Supervised learning for computer vision: Theory and algorithms - Part II

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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 $f \in \mathcal{F}$:

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

Error on data + Regularization

Loss & function space ? Norm ?

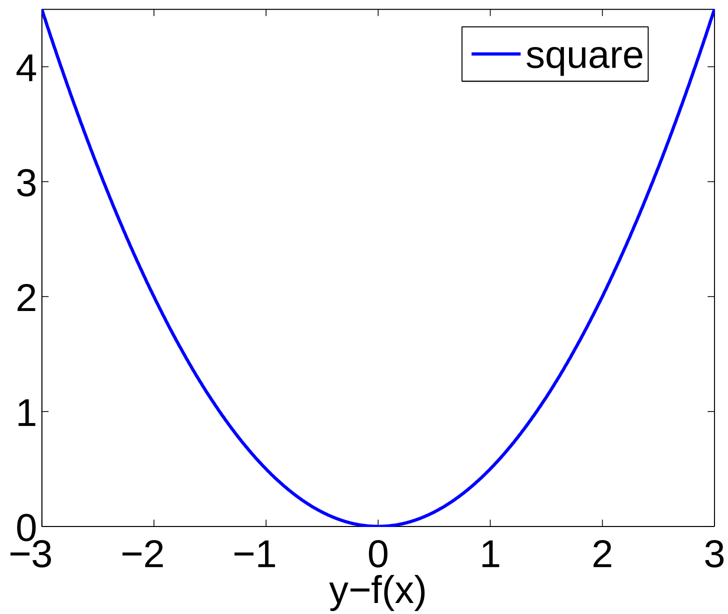
- Two theoretical/algorithmic issues:
  - Loss
  - Function space / norm

Part II - Outline

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

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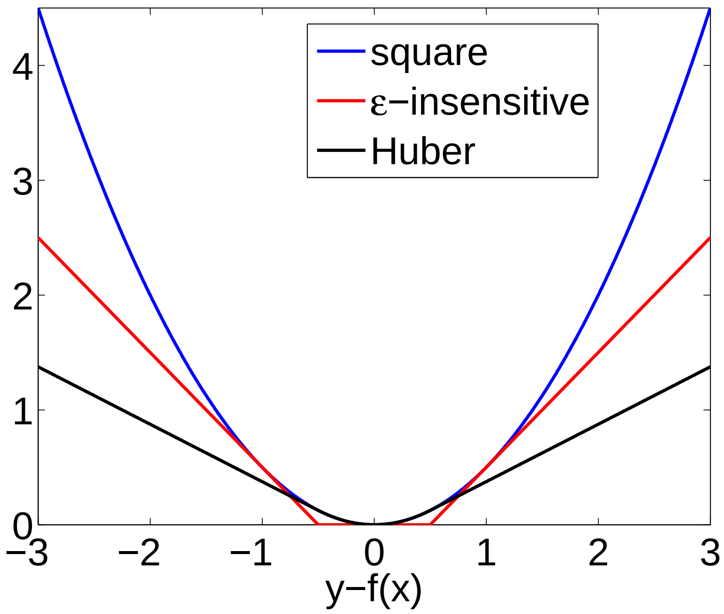
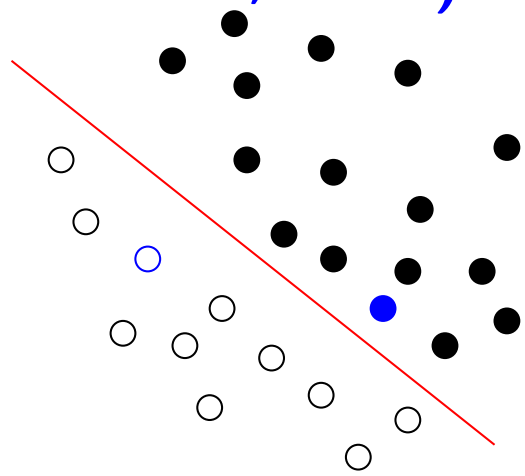
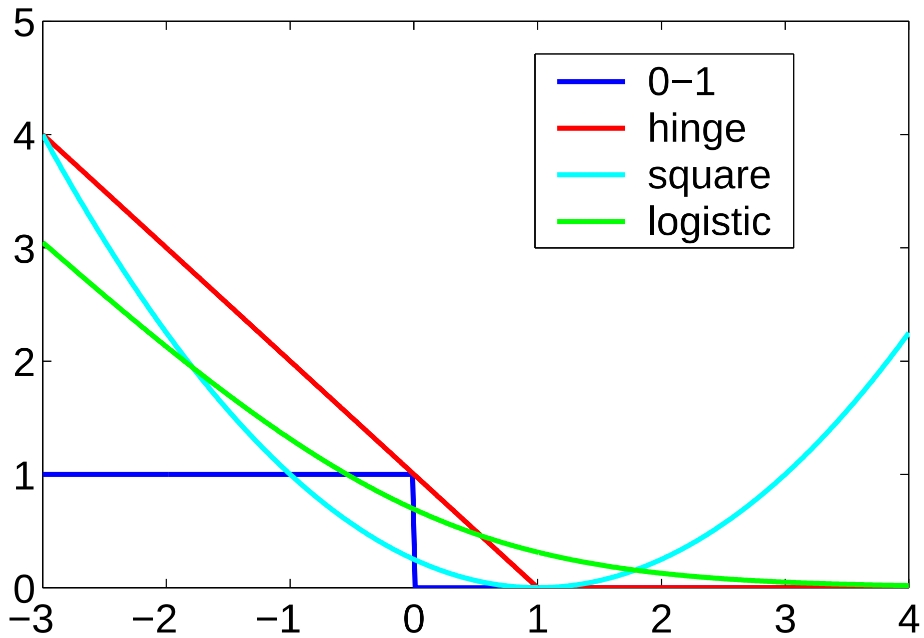
- Other convex losses "with added benefits"
  - ε-insensitive loss $\ell(y, f(x)) = (|y - f(x)| - \varepsilon)_+$
  - Hüber loss (mixed quadratic/linear): robustness to outliers



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

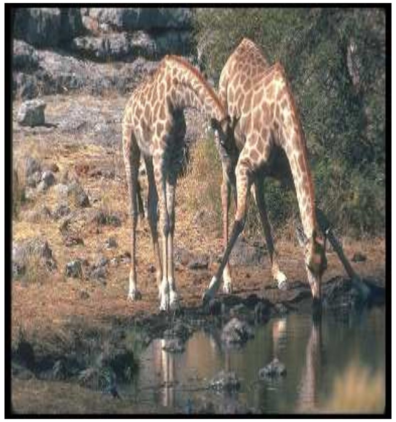


- **Label** : $y \in \{-1, 1\}$, prediction $\hat{y} = \text{sign}(f(x))$
  - loss of the form $\ell(y, f(x)) = \ell(yf(x))$
  - "True" cost: $\ell(yf(x)) = 1_{yf(x)<0}$
  - Usual convex costs:



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

Image annotation ⇒ multi-class classification





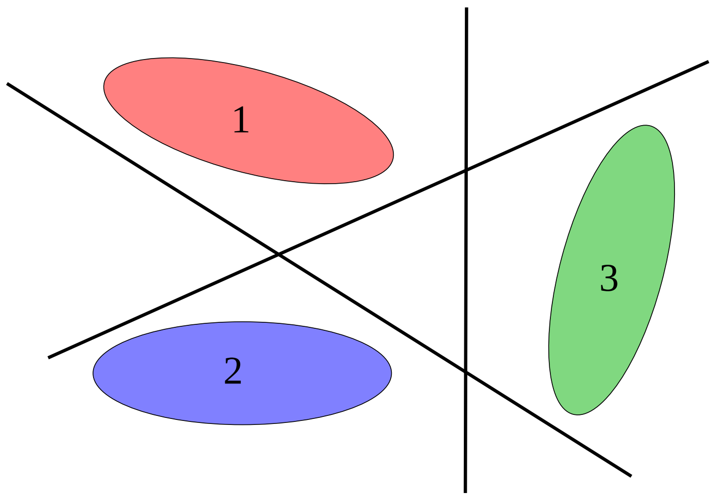
Losses for multi-label classification (Schölkopf and Smola, 2001; Shawe-Taylor and Cristianini, 2004)

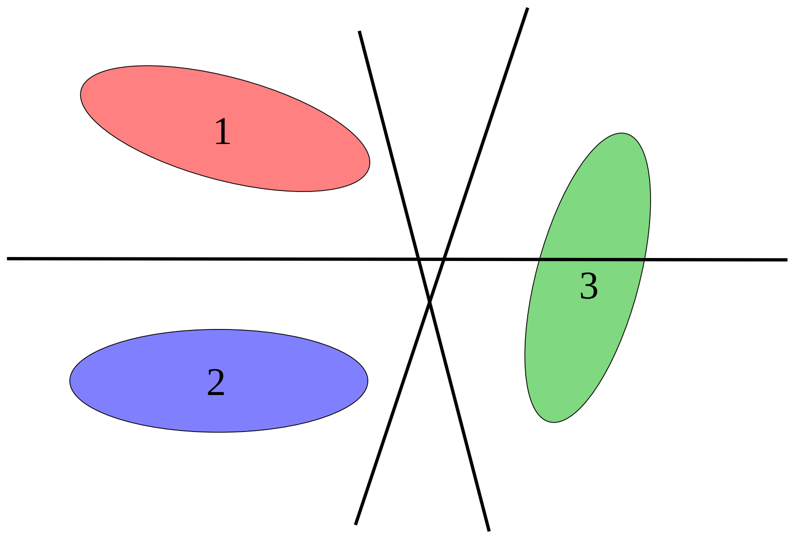
- **Two main strategies** for k classes (with unclear winners)

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")





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
  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

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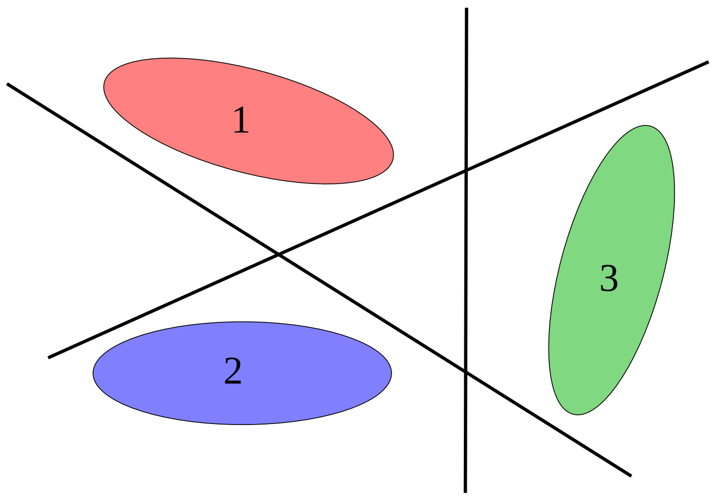
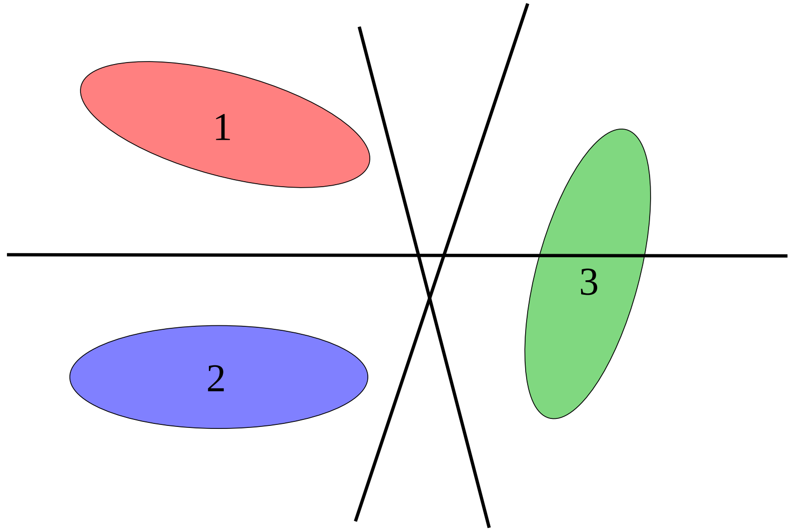




