

Probabilistic Graphical Models

Distributed ADMM for Gaussian Graphical Models

Yaoliang Yu Lecture 29, April 29, 2015

Networks / Graphs







Where do graphs come from?

- Prior knowledge
 - Mom told me "A is connected to B"

• Estimate from data!

- We have seen this in previous classes
- Will see two more today

• Sometimes may also be interested in edge weights

An easier problem

• Real networks are **BIG**

Require distributed optimization



Structural Learning for completely observed MRF (Recall)





 $(x_1^{(M)},...,x_n^{(M)})$

Gaussian Graphical Models

• Multivariate Gaussian density:

$$p(\mathbf{x} \mid \mu, \Sigma) = \frac{1}{(2\pi)^{n/2} |\Sigma|^{1/2}} \exp\left\{-\frac{1}{2} (\mathbf{x} - \mu)^T \Sigma^{-1} (\mathbf{x} - \mu)\right\}$$

• WOLG: let
$$\mu = 0$$
 $Q = \Sigma^{-1}$

$$p(x_1, x_2, \dots, x_p \mid \mu = 0, Q) = \frac{|Q|^{1/2}}{(2\pi)^{n/2}} \exp\left\{-\frac{1}{2} \sum_{i} q_{ii}(x_i)^2 - \sum_{i < j} q_{ij} x_i x_j\right\}$$

• We can view this as a continuous Markov Random Field with potentials defined on every node and edge:

The covariance and the precision matrices

• Covariance matrix Σ

$$\Sigma_{i,j} = 0 \quad \Rightarrow \quad X_i \perp X_j \quad \text{or} \quad p(X_i, X_j) = p(X_i) p(X_j)$$

- Graphical model interpretation?
- Precision matrix $Q = \Sigma^{-1}$

 $Q_{i,j} = 0 \quad \Rightarrow \quad X_i \perp X_j | \mathbf{X}_{-ij} \quad \text{or} \quad p(X_i, X_j | \mathbf{X}_{-ij}) = p(X_i | \mathbf{X}_{-ij}) p(X_j | \mathbf{X}_{-ij})$

• Graphical model interpretation?

Sparse precision vs. sparse covariance in GGM





	(1	6	0	0	0		(0.10	0.15	-0.13	-0.08	0.15
	6	2	7	0	0		0.15	-0.03	0.02	0.01	-0.03
$\Sigma^{-1} =$	0	7	3	8	0	$\Sigma =$	-0.13	0.02	0.10	0.07	-0.12
	0	0	8	4	9		-0.08	0.01	0.07	-0.04	0.07
	0	0	0	9	5		0.15	-0.03	-0.12	0.07	0.08

$$\Sigma_{15}^{-1} = 0 \Leftrightarrow X_1 \perp X_5 | X_{nbrs(1) \text{ or } nbrs(5)}$$

$$\Rightarrow$$

$$X_1 \perp X_5 \Leftrightarrow \Sigma_{15} = 0$$

Another example









- How to estimate this MRF?
- What if *p* >> *n*
 - MLE does not exist in general!
 - What about only learning a "sparse" graphical model?
 - This is possible when s=o(n)
 - Very often it is the structure of the GM that is more interesting ...

Recall lasso



$$\hat{\theta}_i = \arg\min_{\theta_i} l(\theta_i) + \lambda_1 \| \theta_i \|_1$$

where $l(\theta_i) = \log P(y_i | \mathbf{x}_i, \theta_i).$

Graph Regression (Meinshausen & Buhlmann'06)



Neighborhood selection





Graph Regression





Graph Regression



Pros:

- Computationally convenient
- Strong theoretical guarantee (p <= pol(n))

Cons:

- Asymmetry
- Not minimax optimal



The regularized MLE (Yuan & Lin'07)



$\min_{Q} - \log \det Q + \operatorname{tr}(QS) + \lambda \|Q\|_{1}$

- S: sample covariance matrix, may be singular
- ||Q||₁: may exclude the diagonal
- log det Q: implicitly force Q to be PSD symmetric

Pros

- Single step for estimating graph and inverse covariance
- MLE!

