Mathematical Optimization Models and Applications

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Chapters 1, 2.1-2, 6.1-2, 7.2, 11.3, 11.6

What you lean in CME307/MS&E311?

- Present a core element, mathematical optimization theories and algorithms, for the ICME/MS&E disciplines.
- Provide mathematical proofs and in-depth theoretical analyses of optimization/game models/algorithms discussed in MS&E211
- Introduce additional conic and nonlinear/nonconvex optimization/game models/problems comparing to MS&E310.
- Describe new/recent effective optimization/game models/methods/algorithms in Data Science, Machine Learning and AI.
- Emphasis is on nonlinear, nonconvex and stochastic/sample-based optimization theories and practices together with convex analyses.

Mathematical Optimization

The field of optimization is concerned with the study of maximization and minimization of mathematical functions. Very often the arguments of (i.e., variables or unknowns in) these functions are subject to side conditions or constraints. By virtue of its great utility in such diverse areas as applied science, engineering, economics, finance, medicine, and statistics, optimization holds an important place in the practical world and the scientific world. Indeed, as far back as the Eighteenth Century, the famous Swiss mathematician and physicist Leonhard Euler (1707-1783) proclaimed[a] that . . . nothing at all takes place in the Universe in which some rule of maximum or minimum does not appear.

[a]See Leonhardo Eulero, *Methodus Inviendi Lineas Curvas Maximi Minimive Proprietate Gaudentes*, Lausanne & Geneva, 1744, p. 245.

Mathematical Optimization/Programming (MP)

The class of mathematical optimization/programming problems considered in this course can all be expressed in the form

$$\begin{array}{lll} \text{(P)} & \text{minimize} & f(\mathbf{x}) \\ & \text{subject to} & \mathbf{x} \in \mathcal{X} \end{array}$$

where $\mathcal{X}$ usually specified by constraints:

$$\begin{array}{rcll} c_i(\mathbf{x}) & = & 0 & i \in \mathcal{E} \\ c_i(\mathbf{x}) & \leq & 0 & i \in \mathcal{I}. \end{array}$$

If the constraint functions are linear/affine type, then $\mathcal{X}$ is a convex polyhedral set/region.

Model Classifications

Optimization problems are generally divided into Unconstrained, Linear and Nonlinear Programming based upon the objective and constraints of the problem

- Unconstrained Optimization: Ω is the entire space R^n
- Linear Optimization: If both the objective and the constraint functions are linear/affine
- Nonlinear Optimization: If the objective/constraints contain general nonlinear functions
- Convex Optimization: If the objective is a convex function and the constraint region is a convex set
- Conic Linear Optimization: If both the objective and the constraint functions are linear/affine, and variables are in a convex cone.
- (Mixed) Integer Optimization: If the some variables are restricted to be integral
- Stochastic Optimization: Optimize the expected objective function with random parameters
- Fixed-Point or Min-Max Optimization: Optimization of multiple agents with zero-sum objectives

We present a few optimization examples in this lecture that we would cover through out this course.

Structured Optimization: Conic Linear Programming (CLP)

$$\begin{array}{ll} \text{minimize} & \mathbf{c}^T\mathbf{x} \\ \text{subject to} & A\mathbf{x} = \mathbf{b}, \\ & \mathbf{x} \in K. \end{array}$$

Linear Programming (LP): when K is the nonnegative orthant cone

Second-Order Cone Programming (SOCP): when K is the second-order cone

Semidefinite Cone Programming (SDP): when K is the semidefinite matrix cone

$$\begin{array}{ll} \text{min} & 2x_1 + x_2 + x_3 \\ \text{s.t.} & x_1 + x_2 + x_3 = 1, \\ & (x_1; x_2; x_3) \geq \mathbf{0}; \end{array}$$

$$\begin{array}{ll} \text{min} & 2x_1 + x_2 + x_3 \\ \text{s.t.} & x_1 + x_2 + x_3 = 1, \\ & \sqrt{x_2^2 + x_3^2} \leq x_1. \end{array}$$

$$\begin{array}{ll} \text{min} & 2x_1 + x_2 + x_3 \\ \text{s.t.} & x_1 + x_2 + x_3 = 1, \\ & \begin{pmatrix} x_1 & x_2 \\ x_2 & x_3 \end{pmatrix} \succeq \mathbf{0}, \end{array}$$

Facility Location Problem

Let $\mathbf{c}_j$ be the location of client $j = 1, 2, ..., m$, and $\mathbf{y}$ be the location decision of a facility to be built. Then we solve

$$\text{minimize}_{\mathbf{y}} \quad \sum_j \|\mathbf{y} - \mathbf{c}_j\|_p.$$

Or equivalently (?)

$$\begin{array}{ll} \text{minimize} & \sum_j \delta_j \\ \text{subject to} & \mathbf{y} + \mathbf{x}_j = \mathbf{c}_j, \; \|\mathbf{x}_j\|_p \leq \delta_j, \; \forall j. \end{array}$$

This is a p-order conic linear program (POCP) for $p \geq 1$.

In particular, when $p = 2$, it is an SOCP problem.

For simplicity, consider $m = 3$.