- Dedicated loss function

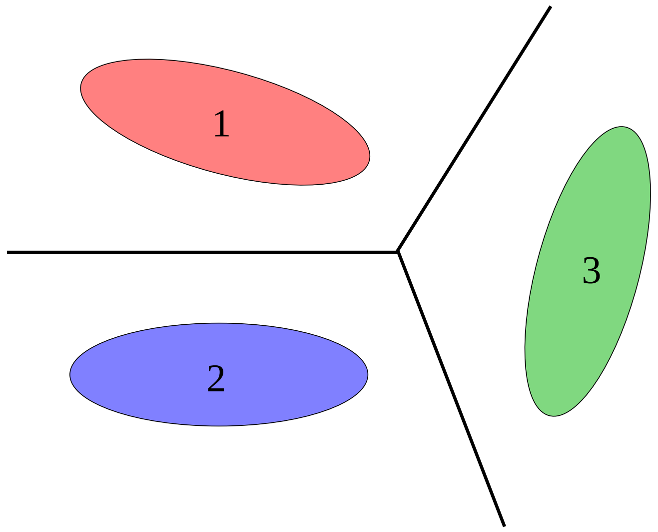
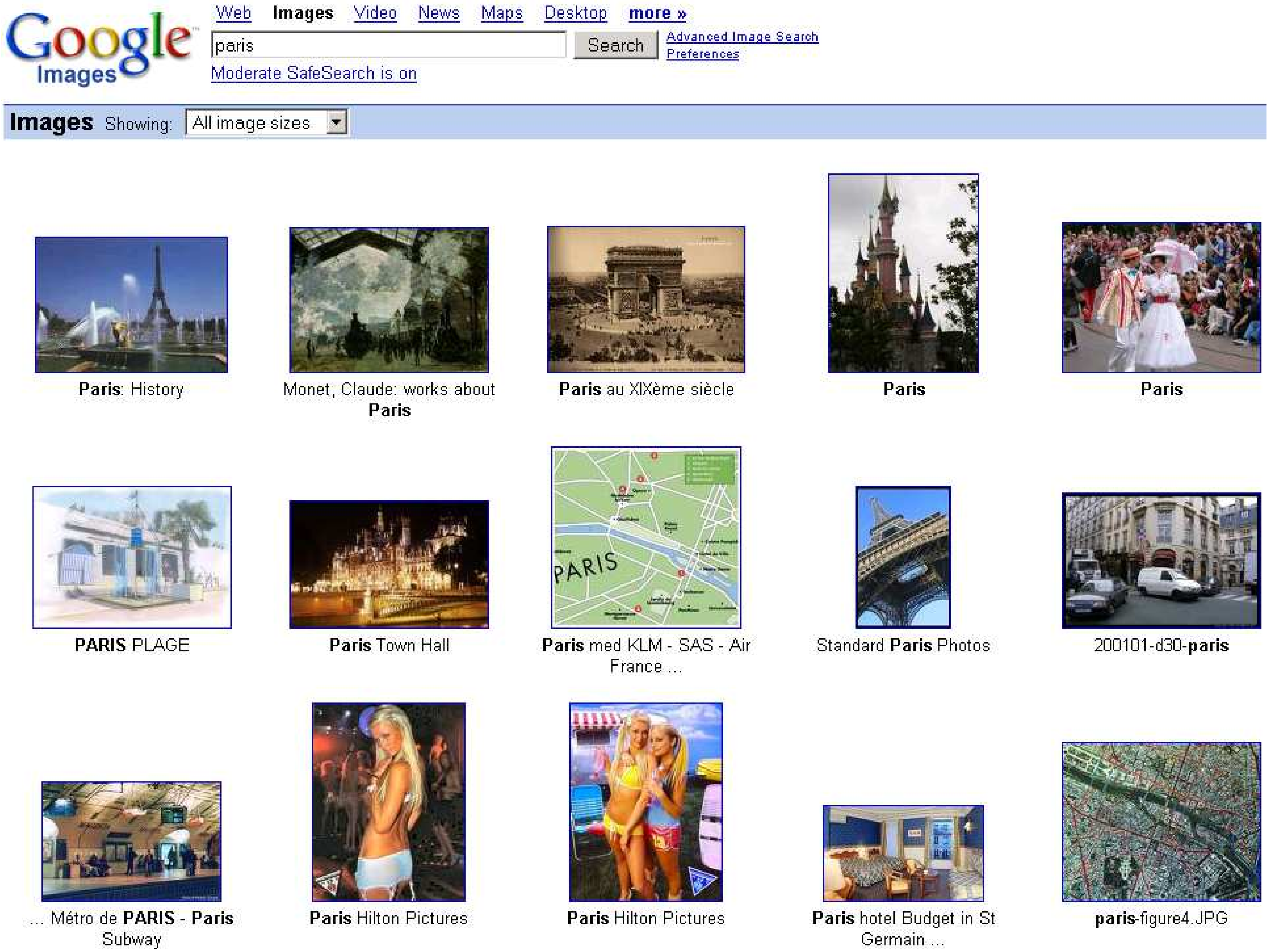


Image retrieval ⇒ ranking

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)

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

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Regularizations

- Main goal: avoid overfitting (see earlier part of the tutorial)

- 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)

- **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 $k(x, y) = \exp(-\alpha \|x - y\|^2)$
  - $\Phi(x) = ??$

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 $x \in \mathbb{R}^d$

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  - 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
$$f = \sum_{j=1}^n \alpha_j \Phi(x_j) = \sum_{j=1}^n \alpha_j k(\cdot, x_j)$$

- $\alpha \in \mathbb{R}^n$ 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

- 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
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  - Linear to non-linear learning methods

- 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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- Dual problem:

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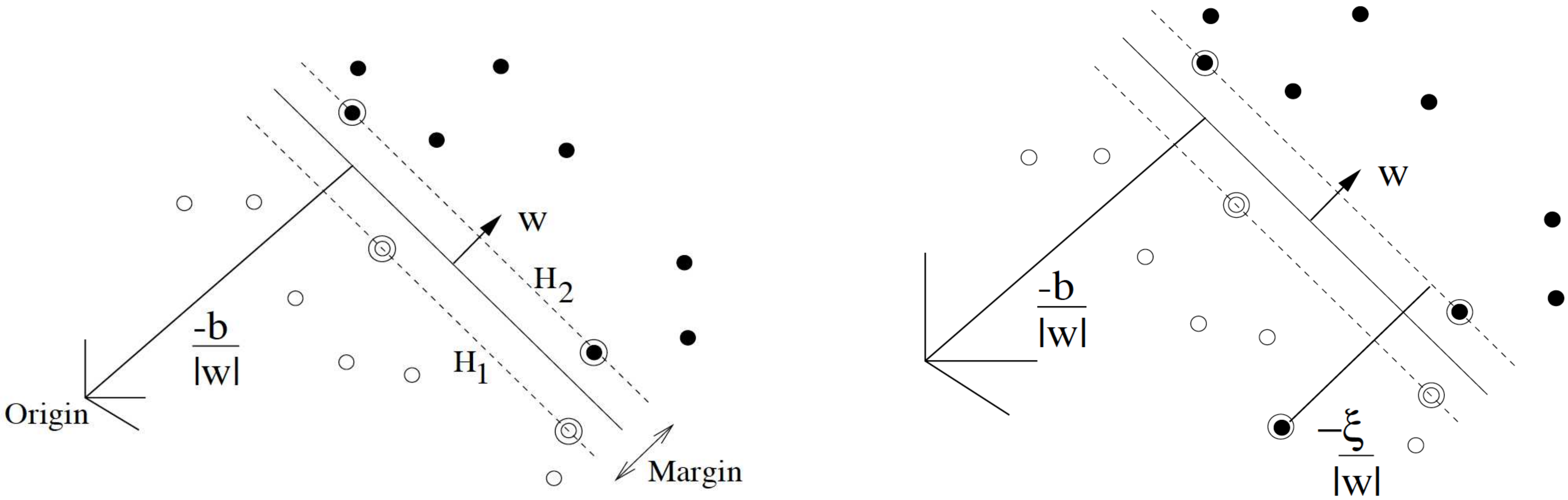
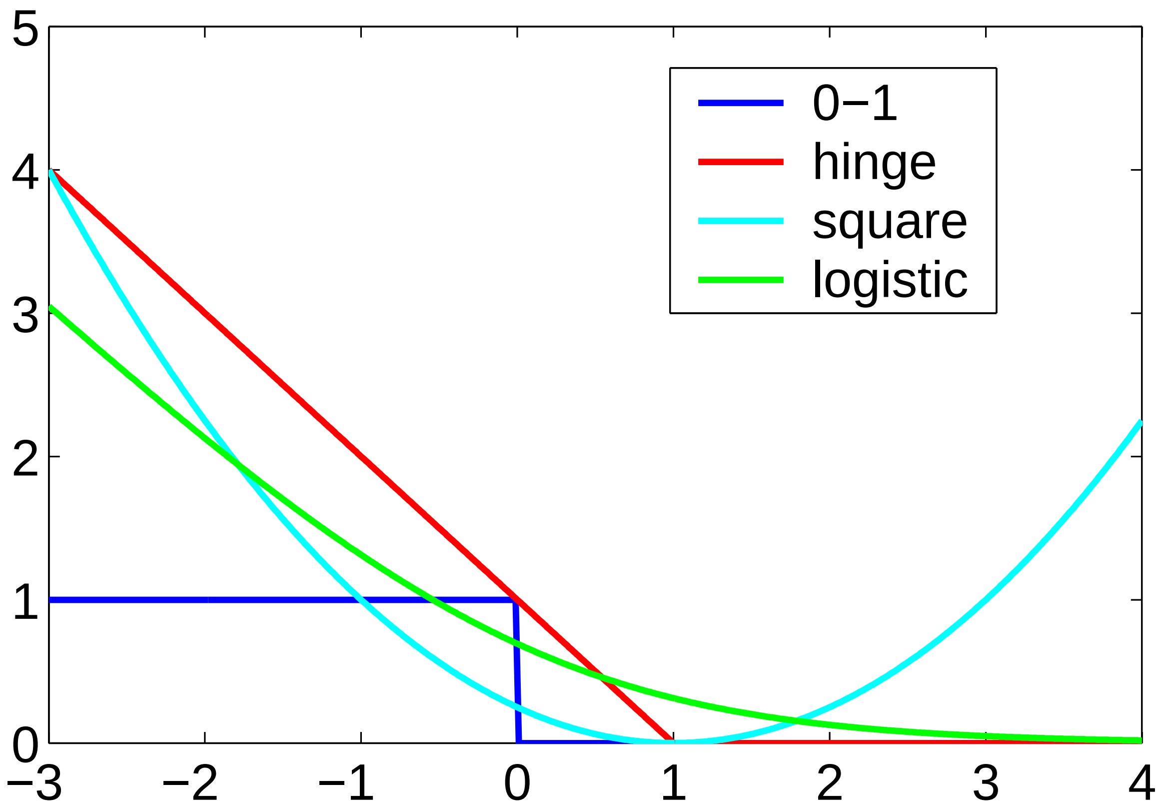
- What about the traditional picture?



