Tractable Big Data and Big Models in Machine Learning

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TAAI 2014

November 2014

Context: Big Data and Big Models

- We are collecting data at unprecedented rates.
  - Seen across many fields of science and engineering.
  - Not gigabytes, but terabytes or petabytes (and beyond).

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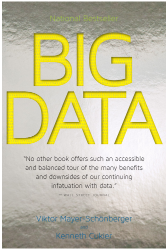

- Many important aspects to the 'big data' puzzle:
  - Distributed data storage and management, parallel computation, software paradigms, data mining, machine learning, privacy and security issues, reacting to other agents, power management, summarization and visualization.

Context: Big Data and Big Models

- Machine learning uses big data to fit richer statistical models:
  - Vision, bioinformatics, speech, natural language, web, social.
  - Developping broadly applicable tools.
  - Output of models can be used for further analysis.

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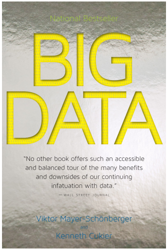

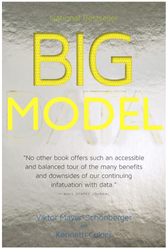

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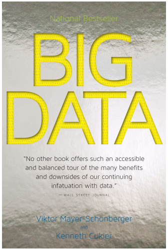

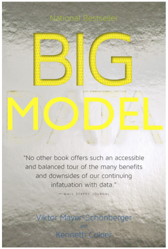

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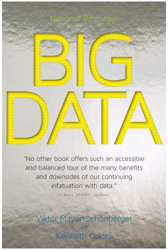

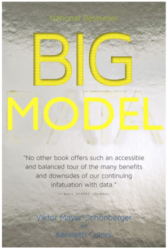

- Numerical optimization is at the core of many of these models.
- But, traditional 'black-box' methods have difficulty with:
  - the large data sizes.
  - the large model complexities.

Two Issues in this Talk

- The first issue is computation:
  - We 'open up the black box', by using the structure of machine models to derive faster large-scale optimization algorithms.
  - Can lead to enormous speedups for big data and complex models.

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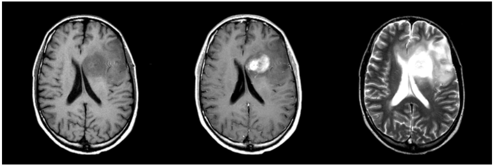
- My research tries to alternate between these two.

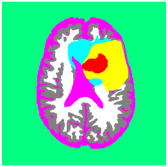
Outline

1. Structured sparsity (inexact proximal-gradient method)
2. Learning dependencies (costly models with simple constraints)
3. Fitting a huge dataset (stochastic average gradient)

Motivation: Automatic Brain Tumor Segmentation

- Task: Segmentation of Multi-Modality MRI Data





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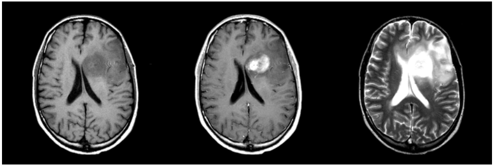

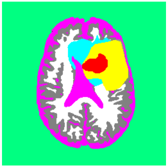

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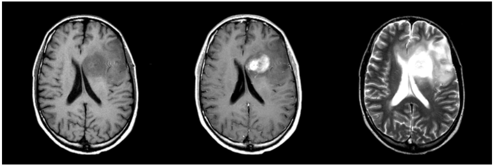

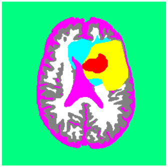

- Applications:
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  - radiation target planning.
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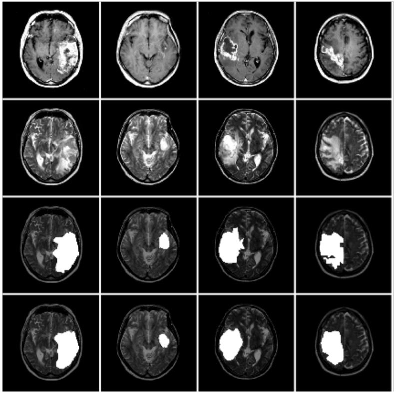
- Challenges:
  - variety of tumor appearances.
  - similarity to normal tissue.

Motivation: Automatic Brain Tumor Segmentation

- Solution strategy:
  1. Incorporate prior knowledge by registration with template.
  2. Pixel-level classifier using image- and template-based features.



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- Problem 2: Designing features.
  - Lots of possible candidate features.
  - Using all features leads to over-fitting.
- Due to slow training time: manual feature selection.

Adding Regularization

- Strange idea: try **all features** with L2-Regularization:

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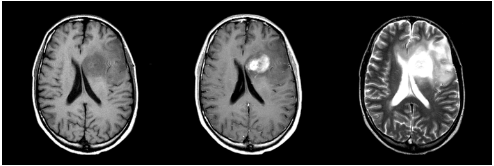
- Another strange idea: try **all features** with L1-Regularization:

$$\min_{x} \frac{1}{N} \sum_{i=1}^{N} f_i(x) + \lambda \sum_{i=1}^{P} |x_i|.$$

  - Still reduces over-fitting.
  - But, solution x is SPARSE (some $x_j = 0$).
  - Feature selection by only training once.

Feature Selection with L1-Regularization (Binary)

- Binary case:
  - Setting variable $x_j = 0$ removes the feature a_j.



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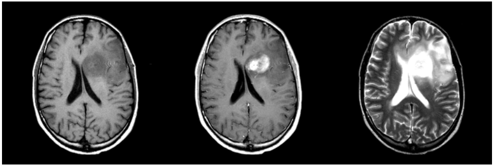

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Variable Selection with L1-Regularization

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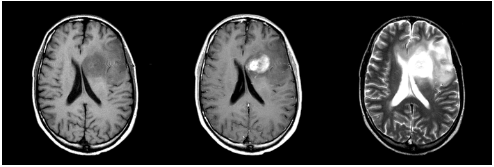

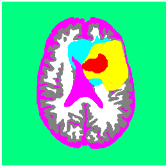

- Because we classify using the maximum of $x_c^T a$:

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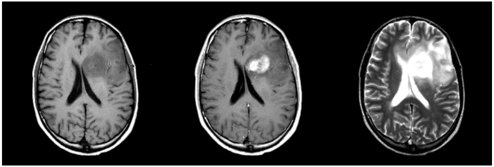

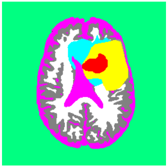

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Feature Selection with Group L1-Regularization

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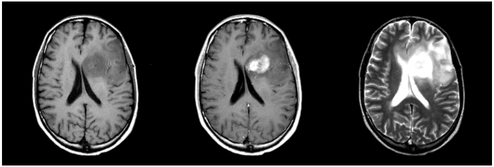

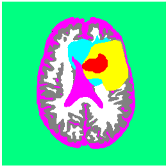

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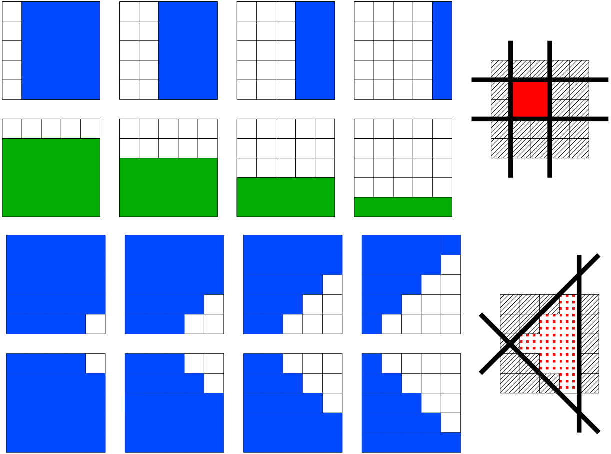
- Structured sparsity generalizes groups to other structures.

