Hierarchical kernel learning

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Outline

- **Supervised learning and regularization**
  - Kernel methods vs. sparse methods
- **MKL: Multiple kernel learning**
  - Non linear sparse methods
- **HKL: Hierarchical kernel learning**
  - Non linear variable selection

Supervised learning and regularization

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

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

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)
     - Non linear predictors
     - Non parametric supervised learning and kernel methods
     - Well developped theory (see, e.g., Wahba, 1990; Schölkopf and Smola, 2001; Shawe-Taylor and Cristianini, 2004)

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   - Non parametric supervised learning and kernel methods
   - Well developped theory (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 "in the making"

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

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- **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: $$\boxed{\min_{\alpha \in \mathbb{R}^n} \sum_{i=1}^n \ell(y_i, (K\alpha)_i) + \frac{\lambda}{2} \alpha^\top K \alpha}$$
  - Kernel matrix $K_{ij} = k(x_i, x_j) = \Phi(x_i)^\top \Phi(x_j)$

Kernel methods: regularization by ℓ^2-norm

- Running time $O(n^2\kappa + n^3)$ where κ complexity of one kernel evaluation (often much less) - **independent of p**

- **Kernel trick**: implicit mapping if $\kappa = o(p)$ by using only $k(x_i, x_j)$ instead of $\Phi(x_i)$

- Examples:
  - Polynomial kernel: $k(x,y) = (1 + x^\top y)^d \Rightarrow \mathcal{F} =$ polynomials
  - Gaussian kernel: $k(x,y) = e^{-\alpha\|x-y\|_2^2} \Rightarrow \mathcal{F} =$ smooth functions
  - Kernels on structured data (see Shawe-Taylor and Cristianini, 2004)

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- $+$: Implicit non linearities and high-dimensionality

- $-$: Problems of interpretability, dimension too high?

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 $w \in \mathbb{R}^p$:

$$\sum_{i=1}^{n} \ell(y_i, w^\top x_i) \quad + \quad \lambda \|w\|_{\mathbf{1}}$$

Error on data + Regularization

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

ℓ^2-norm vs. ℓ^1-norm

- ℓ^1-norms lead to **sparse**/interpretable models
- ℓ^2-norms can be run implicitly with very large feature spaces

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- **Algorithms**:
  - Smooth convex optimization vs. nonsmooth convex optimization
  - First-order methods (Fu, 1998; Wu and Lange, 2008)
  - Homotopy methods (Markowitz, 1956; Efron et al., 2004)

- **Theory**:
  - Advantages of parsimony?
  - Consistent estimation of the support?

Lasso - Two main recent theoretical results

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

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

   where $\mathbf{Q} = \frac{1}{n}\sum_{i=1}^{n} x_i x_i^\top \in \mathbb{R}^{p\times p}$ and $\mathbf{J} = \mathrm{Supp}(\mathbf{w})$.

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- **The Lasso alone cannot find in general the good model**
- Two step-procedures
  - Adaptive Lasso (Zou, 2006; van de Geer et al., 2010)
    $\Rightarrow$ penalize by $\sum_{j=1}^p \frac{|w_j|}{|\hat{w}_j|}$
  - Resampling (Bach, 2008a; Meinshausen and Bühlmann, 2008)
    $\Rightarrow$ use the bootstrap to select the model

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2. **(sub-)exponentially many irrelevant variables** (Zhao and Yu, 2006; Wainwright, 2006; Bickel et al., 2008; Lounici, 2008; Meinshausen and Yu, 2009): under appropriate assumptions, consistency is possible as long as

$$\log p = O(n)$$

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

- Sparse methods are most often linear

- Sparsity with non-linearities
  - replace $f(x) = \sum_{j=1}^{p} w_j^\top x_j$ with $x_j \in \mathbb{R}$ and $w_j \in \mathbb{R}$
  - by $f(x) = \sum_{j=1}^{p} w_j^\top \Phi_j(x)$ with $\Phi_j(x) \in \mathcal{F}_j$ 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 (MKL) (Lanckriet et al., 2004; 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: $f(x) = w_1{}^\top \Phi_1(x) + \cdots + w_p{}^\top \Phi_p(x)$