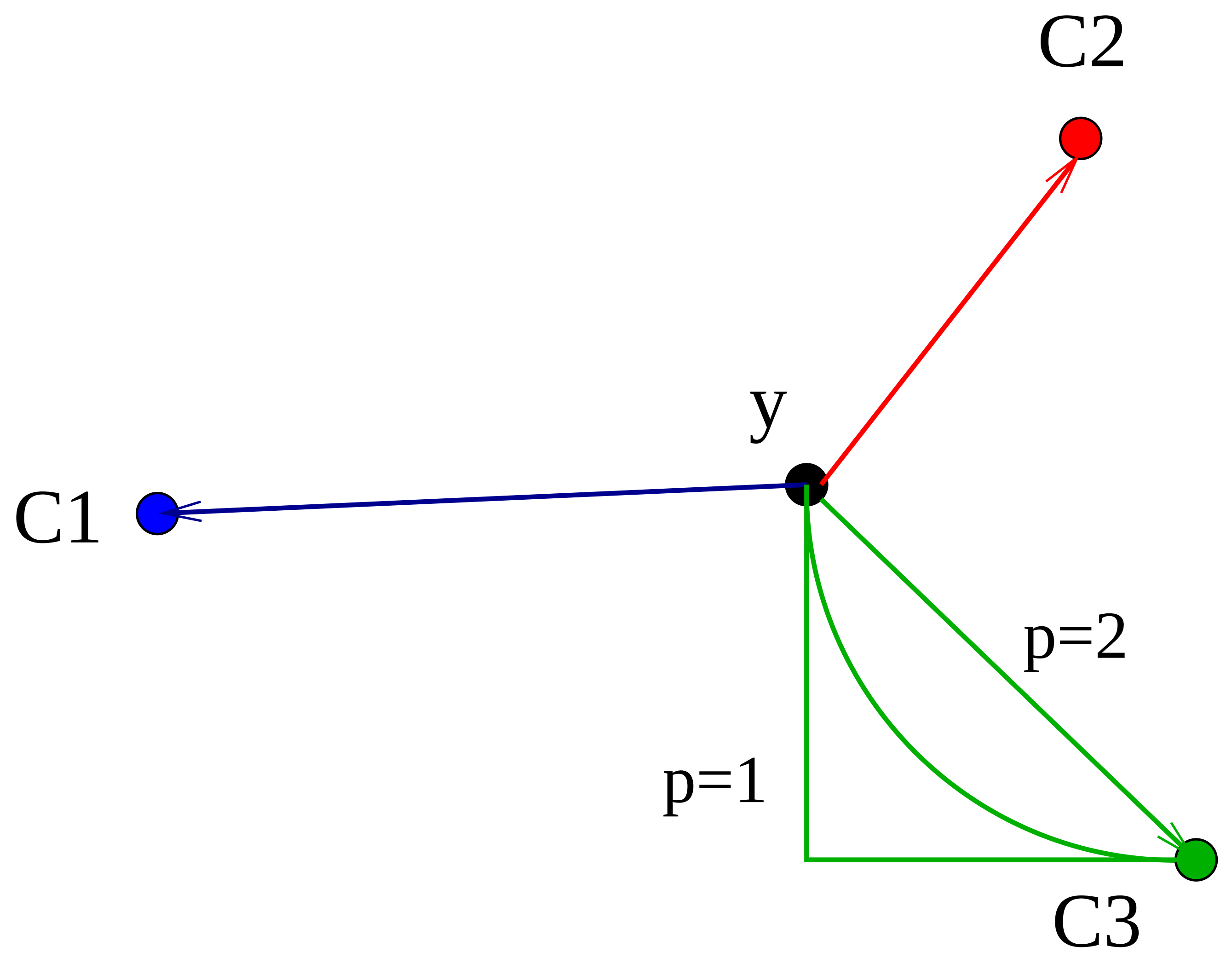


Figure 1: Facility Location at Point $\mathbf{y}$.

Sparse Linear Regression Problems

We want to find a sparsest solution to fit exact data measurements, that is, to minimize the number of non-zero entries in $\mathbf{x}$ such that $A\mathbf{x} = \mathbf{b}$:

$$\begin{array}{ll} \text{minimize} & \|\mathbf{x}\|_0 = |\{j : x_j \neq 0\}| \\ \text{subject to} & A\mathbf{x} = \mathbf{b}. \end{array}$$

Sometimes this objective can be accomplished by LASSO:

$$\begin{array}{ll} \text{minimize} & \|\mathbf{x}\|_1 = \sum_{j=1}^n |x_j| \\ \text{subject to} & A\mathbf{x} = \mathbf{b}. \end{array}$$

It can be equivalently represented by (?)

$$\begin{array}{ll} \text{minimize} & \sum_{j=1}^n y_j \\ \text{subject to} & A\mathbf{x} = \mathbf{b},\ -\mathbf{y} \le \mathbf{x} \le \mathbf{y}; \end{array} \quad \text{or} \quad \begin{array}{ll} \text{minimize} & \sum_{j=1}^n (x'_j + x''_j) \\ \text{subject to} & A(\mathbf{x}' - \mathbf{x}'') = \mathbf{b},\ \mathbf{x}' \ge \mathbf{0},\ \mathbf{x}\text{''} \ge \mathbf{0}. \end{array}$$

Both are linear programs!

Sparsest Data Fitting continued

A better approximation of the objective can be accomplished by

$$\begin{array}{ll} \text{minimize} & \|\mathbf{x}\|_p := \left(\sum_{j=1}^n |x_j|^p\right)^{1/p} \\ \text{subject to} & A\mathbf{x} = \mathbf{b}; \end{array} \quad \text{or} \quad \text{minimize} \quad \|A\mathbf{x} - \mathbf{b}\|^2 + \mu \left(\sum_{j=1}^n |x_j|^p\right)^{1/p}$$

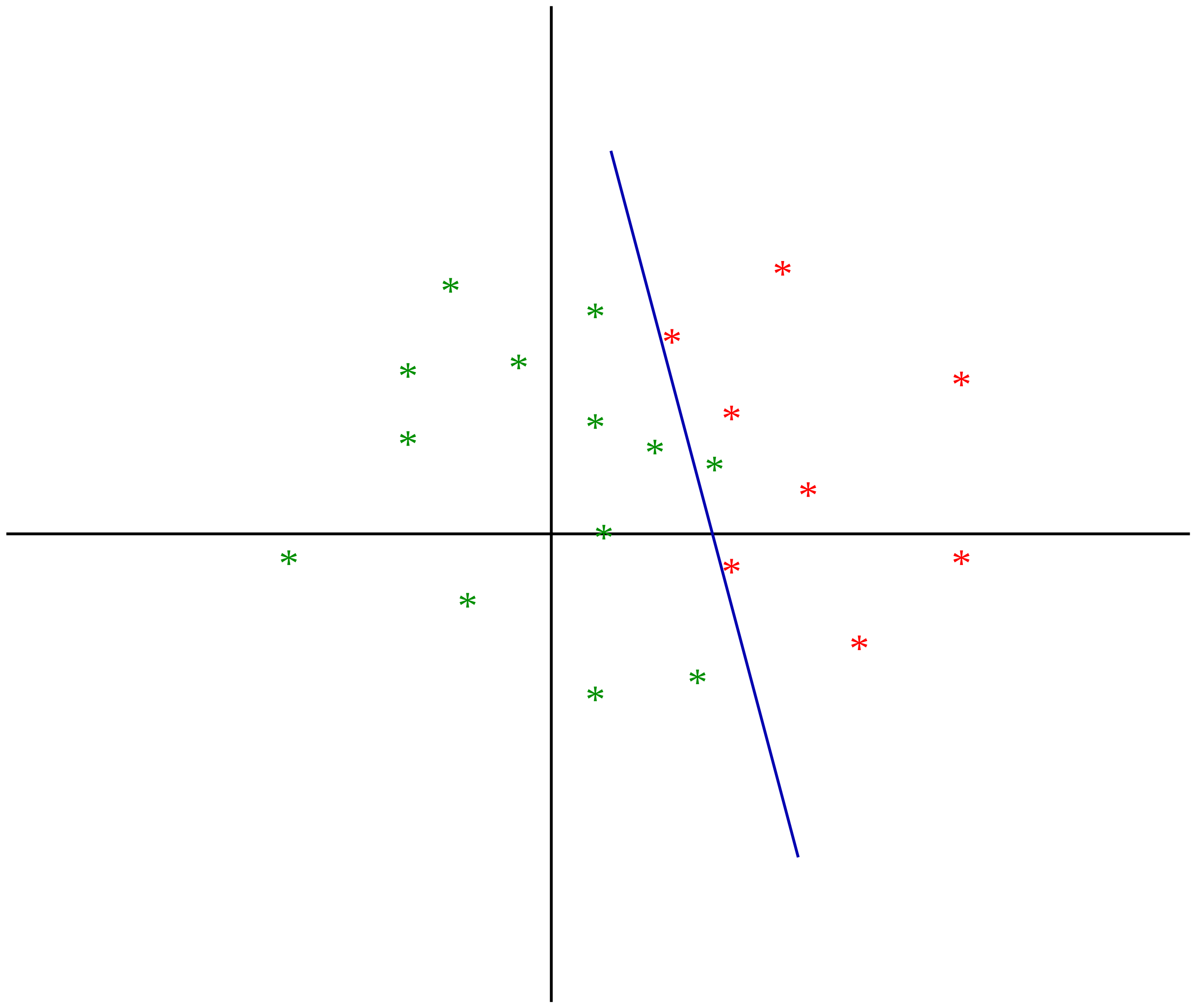
for some $0 < p < 1$, where $\mu > 0$ is a regularization parameter.

