Proximal Newton Methods for Large-Scale Machine Learning

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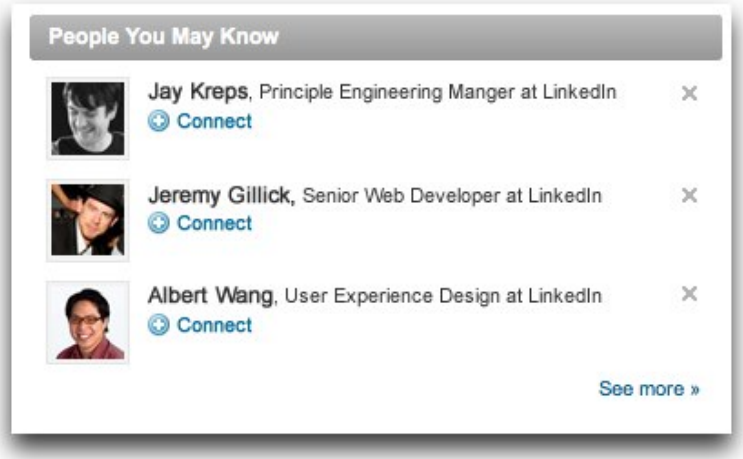
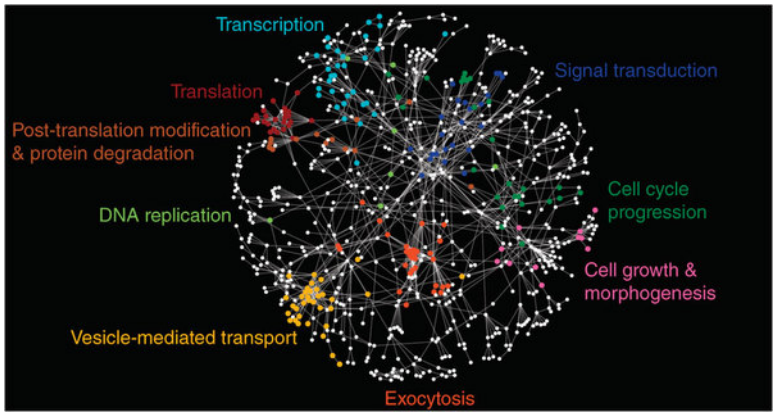
Big Data

Link prediction



LinkedIn.



gene-gene network

fMRI

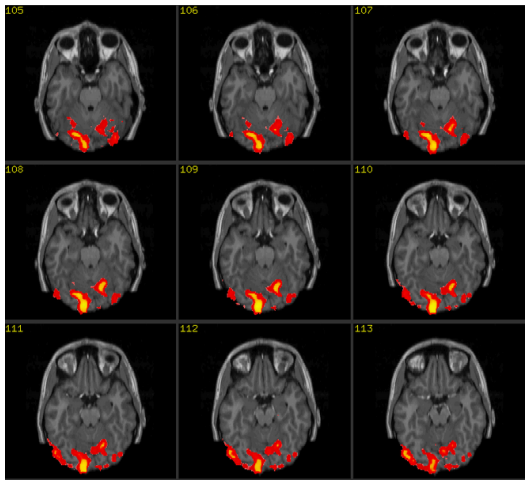
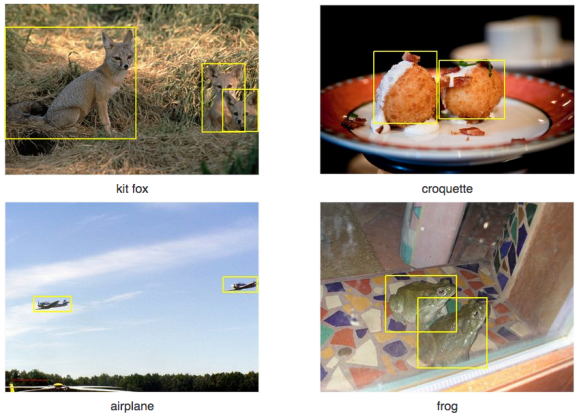
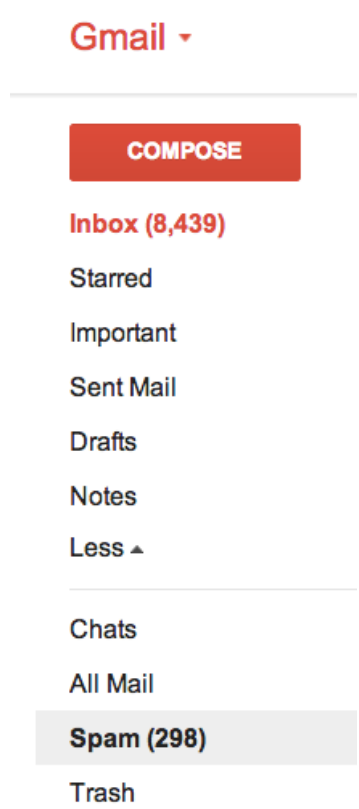


Image classification



Spam classification

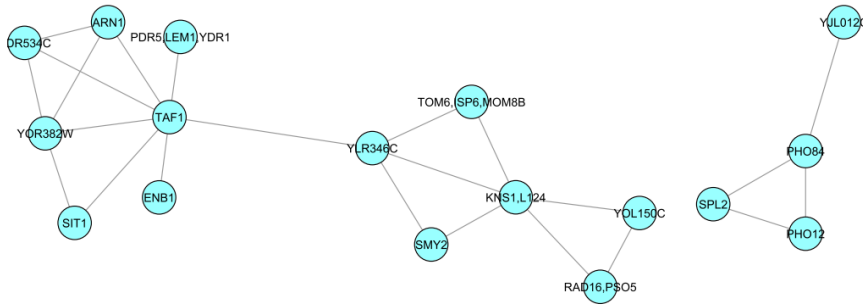


Modern Machine Learning Problems

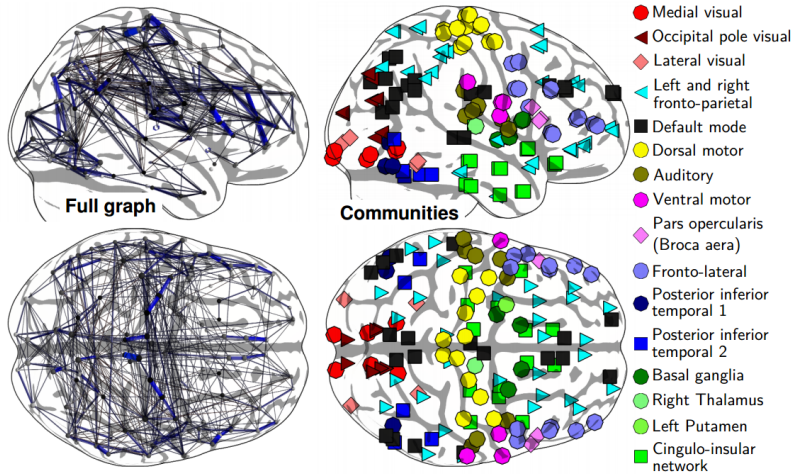
Inverse Covariance Estimation

- Learning graph (structure and/or weights) from data.
- Gene networks, fMRI analysis, stock networks, climate analysis.

Gene network

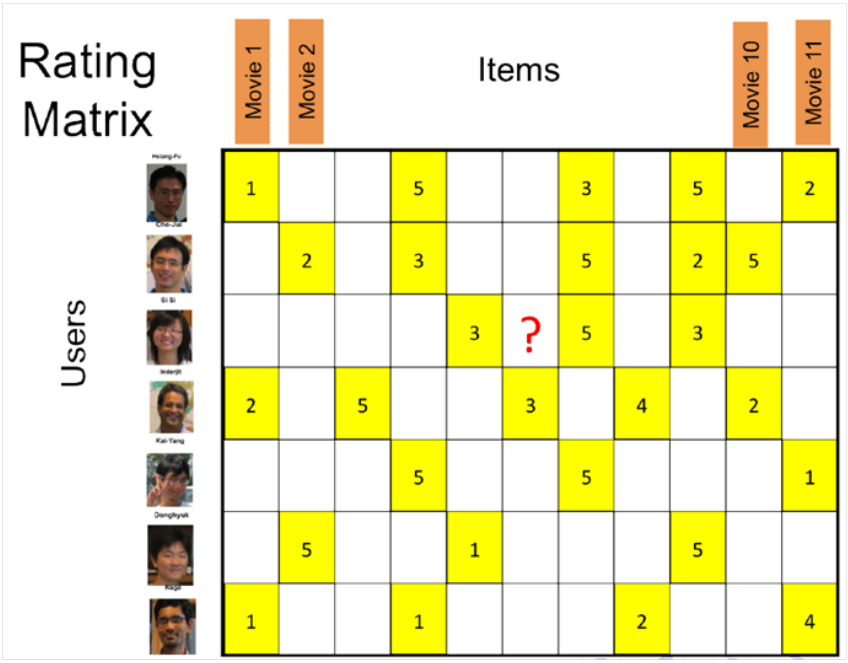


fMRI brain analysis



Matrix Completion

- Missing value estimation for recommender systems.
- Assumption: the underlying matrix is low-rank.



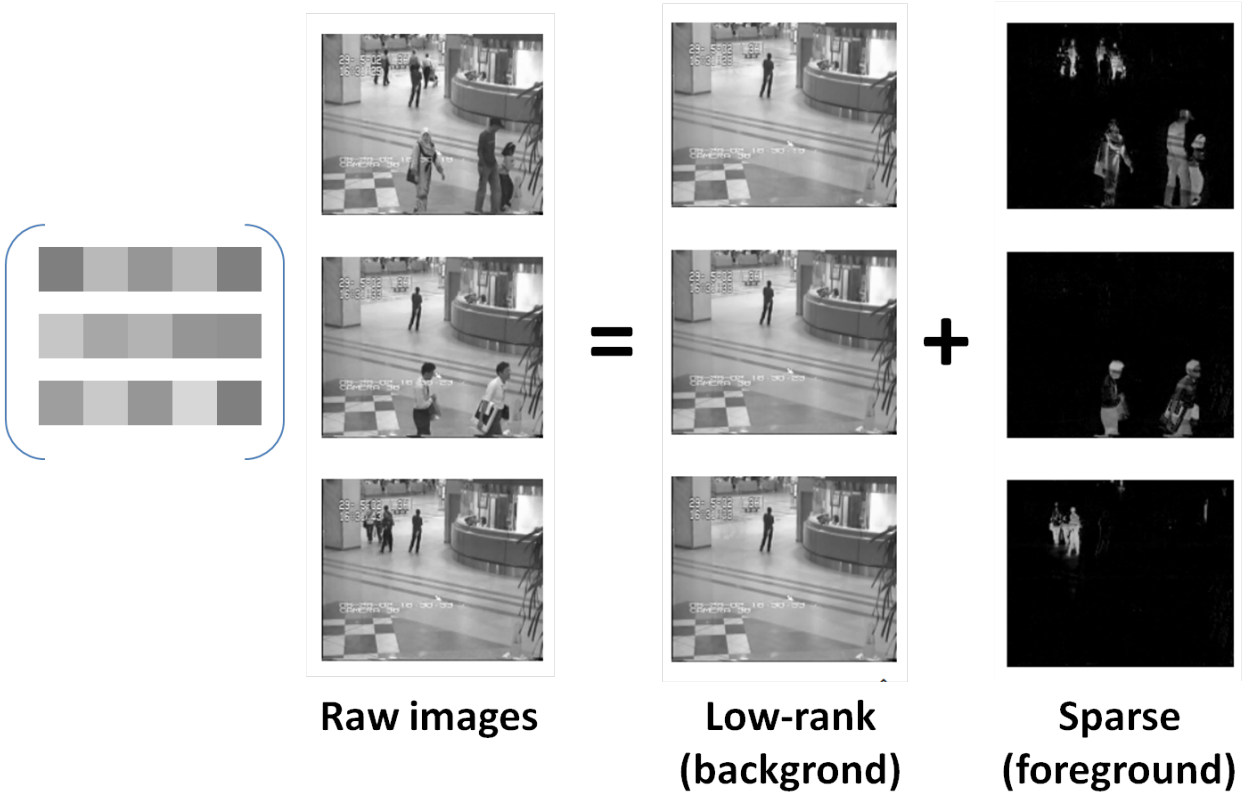
≈

-8.72	0.03	-1.03
-7.56	-0.79	0.62
-4.07	-3.95	2.55
-3.52	3.73	-3.32
-7.78	2.34	2.33
-2.44	-5.29	-3.92
-1.78	1.90	-1.68

-0.07	-0.11	-0.53	-0.46	-0.06	-0.05	-0.53	-0.07	-0.35	-0.19	-0.14
0.13	-0.42	0.45	0.17	-0.25	-0.17	-0.18	0.27	-0.59	0.05	0.14
-0.21	-0.43	-0.23	0.16	0.08	0.17	0.57	-0.39	-0.37	-0.08	-0.15

Robust PCA

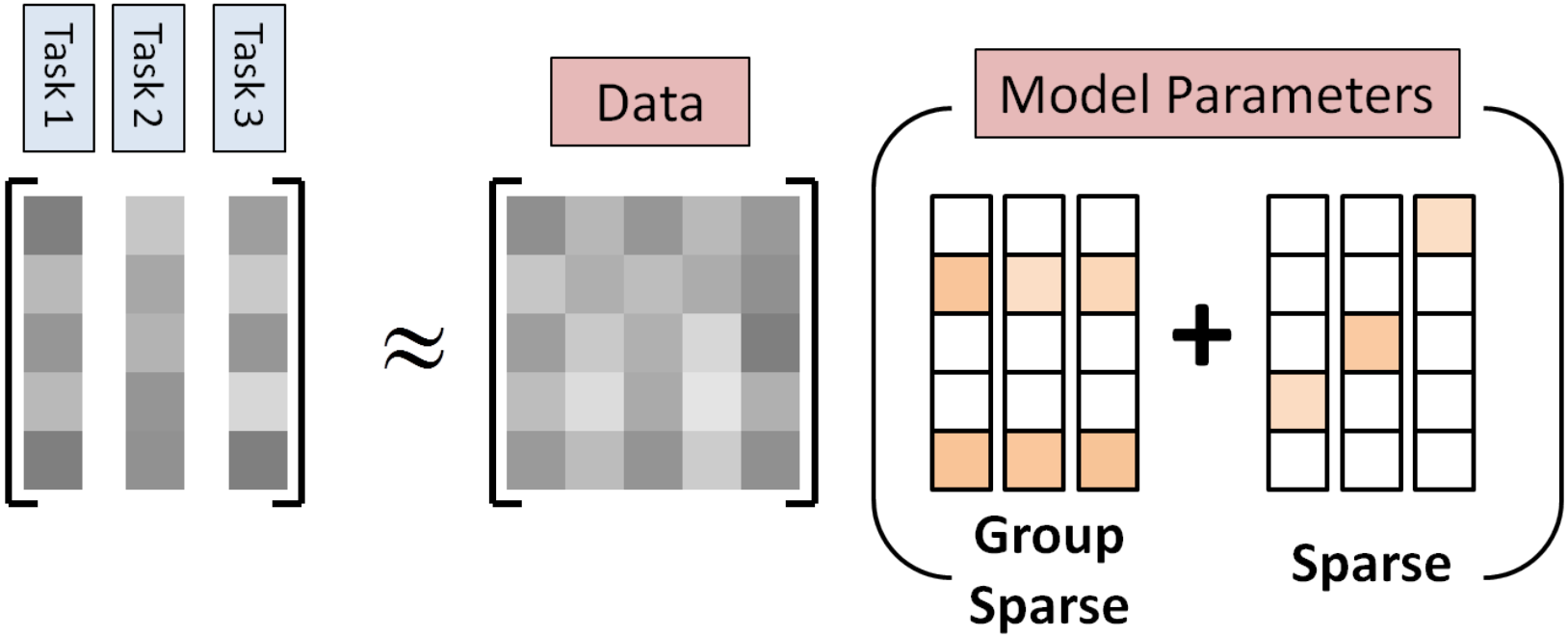
- Image de-noising, face recognition, graphical modeling with latent variables
- Decompose the input matrix as sparse + low-rank matrices.