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

  - Generalized additive models (Hastie and Tibshirani, 1990)
  - **Link between regularization and kernel matrices**

Regularization for multiple features

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

- 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 (Bach et al., 2004a,b; Rakotomamonjy et al., 2008)
  2. Analysis of sparsity inducing properties (Bach, 2008b)
  3. Sparse kernel combinations $\sum_{j=1}^p \eta_j K_j$ (Bach et al., 2004a)
  4. Application to data fusion and hyperparameter learning

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Lasso - Two main recent theoretical results

1. **Support recovery condition**

2. **(sub-)exponentially many irrelevant variables** (Zhao and Yu, 2006; Wainwright, 2006; Bickel et al., 2008; Lounici, 2008; Meinshausen and Yu, 2009): under appropriate assumptions, consistency is possible as long as

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- Question: is it possible to build a sparse algorithm that can learn from more than 10^{80} features?

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- Question: is it possible to build a sparse algorithm that can learn from more than 10^{80} features?
  - **Some type of recursivity/factorization is needed!**

Non-linear variable selection

- Given $x = (x_1, \ldots, x_q) \in \mathbb{R}^q$, find function $f(x_1, \ldots, x_q)$ which depends only on a few variables

- Sparse generalized additive models (e.g., MKL):
  - restricted to $f(x_1, \ldots, x_q) = f_1(x_1) + \cdots + f_q(x_q)$

- Cosso (Lin and Zhang, 2006):
  - restricted to $f(x_1, \ldots, x_q) = \sum_{J \subset \{1,\ldots,q\},\ |J| \leqslant 2} f_J(x_J)$

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- Universally consistent non-linear selection requires all 2^q subsets

$$f(x_1, \dots, x_q) = \sum_{J \subset \{1,\dots,q\}} f_J(x_J)$$

Hierarchical kernel learning (Bach, 2008c)

- Many kernels can be decomposed as a sum of many "small" kernels indexed by a certain set V: $\boxed{k(x,x') = \sum_{v \in V} k_v(x,x')}$

- Example with $x = (x_1, \dots, x_q) \in \mathbb{R}^q$ ($\Rightarrow$ non linear variable selection)
  - Gaussian/ANOVA kernels: $p = \#(V) = 2^q$

$$\prod_{j=1}^{q} \left(1 + e^{-\alpha(x_j - x'_j)^2}\right) = \sum_{J \subset \{1,\dots,q\}} \prod_{j \in J} e^{-\alpha(x_j - x'_j)^2} = \sum_{J \subset \{1,\dots,q\}} e^{-\alpha \|x_J - x'_J\|_2^2}$$

- **Goal**: learning sparse combination $\sum_{v \in V} \eta_v k_v(x,x')$

- Universally consistent non-linear variable selection requires all subsets

Restricting the set of active kernels

- Assume one separate predictor w_v for each kernel k_v
  - Final prediction: $f(x) = \sum_{v \in V} w_v^\top \Phi_v(x)$

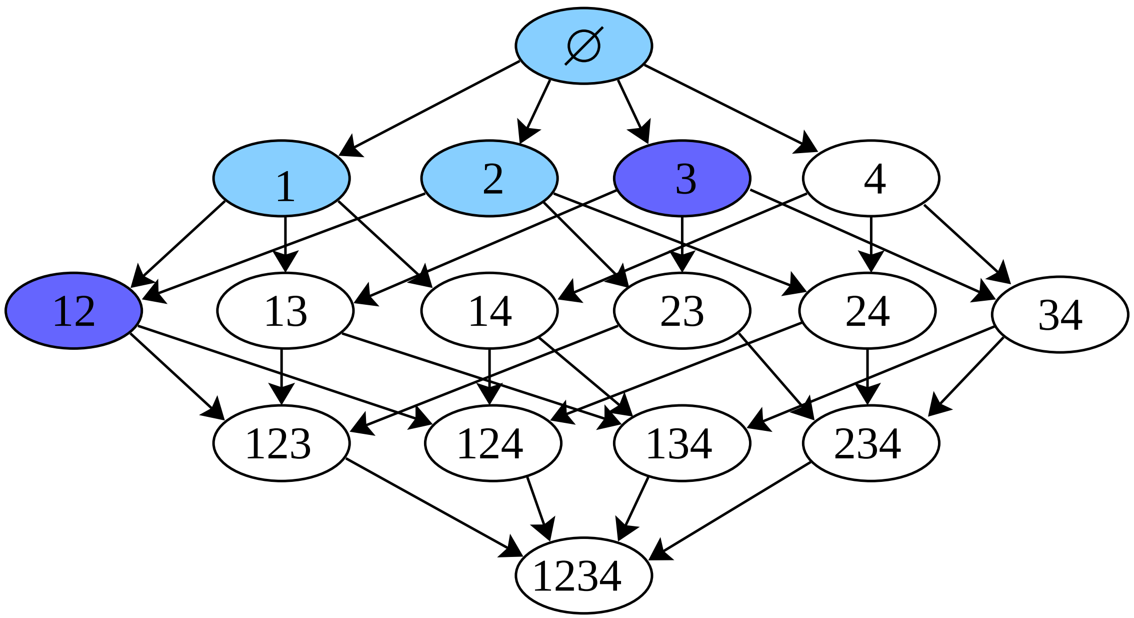
- With flat structure
  - Consider block ℓ_1-norm: $\sum_{v \in V} \|w_v\|_2$
  - cannot avoid being linear in $p = \#(V) = 2^q$