Or simply

$$\begin{array}{ll} \text{minimize} & \|\mathbf{x}\|_p^p := \left(\sum_{j=1}^n |x_j|^p\right) \\ \text{subject to} & A\mathbf{x} = \mathbf{b}; \end{array} \quad \text{or} \quad \text{minimize} \quad \|A\mathbf{x} - \mathbf{b}\|^2 + \beta \left(\sum_{j=1}^n |x_j|^p\right);$$

where the former is a linearly constrained (nonconvex) optimization problem and the latter is an unconstrained (nonconvex) optimization problem

Linear Classifier: Logistic Regression and Support Vector Machine



Data Classification: Supporting Vector Machine I

A powerful binary-classification method is the Supporting Vector Machine (SVM).

Let the first class, say in Red, data points i be denoted by $\mathbf{a}_i \in R^d$, $i = 1, ..., n_1$ and the second class data points j be denoted by $\mathbf{b}_j \in R^d$, $j = 1, ..., n_2$. We like to find a hyperplane, slope vector $\mathbf{x}$ and intersect scalar x_0, to separate the two data classes:

$$\begin{array}{ll} \text{subject to} & \mathbf{a}_i^T\mathbf{x} + x_0 \geq 1, \ \forall i, \\ & \mathbf{b}_j^T\mathbf{x} + x_0 \leq -1, \ \forall j. \end{array}$$

This is a linear program with the null objective!

Data Classification: Supporting Vector Machine II

If strict separation is impossible, we then minimize error variable β

$$\begin{array}{rl} \text{minimize} & \beta \\ \text{subject to} & \mathbf{a}_i^T\mathbf{x} + x_0 + \beta \geq 1,\ \forall i, \\ & \mathbf{b}_j^T\mathbf{x} + x_0 - \beta \leq -1,\ \forall j, \\ & \beta \geq 0. \end{array}$$

Frequently we add the regularization term on the slope vector

$$\begin{array}{rl} \text{minimize} & \beta + \mu\|\mathbf{x}\|^2 \\ \text{subject to} & \mathbf{a}_i^T\mathbf{x} + x_0 + \beta \geq 1,\ \forall i, \\ & \mathbf{b}_j^T\mathbf{x} + x_0 - \beta \leq -1,\ \forall j, \\ & \beta \geq 0, \end{array}$$

where μ is a fixed positive regularization parameter.

This becomes a constrained quadratic program (QP). If $\mu = 0$, then it is a linear program (LP)!

Supporting Vector Machine: Ellipsoidal Separation?

$$\begin{array}{rl} \text{minimize} & \text{trace}(X) + \|\mathbf{x}\|^2 \\ \text{subject to} & \mathbf{a}_i^T X \mathbf{a}_i + \mathbf{a}_i^T \mathbf{x} + x_0 \geq 1, \ \forall i, \\ & \mathbf{b}_j^T X \mathbf{b}_j + \mathbf{b}_j^T \mathbf{x} + x_0 \leq -1, \ \forall j, \\ & X \succeq \mathbf{0}. \end{array}$$

This type of problems is semidefinite programming (SDP). When the problem is not separable:

$$\begin{array}{rl} \text{minimize} & \beta + \mu(\text{trace}(X) + \|\mathbf{x}\|^2) \\ \text{subject to} & \mathbf{a}_i^T X \mathbf{a}_i + \mathbf{a}_i^T \mathbf{x} + x_0 + \beta \geq 1, \ \forall i, \\ & \mathbf{b}_j^T X \mathbf{b}_j + \mathbf{b}_j^T \mathbf{x} + x_0 - \beta \leq -1, \ \forall j, \\ & \beta \geq 0, \\ & X \succeq \mathbf{0}. \end{array}$$

This is a mixed linear and SDP program.

