Optimizing Costly Functions with Simple Constraints: A Limited-Memory Projected Quasi-Newton Algorithm

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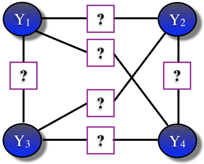
Outline

Motivating Problem: Structure Learning in Discrete MRFs

- We want to fit a Markov random field to discrete data y, but don't know the graph structure



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- Since each edge has multiple parameters, we use group ℓ_1-regularization [Bach et al. 2004, Turlach et al. 2005, Yuan & Lin 2006]:

$$\underset{w}{\text{minimize}} \; -\log p(y|w) \quad \text{subject to} \quad \sum_e ||w_e||_2 \leq \tau$$

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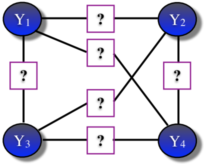

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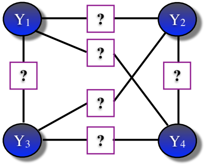

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Optimization Problem Challenges

Solving this optimization problem has 3 complicating factors:

1. the number of parameters is large
2. evaluating the objective is expensive
3. the parameters have constraints

So how should we solve it?

- Interior point methods: the number of parameters is too large
- Projected gradient: evaluating the objective is too expensive
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Extending the L-BFGS Algorithm

Quasi-Newton methods that use L-BFGS updates achieve state of the art performance for unconstrained differentiable optimization [Nocedal 1980, Liu & Nocedal 1989]

L-BFGS updates have also been used for more general problems:

- L-BFGS-B: state of the art performance for bound constrained optimization [Byrd et al. 1995]
- OWL-QN: state of the art performance for ℓ_1-regularized optimization [Andrew & Gao 2007].

The above don't apply since our constraints are not separable

However, the constraints are still simple:

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Our Contribution

This talk presents an extension of L-BFGS that is suitable when:

1. the number of parameters is large
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4. projecting onto the constraints is substantially cheaper than evaluating the objective function

The method uses a two-level strategy

- At the outer level, L-BFGS updates build a constrained local quadratic approximation to the function
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Problem Statement and Assumptions

We address the problem of minimizing a differentiable function $f(x)$ over a convex set $\mathcal{C}$:

$$\underset{x}{\text{minimize}} \quad f(x) \quad \text{subject to} \quad x \in \mathcal{C}$$

We assume you can compute the objective $f(x)$, the gradient $\nabla f(x)$, and the projection $\mathcal{P}_{\mathcal{C}}(x)$:

$$\mathcal{P}_{\mathcal{C}}(x) = \arg\min_{c} \quad \|c - x\|_2 \quad \text{subject to} \quad c \in \mathcal{C}.$$

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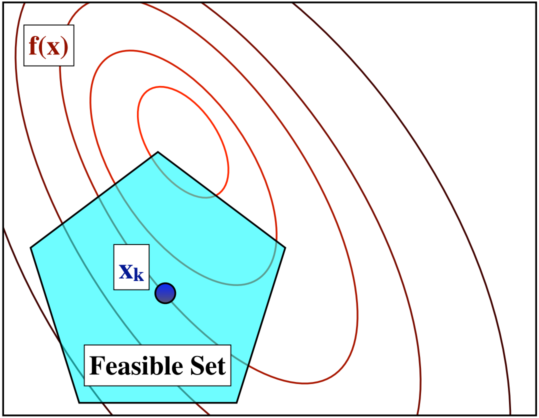
PG: move towards the projection of the negative gradient



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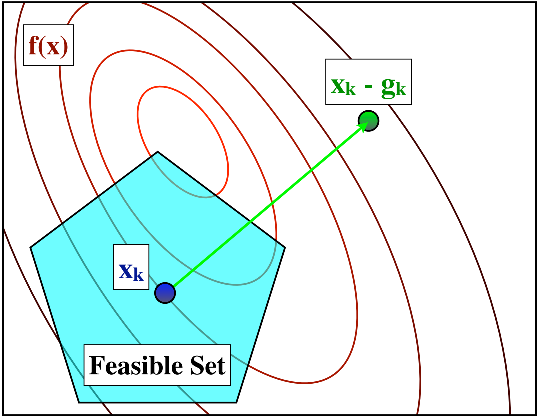

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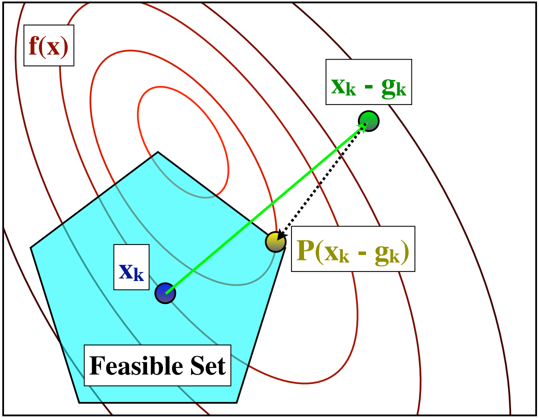

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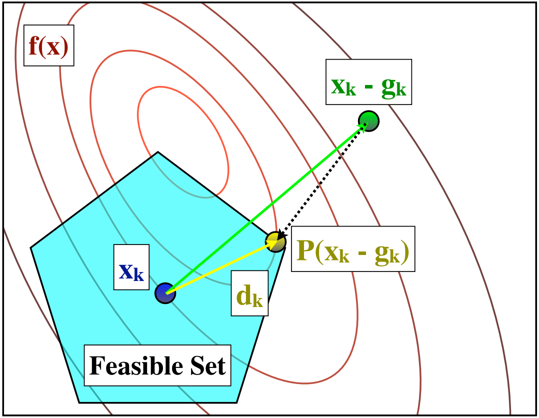

