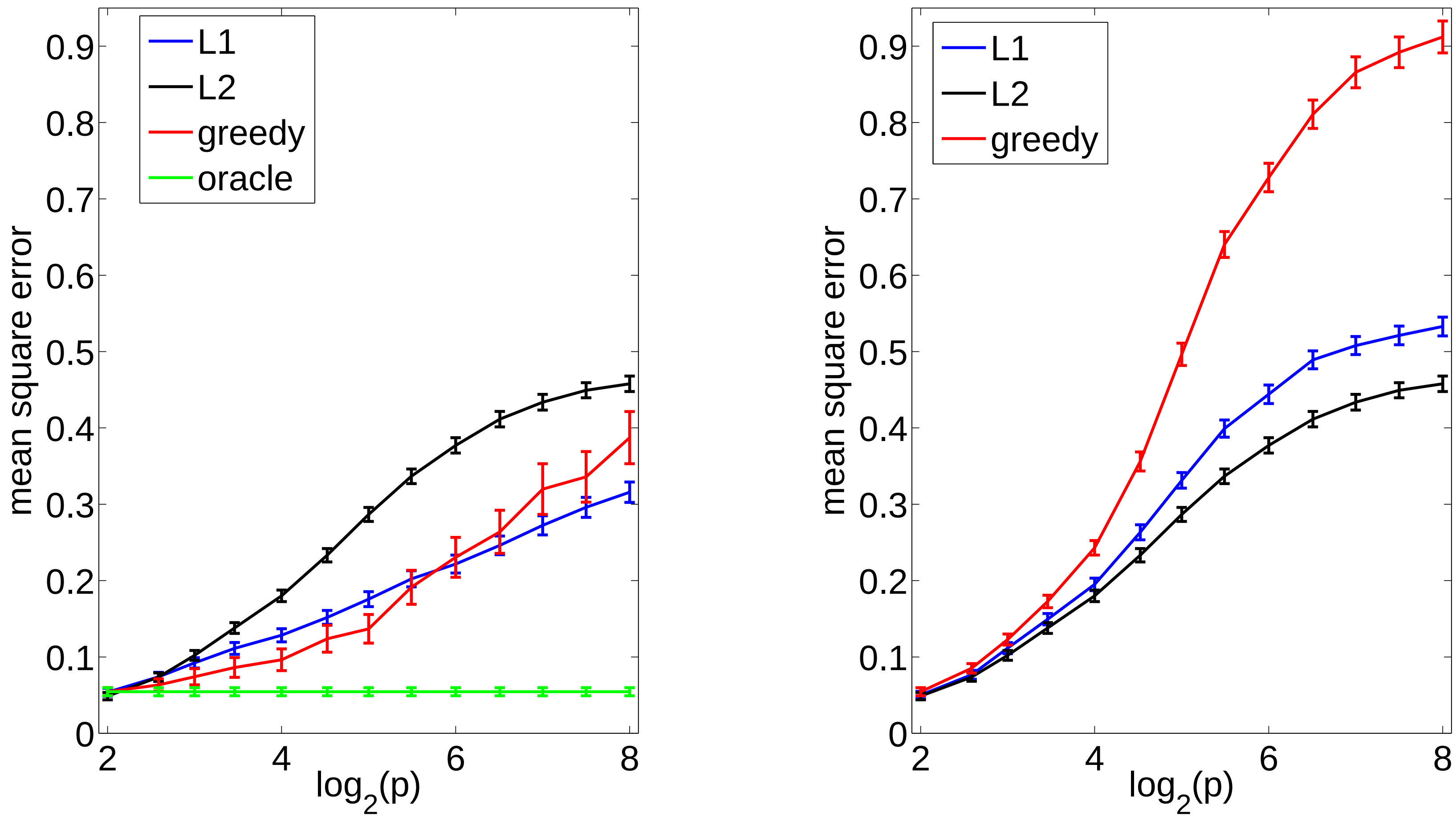
- Compared methods to reach the least-square solution
  - Ridge regression: $\displaystyle \min_{w\in\mathbb{R}^p} \frac{1}{2}\|y - Xw\|_2^2 + \frac{\lambda}{2}\|w\|_2^2$
  - Lasso: $\displaystyle \min_{w\in\mathbb{R}^p} \frac{1}{2}\|y - Xw\|_2^2 + \lambda\|w\|_1$
  - Forward greedy:
    - Initialization with empty set
    - Sequentially add the variable that best reduces the square loss

- Each method builds a path of solutions from 0 to ordinary least-squares solution

- Regularization parameters selected on the test set

Simulation results

- i.i.d. Gaussian design matrix, $k = 4$, $n = 64$, $p \in [2, 256]$, SNR $= 1$
- Note stability to non-sparsity and variability



Sparse	Rotated (non sparse)

Summary
ℓ_1-norm regularization

- ℓ_1-norm regularization leads to **nonsmooth optimization problems**
  - analysis through directional derivatives or subgradients
  - optimization may or may not take advantage of sparsity
- ℓ_1-norm regularization allows **high-dimensional inference**
- Interesting problems for ℓ_1-regularization
  - Stable variable selection
  - Weaker sufficient conditions (for weaker results)
  - Estimation of regularization parameter (all bounds depend on the unknown noise variance σ^2)

Extensions

- **Sparse methods are not limited to the square loss**
  - logistic loss: algorithms (Beck and Teboulle, 2009) and theory (Van De Geer, 2008; Bach, 2009)

- **Sparse methods are not limited to supervised learning**
  - Learning the structure of Gaussian graphical models (Meinshausen and Bühlmann, 2006; Banerjee et al., 2008)
  - Sparsity on matrices (last part of the tutorial)

- **Sparse methods are not limited to variable selection in a linear model**
  - **See next part of the tutorial**

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Penalization with grouped variables (Yuan and Lin, 2006)

- Assume that $\{1, \dots, p\}$ is **partitioned** into m groups $G_1, \dots, G_m$
- Penalization by $\sum_{i=1}^{m} \|w_{G_i}\|_2$, often called ℓ_1-ℓ_2 norm
- Induces group sparsity
  - Some groups entirely set to zero
  - no zeros within groups
- In this tutorial:
  - Groups may have infinite size $\Rightarrow$ **MKL**
  - Groups may overlap $\Rightarrow$ **structured sparsity** (Jenatton et al., 2009)