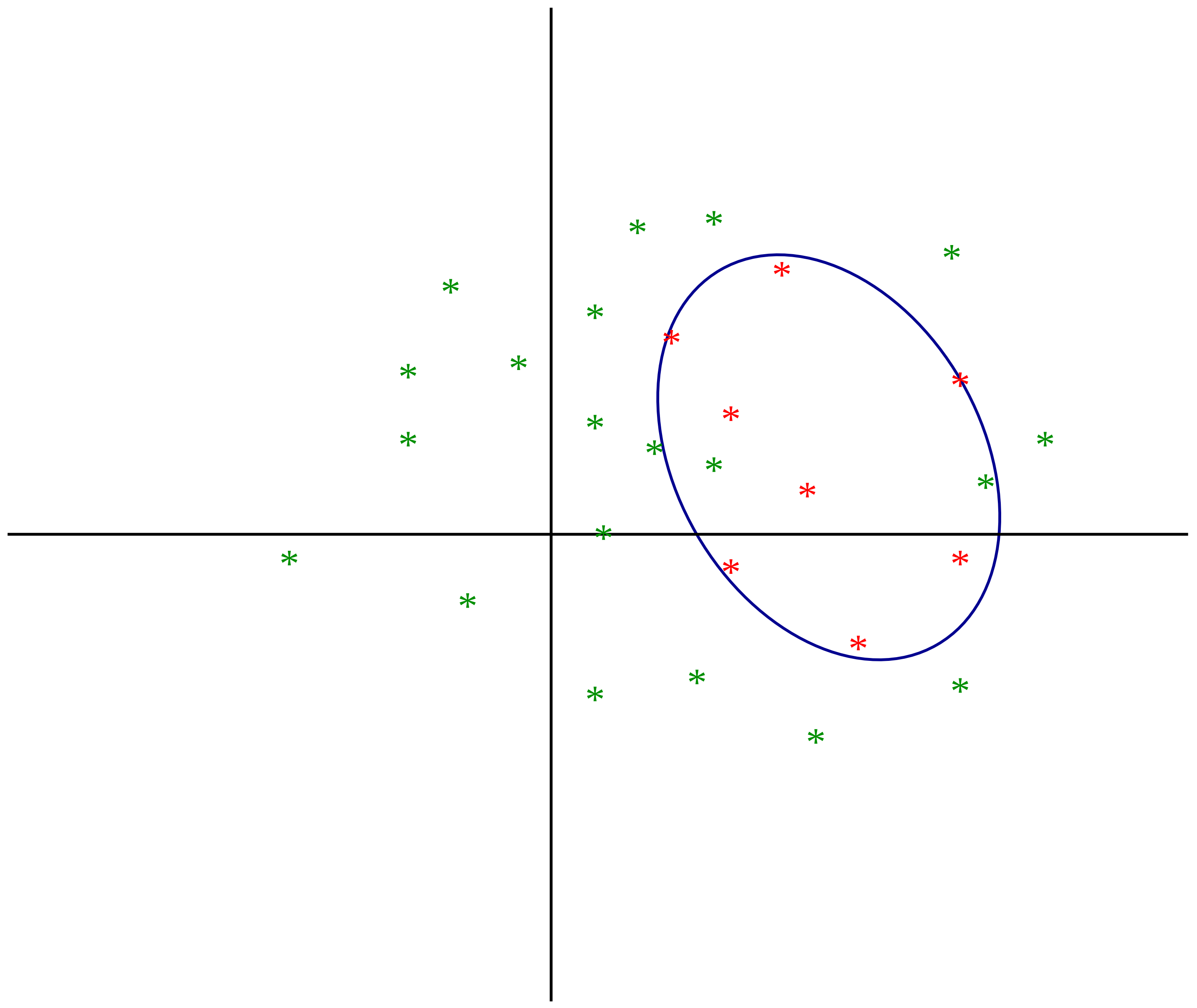


Figure 2: Quadratic Support Vector Machine

Unconstrained Optimization: Logistic Regression I

Similar to SVM, given the two-class discrimination training data points $\mathbf{a}_i \in R^n$, according to the logistic model, the probability that it's in a class C, say in Red, is represented by a linear/affine function with slope-vector $\mathbf{x}$ and intersect scalar x_0:

$$\frac{e^{\mathbf{a}_i^T\mathbf{x}+x_0}}{1+e^{\mathbf{a}_i^T\mathbf{x}+x_0}}.$$

Thus, for some training data points, we like to determine intercept x_0 and slope vector $\mathbf{x} \in R^n$ such that

$$\frac{e^{\mathbf{a}_i^T\mathbf{x}+x_0}}{1+e^{\mathbf{a}_i^T\mathbf{x}+x_0}} = \begin{cases} 1, & \text{if } \mathbf{a}_i \in C \\ 0, & \text{otherwise} \end{cases}.$$

Then the probability to give a "right classification answer" for all training data points is

$$\left(\prod_{\mathbf{a}_i \in C} \frac{e^{\mathbf{a}_i^T\mathbf{x}+x_0}}{1+e^{\mathbf{a}_i^T\mathbf{x}+x_0}}\right)\left(\prod_{\mathbf{a}_i \notin C} \frac{1}{1+e^{\mathbf{a}_i^T\mathbf{x}+x_0}}\right)$$

Logistic Regression II

Therefore, we like to maximize the probability when deciding intercept x_0 and slope vector $\mathbf{x} \in R^n$

$$\left(\prod_{\mathbf{a}_i \in C} \frac{e^{\mathbf{a}_i^T\mathbf{x}+x_0}}{1+e^{\mathbf{a}_i^T\mathbf{x}+x_0}}\right)\left(\prod_{\mathbf{a}_i \notin C} \frac{1}{1+e^{\mathbf{a}_i^T\mathbf{x}+x_0}}\right) = \left(\prod_{\mathbf{a}_i \in C} \frac{1}{1+e^{-\mathbf{a}_i^T\mathbf{x}-x_0}}\right)\left(\prod_{\mathbf{a}_i \notin C} \frac{1}{1+e^{\mathbf{a}_i^T\mathbf{x}+x_0}}\right),$$

which is equivalently to maximize

$$-\left(\sum_{\mathbf{a}_i \in C} \ln(1+e^{-\mathbf{a}_i^T\mathbf{x}-x_0})\right) - \left(\sum_{\mathbf{a}_i \notin C} \ln(1+e^{\mathbf{a}_i^T\mathbf{x}+x_0})\right).$$

Or

$$\min_{x_0,\mathbf{x}} \quad \left(\sum_{\mathbf{a}_i \in C} \ln(1+e^{-\mathbf{a}_i^T\mathbf{x}-x_0})\right) + \left(\sum_{\mathbf{a}_i \notin C} \ln(1+e^{\mathbf{a}_i^T\mathbf{x}+x_0})\right).$$

This is an unconstrained optimization problem, where the objective is a convex function of decision variables: intercept x_0 and slope vector $\mathbf{x} \in R^n$.

More QP Examples: Portfolio Management

For expected return vector $\mathbf{r}$ and co-variance matrix V of an investment portfolio, one management model is:

$$\begin{array}{ll} \text{minimize} & \mathbf{x}^T V \mathbf{x} \\ \text{subject to} & \mathbf{r}^T \mathbf{x} \geq \mu, \\ & \mathbf{e}^T \mathbf{x} = 1,\ \mathbf{x} \geq \mathbf{0}, \end{array} \qquad \text{or simply} \qquad \begin{array}{ll} \text{minimize} & \mathbf{x}^T V \mathbf{x} \\ \text{subject to} & \mathbf{r}^T \mathbf{x} \geq \mu, \\ & \mathbf{e}^T \mathbf{x} = 1, \end{array}$$

where $\mathbf{e}$ is the vector of all ones.