Cons

• Computationally challenging, partly solved by Glasso (Banergee et al'08, Friedman et al'08)

Many many follow-ups





A closer look of RMLE



$$\min_{Q} - \log \det Q + \operatorname{tr}(QS) + \lambda \|Q\|_{1}$$

• Set derivative to 0:

$$-Q^{-1} + S + \lambda \cdot \operatorname{sign}(Q) = 0$$

$$\|Q^{-1} - S\|_{\infty} \leq \lambda$$

• Can we (?!):

$$\min_{Q} \|Q\|_1 \text{ s.t. } \|Q^{-1} - S\|_{\infty} \le \lambda$$

CLIME (Cai et al.'11)

• Further relaxation

$$\min_{Q} \|Q\|_1 \text{ s.t. } \|SQ - I\|_{\infty} \leq \lambda$$

- Constraint controls $Q \approx S^{-1}$
- Objective controls sparsity in Q
- Q is not required to be PSD or symmetric

• Separable! LP!!!

- Both objective and constraint are element-wise separable
- Can be reformulated as LP
- Strong theoretical guarantee
 - Variations are minimax-optimal (Cai et al.'12, Liu & Wang'12)

But for **BIG** problems



$$\min_{Q} \|Q\|_1 \text{ s.t. } \|SQ - I\|_{\infty} \leq \lambda$$

- Standard solvers for LP can be slow
- Embarrassingly parallel:
 - Solve each column of Q independently in each core/machine

$$\min_{q_i} \|q_i\|_1 \text{ s.t. } \|Sq_i - e_i\|_{\infty} \leq \lambda$$

- Thanks for not having PSD constraint on Q
- Still troublesome if S is big
- Need to consider first-order methods



A gentle introduction to alternating direction method of multipliers (ADMM)



- Numerically challenging because
 - Function f or g nonsmooth or constrained (i.e., can take value ∞)
 - Linear constraint couples the variables w and z
 - Large scale, interior point methods NA
- Naively alternating x and z does not work
 - Min w^2 s.t. w + z = 1; optimum clearly is w = 0
 - Start with say $w = 1 \rightarrow z = 0 \rightarrow w = 1 \rightarrow z = 0 \dots$
- However, without coupling, can solve separately w and z
 - Idea: try to decouple vars in the constraint!

Example: Empirical Risk Minimization (ERM)



 $\min_{w} g(w) + \sum_{i=1}^{n} f_i(w)$

- Each i corresponds to a training point (x_i, y_i)
- Loss f_i measures the fitness of the model parameter w
 - least squares: $f_i(w) = (y_i w^{\top} x_i)^2$
 - support vector machines: $f_i(w) = (1 y_i w^{\top} x_i)_+$
 - boosting: $f_i(w) = \exp(-y_i w^\top x_i)$
 - logistic regression: $f_i(w) = \log(1 + \exp(-y_i w^\top x_i))$
- g is the regularization function, e.g. $\lambda_n \|w\|_2^2$ or $\lambda_n \|w\|_1$
- Vars coupled in obj, but not in constraint (none)
 - Reformulate: transfer coupling from obj to constraint
 - Arrive at canonical form, allow unified treatment later

Why canonical form?



ERM:
$$\min_{w} g(w) + \sum_{i=1}^{n} f_i(w)$$

$$\begin{array}{ll} \text{Canonical form:} & \min_{w,z} f(w) + g(z), \quad \text{s.t.} \quad Aw + Bz = c, \\ & \text{where } w \in \mathbb{R}^m, z \in \mathbb{R}^p, A : \mathbb{R}^m \to \mathbb{R}^q, B : \mathbb{R}^p \to \mathbb{R}^q, c \in \mathbb{R}^q \end{array}$$

- ADMM algorithm (to be introduced shortly) excels at solving the canonical form
 - Canonical form is a general "template" for constrained problems
- ERM (and many other problems) can be converted to canonical form through variable duplication (see next slide)