Linear vs. non-linear methods

- All methods in this tutorial are **linear in the parameters**
- By replacing x by features $\Phi(x)$, they can be made **non linear in the data**
- **Implicit vs. explicit features**
  - ℓ_1-norm: explicit features
  - ℓ_2-norm: representer theorem allows to consider implicit features if their dot products can be computed easily (kernel methods)

Kernel methods: regularization by ℓ_2-norm

- Data: $x_i \in \mathcal{X}$, $y_i \in \mathcal{Y}$, $i = 1, \dots, n$, with **features** $\Phi(x) \in \mathcal{F} = \mathbb{R}^p$
  - Predictor $f(x) = w^\top \Phi(x)$ linear in the features

- Optimization problem: $\boxed{\displaystyle \min_{w \in \mathbb{R}^p} \sum_{i=1}^n \ell(y_i, w^\top \Phi(x_i)) + \frac{\lambda}{2} \|w\|_{\mathbf{2}}^2}$

Kernel methods: regularization by ℓ_2-norm

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  - Predictor $f(x) = w^\top \Phi(x)$ linear in the features
- Optimization problem: $\boxed{\displaystyle \min_{w \in \mathbb{R}^p} \sum_{i=1}^n \ell(y_i, w^\top \Phi(x_i)) + \frac{\lambda}{2} \|w\|_{\mathbf{2}}^2}$
- **Representer theorem** (Kimeldorf and Wahba, 1971): solution must be of the form $w = \sum_{i=1}^n \alpha_i \Phi(x_i)$
  - Equivalent to solving: $\boxed{\displaystyle \min_{\alpha \in \mathbb{R}^n} \sum_{i=1}^n \ell(y_i, (K\alpha)_i) + \frac{\lambda}{2} \alpha^\top K \alpha}$
  - Kernel matrix $K_{ij} = k(x_i, x_j) = \Phi(x_i)^\top \Phi(x_j)$

Multiple kernel learning (MKL) (Lanckriet et al., 2004b; Bach et al., 2004a)

- Sparse methods are linear!
- Sparsity with non-linearities
  - replace $f(x) = \sum_{j=1}^{p} w_j^\top x_j$ with $x \in \mathbb{R}^p$ and $w_j \in \mathbb{R}$
  - by $f(x) = \sum_{j=1}^{p} w_j^\top \Phi_j(x)$ with $x \in \mathcal{X}$, $\Phi_j(x) \in \mathcal{F}_j$ an $w_j \in \mathcal{F}_j$
- Replace the ℓ_1-norm $\sum_{j=1}^{p} |w_j|$ by "block" ℓ_1-norm $\sum_{j=1}^{p} \|w_j\|_2$
- Remarks
  - Hilbert space extension of the group Lasso (Yuan and Lin, 2006)
  - Alternative sparsity-inducing norms (Ravikumar et al., 2008)

Multiple kernel learning

- Learning combinations of kernels: $K(\eta) = \sum_{j=1}^{m} \eta_j K_j, \quad \eta \geqslant 0$
  - Summing kernels $\Leftrightarrow$ concatenating feature spaces
  - Assume $k_1(x,y) = \langle \Phi_1(x), \Phi_1(y) \rangle$, $k_2(x,y) = \langle \Phi_2(x), \Phi_2(y) \rangle$

$$k_1(x,y) + k_2(x,y) = \left\langle \binom{\Phi_1(x)}{\Phi_2(x)}, \binom{\Phi_1(y)}{\Phi_2(y)} \right\rangle$$

- Summing kernels $\Leftrightarrow$ generalized additive models

- Relationships with sparse additive models (Ravikumar et al., 2008)

Multiple kernel learning (MKL) (Lanckriet et al., 2004b; Bach et al., 2004a)

- Multiple feature maps / kernels on $x \in \mathcal{X}$:
  - p "feature maps" $\Phi_j : \mathcal{X} \mapsto \mathcal{F}_j$, $j = 1, \dots, p$.
  - Minimization with respect to $w_1 \in \mathcal{F}_1, \dots, w_p \in \mathcal{F}_p$
  - Predictor: $f(x) = w_1{}^\top \Phi_1(x) + \cdots + w_p{}^\top \Phi_p(x)$

$$
\begin{array}{ccccccc}
 & & \Phi_1(x)^\top & w_1 & & & \\
 & \nearrow & \vdots & \vdots & \searrow & & \\
x & \longrightarrow & \Phi_j(x)^\top & w_j & \longrightarrow & w_1^\top \Phi_1(x) + \cdots + w_p^\top \Phi_p(x) \\
 & \searrow & \vdots & \vdots & \nearrow & & \\
 & & \Phi_p(x)^\top & w_p & & &
\end{array}
$$

  - Generalized additive models (Hastie and Tibshirani, 1990)

Regularization for multiple features

$$
\begin{array}{ccccc}
 & & \Phi_1(x)^\top \quad w_1 & & \\
 & \nearrow & \vdots \qquad \vdots & \searrow & \\
x & \longrightarrow & \Phi_j(x)^\top \quad w_j & \longrightarrow & w_1^\top \Phi_1(x) + \cdots + w_p^\top \Phi_p(x) \\
 & \searrow & \vdots \qquad \vdots & \nearrow & \\
 & & \Phi_p(x)^\top \quad w_p & &
\end{array}
$$

- Regularization by $\sum_{j=1}^p \|w_j\|_2^2$ is equivalent to using $K = \sum_{j=1}^p K_j$
  - Summing kernels is equivalent to concatenating feature spaces

Regularization for multiple features

$$
\begin{array}{cccccc}
 & & \Phi_1(x)^\top & w_1 & & \\
 & \nearrow & \vdots & \vdots & \searrow & \\
x & \longrightarrow & \Phi_j(x)^\top & w_j & \longrightarrow & w_1^\top \Phi_1(x) + \cdots + w_p^\top \Phi_p(x) \\
 & \searrow & \vdots & \vdots & \nearrow & \\
 & & \Phi_p(x)^\top & w_p & &
\end{array}
$$

- Regularization by $\sum_{j=1}^{p} \|w_j\|_2^2$ is equivalent to using $K = \sum_{j=1}^{p} K_j$
- Regularization by $\sum_{j=1}^{p} \|w_j\|_2$ imposes sparsity at the group level
- **Main questions when regularizing by block ℓ_1-norm**:
  1. Algorithms
  2. Analysis of sparsity inducing properties (Ravikumar et al., 2008; Bach, 2008c)
  3. Does it correspond to a specific combination of kernels?