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

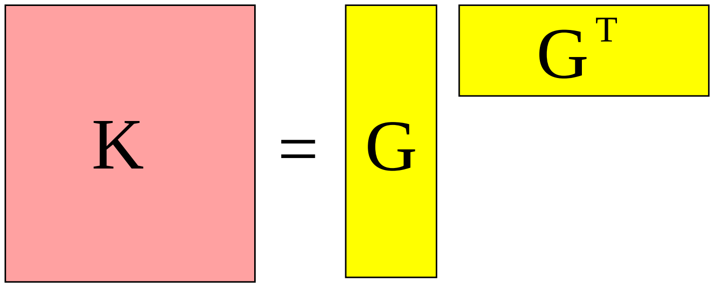
- Larger scale: stochastic gradient descent (Shalev-Shwartz et al., 2007; Bottou and Bousquet, 2008)

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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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**:

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

  - **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 $\displaystyle\sum_{i=1}^{p} \Phi_i(x)\Phi_i(y)$ **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)

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

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**: $\exp\left(-\alpha \sum_i \frac{(h_i - h'_i)^2}{h_i + h'_i}\right)$

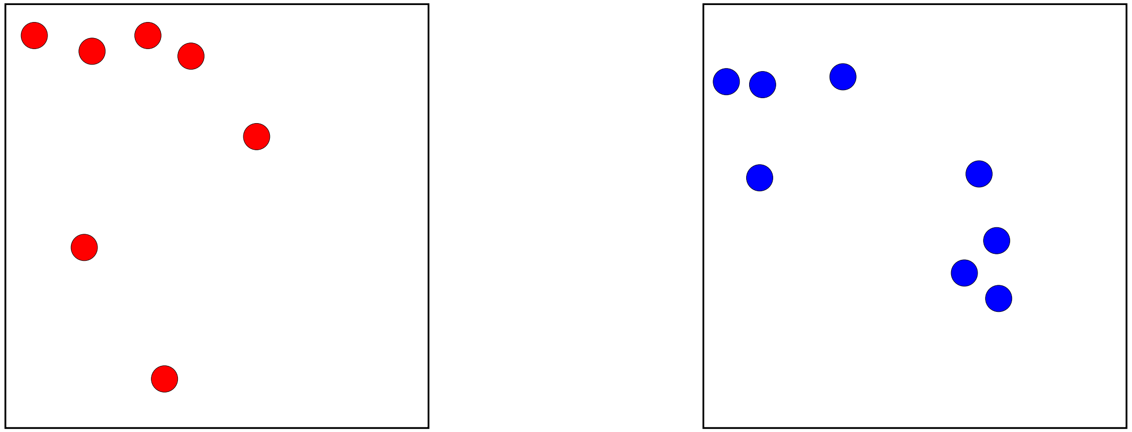
Kernels over (labelled) sets of points

- 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**: $\exp\left(-\alpha \sum_i \frac{(h_i - h'_i)^2}{h_i + h'_i}\right)$
- 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

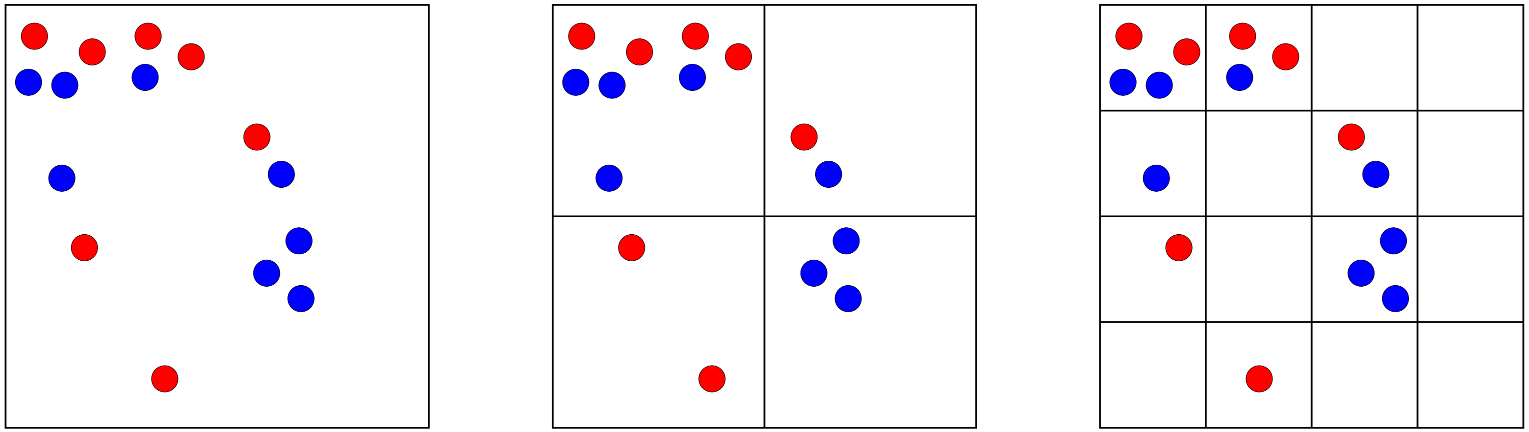
Pyramid match kernel

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

- Two sets of points



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



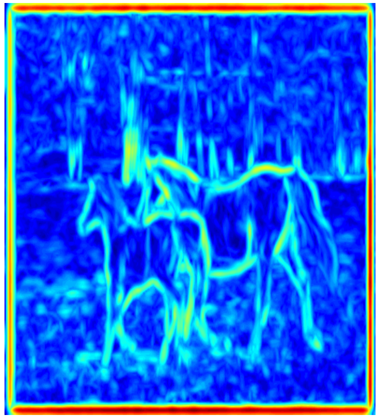
Kernels from segmentation graphs

- 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

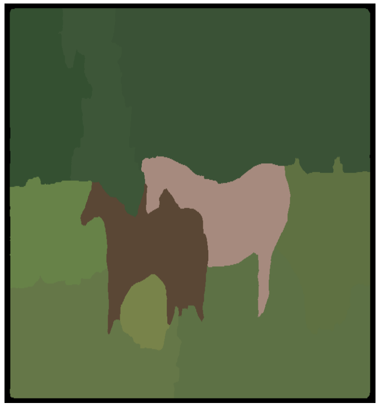


watershed

287 segments

64 segments

10 segments



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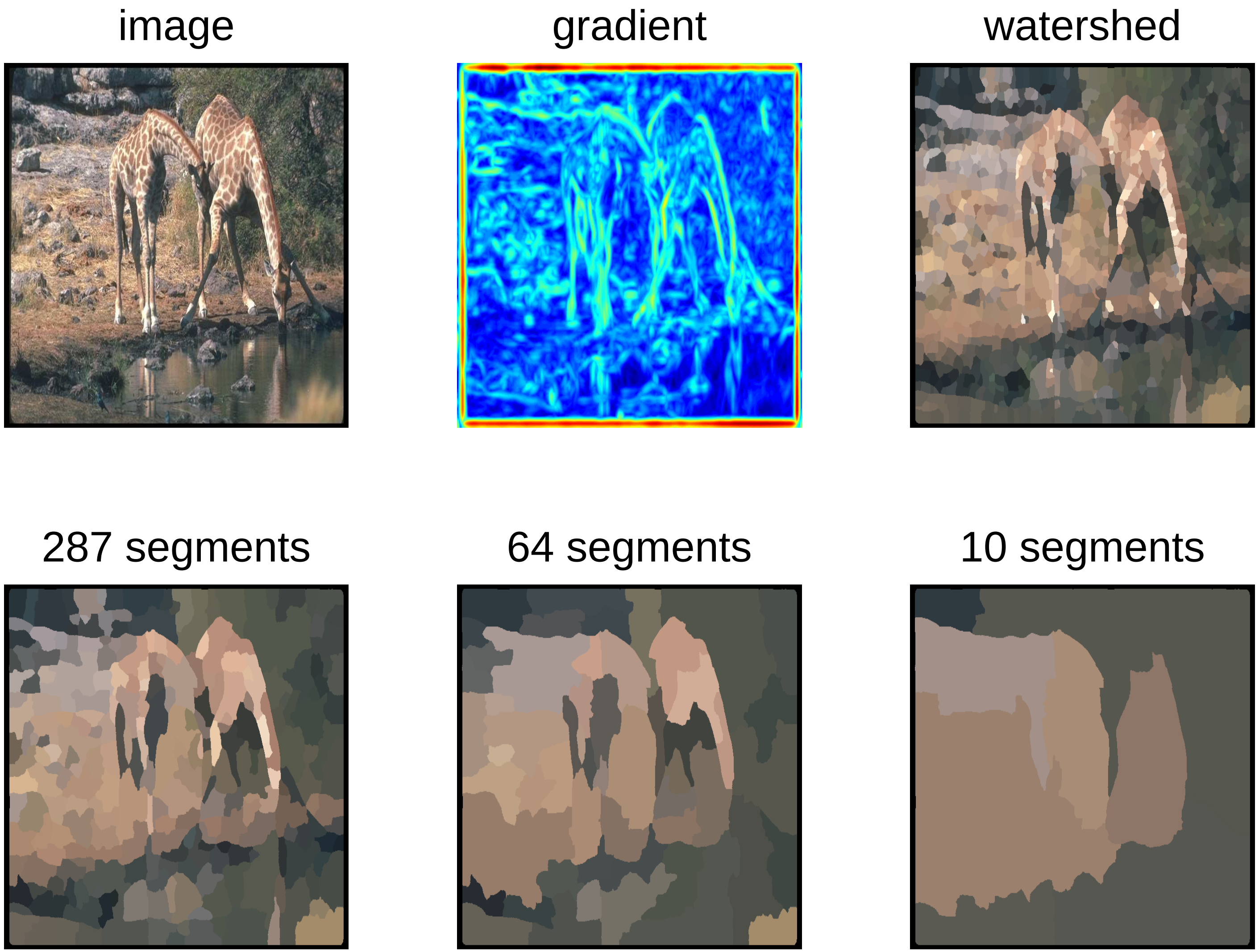


Image as a segmentation graph

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

$\Rightarrow$

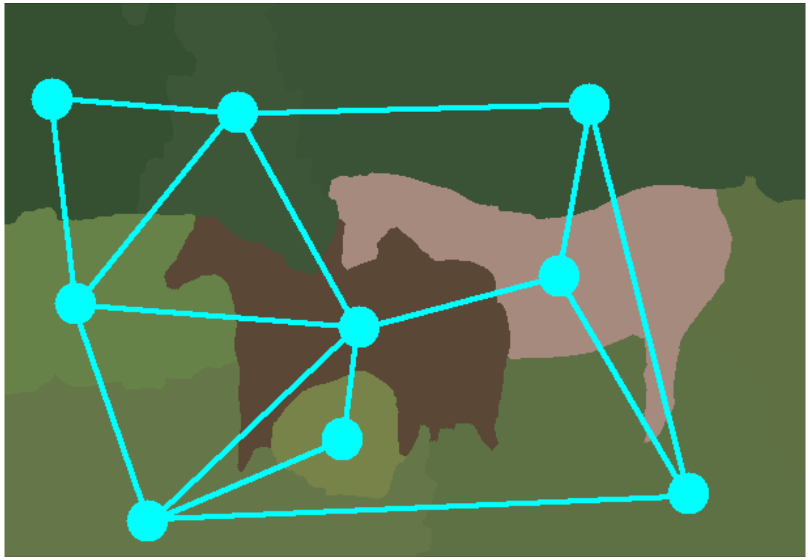


Image as a segmentation graph

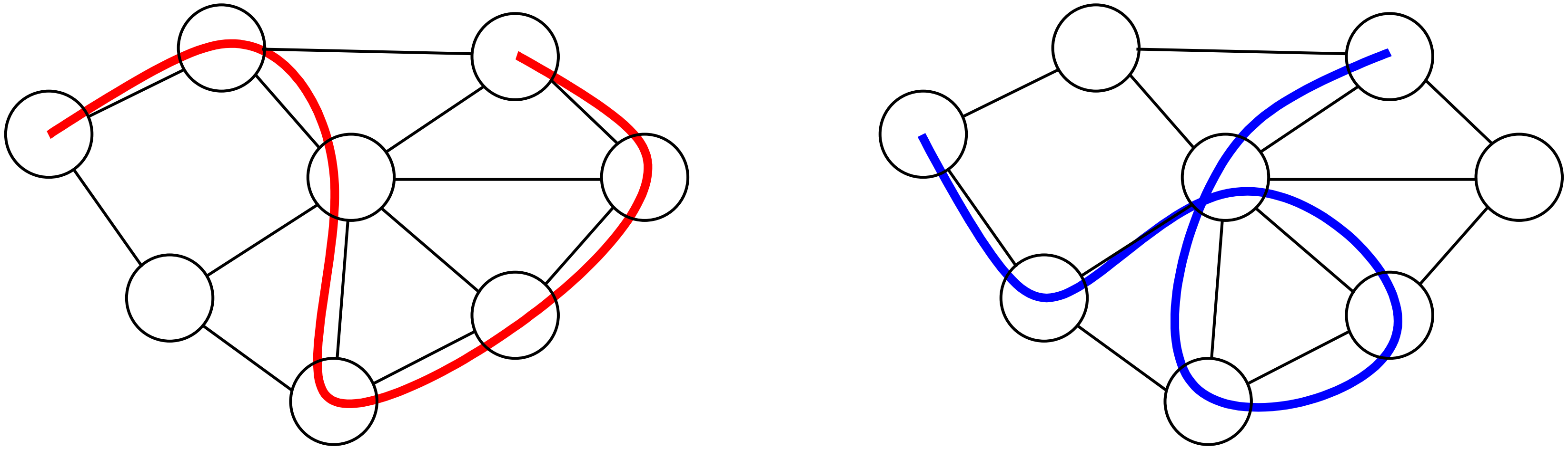
- Labelled undirected graph
  - Vertices: connected segmented regions
  - Edges: between spatially neighboring regions
  - Labels: region pixels
- Difficulties
  - Extremely high-dimensional labels
  - Planar undirected graph
  - Inexact matching
- **Graph kernels** (Gärtner et al., 2003; Kashima et al., 2004; Harchaoui and Bach, 2007) provide an elegant and efficient solution