Figures from (Candès et al, 2009)

Multi-task Learning

- Training T classification tasks together.
- Sparse models: Lasso
- Feature sharing: Group Lasso



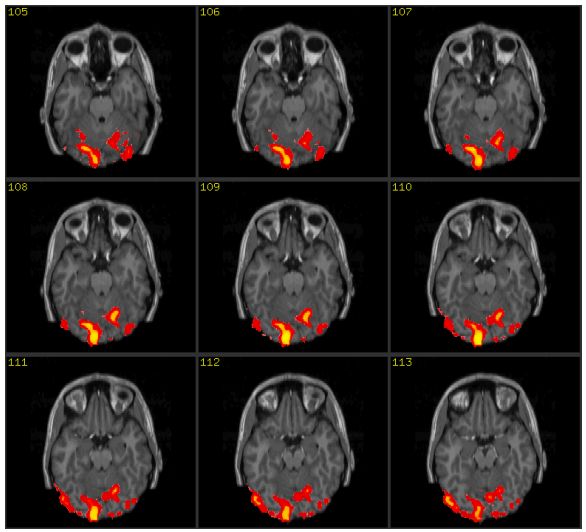
Inverse Covariance Estimation

Estimate Relationships between Variables

- Example: FMRI Brain Analysis.
- Goal: Reveal functional connections between regions of the brain.

(Sun et al, 2009; Smith et al, 2011; Varoquaux et al, 2010; Ng et al, 2011)

Input



Output

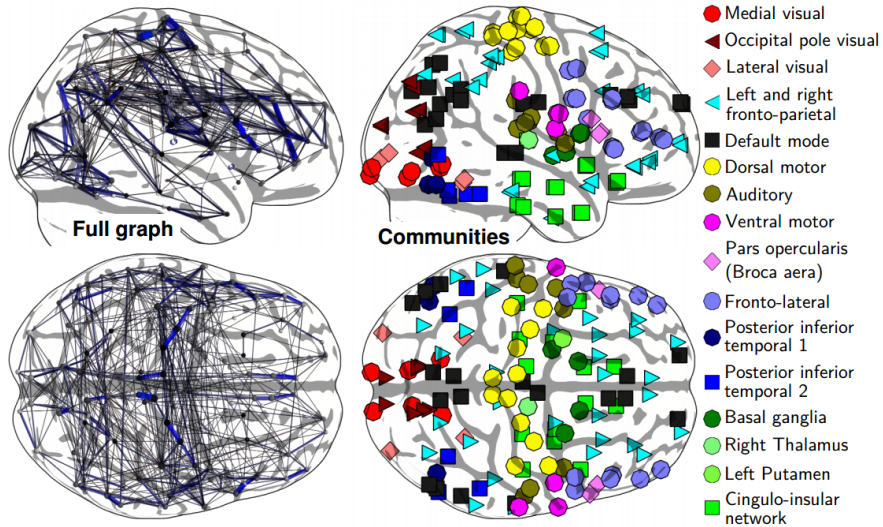


Figure from (Varoquaux et al, 2010)

Estimate Relationships between Variables

- Example: Gene regulatory network discovery.
- Goal: Gene network reconstruction using microarray data.

  (Schafer & Strimmer 2005; Andrei & Kendziorski 2009; Menendez et al, 2010; Yin and Li, 2011)

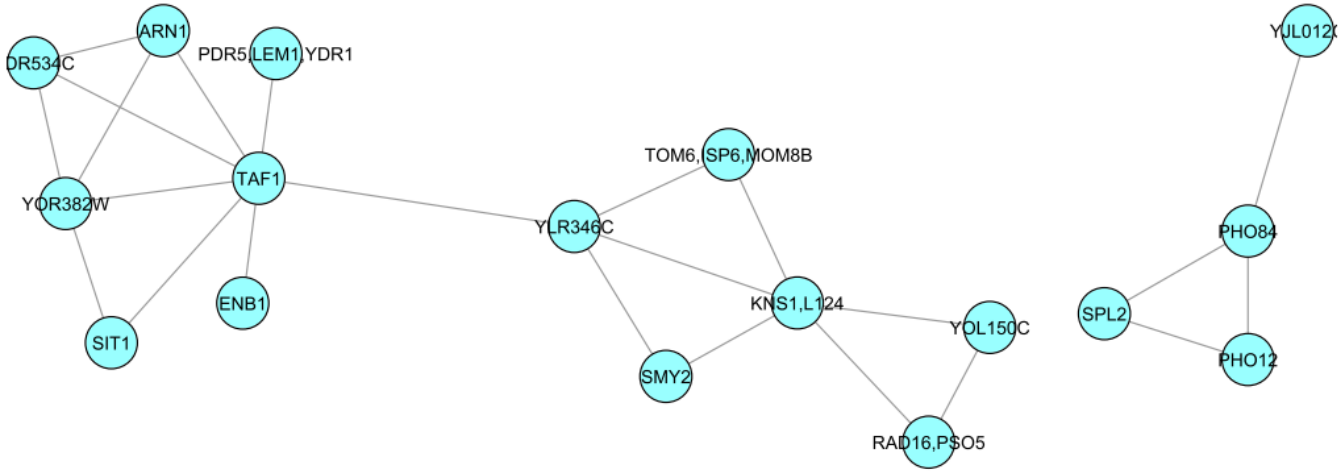


Figure from (Banerjee et al, 2008)

Other Applications

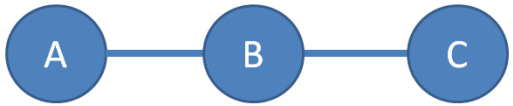
- Financial Data Analysis:
  - Model dependencies in multivariate time series (Xuan & Murphy, 2007).
  - Sparse high dimensional models in economics (Fan et al, 2011).
- Social Network Analysis / Web data:
  - Model co-authorship networks (Goldenberg & Moore, 2005).
  - Model item-item similarity for recommender system(Agarwal et al, 2011).
- Climate Data Analysis (Chen et al., 2010).
- Signal Processing (Zhang & Fung, 2013).
- Anomaly Detection (Ide et al, 2009).

Inverse Covariance Estimation

- Given: n i.i.d. samples $\{\boldsymbol{y_1}, \ldots, \boldsymbol{y_n}\}$, $\boldsymbol{y_i} \in R^p$, $\boldsymbol{y_i} \sim \mathcal{N}(\mu, \Sigma)$,
- Goal: Estimate relationships between variables.
- The sample mean and covariance are given by:

$$\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} \boldsymbol{y_i} \quad \text{and} \quad S = \frac{1}{n}\sum_{i=1}^{n} (\boldsymbol{y_i} - \hat{\mu})(\boldsymbol{y_i} - \hat{\mu})^T.$$

- Covariance matrix Σ may not directly convey relationships.
- An example – Chain graph: $y(j) = 0.5y(j-1) + \mathcal{N}(0,1)$



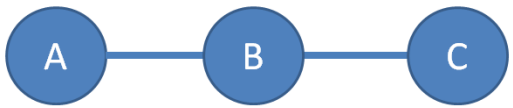
$$\Sigma = \begin{pmatrix} 1.33 & 0.67 & 0.33 \\ 0.67 & 1.33 & 0.67 \\ 0.33 & 0.67 & 1.33 \end{pmatrix}$$

Inverse Covariance Estimation (cont'd)

- Conditional independence is reflected as zeros in Θ $(= \Sigma^{-1})$:

  $\Theta_{ij} = 0 \Leftrightarrow$ $y(i), y(j)$ are conditionally independent given other variables

- Chain graph example: $y(j) = 0.5y(j-1) + \mathcal{N}(0,1)$



$$\Theta = \begin{pmatrix} 1 & -0.5 & 0 \\ -0.5 & 1.25 & -0.5 \\ 0 & -0.5 & 1 \end{pmatrix}$$

- In a GMRF $G = (V, E)$, each node corresponds to a variable, and each edge corresponds to a non-zero entry in Θ.
- Goal: Estimate the inverse covariance matrix Θ from the observations.

Maximum Likelihood Estimator: LogDet Optimization

- Given the n samples, the likelihood is

$$P(\boldsymbol{y_1}, \ldots, \boldsymbol{y_n}; \hat{\boldsymbol{\mu}}, \Theta) \propto \prod_{i=1}^{n} (\det \Theta)^{1/2} \exp\left(-\frac{1}{2} (\boldsymbol{y_i} - \hat{\boldsymbol{\mu}})^T \Theta (\boldsymbol{y_i} - \hat{\boldsymbol{\mu}}) \right)$$

$$= (\det \Theta)^{n/2} \exp\left(-\frac{1}{2} \sum_{i=1}^{n} (\boldsymbol{y_i} - \hat{\boldsymbol{\mu}})^T \Theta (\boldsymbol{y_i} - \hat{\boldsymbol{\mu}}) \right).$$

- The log likelihood can be written as

$$\log(P(\boldsymbol{y_1}, \ldots, \boldsymbol{y_n}; \hat{\boldsymbol{\mu}}, \Theta)) = \frac{n}{2} \log(\det \Theta) - \frac{n}{2} \mathrm{tr}(\Theta S) + \text{constant}.$$

- Maximum likelihood estimator:

$$\Theta^* = \arg\min_{X \succ 0} \{ -\log\det X + \mathrm{tr}(SX) \}.$$

- Problem: when $p > n$, sample covariance matrix S is singular.

L1-regularized inverse covariance selection

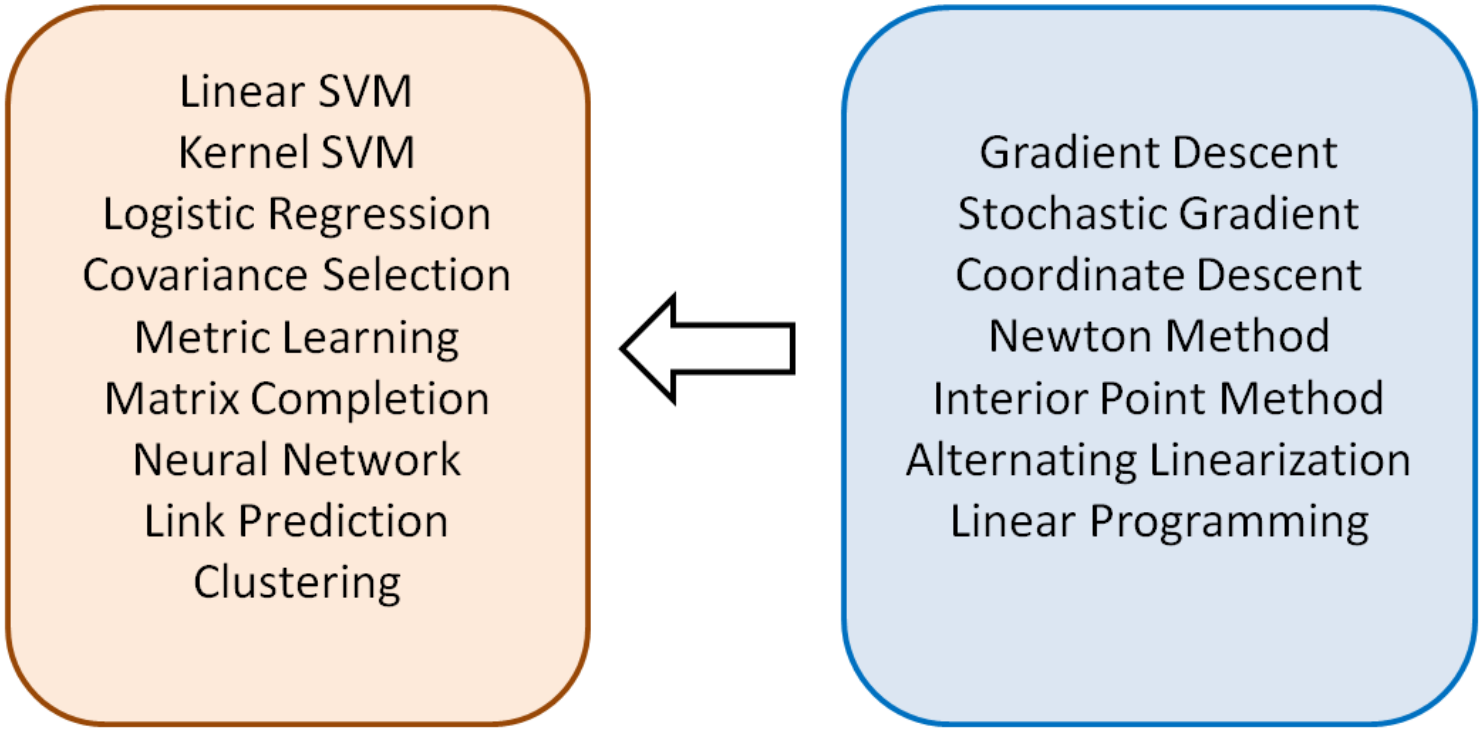
- A sparse inverse covariance matrix is preferred –

  add ℓ_1 regularization to promote sparsity.
- The resulting optimization problem:

$$\Theta = \arg\min_{X \succ 0} \left\{ -\log\det X + \operatorname{tr}(SX) + \lambda \|X\|_1 \right\} = \arg\min_{X \succ 0} f(X),$$

  where $\|X\|_1 = \sum_{i,j=1}^{n} |X_{ij}|$.
- Regularization parameter $\lambda > 0$ controls the sparsity.
- The problem appears hard to solve:
  - Non-smooth log-determinant program.
  - Number of parameters scale quadratically with number of variables.

Optimization in Machine Learning



High-dimensional!

Large number of samples!

Large number of parameters!

Exploiting Structure in Machine Learning Problems

- Regularized Loss Minimization(RLM):

$$\min_{\theta}\{\ \underbrace{g(\theta, X)}_{\text{loss}} + \underbrace{h(\theta)}_{\text{regularization}}\ \} \equiv f(\theta),$$

- Exploiting problem structure:
  - Can we have faster computation?
- Exploiting model structure:
  - Can we avoid un-important search space?
- Exploiting Data distribution:
  - Can we speed up optimization algorithms if we roughly estimate the data distribution?

