Opening up the Black Box: Fast Non-Smooth and Big-Data Optimization

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School of Computing Science
Simon Fraser University

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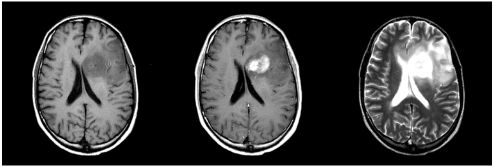
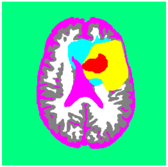
Motivation: Automatic Brain Tumor Segmentation

- Task: Segmentation of Multi-Modality MRI Data





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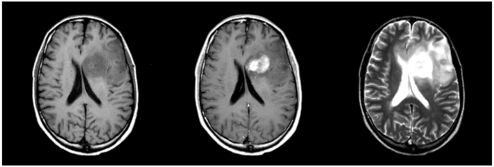

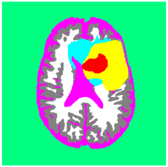

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  - quantifying growth or treatment response.
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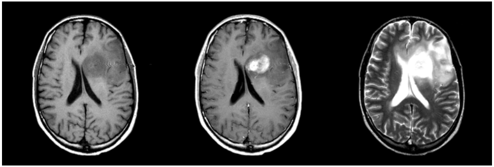

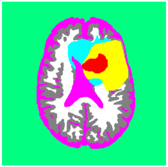

- Various applications:
  - radiation therapy target planning.
  - quantifying growth or treatment response.
  - image-guided surgery.
- Challenges:
  - image noise and intensity inhomogeneity.
  - similarity between tumor and normal tissue.

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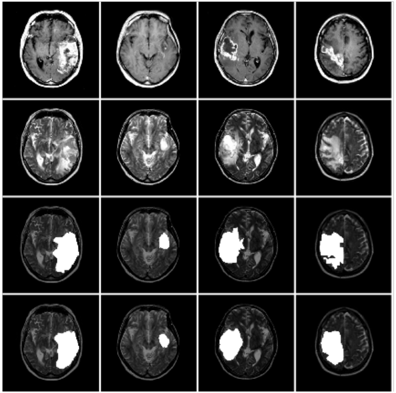
- Solution strategy:
  - Explicit correction of image inhomogeneities.
  - Spatial alignment with template.
  - Image and template-based features.
  - Pixel-level classifier.



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- Problem 1: Estimating x is slow:
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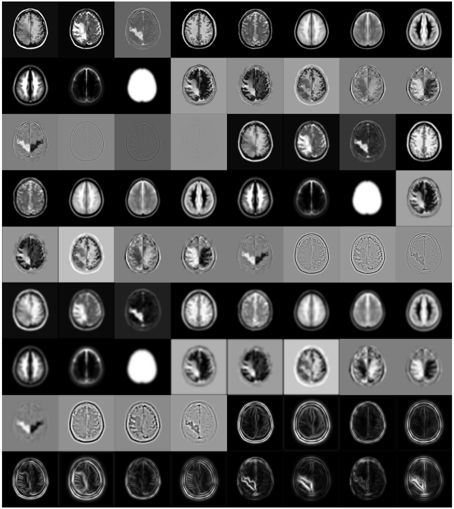
- Problem 2: Designing features.
  - Lots of possible candidate features.
  - Using all features leads to over-fitting.
  - First part of talk: Feature Selection.

Motivation: Automatic Brain Tumor Segmentation



- Training time is too slow for automatic feature selection:
  - forced to use manual feature selection

Optimizing with ℓ_1-Regularzation

- Last day of Master's: try **all features** with ℓ_2-Regularization:

$$\min_x f(x) + \lambda \|x\|^2.$$

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- Amazing! But non-smooth, how do we solve this problem?

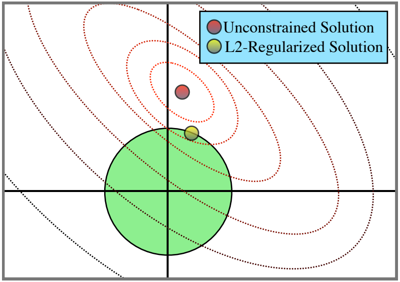
Where does the sparsity come from?

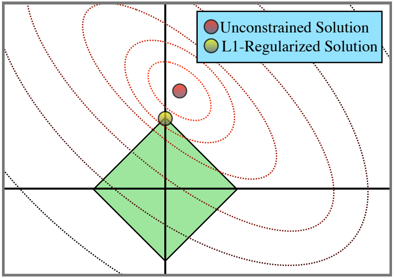
- We can re-write the regularized problem

$$\min_x f(x) + \lambda\|x\|_p$$

as a constrained problem

$$\min_{\|x\|_p \leq \tau} f(x).$$





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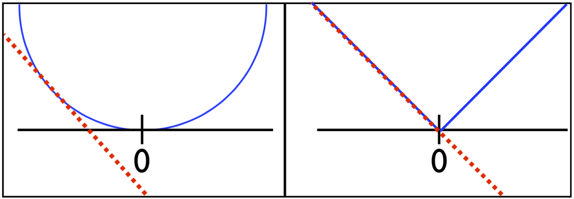

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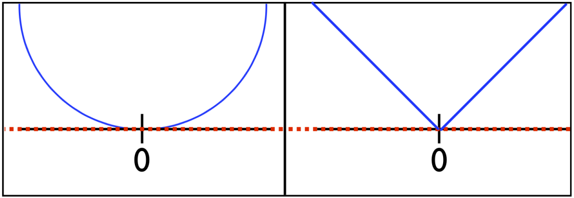

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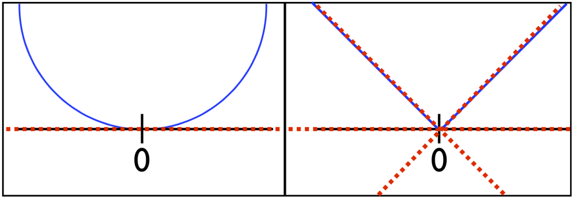

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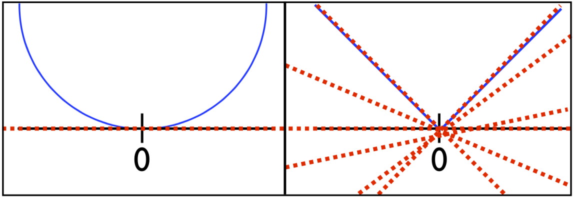

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- Can we extend quasi-Newton methods using this property?

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- Use methods for smooth bound-constrained optimization.

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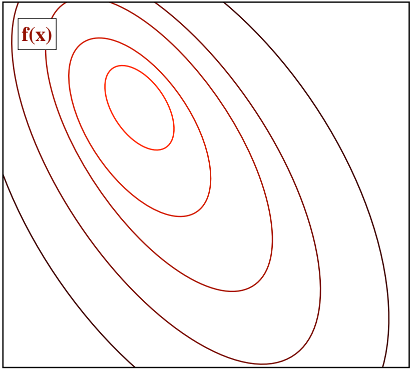

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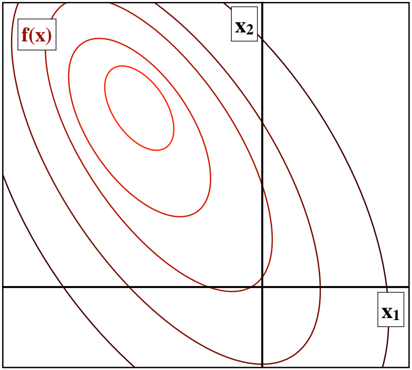

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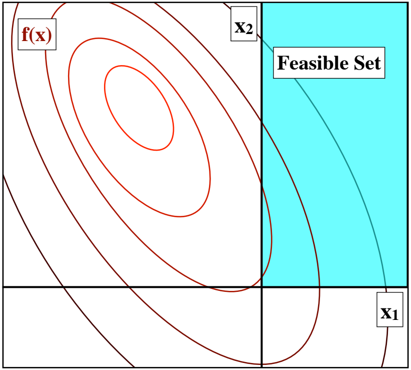

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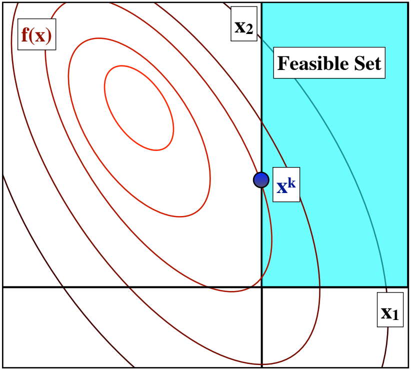

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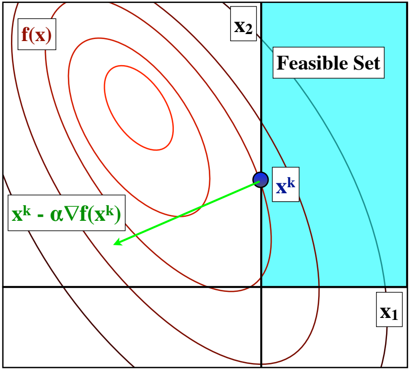

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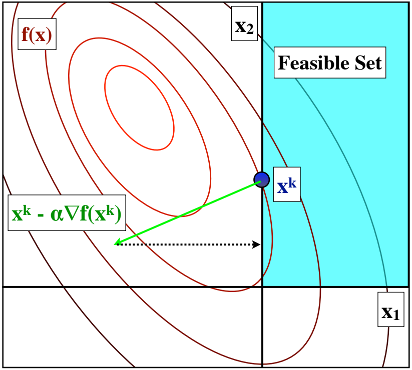

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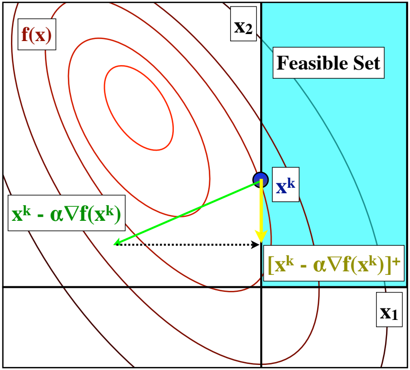

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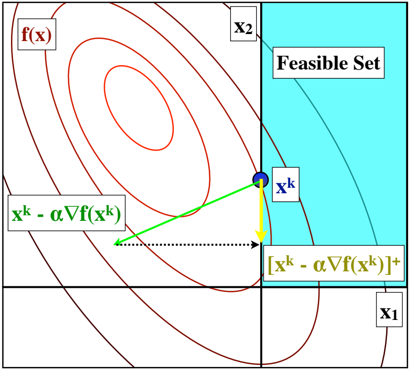

- Convergence properties similar to gradient method.

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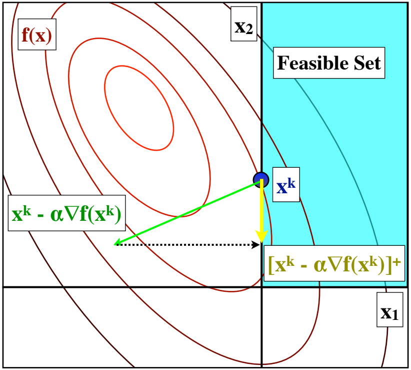

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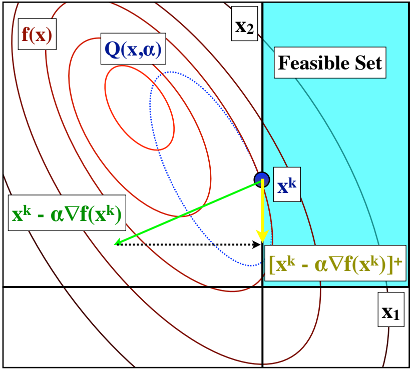

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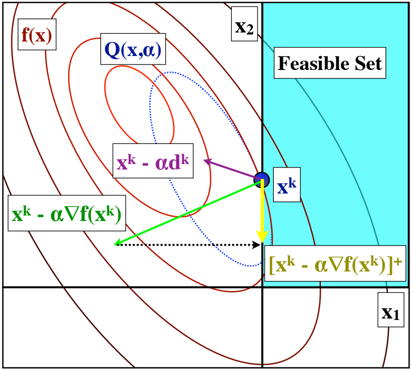

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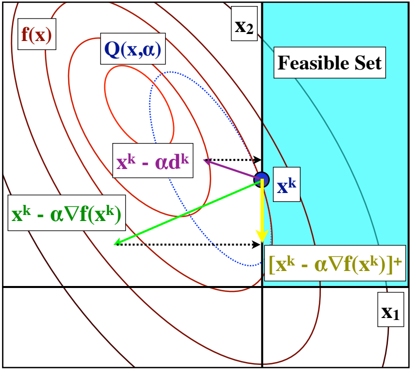

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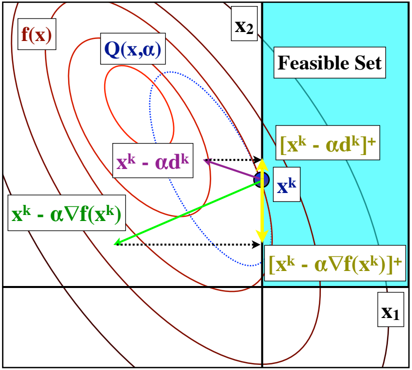

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- $\bar{H}_k$ can be quasi-Newton approximation of $F''(x^k)$.