Kernels between structured objects
Strings, graphs, etc... (Shawe-Taylor and Cristianini, 2004)

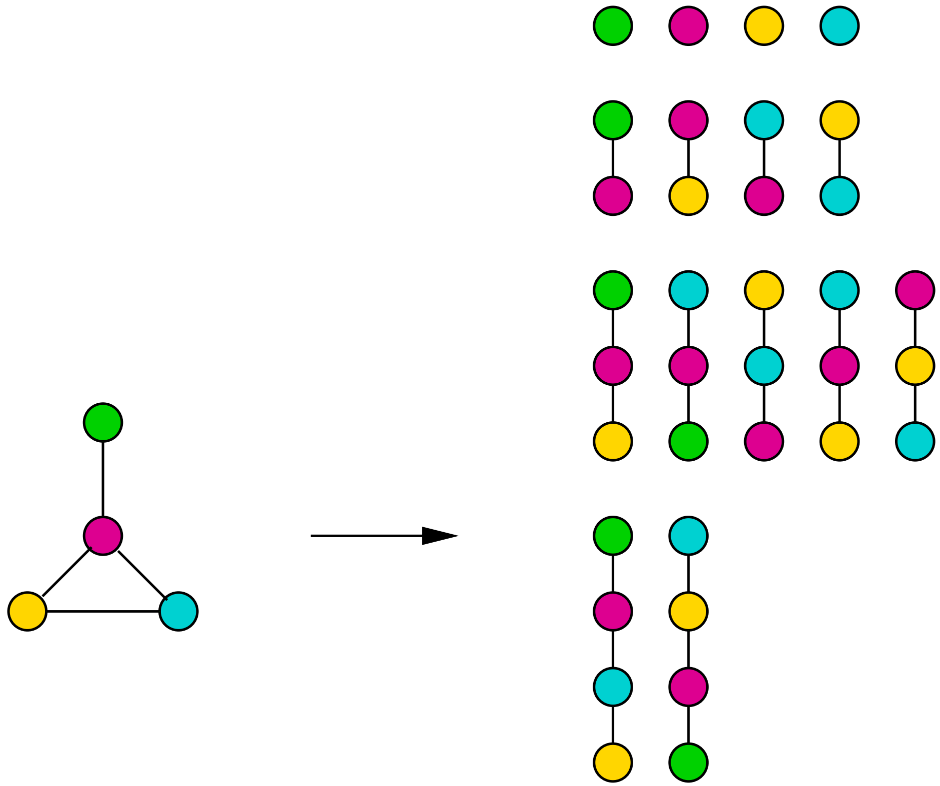
- Numerous applications (text, bio-informatics, speech, vision)
- Common design principle: **enumeration of subparts** (Haussler, 1999; Watkins, 1999)
  - Efficient for strings
  - Possibility of gaps, partial matches, very efficient algorithms
- Most approaches fails for general graphs (even for undirected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

Paths and walks

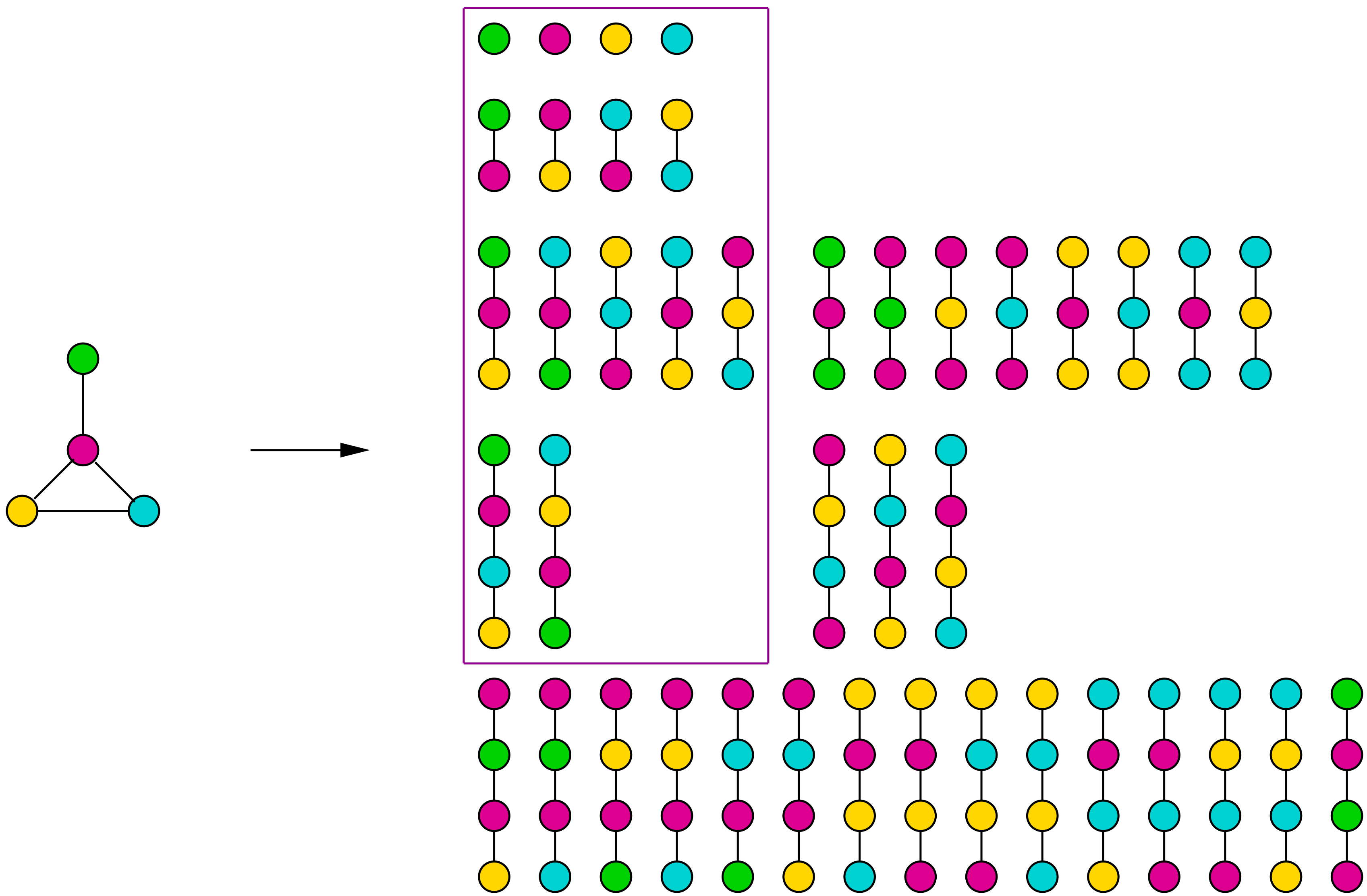
- Given a graph G,
  - A path is a sequence of distinct neighboring vertices
  - A walk is a sequence of neighboring vertices
- Apparently similar notions



Paths



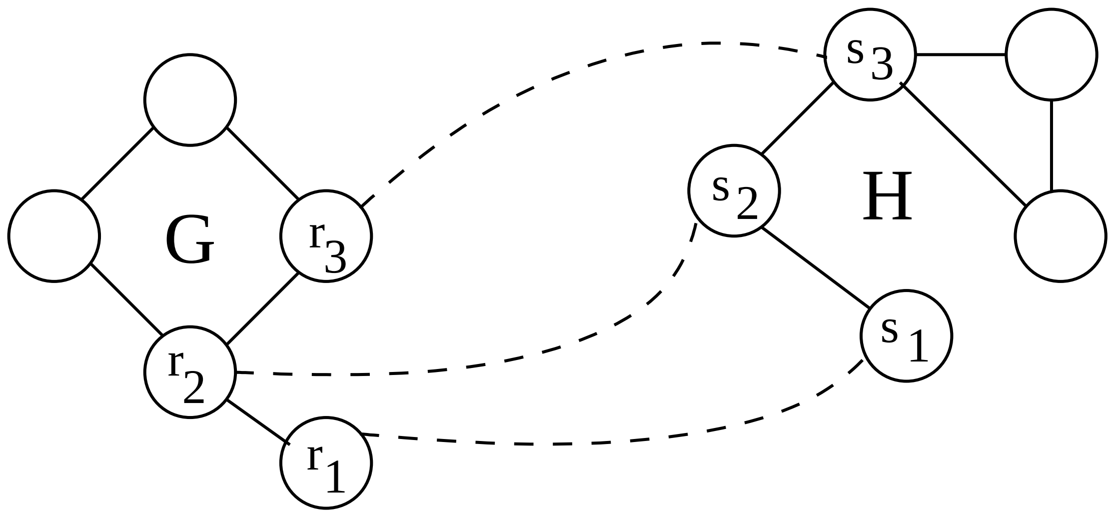
Walks



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

- $\mathcal{W}_{\mathbf{G}}^{p}$ (resp. $\mathcal{W}_{\mathbf{H}}^{p}$) 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:

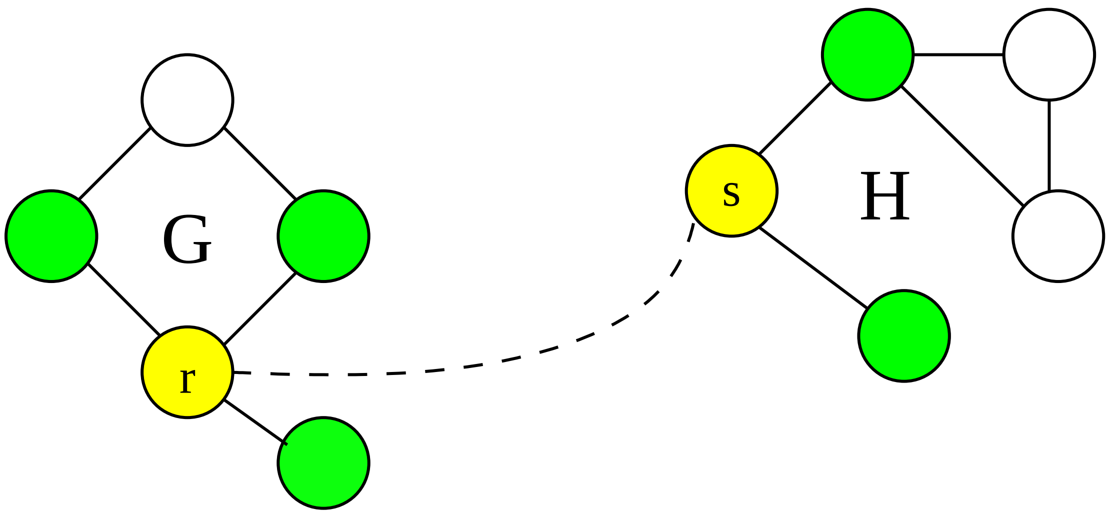
$$k_{\mathcal{W}}^{p}(\mathbf{G}, \mathbf{H}) = \sum_{\substack{(r_1, \ldots, r_p) \in \mathcal{W}_{\mathbf{G}}^{p} \\ (s_1, \ldots, s_p) \in \mathcal{W}_{\mathbf{H}}^{p}}} \prod_{i=1}^{p} k(\ell_{\mathbf{G}}(r_i), \ell_{\mathbf{H}}(s_i)).$$