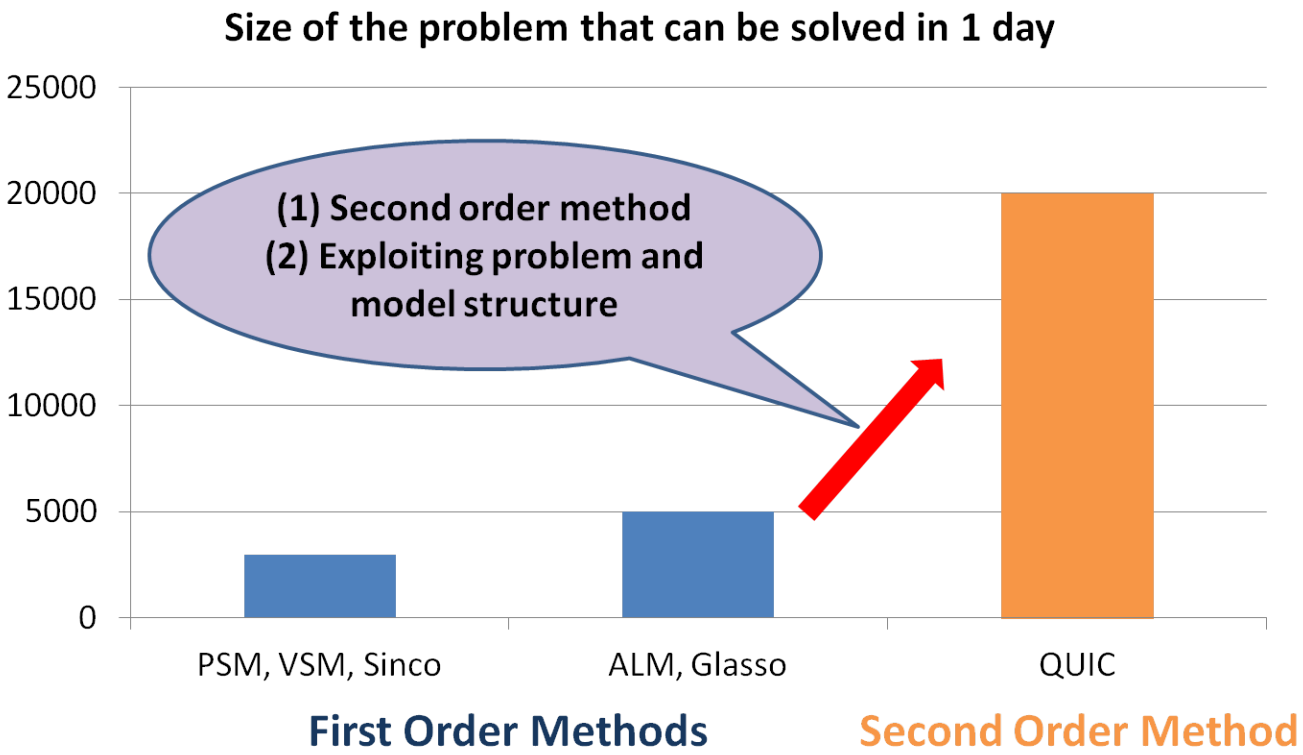
QUIC

QUadratic approximation for Inverse Covariance estimation

Sparse Inverse Covariance Estimation

- p^2 parameters in the non-smooth Log-determinant program:

$$\Theta = \arg\min_{X \succ 0} \{ \underbrace{-\log\det X + \mathrm{tr}(SX)}_{\text{negative log likelihood}} + \lambda \|X\|_1 \}$$

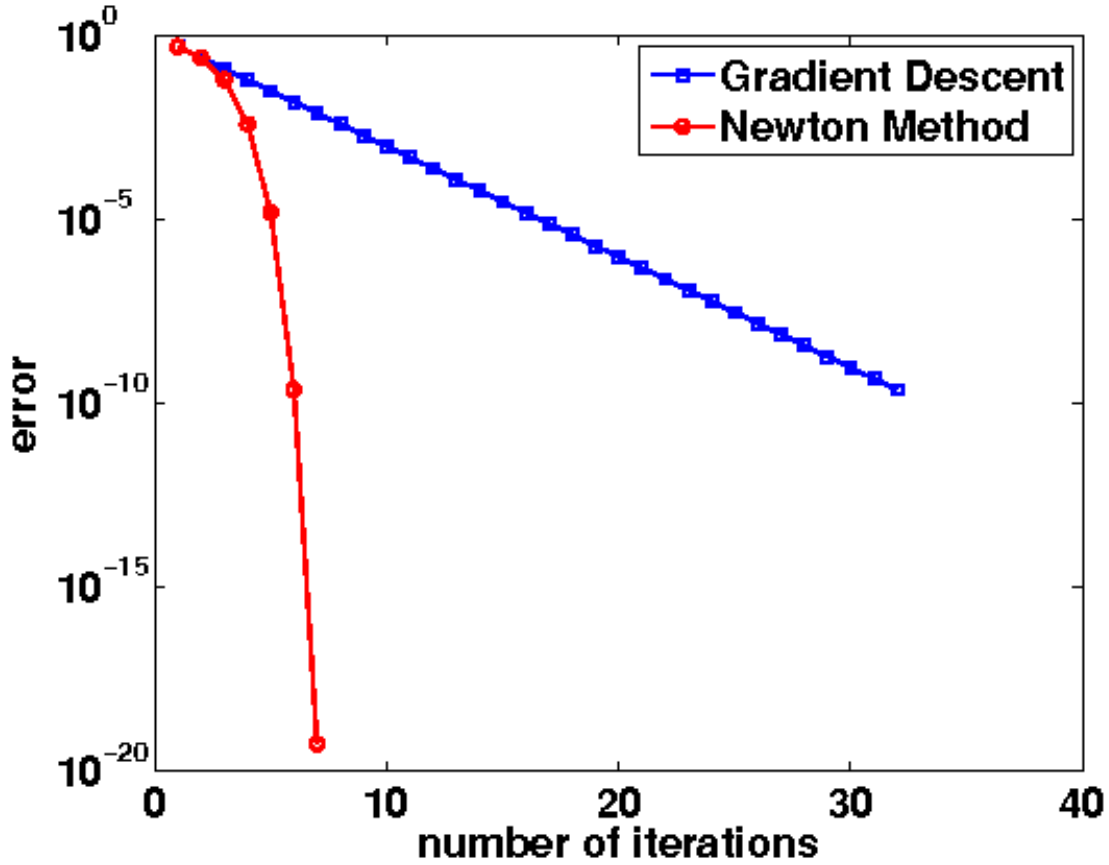


First Order Methods vs Second Order Methods

- Many algorithms have been proposed.
  - Block coordinate descent (Banerjee et al., 2007), (Friedman et al., 2007),
  - Gradient or Accelerate gradient descent (Lu, 2009), (Duchi et al., 2008),
  - Greedy coordinate descent (Scheinberg & Rich., 2009)
  - ADMM (Scheinberg et al., 2009), (Boyd et al., 2011)
- All of them are **first order methods** (only gradient information)
- QUIC: the first **second order method** for this problem (use Hessian information).

$$\nabla f(\boldsymbol{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f(\boldsymbol{x})}{\partial x_d} \end{bmatrix}, \quad H = \nabla^2 f(\boldsymbol{x}) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_d} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_d \partial x_1} & \frac{\partial^2 f}{\partial x_d \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_d^2} \end{bmatrix}$$

First Order Methods vs Second Order Methods



Why do all previous approaches use first order methods?

Second Order Methods for Non-Smooth Functions

- Update rule for Newton method (second order method):

$$\boldsymbol{x} \leftarrow \boldsymbol{x} - \eta(\nabla^2 f(\boldsymbol{x}))^{-1} \nabla f(\boldsymbol{x})$$

- Two difficulties:
  - Time complexity per iteration may be very high.
  - How to deal with non-smooth functions ($\|\boldsymbol{x}\|_1$)?

Second Order Methods for Non-Smooth Functions

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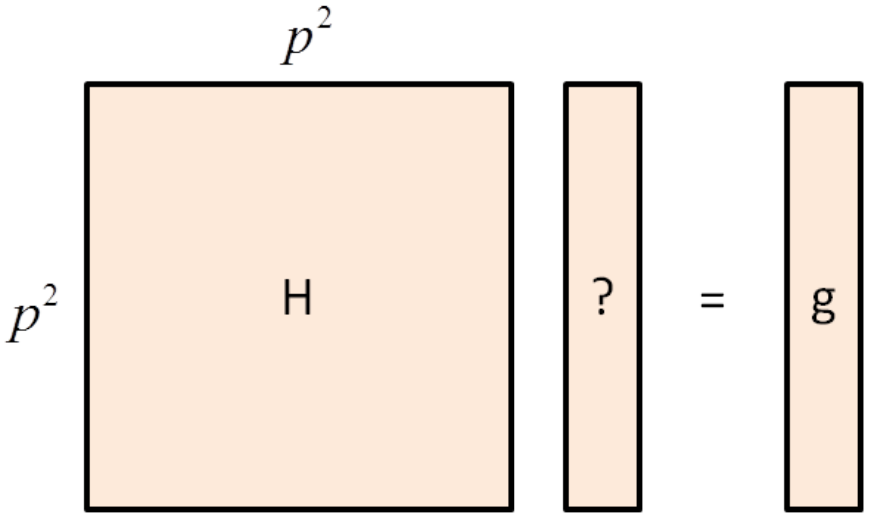
- Two difficulties:
  - Time complexity per iteration may be very high.
  - How to deal with non-smooth functions ($\|\boldsymbol{x}\|_1$)?
- Addressed by (Hsieh, Sustik, Dhillon and Ravikumar, 2011).
- Extensions:
  - Theoretical Analysis: (Lee et al., 2012), (Patrinos and Bemporad., 2013), (Tang and Scheinberg, 2014), (Yen, Hsieh, Ravikumar and Dhillon, 2014), ...
  - Optimization Algorithms: (Olsen et al., 2012), (Dinh et al., 2013), (Treister et al., 2014), (Scheinberg and Tang, 2014), (Zhong et al., 2014), ...

Time Complexity?

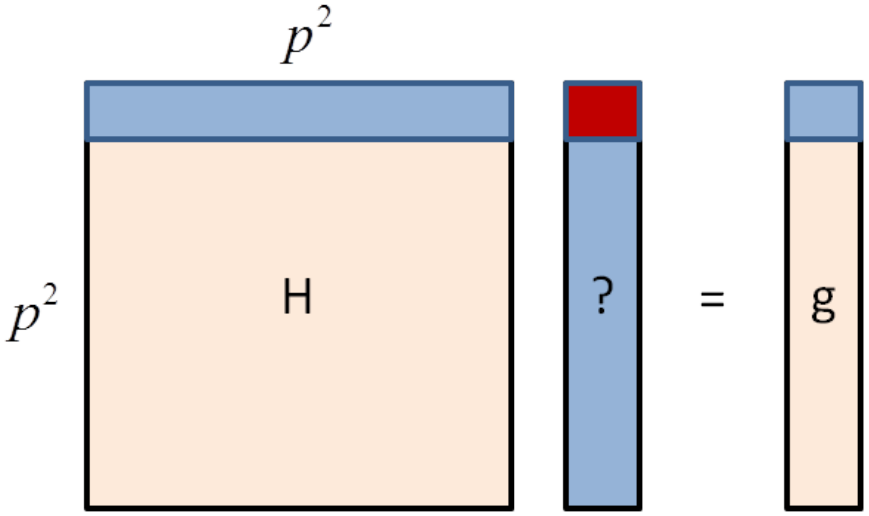
- Newton direction: $H^{-1}\boldsymbol{g}$. (H: Hessian, $\boldsymbol{g}$: gradient)
- Solving the linear system exactly: $O(p^6)$ time.



Appears to be prohibitive to apply a second order method.

Time Complexity?

- Coordinate descent: each time fits one element of $\boldsymbol{g}$.



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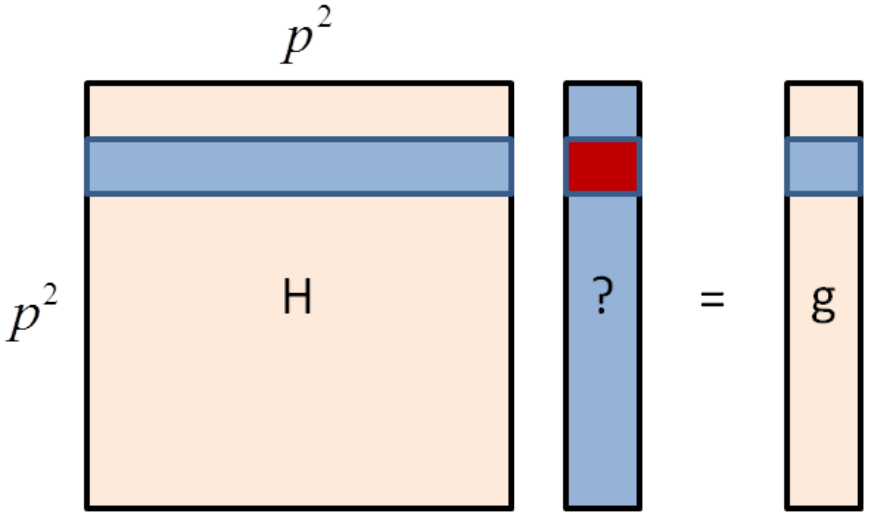
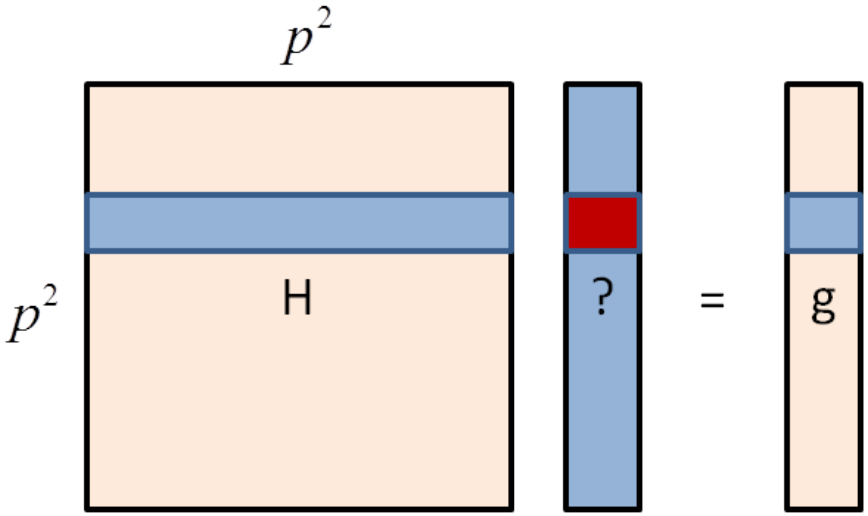


Time Complexity?

- Use iterative solver—coordinate descent

  $O(p^2)$ per coordinate update, $O(p^4)$ for one sweep. $\Rightarrow$ need 40 days for $p = 10^4$ on a 2.83GHz CPU.



Still prohibitive.