This is a (convex) quadratic program.

More CLP Examples: Robust Portfolio Management

In applications, $\mathbf{r}$ and V may be estimated under various scenarios, say $\mathbf{r}_i$ and V_i for $i = 1, ..., m$. Then, we like

$$\begin{array}{rl} \text{minimize} & \max_i \mathbf{x}^T V_i \mathbf{x} \\ \text{subject to} & \min_i \mathbf{r}_i^T \mathbf{x} \geq \mu, \\ & \mathbf{e}^T \mathbf{x} = 1, \ \mathbf{x} \ \geq \ \mathbf{0}. \end{array} \quad \Rightarrow \quad \begin{array}{rl} \text{minimize} & \alpha \\ \text{subject to} & \mathbf{r}_i^T \mathbf{x} \geq \mu, \ \forall i \\ & \sqrt{\mathbf{x}^T V_i \mathbf{x}} \leq \alpha, \ \forall i \\ & \mathbf{e}^T \mathbf{x} = 1, \ \mathbf{x} \ \geq \ \mathbf{0}. \end{array}$$

This is a quadratically constrained quadratic program (QCQP). If factorize $V_i = R_i^T R_i$ and let $\mathbf{y}_i = R_i \mathbf{x}$, we can rewrite the problem as

$$\begin{array}{rl} \text{minimize} & \alpha \\ \text{subject to} & \mathbf{r}_i^T \mathbf{x} \geq \mu, \ \mathbf{y}_i - R_i \mathbf{x} = \mathbf{0}, \ \forall i \\ & \|\mathbf{y}_i\| \leq \alpha, \ \forall i, \ \mathbf{e}^T \mathbf{x} = 1, \ \mathbf{x} \ \geq \ \mathbf{0}, \end{array}$$

which is an SOCP with additional benefits.

Portfolio Selection Problem

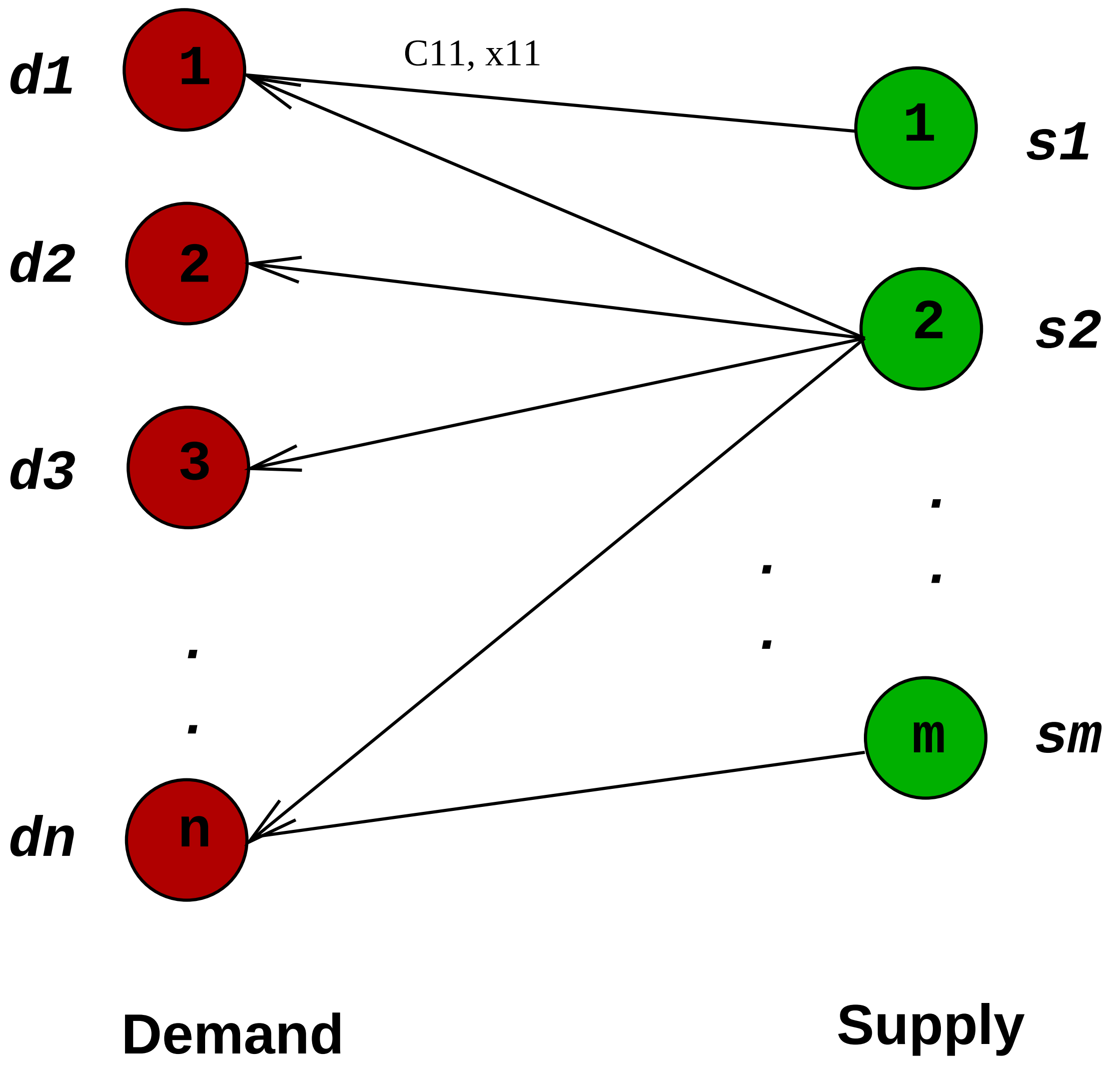
If no more than k stocks can be selected into your portfolio as a policy constraint?

$$\begin{aligned} \text{minimize} \quad & \mathbf{x}^T V \mathbf{x} \\ \text{subject to} \quad & \mathbf{r}^T \mathbf{x} \geq \mu, \\ & \mathbf{e}^T \mathbf{x} = 1, \\ & \mathbf{0} \leq \mathbf{x} \leq \mathbf{y},\ \mathbf{e}^T \mathbf{y} \leq k,\ \mathbf{y} \in \{0,1\}^n \end{aligned}$$

This is a mixed-integer quadratic program (MIP).

If the integer variables are restricted 0 or 1, it is also names as the binary optimization problem.