Dynamic programming for the walk kernel

- Dynamic programming in $O(pd_{\mathbf{G}}d_{\mathbf{H}}n_{\mathbf{G}}n_{\mathbf{H}})$
- $k_{\mathcal{W}}^{p}(\mathbf{G},\mathbf{H},r,s)$ = sum restricted to walks starting at r and s
- recursion between $p-1$-th walk and p-th walk kernel

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



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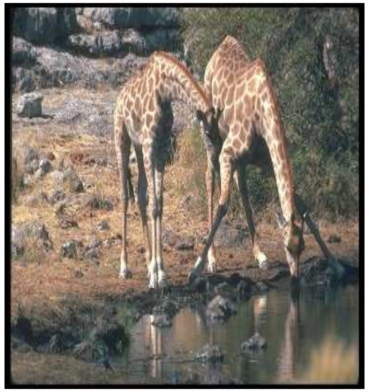
- Kernel obtained as $k_{\mathcal{T}}^{p,\alpha}(\mathbf{G},\mathbf{H}) = \sum_{r \in \mathcal{V}_{\mathbf{G}}, s \in \mathcal{V}_{\mathbf{H}}} k_{\mathcal{T}}^{p,\alpha}(\mathbf{G},\mathbf{H},r,s)$

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)

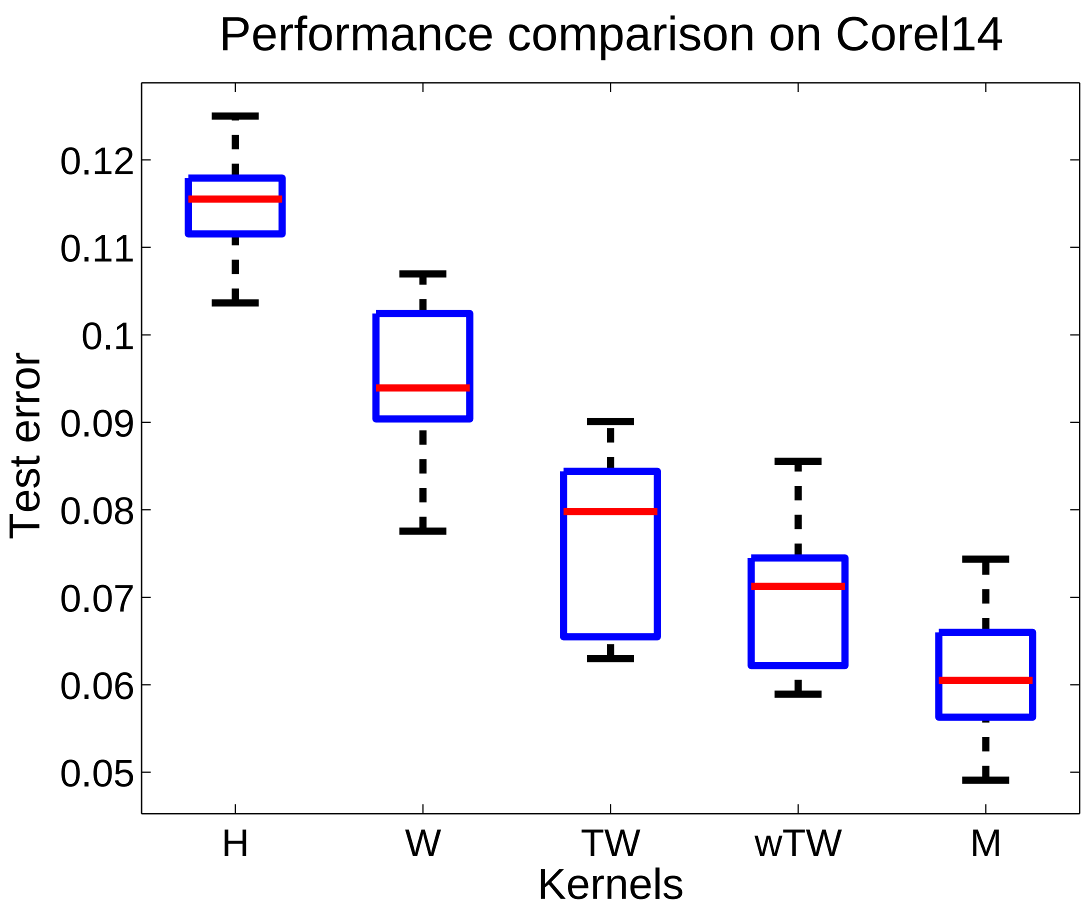
- `Corel14`: 1400 natural images with 14 classes





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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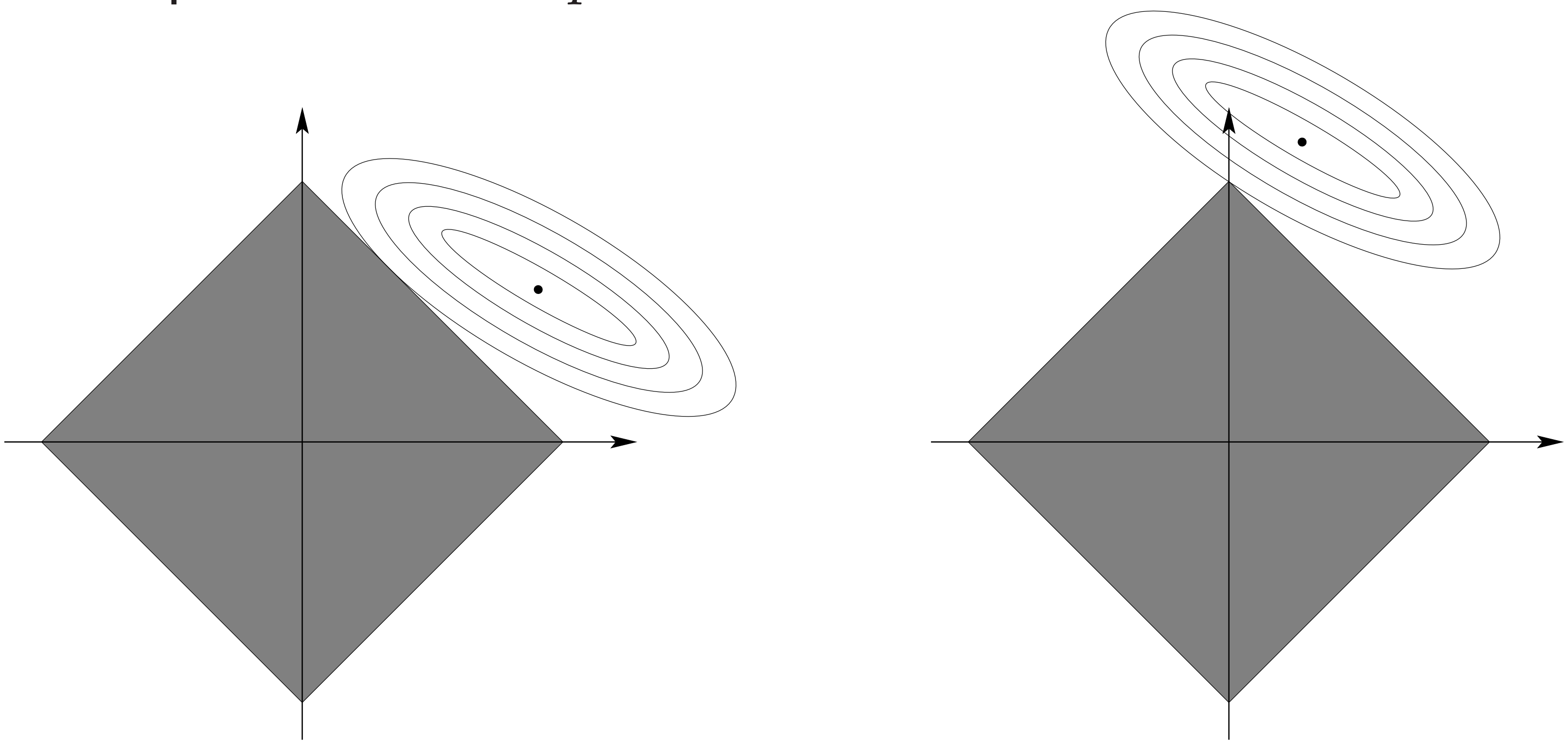
Why ℓ_1-norms lead to sparsity?

- Minimize quadratic objective subjet to constraint

$$\|w\|_1 = \sum_{i=1}^{p} |w_i| \leqslant T$$

  – coupled soft thresolding

- Geometric interpretation with $p = 2$



ℓ_1-norm regularization (linear setting)

- Data: covariates $x_i \in \mathbb{R}^p$, responses $y_i \in \mathcal{Y}$, $i = 1, \dots, n$
- Minimize with respect to loadings/weights $w \in \mathbb{R}^p$:

$$\begin{array}{ccc} \sum_{i=1}^{n} \ell(y_i, w^\top x_i) & + & \lambda \|w\|_1 \\ \text{Error on data} & + & \text{Regularization} \end{array}$$

- Including a constant term b? Penalizing or constraining?
- Assumptions on loss:
  - **convex** and **differentiable** in the second variable
  - NB: with the square loss $\Rightarrow$ basis pursuit (signal processing) (Chen et al., 2001), Lasso (statistics/machine learning) (Tibshirani, 1996)

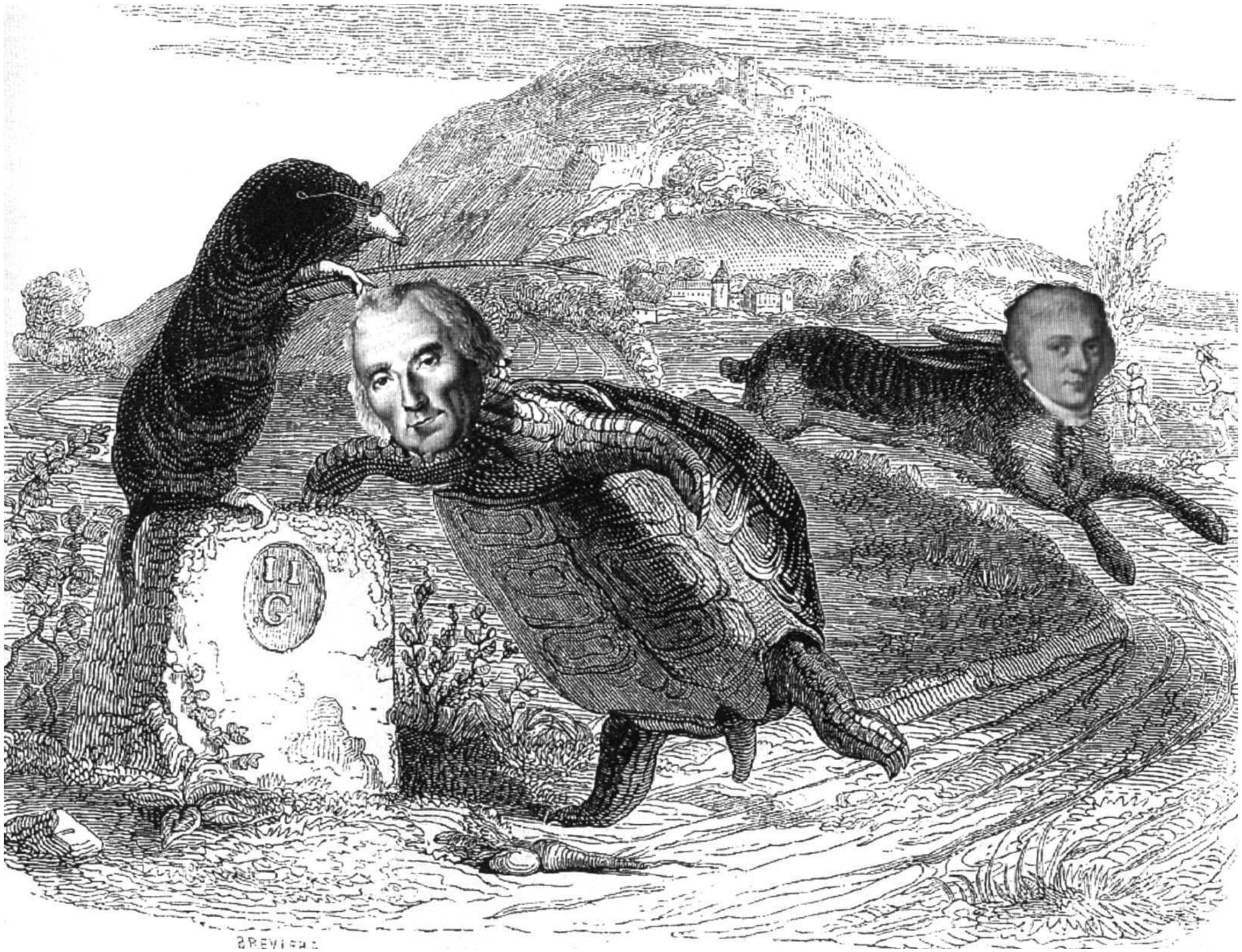
Nonsmooth optimization

- **Simple methods do not always work!**
  - Coordinate/steepest descent might not converge to a local minimum
  - Be careful!