Exploiting Problem Structure

Fast Computation of Newton Direction

$$\min_{X \succ 0} \{ \underbrace{-\log\det X + \operatorname{tr}(SX)}_{\text{problem structure}} + \underbrace{\lambda \|X\|_1}_{\text{regularization}} \}$$

Exploiting Problem Structure

- Structure of the Hessian:

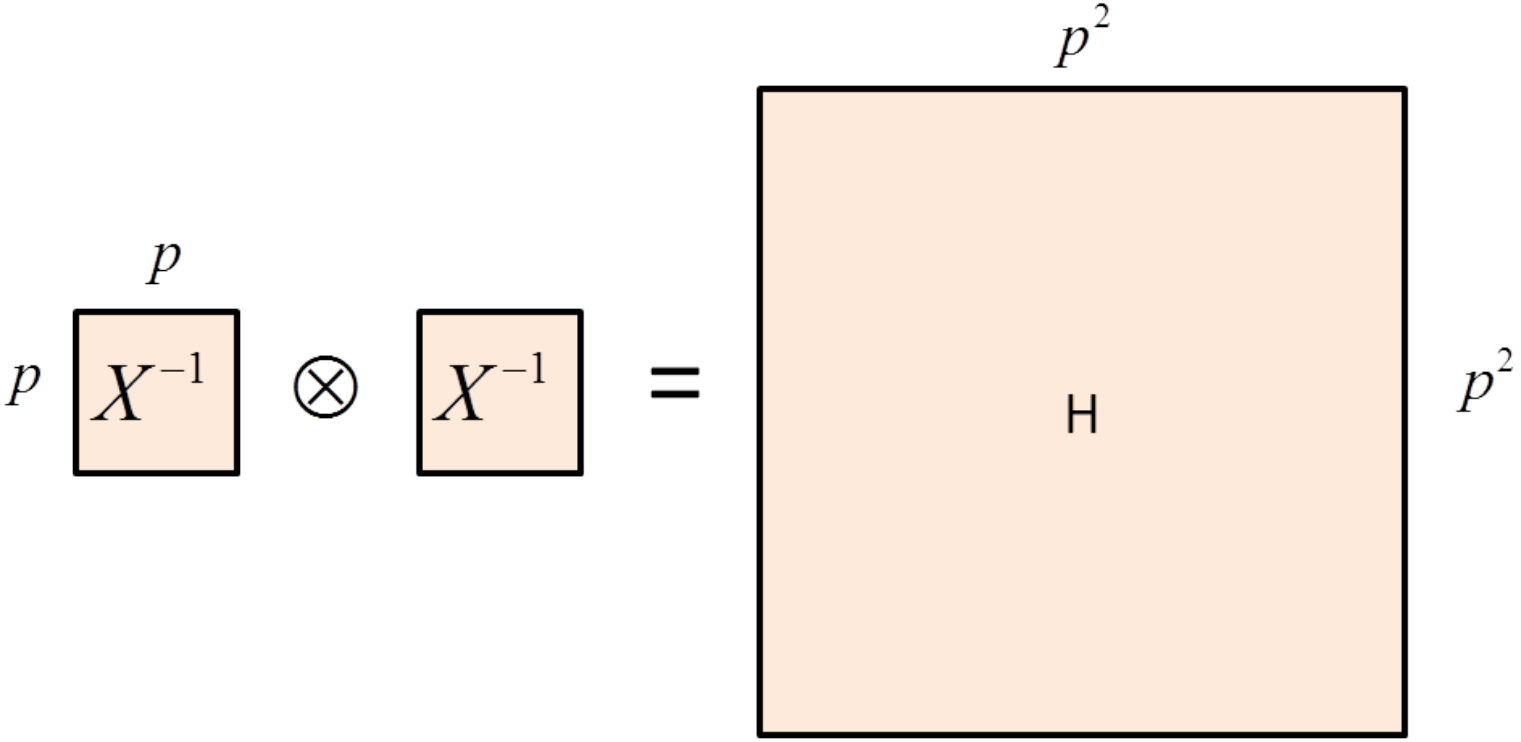
$$H = \frac{\partial^2}{\partial^2 X}(-\log\det X) = X^{-1} \otimes X^{-1}.$$

- The Kronecker product:

$$A \otimes B = \begin{pmatrix} a_{11}B & \cdots & a_{1p}B \\ \vdots & \ddots & \vdots \\ a_{p1}B & \cdots & a_{pp}B \end{pmatrix}$$

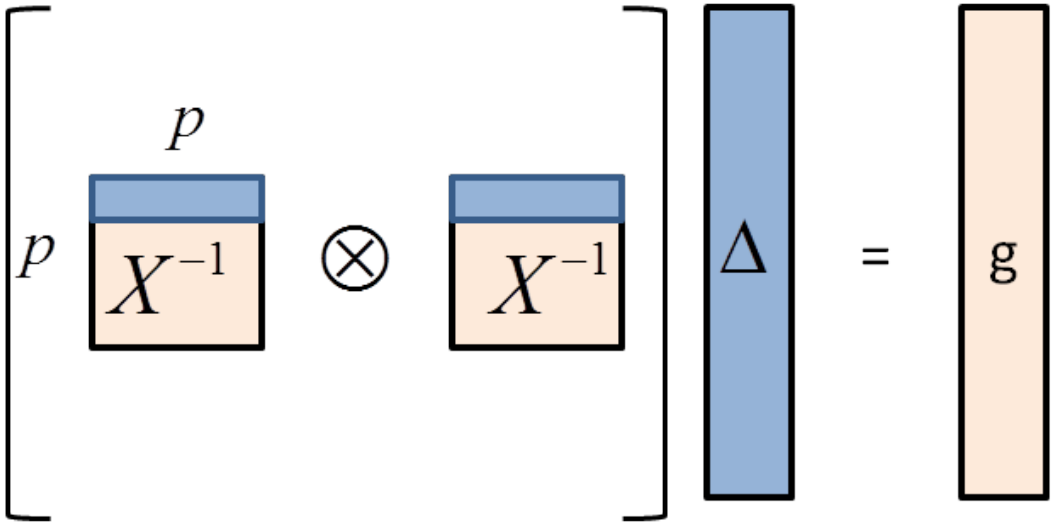
was introduced by G. Zehfuss (1858) and later attributed to L. Kronecker.

Exploiting Problem Structure



The Hessian (p^2 by p^2 matrix) can be represented using p^2 parameters!

Exploiting Problem Structure



- Time complexity: $O(p^2) \Rightarrow O(p)$ for each coordinate update.
  $O(p^4) \Rightarrow O(p^3)$ per sweep.
- At coordinate descent step to update (i, j) element of descent direction:

$$\Big(H \operatorname{vec}(\Delta)\Big)_{ip+j} = \Big((X^{-1} \otimes X^{-1}) \operatorname{vec}(\Delta)\Big)_{ip+j} = \Big(X^{-1} \Delta X^{-1}\Big)_{ij}$$
$$= (X^{-1} U)_{ij},$$

  where $U = \Delta X^{-1}$ is maintained in memory.

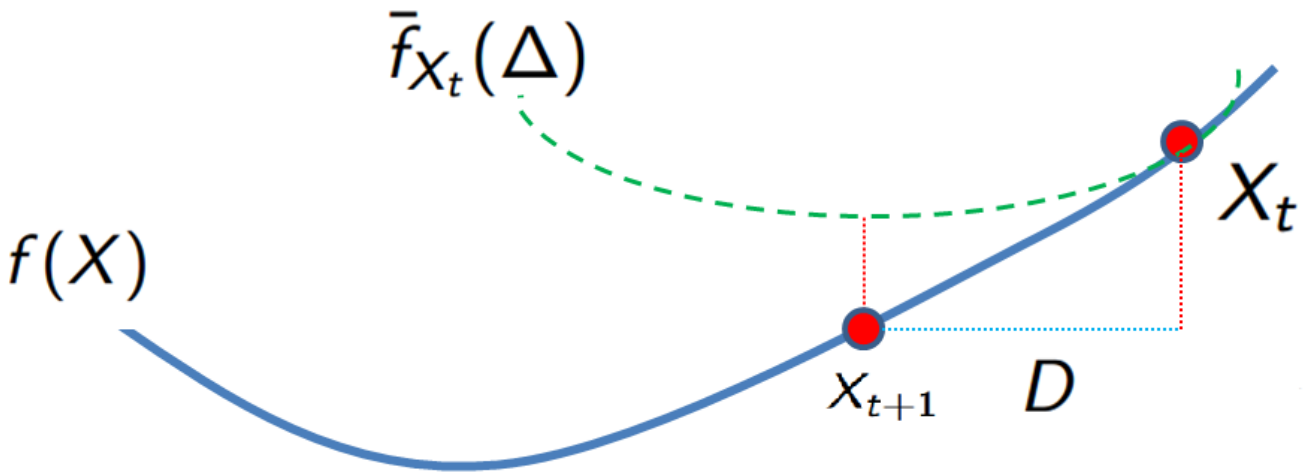
Newton Method for Non-smooth Functions

- Iteration conducts the following updates:
  - Compute the generalized Newton direction

$$D_t = \arg\min_{\Delta} \bar{f}_{X_t}(\Delta)$$

$$= \arg\min_{\Delta} \langle \nabla g(X_t), \mathrm{vec}(\Delta) \rangle + \frac{1}{2} \mathrm{vec}(\Delta)^T \nabla^2 g(X_t) \mathrm{vec}(\Delta) + \lambda \|X_t + \Delta\|_1$$

  - $X_{t+1} \leftarrow X_t + D_t$.



Proximal Newton Method

Proximal Newton for sparse Inverse Covariance estimation

For $t = 0, 1, \ldots$

1. **Compute Proximal Newton direction**: $D_t = \arg\min_{\Delta} \bar{f}_{X_t}(X_t + \Delta)$ (A Lasso problem.)
2. **Line Search**: use an Armijo-rule based step-size selection to get α s.t. $X_{t+1} = X_t + \alpha D_t$ is
   - positive definite,
   - satisfies a sufficient decrease condition $f(X_t + \alpha D_t) \leq f(X_t) + \alpha\sigma\Delta_t$.

Exploiting Problem Structure

Can we scale to $p \approx 20,000$?

- Coordinate descent updates for computing Newton direction.
  - needs $O(p^2)$ storage
  - ~~needs $O(p^4)$ computation per sweep~~
  - needs $O(p^3)$ computation per sweep (by exploiting problem structure)
- Line search (compute determinant using Cholesky factorization).
  - needs $O(p^2)$ storage
  - needs $O(p^3)$ computation

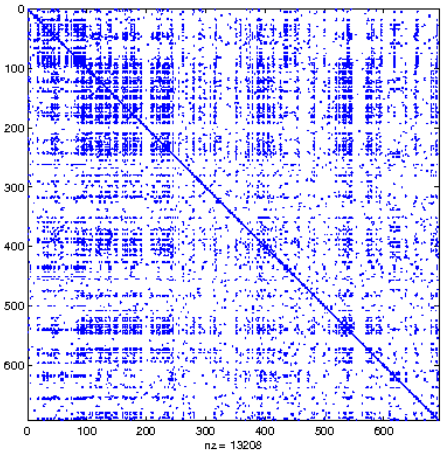
Exploiting Model Structure

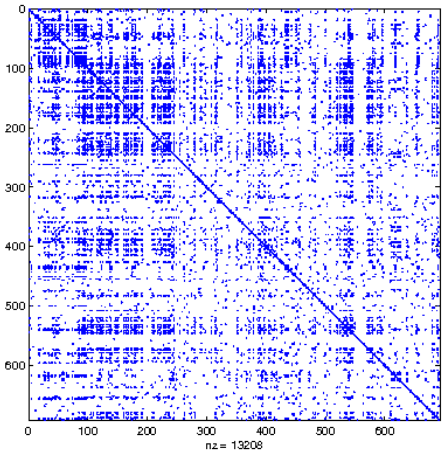
Variable Selection

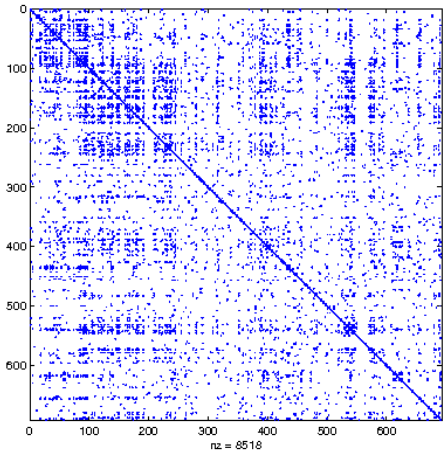
$$\min_{\theta}\{\ \underbrace{-\log\det X + \operatorname{tr}(SX)}_{\text{problem structure}}\ +\ \underbrace{h(\theta)}_{\text{regularization}}\ \} \equiv f(\theta),$$

Sparsity of the Model

ER dataset, $p = 692$, solutions at iteration 1, 3, 5.







Only 2.7% variables become nonzero.

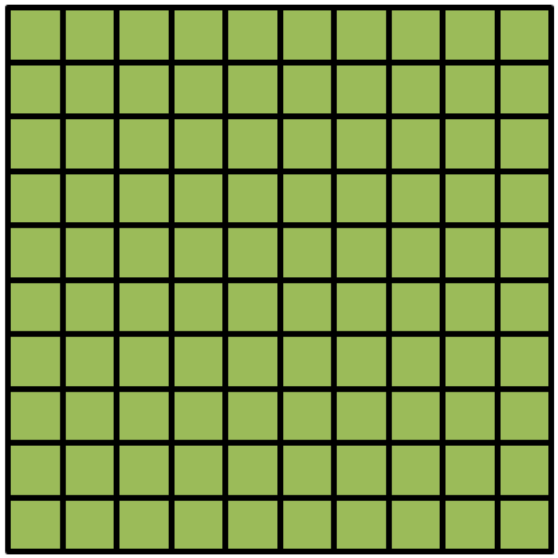
Active Variable Selection

- Strategy: before solving the Newton direction, "guess" the variables that should be updated.
- Fixed set: $S_{fixed} = \{(i,j) \mid X_{ij} = 0 \text{ and } |\nabla_{ij} g(X)| \leq \lambda.\}$.
- Only update the rest of variables (free set).
- Convergence Guaranteed.

  $p = 1869$, number of variables $= p^2 = 3.49$ million. The size of free set drops to $20,000$ very quickly.

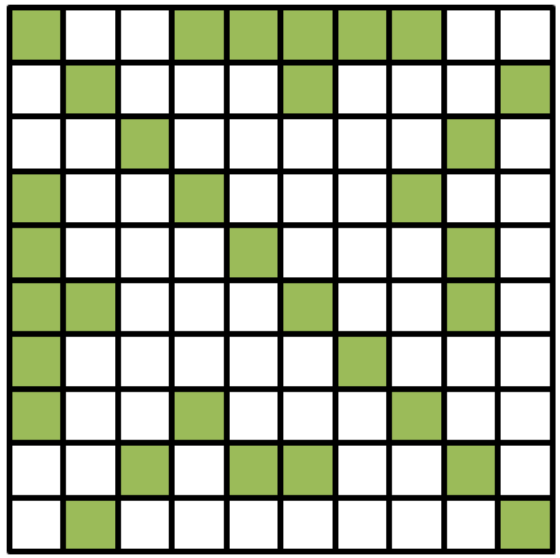
Active Variable Selection

Time complexity: $O(p^3)$ per sweep



Updates on all elements

Time complexity: $O(mp\ )$ per sweep, $m \approx \|X_t\|_0$



Updates on Free Set

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  - ~~needs $O(p^4)$ computation per sweep~~
  - ~~needs $O(p^3)$ computation per sweep (by exploiting problem structure)~~
  - needs $O(mp)$ computation per sweep, where $m \approx \|X\|_0$ (by exploiting problem and model structure)
- Line search (compute determinant using Cholesky factorization).
  - needs $O(p^2)$ storage
  - needs $O(p^3)$ computation

Algorithm

QUIC: QUadratic approximation for sparse Inverse Covariance estimation

Input: Empirical covariance matrix S, scalar λ, initial X_0.