Structured Sparsity Examples

- Examples of structured sparsity:

Structured sparsity to select convex regions:



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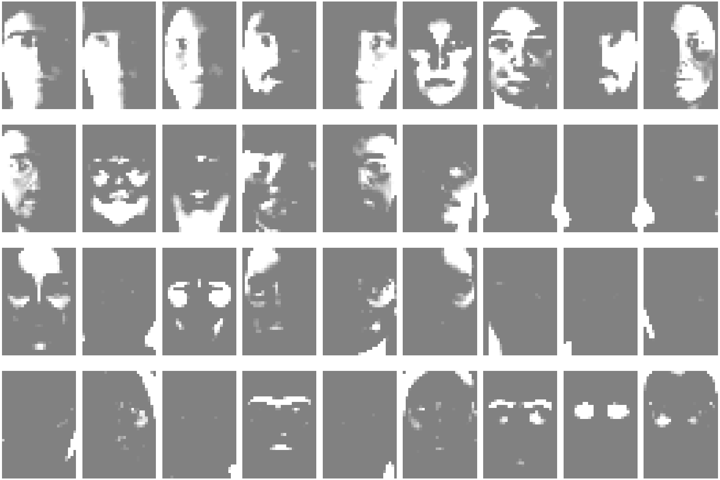
Dictionary learned with non-negative matrix factorization:



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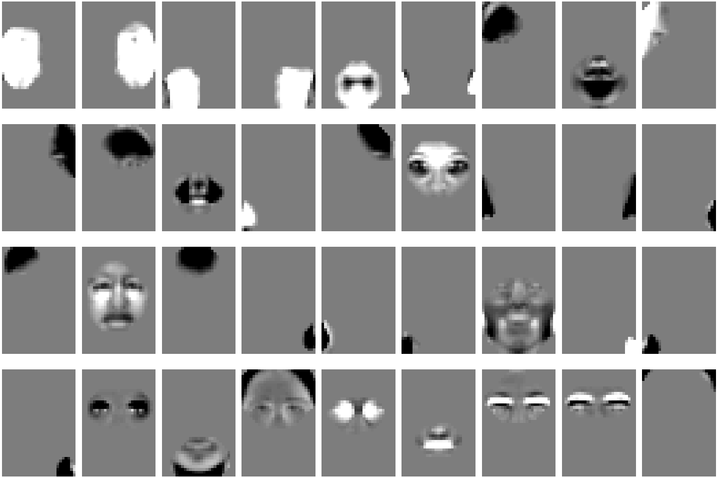

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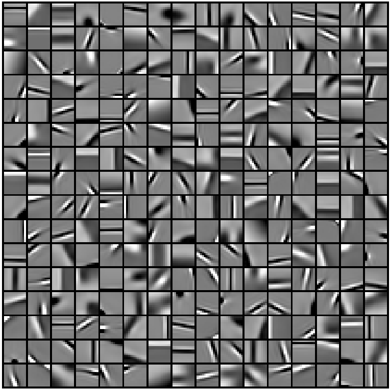
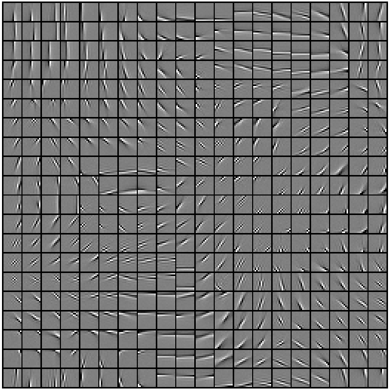
Spatially-structured dictionary with structured sparsity:





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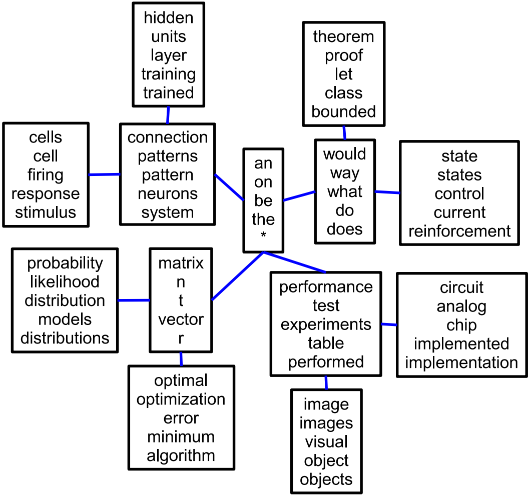
Tree-structured dictionary with structured sparsity:



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  - A linear model with variable interactions:

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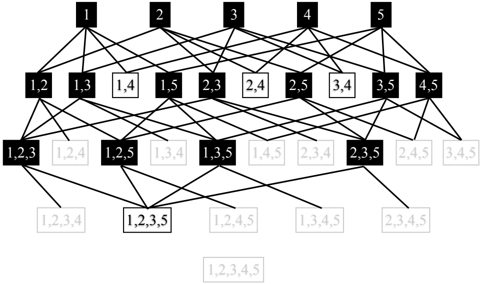
  - Structured sparsity on the hierarchical models.



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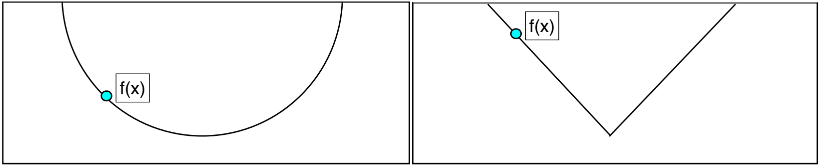

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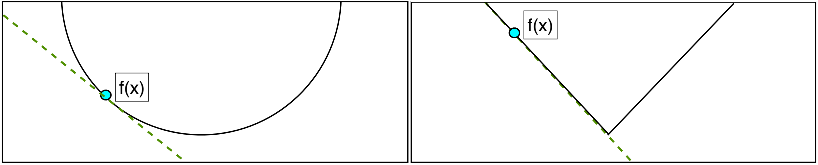

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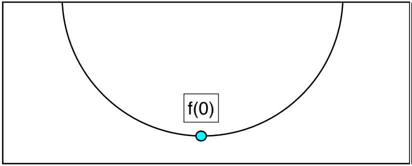

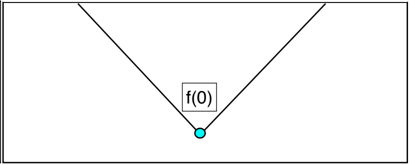

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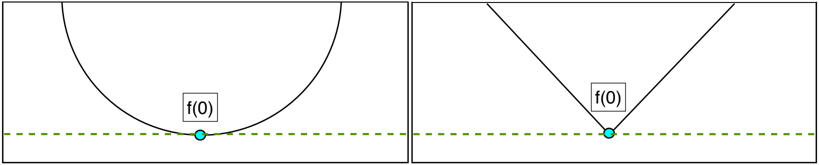

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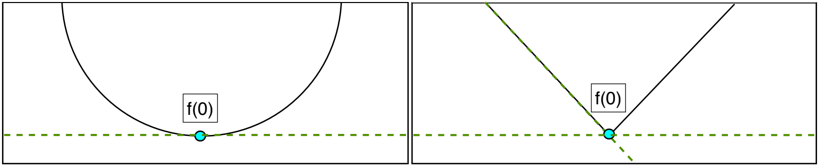

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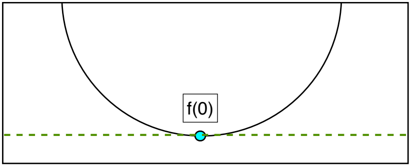

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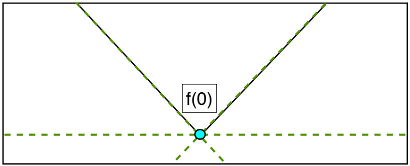

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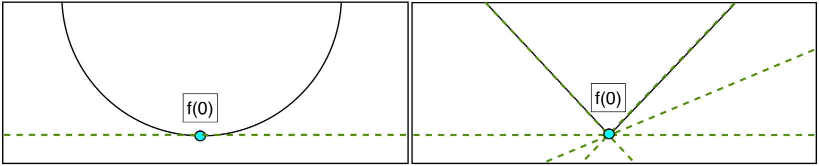

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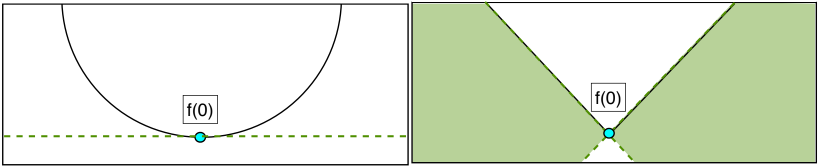

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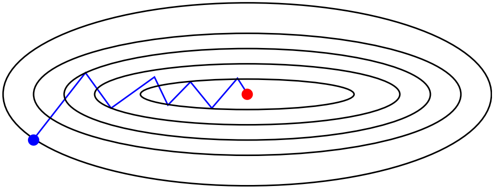

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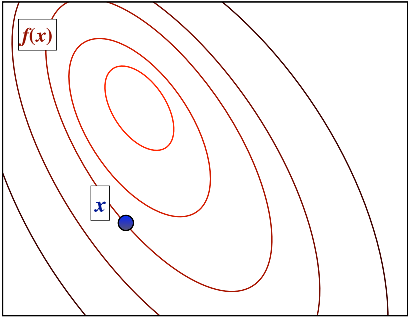