- Using the structure of the small kernels
  1. for computational reasons
  2. to allow more irrelevant variables

Restricting the set of active kernels

- V is endowed with a directed acyclic graph (DAG) structure: **select a kernel only after all of its ancestors have been selected**

- Gaussian kernels: $V =$ power set of $\{1, \ldots, q\}$ with inclusion DAG
  - Select a subset only after all its subsets have been selected

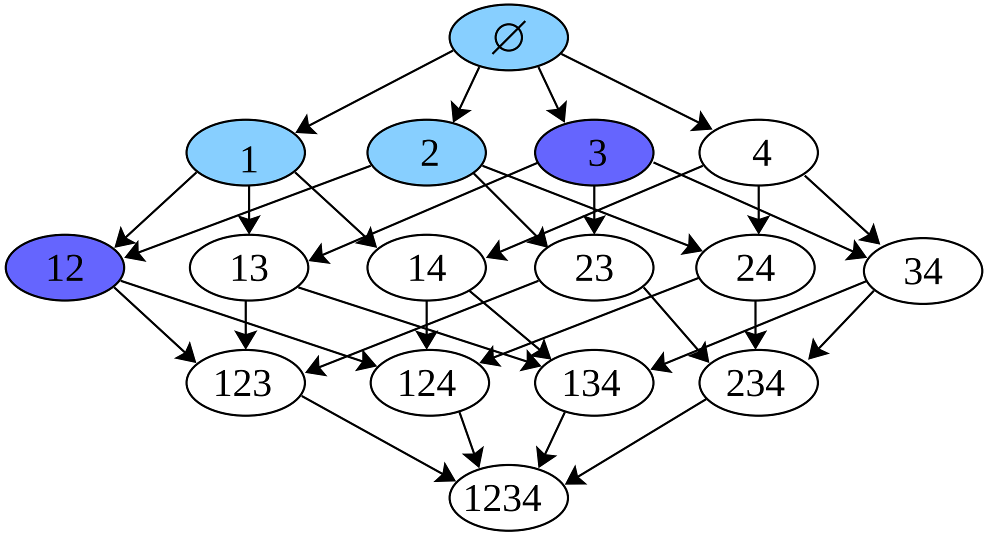