- Optimization algorithms
  - First order methods: good for large scale/low precision
  - Second order methods: good for small scale/high precision

- Books: Boyd and Vandenberghe (2003), Bonnans et al. (2003), Nocedal and Wright (2006), Borwein and Lewis (2000)

Algorithms for ℓ^1-norms: Gaussian hare vs. Laplacian tortoise



Two simple algorithms: one good, one (very) bad

- Coordinate descent (Wu and Lange, 2008)
  - Globaly convergent here under reasonable assumptions!
  - very fast updates (thresholding)

- Quadratic programming formulation for the square loss: minimize

$$\frac{1}{2}\sum_{i=1}^{n}(y_i - w^\top x_i)^2 + \lambda \sum_{j=1}^{p}(w_j^+ + w_j^-) \text{ s.t. } w = w^+ - w^-,\ w^+ \geqslant 0,\ w^- \geqslant 0$$

  - **generic toolboxes $\Rightarrow$ very slow**

Algorithm: Lars/Lasso for the square loss (Efron et al., 2004)

- Goal: Get all solutions for all possible values of the regularization parameter λ

- Property: the regularization path is piecewise linear

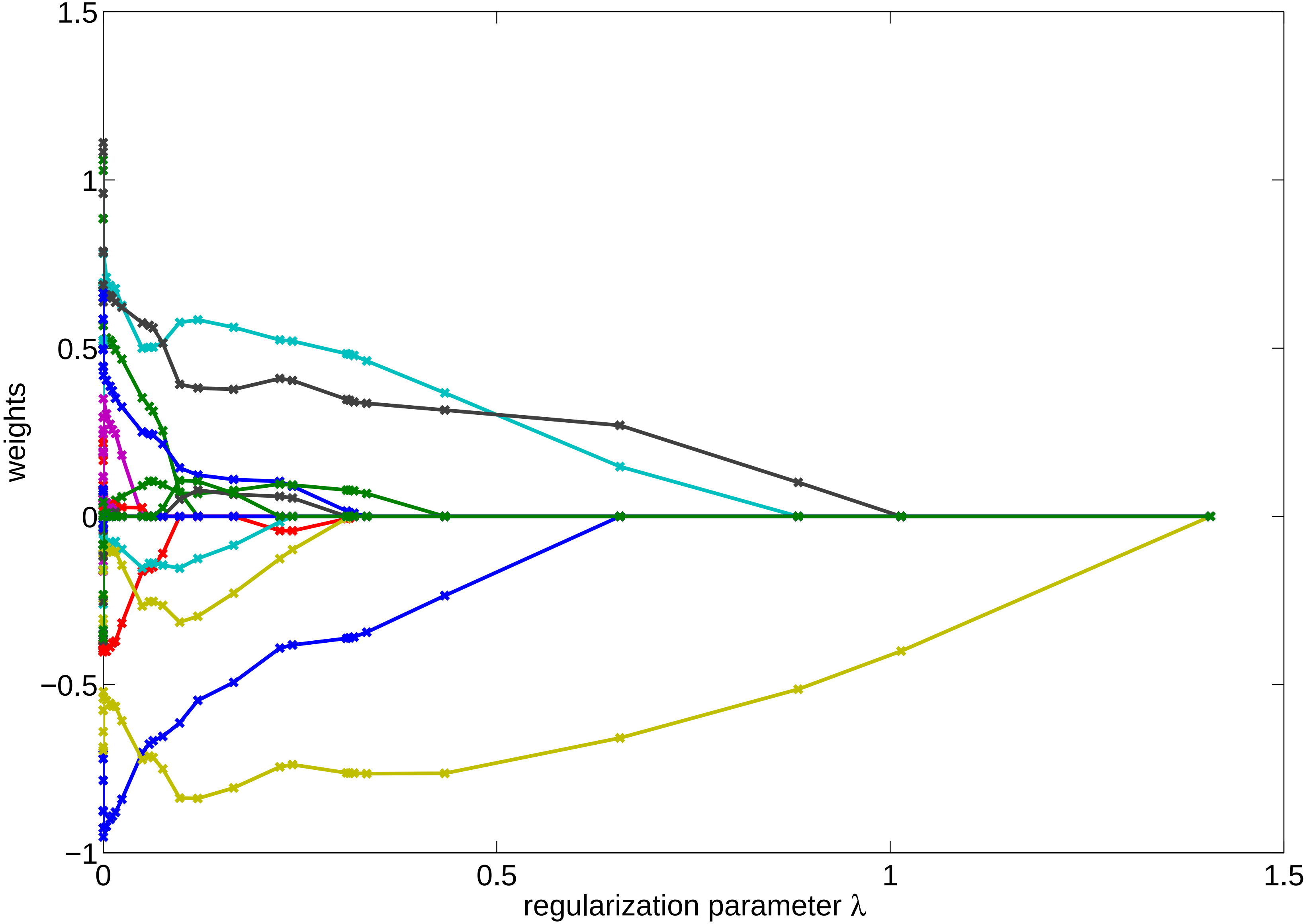
- Simply need to find break points and directions

- Generalizable to many problems (Rosset and Zhu, 2007)

Lasso in action

- Piecewise linear paths
- When is it supposed to work?
  - Simulations with random Gaussians, regularization parameter estimated by cross-validation
  - sparsity is expected or not

Lasso in action

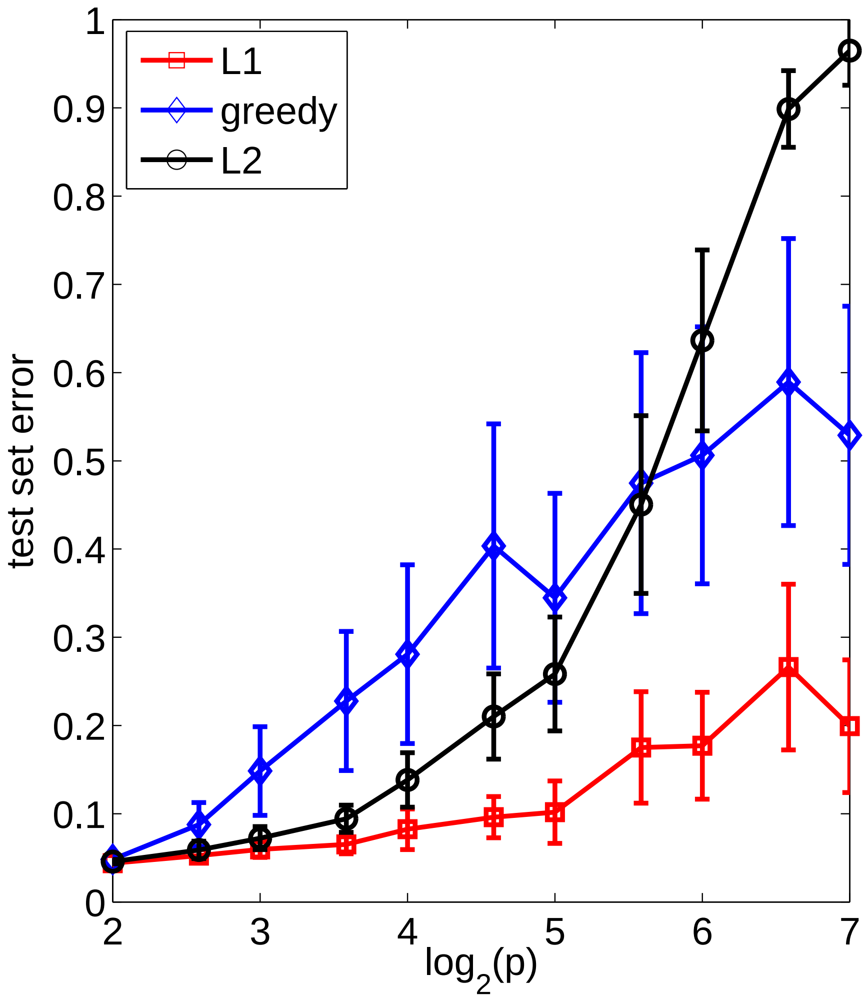


Comparing Lasso and other strategies for linear regression and subset selection

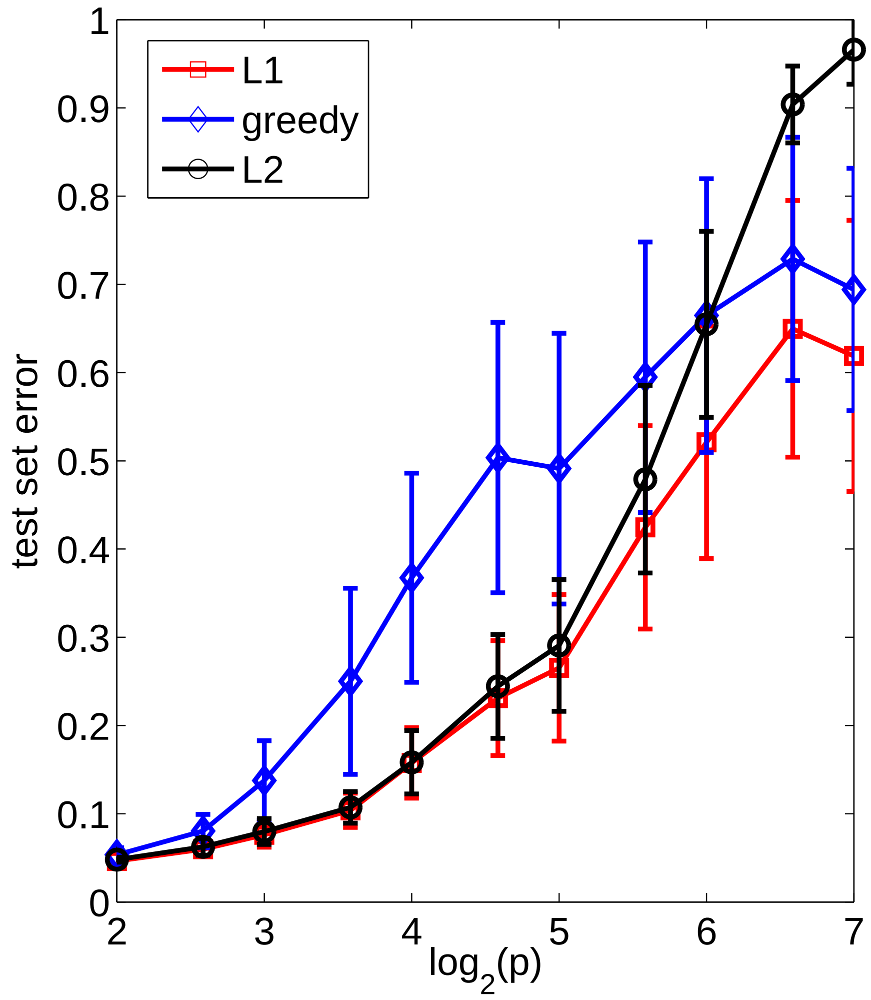
- Compared methods to reach the least-square solution (Hastie et al., 2001)
  - Ridge regression: $\min_w \frac{1}{2}\sum_{i=1}^n (y_i - w^\top x_i)^2 + \frac{\lambda}{2}\|w\|_2^2$
  - Lasso: $\min_w \frac{1}{2}\sum_{i=1}^n (y_i - w^\top x_i)^2 + \lambda\|w\|_1$
  - Forward greedy:
    * Initialization with empty set
    * Sequentially add the variable that best reduces the square loss

- Each method builds a path of solutions from 0 to w_{OLS}

Lasso in action



sparsity is expected



sparsity is not expected

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Kernel learning with convex optimization

- Kernel methods work...