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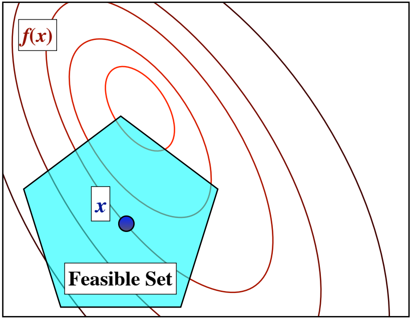

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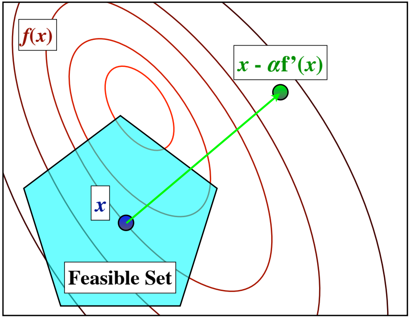

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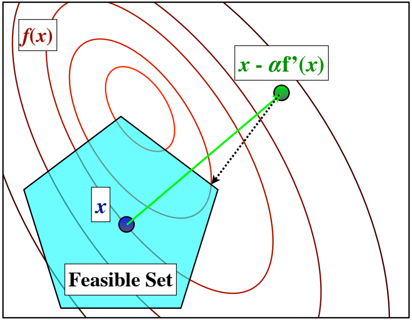

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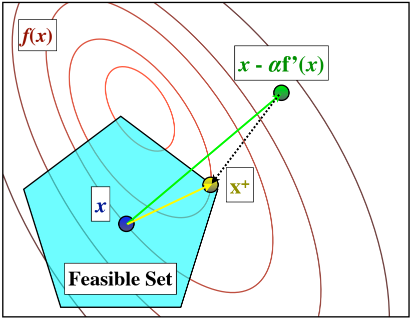

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- For many problems we can not efficiently compute this operator.

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- Do inexact methods have the $O(\kappa \log(1/\epsilon))$ rate?
  - *Yes, if the errors are appropriately controlled*. [Schmidt et al., 2011]

Convergence Rate of Inexact Proximal-Gradient

Proposition *[Schmidt et al., 2011] If the sequences of gradient errors* $\{||e_t||\}$ *and proximal errors* $\{\sqrt{\varepsilon_t}\}$ *are in* $\{O((1-\kappa^{-1})^t)\}$*, then the inexact proximal-gradient method requires* $O(\kappa \log(1/\epsilon))$ *iterations.*

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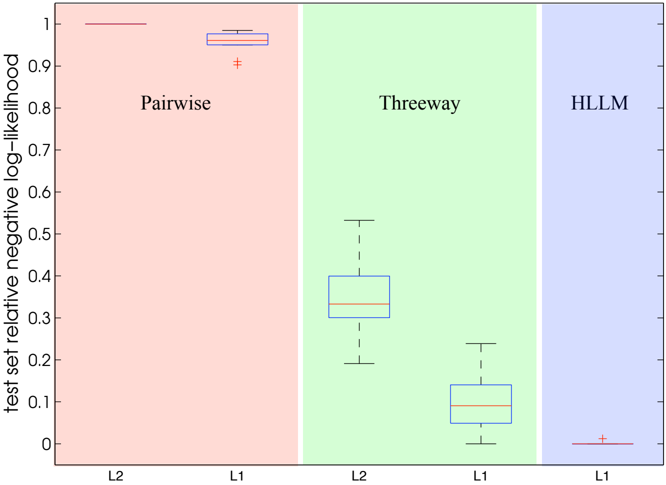
- Classic result as a special case (constants are good).
- The rates degrades gracefully if the errors are larger.
- We also showed the $O(\sqrt{\kappa}\log(1/\epsilon))$ accelerated method rate.
- We also considered weaker convexity assumptions on f.
- Huge improvement in practice over black-box methods.

Flow Cytometry Data

Using structured sparsity to fit a hierarchical log-linear model (HLLM):



Traffic Flow Data

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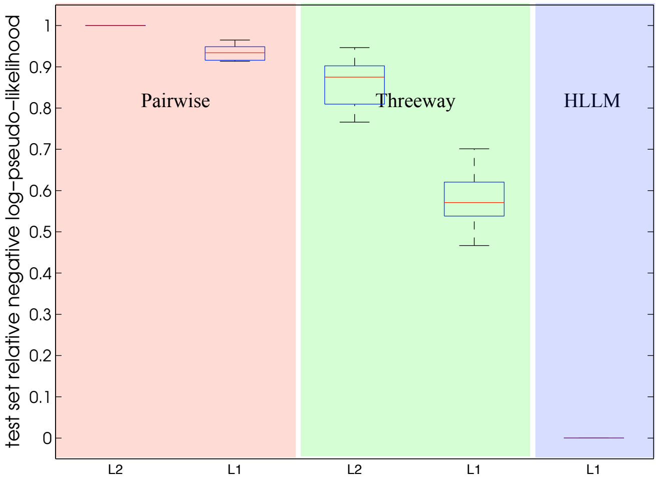

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- But, it assumes computing $f'(x)$ and $\text{prox}_r[x]$ have similar cost.

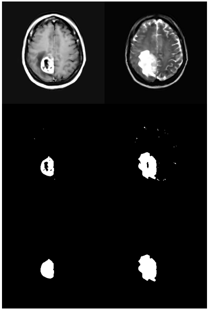
Discussion

- Theoretical justification for what works in practice.
- Significantly extends class of tractable problems.
- Many subsequent applications with inexact proximal operators:
  - Genomic expression, model predictive control, neuroimaging, satellite image fusion, simulating flow fields.

- But, it assumes computing $f'(x)$ and $\text{prox}_r[x]$ have similar cost.
- Often $f'(x)$ is much more expensive:
  - We may have a large dataset.
  - Data-fitting term might be complex.
- Particularly true for structured output prediction:
  - Text, biological sequences, speech, images, matchings, graphs.

Motivation: Automatic Brain Tumor Segmentation

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



- Data-fitting term is solution of 8-million node graph-cut problem.

Outline

1. Structured sparsity (inexact proximal-gradient method)
2. Learning dependencies (costly models with simple constraints)
3. Fitting a huge dataset (stochastic average gradient)

Motivation: Graphical Model Structure Learning

Discovering the dependencies between variables:

car	drive	files	hockey	mac	league	pc	win
0	0	1	0	1	0	1	0
0	0	0	1	0	1	0	1
1	1	0	0	0	0	0	0
0	1	1	0	1	0	0	0
0	0	1	0	0	0	1	1

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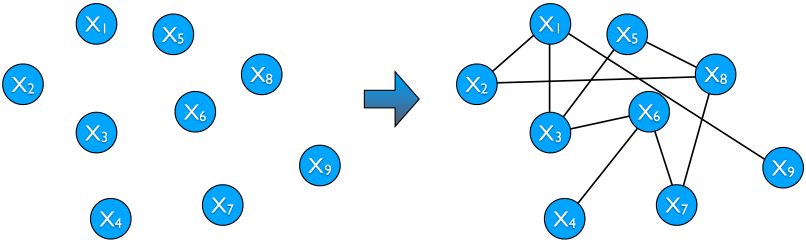
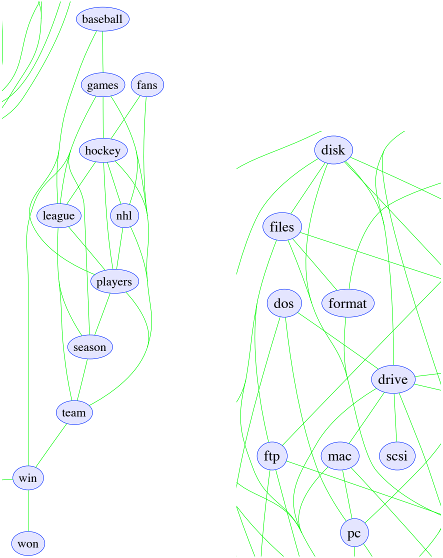
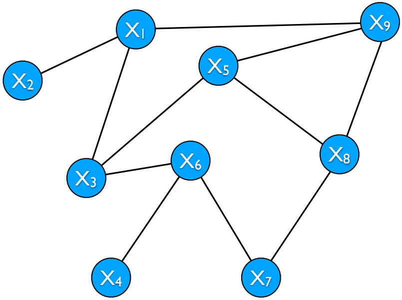


Example: Graphical Model Structure Learning



Structure Learning with ℓ_1-Regularization



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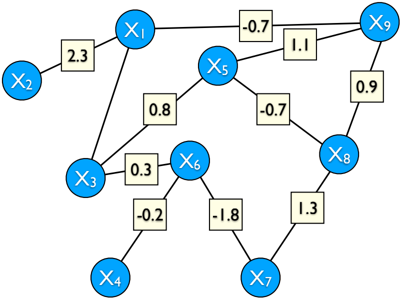