General kernel learning

- **Proposition** (Lanckriet et al, 2004, Bach et al., 2005, Micchelli and Pontil, 2005):

$$
\begin{aligned}
G(K) &= \min_{w \in \mathcal{F}} \textstyle\sum_{i=1}^n \ell(y_i, w^\top \Phi(x_i)) + \frac{\lambda}{2}\|w\|_2^2 \\
&= \max_{\alpha \in \mathbb{R}^n} -\textstyle\sum_{i=1}^n \ell_i^*(\lambda \alpha_i) - \frac{\lambda}{2}\alpha^\top K \alpha
\end{aligned}
$$

  is a **convex** function of the kernel matrix K

- Theoretical learning bounds (Lanckriet et al., 2004, Srebro and Ben-David, 2006)
  - Less assumptions than sparsity-based bounds, but slower rates

Equivalence with kernel learning (Bach et al., 2004a)

- Block ℓ_1-norm problem:

$$\sum_{i=1}^{n} \ell(y_i, w_1^\top \Phi_1(x_i) + \cdots + w_p^\top \Phi_p(x_i)) + \frac{\lambda}{2} (\|w_1\|_2 + \cdots + \|w_p\|_2)^2$$

- **Proposition**: Block ℓ_1-norm regularization is equivalent to minimizing with respect to η the optimal value $G(\sum_{j=1}^{p} \eta_j K_j)$

- (sparse) weights η obtained from optimality conditions

- dual parameters α optimal for $K = \sum_{j=1}^{p} \eta_j K_j$,

- **Single optimization problem for learning both η and α**

Proof of equivalence

$$
\begin{aligned}
& \min_{w_1,\dots,w_p} \sum_{i=1}^n \ell\Big(y_i, \sum_{j=1}^p w_j^\top \Phi_j(x_i)\Big) + \lambda\Big(\sum_{j=1}^p \|w_j\|_2\Big)^2 \\
= \quad & \min_{w_1,\dots,w_p} \min_{\sum_j \eta_j = 1} \sum_{i=1}^n \ell\Big(y_i, \sum_{j=1}^p w_j^\top \Phi_j(x_i)\Big) + \lambda \sum_{j=1}^p \|w_j\|_2^2/\eta_j \\
= \quad & \min_{\sum_j \eta_j = 1} \min_{\tilde{w}_1,\dots,\tilde{w}_p} \sum_{i=1}^n \ell\Big(y_i, \sum_{j=1}^p \eta_j^{1/2} \tilde{w}_j^\top \Phi_j(x_i)\Big) + \lambda \sum_{j=1}^p \|\tilde{w}_j\|_2^2 \text{ with } \tilde{w}_j = w_j \eta_j^{-1/2} \\
= \quad & \min_{\sum_j \eta_j = 1} \min_{\tilde{w}} \sum_{i=1}^n \ell\big(y_i, \tilde{w}^\top \Psi_\eta(x_i)\big) + \lambda \|\tilde{w}\|_2^2 \text{ with } \Psi_\eta(x) = (\eta_1^{1/2}\Phi_1(x), \dots, \eta_p^{1/2}\Phi_p(x))
\end{aligned}
$$

- We have: $\Psi_\eta(x)^\top \Psi_\eta(x') = \sum_{j=1}^p \eta_j k_j(x, x')$ with $\sum_{j=1}^p \eta_j = 1$ (and $\eta \geqslant 0$)

Algorithms for the group Lasso / MKL

- Group Lasso
  - Block coordinate descent (Yuan and Lin, 2006)
  - Active set method (Roth and Fischer, 2008; Obozinski et al., 2009)
  - Nesterov's accelerated method (Liu et al., 2009)

- MKL
  - Dual ascent, e.g., sequential minimal optimization (Bach et al., 2004a)
  - η-trick + cutting-planes (Sonnenburg et al., 2006)
  - η-trick + projected gradient descent (Rakotomamonjy et al., 2008)
  - Active set (Bach, 2008b)

Applications of multiple kernel learning

- **Selection of hyperparameters for kernel methods**
- **Fusion from heterogeneous data sources** (Lanckriet et al., 2004a)
- Two strategies for kernel combinations:
  - Uniform combination $\Leftrightarrow$ ℓ_2-norm
  - Sparse combination $\Leftrightarrow$ ℓ_1-norm
  - MKL always leads to more interpretable models
  - MKL does not always lead to better predictive performance
    * In particular, with few well-designed kernels
    * Be careful with normalization of kernels (Bach et al., 2004b)

Applications of multiple kernel learning

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    - In particular, with few well-designed kernels
    - Be careful with normalization of kernels (Bach et al., 2004b)
- **Sparse methods**: new possibilities and new features