  ...with the good kernel!

  $\Rightarrow$ Why not learn the kernel directly from data?

Kernel learning with convex optimization

- Kernel methods work...

  ...with the good kernel!

  $\Rightarrow$ Why not learn the kernel directly from data?

- **Proposition** (Lanckriet et al., 2004b; Bach et al., 2004a):

$$
\begin{aligned}
G(K) &= \min_{f \in \mathcal{F}} \sum_{i=1}^{n} \varphi_i(f^\top \Phi(x_i)) + \frac{\lambda}{2}\|f\|^2 \\
&= \max_{\alpha \in \mathbb{R}^n} -\sum_{i=1}^{n} \psi_i(\lambda \alpha_i) - \frac{\lambda}{2}\alpha^\top K \alpha
\end{aligned}
$$

  is a convex function of the Gram (a.k.a. kernel) matrix K

- Theoretical learning bounds (Lanckriet et al., 2004b)

MKL framework

- Minimize with respect to the kernel matrix K

$$G(K) = \max_{\alpha \in \mathbb{R}^n} - \sum_{i=1}^{n} \psi_i(\lambda \alpha_i) - \frac{\lambda}{2} \alpha^\top K \alpha$$

- Optimization domain:
  - K positive semi-definite in general : very large set!
  - The set of kernel matrices is a cone $\Rightarrow$ conic representation

$$\boxed{K(\eta) = \sum_{j=1}^{m} \eta_j K_j, \quad \eta \geqslant 0}$$

  - Trace constraints: $\operatorname{tr} K = \sum_{j=1}^{m} \eta_j \operatorname{tr} K_j = 1$

- Optimization:
  - In most cases, representation in terms of SDP, QCQP or SOCP
  - Optimization by generic toolbox is costly (Lanckriet et al., 2004b)

MKL - "reinterpretation" (Bach et al., 2004a)

- Framework limited to $K = \sum_{j=1}^{m} \eta_j K_j$, $\eta \geqslant 0$

- Summing kernels is equivalent to concatenating feature spaces
  - m "feature maps" $\Phi_j : \mathcal{X} \mapsto \mathcal{F}_j$, $j = 1, \dots, m$.
  - Minimization with respect to $f_1 \in \mathcal{F}_1, \dots, f_m \in \mathcal{F}_m$
  - Predictor: $f(x) = f_1{}^\top \Phi_1(x) + \cdots + f_m{}^\top \Phi_m(x)$

$$
\begin{array}{ccccccc}
 & & \Phi_1(x)^\top & f_1 & & & \\
 & \nearrow & \vdots & \vdots & \searrow & & \\
x & \longrightarrow & \Phi_j(x)^\top & f_j & \longrightarrow & f_1^\top \Phi_1(x) + \cdots + f_m^\top \Phi_m(x) \\
 & \searrow & \vdots & \vdots & \nearrow & & \\
 & & \Phi_m(x)^\top & f_m & & &
\end{array}
$$

  - **Which regularization?**

Regularization for multiple kernels

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- Regularization by $\sum_{j=1}^m \|f_j\|^2$ is equivalent to using $K = \sum_{j=1}^m K_j$

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- Regularization by $\sum_{j=1}^m \|f_j\|$ should impose sparsity at the group level

- **Main questions when regularizing by block ℓ^1-norm**:

1. Equivalence with previous formulations
2. Algorithms
3. Analysis of sparsity inducing properties (Bach, 2008c)

MKL - equivalence with general kernel learning (Bach et al., 2004a)

- Block ℓ^1-norm problem:

$$\sum_{i=1}^{n} \varphi_i(f_1^\top \Phi_1(x_i) + \cdots + f_m^\top \Phi_m(x_i)) + \frac{\lambda}{2} (\|f_1\| + \cdots + \|f_m\|)^2$$

- **Proposition**: It is equivalence to minimize with respect to η the optimal value $G(K(\eta))$ of the supervised learning problem (Bach et al., 2004a)

- Kernel weights obtained from optimality conditions and Lagrange multipliers

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

Algorithms for MKL

- (very) costly optimization with SDP, QCQP ou SOCP
  - $n \geqslant 1,000 - 10,000$, $m \geqslant 100$ not possible
  - "loose" required precision $\Rightarrow$ first order methods
- Dual coordinate ascent (SMO) with smoothing (Bach et al., 2004a)
- Optimization of $G(K)$ by cutting planes (Sonnenburg et al., 2006)
- Optimization of $G(K)$ with steepest descent with smoothing (Rakotomamonjy et al., 2008)
- Regularization path (Bach et al., 2004b)

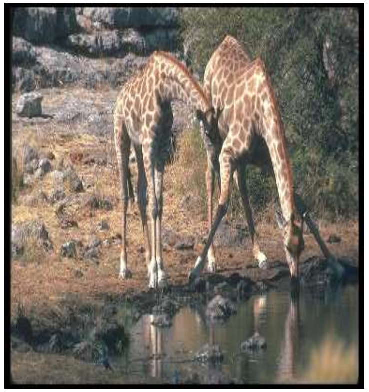
Applications

- Several applications
  - Bioinformatics (Lanckriet et al., 2004a)
  - Speech processing (Longworth and Gales, 2008)
  - Image annotation (Harchaoui and Bach, 2007; Varma and Ray, 2007; Bosch et al., 2008)

- Two potential uses
  - Fusion of heterogeneous data sources
  - Learning hyperparameters
  - Sparsity in non-linear settings

Performance on Corel14 (Harchaoui and Bach, 2007)

- Corel14: 1400 natural images with 14 classes



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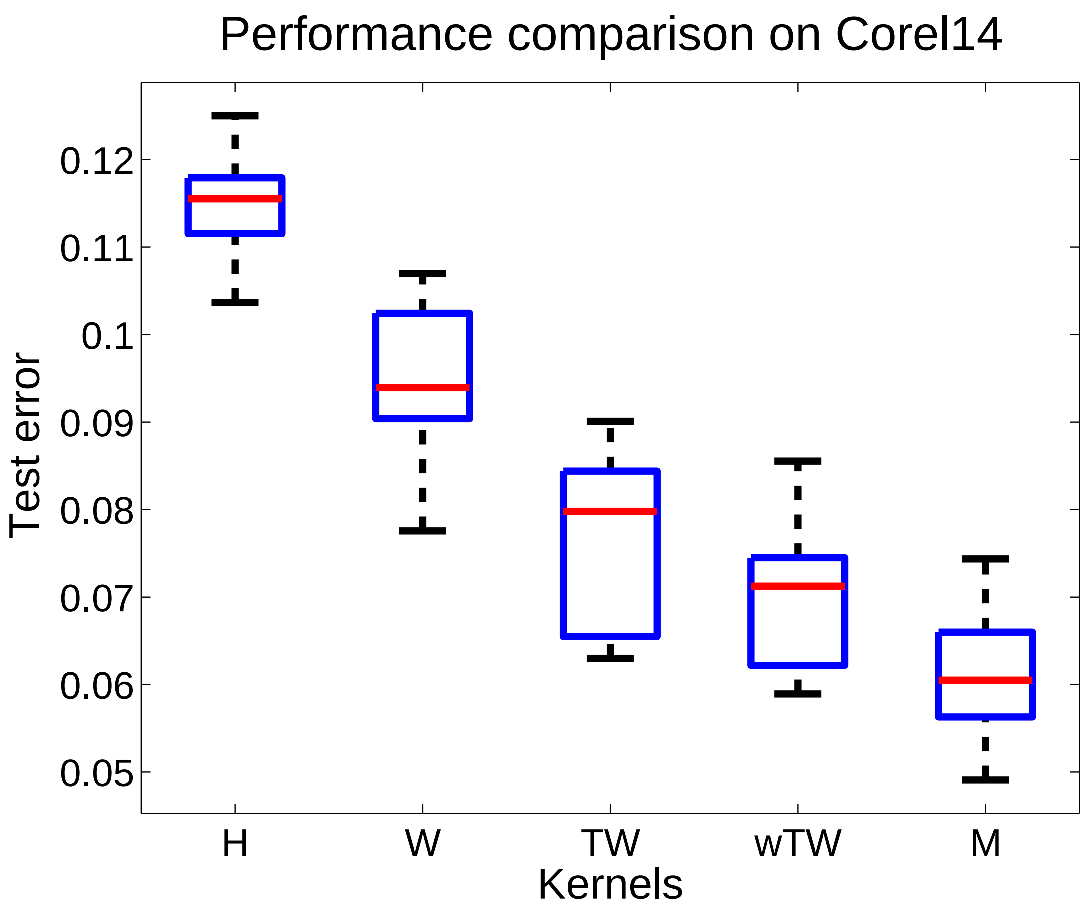
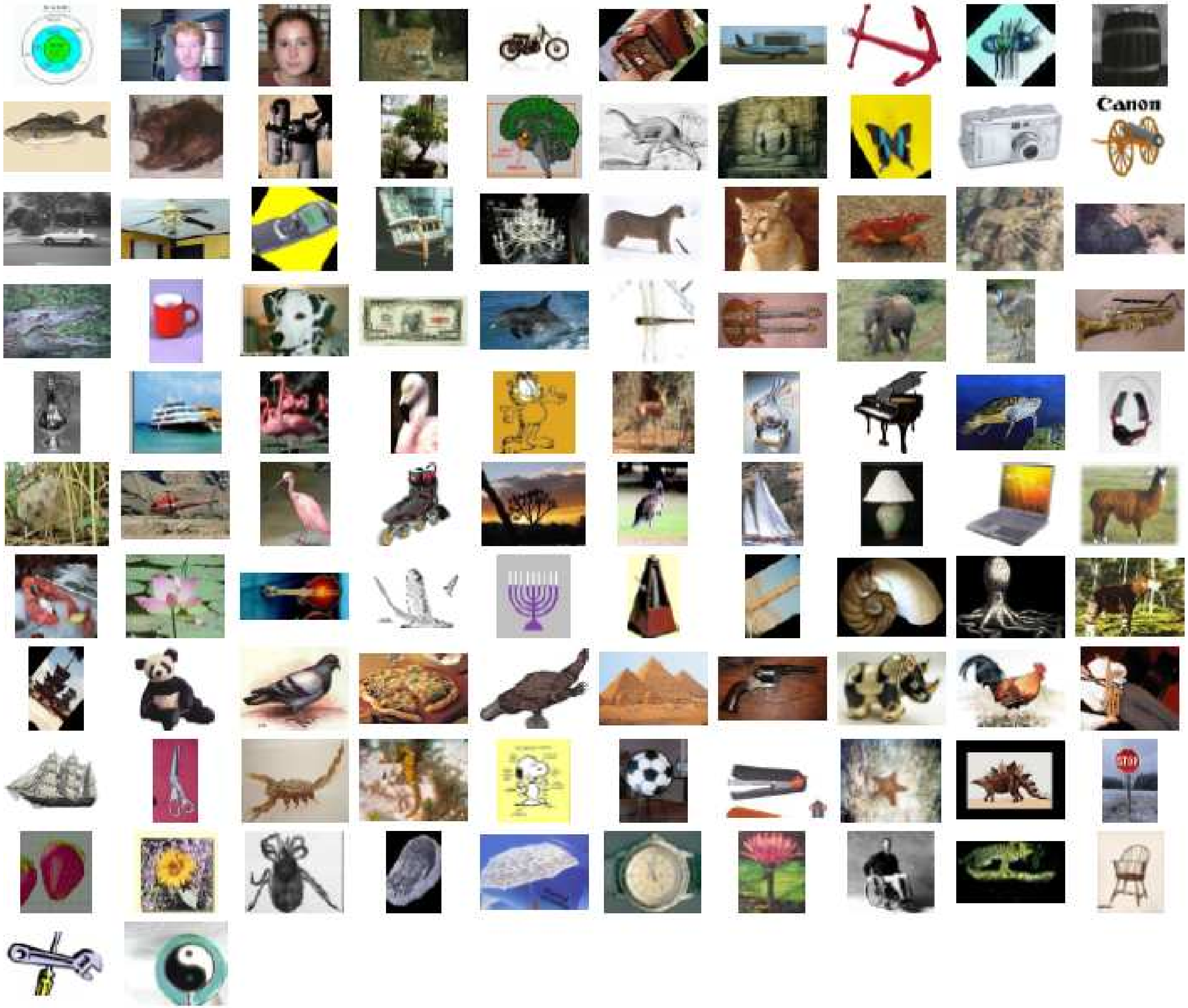