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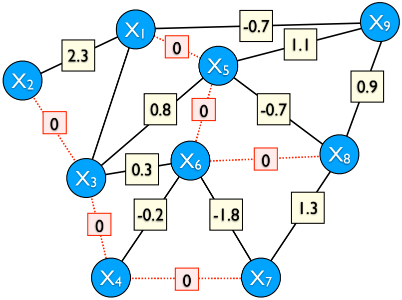

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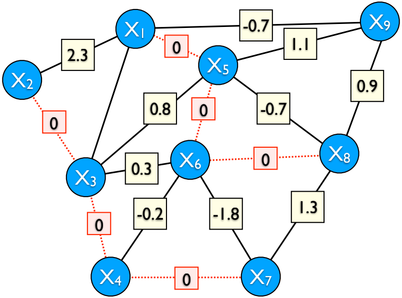
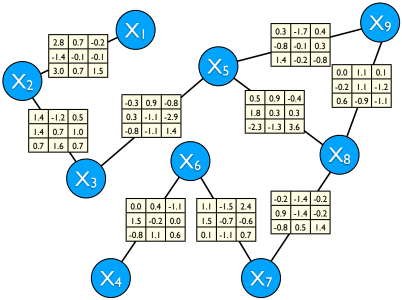


- We want to fit a Markov random field with unknown structure.
- Learn a sparse structure by ℓ_1-regularization of edge weights.

Structure Learning with Group ℓ_1-Regularization



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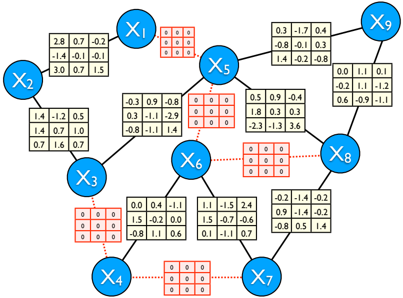

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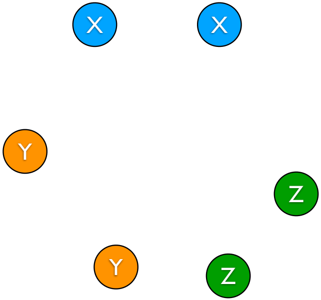

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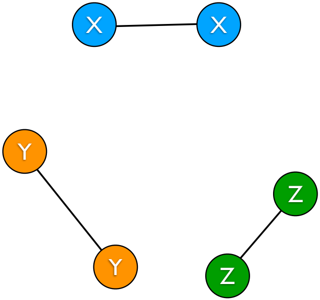

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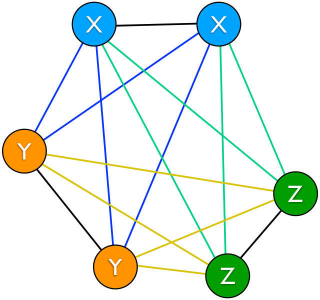

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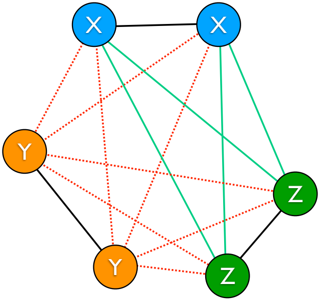

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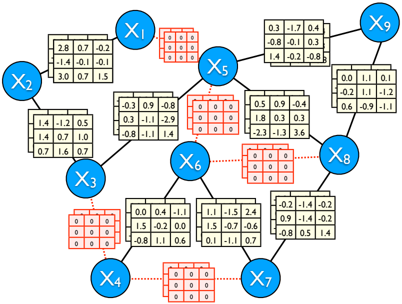

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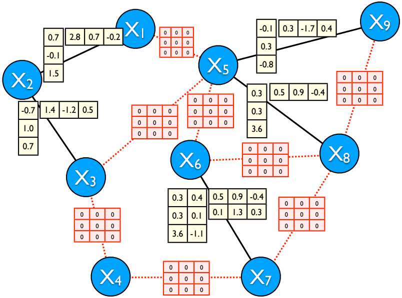

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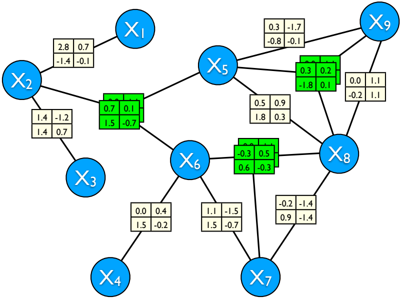

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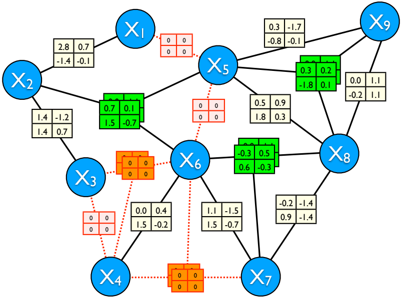

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Costly Data-Fitting Term, Simple Regularizer

- These problems and many others have the form:

$$\min_{x \in \mathbb{R}^P} \quad \frac{1}{N}\sum_{i=1}^{N} f_i(x) \quad + \quad r(x)$$

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- Inspiration from the smooth case:
  - For smooth high-dimensional problems, L-BFGS outperform accelerated/spectral gradient methods.

Quasi-Newton Methods

- Gradient method for optimizing a smooth f:

$$x^+ = x - \alpha f'(x).$$

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- Newton-like methods alternatively use:

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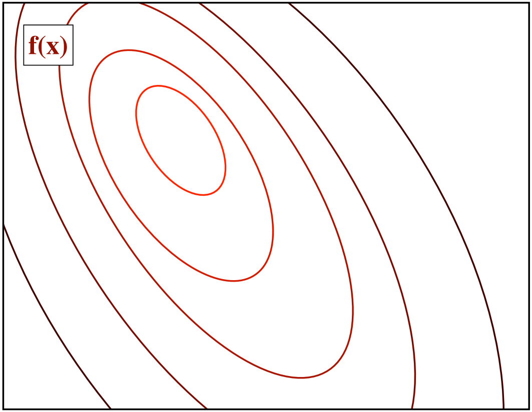
- H approximates the second-derivative matrix.
- L-BFGS is a particular strategy to choose the H values:
  - Based on gradient differences.
  - Linear storage and linear time.

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

Gradient Method and Newton’s Method



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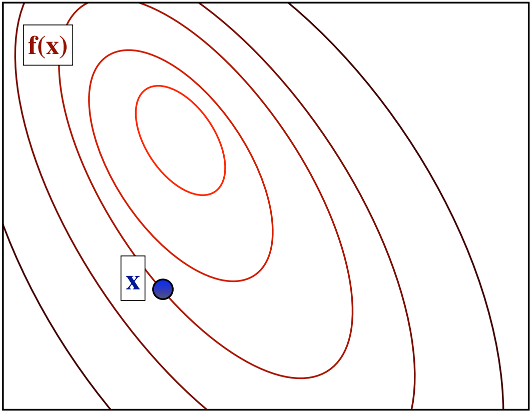

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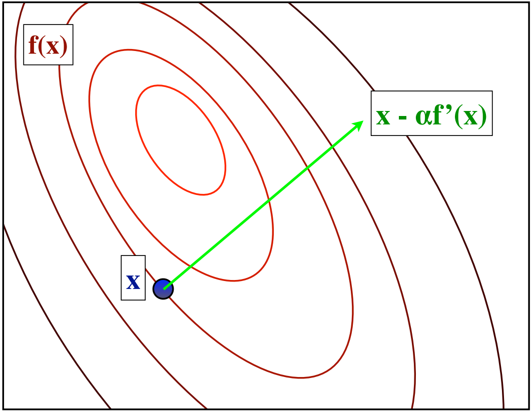

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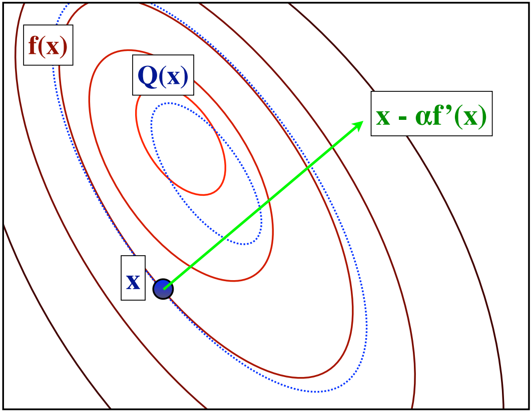