Course outline

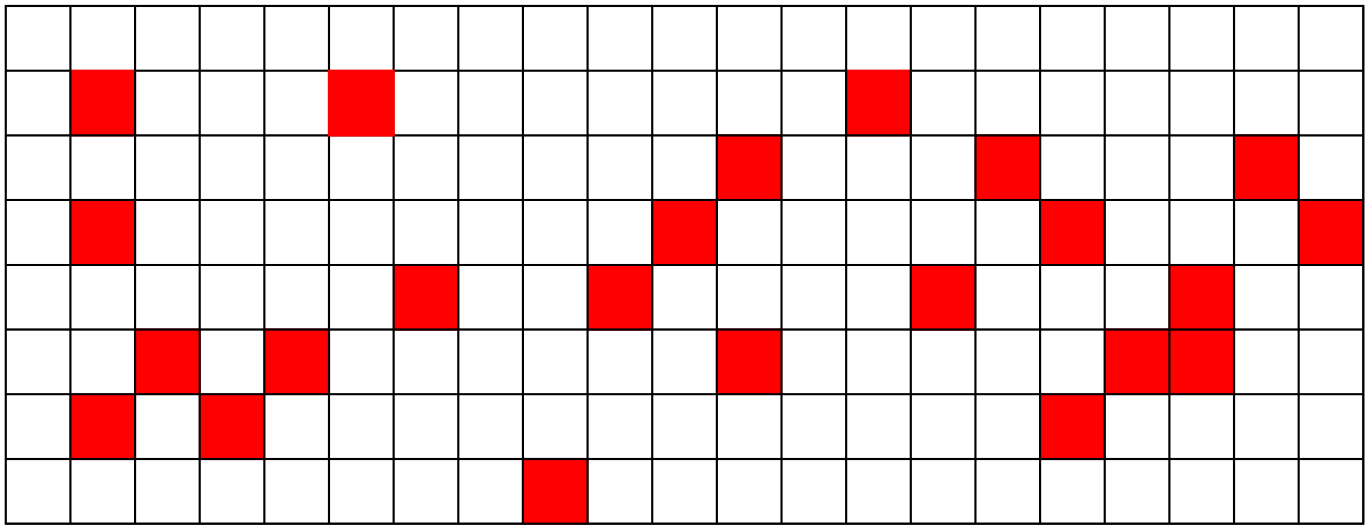
1. **Losses for particular machine learning tasks**
   - Classification, regression, etc...
2. **Regularization by Hilbert norms (kernel methods)**
   - Kernels and representer theorem
   - Convex duality, optimization and algorithms
   - Kernel methods
   - Kernel design
3. **Regularization by sparsity-inducing norms**
   - ℓ_1-norm regularization
   - Multiple kernel learning
   - Theoretical results
   - Learning on matrices

Learning on matrices - Image denoising

- Simultaneously denoise all patches of a given image
- Example from Mairal, Bach, Ponce, Sapiro, and Zisserman (2009)

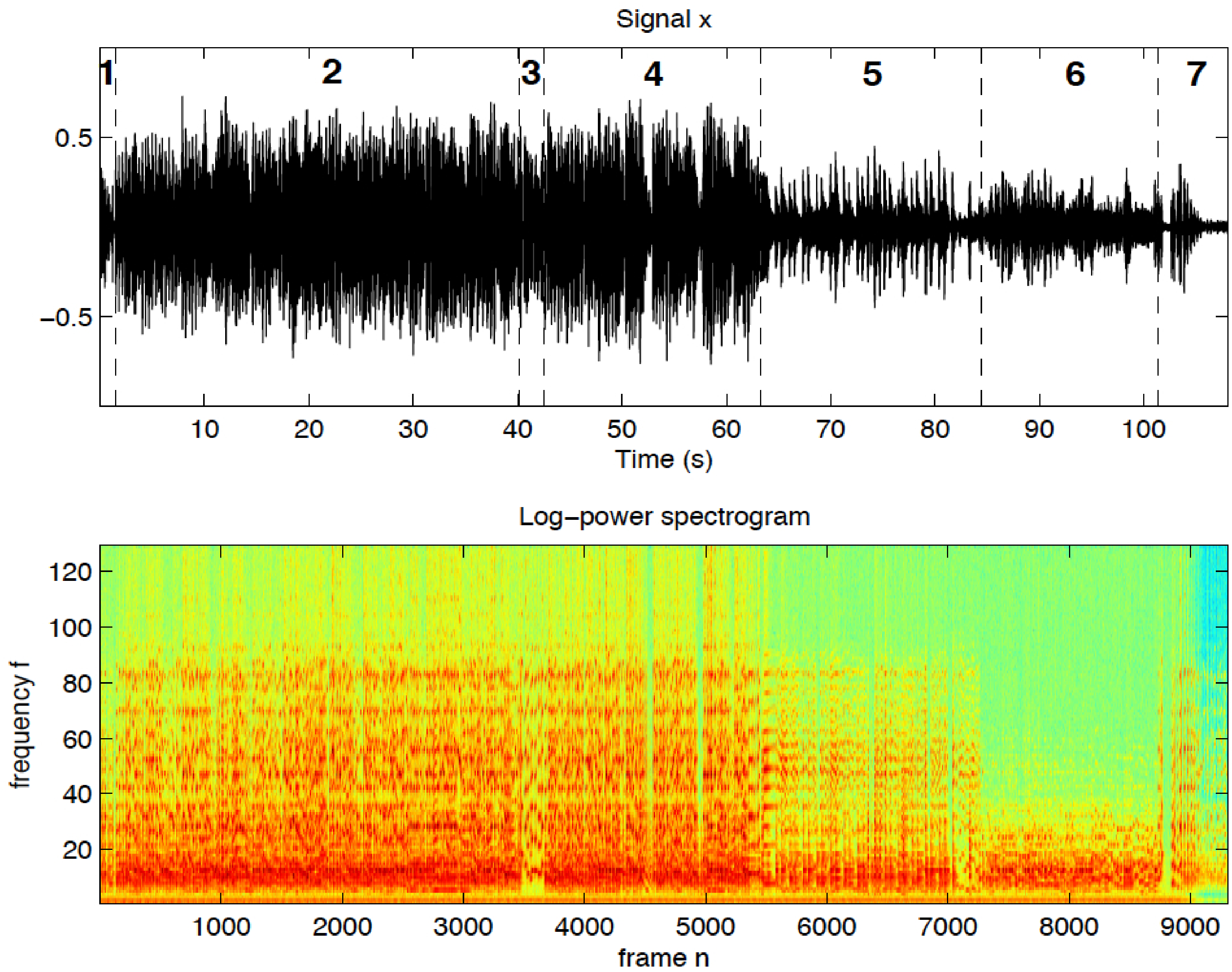

Learning on matrices - Collaborative filtering

- Given $n_{\mathcal{X}}$ "movies" $\mathbf{x} \in \mathcal{X}$ and $n_{\mathcal{Y}}$ "customers" $\mathbf{y} \in \mathcal{Y}$,
- predict the "rating" $z(\mathbf{x}, \mathbf{y}) \in \mathcal{Z}$ of customer $\mathbf{y}$ for movie $\mathbf{x}$
- Training data: large $n_{\mathcal{X}} \times n_{\mathcal{Y}}$ incomplete matrix $\mathbf{Z}$ that describes the known ratings of some customers for some movies
- **Goal**: complete the matrix.