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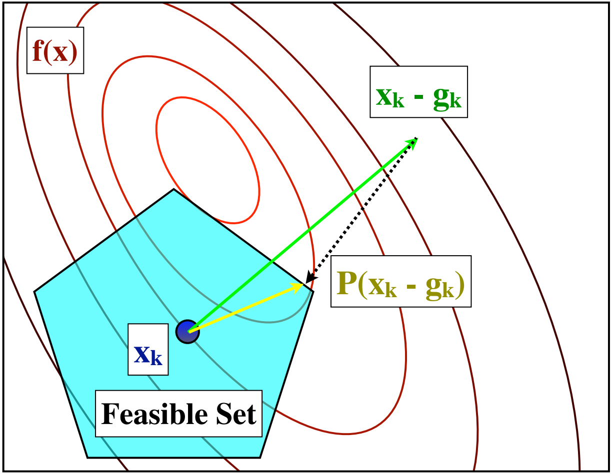

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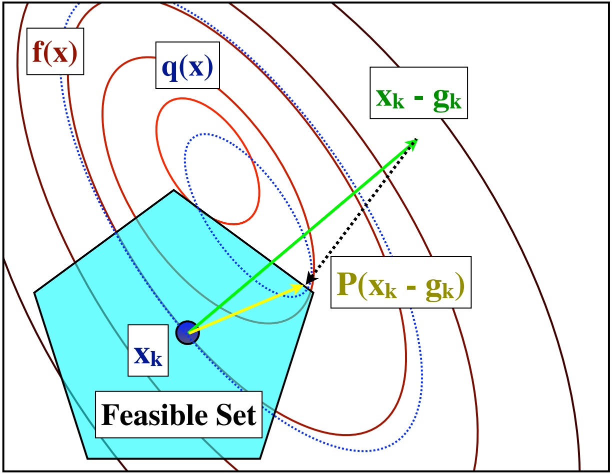

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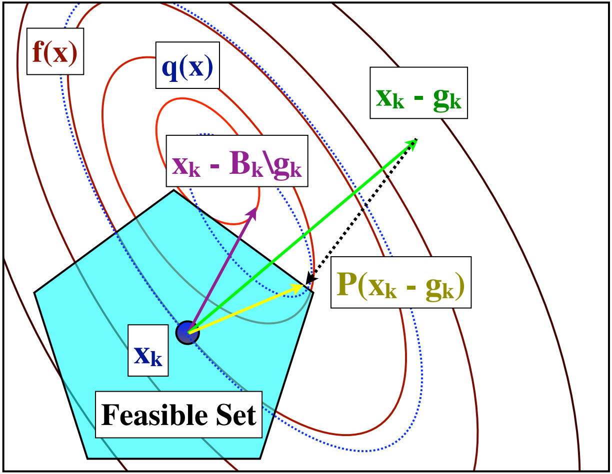

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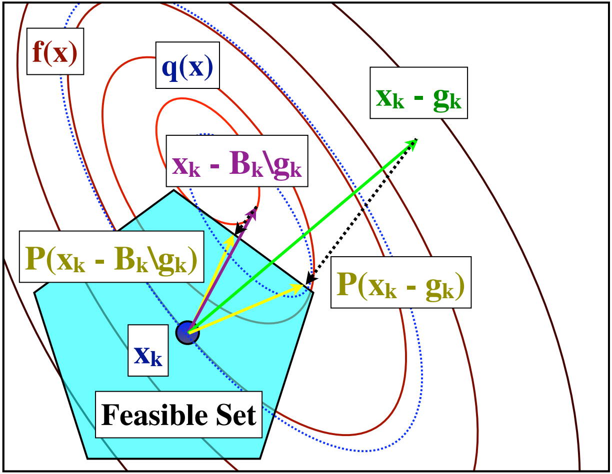

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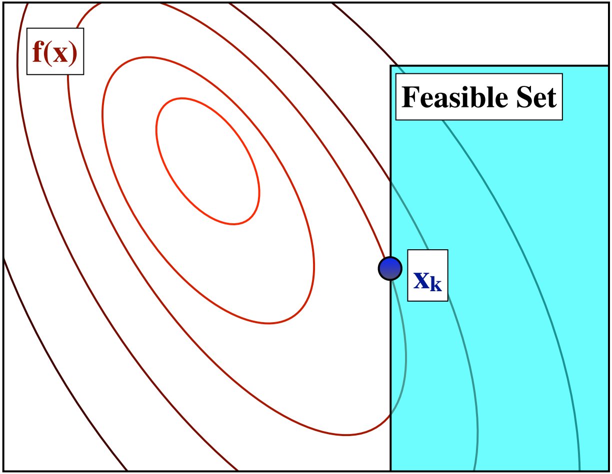

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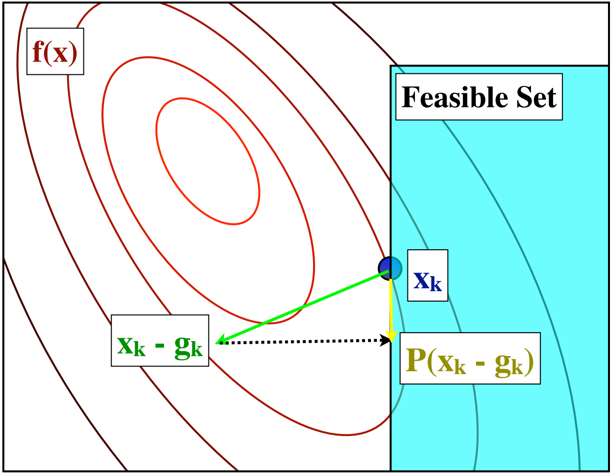