Discussion of Two-Metric Projection

- Outperforms 11 other methods in Schmidt et al. [2007]:
  - Iterations only require linear time and space.
  - Many variables can be made zero/non-zero at once.
  - Allows warm-starting.
  - Eventually becomes quasi-Newton on the non-zeroes.

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- Can we use the same tricks on the original problem?

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- We could use the steepest descent direction $-z^k$.

Non-Smooth Steepest Descent

- The original problem:

$$\min_x F(x) = f(x) + \lambda \|x\|_1.$$

- If f is smooth, F has directional derivatives everywhere.
- We could use the steepest descent direction $-z^k$.
- For convex problems, z^k is the minimum-norm sub-gradient:

$$z^k = \arg\min_{z \in \partial F(x^k)} ||z||$$

Non-Smooth Steepest Descent

- The steepest descent direction for ℓ_1-Regularization problems,

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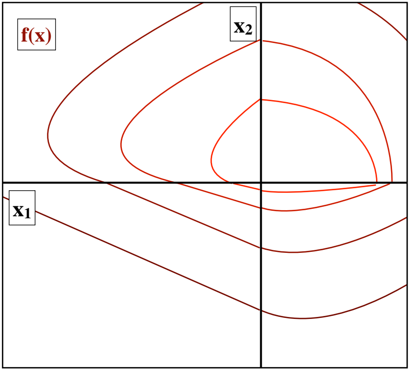
- However, there are two problems with this step:
  1. It may not decrease the objective.
  2. The iterations are not sparse.

Orthant Projection

- Use orthant projection to get sparse iterates:

$$x^{k+1} \leftarrow \mathcal{P}_{\mathcal{O}(x^k)}[x^k - \alpha[H_k]^{-1} z^k],$$

[Osborne et al., 2000, Andrew & Gao, 2007]



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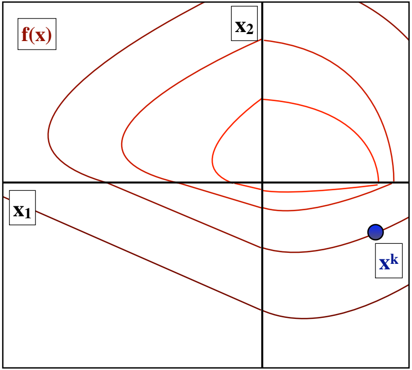

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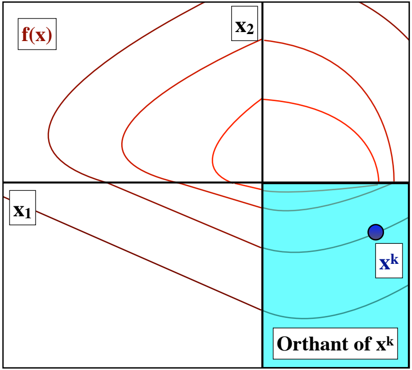

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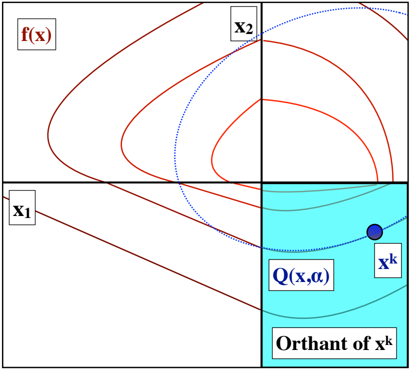

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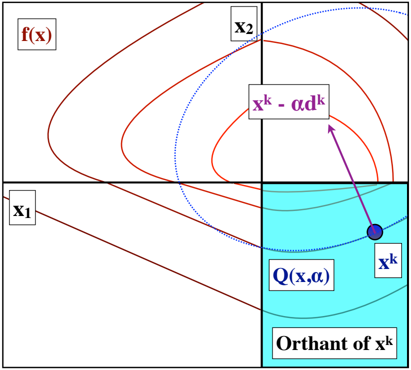

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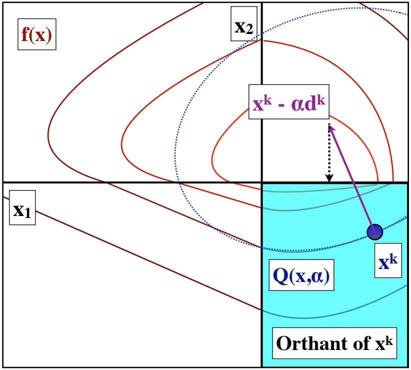

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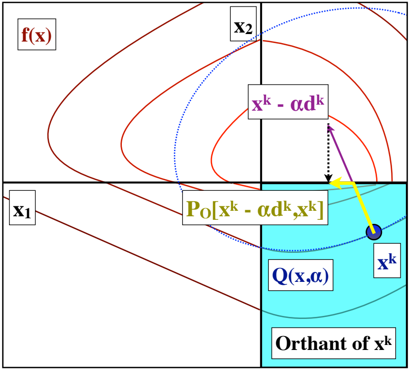

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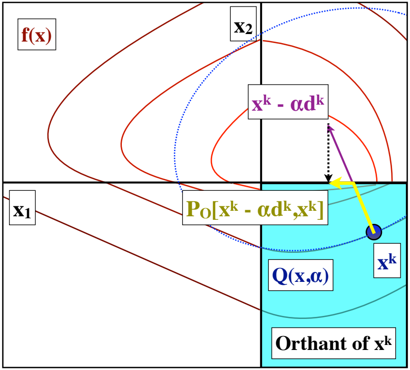

- Variables that change sign become exactly zero.

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- We can guarantee descent using diagonal scaling:

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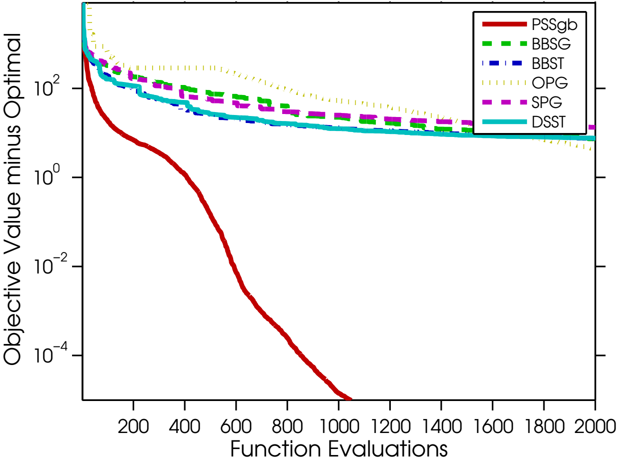
- Quasi-Newton method with separable non-smooth regularization.

Comparing to non-L-BFGS methods

Comparing to methods not based on L-BFGS (sido data):



Discussion

- Similar ideas used in many ℓ_1-Regularization solvers.

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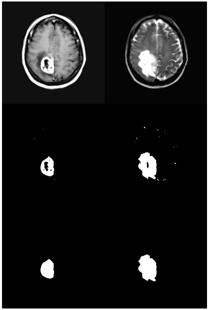
- Generalizes to separable A.E.-differentiable regularizers.
- Exist two-metric projection for simplex constraints.

Motivation:Automatic Brain Tumor Segmentation

- Independent pixel classifier ignores correlations.
- Conditional random fields (CRFs) generalize logistic regression to multiple labels.



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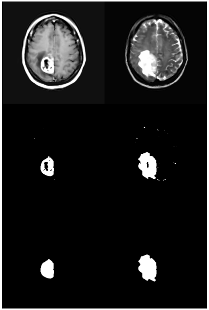


- Can use exact same optimizer for ℓ_1-regularized CRFs.

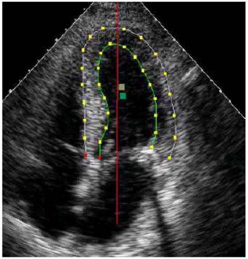
`http://www.di.ens.fr/~mschmidt/Software/L1General.html`

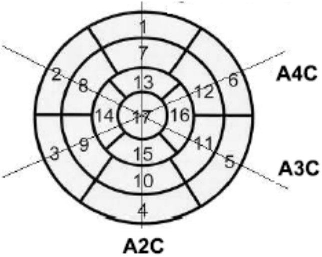
Outline

1. Sparsity
2. Group Sparsity
3. Structured Sparsity
4. Big-N Problems

Motivation: Structure Learning in CRFs

- Task: early detection of coronoary heart disease.





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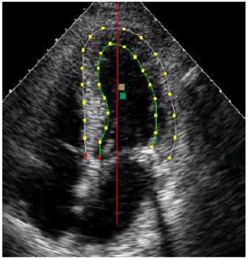

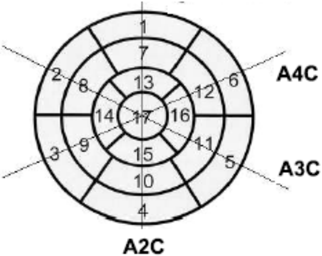

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- But, do not know the best correlation structure.

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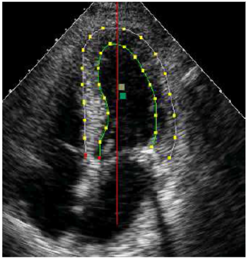

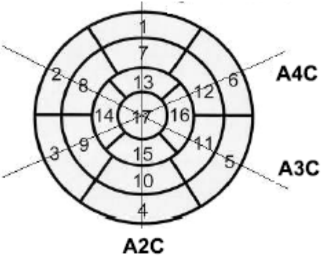

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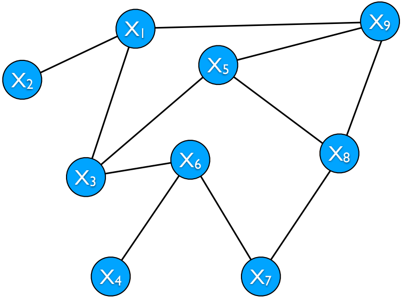
- But, do not know the best correlation structure.
- Perform structure learning with ℓ_1-regularization.

Structure Learning with ℓ_1-Regularization



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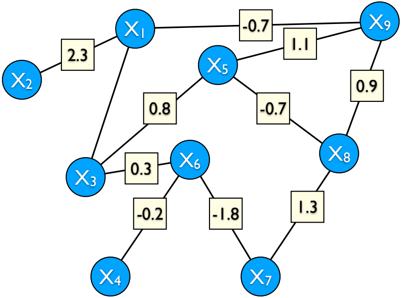

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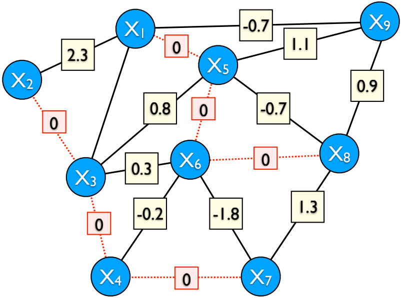

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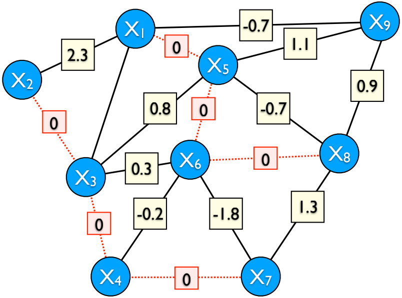
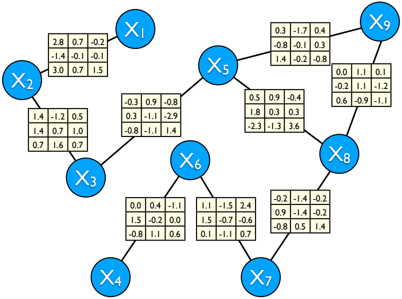


- We want to fit a Markov random field with unknown structure.
- Learn a sparse structure by ℓ_1-regularization of edge weights.