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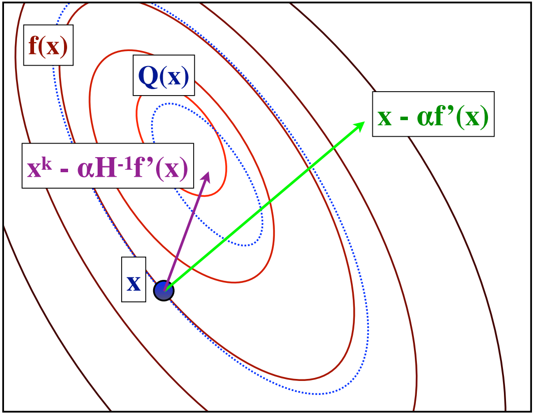

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- Proximal-gradient method:

$$x^+ = \text{prox}_{\alpha r}[x - \alpha f'(x)].$$

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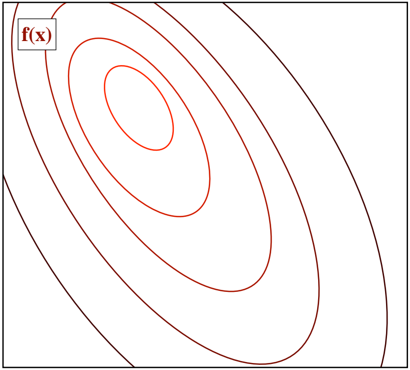

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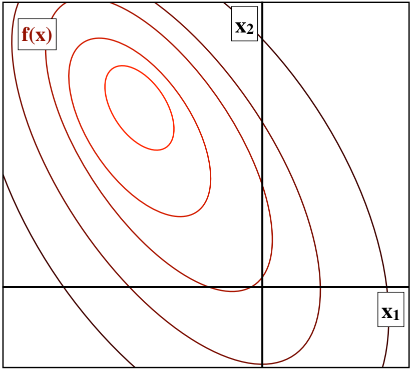

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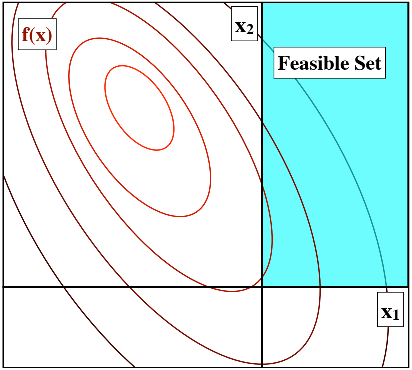

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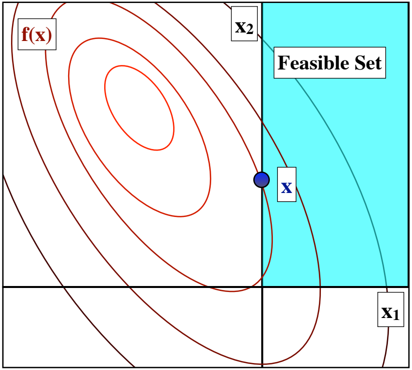

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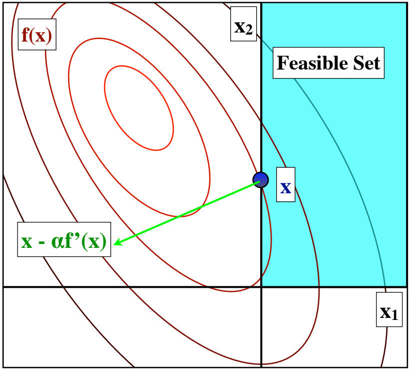

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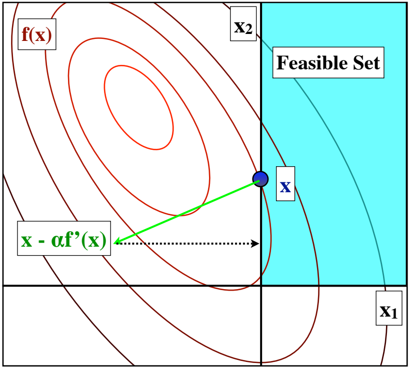

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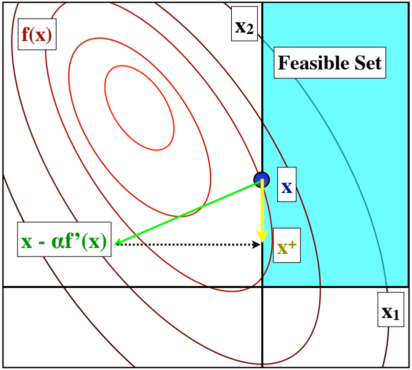

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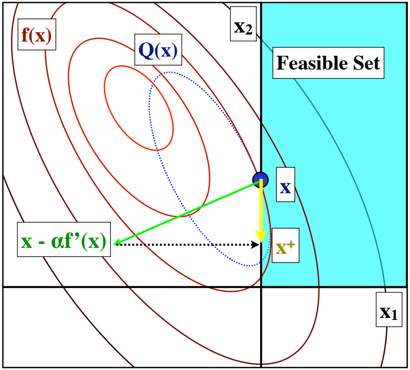

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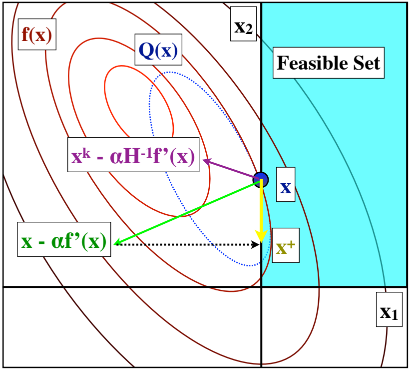

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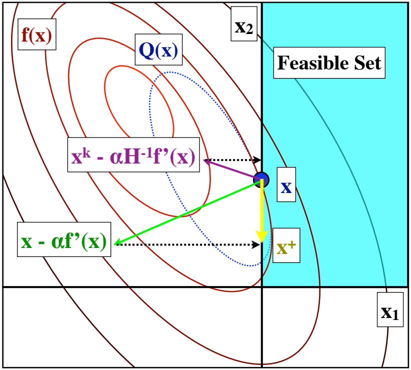

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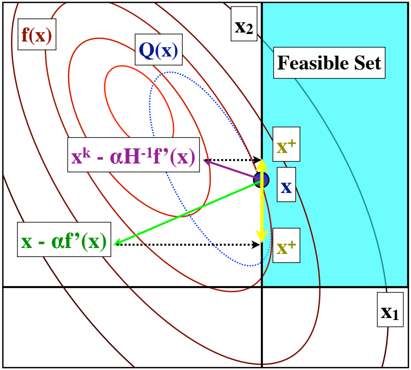


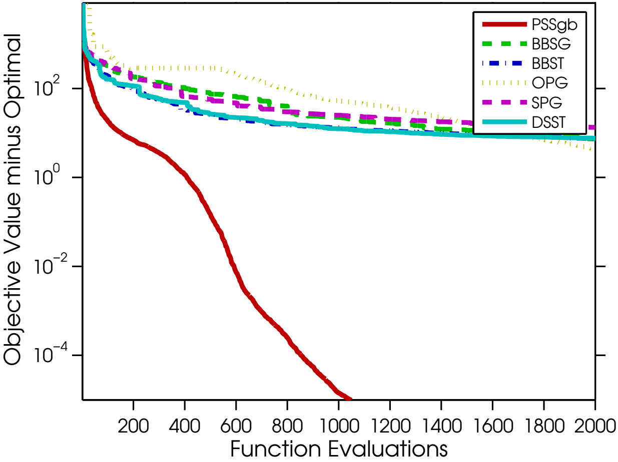
Two-Metric (Sub)Gradient Projection

- In some cases, we can modify H to make this work:
  - Bound constraints.
  - Probability constraints.
  - L1-regularization.
- Two-metric (sub)gradient projection.

  [Gafni & Bertskeas, 1984, Schmidt, 2010].

Comparing to accelerated/spectral/diagonal gradient

Comparing to methods that do not use L-BFGS (sido data):



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

Inexact Proximal-Newton

- The broken proximal-Newton method:

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with the Euclidean proximal operator:

$$\text{prox}_r[y] = \mathop{\arg\min}_{x \in \mathbb{R}^P} \; r(x) + \frac{1}{2}\|x - y\|^2,$$

Inexact Proximal-Newton

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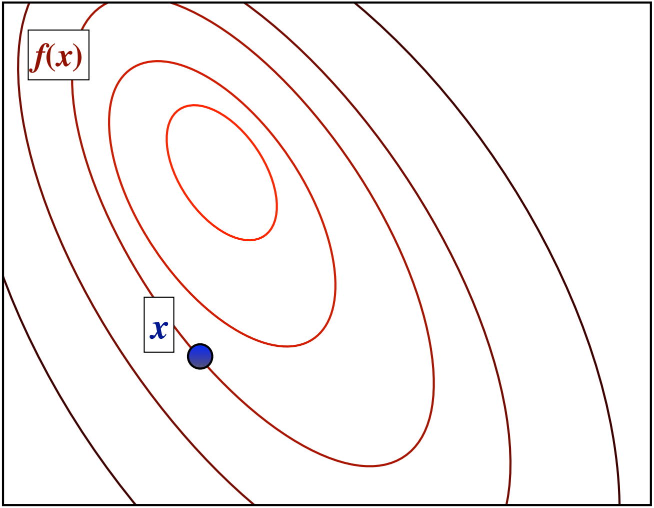
- Non-smooth Newton-like method
- Same convergence properties as smooth case.
- But, the prox is expensive even with a simple regularizer.
- Solution: use a cheap approximate solution.