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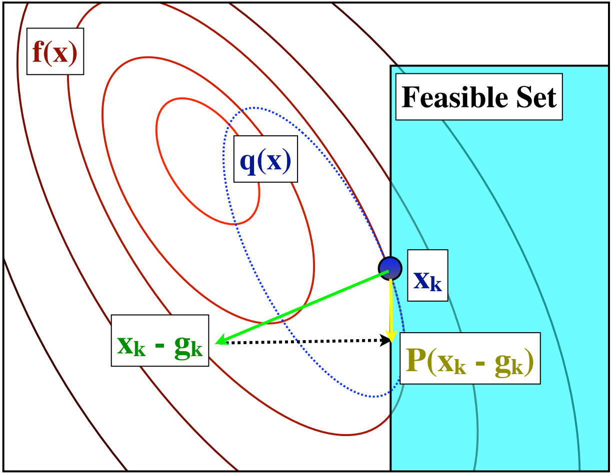

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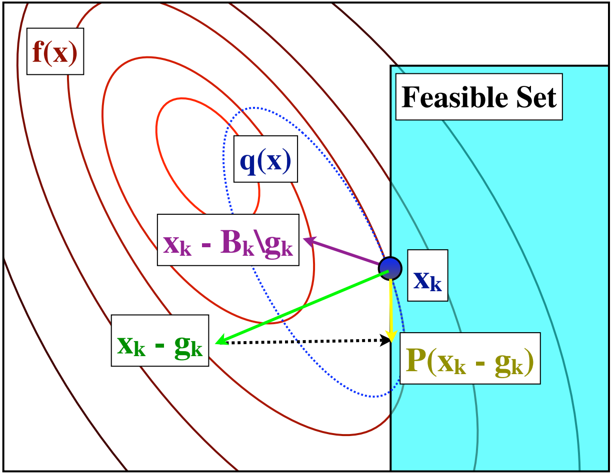

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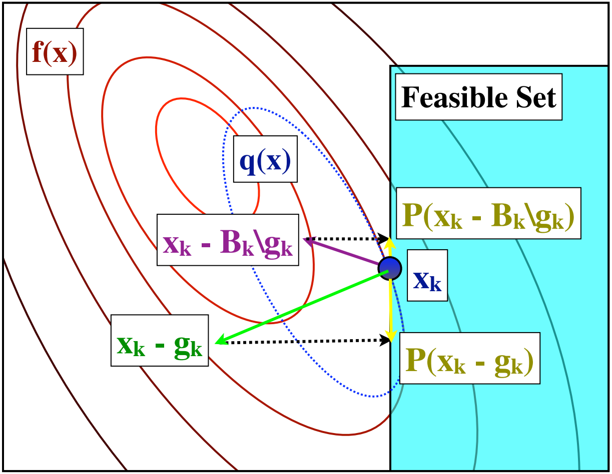

Correct Projected Newton Algorithm

- In projected Newton methods, we form a quadratic approximation to the function around x_k:

$$q_k(x) \triangleq f_k + (x - x_k)^T \nabla f(x_k) + \frac{1}{2}(x - x_k)^T B_k (x - x_k)$$

- At each iteration, we minimize this function over the set:

$$\underset{x}{\text{minimize}} \quad q_k(x) \quad \text{subject to} \quad x \in \mathcal{C}$$

- NOT the same as projecting the unconstrained Newton step
- This generates a feasible descent direction $d_k \triangleq x - x_k$
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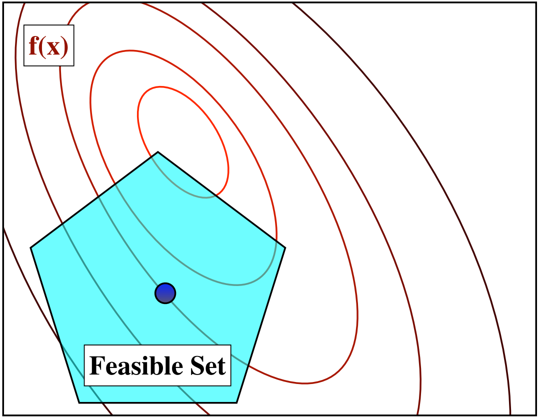

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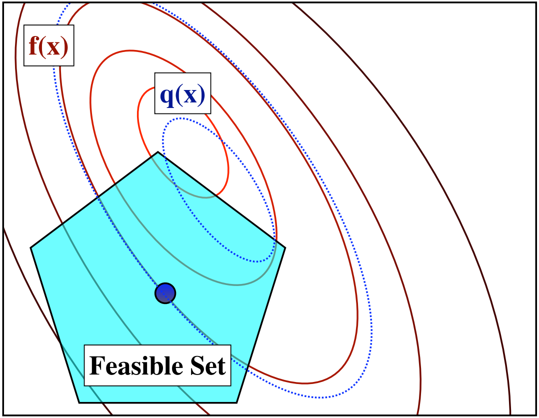

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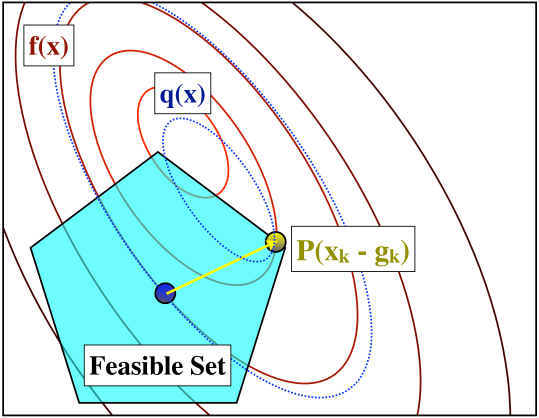

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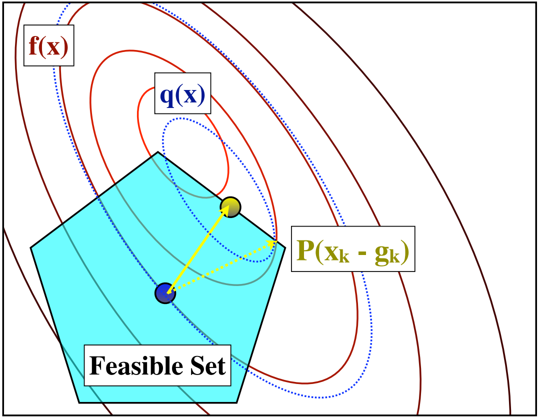