[Lee et al. 2006, Wainwright et al. 2006]

Structure Learning with Group ℓ_1-Regularization



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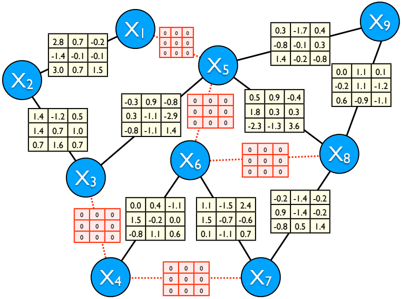

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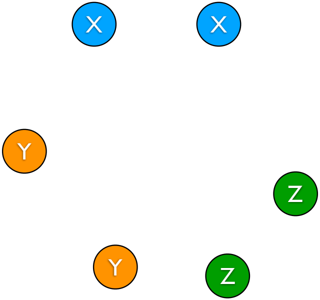

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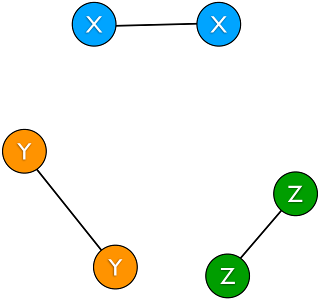

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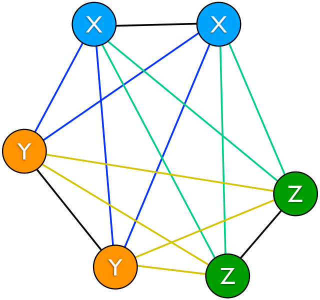

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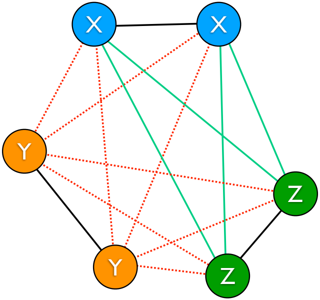

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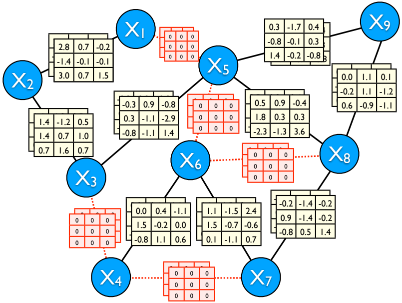

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Structure Learning with Group ℓ_1-Regularization

- Encourage group sparsity using group ℓ_1-regularization:

$$\min_x f(x) + \lambda \|x\|_{1,p},$$

where

$$\|x\|_{1,p} = \sum_g \|x_g\|_p.$$

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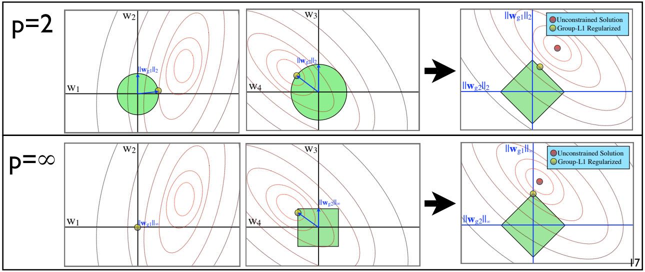
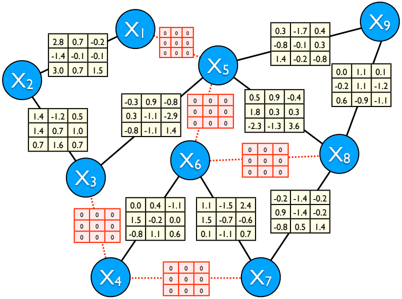
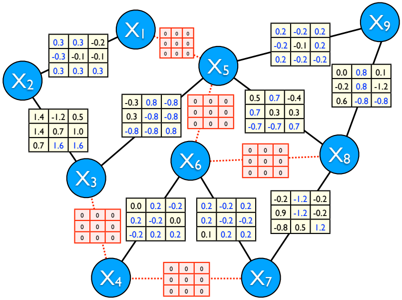


Effect of Different Group Norms



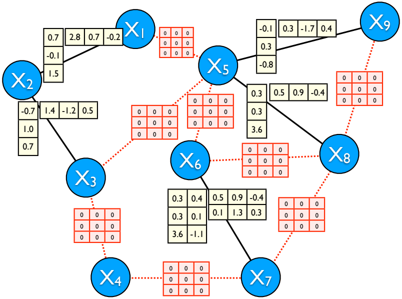
- Group ℓ_1-Regularization with the ℓ_2 group norm.
- Encourages group sparsity.

Effect of Different Group Norms



- Group ℓ_1-Regularization with the ℓ_∞ group norm.
- Encourages group sparsity and parameter tieing.

Effect of Different Group Norms



- Group ℓ_1-Regularization with the nuclear group norm.
- Encourages group sparsity and low-rank.

Optimization with Group ℓ_1-Regularization

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where f is the CRF (expensive) objective.

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- But the regularizer is simple.
- Can we extend quasi-Newton methods using this property?

Converting to a Constrained Problem

- We can re-write the non-smooth objective

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as a smooth objective with norm-cone constraints:

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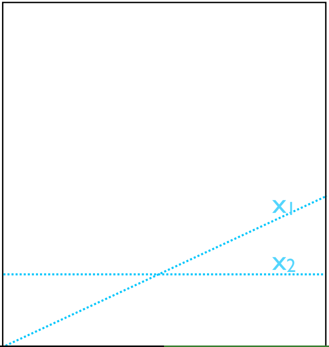

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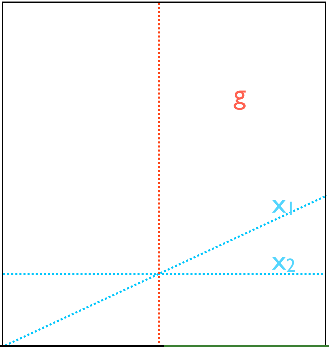

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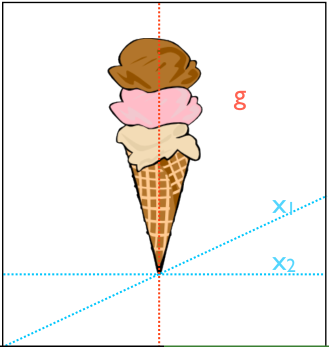

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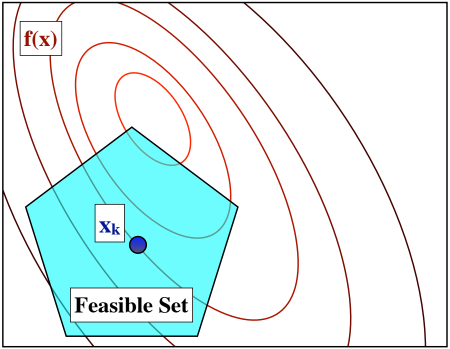

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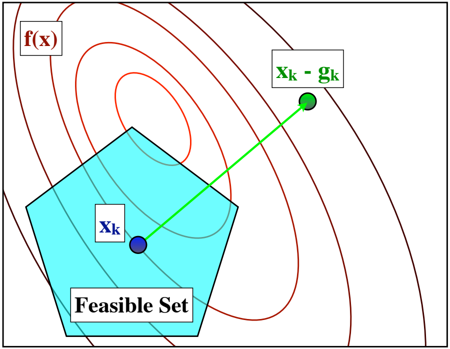

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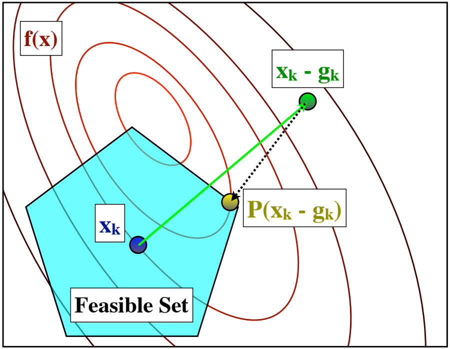

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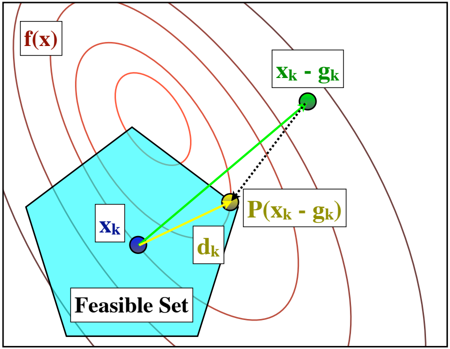

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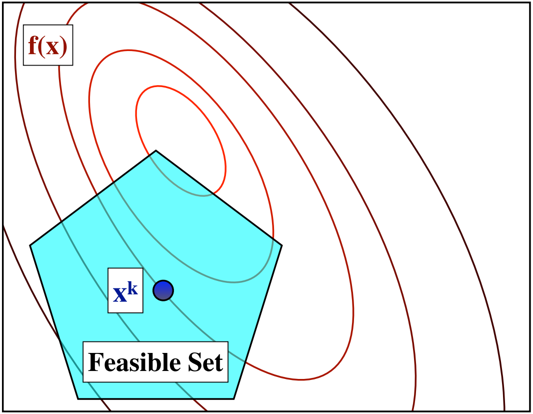

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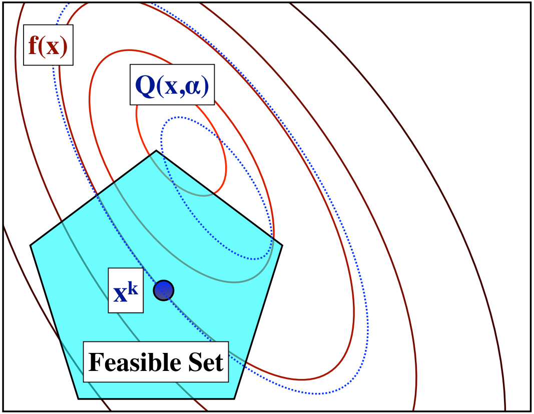

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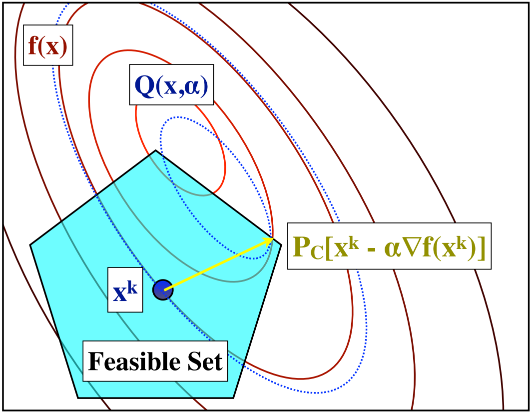

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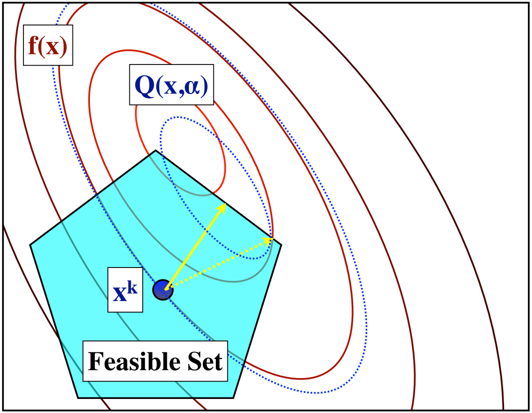