For $t = 0, 1, \ldots$

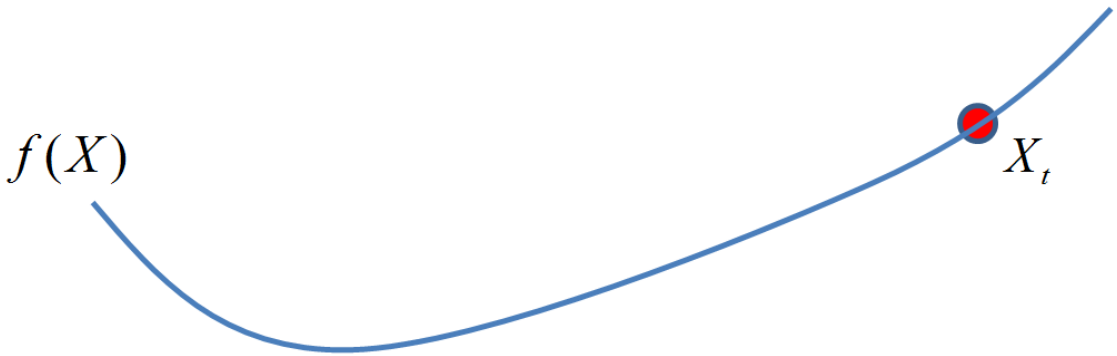
1. Variable selection: select a *free* set of $m \ll p^2$ variables.
2. Use coordinate descent to find descent direction:
   $D_t = \arg\min_\Delta \bar{f}_{X_t}(X_t + \Delta)$ over set of free variables, (A Lasso problem.)
3. Line Search: use an Armijo-rule based step-size selection to get α s.t. $X_{t+1} = X_t + \alpha D_t$ is
   - positive definite,
   - satisfies a sufficient decrease condition $f(X_t + \alpha D_t) \leq f(X_t) + \alpha\sigma\Delta_t$.

   (Cholesky factorization of $X_t + \alpha D_t$)

QUIC can solve $p = 20,000$ in about 2.3 hours.

Algorithm

- Current iterate X_t.

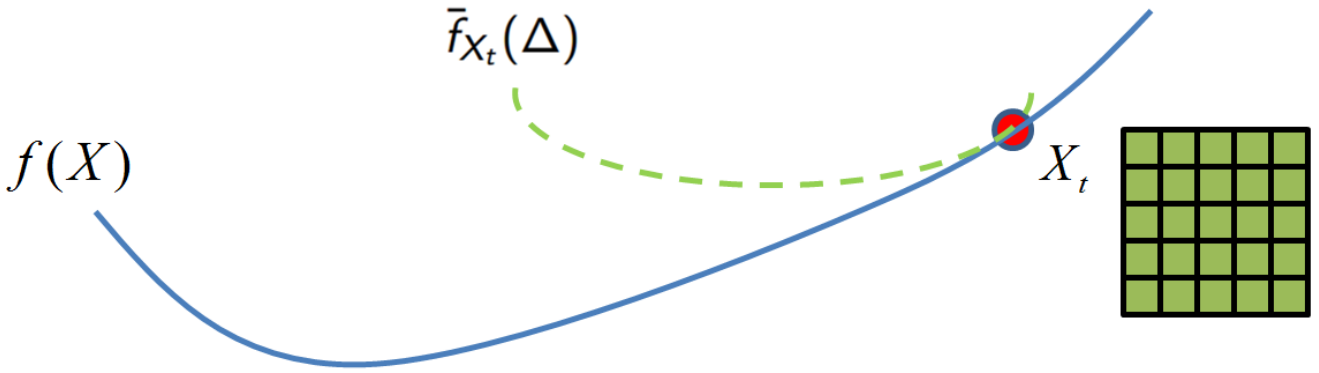


Algorithm

- Form the quadratic approximation $\bar{f}_{X_t}(\Delta)$.

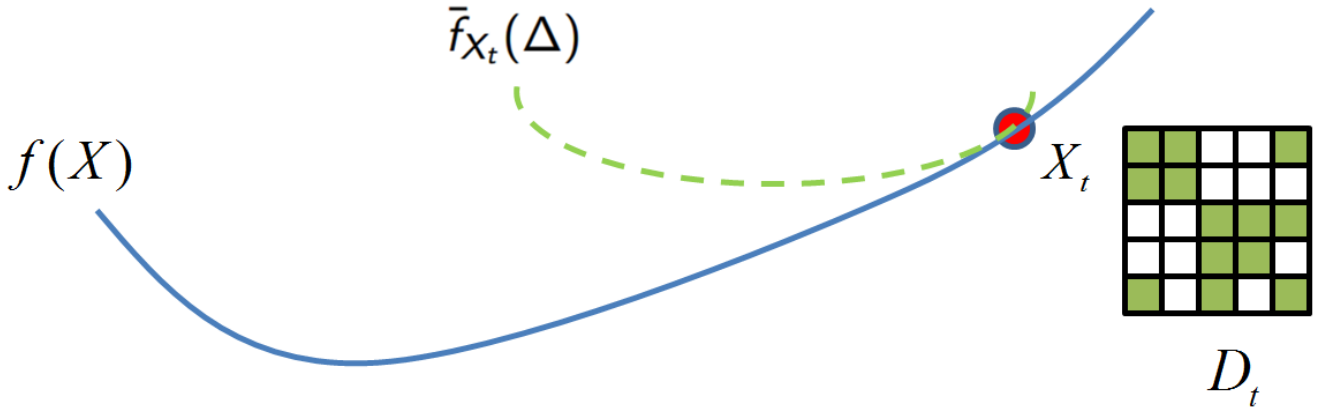
$$f(X) = g(X) + \lambda \|X\|_1$$

$$\bar{f}_{X_t}(\Delta) = f(X_t) + \langle \nabla g(X), \Delta \rangle + \frac{1}{2} \mathrm{vec}(\Delta)^T \nabla^2 g(X) \mathrm{vec}(\Delta) + \lambda \|X + \Delta\|_1$$



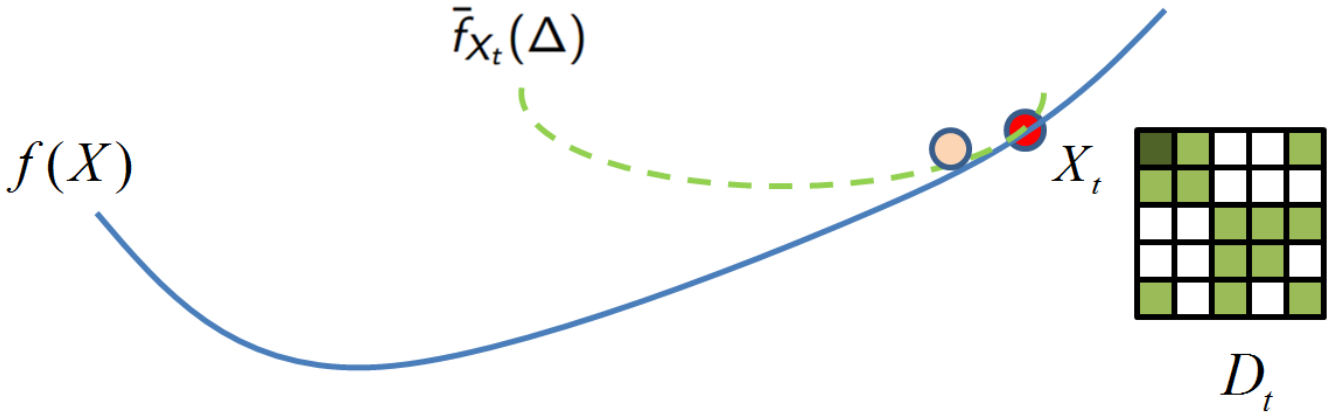
Algorithm

- Form the quadratic approximation $\bar{f}_{X_t}(\Delta)$.
- Free set selection.



Algorithm

- Form the quadratic approximation $\bar{f}_{X_t}(\Delta)$.
- Free set selection.
- Coordinate descent to minimize $\bar{f}_{X_t}(\Delta)$



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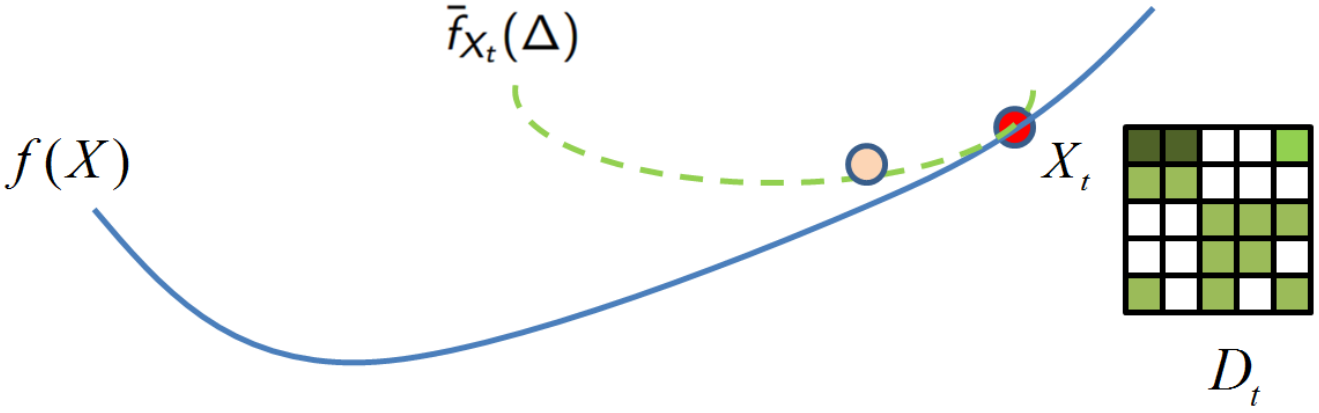
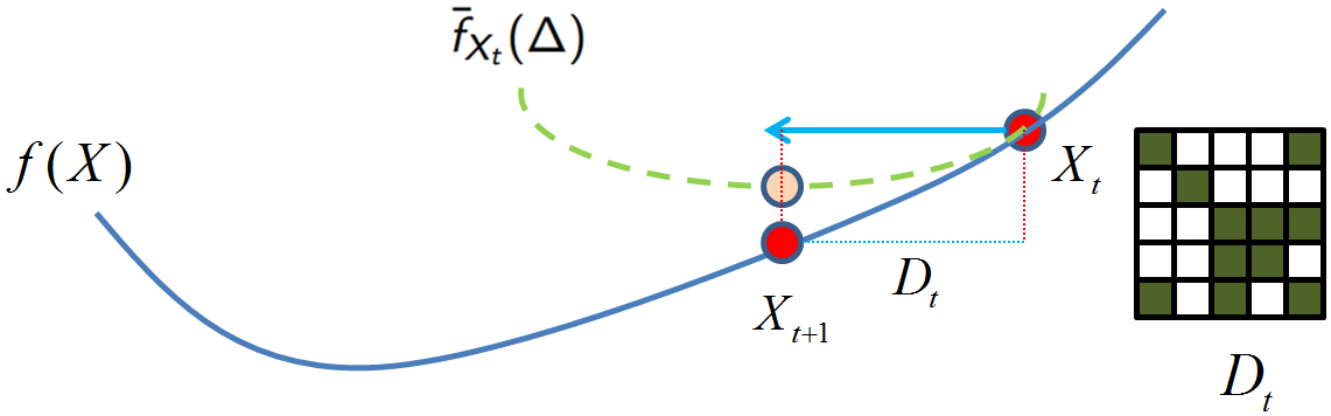


Algorithm

- Form the quadratic approximation $\bar{f}_{X_t}(\Delta)$.
- Free set selection.
- Coordinate descent to minimize $\bar{f}_{X_t}(\Delta)$
- $X_{t+1} \leftarrow X_t + D_t$



Theoretical Guarantee

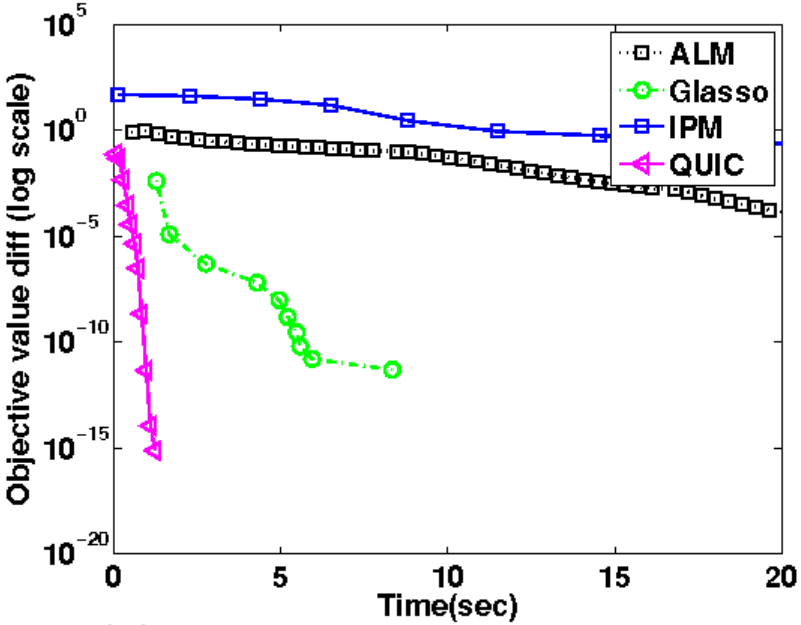
Theorem: Quadratic Convergence Rate for QUIC

Suppose $g(\cdot)$ is strongly convex and the quadratic subproblem at each iteration is solved exactly, QUIC converges to the global optimum with an asymptotic quadratic convergence rate:

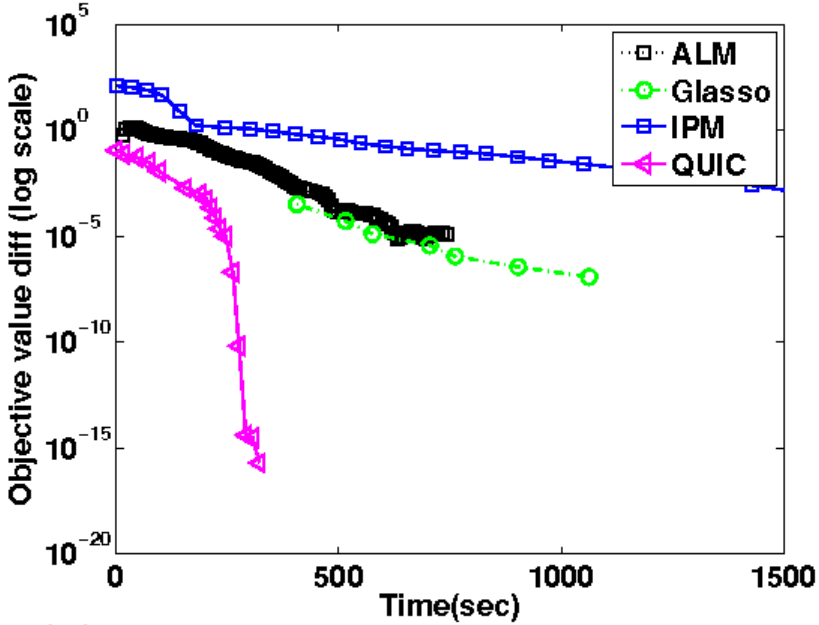
$$\lim_{t \to \infty} \frac{\|X_{t+1} - X^*\|_F}{\|X_t - X^*\|_F^2} = \kappa,$$

where κ is a constant.