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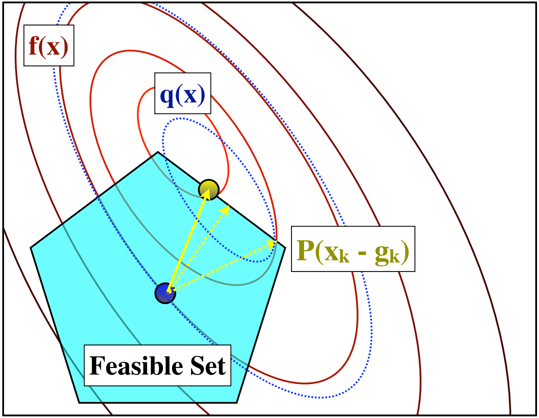

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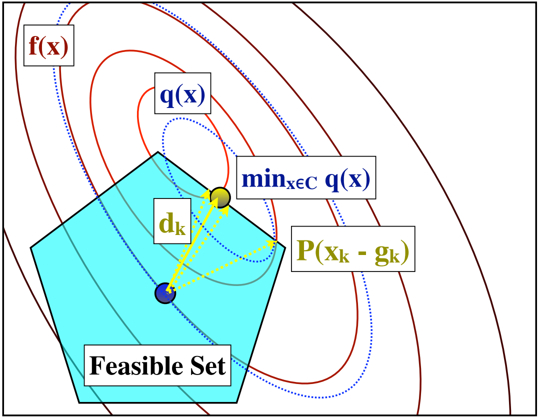

Problems with the Projected Newton Algorithm

Unfortunately, the projected Newton method can be inefficient:

- Computing d_k may be very expensive
- Using a general n-by-n matrix B_k is impratical

Our algorithm is a projected quasi-Newton algorithm where:

- L-BFGS updates construct a diagonal plus low-rank B_k
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Broyden-Fletcher-Goldfarb-Shanno (BFGS) Updates

Quasi-Newton methods work with parameter and gradient differences between iterations:

$$s_k \triangleq x_{k+1} - x_k \quad \text{and} \quad y_k \triangleq g_{k+1} - g_k$$

They start with an initial approximation $B_0 \triangleq \sigma I$, and choose B_{k+1} to interpolate the gradient difference:

$$B_{k+1} s_k = y_k$$

Since B_{k+1} is not unique, the BFGS method chooses the matrix whose difference with B_k minimizes a weighted Frobenius norm:

$$B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{y_k^T s_k}$$

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L-BFGS: Limited-Memory BFGS

Instead of storing B_k, the limited-memory BFGS (L-BFGS) method just stores the previous m differences s_k and y_k.
[Nocedal 1980, Liu & Nocedal 1989]

These updates applied to $B_0 = \sigma_k I$ can be written compactly in a diagonal plus low-rank form [Byrd et al. 1994]:

$$B_m = \sigma_k I - NM^{-1}N^T$$

This representations makes multiplication with B_k cost $\mathcal{O}(mn)$.

SPG: Spectral Projected Gradient

Recall the projected quasi-Newton sub-problem:

$$\underset{x}{\text{minimize}} \quad f_k + (x - x_k)^T \nabla f(x_k) + \frac{1}{2}(x - x_k)^T B_k (x - x_k)$$
$$\text{subject to } x \in \mathcal{C}$$

With the L-BFGS representation of B_k, we can compute the objective function and gradient in $\mathcal{O}(mn)$.

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SPG: Spectral Projected Gradient

The classic projected gradient takes steps of the form

$$x_{k+1} = \mathcal{P}_{\mathcal{C}}(x_k - \alpha g_k)$$

SPG has two enhancements [Birgin et al. 2000]:

- It uses the Barzilai and Borwein [1988] 'spectral' step length:

$$\alpha_{bb} = \frac{\langle y_{k-1}, y_{k-1}\rangle}{\langle s_{k-1}, y_{k-1}\rangle}$$

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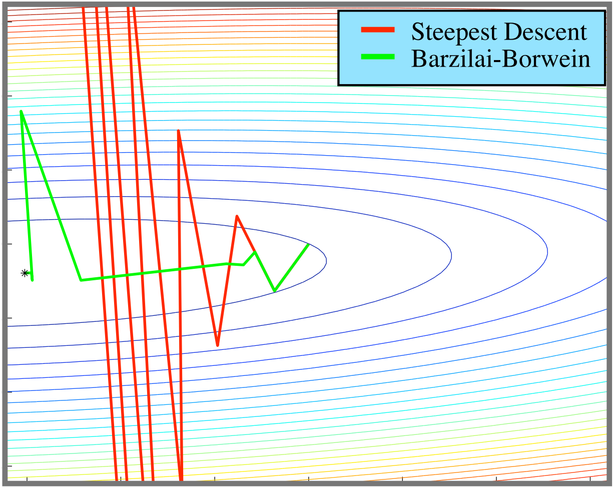
Barzilai & Borwein Step Size



SPG: Spectral Projected Gradient

- There is growing interest in SPG for constrained optimization [Dai & Fletcher 2005, van den Berg & Friedlander 2008]

- We apply SPG to minimize the strictly convex constrained quadratic approximations
- Friedlander et al. [1999] show that SPG has a superlinear convergence rate for minimizing strictly convex quadratics

- Instead of 'solving' the sub-problem, we could just perform k iterations of SPG to improve the steepest descent direction.
- In this case, solving the sub-problems is in $\mathcal{O}(mnk)$, plus the cost of computing the projection k times.