The Transportation Problem



Mathematical Optimization Model:

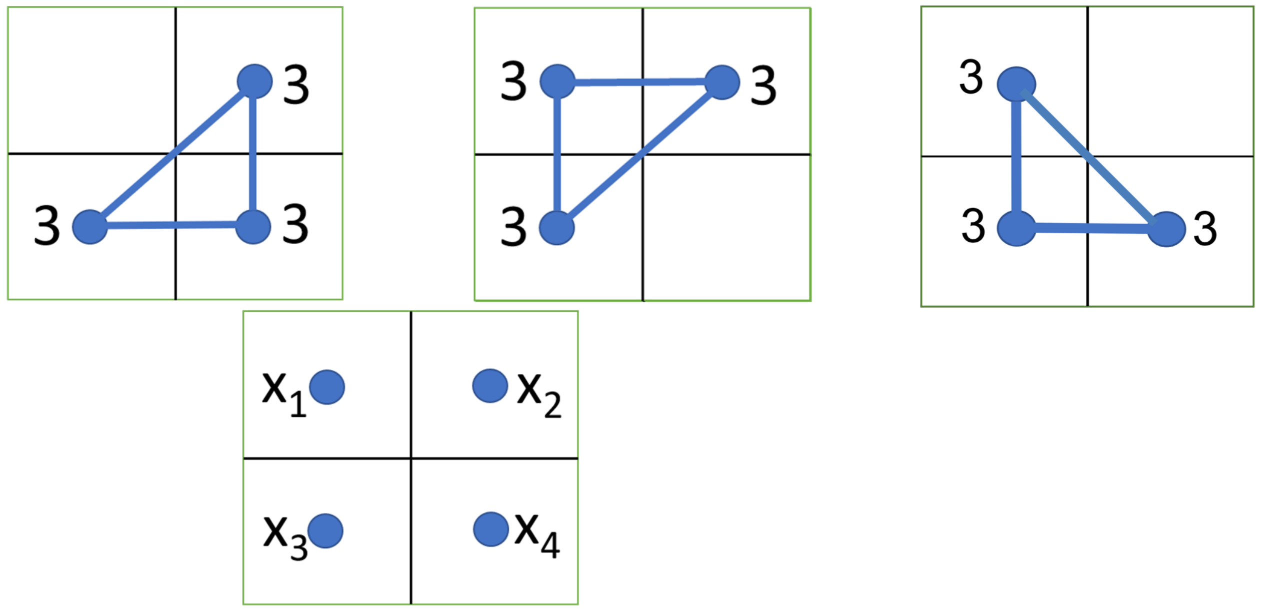
$$
\begin{array}{lll}
\min & \sum_{i=1}^{m}\sum_{j=1}^{n} c_{ij}x_{ij} & \\
\text{s.t.} & \sum_{j=1}^{n} x_{ij} & = s_i,\ \forall i = 1, ..., m \\
& \sum_{i=1}^{m} x_{ij} & = d_j,\ \forall j = 1, ..., n \\
& x_{ij} & \geq 0,\ \forall i, j.
\end{array}
$$

The minimal transportation cost is called the Wasserstein Distance (WD) between supply distribution $\mathbf{s}$ and demand distribution $\mathbf{d}$ (can be interpreted as two probability distributions after normalization). This is a linear program!

What happen if supplies $\mathbf{s}$ are also decision variables?

The Wasserstein Barycenter Problem is to find a distribution such that the sum of its Wasserstein Distance to each of a set of distributions would be minimized.

A Wassestein Barycenter Application: Stochastic Optimization



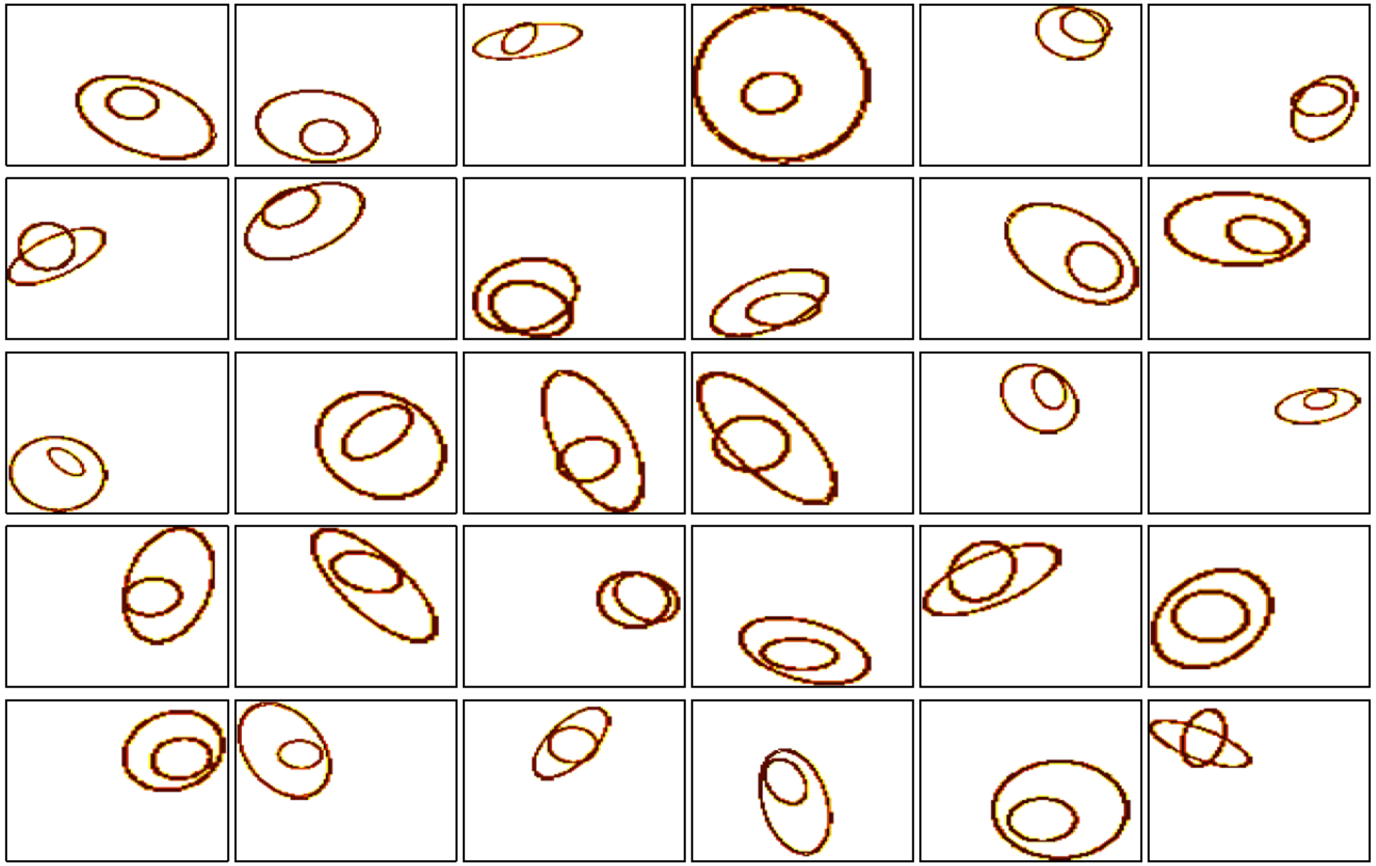
Find distribution of $s_i, i = 1,2,3,4$ to minimize