QUIC Results: Data from Biology Applications



(a) Time for Estrogen, $p = 692$



(b) Time for hereditarybc, $p = 1,869$

QUIC & DIRTY

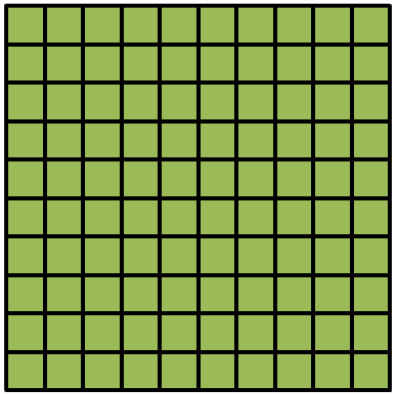
Active Subspace Selection for Dirty Statistical Models

Exploiting Model Structure

$$\min_X \{ \underbrace{\text{Loss}(X; \text{Data})}_{\text{problem structure}} + \underbrace{\text{Regularization}(X)}_{\text{model structure}} \}$$

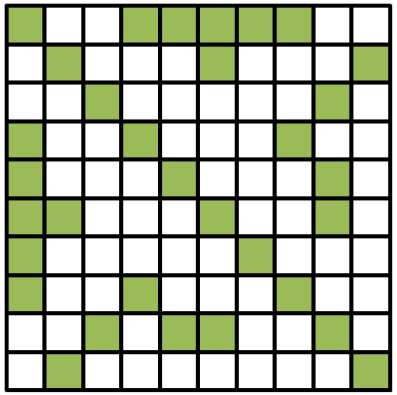
- If $h(X) = \|X\|_1$, the solution is expected to be sparse.
- Active Variable Selection:

Time complexity: $O(p^3)$ per sweep



Updates on all elements

Time complexity: $O(mp^2)$ per sweep, $m \approx \|X_t\|_0$

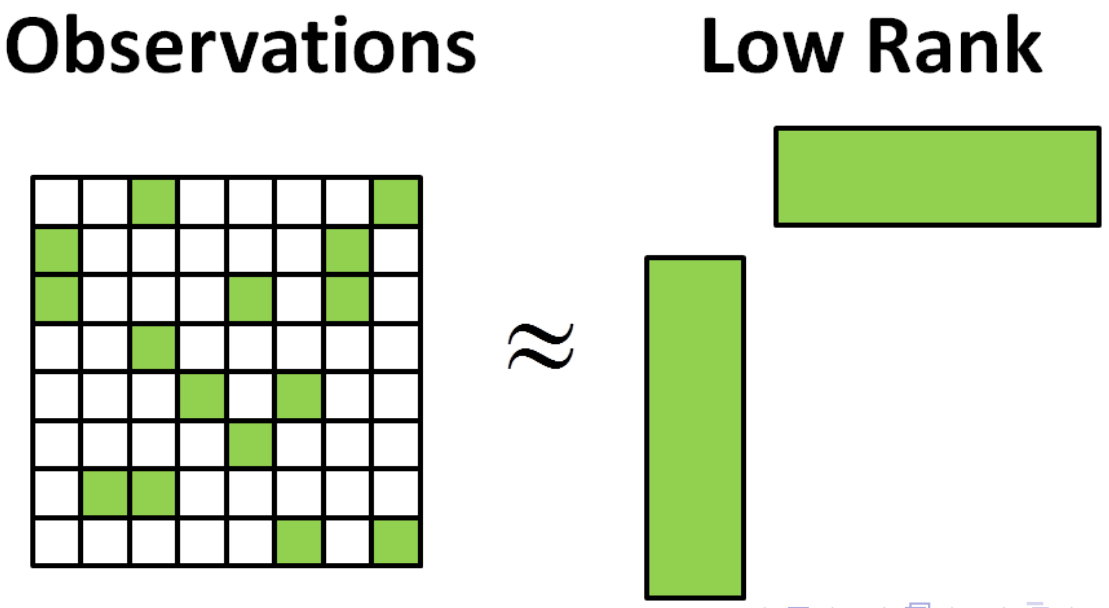


Updates on Free Set

Matrix Completion Problems

$$\min_X \{ \; g(X) \; + \; \lambda \|X\|_* \; \}$$

- $\|X\|_*$: a nuclear norm regularization to promote the low rank structure.
- Active variable selection $\Rightarrow$ Active subspace selection
  (identify the low-dimensional subspace)



Active Subspace Selection

- Given current iterate $X = U\Sigma V^T$, the "active subspace" is:

$$\mathcal{A} = \{\mathbf{u}\mathbf{v}^T \mid \mathbf{u}^T X \mathbf{v} \neq 0 \ \text{ or } \ |\mathbf{u}^T \nabla X \mathbf{v}| > \lambda\}.$$

- Step 1: Active subspace selection:
  - $U_G \Sigma_G V_G^\top = S_\lambda(X - \nabla g(X))$.
  - $U_A := \text{span}(U, U_G)$, $V_A := \text{span}(V, V_G)$.
  - $\mathcal{A} = \{\mathbf{u}\mathbf{v}^T \mid \mathbf{u} \in U_A, \mathbf{v} \in \mathcal{V}_A\}$.
- Step 2: Solve the reduced-sized problem:

$$\underset{S \in \mathbb{R}^{k \times k}}{\text{argmin}} \, \bar{g}_X(U_A S V_A^\top) + \lambda \|S\|_*,$$

  $\bar{g}_X(\cdot)$ is the quadratic approximation of $g(\cdot)$ at current iterate X
- Iterate steps 1 and 2.

- Subspace selection can be generalized to settings where the regularizer is a "decomposable norm" at the solution

Active Subspace Selection for Decomposable Norms

- A norm $\|\cdot\|$ is **decomposable** at $\boldsymbol{x}$ if there is a subspace $\mathcal{T}$ and vector $\boldsymbol{e} \in \mathcal{T}$ such that the sub differential at $\boldsymbol{x}$ is

$$\partial\|\boldsymbol{x}\|_r = \{\boldsymbol{\rho} \in \mathbb{R}^n \mid \Pi_{\mathcal{T}}(\boldsymbol{\rho}) = \boldsymbol{e} \text{ and } \|\Pi_{\mathcal{T}^\perp}(\boldsymbol{\rho})\|_r^* \leq 1\},$$

- Examples: ℓ_1 norm, nuclear norm, group lasso, ...
- **Active subspace selection**:
  - Divide the space into "fixed" subspace and "free subspace":

$$\mathcal{S}_{\text{free}} := [\mathcal{T}(\boldsymbol{\theta})] \cup [\mathcal{T}(\text{prox}_{\lambda_r}(G))], \quad \mathcal{S}_{\text{fixed}} = \mathcal{S}_{\text{free}}{}^{\perp},$$

    where $\mathcal{T}(\cdot)$ is the support of the decomposable norm.
  - Solve the reduced sized problem.

Active Subspace Selection for Dirty Models

- Superposition-structured models or "dirty models":

$$\min_{\{\boldsymbol{\theta}^{(r)}\}_{r=1}^{k}} \left\{ g\left(\sum_r \boldsymbol{\theta}^{(r)} \right) + \sum_r \lambda_r h^{(r)}(\boldsymbol{\theta}^{(r)}) \right\},$$

- Examples:
  - Sparse + low-rank graphical model learning
  - Multi-task learning (sparse + group-sparse or sparse + low-rank).
- Select active subspace for each $\boldsymbol{\theta}^{(r)}$.

Proximal Newton Method

Proximal Newton for Dirty Models (QUIC & DIRTY)

For $t = 0, 1, \ldots$

1. Compute $\bar{\boldsymbol{\theta}} = \sum_{r=1}^{k} \boldsymbol{\theta}^{(r)}$
2. Compute the current gradient $G = \nabla g(\bar{\boldsymbol{\theta}})$
3. Select free set by

$$\mathcal{S}_{\text{free}}^{(r)} := [\mathcal{T}(\boldsymbol{\theta}^{(r)})] \cup [\mathcal{T}(\text{prox}_{\lambda_r}^{(r)}(G))], \quad \mathcal{S}_{\text{fixed}}^{(r)} = \mathcal{S}_{\text{free}}^{(r)\,\perp},$$

4. For $r = 1, \ldots, k$
   - Solve the subproblem

$$\Delta^{(r)} = \underset{\boldsymbol{d} \in \mathbb{R}^n}{\text{argmin}} \langle \boldsymbol{d}, G + \sum_{t \neq r} H\Delta^{(t)} \rangle + \frac{1}{2} \boldsymbol{d}^T H \boldsymbol{d} + \lambda_r \|\boldsymbol{\theta}^{(r)} + \boldsymbol{d}\|_r.$$

5. **Line Search**: use an Armijo-rule based step-size selection to get α s.t. $\boldsymbol{\theta} = \boldsymbol{\theta} + \alpha\Delta$ sufficient decrease the objective function value.

Theoretical Guarantee

Theorem: Quadratic Convergence Rate for QUIC & DIRTY

Suppose $g(\cdot)$ is strongly convex and the quadratic subproblem at each iteration is solved exactly, QUIC & DIRTY converges to the global optimum with an asymptotic quadratic convergence rate:

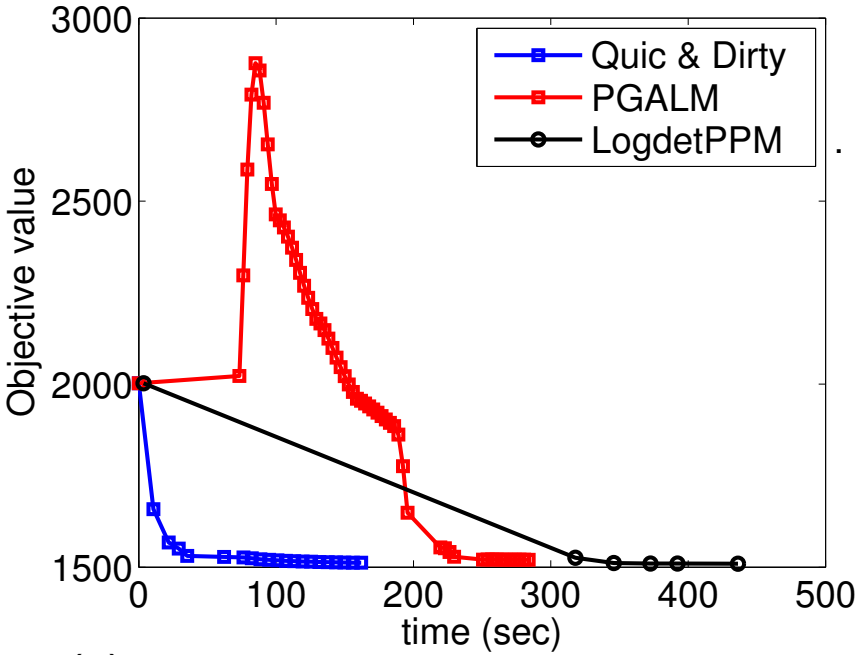
$$\lim_{t \to \infty} \frac{\|X_{t+1} - X^*\|_F}{\|X_t - X^*\|_F^2} = \kappa,$$

where κ is a constant.

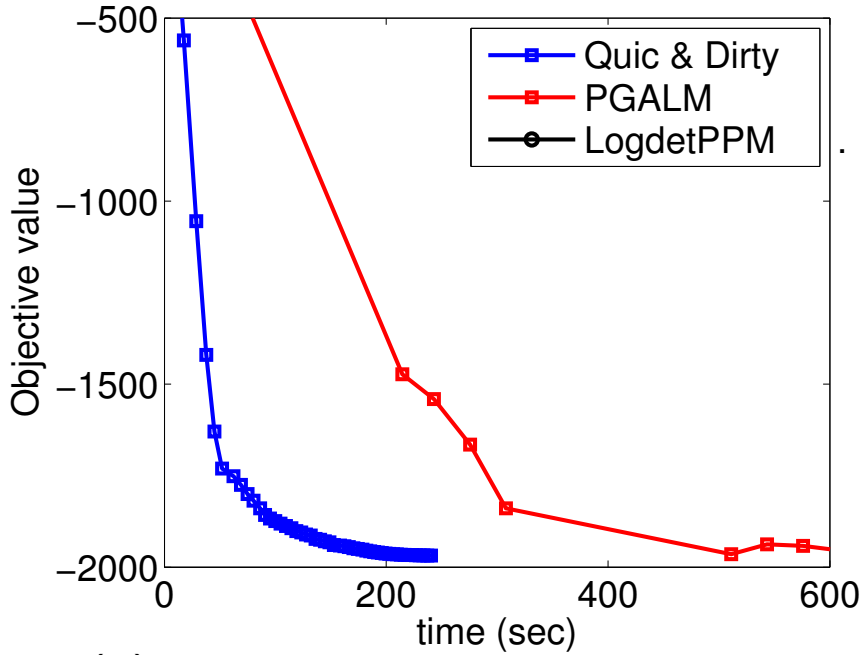
Results: Data from Biology Applications

Sparse + low rank graphical model learning

$$\min_{S,L:L\succeq 0,S-L\succ 0} -\log\det(S-L)+\langle S-L,\Sigma\rangle+\lambda_S\|S\|_1+\lambda_L\,\mathrm{tr}(L).$$



(c) Time for Leukemia, $p = 1,255$



(d) Time for Rosetta, $p = 2,000$

Application: Multi-task Learning

- Multi-task (multi-class) learning with sparse + group sparse structure.

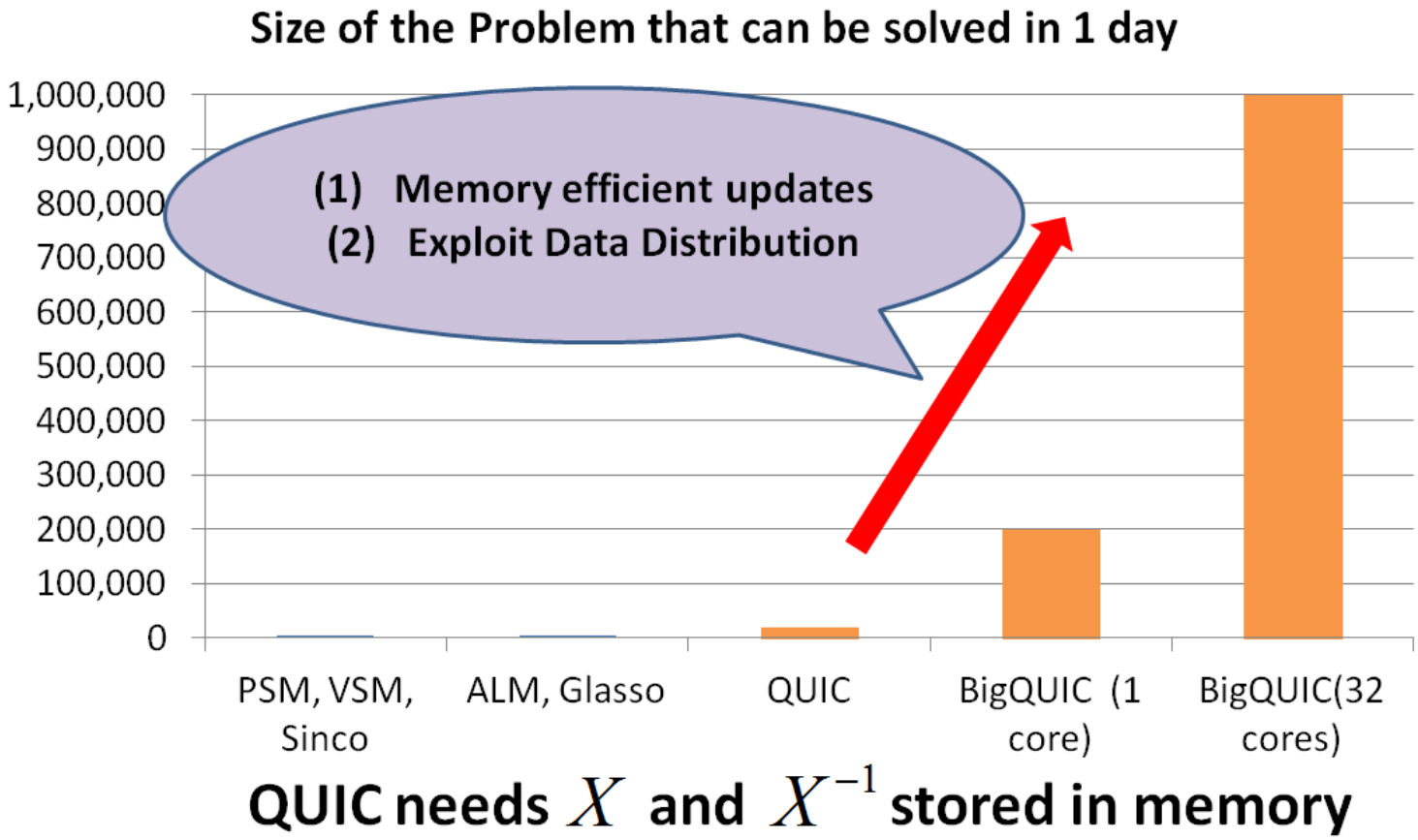
$$\sum_{r=1}^{k} \ell(y^{(r)}, X^{(r)}(S^{(r)} + B^{(r)})) + \lambda_S \|S\|_1 + \lambda_B \|B\|_{1,2},$$

dataset	number of training data	Dirty Models (sparse + group sparse)			Other Models	
		QUIC & DIRTY	proximal gradient	ADMM	Lasso	Group Lasso
USPS	100	7.47% / **0.75s**	7.49% / 10.8s	7.47% / 4.5s	10.27%	8.36%
	400	2.5% / **1.55s**	2.5% / 35.8	2.5% / 11.0s	4.87%	2.93%
RCV1	1000	18.45% / **23.1s**	18.49% / 430.8s	18.5% / 259s	22.67%	20.8%
	5000	10.27% / **87s**	10.27% / 2254s	10.27% / 1191s	13.67%	12.25%