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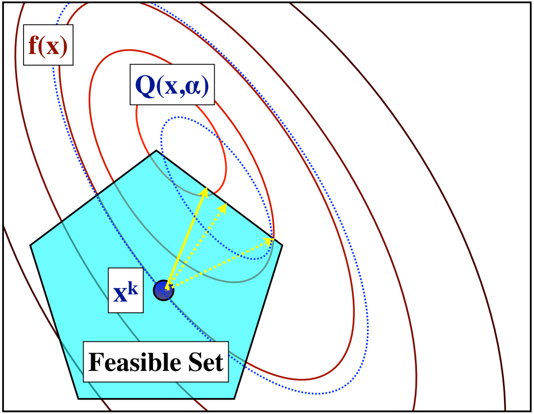

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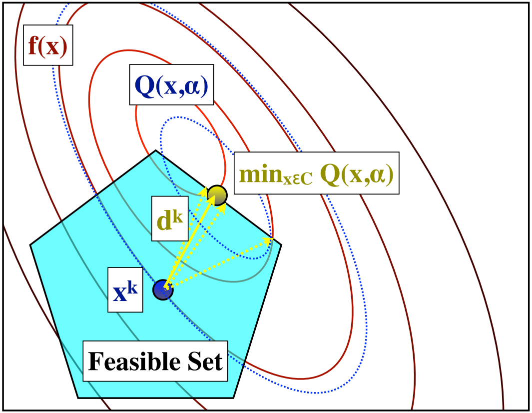

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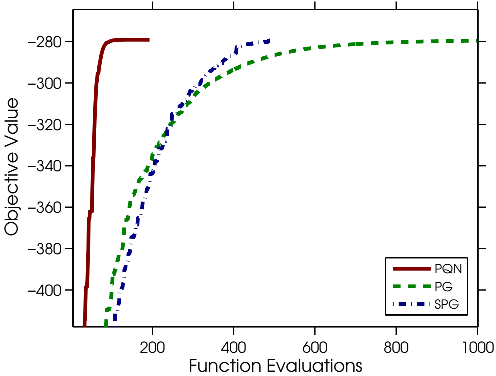
- The projected quasi-Newton (PQN) approach:
  - Best paper prize at AI/Stats.
  - "The projected quasi-Newton (PQN) algorithm [19, 20] is perhaps the most elegant and logical extension of quasi-Newton methods, but it involves solving a sub-iteration." [Becker and Fadili, 2012].
  - "PQN is an implementation that uses a limited-memory quasi-Newton update and has both excellent empirical performance and theoretical properties." [Lee et al., 2012].
  - `http://www.di.ens.fr/~mschmidt/Software/PQN.html`

Graphical Model Structure Learning with Groups

Comparing PQN to first-order methods on a graphical model structure learning problem. [Gasch et al., 2000, Duchi et al., 2008].



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- Yes, with proximal-gradient methods.

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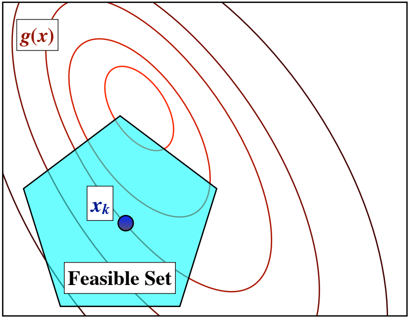

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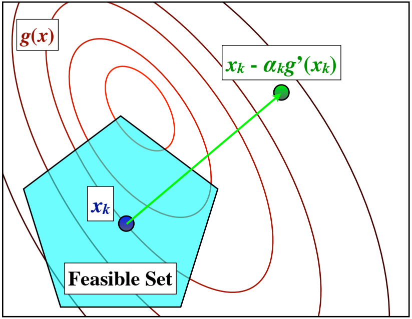

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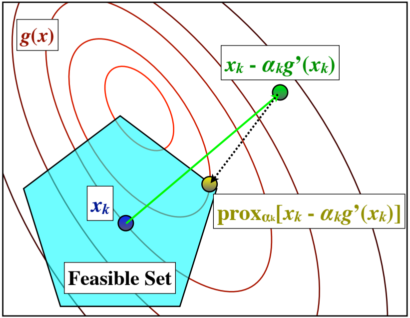

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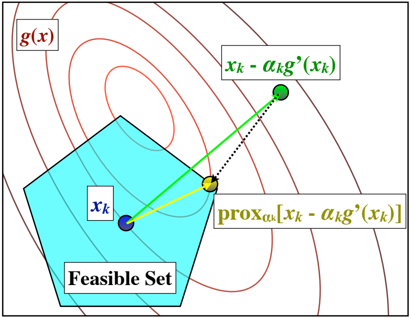

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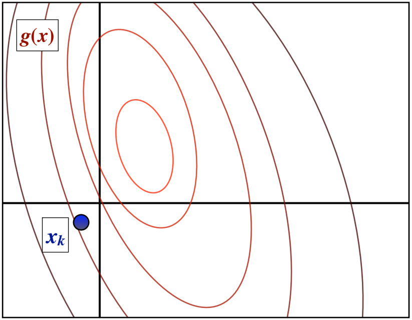

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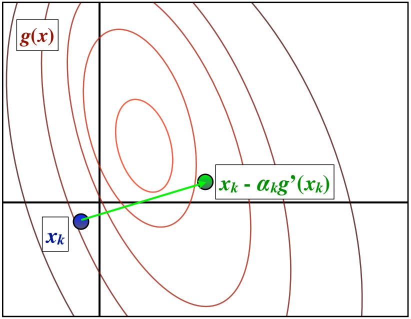

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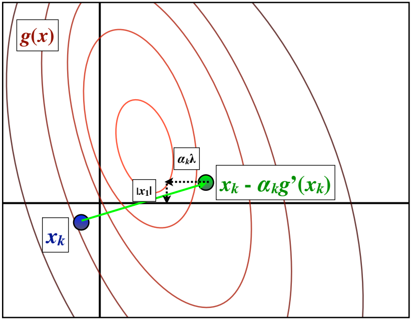

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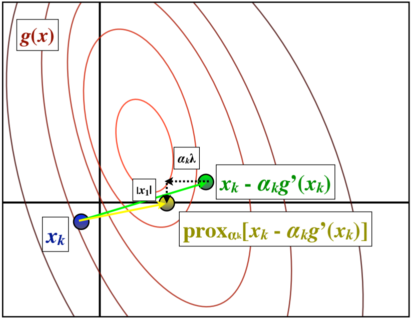

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Proximal Gradient for Group ℓ_1-Regularization

- The group ℓ_1-regularizer is simple; we can compute the proximal operator in linear time. [Wright et al., 2009]

$$\mathrm{prox}_{\alpha||x_g||}[x_g] = \arg\min_x \frac{1}{2}||x - x_g||^2 + \alpha||x||$$
$$= \frac{x_g}{||x_g||}\max\{0, ||x_g|| - \alpha\}$$

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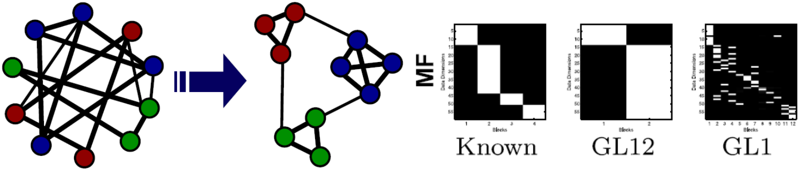
- Proximal-Newton is increasing in popularity, e.g. NIPS 2012:
  - Becker & Fadili, Hsieh et al., Lee et al., Olsen et al., Pacheco & Sudderth.

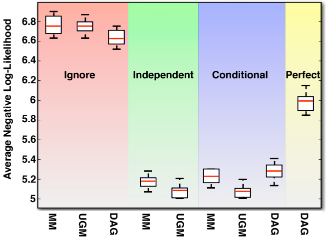
Motivation: Structure Learning in Graphical Models

PQN has been used in other structure learning applications:

- Learning variable groups [Marlin et al., 2009].



- Non-DAG approaches to causality [Duvenaud et al., 2010].



Outline

1. Sparsity
2. Group Sparsity
3. Structured Sparsity
4. Big-N Problems

Structure Learning with ℓ_1-Regularization

A list of papers on this topic (incomplete):

[Li & Yang, 2004], [Li & Yang, 2005], [Banerjee et al., 2006], [Huang et al., 2006], [Lee et al., 2006], [Meinshausen & Bühlmann, 2006], [Wainwright et al., 2006], [Dahinden et al., 2007], [Schmidt et al., 2007], [Shimamura et al., 2007], [Yuan & Lin, 2007], [d' Aspremont et al., 2008], [Banerjee et al., 2008], [Dahl et al., 2008], [Duchi et al., 2008], [Friedman et al., 2008], [Kolar & Xing, 2008], [Levina et al., 2008], [Schmidt et al., 2008], [Fan & Feng, 2009], [Höling & Tibshirani, 2009], [Krishnamurphy & d'Aspremont, 2009], [Lu, 2009a], [Lu, 2009b], [Marlin et al., 2009a], [Marlin et al., 2009b], [Schmidt et al., 2009], [Schmidt & Murphy, 2009], [Schnitzspan et al., 2009], [Yuan, 2009]. Many more since 2009...

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- We want to go beyond pairwise potentials.

General Log-Linear Models

- Log-linear models write the probability of a vector x as

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- Setting $w_A = 0$ is equivalent to removing the potential.
- In pairwise models we assume $w_A = 0$ if $|A| > 2$.

Group ℓ_1-Regularization for Log-Linear Models

- We can extend group ℓ_1-regularization to the general case:

$$\min_w f(w) + \sum_{A \subseteq S} \lambda_A ||w_A||.$$

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  - Setting $w_A = 0$ does not give conditional independence.
- Prior work restricted the cardinality (e.g., threeway models).

[Dahinden et al., 2007]

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  - Group-sparsity corresponds to conditional independence.
- But, how can we encourage this structured sparsity?

Structured Sparsity for Hierarchical Constraints

- Can enforce a hierarchy with overlapping group ℓ_1-regularization.

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$$\lambda_{\{B\}}||w_B||_2 + \lambda_{\{A,B\}}||w_{A,B}||_2.$$

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- We can learn hierarchical models by solving

$$\min_w f(w) + \sum_{A \subseteq S} \lambda_A \|w_{A^*}\|,$$

where $A^* = \{B | A \subseteq B\}$. [Schmidt & Murphy, 2010]

Active Set Method

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- Heuristic: only consider adding groups that satisfy hierarchichy.
  (And that are sub-optimal. E.g., poorly estimated by the model.)
- Convex analogue of [Cheeseman, 1983, Gevarter, 1987].
- Guarantees weak form of global optimality.

Example of Active Set Method

Initial boundary groups.

1 2 3 4 5

1,2 1,3 1,4 1,5 2,3 2,4 2,5 3,4 3,5 4,5

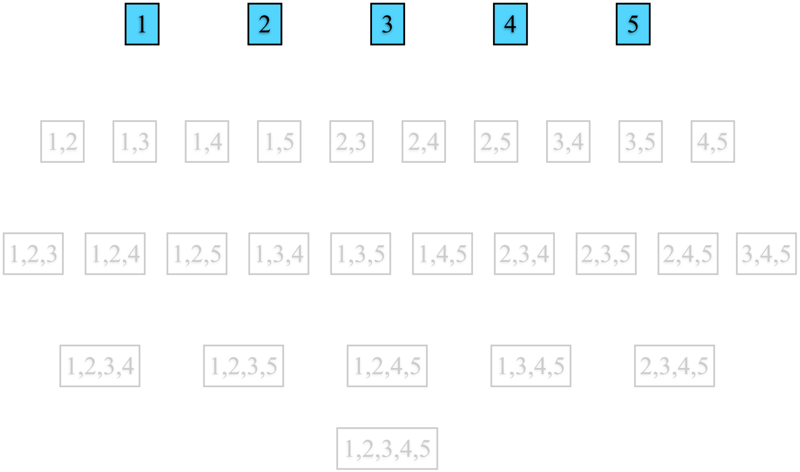
1,2,3 1,2,4 1,2,5 1,3,4 1,3,5 1,4,5 2,3,4 2,3,5 2,4,5 3,4,5

1,2,3,4 1,2,3,5 1,2,4,5 1,3,4,5 2,3,4,5

1,2,3,4,5

Example of Active Set Method

Optimize initial boundary groups.