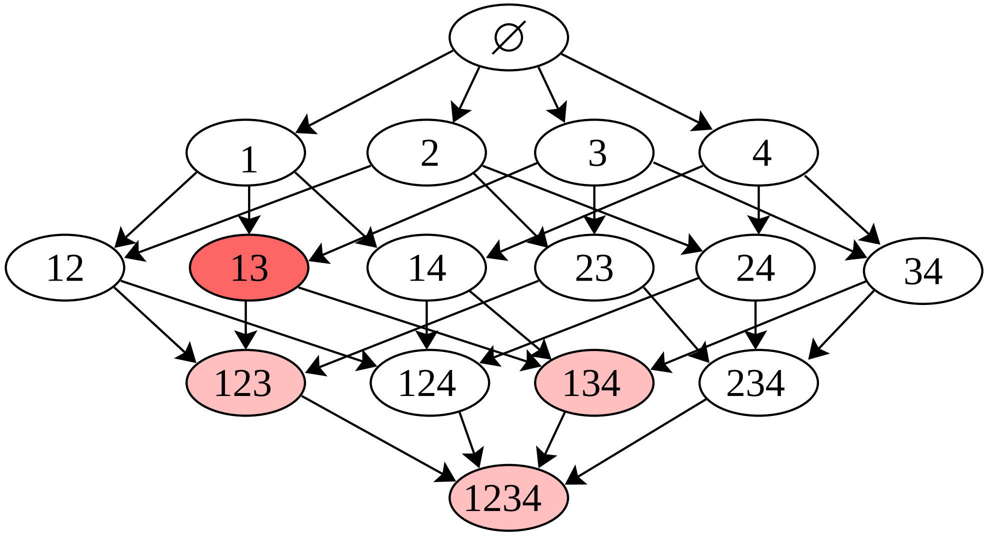
DAG-adapted norm (Zhao & Yu, 2008)

- Graph-based structured regularization
  - $\mathrm{D}(v)$ is the set of descendants of $v \in V$:

$$\sum_{v \in V} \|w_{\mathrm{D}(v)}\|_2 = \sum_{v \in V} \left(\sum_{t \in \mathrm{D}(v)} \|w_t\|_2^2 \right)^{1/2}$$

- Main property: If v is selected, so are all its ancestors





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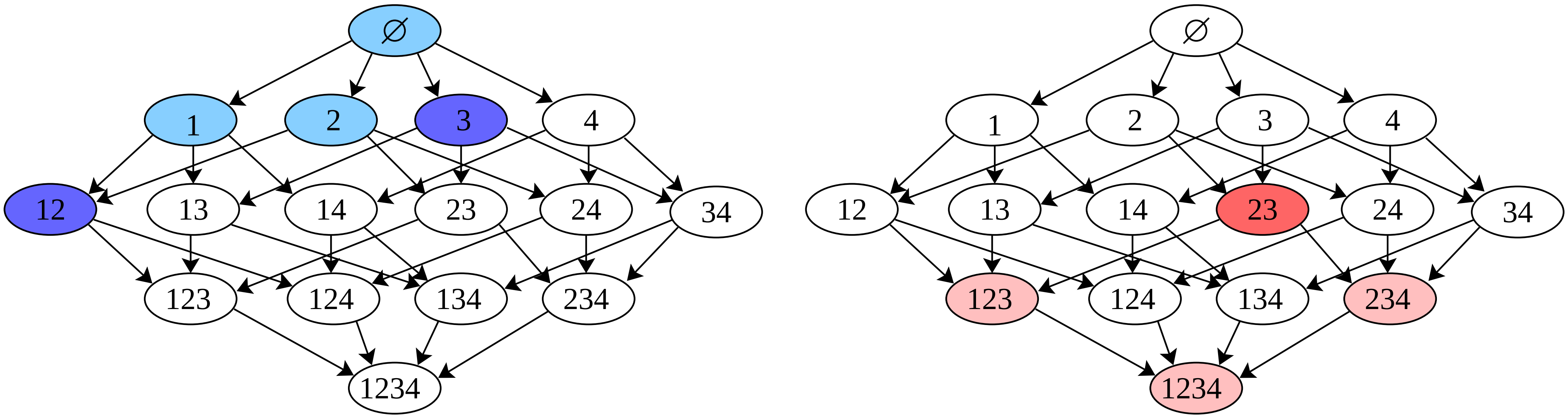