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- Instead of 'solving' the sub-problem, we could just perform k iterations of SPG to improve the steepest descent direction.
- In this case, solving the sub-problems is in $\mathcal{O}(mnk)$, plus the cost of computing the projection k times.

Outline of the Method

The projected quasi-Newton (PQN) method:

1. Evaluate the current objective function and gradient
2. Add/remove difference vectors for L-BFGS
3. Run SPG to compute the projected quasi-Newton direction d_k
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Outline

Projection onto Norm-Balls

We are interested in projecting onto balls induced by norms:

$$\mathcal{C} \equiv \{x \mid \|x\| \leq \tau\}$$

This projection can be computed in linear-time for many ℓ_p-norms, such as the ℓ_2-, ℓ_∞-, and ℓ_1-norms [Duchi et al. 2008]

We are also interested in the case of the mixed p, q-norm balls that arise in group variable selection:

$$\|x\|_{p,q} = \left(\sum_i \|x_{\sigma_i}\|_q^p\right)^{1/p}$$

The group-lasso is the special case where $p = 1$, $q = 2$:

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Projection onto Mixed Norm-Balls

The following proposition leads to an expected linear-time randomized algorithm for group-lasso projection:

Proposition

Consider $c \in \mathbb{R}^n$ and a set of g disjoint groups $\{\sigma_i\}_{i=1}^g$ such that $\cup_i \sigma_i = \{1, \ldots, n\}$. Then the Euclidean projection $\mathcal{P}_{\mathcal{C}}(c)$ onto the $\ell_{1,2}$-norm ball of radius τ is given by

$$x_{\sigma_i} = \operatorname{sgn}(c_{\sigma_i}) \cdot w_i, \qquad i = 1, \ldots, g,$$

where $w = \mathcal{P}(v)$ is the projection of vector v onto the ℓ_1-norm ball of radius τ, with $v_i = \|c_{\sigma_i}\|_2$.

Outline

Experiments

We performed several experiments to test the new method:

- We first compared to other extensions of L-BFGS [see paper]
- We then compared to state of the art methods for graph structure learning

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Gaussian Graphical Model Structure Learning

We looked at training a Gaussian graphical model with an ℓ_1 penalty on the precision matrix elements to induce a sparse structure [Banerjee et al. 2006, Friedman et al. 2007]:

$$\underset{K \succ 0}{\text{minimize}} \quad -\log\det(K) + \mathrm{tr}(\hat{\Sigma}K) + \lambda\|K\|_1,$$

We used the Gasch et al. [2000] data with the pre-processing of Duchi et al. [2008], and as with previous work we solve the dual problem:

$$\begin{array}{ll} \underset{W}{\text{maximize}} & \log\det(\hat{\Sigma} + W) \\ \text{subject to} & \hat{\Sigma} + W \succ 0,\ \|W\|_\infty \leq \lambda \end{array}$$

We compared to a projected gradient method [Duchi et al. 2008].

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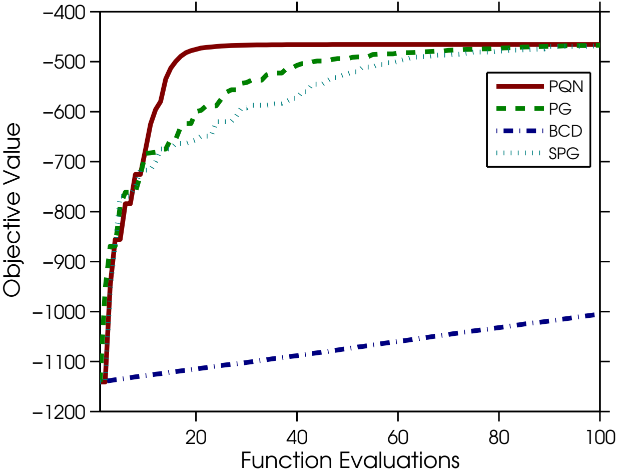

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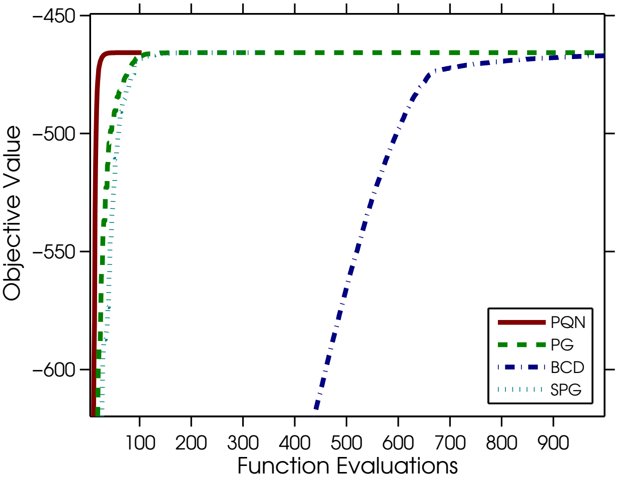

Gaussian Graphical Model Structure Learning with Groups

We also compared the methods when we induce a group-sparse precision matrix using the $\ell_{1,\infty}$-norm [Duchi et al. 2008]:

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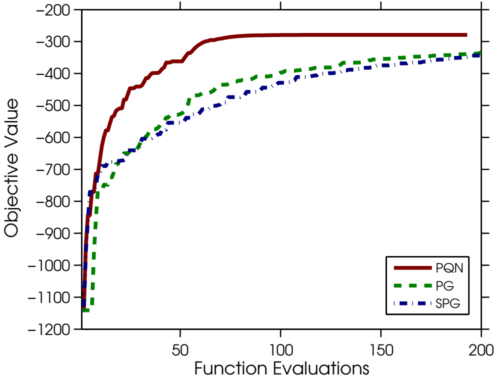