How to: variable duplication

• Duplicate variables to achieve canonical form

$$\min_{w} g(w) + \sum_{i=1}^{n} f_i(w)$$

$$\downarrow v = [w_1, \dots, w_n]^{\top}$$

$$\min_{v, z} \quad g(z) + \underbrace{\sum_{i} f_i(w_i)}_{f(v)}, \quad \text{s.t.} \quad \underbrace{w_i = z, \forall i}_{v - [I, \dots, I]^{\top} z = 0}$$

• Global consensus constraint: $orall i, w_i = z$

- All w_i must (eventually) agree
- Downside: many extra variables, increase problem size
 - Implicitly maintain duplicated variables

Augmented Lagrangian



Canonical form:
$$\min_{\mathbf{w}, \mathbf{z}} f(\mathbf{w}) + g(\mathbf{z}), \quad \text{s.t.} \quad A\mathbf{w} + B\mathbf{z} = \mathbf{c},$$

where $\mathbf{w} \in \mathbb{R}^m, \mathbf{z} \in \mathbb{R}^p, A : \mathbb{R}^m \to \mathbb{R}^q, B : \mathbb{R}^p \to \mathbb{R}^q, \mathbf{c} \in \mathbb{R}^q$

• Intro Lagrangian multiplier λ to decouple variables

$$\min_{\mathbf{w},\mathbf{z}} \max_{\boldsymbol{\lambda}} \underbrace{f(\mathbf{w}) + g(\mathbf{z}) + \boldsymbol{\lambda}^{\top} (A\mathbf{w} + B\mathbf{z} - \mathbf{c}) + \frac{\mu}{2} \|A\mathbf{w} + B\mathbf{z} - \mathbf{c}\|_{2}^{2}}_{L_{\mu}(\mathbf{w},\mathbf{z};\boldsymbol{\lambda})}$$

- L_{μ} : augmented Lagrangian
- More complicated min-max problem, but no coupling constraints

Why Augmented Lagrangian?

• Quadratic term gives numerical stability

$$\min_{\mathbf{w},\mathbf{z}} \max_{\boldsymbol{\lambda}} \underbrace{f(\mathbf{w}) + g(\mathbf{z}) + \boldsymbol{\lambda}^{\top} (A\mathbf{w} + B\mathbf{z} - \mathbf{c}) + \frac{\mu}{2} \|A\mathbf{w} + B\mathbf{z} - \mathbf{c}\|_{2}^{2}}_{L_{\mu}(\mathbf{w}, \mathbf{z}; \boldsymbol{\lambda})}$$

- May lead to strong convexity in w or z
 - Faster convergence when strongly convex
- Allows larger step size (due to higher stability)
- Prevents subproblems diverging to infinity (again, stability)
- But sometimes better to work with normal Lagrangian

ADMM Algorithm

$$\min_{\mathbf{w},\mathbf{z}} \max_{\boldsymbol{\lambda}} \underbrace{f(\mathbf{w}) + g(\mathbf{z}) + \boldsymbol{\lambda}^{\top} (A\mathbf{w} + B\mathbf{z} - \mathbf{c}) + \frac{\mu}{2} \|A\mathbf{w} + B\mathbf{z} - \mathbf{c}\|_{2}^{2}}_{L_{\mu}(\mathbf{w}, \mathbf{z}; \boldsymbol{\lambda})}$$

• Fix dual $\boldsymbol{\lambda}$, block coordinate descent on primal w, z

$$\begin{split} \mathbf{w}^{t+1} \leftarrow \arg\min_{\mathbf{w}} L_{\mu}(\mathbf{w}, \mathbf{z}^{t}; \boldsymbol{\lambda}^{t}) &\equiv f(\mathbf{w}) + \frac{\mu}{2} \|A\mathbf{w} + B\mathbf{z}^{t} - \mathbf{c} + \boldsymbol{\lambda}^{t}/\mu\|^{2} \\ \mathbf{z}^{t+1} \leftarrow \arg\min_{\mathbf{z}} L_{\mu}(\mathbf{w}^{t+1}, \mathbf{z}; \boldsymbol{\lambda}^{t}) &\equiv g(\mathbf{z}) + \frac{\mu}{2} \|A\mathbf{w}^{t+1} + B\mathbf{z} - \mathbf{c} + \boldsymbol{\lambda}^{t}/\mu\|^{2} \end{split}$$