Big & Quic

Sparse Inverse Covariance Estimation with 1 Million Random Variables

Big & Quic


Size of the Problem that can be solved in 1 day
1,000,000
900,000
800,000
700,000
600,000
500,000
400,000
300,000
200,000
100,000
0
(1) Memory efficient updates
(2) Exploit Data Distribution
PSM, VSM, Sinco
ALM, Glasso
QUIC
BigQUIC (1 core)
BigQUIC(32 cores)
QUIC needs X and X^{-1} stored in memory

Difficulties in Scaling QUIC

- Coordinate descent requires X_t and X_t^{-1},
  - needs $O(p^2)$ storage
  - needs $O(mp)$ computation per sweep, where $m = \|X_t\|_0$
- Line search (compute determinant of a big sparse matrix).
  - needs $O(p^2)$ storage
  - needs $O(p^3)$ computation

Line Search

- Given sparse matrix $A = X_t + \alpha D$, we need to
  1. Check its positive definiteness.
  2. Compute $\log\det(A)$.
- Cholesky factorization in QUIC requires $O(p^3)$ computation.
- If $A = \begin{pmatrix} a & \boldsymbol{b}^T \\ \boldsymbol{b} & C \end{pmatrix}$,
  - $\det(A) = \det(C)(a - \boldsymbol{b}^T C^{-1} \boldsymbol{b})$
  - A is positive definite iff C is positive definite and $(a - \boldsymbol{b}^T C^{-1} \boldsymbol{b}) > 0$.
- C is sparse, so can compute $C^{-1}\boldsymbol{b}$ using Conjugate Gradient (CG).
- Time complexity: $T_{CG} = O(mT)$, where T is number of CG iterations.

Difficulties in Scaling QUIC

- Coordinate descent requires X_t and X_t^{-1},
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- Line search (compute determinant of a big sparse matrix).
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  - needs $O(mp)$ computation

Back-of-the-envelope calculations

- Co-ordinate descent requires m computations of $\boldsymbol{w}_i^T D \boldsymbol{w}_j$.
- To solve a problem of size $p = 10^4$ (avg degree=10), QUIC takes 12 minutes
- Extrapolate: to solve a problem with $p = 10^6$, QUIC would take $12\text{min} \times 10^4 = 83.33$ days (2.6 days using 32 cores).
- p^2 memory means 8 Terabyte main memory for $p = 10^6$.
- Naive solution that has $O(m)$ memory requirement:
  - Compute $\boldsymbol{w}_i, \boldsymbol{w}_j$ by solving two linear systems by CG,
  - $O(T_{CG})$ computation per coordinate update
  - $O(mT_{CG})$ computation per sweep.
  - Would need 8,333 days to solve the problem for $p = 10^6$ (260 days using 32 cores).

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- BigQUIC solves problems of size $p = 10^6$ in one day on 32 cores.

Coordinate Updates with Memory Cache

- Assume we can store M columns of W in memory.
- Coordinate descent update (i, j): compute $\boldsymbol{w}_i^T D \boldsymbol{w}_j$.
- If $\boldsymbol{w}_i, \boldsymbol{w}_j$ are not in memory: recompute by CG:

  $X\boldsymbol{w}_i = \boldsymbol{e}_i$: $O(T_{CG})$ time.

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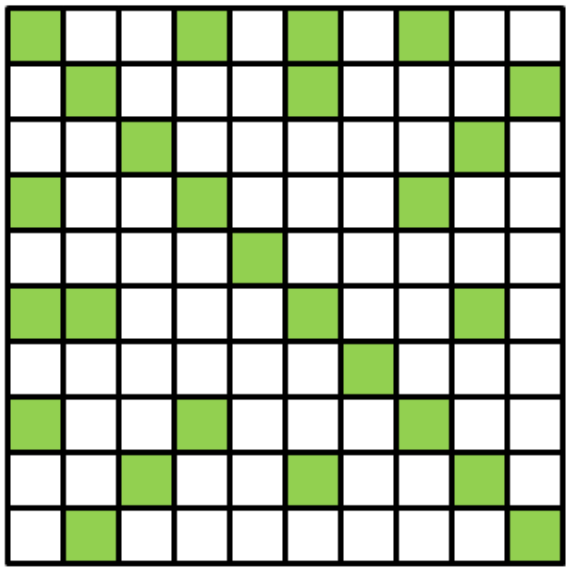

Free Set

Memory Cache
(M=4)

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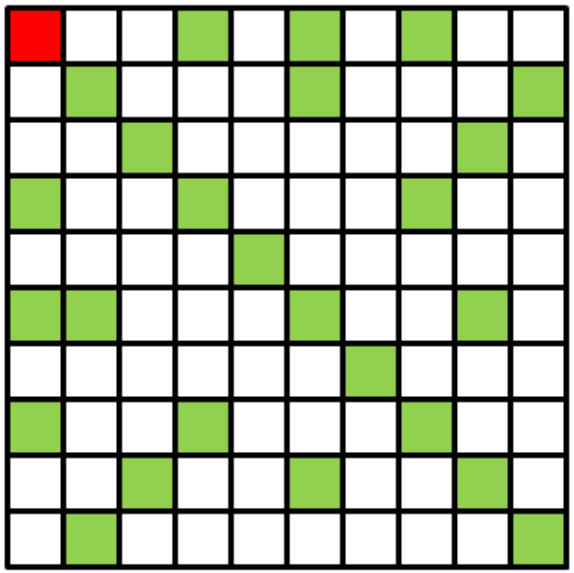
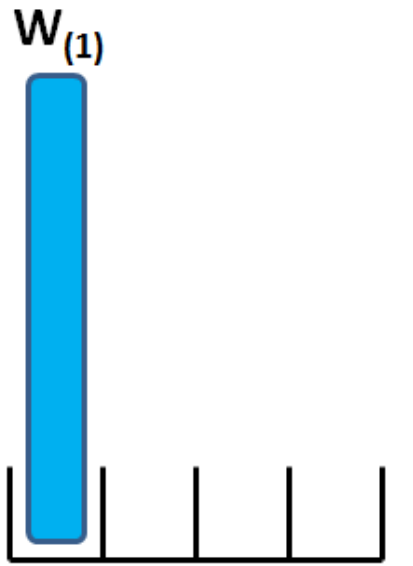


Update (1,1)



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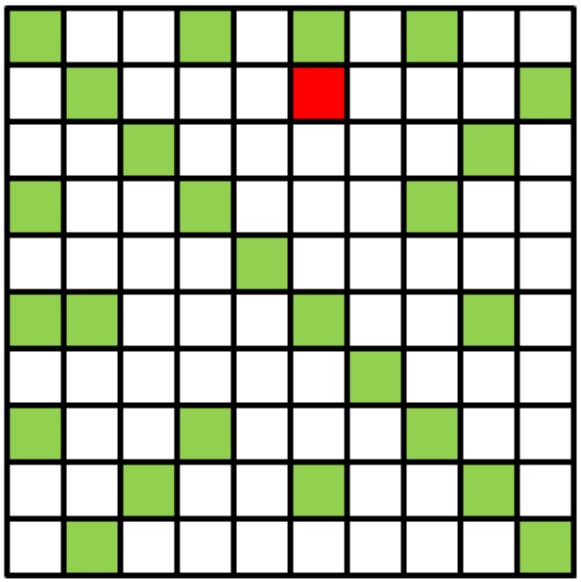
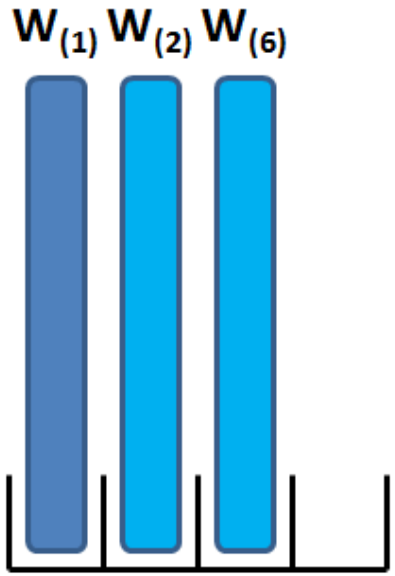


Update (2,6)



Memory Cache
(M=4)

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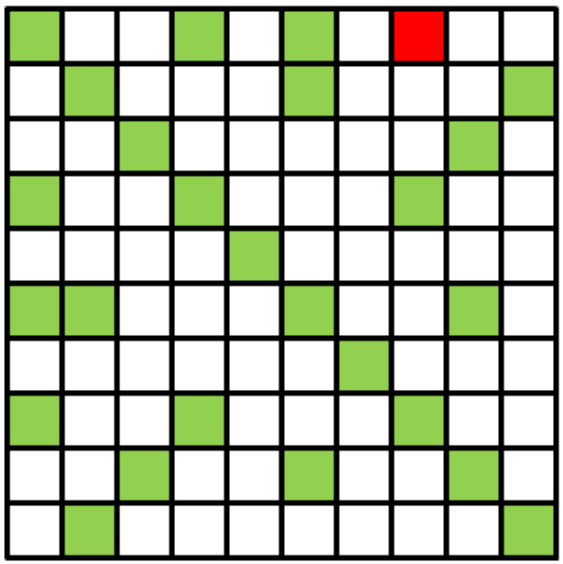
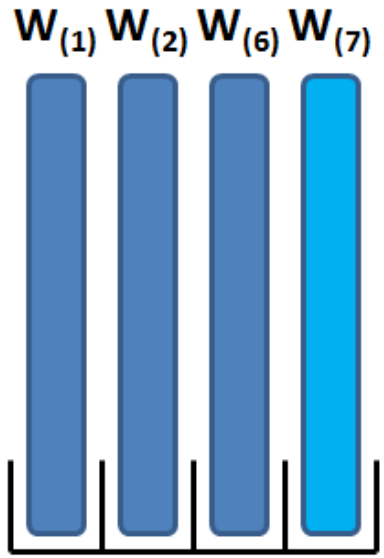


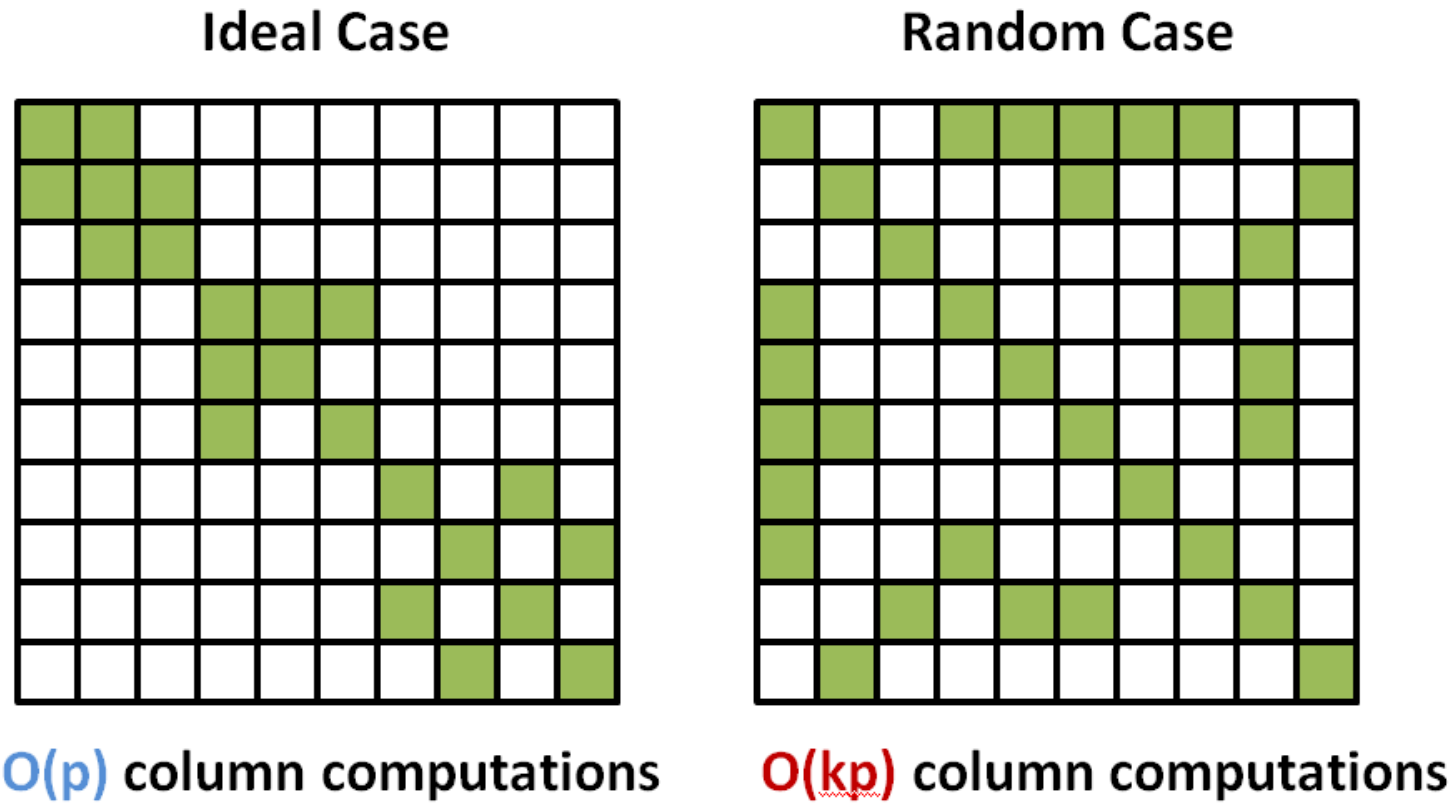
Update (1,7)



Memory Cache
(M=4)

Coordinate Updates – ideal case

- Want to find update sequence that minimizes number of cache misses: probably NP Hard.
- Our strategy: update variables **block by block** (assume $k = p/M$ blocks).