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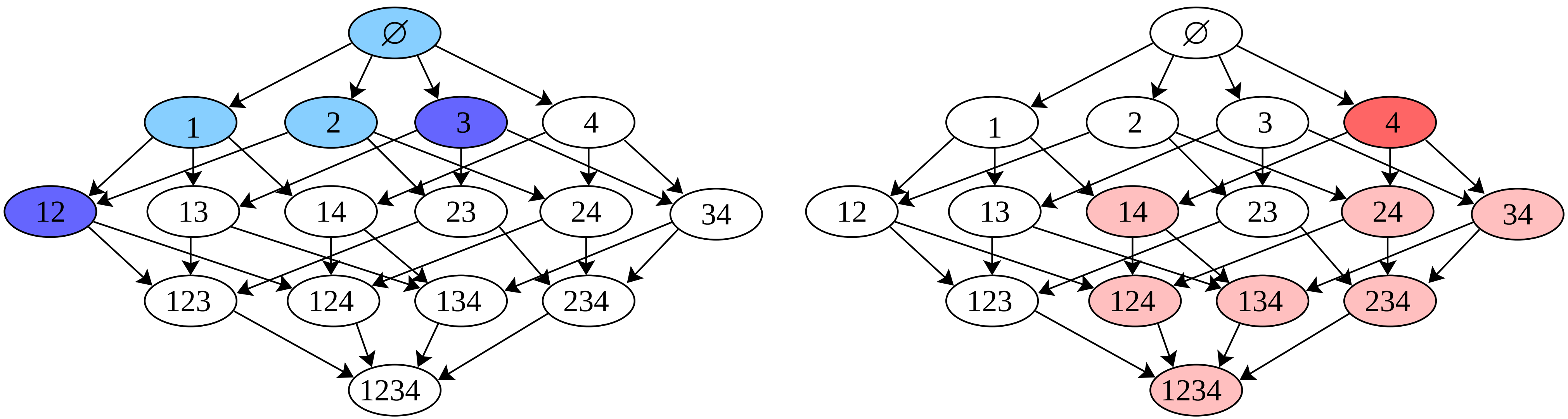

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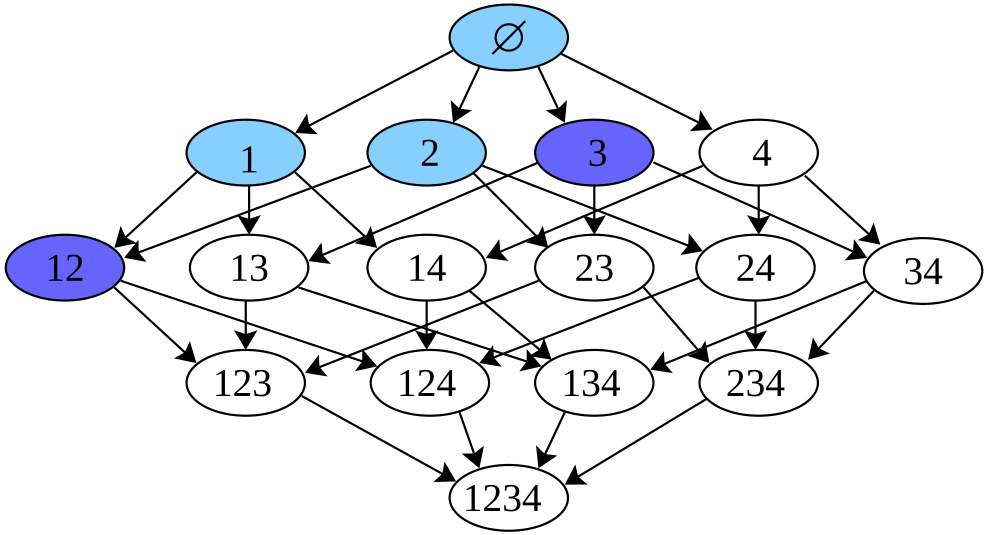