Learning on matrices - Source separation

- Single microphone (Benaroya et al., 2006; Févotte et al., 2009)

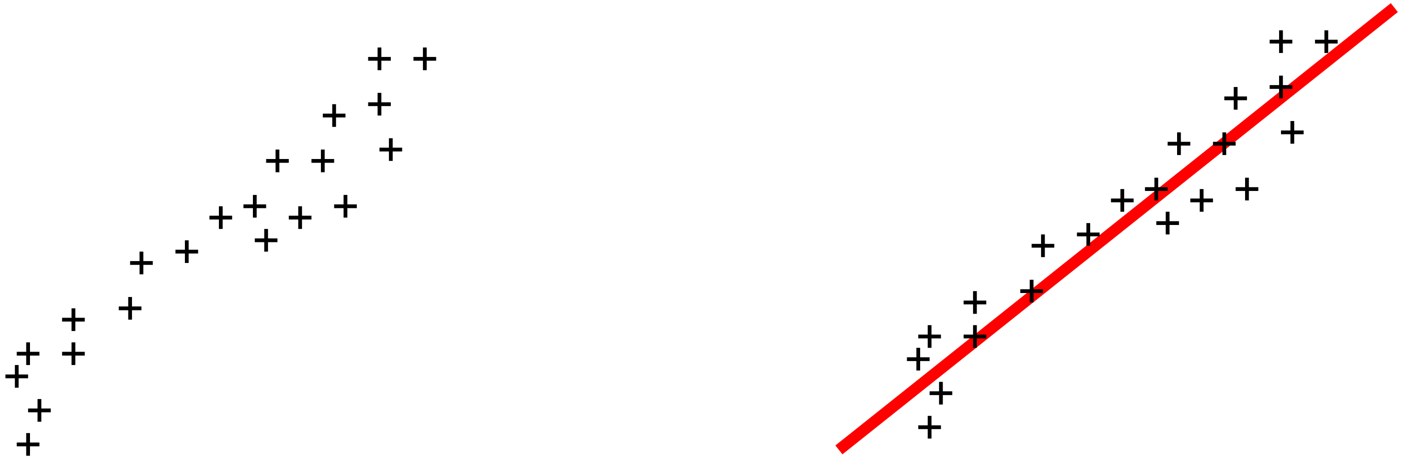


Learning on matrices - Multi-task learning

- k linear prediction tasks on same covariates $\mathbf{x} \in \mathbb{R}^p$
  - k weight vectors $\mathbf{w}_j \in \mathbb{R}^p$
  - Joint matrix of predictors $\mathbf{W} = (\mathbf{w}_1, \dots, \mathbf{w}_k) \in \mathbb{R}^{p \times k}$
- Classical application
  - Multi-category classification (one task per class) (Amit et al., 2007)
- **Share parameters between tasks**
- **Joint variable selection** (Obozinski et al., 2009)
  - Select variables which are predictive for all tasks
- **Joint feature selection** (Pontil et al., 2007)
  - Construct linear features common to all tasks

Matrix factorization - Dimension reduction

- Given data matrix $\mathcal{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_n) \in \mathbb{R}^{p \times n}$
  - **Principal component analysis**: $\boxed{\mathbf{x}_i \approx \mathbf{D}\boldsymbol{\alpha}_i \Rightarrow \mathbf{X} = \mathbf{DA}}$

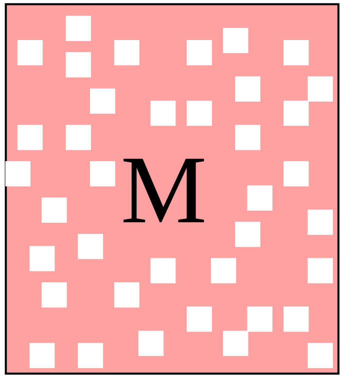


  - **K-means**: $\boxed{\mathbf{x}_i \approx \mathbf{d}_k \Rightarrow \mathbf{X} = \mathbf{DA}}$

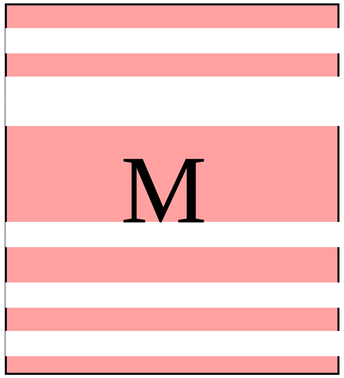
Two types of sparsity for matrices $\mathbf{M} \in \mathbb{R}^{n \times p}$