Example of Active Set Method

Find new **active groups**.

1 2 3 4 5

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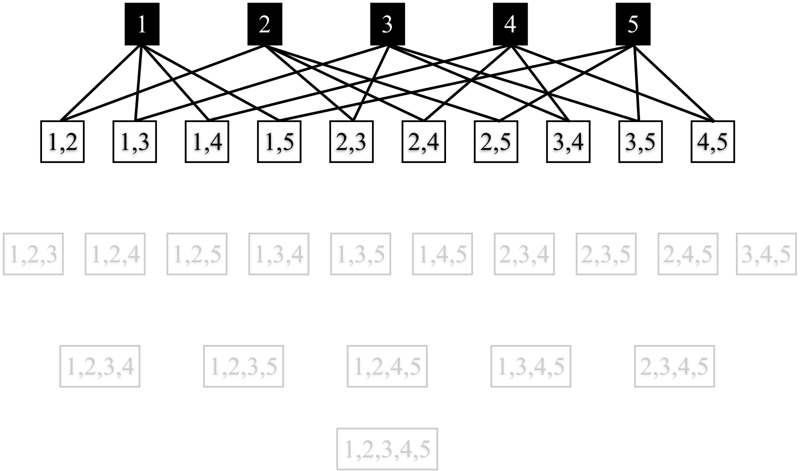

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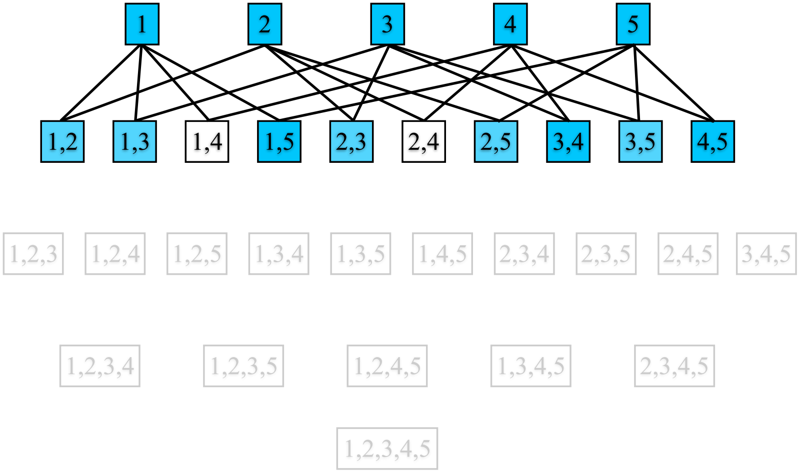
Optimize active groups and sub-optimal boundary groups.



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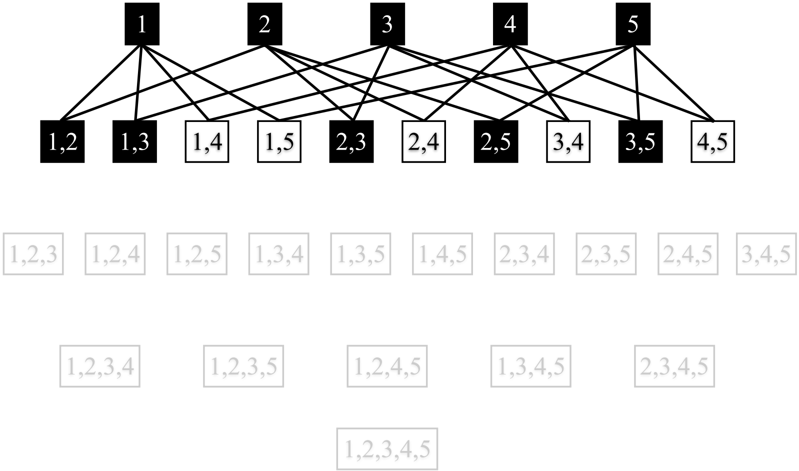

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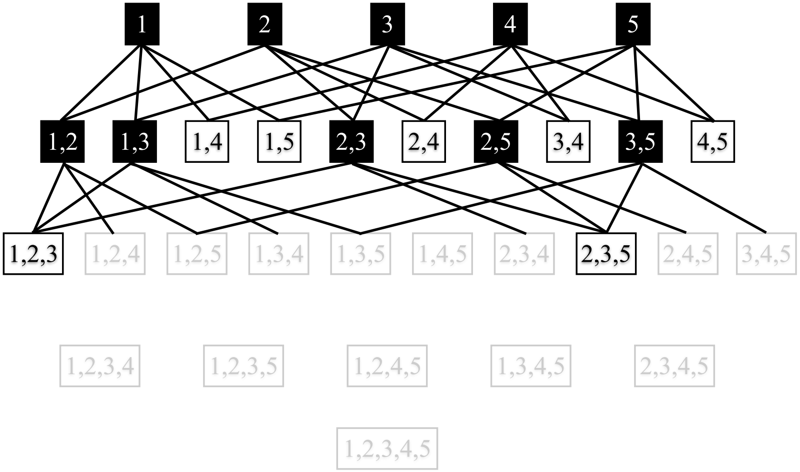

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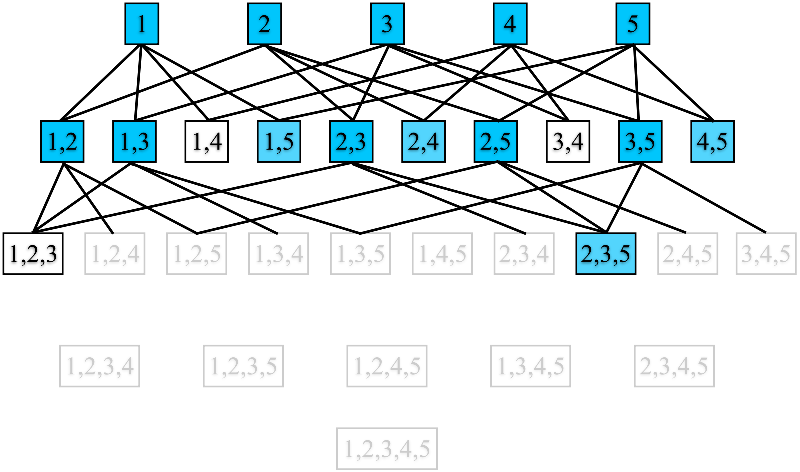

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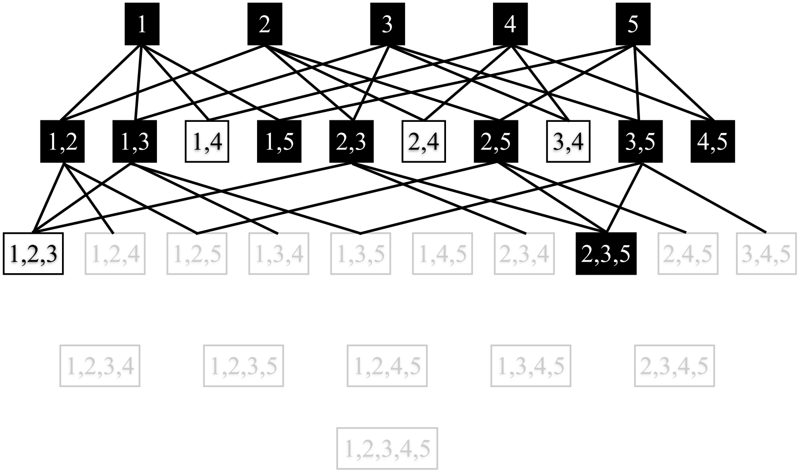

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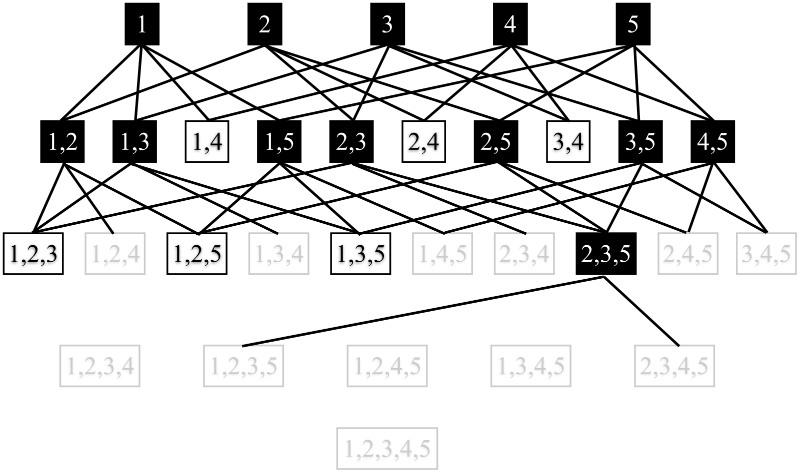

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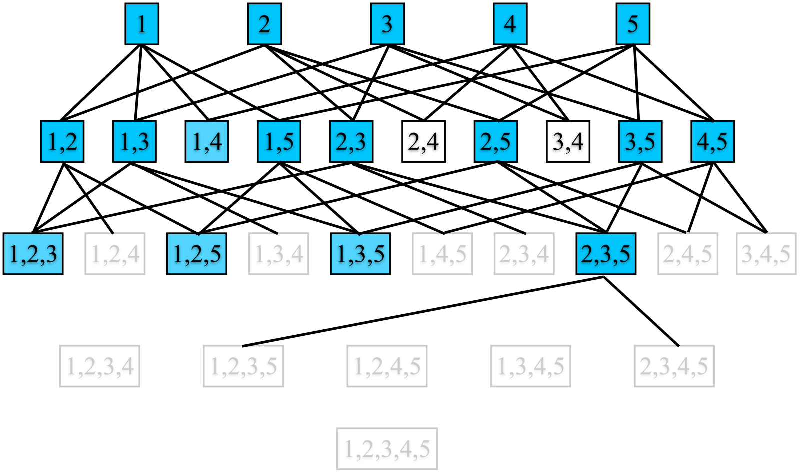

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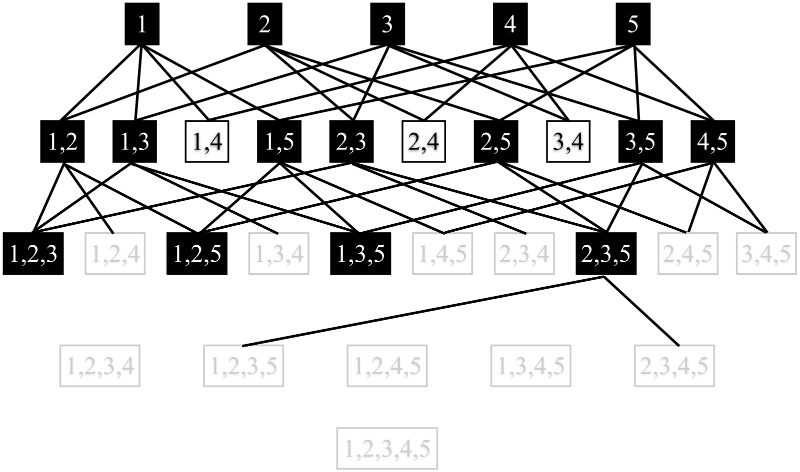

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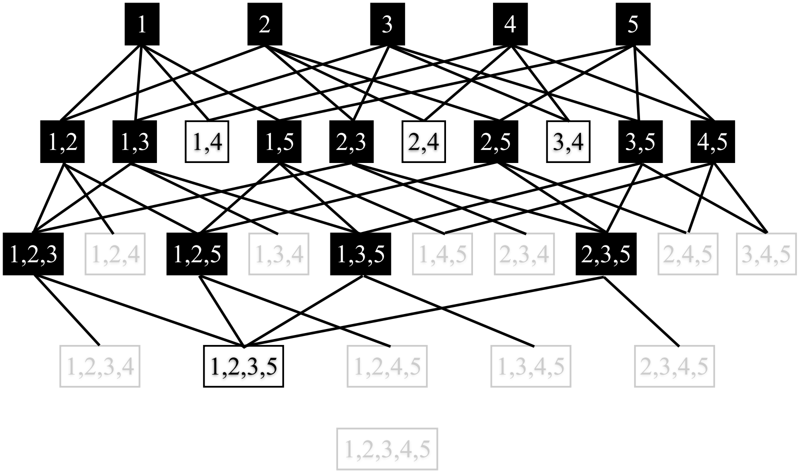