(e.g., spectral proximal-gradient)

Inexact Projected Newton



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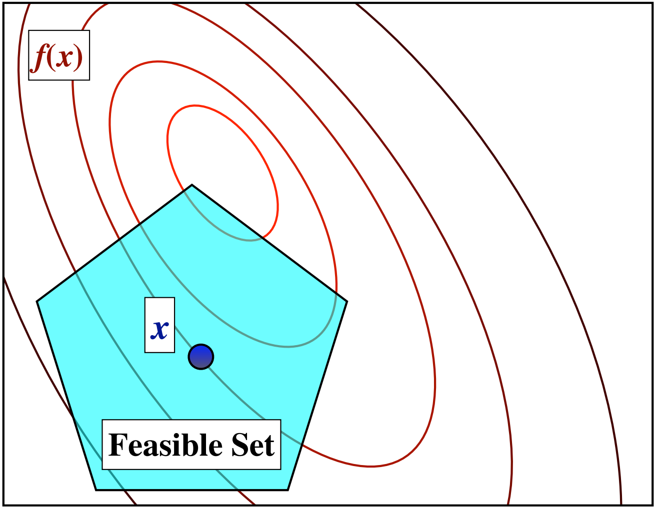

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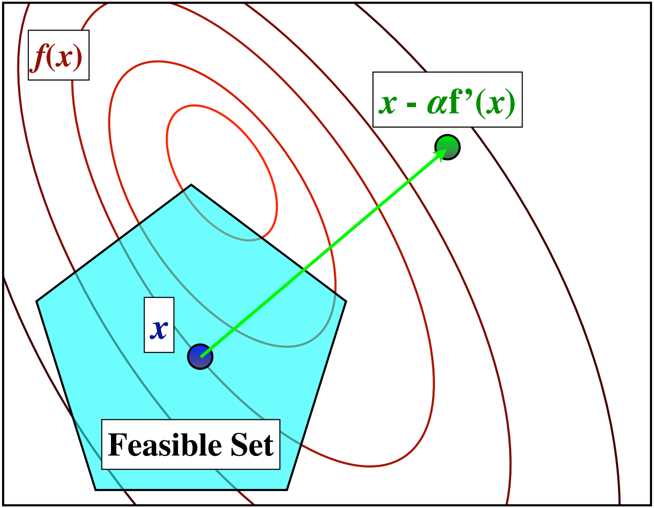

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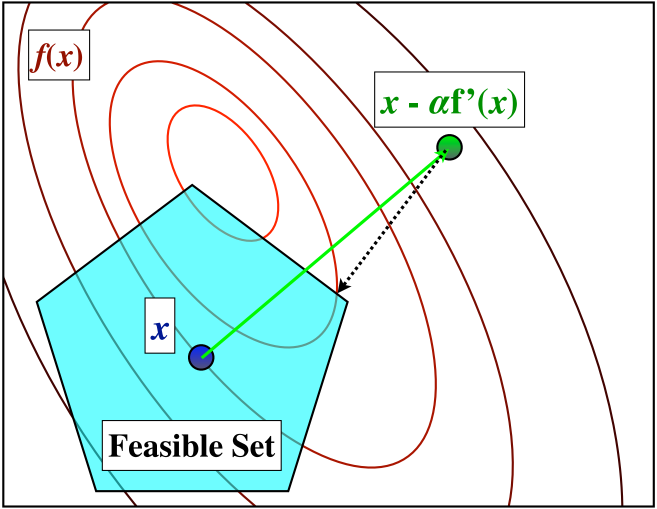

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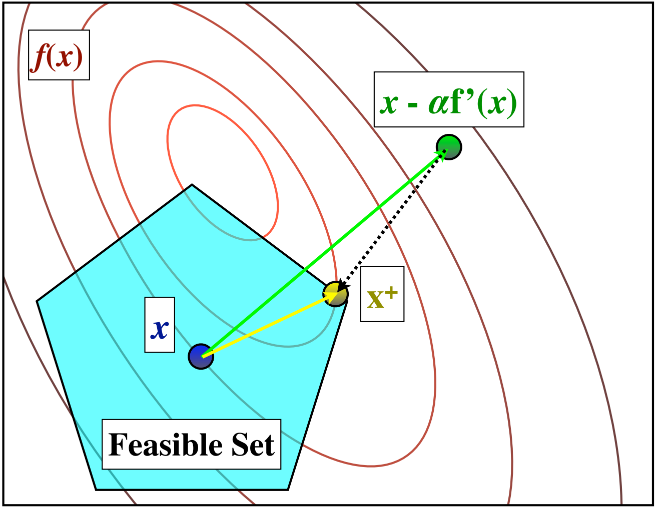

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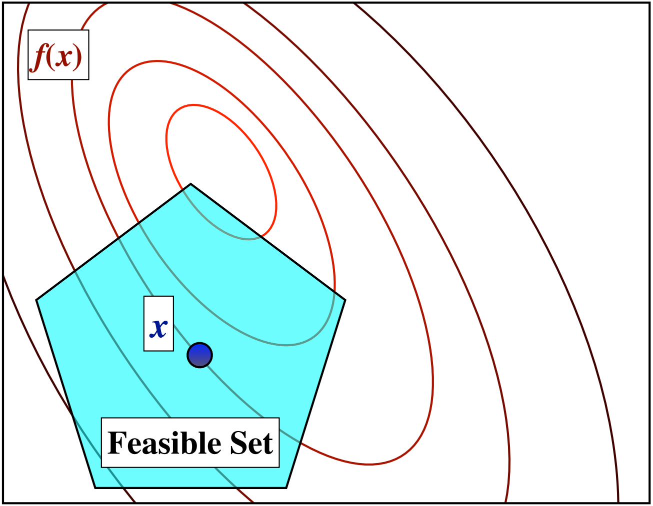

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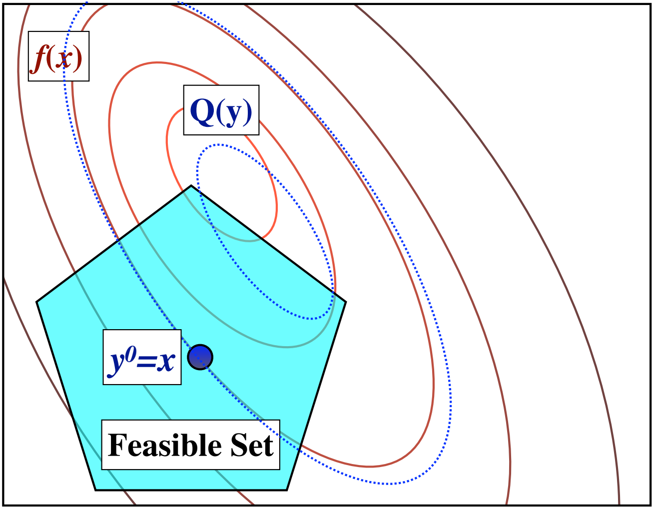

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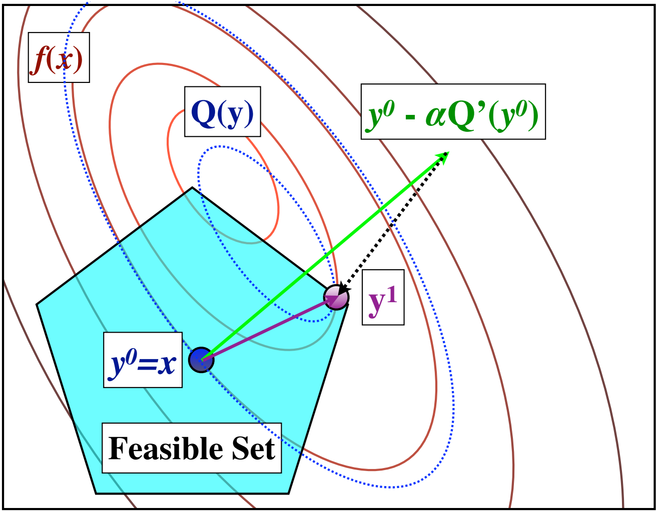