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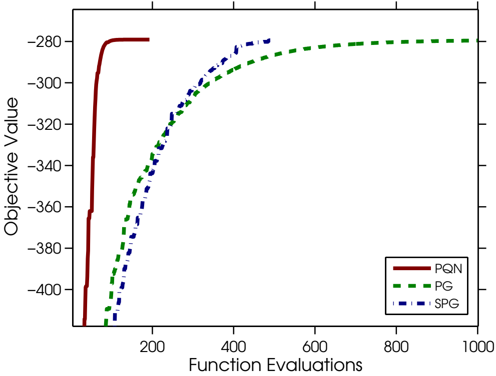

Gaussian Graphical Model Structure Learning with Groups

We also used PQN to look at the performance if we replace the $\ell_{1,\infty}$-norm [Duchi et al. 2008] with the $\ell_{1,2}$-norm:

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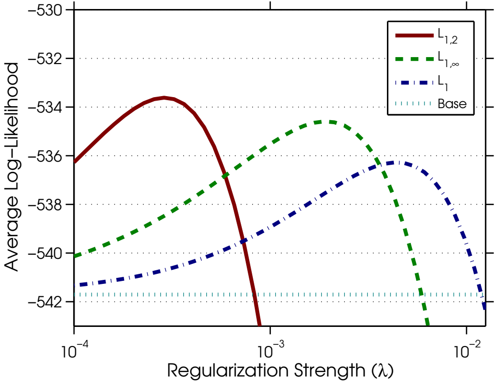

Markov Random Field Structure Learning

Finally, we looked at learning a sparse Markov random field:

$$\underset{w}{\text{minimize}} \; -\log p(y|w) \quad \text{subject to} \quad \sum_e ||w_e||_2 \leq \tau$$

We used the trinary data from [Sachs et al. 2005], and compared to Grafting [Lee et al. 2006] and applying SPG to a second-order cone reformulation [Schmidt et al. 2008].

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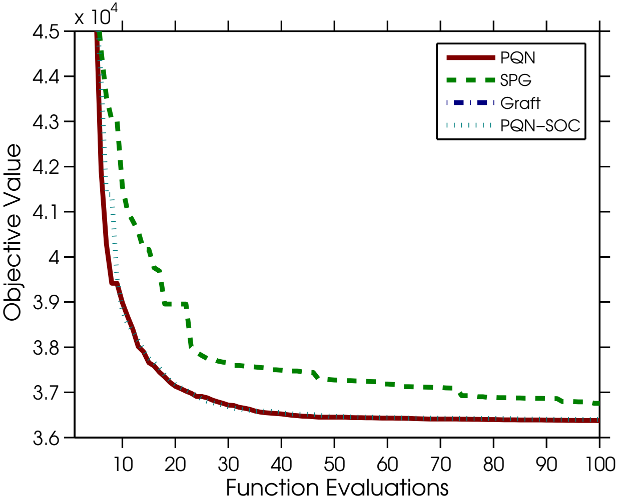

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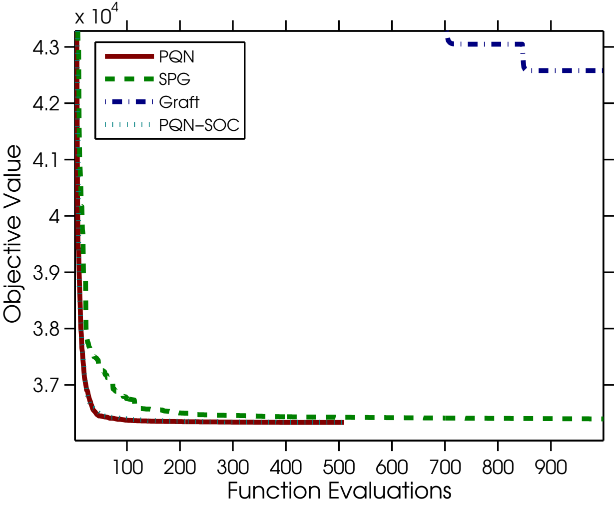

Extensions to Other Problems

There are many other cases where we can efficiently compute projections:

- Projection onto bounds, hyper-planes, or half-spaces is trivial
- Projecting onto the probability simplex can be done in $\mathcal{O}(n \log n)$
- Projecting onto the positive semi-definite cone involves truncating the spectral decomposition
- Projecting onto second-order cones of the form $\|x\|_2 \leq y$ can be done in $\mathcal{O}(n)$
- Dykstra's algorithm can be used for combinations of simple constraints [Dykstra, 1983]

A similar method can also be used for objectives with a 'simple' non-differentiable component.

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A similar method can also be used for objectives with a 'simple' non-differentiable component.

Summary

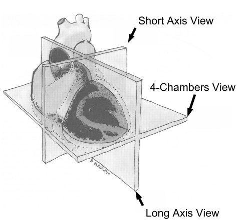
PQN is an extension of L-BFGS that is suitable when:

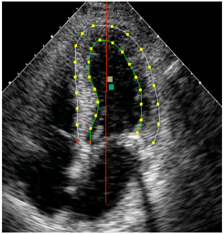
1. the number of parameters is large
2. evaluating the objective is expensive
3. the parameters have constraints
4. projecting onto the constraints is substantially cheaper than evaluating the objective function

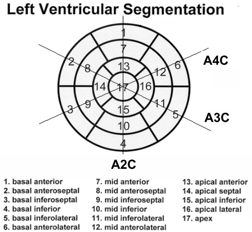
We have found the algorithm useful for a variety of problems, and it is likely useful for others (code online)

Outline

Structure Learning in Conditional Random Fields for Heart Motion Abnormality Detection



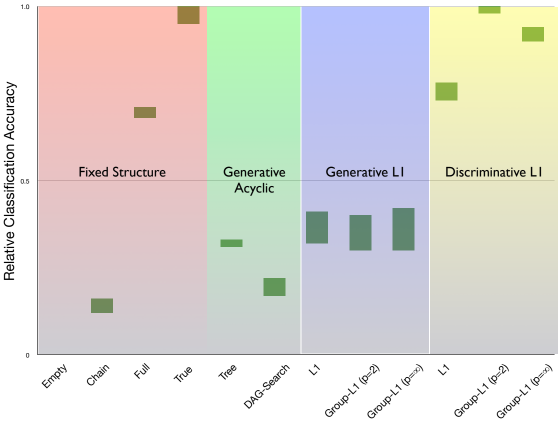




- We built a classifier that detects coronary heart disease from the motion of 16 left ventricle segments in ultrasound video.
- We use group ℓ_1-regularization to simultaneously learn the parameters and structure of a conditional random field.