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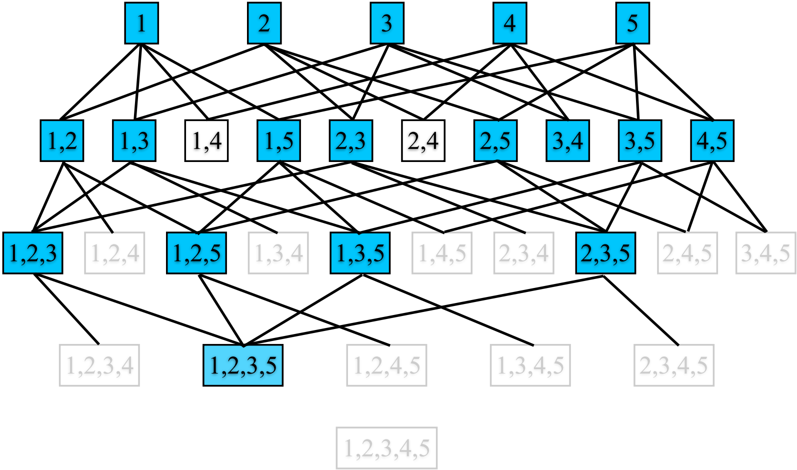

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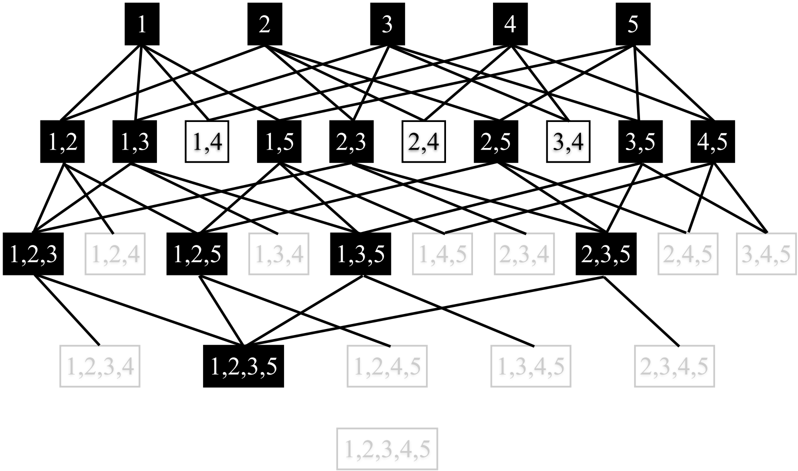
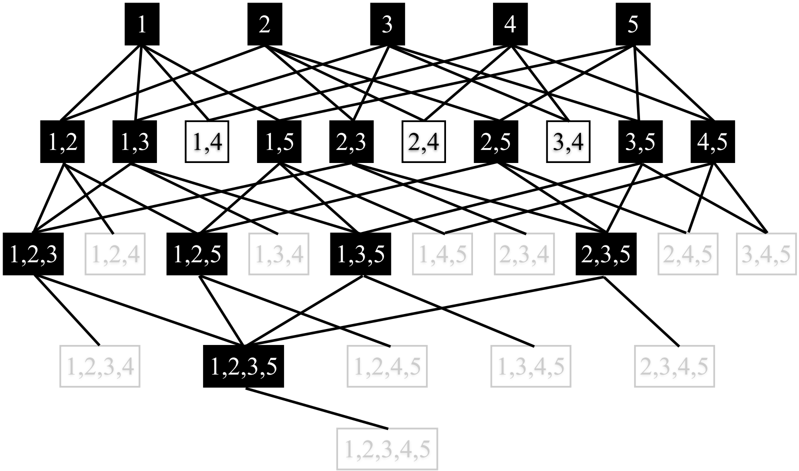


Example of Active Set Method

No new boundary groups, so we are done.



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- We only considered:
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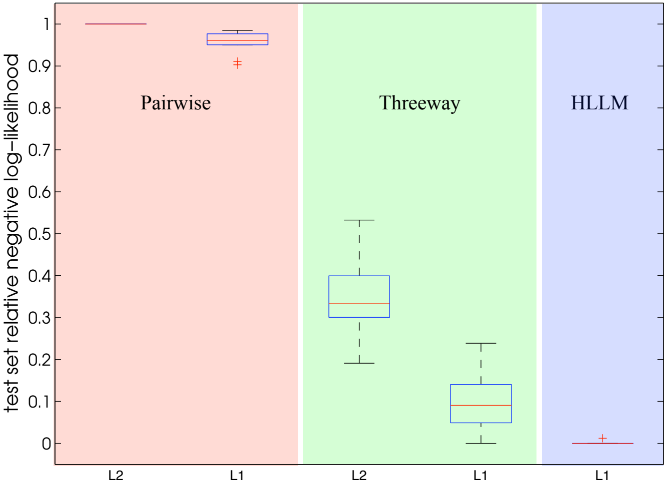
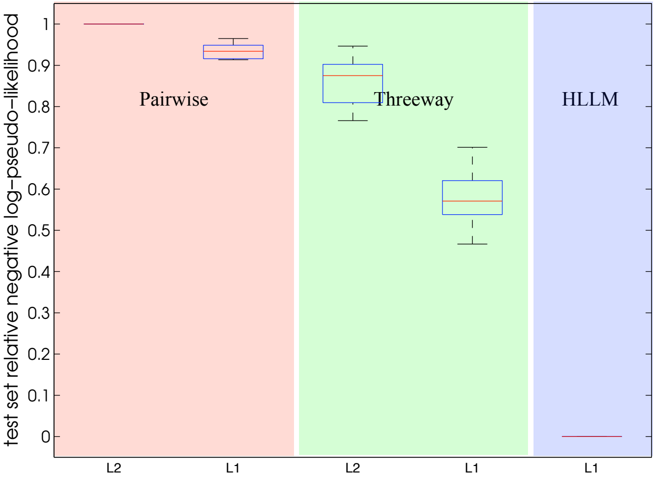
- In practice, do the heuristic and higher-order potentials help?

Flow Cytometry Data



Traffic Flow Data



Structured Sparsity for Hierarchical Constraints

- We now turn to the overlapping group ℓ_1-regularization problem,

$$\min_x f(x) + \lambda \sum_g ||x_g||,$$

  where the groups g may not overlap.

- Non-smooth is regularizer is not simple.
- But we can use that each term is simple.

Converting to a Constrained Problem

- Constrained re-formulation:

$$\min_{\|x_g\| \leq t_g} f(x) + \lambda \sum_g t_g.$$

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- But projections aren't independent since groups overlap.
- We want the projection onto the intersection of simple sets.

Cyclic Projection Algorithms

Projecting onto the intersection of simple sets is a classic problem:

Cyclic Projection Algorithms

Projecting onto the intersection of simple sets is a classic problem:

- Cyclically projecting onto two subspaces converges to the projection onto their intersections. [von Neumann, 1933]

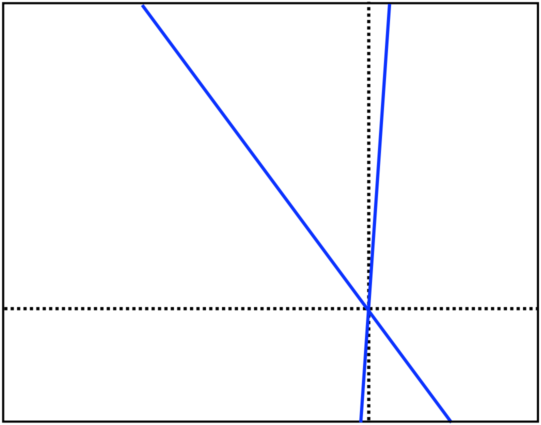
von Neumann's Result

Definition 13.7: If $\phi_1, \phi_2, \ldots$ is a sequence $\sum$ of s.v. operators, if f is an element of $\prod_{n=1}^{\infty} D(\phi_n)$ such that $\lim_{n\to\infty} \phi_n f$ exists, and if D is the set of all such elements f, then $\sum$ is said to have a limit ϕ over D, and, for $f \in D = D(\phi)$, $\phi f = \lim_{n\to\infty} \phi_n f$.

THEOREM 13.7. If $E = P_M$ and $F = P_N$, then the sequence $\sum_1$ of operators $E, FE, EFE, FEFE, \ldots$ has a limit G, the sequence $\sum_2$: $F, EF, FEF, \ldots$ has the same limit G, and $G = P_{MN}$. (The condition $EF = FE$ need not hold.)

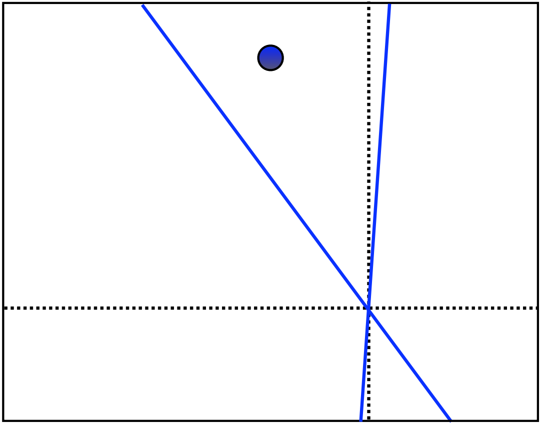
Proof: Let A_n be the n^{th} operator of the sequence $\sum_1$. Then $(A_m f, A_n g) = (A_{m+n-\varepsilon} f, g)$, where $\varepsilon = 1$ if m and n have the same parity and $\varepsilon = 0$ if m and n have opposite parity. It must be shown that if f is any element of S, then $\lim_{n\to\infty} A_n f$ exists. But $\|A_m f - A_n f\|^2 = (A_m f - A_n f, A_m f - A_n f) =$

Take two intersecting subspaces.



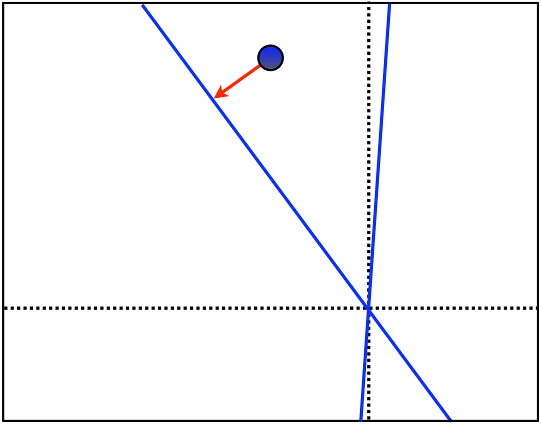
von Neumann's Result

We want to project a point onto their intersection.



von Neumann's Result

Project onto subspace 1.



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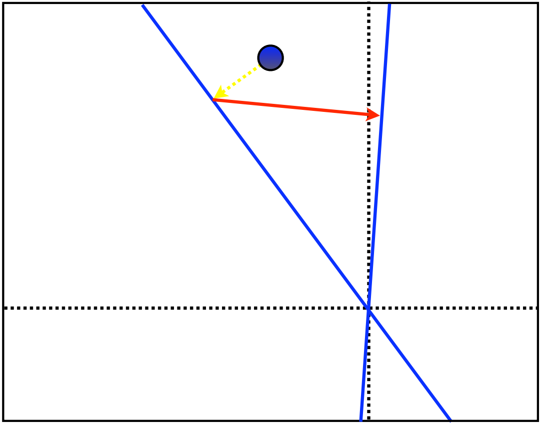
Project onto subspace 2.