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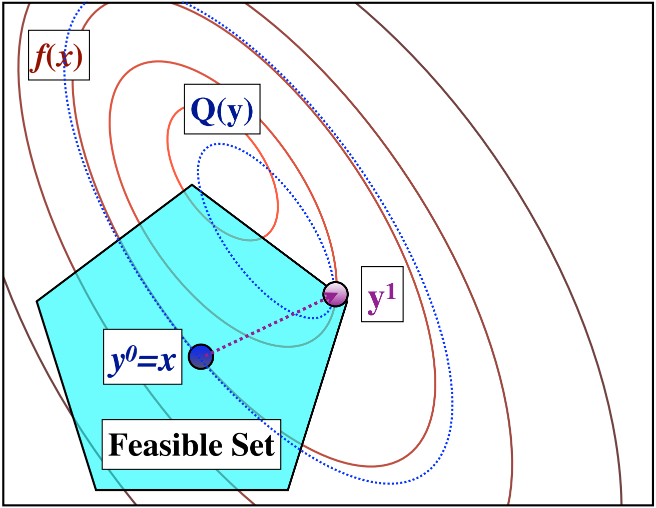

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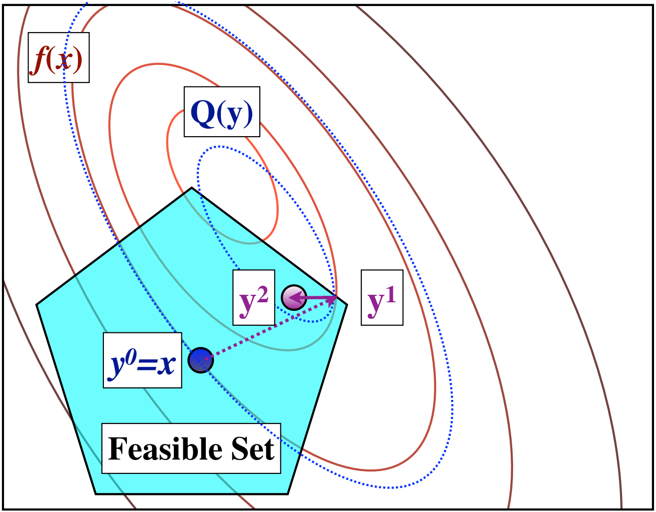

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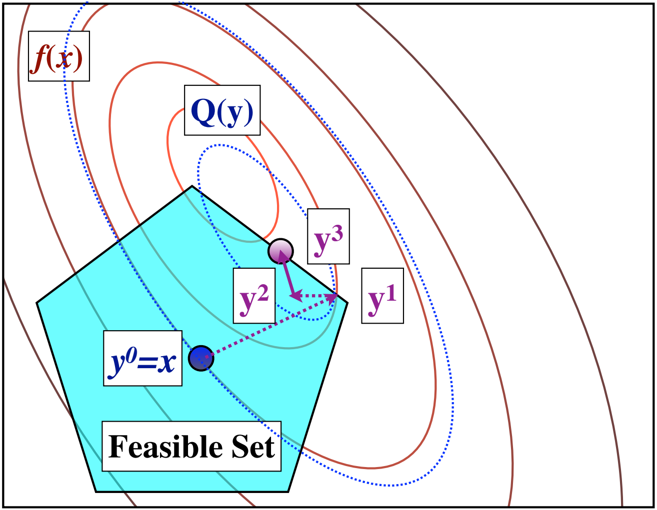

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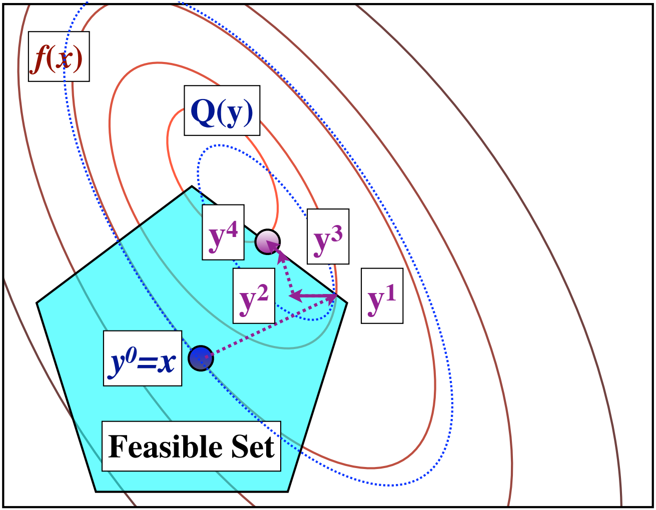

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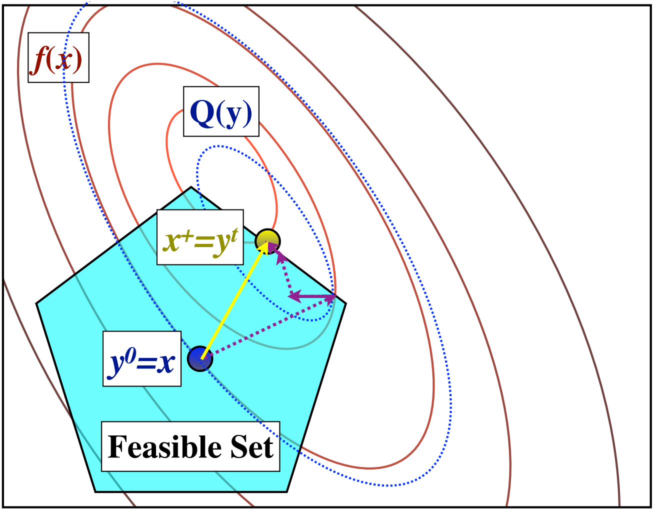

Projected Quasi-Newton (PQN) Algorithm

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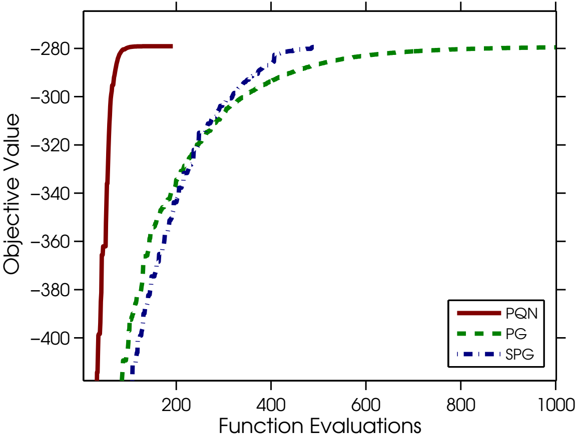
Graphical Model Structure Learning with Groups

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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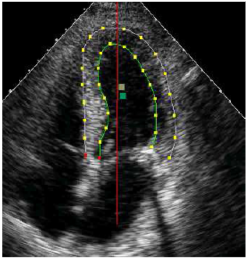
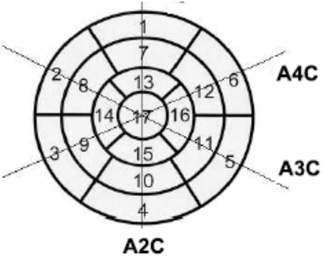
  - Proximal-Newton methods are becoming optimization workhorse, e.g. NIPS 2012:
    - Becker & Fadili, Hsieh et al., Lee et al., Olsen et al., Pacheco & Sudderth.
  - `http://www.di.ens.fr/~mschmidt/Software/PQN.html`

Motivation: Structure Learning in CRFs

- Task: early detection of coronoary heart disease.





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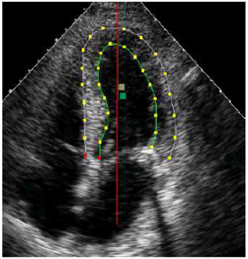
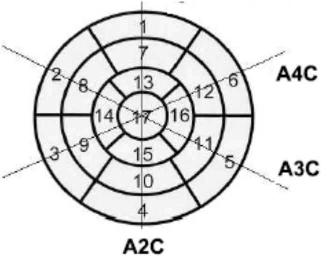
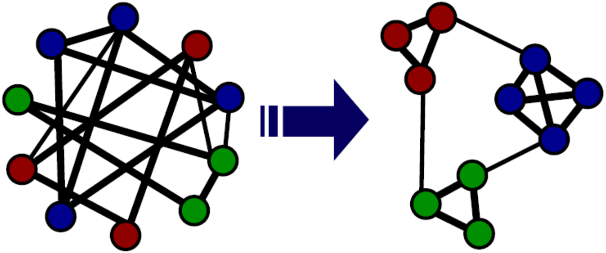




- Assess motion of heart segments using structured prediction.
- Data-fitting function is dynamic program.