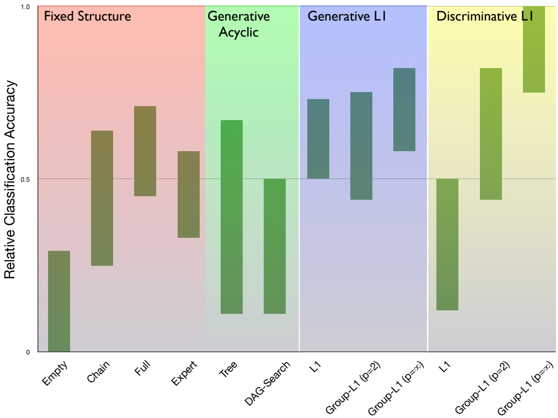
Structure Learning in Conditional Random Fields for Heart Motion Abnormality Detection

Synthetic CRF data [Schmidt, Murphy, Fung, Rosales. CVPR '08].



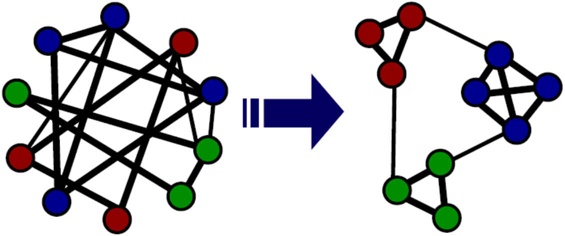
Structure Learning in Conditional Random Fields for Heart Motion Abnormality Detection

Heart data [Schmidt, Murphy, Fung, Rosales. CVPR '08]



Group Sparse Priors for Covariance Estimation

Earlier we discussed learning learning group-sparse GGMs



What if the correlations between groups aren't completely sparse?

What if we don't know the variable groups?

We give bounds on integrals of priors over the positive-definite cone, and use them in a variational methods that learns the groups [Marlin, Schmidt, Murphy, UAI '09]

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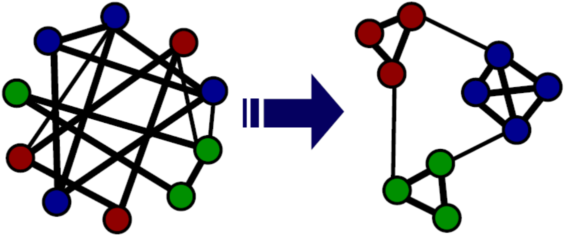

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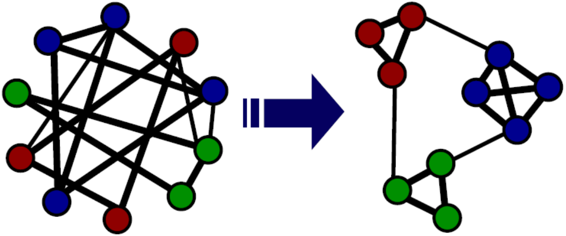

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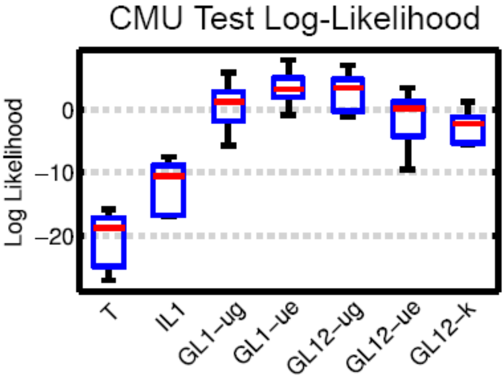
Group Sparse Priors for Covariance Estimation

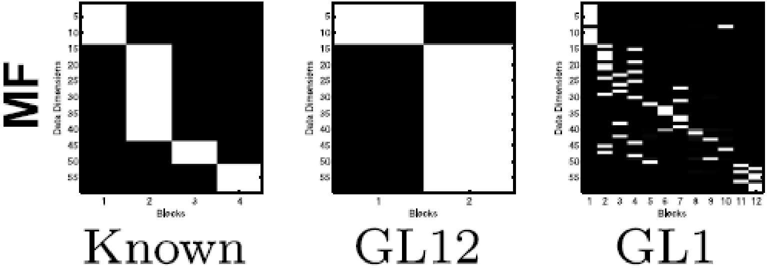
Results on data from the CMU motion capture library:



Learning a set of groups does better than knowing the groups.

Group Sparse Priors for Covariance Estimation

Mutual fund data [Scott and Carvalho, 2008]:



The methods discover the 'stocks' and 'bonds' groups.

Optimization Methods for ℓ_1-Regularization

There are a large number of optimizers for ℓ_1-regularization:

- Coordinate descent
- Active set methods
- Orthant-wise methods
- Smoothing
- Bound optimization (EM)
- Interior point methods
- Projection methods
- Many others...

In [Schmidt, Fung, Rosales, TR '09], we discuss these methods' advantages/disadvantages, and compare them experimentally.