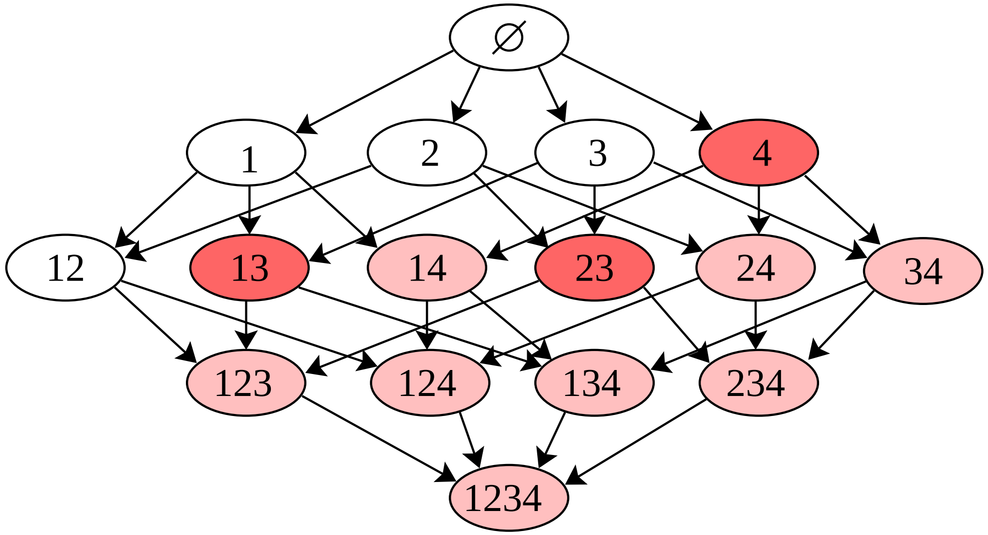

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- **Hierarchical kernel learning** (Bach, 2008c) :
  - **polynomial-time** algorithm for this norm
  - **necessary/sufficient conditions** for consistent kernel selection
  - **Scaling between p, q, n** for consistency
  - **Applications** to variable selection or other kernels

Scaling between p, n and other graph-related quantities

$$
\begin{aligned}
n &= \text{number of observations} \\
p &= \text{number of vertices in the DAG} \\
\deg(V) &= \text{maximum out degree in the DAG} \\
\operatorname{num}(V) &= \text{number of connected components in the DAG}
\end{aligned}
$$

- **Proposition** (Bach, 2009): Assume consistency condition satisfied, Gaussian noise and data generated from a sparse function, then the support is recovered with high-probability as soon as:

$$\log \deg(V) + \log \operatorname{num}(V) = O(n)$$

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- Unstructured case: $\mathrm{num}(V) = p \Rightarrow \boxed{\log p = O(n)}$

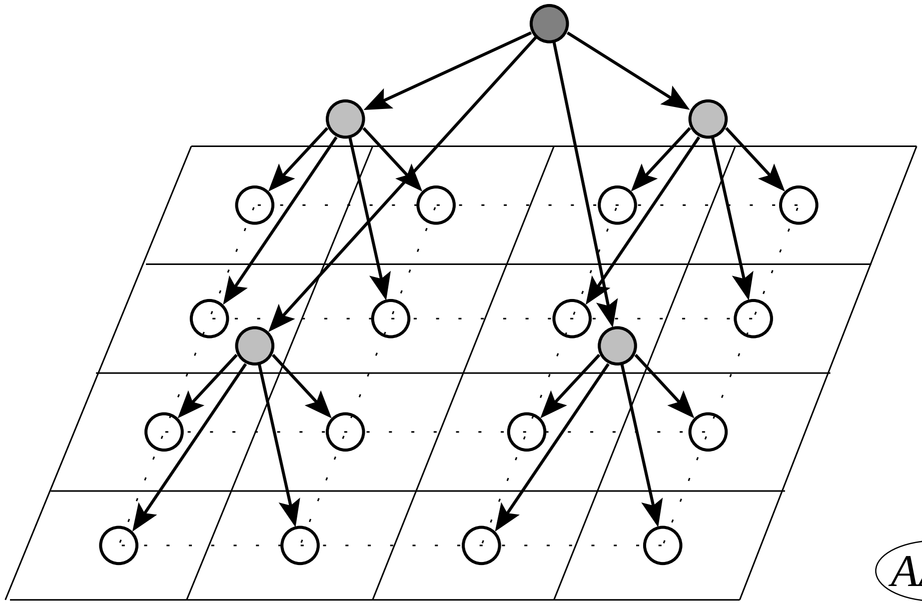
- Power set of q elements: $\deg(V) = q \Rightarrow \boxed{\log q = \log \log p = O(n)}$