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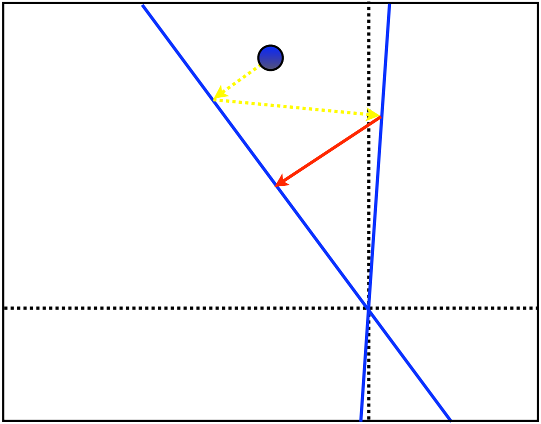

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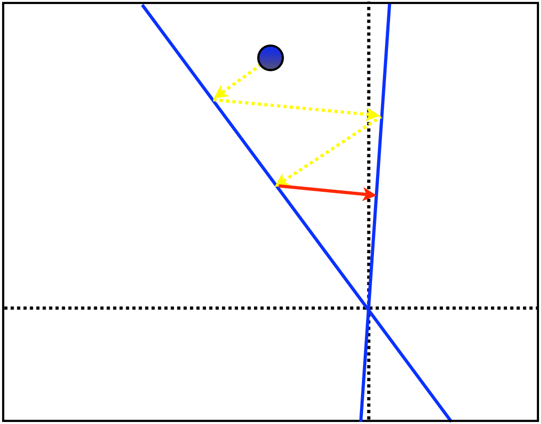

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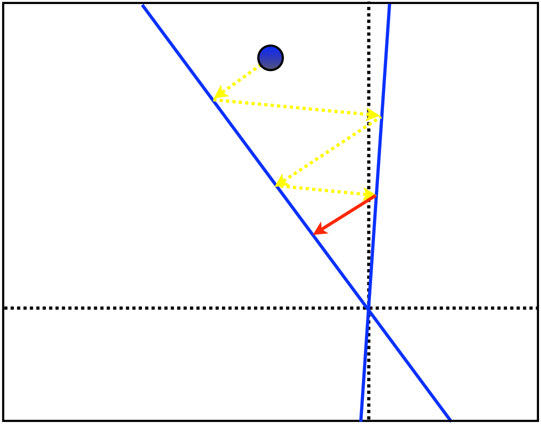

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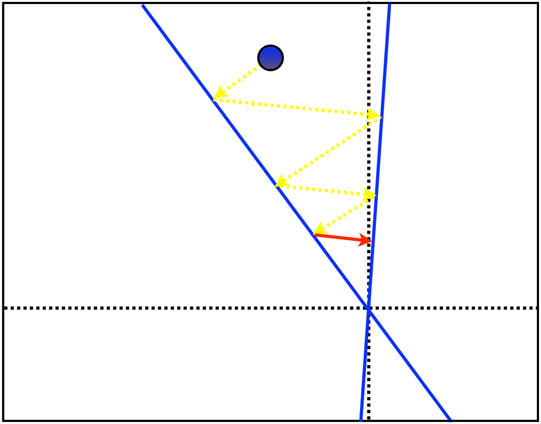

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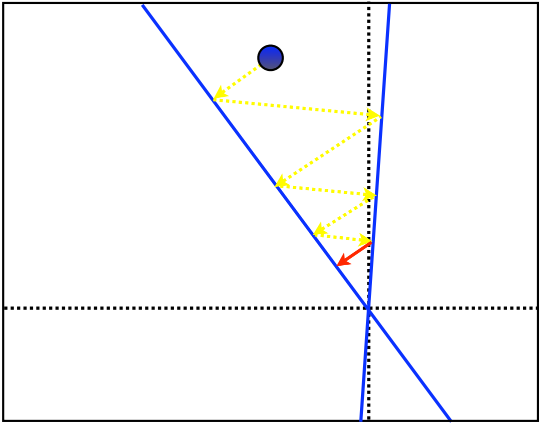
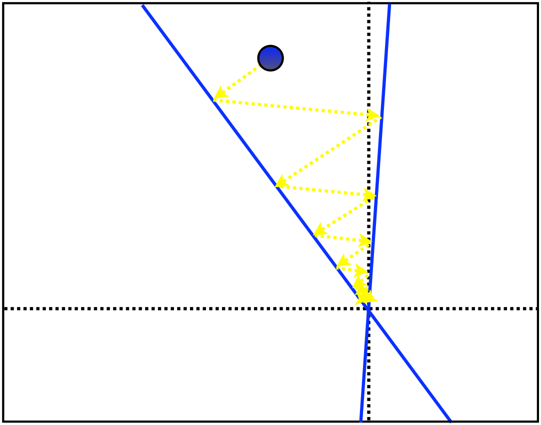


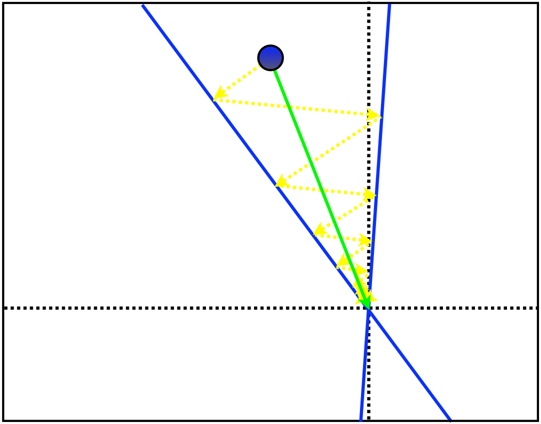
von Neumann's Result

And keep going...



von Neumann's Result

The limit is the projection onto the intersection.



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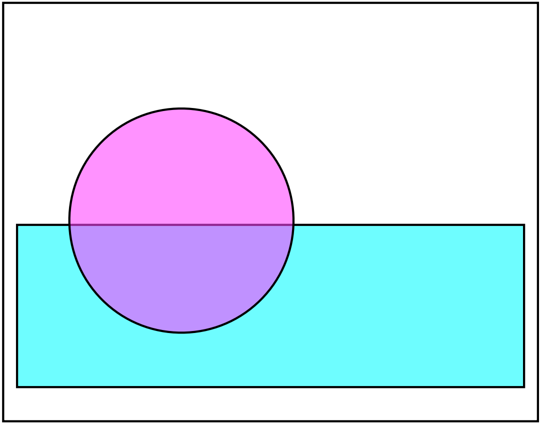
Projecting onto the intersection of simple sets is a classic problem:

- Cyclically projecting onto two subspaces converges to the projection onto their intersections. [von Neumann, 1933]
- Cyclically projecting onto convex sets converges to a point in their interesections. [Bregman, 1965]

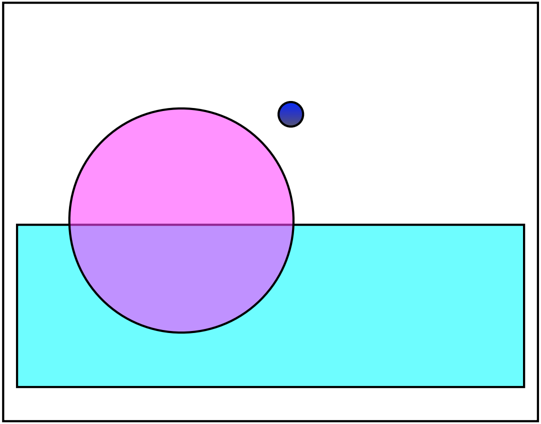
Bregman's Algorithm

We have an arbitrary number of convex sets.



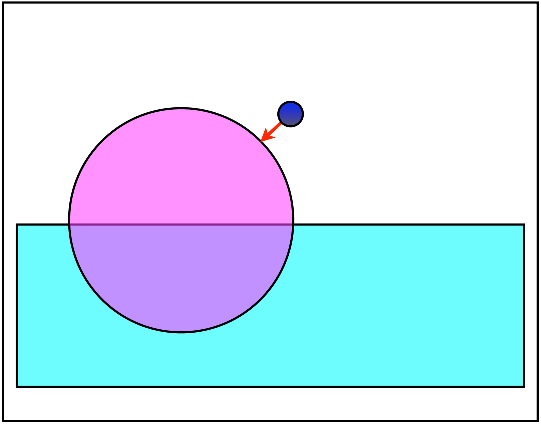
Bregman's Algorithm

Start with some initial point.



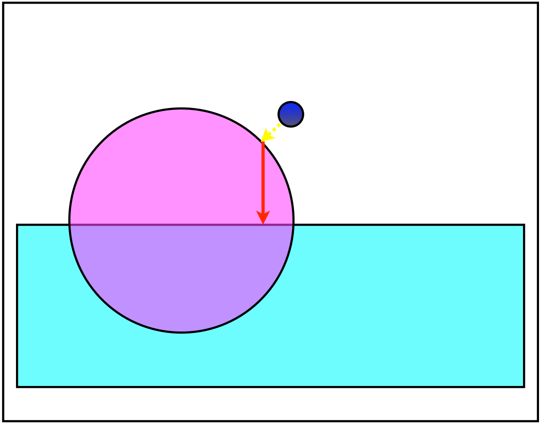
Bregman's Algorithm

Project onto convex set 1.



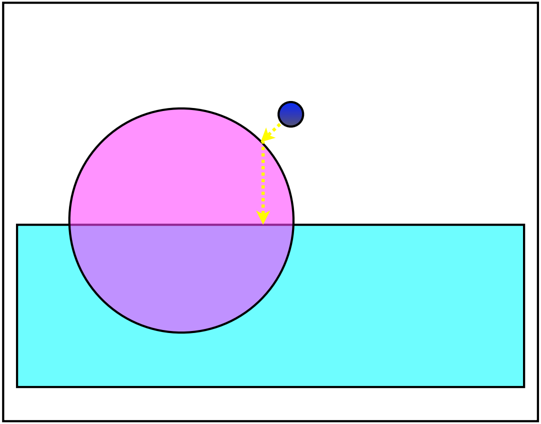
Bregman's Algorithm

Project onto convex set 2.



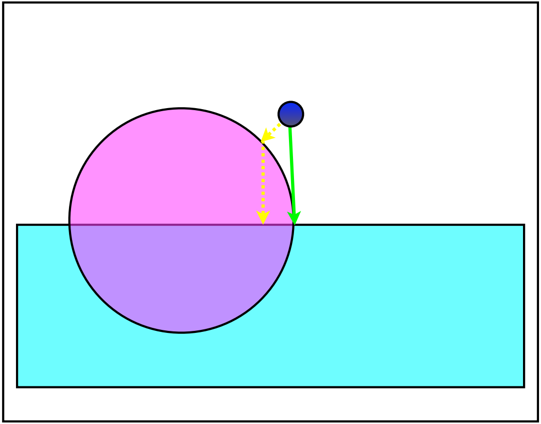
Bregman's Algorithm

The limit is a point in the intersection.



Bregman's Algorithm

In general, the limit is not the projection.



Cyclic Projection Algorithms

Projecting onto the intersection of simple sets is a classic problem:

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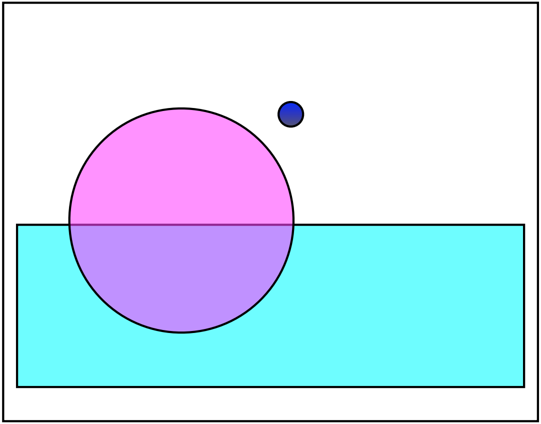

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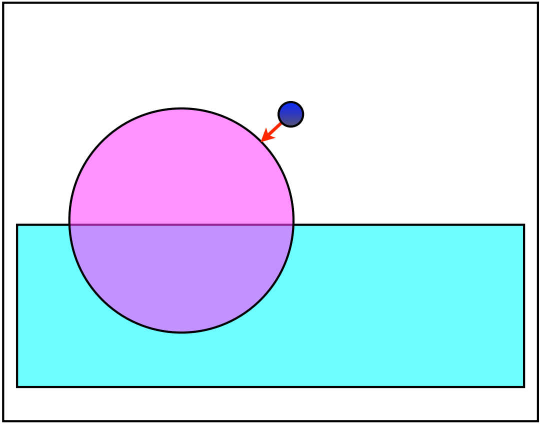
Project onto convex set 1, and store the difference.