I - Directly on the elements of $\mathbf{M}$

- Many zero elements: $\mathbf{M}_{ij} = 0$



- Many zero rows (or columns): $(\mathbf{M}_{i1}, \ldots, \mathbf{M}_{ip}) = 0$

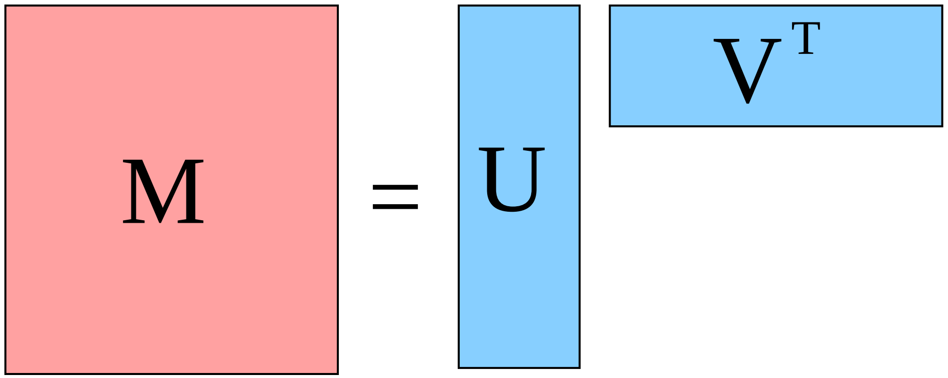


Two types of sparsity for matrices $\mathbf{M} \in \mathbb{R}^{n \times p}$

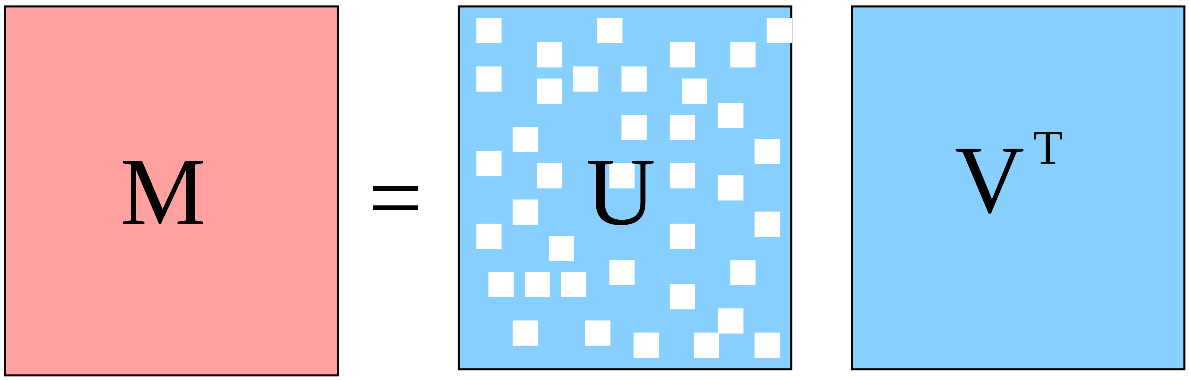
II - Through a factorization of $\mathbf{M} = \mathbf{U}\mathbf{V}^\top$

- Matrix $\mathbf{M} = \mathbf{U}\mathbf{V}^\top$, $\mathbf{U} \in \mathbb{R}^{n \times k}$ and $\mathbf{V} \in \mathbb{R}^{p \times k}$

- **Low rank**: m small



- **Sparse decomposition**: $\mathbf{U}$ sparse



Structured sparse matrix factorizations

- Matrix $\mathbf{M} = \mathbf{U}\mathbf{V}^\top$, $\mathbf{U} \in \mathbb{R}^{n\times k}$ and $\mathbf{V} \in \mathbb{R}^{p\times k}$

- **Structure on $\mathbf{U}$ and/or $\mathbf{V}$**
  - Low-rank: $\mathbf{U}$ and $\mathbf{V}$ have few columns
  - Dictionary learning / sparse PCA: $\mathbf{U}$ has many zeros
  - Clustering (k-means): $\mathbf{U} \in \{0,1\}^{n\times m}$, $\mathbf{U}\mathbf{1} = \mathbf{1}$
  - Pointwise positivity: non negative matrix factorization (NMF)
  - Specific patterns of zeros (Jenatton et al., 2010)
  - Low-rank + sparse (Candès et al., 2009)
  - etc.

- **Many applications**

- **Many open questions** (Algorithms, identifiability, etc.)

Multi-task learning

- Joint matrix of predictors $W = (w_1, \ldots, w_k) \in \mathbb{R}^{p \times k}$
- **Joint variable selection** (Obozinski et al., 2009)
  - Penalize by the sum of the norms of rows of W (group Lasso)
  - Select variables which are predictive for all tasks

Multi-task learning

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- **Joint variable selection** (Obozinski et al., 2009)
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  - Select variables which are predictive for all tasks

- **Joint feature selection** (Pontil et al., 2007)
  - Penalize by the trace-norm (see later)
  - Construct linear features common to all tasks

- Theory: allows number of observations which is sublinear in the number of tasks (Obozinski et al., 2008; Lounici et al., 2009)

- Practice: more interpretable models, slightly improved performance

Low-rank matrix factorizations
Trace norm

- Given a matrix $\mathbf{M} \in \mathbb{R}^{n \times p}$
  - Rank of $\mathbf{M}$ is the minimum size m of **all** factorizations of $\mathbf{M}$ into $\mathbf{M} = \mathbf{U}\mathbf{V}^\top$, $\mathbf{U} \in \mathbb{R}^{n \times m}$ and $\mathbf{V} \in \mathbb{R}^{p \times m}$
  - Singular value decomposition: $\mathbf{M} = \mathbf{U}\,\mathrm{Diag}(\mathbf{s})\mathbf{V}^\top$ where $\mathbf{U}$ and $\mathbf{V}$ have orthonormal columns and $\mathbf{s} \in \mathbb{R}_+^m$ are singular values

- Rank of $\mathbf{M}$ equal to the number of non-zero singular values

Low-rank matrix factorizations
Trace norm

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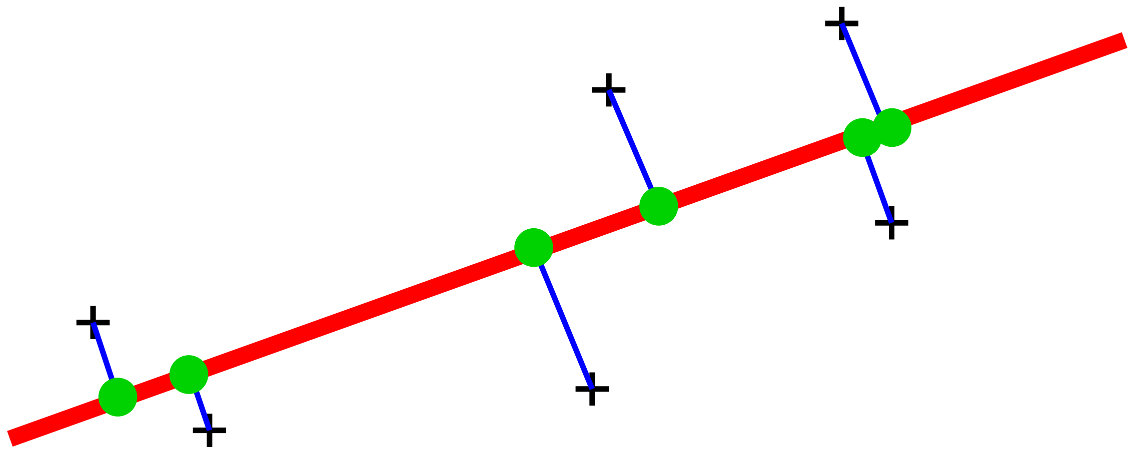
- Rank of $\mathbf{M}$ equal to the number of non-zero singular values
- **Trace-norm (a.k.a. nuclear norm)** $=$ sum of singular values
- Convex function, leads to a semi-definite program (Fazel et al., 2001)
- First used for collaborative filtering (Srebro et al., 2005)

