# Matrix Algebra and Optimization for Statistics and Machine Learning

#### Yiyuan She

Department of Statistics, Florida State University

▶ Convexity and convex optimization

#### Convex functions

•  $f: \mathbb{R}^n \to \mathbb{R}$  is convex if dom f is a convex set and

$$\theta f(x) + (1 - \theta)f(y) - f(\theta x + (1 - \theta)y) \ge 0$$

holds for any  $x, y \in \text{dom} f$  and any  $\theta \in [0, 1]$ .

- Equivalently, f(x+tv) as a function of  $t \in \mathbb{R}$  is convex
- The RHS defines a useful operator  $\mathbf{C}_f(x, y, \theta)$ .
- ightharpoonup  $\Leftrightarrow$  Convexity of  $\{(x,t)|t\geq f(x),x\in\mathrm{dom}f\}$  (epigraph)
- $\blacktriangleright$  When f is differentiable, an equivalent definition is

$$\mathbf{D}_f(y,x) \triangleq f(y) - f(x) - \langle \nabla f(x), y - x \rangle \ge 0, \forall x, y \in \text{dom} f$$



- ▶ We often consider f as an extended convex function on  $\mathbb{R}^n$ :  $\tilde{f}(x) = f(x)$  if  $x \in \text{dom } f$  and  $+\infty$  otherwise
- ▶ Given a convex set A, say  $A = \{||x|| \le 1\}$ , the indicator function,  $\iota_A(x) = 0$  if  $x \in A$  and  $+\infty$  o/w, is convex
  - Constrained objective  $\rightarrow$  penalized objective
- ▶ Jensen's inequality: Let X be a random variable, f a convex function and  $X \in \text{dom } f$ , then  $f(\mathbb{E}X) \leq \mathbb{E}f(X)$

#### Strict/strong convexity

- $\blacktriangleright$  Assume f is convex and differentiable. Then
  - f is strictly convex means  $\mathbf{D}_f(y,x) > 0$  for  $x \neq y$
  - f is  $\alpha$ -strongly convex with  $\alpha > 0$  means  $\mathbf{D}_f(y, x) \ge \alpha \mathbf{D}_2(y, x) = \alpha \|y x\|^2 / 2$
- ▶ We do not have to assume differentiability if using  $\mathbf{C}_f$ . [Strict:  $\mathbf{C}_f(x, y, \theta) > 0 \ \forall x \neq y$ ; strong:  $\mathbf{C}_f \geq \alpha \mathbf{C}_2$ ]
- ▶ When  $f \in \mathcal{C}^{(2)}$ , convexity  $\iff \nabla^2 f(x) \succeq 0$ 
  - Strong convexity  $\Leftrightarrow \nabla^2 f(x) \succeq \alpha I$
  - Strict convexity is implied by  $\nabla^2 f(x) > 0$

## Optimality and convexity

- ▶ Let  $x^o$  be a (local) minimizer of f(x) with f differentiable. Then  $\langle \nabla f(x^o), x x^o \rangle \geq 0$ ,  $\forall x$  (feasible)
- ▶ It follows that  $f(x) f(x^o) \ge \mathbf{D}_f(x, x^o) \ \forall$  feasible x
  - If f is convex,  $x^o$  is a global minimizer; if f is strictly convex,  $x^o$  is unique!  $(\mathbf{D}_f(y,x) = 0 \to x = y)$
- ▶ Q: Does lasso min  $||y X\beta||_2^2/2 + \lambda ||\beta||_1$  always lead to a unique solution? How about graphical lasso?

#### Examples

- $ightharpoonup \exp(ax), |x|^a \text{ with } a \ge 1, -\log x, x \log x$
- ▶ Norm functions
- ▶ The max function  $f(x) = \max_i x_i$
- $ightharpoonup \log \sum \exp(a_i x_i)$  (multinomial)
  - Logistic regression:  $-y^T X \beta + \sum \log(1 + \exp(\tilde{x}_i^T \beta))$
- $ightharpoonup \log \det(X) \ (X \succeq 0)$ 
  - It suffices to show  $-\log \det(Z + tV)$  is convex in t
- ▶ Question: Are the last two strictly convex?