Fix primal w, z, gradient ascent on dual $\boldsymbol{\lambda}$

$$\boldsymbol{\lambda}^{t+1} \leftarrow \boldsymbol{\lambda}^t + \eta (A \mathbf{w}^{t+1} + B \mathbf{z}^{t+1} - \mathbf{c})$$

- Step size η can be large, e.g. $\eta = \mu$
 - Usually rescale $oldsymbol{\lambda} \leftarrow oldsymbol{\lambda}/\eta~$ to remove η

ERM revisited



• Reformulate by duplicating variables

$$\min_{\mathbf{v},\mathbf{z}} \quad g(\mathbf{z}) + \underbrace{\sum_{i} f_i(\mathbf{w}_i)}_{f(\mathbf{v})}, \quad \text{s.t.} \quad \underbrace{\mathbf{w}_i = \mathbf{z}, \forall i}_{\mathbf{v} - [I, \dots, I]^\top \mathbf{z} = 0}$$

• ADMM x-step:

$$\mathbf{w}^{t+1} \leftarrow \arg\min_{\mathbf{w}} L_{\mu}(\mathbf{w}, \mathbf{z}^{t}; \boldsymbol{\lambda}^{t}) \equiv f(\mathbf{w}) + \frac{\mu}{2} \|A\mathbf{w} + B\mathbf{z}^{t} - \mathbf{c} + \boldsymbol{\lambda}^{t}/\mu\|^{2}$$
$$= \sum_{i} f_{i}(\mathbf{w}_{i}) + \frac{\mu}{2} \|\mathbf{w}_{i} - \mathbf{z}^{t} + \boldsymbol{\lambda}^{t}_{i}\|^{2}$$

• Thanks to duplicating



- Completely decoupled
- Parallelizable
- Closed-form if f_i is "simple"

ADMM: History and Related



- Augmented Lagrangian Method (ALM): solve w, z jointly even though coupled
 - (Bertsekas'82) and refs therein
- Alternating Direction of Multiplier Method (ADMM): alternate w and z as previous slide
 - (Boyd et al.'10) and refs therein
 - Operator splitting for PDEs: Douglas, Peaceman, and Rachford (50s-70s)
 - Glowinsky et al.'80s, Gabay'83; Spingarn'85
 - (Eckstein & Bertsekas'92; He et al.'02) in variational inequality
 - Lots of recent work.

ADMM: Linearization



- Demanding step in each iteration of ADMM (similar for z):
- $x_{t+1} \leftarrow \arg\min_{x} L_{\mu}(x, z_t; y_t) = f(x) + g(z_t) + y_t^{\mathsf{T}}(Ax + Bz_t c) + \frac{\mu}{2} \|Ax + Bz_t c\|_2^2$
 - Diagonal A: reduce to proximal map (more later) of f
 - $f(x) = ||x||_1$, soft-shrinkage: $\operatorname{sign}(x) \cdot (|x| \mu)_+$
 - Non-diagonal A: no closed-form, messy inner loop
 - Instead, reduce to diagonal A by
 - A single gradient step: $x_{t+1} \leftarrow x_t \eta \partial f(x_t) + A^\top y_t + \mu A^\top (Ax_t + Bz_t c)$
 - Or, linearize the quadratic at x_t :

 $x_{t+1} \leftarrow \arg\min_{x} \underbrace{f(x) + y_t^{\top} A x + (x - x_t)^{\top} \mu A^{\top} (A x_t + B z_t - c) + \frac{\mu}{2} \|x - x_t\|_2^2}_{2}$