Caltech101 database (Fei-Fei et al., 2006)



Kernel combination for Caltech101 (Varma and Ray, 2007)

Classification accuracies

	1- NN	SVM (1 vs. 1)	SVM (1 vs. rest)
Shape GB1	39.67 ± 1.02	57.33 ± 0.94	62.98 ± 0.70
Shape GB2	45.23 ± 0.96	59.30 ± 1.00	61.53 ± 0.57
Self Similarity	40.09 ± 0.98	55.10 ± 1.05	60.83 ± 0.84
PHOG 180	32.01 ± 0.89	48.83 ± 0.78	49.93 ± 0.52
PHOG 360	31.17 ± 0.98	50.63 ± 0.88	52.44 ± 0.85
PHOWColour	32.79 ± 0.92	40.84 ± 0.78	43.44 ± 1.46
PHOWGray	42.08 ± 0.81	52.83 ± 1.00	57.00 ± 0.30
MKL Block ℓ^1		$\mathbf{77.72 \pm 0.94}$	$\mathbf{83.78 \pm 0.39}$
(Varma and Ray, 2007)		$\mathbf{81.54 \pm 1.08}$	$\mathbf{89.56 \pm 0.59}$

- See also Bosch et al. (2008)

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Learning on matrices

- Example 1: **matrix completion**
  - Given a matrix $M \in \mathbb{R}^{n \times p}$ and a subset of observed entries, estimate all entries
  - Many applications: graph learning, collaborative filtering (Breese et al., 1998; Heckerman et al., 2000; Salakhutdinov et al., 2007)

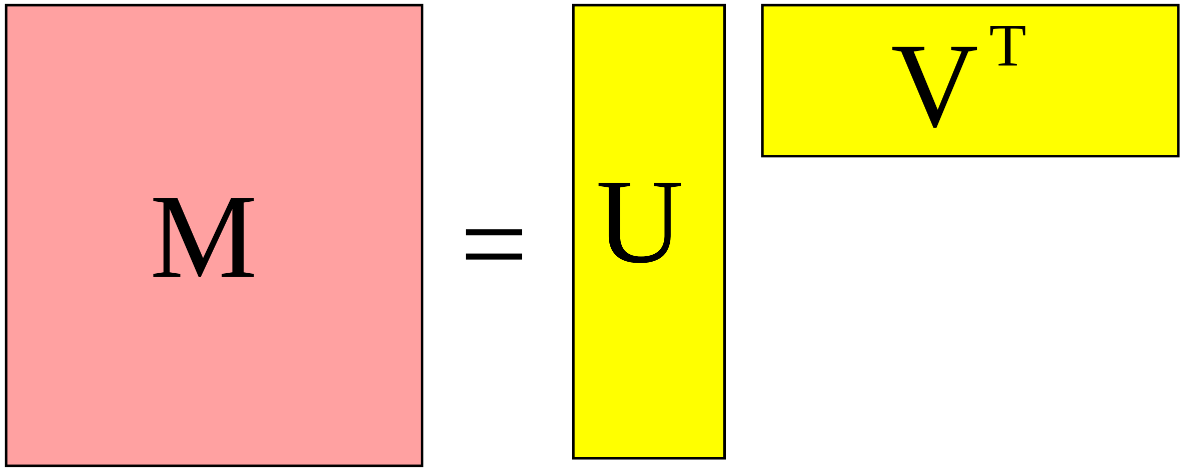
- Example 2: **multi-task learning** (Obozinski et al., 2007; Pontil et al., 2007)
  - Common features for m learning problems $\Rightarrow$ m different weights, i.e., $W = (w_1, \dots, w_m) \in \mathbb{R}^{p \times m}$
  - Numerous applications

- Example 3: **image denoising** (Elad and Aharon, 2006; Mairal et al., 2008)
  - Simultaneously denoise all patches of a given image

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

1. A lot of zero elements
   - does not use the matrix structure!

2. A small rank
   - $M = UV^\top$ where $U \in \mathbb{R}^{n \times m}$ and $V \in \mathbb{R}^{n \times m}$, m small
   - **Trace norm**



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   - **Trace norm** (Srebro et al., 2005; Fazel et al., 2001; Bach, 2008d)

3. A decomposition into sparse (but large) matrix $\Rightarrow$ redundant dictionaries
   - $M = UV^\top$ where $U \in \mathbb{R}^{n \times m}$ and $V \in \mathbb{R}^{n \times m}$, U sparse
   - **Dictionary learning** (Elad and Aharon, 2006; Mairal et al., 2008)

Trace norm (Srebro et al., 2005; Bach, 2008d)

- Singular value decomposition: $M \in \mathbb{R}^{n \times p}$ can always be decomposed into $M = U \operatorname{Diag}(s) V^\top$, where $U \in \mathbb{R}^{n \times m}$ and $V \in \mathbb{R}^{n \times m}$ have orthonormal columns and s is a positive vector (of singular values)

- ℓ^0 norm of singular values = rank

- ℓ^1 norm of singular values = trace norm

- Similar properties than the ℓ^1-norm
  - Convexity
  - Solutions of penalized problem have low rank
  - Algorithms

Dictionary learning

(Elad and Aharon, 2006; Mairal et al., 2008)

- Given $X \in \mathbb{R}^{n \times p}$, i.e., n vectors in $\mathbb{R}^p$, find
  - m dictionary elements in $\mathbb{R}^p$: $V = (v_1, \dots, v_m) \in \mathbb{R}^{p \times m}$
  - m set of decomposition coefficients: $U = \in \mathbb{R}^{n \times m}$
  - such that U is sparse and small reconstruction error, i.e., $\|X - UV^\top\|_F^2 = \sum_{i=1}^n \|X(i,:) - U(i,:)V^\top\|_2^2$ is small

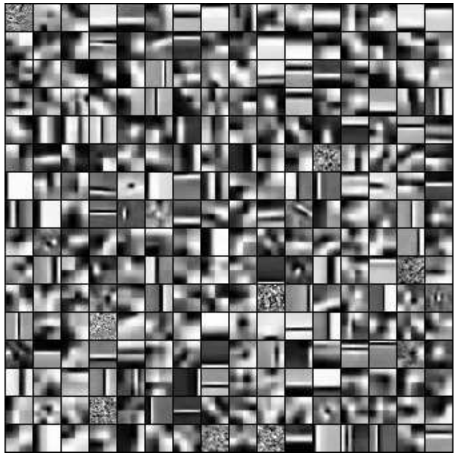
- NB: Opposite view, i.e., not sparse in term of ranks, sparse in terms of decomposition coefficients

- Minimize with respect to U and V, such that $\|V(:,i)\|_2 = 1$,

$$\frac{1}{2}\|X - UV^\top\|_F^2 + \lambda \sum_{i=1}^N \|U(i,:)\|_1$$

  - non convex, alternate minimization

Dictionary learning - Denoising (Mairal et al., 2008)



Dictionary

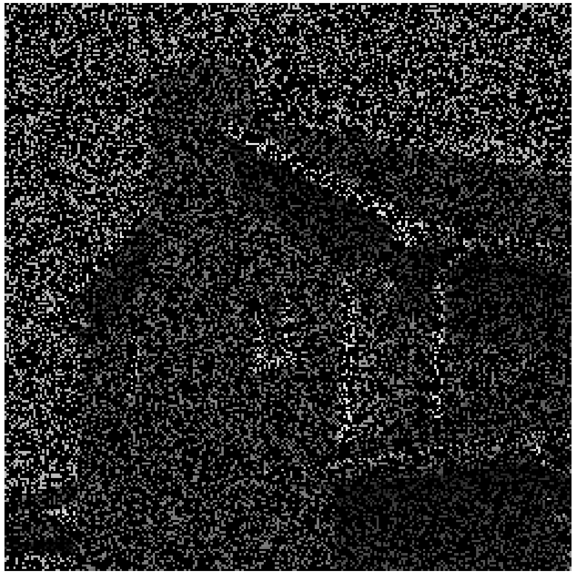
Original

Noisy

Denoised

Dictionary learning - Inpainting (Mairal et al., 2008)

Original



Missing pixels

Denoised

Theory: model consistency of the Lasso

- Sparsity-inducing norms often used heuristically
- If the responses $y_1, \ldots, y_n$ are such that $y_i = \mathbf{w}^\top x_i + \varepsilon_i$ where ε_i are i.i.d. and $\mathbf{w}$ is sparse, do we get back the correct pattern of zeros?
- Intuitive answer: yes **if and ony if** some consistency condition on the generating covariance matrices is satisfied (Zhao and Yu, 2006; Yuan and Lin, 2007; Zou, 2006; Wainwright, 2006)

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

where $\mathbf{J}$ = indices of relevant variables, $\mathbf{w}$ = true loading vector

- What if condition not satisfied?
  - Adaptive versions (Zou, 2006) or resampling methods (Bach, 2008a)

High-dimensional setting

- If consistency condition is satisfied, the Lasso is indeed consistent as long as $\log(p) \ll n$

- A lot of on-going work (Meinshausen and Yu, 2008; Wainwright, 2006; Lounici, 2008)

High-dimensional setting (Lounici, 2008)

- Assumptions
  - $y_i = \mathbf{w}^\top x_i + \varepsilon_i$, ε i.i.d. normal with mean zero and variance σ^2
  - $Q = X^\top X/n$ with unit diagonal and cross-terms less than $\frac{1}{14s}$
  - **Theorem**: if $\|\mathbf{w}\|_0 \leqslant s$, and $A > 8^{1/2}$, then

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

- Get the correct sparsity pattern if $\min_{j,\mathbf{w}_j \neq 0} |\mathbf{w}_j| > C\sigma \left(\frac{\log p}{n}\right)^{1/2}$
- Can have a lot of irrelevant variables!

High-dimensional setting

- If consistency condition is satisfied, the Lasso is indeed consistent as long as $\log(p) \ll n$
- A lot of on-going work (Meinshausen and Yu, 2008; Wainwright, 2006; Lounici, 2008)
- Link with compressed sensing (Baraniuk, 2007; Candès and Wakin, 2008)
  - Goal of compressed sensing: recover a signal $w \in \mathbb{R}^p$ from only n measurements $y = Xw \in \mathbb{R}^n$
  - Assumptions: the signal is k-sparse, $k \ll p$
  - Algorithm: $\min_{w \in \mathbb{R}^p} \|w\|_1$ such that $y = Xw$
  - X is not given but may be chosen (deterministic or random)!

Summary - sparsity-inducing norms

- Sparsity through non Euclidean norms

- Alternative approaches to sparsity
  - greedy approaches - Bayesian approaches

- Important (often non treated) question: when does sparsity actually help?

- Current research directions
  - Algorithms, algorithms, algorithms!
  - Structured norm for structured situations (variables are usually not created equal) $\Rightarrow$ hierarchical Lasso or MKL (Zhao et al., 2008; Bach, 2008b)

Conclusion - Course Outline

1. **Theory**
   - Probabilistic model and universal consistency
   - Local averaging methods
   - Empirical risk minimization

2. **Algorithms**
   - Losses for particular machine learning tasks
   - Regularization by Hilbert norms (kernel methods)
     – Algorithms
     – Kernel design
   - Regularization by sparsity-inducing norms
     – ℓ_1-norm regularization
     – Multiple kernel learning

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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
  www.dsp.ece.rice.edu/cs

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

Conclusion - Interesting problems

- 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