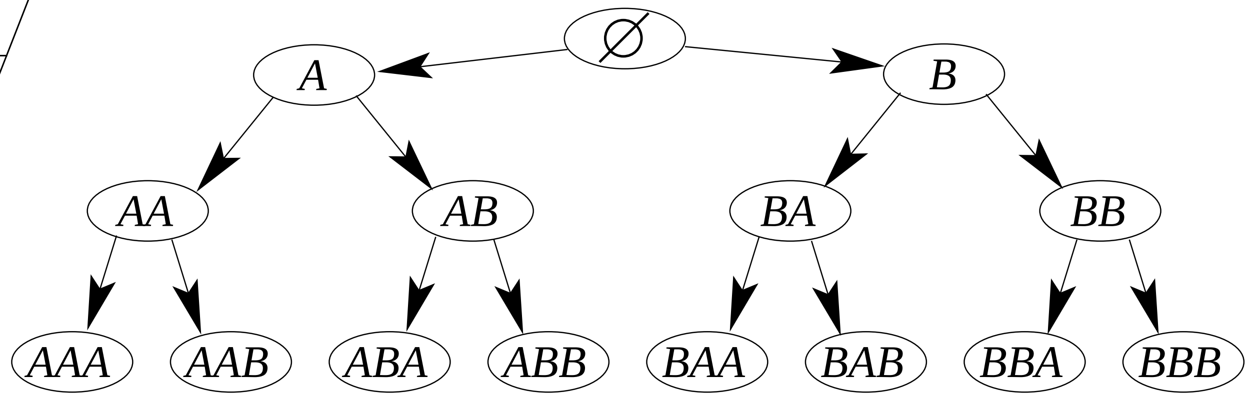
Mean-square errors (regression)

dataset	n	p	k	$\#(V)$	L2	greedy	MKL	HKL
abalone	4177	10	pol4	$\approx 10^{7}$	44.2±1.3	43.9±1.4	44.5±1.1	**43.3±1.0**
abalone	4177	10	rbf	$\approx 10^{10}$	**43.0±0.9**	45.0±1.7	43.7±1.0	43.0±1.1
boston	506	13	pol4	$\approx 10^{9}$	**17.1±3.6**	24.7±10.8	22.2±2.2	18.1±3.8
boston	506	13	rbf	$\approx 10^{12}$	**16.4±4.0**	32.4±8.2	20.7±2.1	17.1±4.7
pumadyn-32fh	8192	32	pol4	$\approx 10^{22}$	57.3±0.7	56.4±0.8	**56.4±0.7**	56.4±0.8
pumadyn-32fh	8192	32	rbf	$\approx 10^{31}$	57.7±0.6	72.2±22.5	56.5±0.8	**55.7±0.7**
pumadyn-32fm	8192	32	pol4	$\approx 10^{22}$	6.9±0.1	6.4±1.6	7.0±0.1	**3.1±0.0**
pumadyn-32fm	8192	32	rbf	$\approx 10^{31}$	5.0±0.1	46.2±51.6	7.1±0.1	**3.4±0.0**
pumadyn-32nh	8192	32	pol4	$\approx 10^{22}$	84.2±1.3	73.3±25.4	83.6±1.3	**36.7±0.4**
pumadyn-32nh	8192	32	rbf	$\approx 10^{31}$	56.5±1.1	81.3±25.0	83.7±1.3	**35.5±0.5**
pumadyn-32nm	8192	32	pol4	$\approx 10^{22}$	60.1±1.9	69.9±32.8	77.5±0.9	**5.5±0.1**
pumadyn-32nm	8192	32	rbf	$\approx 10^{31}$	15.7±0.4	67.3±42.4	77.6±0.9	**7.2±0.1**

Extensions to other kernels

- Extension to graph kernels, string kernels, pyramid match kernels





- Exploring large feature spaces with structured sparsity-inducing norms
  - Opposite view than traditional kernel methods
  - Interpretable models

- **Other structures than hierarchies** (Jenatton et al., 2009a)

Conclusion

- **Structured sparsity**
  - Sparsity-inducing norms
  - Supervised learning: high-dimensional non-linear variable selection
  - Unsupervised learning: sparse principal component analysis (Jenatton et al., 2009b) and dictionary learning (Mairal et al., 2009)

- **Further/current work**
  - Universal consistency of non-linear variable selection
  - Algorithms (Jenatton, Mairal, Obozinski, and Bach, 2010)
  - Norm design, norms on matrices

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