 $f(x) + \frac{\mu}{2} \|x - x_t + A^\top (Ax_t + Bz_t - c + y_t/\mu)\|_2^2$

- Intuition: x re-computed in the next iteration anyways
 - No need for "perfect" x

Convergence Guarantees: Fixedpoint theory

• Recall some definitions

proximal map
$$\mathsf{P}_{f}^{\mu}(w) := \arg\min_{z} \frac{1}{2\mu} \|z - w\|_{2}^{2} + f(z)$$

reflection map $\mathsf{R}^{\mu}_{f}(w) := 2\mathsf{P}^{\mu}_{f}(w) - w$

- well-defined for convex f, non-expansive: $||T(x) T(y)||_2 \le ||x y||_2$
- proximal map generalizes the Euclidean projection

• Lagrangian:
$$L_0(x, z; y) = \underbrace{\min_x \left(f(x) + y^\top Ax \right)}_{d_1(y)} + \underbrace{\min_z \left(g(z) + y^\top (Bz - c) \right)}_{d_2(y)}$$

ADMM = Douglas-Rachford splitting

$$w \leftarrow \frac{1}{2}(w + \mathsf{R}^{\mu}_{d_2}(\mathsf{R}^{\mu}_{d_1}(w))); \quad y \leftarrow \mathsf{P}^{\mu}_{d_2}(w)$$

- Fixed-point iteration!
 - convergence follows, e.g. (Bauschke & Combettes'13)
 - explains why dual y, not primal x or z, always converges



ADMM for CLIME

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Apply ADMM to CLIME



$$\min_{Q} \|Q\|_1 \text{ s.t. } \|SQ - E\|_{\infty} \leq \lambda$$

- Solve a block of columns of Q in each core/machine
 - E is the corresponding block in I
- Step 1: reduce to ADMM canonical form
 - Use variable duplicating

 $\min_{Q,Z} \|Q\|_1 \text{ s.t. } \|Z - E\|_{\infty} \leq \lambda, \quad Z = SQ$ $\lim_{Q,Z} \|Q\|_1 + [\|Z - E\|_{\infty} \leq \lambda] \quad \text{s.t. } Z = SQ$

Apply ADMM to CLIME (cont')

• Step 2: Write out augmented Lagrangian

 $L(Q, Z; Y) = \|Q\|_1 + [\|Z - E\|_{\infty} \le \lambda] + \rho \operatorname{tr}[(SQ - Z)Y] + \frac{\rho}{2} \|SQ - Z\|_F^2$

• Step 3: Perform primal-dual updates

$$Q \leftarrow \arg\min_{Q} \|Q\|_{1} + \frac{\rho}{2} \|SQ - Z + Y\|_{F}^{2}$$
$$Z \leftarrow \arg\min_{Z} [\|Z - E\|_{\infty} \leq \lambda] + \frac{\rho}{2} \|SQ - Z + Y\|_{F}^{2}$$
$$= \arg\min_{\|Z - E\|_{\infty} \leq \lambda} \frac{\rho}{2} \|SQ - Z + Y\|_{F}^{2}$$
$$Y \leftarrow Y + SQ - Z$$

Apply ADMM to CLIME (cont")

• Step 4: Solve the subproblems

- Lagrangian dual Y: trivial
- Primal Z: projection to I_inf ball, separable, easy
- Primal Q: easy if S is orthogonal, in general a lasso problem
- Bypass double loop by linearization
 - Intuition: wasteful to solve Q to death

$$\min_{Q} \|Q\|_{1} + \rho \operatorname{tr}(Q^{\top}S(Y + SQ_{t} - Z)) + \frac{\eta}{2} \|Q - Q_{t}\|_{F}^{2}$$

- Soft-thresholding
- Putting things together

$$Q \leftarrow \arg\min_{Q} \|Q\|_{1} + \frac{\rho}{2} \|SQ - Z + Y\|_{F}^{2}$$
$$Z \leftarrow \arg\min_{Z} [\|Z - E\|_{\infty} \le \lambda] + \frac{\rho}{2} \|SQ - Z + Y\|_{F}^{2}$$
$$= \arg\min_{\|Z - E\|_{\infty} \le \lambda} \frac{\rho}{2} \|SQ - Z + Y\|_{F}^{2}$$
$$Y \leftarrow Y + SQ - Z$$