Sparse principal component analysis

- Given data $\mathcal{X} = (\mathbf{x}_1^\top, \dots, \mathbf{x}_n^\top) \in \mathbb{R}^{p \times n}$, two views of PCA:
  - **Analysis view**: find the projection $\mathbf{d} \in \mathbb{R}^p$ of maximum variance (with deflation to obtain more components)
  - **Synthesis view**: find the basis $\mathbf{d}_1, \dots, \mathbf{d}_k$ such that all $\mathbf{x}_i$ have low reconstruction error when decomposed on this basis

- For regular PCA, the two views are equivalent



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- For regular PCA, the two views are equivalent

- **Sparse extensions**
  - Interpretability
  - High-dimensional inference
  - Two views are differents
    - For analysis view, see d'Aspremont, Bach, and El Ghaoui (2008)

Sparse principal component analysis
Synthesis view

- Find $\mathbf{d}_1, \ldots, \mathbf{d}_k \in \mathbb{R}^p$ **sparse** so that

$$\sum_{i=1}^{n} \min_{\boldsymbol{\alpha}_i \in \mathbb{R}^m} \left\| \mathbf{x}_i - \sum_{j=1}^{k} (\boldsymbol{\alpha}_i)_j \mathbf{d}_j \right\|_2^2 = \sum_{i=1}^{n} \min_{\boldsymbol{\alpha}_i \in \mathbb{R}^m} \left\| \mathbf{x}_i - \mathbf{D}\boldsymbol{\alpha}_i \right\|_2^2 \text{ is small}$$

  – Look for $\mathbf{A} = (\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_n) \in \mathbb{R}^{k \times n}$ and $\mathbf{D} = (\mathbf{d}_1, \ldots, \mathbf{d}_k) \in \mathbb{R}^{p \times k}$ such that $\mathbf{D}$ is sparse and $\|\mathcal{X} - \mathbf{D}\mathbf{A}\|_F^2$ is small

Sparse principal component analysis
Synthesis view

- Find $\mathbf{d}_1, \dots, \mathbf{d}_k \in \mathbb{R}^p$ **sparse** so that

$$\sum_{i=1}^{n} \min_{\boldsymbol{\alpha}_i \in \mathbb{R}^m} \left\| \mathbf{x}_i - \sum_{j=1}^{k} (\boldsymbol{\alpha}_i)_j \mathbf{d}_j \right\|_2^2 = \sum_{i=1}^{n} \min_{\boldsymbol{\alpha}_i \in \mathbb{R}^m} \left\| \mathbf{x}_i - \mathbf{D}\boldsymbol{\alpha}_i \right\|_2^2 \text{ is small}$$

  – Look for $\mathbf{A} = (\boldsymbol{\alpha}_1, \dots, \boldsymbol{\alpha}_n) \in \mathbb{R}^{k \times n}$ and $\mathbf{D} = (\mathbf{d}_1, \dots, \mathbf{d}_k) \in \mathbb{R}^{p \times k}$ such that $\mathbf{D}$ is sparse and $\|\mathcal{X} - \mathbf{DA}\|_F^2$ is small

- Sparse formulation (Witten et al., 2009; Bach et al., 2008)

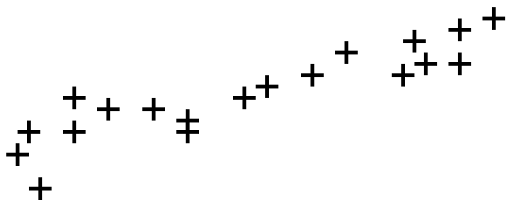
  – Penalize/constrain $\mathbf{d}_j$ by the ℓ_1-norm for sparsity

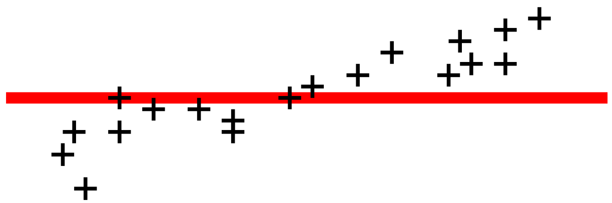
  – Penalize/constrain $\boldsymbol{\alpha}_i$ by the ℓ_2-norm to avoid trivial solutions

$$\min_{\mathbf{D},\mathbf{A}} \sum_{i=1}^{n} \|\mathbf{x}_i - \mathbf{D}\boldsymbol{\alpha}_i\|_2^2 + \lambda \sum_{j=1}^{k} \|\mathbf{d}_j\|_1 \text{ s.t. } \forall i, \|\boldsymbol{\alpha}_i\|_2 \leqslant 1$$

Sparse PCA vs. dictionary learning

- **Sparse PCA**: $\mathbf{x}_i \approx \mathbf{D}\boldsymbol{\alpha}_i$, $\mathbf{D}$ sparse