# 'Convex' operations

- ▶ If  $f_i$  are convex, so is  $\sum a_i f_i$  as long as  $a_i \geq 0$
- ▶ If f is convex, g(x) = f(Ax + b) is convex
- ▶ If  $f_i$  are convex, so is  $f(x) = \max_i f_i(x)$ . In fact,  $f(\cdot, l)$  is convex,  $\forall l \in L \Rightarrow \sup_{l \in L} f(x, l)$  is convex
- ▶ If h is convex and (its extension) is increasing, and g is convex, then f(x) = h(g(x)) is convex
  - Vector:  $h(g(x) = h(g_1(x), ..., g_n(x))$  is convex if  $g_i$  are convex, h is convex and increasing in each argument
- ▶ If f(x, y) is (jointly) convex, and C is a nonempty convex set, then  $g(x) = \inf_{y \in C} f(x, y)$  is convex

#### Examples

- ▶ If f(x) is convex, f(-x) is convex (& -f(x) is concave)
- ▶  $\log(\sum_k \exp(g_k(x)))$  is convex in x, if  $g_k$  are convex

▶ Courant-Fischer minimax theorem states that the k-th largest eigenvalue  $\lambda_i$  of a symmetric  $A \in \mathbf{S}^n$  is

$$\lambda_k(A) = \sup_{V: \dim V = k} \inf_{v \in V: ||v||_2 = 1} v^T A v$$
  
=  $\inf_{\dim V = n - k + 1} \sup_{v \in V: ||v||_2 = 1} v^T A v$ 

- ▶ Intuition: k = 2:  $V = V_{\lambda_1} \oplus V_{\lambda_2}, V_{\lambda_2} \oplus V_{\lambda_3}, V_{\lambda_1} \oplus V_{\lambda_n}, \dots$
- ▶ When k = 1,  $\lambda_1(A) = \sup_{v:||v||_2=1} v^T A v$  is a convex function. Indeed  $\lambda_1(A)$  gives the matrix norm  $||A||_2$

- ▶ Similarly, we know  $\lambda_n(A)$  is concave in A (and any induced matrix-norm is convex)
- $\triangleright$  A related fact (where  $\mathcal{P}_V$  is the projection onto V)

$$\lambda_1(A) + \dots + \lambda_k(A) = \sup_{\dim(V)=k} tr(A\mathcal{P}_V)$$

$$\lambda_n(A) + \dots + \lambda_{n-k+1}(A) = \inf_{\dim(V)=k} tr(A\mathcal{P}_V)$$

$$\Rightarrow \lambda_1(A) + \cdots + \lambda_k(A)$$
 is convex given any  $1 \le k \le n$ 

- So is  $w_1\lambda_1(A) + \cdots + w_k\lambda_k(A)$  if  $w_1 \ge \cdots \ge w_k \ge 0$
- ▶ A special case: A is diagonal. Extension:  $A \in \mathbb{R}^{n \times p}$ ?

## Sorted $\ell_1$ norm for high-dimensional **inference**

- ▶ Benjamini-Hochberg (BH) is widely used in multiple testing and controls the FDR level q
- ▶ Interestingly, BH can be characterized from an optimization perspective (Abramovich et al 13)
- ▶ In the regression setting, let  $\lambda_j = \sigma \Phi^{-1}(1 jq/2n)$  (1 ≤  $j \le p$ ). SLOPE minimizes the following objective

$$\frac{1}{2}||y - X\beta||_2^2 + \sum \lambda_j |\beta|_{(j)}$$

► Can you see the convex relaxation? Q: Study how SNR and dependencies affect the power; unknown scale.

# Conjugate

• Given  $f: \mathbb{R}^n \to \mathbb{R}$ , define its conjugate

$$f^*(y) = \sup_{x \in \text{dom}f} \{y^T x - f(x)\}\$$

where  $y \in \mathbb{R}^n : y^T x - f(x) < +\infty$  (domain!)

- $f^*$  is convex and closed (whether or not f is convex)
  - Closedness refers to the epigraph
- ▶ Surely it has a close connection to Lagrangian, and we have  $\langle x, y \rangle \leq f(x) + f^*(y)$  (Fenchel's inequality)

- ► Examples:
  - Support function of A: given A,  $\iota_A^*(y) = \sup_{x \in A} \langle y, x \rangle$
  - $f(x) = x^T Qx/2$  with Q pd  $\Rightarrow f^*(y) = y^T Q^{-1}y/2$
  - $f(x) = ax + b \Rightarrow f^*(y) = -b + \iota_{\{y=a\}}$
  - $f(x) = \lambda ||x|| (\lambda \ge 0) \Rightarrow f^*(y) = \iota_{||y||_* \le \lambda}$ . This is due to Holder's inequality  $\langle x, y \rangle \le ||x|| ||y||_*$
- ► Recognizing the conjugate can often facilitate the derivation of the dual problem

## Entropy functions

- Let  $f(x) = \log \sum_{1}^{n} \exp(x_i)$ . Then  $f^*(y) = \sum y_i \log y_i$ , where  $y \in \mathbb{R}^n : y_i \ge 0$  and  $1^T y = 1$  (negative entropy)
- ▶ **KL** divergence:  $D(p,q) = \sum p_i \log(p_i/q_i)$  for two discrete probabilities p, q (also called relative entropy)
  - Finiteness needs  $q_i = 0 \rightarrow p_i = 0$  and  $0 \log 0 := 0$
  - Un-normalized:  $D(p,q) = \sum \{p_i \log(p_i/q_i) p_i + q_i\},$ the Bregman divergence of  $\sum t_i \log t_i$
- ▶  $D(p,q) = -\sum p_i \log q_i + \sum p_i \log p_i = H(p,q) H(p)$ (cross-entropy minus entropy) and is convex (jointly)



- ▶ log{1/P(A)}: information or surprisal of event A
   No surprise, no information
- ▶ Entropy tells the average information of a r.v., and offers a measure of uncertainty or disorder (diversity)
- ► The principle of maximum entropy: Find a distribution satisfying all given constraints (but no more)
  - No additional knowledge is to be assumed (no bias)
  - Hence we would like to **maximize** the (remaining) uncertainty or information of the distribution

#### Maximum entropy

- ▶ One rolled a die many times and got an average of 5
- ▶ 5 > 3.5.. The die might not be fair. Then what could be a reasonable estimate of the distribution of X?
- ► Formulate the optimization problem as

$$\min_{p} \sum p_i \log p_i \text{ s.t. } p_i \ge 0, \sum p_i = 1, \sum i p_i = 5$$

or 
$$\min_{p} D(\{p_i\}, \{1/6\})$$
 s.t.  $p_i \ge 0, \sum p_i = 1, \sum i p_i = 5$ 

▶ The prior pmf  $\{1/6\}$  can be changed. Constraints extend to  $\mathbb{E}f_k(X) = 0$ ,  $1 \le k \le K$  (with  $f_k$  known)



## Most uncertain(informative) vs. most probable

► Constrained multinomial MLE:

$$\max \Pi p_i \text{ s.t. } p_i \ge 0, \sum p_i = 1, \sum i p_i = 5$$

- ▶ Empirical likelihood: Similarly, we can add a baseline to minimize  $-2 \log(\Pi p_i/\Pi(1/6)) = 2 \sum \{(1/6) \log(1/6) (1/6) \log p_i\} \propto D(\{1/6\}, \{p_i\}),$  subject to the same linear constraints (also convex)
- ► There is a large body of literature studying these optimization problems and the solutions' asymptotics
- ▶ The Cressie-Read (CR) family of divergence measures

# Constrained entropy & Poisson GLM

Let  $\mu_i$  be the unknowns (i = 1, ..., n),  $q_i \ge 0$  be the prior,  $x_j$  (j = 1, ..., p) be the features. Consider

$$\min_{\mu} D(\mu, q) = \sum_{i} \mu_{i} \log(\mu_{i}/q_{i}) - \mu_{i} + q_{i}$$
s.t.  $x_{j}^{T} \mu = \alpha_{j}, 1 \leq j \leq p, \mu_{i} \geq 0$ 

From the dual, it is equivalent to (non-rigorous for  $q_i = 0$ )

$$\min_{\beta} \langle q, \exp(X\beta) \rangle - \langle \alpha, \beta \rangle$$

which is the Poisson MLE when  $\alpha = X^T y, q = 1$ 



- ▶ Note the difference and relation between  $\mu, q, y$ 
  - A good example: iterative proportional scaling
- ▶ We can extend the result to derive distributions in the *exponential* family (by varying the support and moment constraints)
- ► Another note: "Least informative" priors refer to those containing least information in the <u>constraints</u> (but have maximum entropy or information)

#### Log-concave functions

- ▶ f(x) > 0 and  $-\log f$  is convex. (It is convenient to use the extended-value function here)
- Assume  $\operatorname{vec}(X) \sim \mathcal{N}(0, \Sigma_p \otimes I_n)$ . Then  $W = X^T X \sim W_p(\Sigma, n)$  (Wishart); its density is log-concave in W

$$\propto (\det W)^{(n-p-1)/2} (\det \Sigma)^{-n/2} \exp(-\frac{1}{2} tr(\Sigma^{-1} W))$$

▶ Also, the reparametrization  $\Omega = \Sigma^{-1}$  ensures the log-concavity of the **likelihood** in  $\Omega$ 



- ► Statisticians frequently encounter log-concave densities/distributions
  - Gibbs random fields, Monte Carlo, majorization, etc.
- ► A log-concave density is sub-exponential and unimodal
- ► The product of two log-concave functions is log-concave
- ▶ A nice & deep result: If  $f(\cdot, \cdot)$  is (jointly) log-concave, then  $g(x) = \int f(x, y) dy$  is also log-concave

- ► Therefore, all marginal densities of a log-concave density are necessarily log-concave
- ► Also, log-concavity is closed under convolution  $(f * g)(x) = \int f(x y)g(y) dy$
- ► The distribution of a log-concave density is log concave– $F(x) = \int_{-\infty}^{x} f(t) dt = \int_{-\infty}^{\infty} 1_{\geq 0}(x-t)f(t) dt$

## Moment/cumulant generating functions

- ▶ Due to the composition rules, the sum of log-convex functions is still log-convex (so is their product)
- ▶ So  $M_X(t) := \mathbb{E}_X \exp\langle t, X \rangle = \int \exp\langle t, X \rangle dF(x)$  is always log-convex!
- ▶ Under some regularity conditions,  $\nabla M(0) = [\mathbb{E}_X(\exp\langle t, X \rangle)']_{t=0} = \mathbb{E}X,$   $\nabla^2 M(0) = [\mathbb{E}_X \nabla (\exp\langle t, X \rangle X^T)]_{t=0} = \mathbb{E}[XX^T]$
- ▶  $m_X(t) = \log M_X(t)$  is convex and  $\nabla \log M(0) = \mathbb{E}X$ ,  $\nabla^2 \log M(0) = \mathbb{E}[(X - \mathbb{E}X)(X - \mathbb{E}X)^T]$
- ▶ We will define and study the derivatives later

- ▶ Consider bounding  $\mathbb{P}[X \in A]$  (A may not be convex)
- Similar to the proof of Markov inequality,

$$\mathbb{P}[X \in A] = \mathbb{E}1_A(X) \le \mathbb{E}\exp(\langle t, X \rangle) + \mu),$$

where  $\mu : \mu + \langle t, x \rangle \ge 0, \, \forall x \in A$ 

▶ We can solve a convex problem to get a bound, since

$$\mathbb{P}[X \in A] \le \exp\{\log \mathbb{E} \exp(\langle t, X \rangle) + \sup_{x \in A} (-\langle x, t \rangle)\}$$
$$= \exp(m_X(t) + \iota_A^*(-t))$$

where  $\iota_A^*$  is the support function (conjugate) of A

#### Generalized convexity

▶ Given a proper cone  $K \subseteq \mathbb{R}^m$  with associated inequality  $\leq_K$ ,  $f : \mathbb{R}^n \to \mathbb{R}^m$  is K-convex if

$$f(\theta x + (1-\theta)y) \preceq_K \theta f(x) + (1-\theta)f(y), \forall x, y, \theta \in [0,1]$$

- ► Matrix convexity for  $f : \mathbb{R}^n \to \mathbf{S}^m : \mathbf{C}_f(x, y, \theta) \succeq 0$ , where  $\mathbf{S}^m = \{X \in \mathbb{R}^{m \times m} : X = X^T\}$
- ▶ Generalized inequalities are used on matrix functions

## Generalized inequalities

- Let  $K \in \mathbb{R}^n$  be a proper cone satisfying (a) cone: for any  $x \in C$ ,  $\theta \ge 0$ ,  $\theta x \in C$ ; (b) convex; (c) closed; (d) solid (int $K \ne \phi$ ); (e) pointed (containing no line)
- ▶  $K = \mathbb{R}^n_+$ . Norm cones:  $C = \{(x, t) : ||x|| \le t\} \in \mathbb{R}^{n+1}$ . Positive semidefinite cone:  $\mathbf{S}^n_+ = \{X \in \mathbf{S}^n : X \succeq 0\}$
- ▶ K defines a partial ordering on  $\mathbb{R}^n$ :  $y \succeq_K 0 \Leftrightarrow y \in K$ ,  $x \preceq_K y \Leftrightarrow y x \in K$ ,  $x \prec_K y \Leftrightarrow y x \in \text{int}K$ .
- ▶ In particular, for two symmetric matrices  $X, Y \in \mathbf{S}^n$ ,  $X \succeq Y$  (associated with  $\mathbf{S}^n_+$ ) means X Y is psd

#### Convex optimization

► Consider the optimization problem:

$$\min f_0(x)$$
 s.t.  $f_i(x) \le 0, 1 \le i \le m, h_j(x) = 0, 1 \le j \le p$ 

- ► Feasibility problems:  $f_0 = 0$ . So the optimal value  $p^* \triangleq \inf\{f_0(x) : f_i(x) \leq 0, 1 \leq i \leq m, \ h_j(x) = 0, 1 \leq j \leq p\}$  is either 0 or  $+\infty$  (if the feasible set is empty)
- ▶ Convex optimization:  $f_0, f_1, ..., f_m$  are convex and the equality constraints are **affine**:  $a_j^T x = b_j$ ,  $1 \le j \le p$

# Examples of convex programming

- Linear program:  $\min c^T x + d$  s.t.  $Gx \leq h, Ax = b$ . Standard form LP:  $\min c^T x$  s.t.  $Ax = b, x \geq 0$
- ▶ Quadratic program (QP):  $\min x^T Px/2 + q^T x + r$  s.t.  $Gx \leq h, Ax = b$ , where P is psd  $(P \in S_+^n)$
- ▶ Quadratically constrained quadratic program (QCQP):  $\min x^T Px/2 + q^T x + r$  s.t.  $x^T P_i x/2 + q_i^T x + r_i \le 0, 1 \le i \le m, Ax = b$ , where  $P, P_i$  are psd
- Second-order cone program (SOCP): min  $f^T x$  s.t.  $||A_i x + b_i||_2 \le c_i^T x + d_i, 1 \le i \le m, F x = g.$ 
  - Note the second-order (norm) cone in form of  $||x||_2 \le t$

## Semidefinite programming

- Convex optimization with generalized inequality constraints: min  $f_0(x)$  s.t.  $f_i(x) \leq_{\mathbf{K}_i} 0$ ,  $1 \leq i \leq m$ , Ax = b, where  $K_i$  are proper cones,  $f_0$ ,  $f_i$  are convex
  - Ordinary convex programming:  $K_i = \mathbf{R}_+$
- ▶ Conic-form problems:  $\min c^T x$  s.t. $Fx + g \leq_K 0, Ax = b$
- ▶ SDP:  $K = \mathbf{S}_+^k$ , i.e., for  $x \in \mathbb{R}^n$ ,  $F_i, G \in \mathbf{S}^k$ ,  $A \in \mathbb{R}^{\times n}$  $\min c^T x \text{ s.t. } x_1 F_1 + \dots + x_n F_n + G \leq 0, Ax = b$
- ▶ Note the linear matrix inequality (& linear objective)



▶ Standard form SDP (with a matrix variable):

$$\min tr(CX)$$
 s.t.  $tr(A_iX) = b_i(1 \le i \le p), X \succeq 0$ 

where  $X, C, A_i$  are symmetric matrices of the same size

- ▶  $LP \subset QP \subset QCQP \subset SOCP \subset SDP$ 
  - QCQP  $\subset$  SOCP: Convex quadratic constraint can be written as SOC; min t s.t.  $x^T P x / 2 + 0 \cdot t^2 + q^T x t + r \le 0, x^T P_i x / 2 + q_i^T x + r_i \le 0, 1 \le i \le m, Ax = b$
  - SOCP ⊂ SDP: <u>2nd-order</u> constraints can be converted to LMI using the (generalized) <u>Schur complement</u>:

$$||x||_2 \le t \Leftrightarrow t - x^T t^+ x \succeq 0, t \succeq 0, (1 - tt^+) x = 0 \Leftrightarrow \begin{bmatrix} t & x^T \\ x & tI \end{bmatrix} \succeq 0$$

- ► SDP can be efficiently solved by say interior point methods, and has very good software support
  - SeDuMi, SDPT3, SDPA, ...
  - Also, check CVX, CVXOPT
- ► However, the guaranteed polynomial-complexity is still prohibitive on large (or even moderate) problems

#### Robust programming

- ▶ Let's start with an LP:  $\min c^T x$  s.t.  $a_i^T x \leq b_i, 1 \leq i \leq n$
- ▶ Assume  $a_i$  are Gaussian **random** vectors  $\mathcal{N}(\bar{a}_i, \Sigma_i)$  and each constraint holds with probability at least  $\eta$

$$\min c^T x \text{ s.t. } \mathbb{P}(a_i^T x \le b_i) \ge \eta, 1 \le i \le n$$

▶ Since  $\mathbb{P}(z \leq b) \geq \eta \Leftrightarrow b \geq F_z^{-1}(\eta)$ , we get an SOCP

$$\min c^T x \text{ s.t. } \bar{a}_i^T x + \Phi^{-1}(\eta) \| \sum_{i=1}^{1/2} x \|_2 \le b_i, 1 \le i \le n$$



#### A latent variable model for classification

Let 
$$y_i = \begin{cases} 1, & \tilde{x}_i^T \beta + \epsilon_i > 0 \\ 0, & \tilde{x}_i^T \beta + \epsilon_i \le 0 \end{cases}$$
, where  $\epsilon_i \stackrel{iid}{\sim} F$ 

- $\triangleright$  Assume F has a log-concave density f
- $y_i$  is Bernoulli:  $\pi_i = 1 F(-\tilde{x}_i^T \beta) = F((-\tilde{x}_i^T \beta, +\infty))$
- $L(\beta) = -\sum \log(1 \pi_i) \sum y_i \log(\pi_i/(1 \pi_i)) = -\sum y_i \log F(-\tilde{x}_i^T \beta) \sum (1 y_i) \log(F((-\tilde{x}_i^T \beta, +\infty)))$
- ▶ L is always convex in  $\beta$  (why?)
- A perhaps more convenient way:  $y_i = 1_{\tilde{x}_i^T \beta \geq \varepsilon_i}$ ,  $\varepsilon_i \stackrel{iid}{\sim} F$

Some special cases (with different tails & symmetry)

- $F = \Phi$  gives Probit models  $(F^{-1}(\pi_i) = \tilde{x}_i^T \beta)$
- ▶ Assuming a logistic distribution for  $\epsilon_i$  (symmetric):

$$f(x) = \frac{\exp(-x)}{(1 + \exp(-x))^2}, \ F(x) = \frac{1}{1 + \exp(-x)}$$

we get the logistic regression

- ► Gumbel distribution:  $F(t) = \exp(-\exp(-t))$ ,  $f(t) = \exp(-t \exp(-t))$  (nonsymmetric but log-concave) → negative log-log link  $g = -\log(-\log(\pi))$
- ▶ Choice? Relate the link function to  $\varepsilon_i$ 's distribution!

#### Max cut

- ▶ let G be an undirected graph with n nodes and  $n^2$  weights  $a_{ij} \ge 0$  placed on the edges  $(a_{ij} = a_{ji})$
- ▶ The problem is to find a partition  $S \cup S^C = [n]$  to maximize the sum of the weights of the 'crossing' edges
- ▶ Let  $S = \{i \in [n] : x_i = 1\}$  and  $S^c = \{i \in [n] : x_i = -1\}.$

$$\max_{x \in \{-1,1\}^n} \frac{1}{2} \sum_{i,j} a_{ij} 1_{x_i x_j = -1} = \frac{1}{4} \sum_{i,j} a_{ij} (1 - x_i x_j)$$

• Equivalent to  $\min_{x \in \{-1,1\}^n} x^T A x$ .



- ▶ The IP is well known to be NP-hard. Convex relation?
  - Replace the constraints by  $-1 \le x_i \le 1$  (and use  $A + \lambda I$  in place of A?  $||x||_2^2 = n$  on  $\{-1, 1\}^n$ )
- ▶ To make a better one, introduce  $X = xx^T$  which satisfies  $X \succeq 0$ ,  $X_{i,i} = 1$ , and rank(X) = 1. Consider

$$\min_{X \in \mathbf{S}^n} \langle A, X \rangle \text{ s.t. } X_{i,i} = 1, X \succeq 0$$

► The SDP gives impressive bounds on the optimal value. Need an extra rounding to get an approximate solution

#### Nuclear norm minimization

▶ Let's consider a matrix completion problem

$$\min_{X \in \mathbb{R}^{n \times m}} \operatorname{rank}(X) \text{ s.t. } \mathcal{A}(X) = b$$

where  $\mathcal{A}(\cdot)$  denotes a linear mapping

- ▶ Enforcing low rank is natural and effective
  - Robust PCA, video inpainting, recommender systems
- ▶ A convex relaxation can be made with nuclear norm

$$\min_{X \in \mathbb{R}^{n \times m}} \|X\|_* \text{ s.t. } \mathcal{A}(X) = b$$

▶ How to deal with the nondifferentiable objective?



- ► Fazel (02):  $||X||_* \le t \iff tr(W_1)/2 + tr(W_2)/2 \le t$  for some  $W_i$  satisfying  $\begin{bmatrix} W_1 & X \\ X^T & W_2 \end{bmatrix} \succeq 0$ . (Use SDP duals!)
- ▶ Hence we get an **SDP** as follows

$$\min_{X \in \mathbb{R}^{n \times m}, W_1 \in \mathbf{S}^n, W_2 \in \mathbf{S}^m} tr(W_1)/2 + tr(W_2)/2$$
s.t.  $\mathcal{A}(X) = b$ ,  $\begin{bmatrix} W_1 & X \\ X^T & W_2 \end{bmatrix} \succeq 0$ 

► Other ways exist to solve it (e.g., **proximal** methods)

## A sparse PCA

- ▶ Recall that given  $X = UDV^T$ ,  $XV_rV_r^T$  gives the best rank-r approximation to X in the sense of F-norm
- ▶ We can minimize  $||X X\mathbf{P}||_F^2$  over all rank-r projection matrices, or equivalently,  $\max_{\mathbf{P} \in \mathcal{P}^r} \langle \Sigma, \mathbf{P} \rangle$
- Here,  $\Sigma = X^T X$ ,  $\mathcal{P}^r = \{P : P^2 = P, P^T = P, r(P) = r\}$
- ▶ A formulation of the sparse PCA problem is

$$\max_{\mathbf{P} \in \frac{\mathcal{P}^r}{}} \langle \Sigma, \mathbf{P} \rangle - \lambda \| \operatorname{vec}(\mathbf{P}) \|_{\mathbf{1}}$$

 $\blacktriangleright$  A convex relation (**Fantope** of order r, Vu et al 13):

$$\mathcal{F}^r = \{ P : 0 \le P \le I, tr(P) = r \}$$

- ► The resulting problem is an SDP. (Of course, we can solve it using other methods, such as ADMM.)
- ▶ Do you think if pursuing sparsity in **P** makes sense? Later we will introduce other forms of sparse PCA.