Exploring structure



- Expensive step in ADMM-CLIME:
 - Matrix-matrix multiplication: SQ and alike

- If p >> n, S is size p x p but of rank at most n $A = \begin{bmatrix} Y_1 & Y_2 \end{bmatrix} \subset \mathbb{R}^{p \times r}$
 - Write S = AA', and do A(A'Q) $A = [X_1, \dots, X_n] \in \mathbb{R}^{p imes n}$
- Matrix * matrix >> for loop of matrix * vector
 - Preferable to solve a balanced block of columns

Parallelization (Wang et al'13)

- Embarrassingly parallel
 - If A fits into memory
- Chop A into small blocks and distribute
 - Communication may be high





Numerical results (Wang et al'13)





Numerical results cont' (Wang et al'13)

node ×core	k = 1	k = 5	k = 10	k = 50	k = 100	k = 500	k = 1000
100×1	0.56	1.26	2.59	6.98	13.97	62.35	136.96
25×4	1.02	2.40	3.42	8.25	16.44	84.08	180.89
200×1	0.37	0.68	1.12	3.48	6.76	33.95	70.59
50×4	0.74	1.44	2.33	4.49	8.33	48.20	103.87



Nonparanormal extensions

Nonparanormal (Liu et al.'09)

$$Z_i = f_i(X_i), \quad i = 1, \dots, p$$

 $(Z_1, \dots, Z_p) \sim \mathcal{N}(0, \Sigma)$

- f_{i:} unknown monotonic functions
- Observe X, but not Z
- Independence preserved under transformations $X_i \perp X_j | X_{rest} \iff Z_i \perp Z_j | Z_{rest} \iff Q_{ij} = 0$
- Can estimate f_i first, then apply glasso on $f_i(X_i)$
 - Estimating functions can be slow, nonparametric rate

A neat observation

- Since f_i is monotonic
 - Z_{i,:} comonotone / concordant with X_{i,:}
- Use rank estimator !

$$Z_{i,1}, Z_{i,2}, \dots, Z_{i,n}$$

 $R_{i,1}, R_{i,2}, \dots, R_{i,n}$
 $X_{i,1}, X_{i,2}, \dots, X_{i,n}$

• Want \sum , but do not observe Z

• Maybe ???

$$\Sigma_{ij} = \frac{1}{n} \sum_{k=1}^{n} Z_{i,k} Z_{j,k} \stackrel{?}{=} \frac{1}{n} \sum_{k=1}^{n} R_{i,k} R_{j,k}$$

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 $Z_i = f_i(X_i), \quad i = 1, \dots, p$ $(Z_1, \dots, Z_p) \sim \mathcal{N}(0, \Sigma)$



Kendall's tau

• Assuming no ties:

$$\tau_{ij} = \frac{1}{n(n-1)} \sum_{k,\ell} \operatorname{sign}[(R_{i,k} - R_{i,\ell})(R_{j,k} - R_{j,\ell})]$$

• Complexity of computing Kendall's tau?

• Key:
$$\Sigma_{ij} = 2\sin(\frac{\pi}{6}\mathbb{E}(\tau_{ij}))$$

- Genuine, asymptotically unbiased estimate of \sum
- $t \mapsto 2\sin(\frac{\pi}{6}t)$ is a contraction, preserving concentration
- After having \sum , use whatever glasso, e.g., CLIME
 - Can also use other rank estimator, e.g., Spearman's rho

Summary



• Gaussian graphical model selection

- Neighborhood selection, Regularized MLE, CLIME
- Implicit PSD vs. Explicit PSD

• Distributed ADMM

- Generic procedure
- Can distribute matrix product

Nonparanormal Gaussian graphical model

- Rank statistics
- Plug-in estimator

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