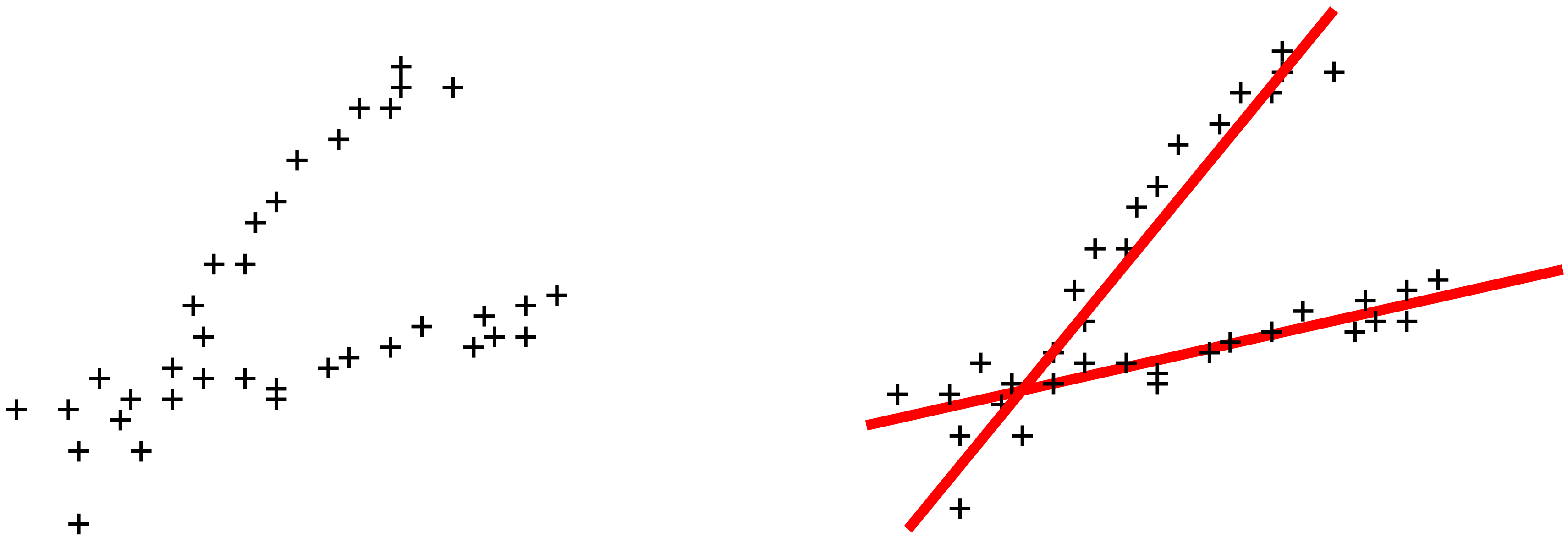




Sparse PCA vs. dictionary learning

- **Sparse PCA**: $\mathbf{x}_i \approx \mathbf{D}\boldsymbol{\alpha}_i$, $\mathbf{D}$ sparse

- **Dictionary learning**: $\mathbf{x}_i \approx \mathbf{D}\boldsymbol{\alpha}_i$, $\boldsymbol{\alpha}_i$ sparse



Structured matrix factorizations (Bach et al., 2008)

$$\min_{\mathbf{D},\mathbf{A}} \sum_{i=1}^{n} \|\mathbf{x}_i - \mathbf{D}\boldsymbol{\alpha}_i\|_2^2 + \lambda \sum_{j=1}^{k} \|\mathbf{d}_j\|_{\star} \text{ s.t. } \forall i, \|\boldsymbol{\alpha}_i\|_{\bullet} \leqslant 1$$

$$\min_{\mathbf{D},\mathbf{A}} \sum_{i=1}^{n} \|\mathbf{x}_i - \mathbf{D}\boldsymbol{\alpha}_i\|_2^2 + \lambda \sum_{i=1}^{n} \|\boldsymbol{\alpha}_i\|_{\bullet} \text{ s.t. } \forall j, \|\mathbf{d}_j\|_{\star} \leqslant 1$$

- Optimization by alternating minimization (non-convex)
- $\boldsymbol{\alpha}_i$ decomposition coefficients (or "code"), $\mathbf{d}_j$ dictionary elements
- Two related/equivalent problems:
  - **Sparse PCA = sparse dictionary** (ℓ_1-norm on $\mathbf{d}_j$)
  - **Dictionary learning = sparse decompositions** (ℓ_1-norm on $\boldsymbol{\alpha}_i$) (Olshausen and Field, 1997; Elad and Aharon, 2006; Lee et al., 2007)

Dictionary learning for image denoising

$$\underbrace{\mathbf{x}}_{\text{measurements}} = \underbrace{\mathbf{y}}_{\text{original image}} + \underbrace{\varepsilon}_{\text{noise}}$$

Sparse methods for machine learning
Why use sparse methods?

- **Sparsity as a proxy to interpretability**
  - Structured sparsity
- **Sparsity for high-dimensional inference**
  - Influence on feature design
- **Sparse methods are not limited to least-squares regression**
- **Faster training/testing**
- **Better predictive performance?**
  - Problems are sparse if you look at them the right way

Conclusion - Interesting questions/issues

- Implicit vs. explicit features
  - Can we algorithmically achieve $\log p = O(n)$ with explicit unstructured features?
- Norm design
  - What type of behavior may be obtained with sparsity-inducing norms?
- Overfitting convexity
  - Do we actually need convexity for matrix factorization problems?

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   - Kernel methods
   - Kernel design
3. **Regularization by sparsity-inducing norms**
   - ℓ_1-norm regularization
   - Multiple kernel learning
   - Theoretical results
   - Learning on matrices

Conclusion - Interesting problems (machine learning)

- Kernel design for computer vision
  - Benefits of "kernelizing" existing representations
  - Combining kernels
- Sparsity and computer vision
  - Going beyond image denoising
- Large numbers of classes
  - Theoretical and algorithmic challenges
- Structured output

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Code

- SVM and other supervised learning techniques
  `www.shogun-toolbox.org`
  `http://gaelle.loosli.fr/research/tools/simplesvm.html`
  `http://www.kyb.tuebingen.mpg.de/bs/people/spider/main.html`

- ℓ^1-penalization: Matlab/C/R codes available from

  – SPAMS (SPArse Modeling Software)
    `http://www.di.ens.fr/willow/SPAMS/`

- Multiple kernel learning:
  `asi.insa-rouen.fr/enseignants/~arakotom/code/mklindex.html`
  `www.stat.berkeley.edu/~gobo/SKMsmo.tar`