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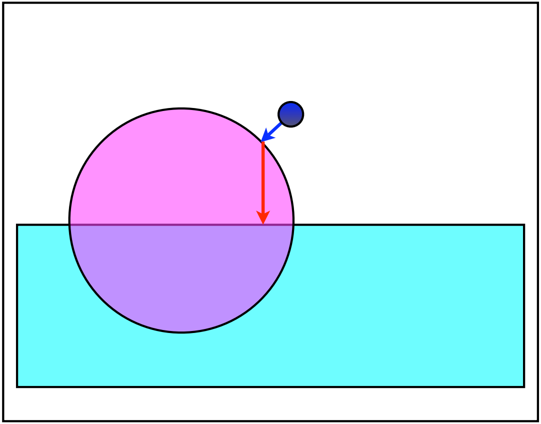
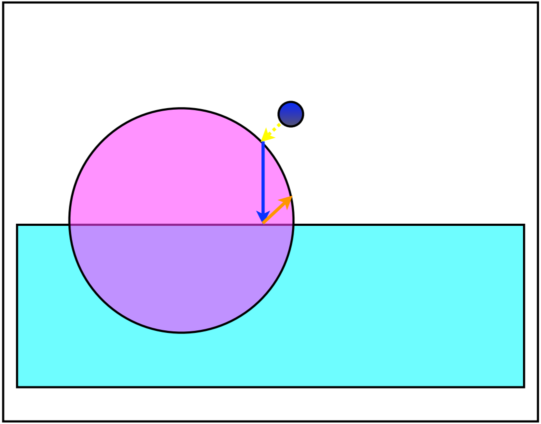


Dykstra's Algorithm

Remove the difference from projecting on convex set 1.



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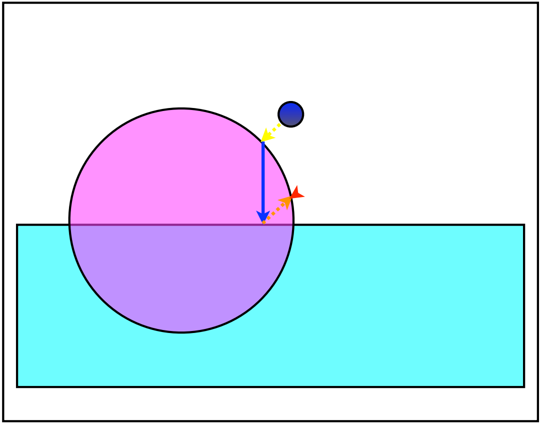

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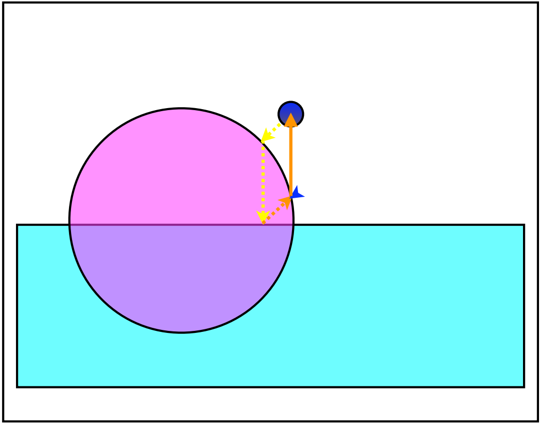

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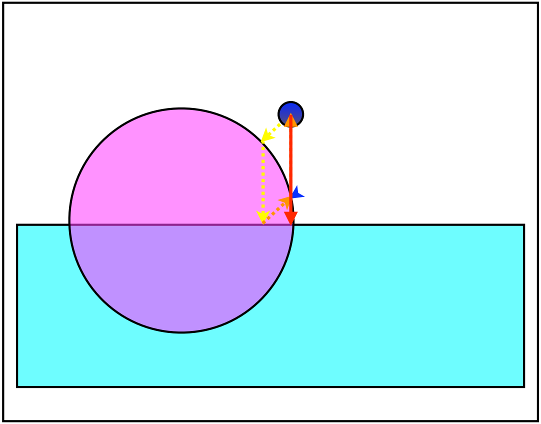

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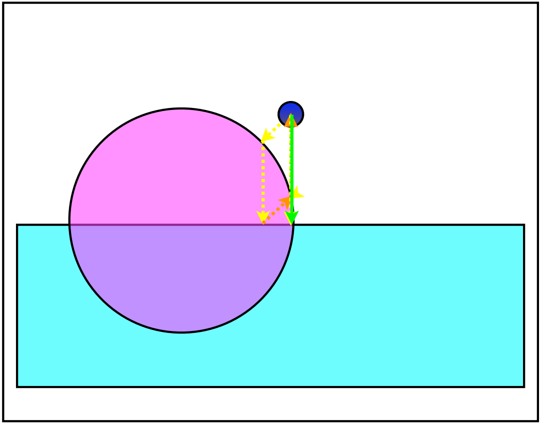

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- Proximal versions of Dykstra's algorithm have recently been developed. [Bauschke and Combettes, 2008]

Exact and Inexact Proximal-Gradient Methos

- We can efficiently compute the proximity operator for:
  1. ℓ_1-*Regularization*.
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- We show analogous results for accelerated proximal-gradient methods, including when $\mu = 0$. [Schmidt et al., 2011]

Outline

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2. Group Sparsity
3. Structured Sparsity
4. Big-N Problems

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- Main practical challenges:
  - Designing/learning good features.
  - Efficiently solving the problem when N or P are very large.

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- Simple example is ℓ_2-regularized least-squares,

$$f_i(x) := (a_i^T x - b_i)^2 + \frac{\lambda}{2} \|x\|^2.$$

- Other examples include any ℓ_2-regularized convex loss:
  - logistic regression, Huber regression, smooth SVMs, CRFs, etc.

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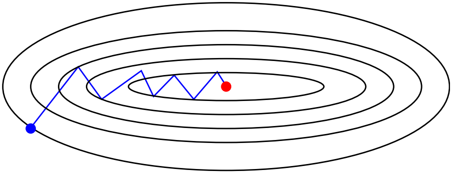

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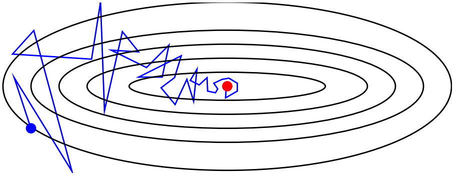
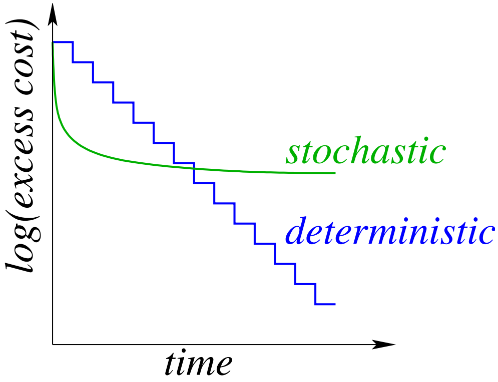


Motivation for New Methods

- FG method has $O(N)$ cost with $O(\rho^k)$ rate.
- SG method has $O(1)$ cost with $O(1/k)$ rate.



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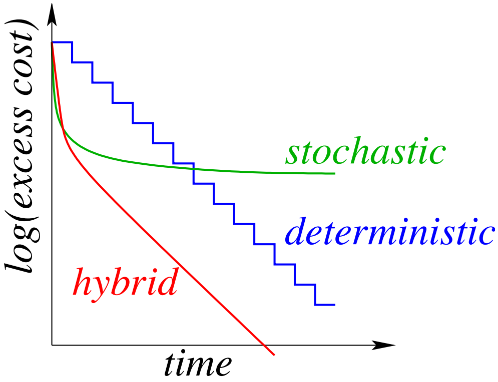

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Prior Work on Speeding up SG Methods

A variety of methods have been proposed to speed up SG methods:

- **Momentum, gradient/iterate averaging**
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- None of these methods improve on the $O(1/t)$ rate

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Existing linear convergence results:

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- **Special Problems Classes**
  - Collins et al. (2008), Strohmer & Vershynin (2009), Schmidt and Le Roux (2012), Shalev-Shwartz and Zhang (2012)
  - Linear rate but limited choice for the f_i's

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  - Stochastic variant of increment average gradient (IAG).

    [Blatt et al. 2007]
  - $O(NP)$ memory requirements reduced to $O(N)$ for many problems.

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- **Convergence rate of $O(\rho^t)$ with cost of $O(1)$** (true for $\alpha \leq \frac{1}{16L}$).
- This rate is "very fast":
  - Well-conditioned problems: constant non-trivial reduction per pass:

$$\left(1 - \frac{1}{8N}\right)^N \leq \exp\left(-\frac{1}{8}\right) = 0.8825.$$

  - Badly-conditioned problems, almost same as deterministic method. (deterministic has rate $\left(1 - \frac{\mu}{L}\right)^{2t}$ with $\alpha = \frac{1}{L}$, but N times slower)

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  - *Fastest possible deterministic method:* $\left(\frac{\sqrt{L}-\sqrt{\mu}}{\sqrt{L}+\sqrt{\mu}}\right)^2 = 0.99048$.
- *SAG beats two lower bounds:*
  - *Stochastic gradient bound (of $O(1/t)$).*
  - *Deterministic gradient bound (for typical L, μ, and N).*

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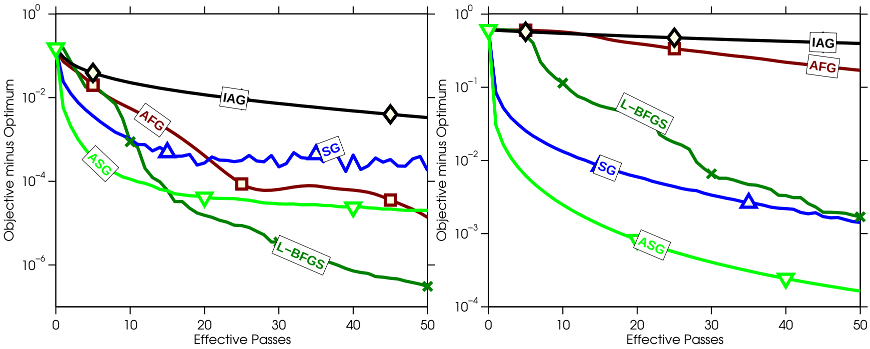
- **Faster than SG lower bound of $O(1/\sqrt{N})$.**
- Same algorithm and step-size as strongly-convex case:
  - Algorithm is adaptive to strong-convexity.
  - Faster convergence rate if μ is locally bigger around x^*.

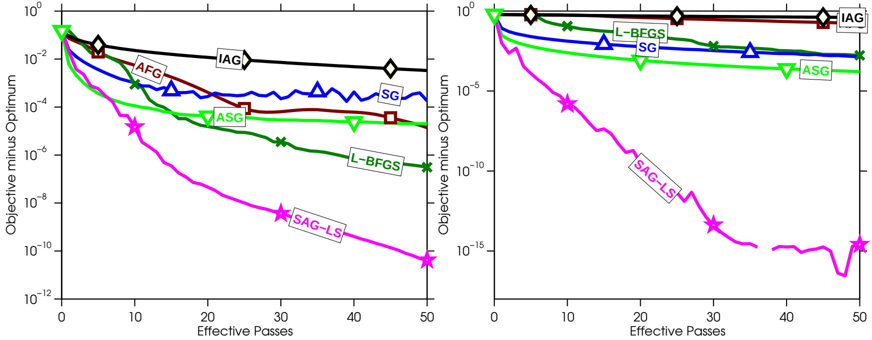
Comparing FG and SG Methods

- quantum ($n = 50000$, $p = 78$) and rcv1 ($n = 697641$, $p = 47236$)



SAG Compared to FG and SG Methods

- quantum ($n = 50000$, $p = 78$) and rcv1 ($n = 697641$, $p = 47236$)



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- Thanks for coming!