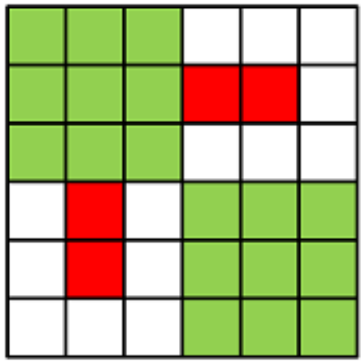
General case: block diagonal + sparse

- If the block partition is not perfect:

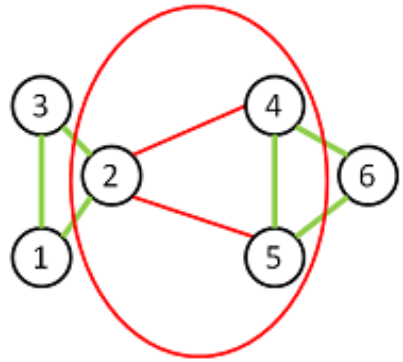
  extra column computations can be characterized by boundary nodes.
- Given a partition $\{S_1, \ldots, S_k\}$, we define boundary nodes as

$$B(S_q) \equiv \{j \mid j \in S_q \text{ and } \exists i \in S_z, z \neq q \text{ s.t. } F_{ij} = 1\},$$

where F is adjacency matrix of the free set.



Free Set



boundary nodes

Graph Clustering Algorithm

- The number of columns to be computed in one sweep is

$$p + \sum_q |B(S_q)|.$$

- Can be upper bounded by

$$p + \sum_q |B(S_q)| \leq p + \sum_{z \neq q} \sum_{i \in S_z, j \in S_q} F_{ij}.$$

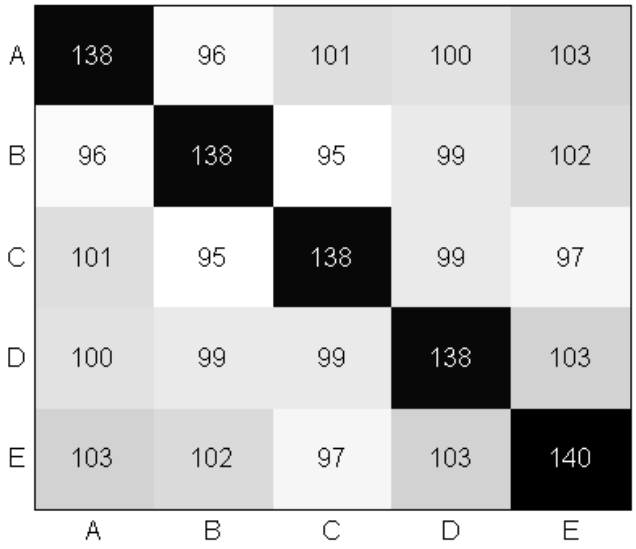
- Minimize the right hand side $\rightarrow$ minimize off-diagonal entries.

  Use Graph Clustering (METIS or Graclus) to find the partition.

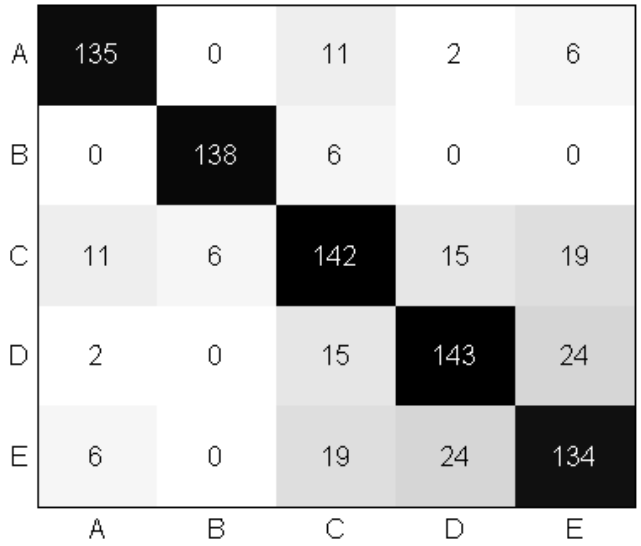
Size of boundary nodes in real datasets

ER dataset with $p = 692$.

Random partition
compute 1687 columns



Partition by clustering
compute 775 columns



$O(kpT_{CG}) \rightarrow O(pT_{CG})$ flops per sweep.

BigQUIC

- Block co-ordinate descent with clustering,
  - needs $O(m + p^2/k)$ storage
  - needs $O(mp)$ computation per sweep, where $m = \|X_t\|_0$
- Line search (compute determinant of a big sparse matrix).
  - needs $O(p)$ storage
  - needs $O(mp)$ computation

Convergence Guarantees for QUIC

Theorem (Hsieh, Sustik, Dhillon & Ravikumar, NIPS, 2011)

QUIC converges quadratically to the global optimum, that is for some constant $0 < \kappa < 1$*:*

$$\lim_{t \to \infty} \frac{\|X_{t+1} - X^*\|_F}{\|X_t - X^*\|_F^2} = \kappa.$$

BigQUIC Convergence Analysis

- Recall $W = X^{-1}$.
- When each $\boldsymbol{w}_i$ is computed by CG ($X\boldsymbol{w}_i = \boldsymbol{e}_i$):
  - The gradient $\nabla_{ij} g(X) = S_{ij} - W_{ij}$ on free set can be computed once and stored in memory.
  - Hessian ($\boldsymbol{w}_i^T D \boldsymbol{w}_j$ in coordinate updates) needs to be repeatedly computed.
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Theorem (Hsieh, Sustik, Dhillon, Ravikumar & Poldrack, 2013)

If $\nabla g(X)$ is computed exactly and $\bar{\eta} I \succeq \hat{H}_t \succeq \eta I$ for some constant $\bar{\eta}, \eta > 0$ at every Newton iteration, then BigQUIC *converges to the global optimum.*

BigQUIC Convergence Analysis

- To have super-linear convergence rate, we require the Hessian computation to be more and more accurate as X_t approaches X^*.
- Measure the accuracy of Hessian computation by $R = [\boldsymbol{r}_1 \ldots, \boldsymbol{r}_p]$, where $\boldsymbol{r}_i = X\boldsymbol{w}_i - \boldsymbol{e}_i$.
- The optimality of X_t can be measured by

$$\nabla^S_{ij} f(X) = \begin{cases} \nabla_{ij} g(X) + \text{sign}(X_{ij})\lambda & \text{if } X_{ij} \neq 0, \\ \text{sign}(\nabla_{ij} g(X)) \max(|\nabla_{ij} g(X)| - \lambda, 0) & \text{if } X_{ij} = 0. \end{cases}$$

Theorem (Hsieh, Sustik, Dhillon, Ravikumar & Poldrack, 2013)

In BigQUIC, *if residual matrix* $\|R_t\| = O(\|\nabla^S f(X_t)\|^\ell)$ *for some* $0 < \ell \leq 1$ *as* $t \to \infty$, *then* $\|X_{t+1} - X^*\| = O(\|X_t - X^*\|^{1+\ell})$ *as* $t \to \infty$.

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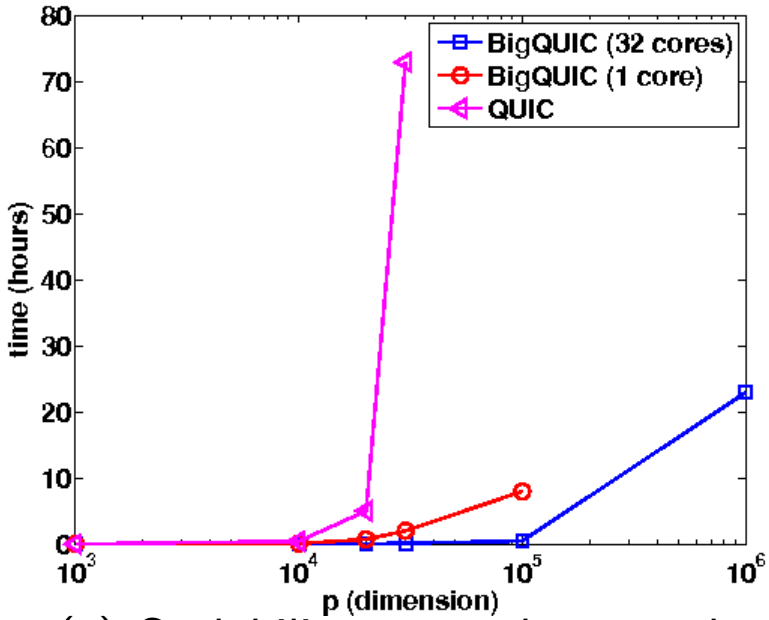
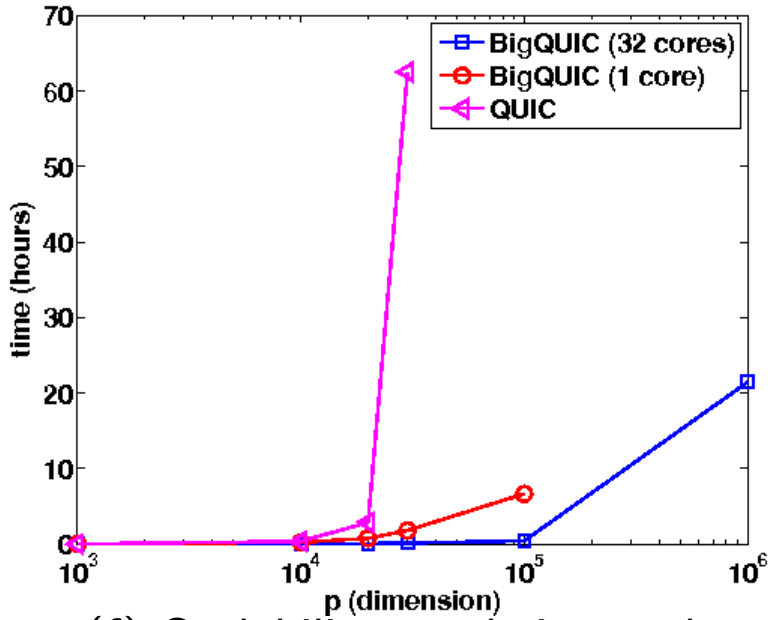
- When $\|R_t\| = O(\|\nabla^S f(X_t)\|)$, BigQUIC has asymptotic quadratic convergence rate.

Experimental results (scalability)



(e) Scalability on random graph



(f) Scalability on chain graph

Figure: BigQUIC can solve one million dimensional problems.

Experimental results

BigQUIC is faster even for medium size problems.

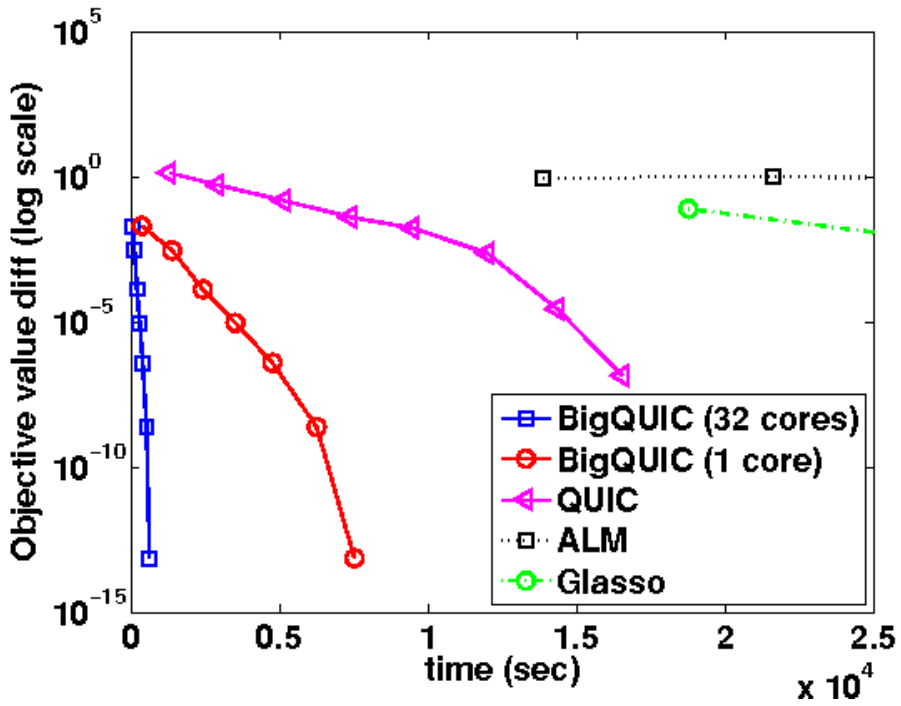
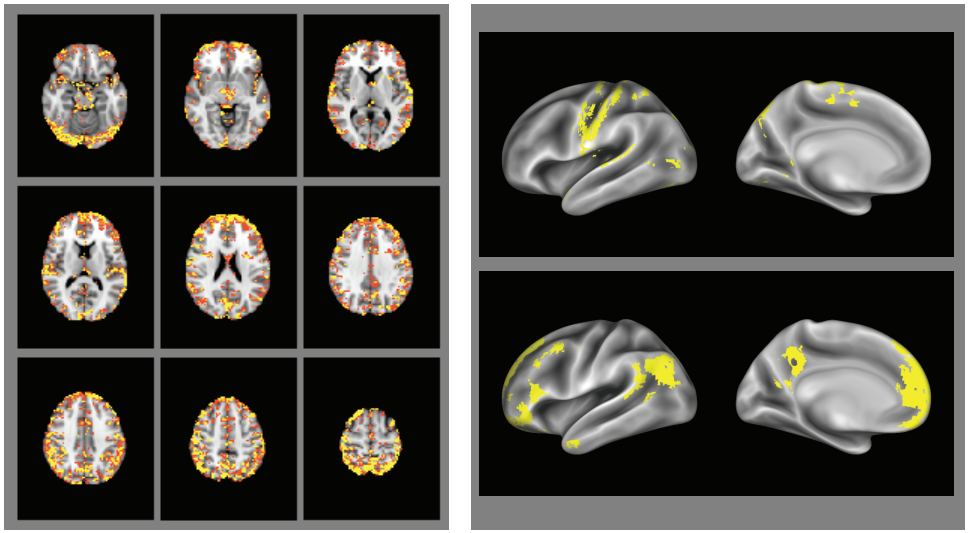


Figure: Comparison on FMRI data with a $p = 20000$ subset (maximum dimension that previous methods can handle).

Results on FMRI dataset

- 228,483 voxels, 518 time points.
- $\lambda = 0.6 \Longrightarrow$ average degree 8, BigQUIC took 5 hours.

  $\lambda = 0.5 \Longrightarrow$ average degree 38, BigQUIC took 21 hours.
- Findings:
  - Voxels with large degree were generally found in the gray matter.
  - Can detect meaningful brain modules by modularity clustering.



Conclusions

- **Proximal Newton method**: a second order method for optimizing a smooth convex function plus a non-smooth regularizer.
- How to develop an efficient proximal Newton method?

  Exploit problem structure and geometry of problem
- For sparse inverse covariance estimation problem, our proposed algorithm (BigQuic) can solve a 1-million dimensional problem in 1-day on a single 32-core machine.
- Main ingredients for BigQuic:
  - Fast coordinate descent solver for computing Newton direction.
  - Avoid un-important updates by **active subspace selection**.
  - Memory efficient coordinate descent updates.
- Quic & Dirty: extension to "Dirty" Statistical Models.

Future Work

- "Effective" order of Newton-like methods for specific problems?
- Multi-core Computation? "Wild" Co-ordinate Descent?
- Prioritized Scheduling (Co-ordinate Descent)?
- Suitability for Distributed for Out-of-core Computing?

- Develop scalable & reliable software
- No dearth of interesting applications!

References

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