Example: Learning Variable Groupings

Discovering variable groupings:



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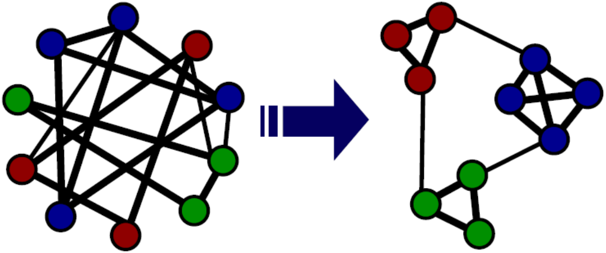

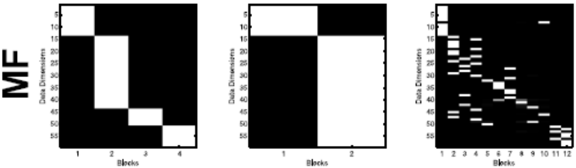

Known GL12 GL1

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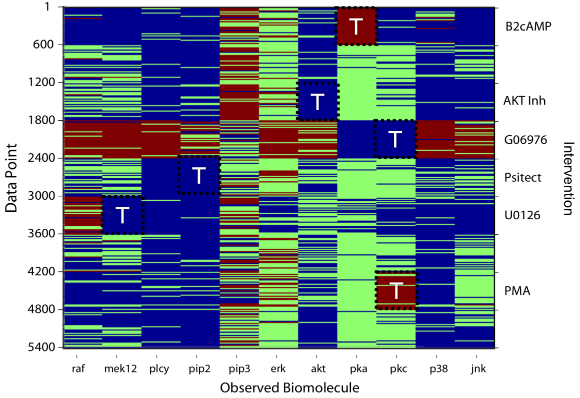
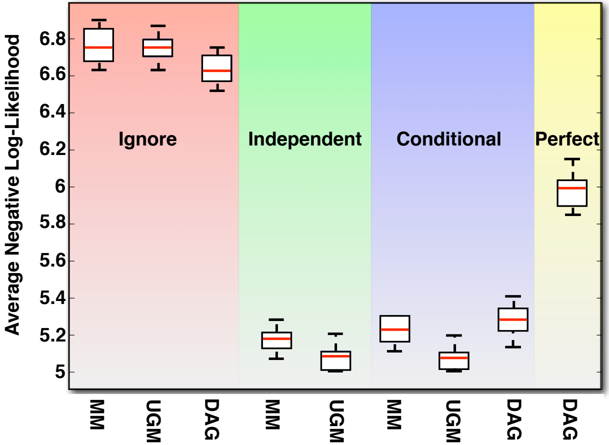


Example: Modeling Interventional Data

Using structured prediction to model interventions:



Outline

1. Structured sparsity (inexact proximal-gradient method)
2. Learning dependencies (costly models with simple constraints)
3. Fitting a huge dataset (stochastic average gradient)

Big-N Problems

- We want to minimize the sum of a finite set of smooth functions:

$$\min_{x \in \mathbb{R}^P} f(x) := \frac{1}{N} \sum_{i=1}^{N} f_i(x).$$

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- Simple example is least-squares,

$$f_i(x) := (a_i^T x - b_i)^2.$$

- Other examples:
  - logistic regression, Huber regression, smooth SVMs, CRFs, etc.

Stochastic vs. Deterministic Gradient Methods

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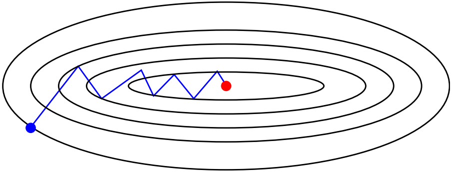

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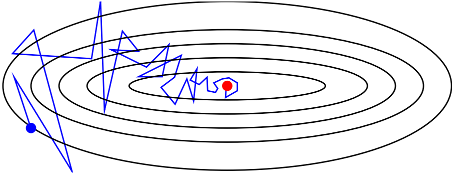

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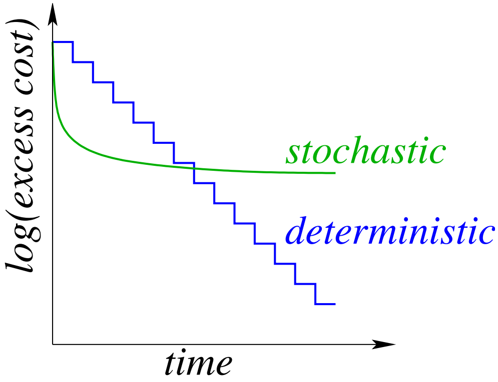

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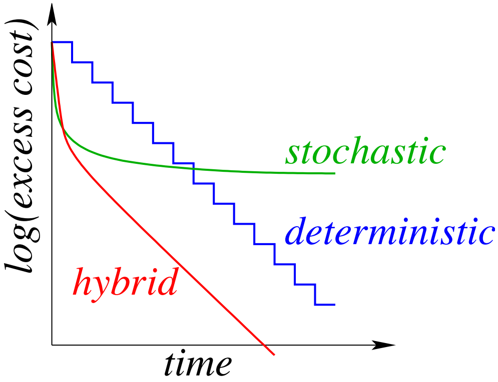

- Goal is requiring $O(\log(1/\epsilon))$ iterations with $O(1)$ cost.

Prior Work on Speeding up SG Methods

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

- **Step-size strategies, momentum, gradient/iterate averaging**
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- **Hybrid methods, incremental average gradient**
  - Bertsekas (1997), Blatt et al. (2007), Friedlander and Schmidt (2012)
  - $O(\log(1/\epsilon))$ iterations but eventually requires full passes.

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  - Assumes gradients of non-selected examples don't change.
  - Assumption becomes accurate as $||x^{t+1} - x^t|| \to 0$.
  - Memory requirements reduced to $O(N)$ for many problems.

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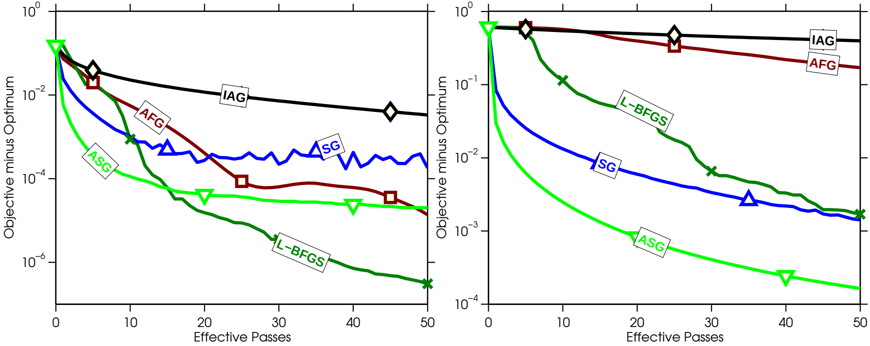
  - SAG: $O(\max\{N, \kappa\}\log(1/\epsilon))$.
- SAG beats two lower bounds:
  - Stochastic gradient bound of $O(1/\epsilon)$.
  - Deterministic gradient bound of $O(N\sqrt{\kappa}\log(1/\epsilon))$ (large N and κ).

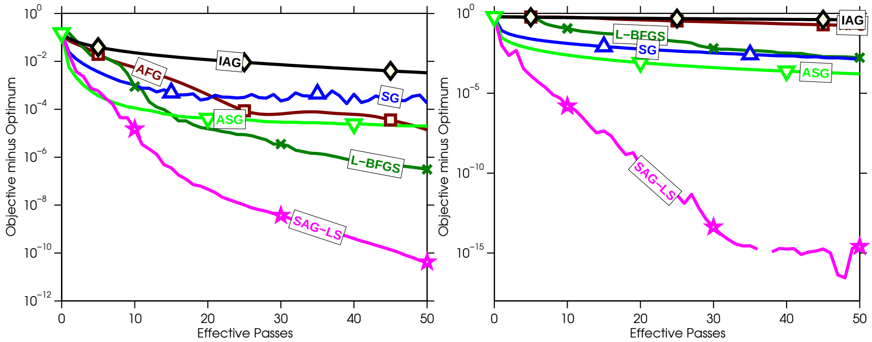
Comparing FG and SG Methods

- 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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- Various extensions:
  - Non-uniform sampling.

    [Schmidt et al., 2013]
  - Non-smooth problems.

    [Mairal, 2013, Wong et al., 2013, Mairal, 2014, Xiao and Zhang, 2014, Defazio et al., 2014]
  - Memory-free methods.

    [Mahdavi et al., 2013, Johnson and Zhang, 2013, Zhang et al., 2013, Konecny and Richtarik, 2013, Xiao and Zhang, 2014]
  - Quasi-Newton methods.

    [Sohl-Dickstein et al., 2014]