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Increased Discrimination in Level Set Methods with Embedded Conditional Random Fields

Conditional random fields (CRFs):

- **discriminative model, models neighbor's correlation**
- **feature-based edge regularization**
- Markov assumption on labels

Level set methods:

- generative model, assumes neighbor independence
- image-based regularization
- **allows non-Markov priors**

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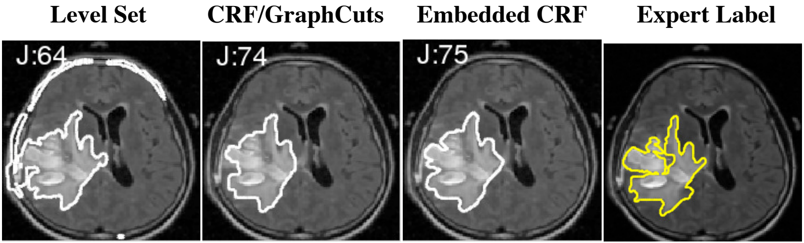
Experiments on brain tumor segmentation in multi-modal MRI
[Cobzas and Schmidt, CVPR '09]



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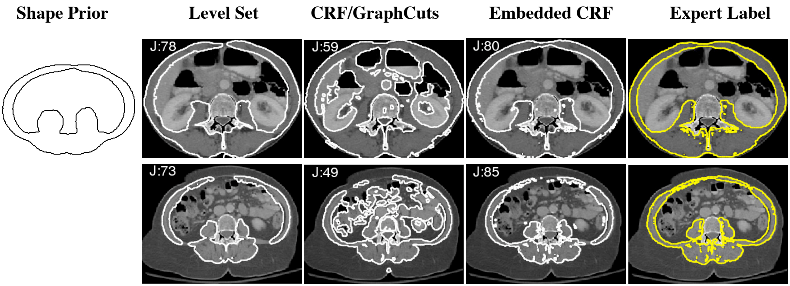
Experiments on CT muscle segmentation with a shape prior [Cobzas and Schmidt, CVPR '09]



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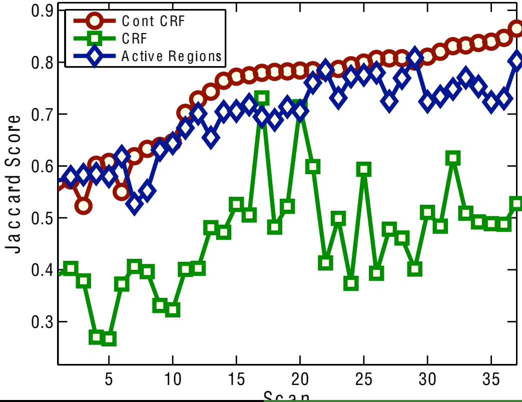

Modeling Discrete Interventional Data using Directed Cyclic Graphical Models

The difference between conditioning by observation and conditioning by intervention in the 'hungry at work' problem:

- If I see that my watch says 11:55, then it's almost lunch time
- If I set my watch so it says 11:55, it doesn't help

So how should we model interventional data?

- DAGs can model interventions, but don't allow cycles
- UGs allow cycles, but can't model interventions

We define a model that allows cycles and can model interventions. [Schmidt and Murphy, UAI '09]

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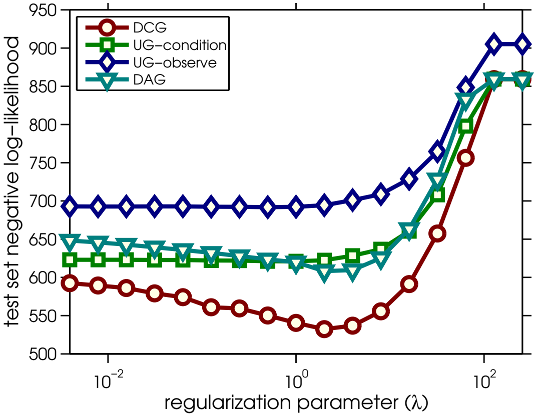
Synthetic Directed Cyclic Interventional Data



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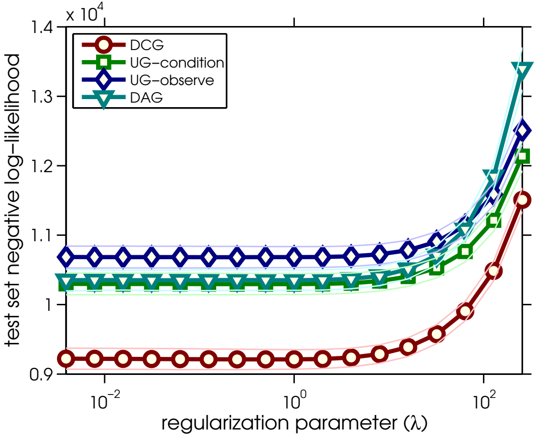
Interventional Cell Signaling Data [Sachs et al., 2005]



Causal Learning without DAGs

Causal learning methods are usually evaluated in terms of a ‘true’ underlying DAG.

For real data, the structure may not be known, or a DAG

Why not evaluate causal models in terms of predicting the effects of interventions?

Given this task, there are a variety of approaches to causality.

[Duvenaud, Eaton, Murphy, Schmidt, JMLR WCP ’09]

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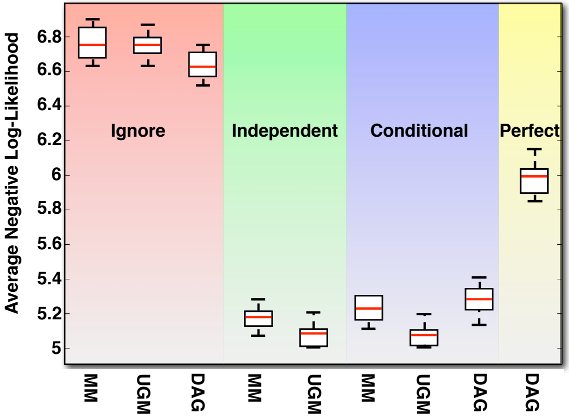

Causal Learning without DAGs

Predicting the effects of new actions in a SEM: