Chapter 6: Optimization for Data Science
Optimization in Machine Learning and Statistics

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Maximum likelihood estimation

Distribution estimation: Estimate a probability density $p(y)$ of a random variable from observed data

Parametric distribution estimation: Choose from a family of densities $p_\beta(y)$ parametrized in β

Maximum likelihood estimation: Observations y_i for $i = 1, \ldots, m$. Assume the values are iid samples from $p_\beta(\cdot)$. Then, the likelihood to observe y_i, $i = 1, \ldots, m$ is

$$\ell(\beta) = \prod_{i=1}^{m} p_\beta(y_i).$$

The parameters most likely to have generated the observations are found by solving $\max_\beta \ell(\beta)$ or, equivalently, $\max_\beta \log \ell(\beta)$.

$$L(\beta) = \log \ell(\beta) = \sum_{i=1}^{m} \log(p_\beta(y_i))$$

is the log-likelihood function.

Linear measurement model

$$y_i = x_i^\top \beta + v_i$$

- (y_i, x_i) observations
- β unknown parameters
- $v_i \sim p(\cdot)$ noise

The maximum likelihood (ML) estimate is an optimal solution of

$$\max_{\beta} L(\beta) = \max_{\beta} \sum_{i=1}^{m} \log(p(y_i - x_i^\top \beta))$$

Example: Gaussian noise: $p(v) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{v^2}{2\sigma^2}} \quad (\sigma > 0)$

$$\Longrightarrow L(\beta) = -\frac{m}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\|y - X\beta\|_2^2,$$

where $X = [x_1, \ldots, x_m]^\top$ and $y = [y_1, \ldots, y_m]^\top$

Linear measurement model

$$y_i = x_i^\top \beta + v_i$$

- (y_i, x_i) observations
- β unknown parameters
- $v_i \sim p(\cdot)$ noise

The maximum likelihood (ML) estimate is an optimal solution of

$$\max_\beta L(\beta) = \max_\beta \sum_{i=1}^{m} \log(p(y_i - x_i^\top \beta))$$

Example: Laplacian noise: $p(v) = \frac{1}{2a} e^{-\frac{|v|}{a}} \quad (a > 0)$

$$\implies L(\beta) = -m \log(2a) - \frac{1}{a} \|y - X\beta\|_1,$$

where $X = [x_1, \ldots, x_m]^\top$ and $y = [y_1, \ldots, y_m]^\top$

Linear measurement model

$$y_i = x_i^\top \beta + v_i$$

- (y_i, x_i) observations
- β unknown parameters
- $v_i \sim p(\cdot)$ noise

The maximum likelihood (ML) estimate is an optimal solution of

$$\max_\beta L(\beta) = \max_\beta \sum_{i=1}^{m} \log(p(y_i - x_i^\top \beta))$$

Example: Uniform noise: $p(v) = \begin{cases} \frac{1}{2a}, & \text{if } v \in [-a, a], \quad (a > 0) \\ 0 & \text{else} \end{cases}$

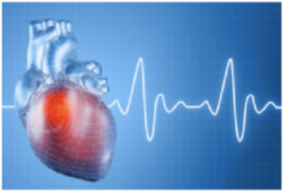
$$\implies L(\beta) = \begin{cases} -m \log(2a), & \text{if } \|y - X\beta\|_\infty \leq a \\ -\infty, & \text{else} \end{cases}$$

where $X = [x_1, \ldots, x_m]^\top$ and $y = [y_1, \ldots, y_m]^\top$

Logistic regression

Predicting the probability of a heart attach based on

- age
- height
- weight
- blood pressure
- cholesterol level
- etc.



$$\text{Label:} \quad y = \begin{cases} +1 & \text{person } x \text{ has a heart attack} \\ -1 & \text{person } x \text{ is healthy} \end{cases}$$

$$\text{Model:} \quad p_\theta(y|x) = \frac{1}{1 + \exp(-y \cdot \theta^\top x)} \qquad \theta \text{ unknown parameter}$$

Logistic regression (cont'd)

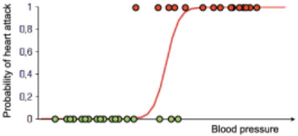
- Training data: $\{(x_i, y_i)\}_{i=1}^m$
- Log-likelihood function:

$$L(\theta) = \log \prod_{i=1}^{m} (1+\exp(-y_i \cdot \theta^\top x_i))^{-1} = -\sum_{i=1}^{m} \log(1+\exp(-y_i \cdot \theta^\top x_i))$$

- Logloss function: $l(z) = \log(1 + \exp(-z))$
  - smooth overestimation of $\max\{-z, 0\}$
  - special case of a log-sum-exp function $\Longrightarrow$ convex

ML estimation $\Longleftrightarrow$ empirical logloss minimization

$$\min_\theta \frac{1}{m} \sum_{i=1}^{m} l(y_i \cdot \theta^\top x_i)$$



Covariance estimation for Gaussian variables

- $y \in \mathbb{R}^n$ is Gaussian with mean zero and covariance matrix R. Its density is

$$p_R(y) = \frac{1}{\sqrt{(2\pi)^n \det R}} e^{-\frac{1}{2} y^\top R^{-1} y}$$

- Log-likelihood function for observations y_i, $i = 1, \ldots, m$

$$L(R) = -\frac{mn}{2} \log(2\pi) - \frac{m}{2} \log(\det R) - \frac{m}{2} \mathrm{tr}(YR^{-1}),$$

where $Y = \frac{1}{m} \sum_{i=1}^{m} y_i y_i^\top$ is the sample covariance matrix

Note: This log-likelihood function is not concave

Covariance estimation for Gaussian variables (cont'd)

- Information matrix: $S = R^{-1} \quad (S \succ 0 \iff R \succ 0)$
- Using S instead of R as the parameter, we find

$$L(S) = -\frac{mn}{2}\log(2\pi) + \frac{m}{2}\log(\det S) - \frac{m}{2}\mathrm{tr}(YS),$$

which is concave

- The ML estimate of S (and thus R) is found by solving

$$\begin{cases} \max & \log(\det S) - \mathrm{tr}(YS) \\ \text{s.t.} & S \in \mathcal{S}, \end{cases}$$

where $\mathcal{S}$ contains all constraints that capture prior structural information

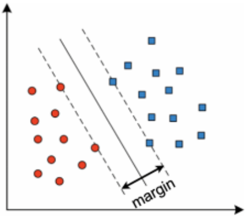
- If $\mathcal{S} = \mathbb{S}^n_{++}$, then $S = Y^{-1} \iff R = Y$ at optimality
(Recall that $\nabla \log(\det S) = S^{-1}$)

Support Vector Machines (SVM)

Classification problem: Given labelled data pairs (x_i, y_i), $i = 1, \dots, m$, where $x_i \in \mathbb{R}^d$ are the features (e.g., age, blood pressure, ...) and $y_i \in \{1, -1\}$ are the labels (e.g., healthy vs. heart attack, red vs. blue,...)

Goal: Predict the label of a new feature $x \in \mathbb{R}^n$

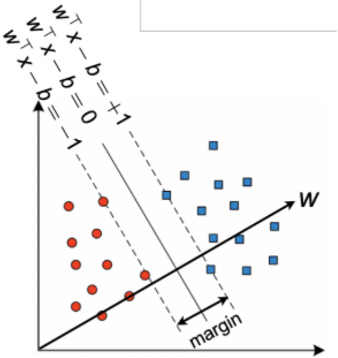
Idea: Find a hyperplane that separates the " blue" and "red" points with maximum margin. Predict labels of new points x depending on which side of the hyperplane they fall



Hard margin SVM

Hyperplane: $w^\top x - b = 0, w \neq 0$

We require: $w_i^\top x - b \geq 1 \quad \forall i$ with $y_i = 1$ (blue)
$w_i^\top x - b \leq -1 \ \forall i$ with $y_i = -1$ (red)



Margin $= \frac{2}{\|w\|_2}$

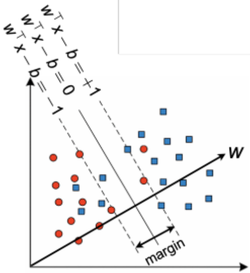
Hyperplane is found via the QP

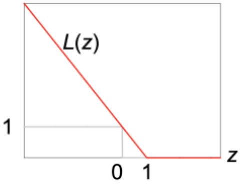
$$\begin{cases} \min_{w,b} & \frac{1}{2}\|w\|_2^2 \\ \text{s.t.} & y_i(w^\top x_i - b) \geq 1 \ \forall i \end{cases}$$

Soft margin SVM

What if the blue and red points are not linearly separable?

$$\min_{w,b} \underbrace{\frac{1}{m}\sum_{i=1}^{m} \max\{0, 1 - y_i(w^\top x_i - b)\}}_{\text{empirical Hinge loss}} + \underbrace{\frac{\rho}{2}\|w\|_2^2}_{\text{regularization term}}$$





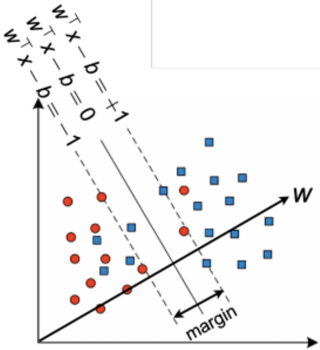
Hinge loss: $L(z) = \max\{0, 1 - z\}$

Signal: $z = y_i(w^\top x_i - b)$

- When $w^\top x_i - b$ and y_i have the same sign (i.e., y_i predicts the right class) and $|w^\top x_i - b| \geq 1$, then $L(z) = 0$

Soft margin SVM

What if the blue and red points are not linearly separable?



Replace Hinge loss of $i^t h$ sample with s_i

$$\begin{cases} \min_{w,b,s} & \frac{1}{m}\sum_{i=1}^{m} s_i + \frac{\rho}{2}\|w\|_2^2 \\ \text{s. t.} & y_i(w^\top x_i - b) + s_i \geq 1 \ \forall i \\ & s_i \geq 0 \ \forall i \end{cases}$$

Soft margin SVM

Primal QP:
$$\begin{cases} \min\limits_{w,b,s} & \frac{1}{m}\sum_{i=1}^m s_i + \frac{\rho}{2}\|w\|_2^2 \\ \text{s. t.} & y_i(w^\top x_i - b) + s_i \geq 1,\ s_i \geq 0,\ \forall i \end{cases}$$

Lagrangian:
$$L(w,b,s,\lambda,\gamma) = \frac{1}{m}\sum_{i=1}^m s_i + \frac{\rho}{2}\|w\|_2^2 - \sum_{i=1}^m \gamma_i s_i + \sum_{i=1}^m \lambda_i(1 - s_i - y_i(w^\top x_i - b))$$

Dual QP:
$$\begin{cases} \max\limits_{\lambda} & \sum_{i=1}^m \lambda_i - \frac{1}{2\rho}\sum_{i,j=1}^m \lambda_i\lambda_j y_i y_j x_i^\top x_j \\ \text{s. t.} & \sum_{i=1}^m y_i\lambda_i = 0, 0 \leq \lambda_i \leq \frac{1}{m},\ \forall i \end{cases}$$

KKT allows us to construct w and b from the dual solution.

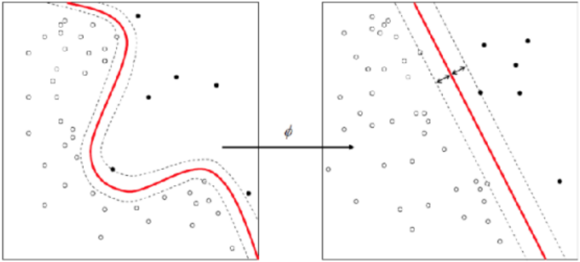
$$\nabla_w L(w,b,s,\lambda,\gamma) = 0 \qquad \Longrightarrow w = \frac{1}{\rho}\sum_{i=1}^m \lambda_i y_i x_i$$

$$\left.\begin{array}{l} \lambda_i(1 - s_i - y_i(w^\top x_i - b)) = 0 \\ (1/m - \lambda_i)s_i = 0 \end{array}\right\} \Longrightarrow \begin{cases} b = w^\top x_i - y_i \text{ for any } i \\ \text{with } 0 < \lambda_i < 1/m \end{cases}$$

Primal learns d and dual m parameters. Dual is easier if $m \ll d$

Kernel trick

- Improve classification via nonlinear separators.
- Use feature map $\phi : \mathbb{R}^d \to \mathbb{R}^D$ to lift the problem to a high-dimensional feature space $\mathbb{R}^D$, $D \gg d$



$x_1, \ldots, x_m$ $\qquad$ $x'_1 = \Phi(x_1), \ldots, x'_m = \Phi(x_m)$

Image source: Wikipedia

Nonlinear dimensionality reduction

SVM in high-dimensional space:

Primal QP:
$$\begin{cases} \min\limits_{w,b,s} & \frac{1}{m}\sum_{i=1}^{m} s_i + \frac{\rho}{2}\|w\|_2^2 \\ \text{s. t.} & y_i(w^\top \phi(x_i) - b) + s_i \geq 1,\ s_i \geq 0,\ \forall i \end{cases}$$

Dual QP:
$$\begin{cases} \max\limits_{\lambda} & \frac{1}{m}\lambda_i - \frac{1}{2\rho}\sum_{i,j=1}^{m} \lambda_i\lambda_j y_i y_j \phi(x_i)^\top \phi(x_j) \\ \text{s. t.} & \sum_{i=1}^{m} y_i\lambda_i = 0, 0 \leq \lambda_i \leq \frac{1}{m},\ \forall i \end{cases}$$

- The label of any new point x is predicted as

$$y = \text{sign}(w^\top \phi(x) - b) = \text{sign}\left(\frac{1}{\rho}\sum_{i=1}^{m} \lambda_i y_i \phi(x_i)^\top \phi(x) - b\right)$$

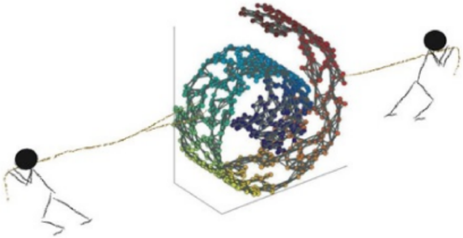
- Kernel function $K(x, x') = \phi(x)^\top \phi(x')$

The size of the dual QP is independent of the feature dimension D. Never evaluate inner products explicitly!

Nonlinear dimensionality reduction (cont'd)

Dimensionality reduction: Find meaningful low-dimensional structures hidden in high-dimensional observations (e.g., digital images, human genes, climate patterns etc.)

Example: Unwinding a Euro bill



The unwound Euro bill is flat ⇒ reduction from 3 to 2 dimensions

Nonlinear dimensionality reduction (cont'd)

Input: $y_i \in \mathbb{R}^d, \ i = 1, \ldots, m$

Construct a k-nearest neighbourhood graph $G = (V, E)$ with nodes $V = \{1, \ldots, m\}$ and edges E, where $(i, j) \in E$ if and only if y_i is among the k nearest neighbours of y_j

Example:

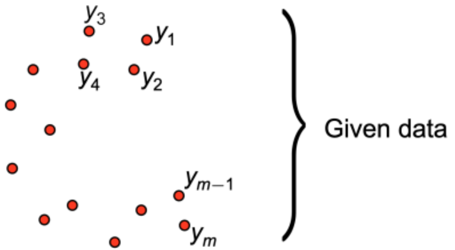


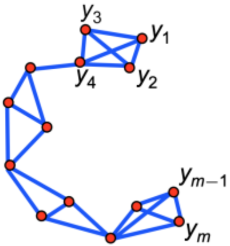
Figure:

Nonlinear dimensionality reduction (cont'd)

Input: $y_i \in \mathbb{R}^d,\ i = 1, \ldots, m$

Construct a k-nearest neighbourhood graph $G = (V, E)$ with nodes $V = \{1, \ldots, m\}$ and edges E, where $(i, j) \in E$ if and only if y_i is among the k nearest neighbours of y_j

Example:

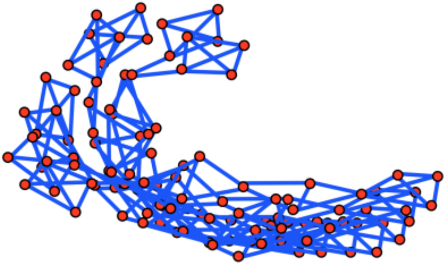


connect every node with its 3 nearest neighbors

Nonlinear dimensionality reduction (cont'd)

Idea: Spread out the data points as much as possible while keeping the distances between nearest neighbours fixed

Example:

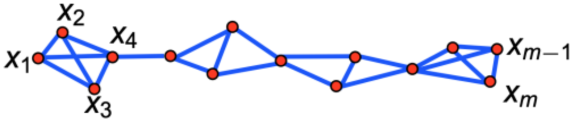


Nonlinear dimensionality reduction (cont'd)

Idea: Spread out the data points as much as possible while keeping the distances between nearest neighbours fixed

This can be done with and SDP !

Example: Let x_i, $i = 1, \ldots, m$ be the new positions of the data points (after spreading them out)



Nonlinear dimensionality reduction (cont'd)

Optimization problem for unfolding the kNN graph:

$$\begin{cases} \max\limits_{x} & \sum_{i=1}^{m} \|x_i\|_2^2 \\ \text{s.t.} & \sum_{i=1}^{m} x_i = 0 \\ & \|x_i - x_j\|_2^2 = \|y_i - y_j\|_2^2 \quad \forall (i,j) \in E \end{cases} \tag{1}$$

Maximize the variance of new positions. Require that mean is zero (eliminate translational degree of freedom) and require that distances between nearest neighbours are kept fixed.

Introduce Gram matrix $X \in \mathbb{S}_+^m$ with $X_{ij} = x_i^\top x_j$. We then have

- $\sum_{i=1}^{m} \|x_i\|_2^2 = \mathrm{tr}(X)$
- $\sum_{i=1}^{m} x_i = 0 \iff (\sum_{i=1}^{m} x_i)^\top (\sum_{j=1}^{m} x_j) = \sum_{i,j=1}^{m} X_{ij} = 0$
- $\|x_i - x_j\|_2^2 = X_{ii} - 2X_{ij} + X_{jj} = \|y_i - y_j\|_2^2 \quad \forall (i,j) \in E$

Nonlinear dimensionality reduction (cont'd)

Theorem: The "unfolding problem" (1) is equivalent to

$$\begin{cases} \max\limits_{X} & \mathrm{tr}(X) \\ \text{s. t.} & \sum_{i,j=1}^{m} X_{ij} = 0 \\ & X_{ii} - 2X_{ij} + X_{jj} = \|y_i - y_j\|_2^2 \quad \forall (i,j) \in E \\ & X \succeq 0, \mathrm{rank}(X) \leq d \end{cases} \tag{2}$$

Proof sketch: If x_i, $i = 1, \ldots, m$ is feasible in (1), then X defined via $X_{ij} = x_i^\top x_j$ is feasible in (2) with the same objective value. Note that

$$X = \begin{pmatrix} x_1^\top \\ \vdots \\ x_m^\top \end{pmatrix} (x_1 \ldots x_m) \succeq 0$$

Nonlinear dimensionality reduction (cont'd)

Theorem: The "unfolding problem" (1) is equivalent to

$$\begin{cases} \max\limits_{X} & \mathrm{tr}(X) \\ \text{s. t.} & \sum_{i,j=1}^{m} X_{ij} = 0 \\ & X_{ii} - 2X_{ij} + X_{jj} = \|y_i - y_j\|_2^2 \quad \forall (i,j) \in E \\ & X \succeq 0, \mathrm{rank}(X) \leq d \end{cases}$$

Proof sketch: If X is feasible in (2), then $X = RDR^\top$, where $D \in \mathbb{R}^{r\times r}$ is the diagonal matrix of all positive eigenvalues of X, the columns of $R \in \mathbb{R}^{m\times r}$ contain the corresponding orthonormal eigenvectors, and $r \leq \min\{d, m\}$ is the rank of X. Define x_i as the i^{th} row of $RD^{1/2}$. By construction, $X = (RD^{1/2})(RD^{1/2})^\top = (x_1 \dots x_m)^\top (x_1 \dots x_m)$ is the Gram matrix of the recovered x_i. Thus, the x_i are feasible in (1) and attain the same objective value as X in (2).

Nonlinear dimensionality reduction (cont'd)

The "unfolding problem" (1) is approximated by the SDP

$$\begin{cases} \max\limits_{X} & \mathrm{tr}(X) \\ \text{s. t.} & \sum_{i,j=1}^{m} X_{ij} = 0 \\ & X_{ii} - 2X_{ij} + X_{jj} = \|y_i - y_j\|_2^2 \quad \forall (i,j) \in E \\ & X \succeq 0, \cancel{\mathrm{rank}(X) \leq d} \end{cases} \tag{3}$$

How to recover a low-dimensional solution $x_i \in \mathbb{R}^r$, $i = 1, \ldots, m$ with $r \ll \min\{d, m\}$ from a solution X of the SDP (3)?

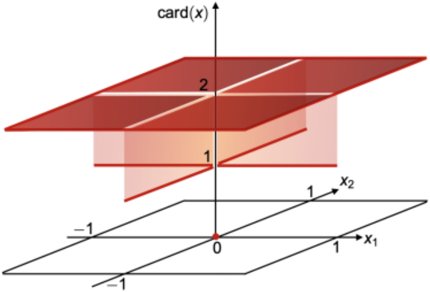
Heuristic approach: Let $D \in \mathbb{R}^{r \times r}$ be the diagonal matrix of the r largest eigenvalues of X, and let $R \in \mathbb{R}^{m \times r}$ be the matrix whose columns are the corresponding eigenvectors. Define x_i as the i^{th} row of $RD^{1/2}$. As small eigenvalues are ignored, we have

$$X \approx (RD^{1/2})(RD^{1/2})^\top = (x_1 \ldots x_m)^\top (x_1 \ldots x_m),$$

and thus the x_i are nearly feasible and optimal in (1).

Cardinality

Definition: The cardinality $\mathrm{card}(x)$ of $x \in \mathbb{R}^n$ is the number of non-zero entries of x.



The cardinality function is non-convex !

Convex cardinality problems

A convex cardinality problem is a convex except for a single cardinality function in the objective or in the constraints.

Assume that $C \subset \mathbb{R}^n$ is a convex set, and $f : \mathbb{R}^n \to \mathbb{R}$ is a convex function.

Convex minimum cardinality problem

$$\begin{cases} \min\limits_{x} & \operatorname{card}(x) \\ \text{s.t.} & x \in C \end{cases}$$

Convex problem with cardinality constraint:

$$\begin{cases} \min\limits_{x} & f(x) \\ \text{s.t.} & x \in C,\ \operatorname{card}(x) \leq k \end{cases}$$

Examples: Statistics

Regressor selection: Fit $b \in \mathbb{R}^m$ as a linear combination of k out of n possible columns of $A \in \mathbb{R}^{m \times n}$

$$\begin{cases} \min\limits_{x} & \|Ax - b\|_2 \\ \text{s. t.} & \operatorname{card}(x) \leq k \end{cases}$$

Linear classification with fewest errors: Replace the objective of the soft margin SVM with card(s)

$$\begin{cases} \min\limits_{w,b,s} & \operatorname{card}(s) \\ \text{s. t.} & y_i(w^\top x_i - b) + s_i \geq 1, \ s_i \geq 0, \ \forall i \end{cases}$$

Example: Minimum number of violations

Find $x \in C$ that violates as few of the following m convex inequalities as possible:

$$f_1(x) \leq 0, \ldots f_m(x) \leq 0$$

Such an x can be found by solving

$$\begin{cases} \min\limits_{x,t} & \mathrm{card}(t) \\ \text{s.t.} & x \in C,\ t \geq 0 \\ & f_i(x) \leq t_i \quad \forall i = 1, \ldots, m \end{cases}$$

Example: Sparse design

Find the sparsest design vector that satisfies a set of specifications

$$\begin{cases} \min\limits_{x} & \mathrm{card}(x) \\ \text{s.t.} & x \in C \end{cases}$$

Examples:

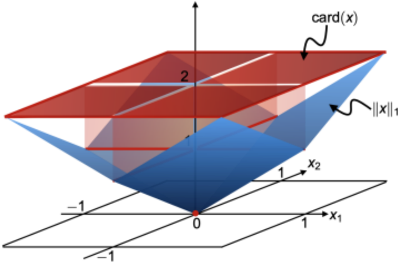
- finite impulse response filter design (zero entires reduce the required hardware)
- antenna array beamforming (zero entries correspond to unneeded antenna elements)
- truss design (zero entries correspond to unneeded bars)
- wire sizing (zero entries correspond to unneeded wires)

Exact solution of convex cardinality problems

- The decision $x \in \mathbb{R}^n$ has 2^n sparsity patterns (each component of x can be zero or nonzero)
- A convex cardinality problem can thus be solved exactly by solving 2^n convex problems (each enforcing a sparsity pattern)
- This may be practical for $n \leq 10$ but impractical for $n \geq 15$

ℓ_1-Norm heuristic

Replace $\text{card}(x)$ with $\gamma\|x\|_1$ or add a regularization term $\gamma\|x\|_1$ to the objective. Tune $\gamma > 0$ to achieve the desired sparsity



Note: $\|x\|_1$ is the convex envelope of $\text{card}(x)$ on $\{x : \|x\|_\infty \leq 1\}$

ℓ_1-Norm heuristic (cont'd)

Convex minimum cardinality problem:

$$\begin{cases} \min\limits_{x} & \mathrm{card}(x) \\ \text{s. t.} & x \in C \end{cases} \implies \begin{cases} \min\limits_{x} & \|x\|_1 \\ \text{s. t.} & x \in C \end{cases}$$

Convex problem with cardinality constraint:

$$\begin{cases} \min\limits_{x} & f(x) \\ \text{s. t.} & x \in C,\ \mathrm{card}(x) \le k \end{cases} \implies \begin{cases} \min\limits_{x} & f(x) \\ \text{s. t.} & x \in C,\ \|x\|_1 \le \beta \end{cases}$$

β can be tuned to ensure that $\mathrm{card}(x) \le k$.