$$\begin{array}{ll} \min & WD_l(\mathbf{s},\mathbf{d}_l) + WD_m(\mathbf{s},\mathbf{d}_m) + WD_r(\mathbf{s},\mathbf{d}_r) \\ \text{s.t.} & s_1+s_2+s_3+s_4 = 9, \qquad s_i \ge 0,\ i=1,2,3,4. \end{array}$$

The objective is a nonlinear function, but its gradient vector $\nabla WD_l(\mathbf{s},\mathbf{d}_l)$, $\nabla WD_m(\mathbf{s},\mathbf{d}_m)$ and $\nabla WD_r(\mathbf{s},\mathbf{d}_r)$ are shadow prices of the three sub-transportation problems –popularly used in Hierarchy Optimization.

The Wasserstein Barycenter (Mean) Problem in Data Science

What is the "mean or consensus" image from a set of images/distributions:



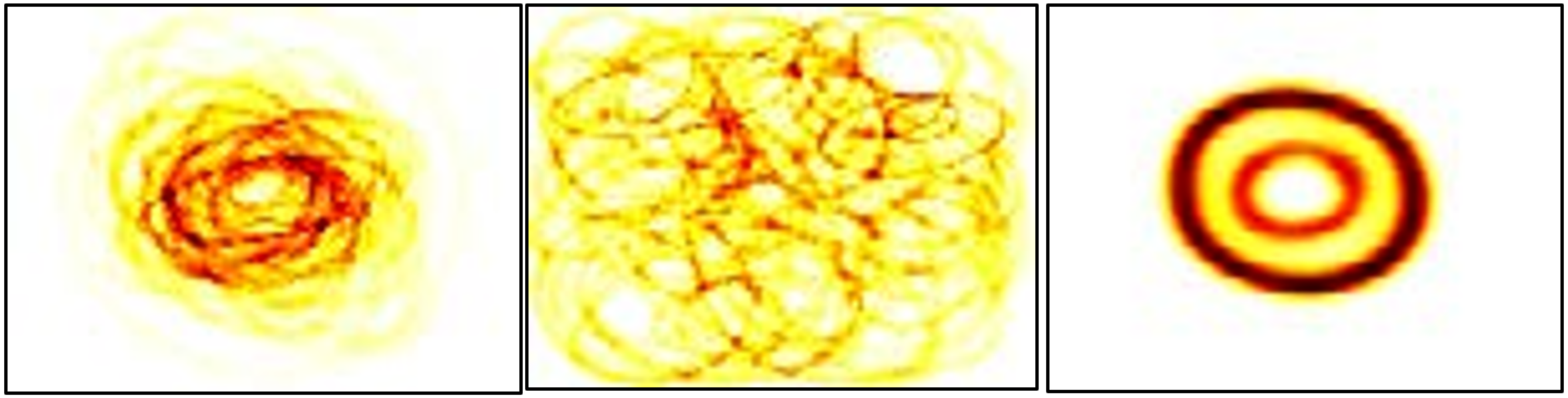


Figure 3: Mean picture constructed from the (a) Euclidean mean after re-centering images (b) Euclidean mean (c) Wasserstein Barycenter (self recenter, resize and rotate)

Euclidean Mean/Center:

$$\mathbf{x} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{a}_i, \quad \text{or} \quad \min_{\mathbf{x}} \sum_{i=1}^{n} \|\mathbf{x} - \mathbf{a}_i\|_2^2,$$

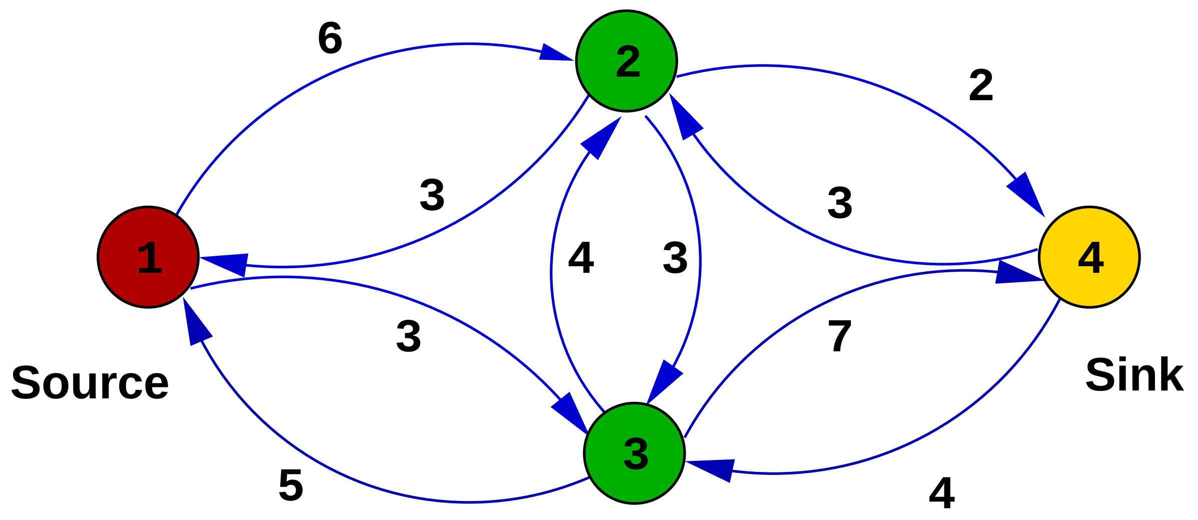
which is an unconstrained optimization, or least-squares, problem

Max-Flow Problem

Given a directed graph with nodes $1, ..., m$ and edges $\mathcal{A}$, where node 1 is called source and node m is called the sink, and each edge (i, j) has a flow rate capacity k_{ij}. The Max-Flow problem is to find the largest possible flow rate from source to sink.

Let x_{ij} be the flow rate from node i to node j. Then the problem can be formulated as

$$\begin{array}{ll} \text{maximize} & x_{m1} \\ \text{subject to} & \sum_{j:(j,1)\in\mathcal{A}} x_{j1} - \sum_{j:(1,j)\in A} x_{1j} + x_{m1} = 0, \\ & \sum_{j:(j,i)\in\mathcal{A}} x_{ji} - \sum_{j:(i,j)\in\mathcal{A}} x_{ij} = 0, \forall i = 2, ..., m-1, \\ & \sum_{j:(j,m)\in\mathcal{A}} x_{jm} - \sum_{j:(m,j)\in\mathcal{A}} x_{mj} - x_{m1} = 0, \\ & 0 \leq x_{ij} \leq k_{ij}, \ \forall (i,j) \in \mathcal{A}. \end{array}$$



6
2
2
3
3
4
3
1
3
4
3
7
Source
Sink
5
3
4

Prediction Market I: World Cup Information Market

Order:	#1	#2	#3	#4	#5
Argentina	1	0	1	1	0
Brazil	1	0	0	1	1
Italy	1	0	1	1	0
Germany	0	1	0	1	1
France	0	0	1	0	0
Bidding Prize:π	0.75	0.35	0.4	0.95	0.75
Quantity limit:$\mathbf{q}$	10	5	10	10	5
Order fill:$\mathbf{x}$	x_1	x_2	x_3	x_4	x_5

Prediction Market II: Call Auction Mechanism

Given m potential states that are mutually exclusive and exactly one of them will be realized at the maturity.

An order is a bet on one or a combination of states, with a price limit (the maximum price the participant is willing to pay for one unit of the order) and a quantity limit (the maximum number of units or shares the participant is willing to accept).

A contract on an order is a paper agreement so that on maturity it is worth a notional $\$1$ dollar if the order includes the winning state and worth $\$0$ otherwise.

There are n orders submitted now.

Prediction Market III: Input Order Data

The ith order is given as $(\mathbf{a}_{i\cdot} \in R^m_+,\ \pi_i \in R_+,\ q_i \in R_+)$: $\mathbf{a}_{i\cdot}$ is the betting indication row vector where each component is either 1 or 0

$$\mathbf{a}_{i\cdot} = (a_{i1},\ a_{i2},\ ...,\ a_{im})$$

where 1 is winning state and 0 is non-winning state; π_i is the price limit for one unit of such a contract, and q_i is the maximum number of contract units the better like to buy.

Prediction Market IV: Output Order-Fill Decisions

Let x_i be the number of units or shares awarded to the ith order. Then, the ith bidder will pay the amount $\pi_i \cdot x_i$ and the total amount collected would be $\pi^T \mathbf{x} = \sum_i \pi_i \cdot x_i$.

If the jth state is the winning state, then the auction organizer need to pay the winning bidders

$$\left(\sum_{i=1}^{n} a_{ij} x_i \right) = \mathbf{a}_{.j}^T \mathbf{x}$$

where column vector

$$\mathbf{a}_{.j} = (a_{1j};\ a_{2j};\ ...;\ a_{nj})$$

The question is, how to decide $\mathbf{x} \in R^n$, that is, how to fill the orders.

Prediction Market V: Worst-Case Profit Maximization

$$
\begin{array}{rrl}
\max & \pi^T \mathbf{x} - \max_j \{\mathbf{a}_{\cdot j}^T \mathbf{x}\} & \\
\text{s.t.} & \mathbf{x} & \leq \mathbf{q}, \\
 & \mathbf{x} & \geq \mathbf{0}.
\end{array}
$$

$$
\begin{array}{rrl}
\max & \pi^T \mathbf{x} - \max(A^T \mathbf{x}) & \\
\text{s.t.} & \mathbf{x} & \leq \mathbf{q}, \\
 & \mathbf{x} & \geq \mathbf{0}.
\end{array}
$$

This is NOT a linear program.

Prediction Market VI: LP Representation

However, the problem can be rewritten as

$$\begin{array}{rrl} \max & \pi^T \mathbf{x} - y & \\ \text{s.t.} & A^T\mathbf{x} - \mathbf{e}\cdot y & \leq \mathbf{0}, \\ & \mathbf{x} & \leq \mathbf{q}, \\ & \mathbf{x} & \geq \mathbf{0}, \end{array}$$

where $\mathbf{e}$ is the vector of all ones. This is a linear program.

$$\begin{array}{rrl} \max & \pi^T \mathbf{x} - y & \\ \text{s.t.} & A^T\mathbf{x} - \mathbf{e}\cdot y + s_0 & = \mathbf{0}, \\ & \mathbf{x} + \mathbf{s} & = \mathbf{q}, \\ & (\mathbf{x}, s_0, \mathbf{s}) & \geq \mathbf{0}, \quad y \text{ free}, \end{array}$$

Graph Realization and Sensor Network Localization

Given a graph $G = (V, E)$ and sets of non–negative weights, say $\{d_{ij} : (i, j) \in E\}$, the goal is to compute a realization of G in the Euclidean space $\mathbf{R}^d$ for a given low dimension d, where the distance information is preserved.

More precisely: given anchors $\mathbf{a}_k \in \mathbf{R}^d$, $d_{ij} \in N_x$, and $\hat{d}_{kj} \in N_a$, find $\mathbf{x}_i \in \mathbf{R}^d$ such that

$$\begin{aligned} \|\mathbf{x}_i - \mathbf{x}_j\|^2 &= d_{ij}^2, \ \forall\,(i,j) \in N_x,\ i < j, \\ \|\mathbf{a}_k - \mathbf{x}_j\|^2 &= \hat{d}_{kj}^2, \ \forall\,(k,j) \in N_a. \end{aligned}$$

This is a set of Quadratic Equations, which can be represented as an optimization problem:

$$\min_{\mathbf{x}_i \forall i} \sum_{(i,j)\in N_x} (\|\mathbf{x}_i - \mathbf{x}_j\|^2 - d_{ij}^2)^2 + \sum_{(k,j)\in N_a} (\|\mathbf{a}_k - \mathbf{x}_j\|^2 - \hat{d}_{kj}^2)^2.$$

Does the system have a localization or realization of all $\mathbf{x}_j$'s? Is the localization unique? Is there a certification for the solution to make it reliable or trustworthy? Is the system partially localizable with a certification?

It can be relaxed to SOCP (change "$=$" to "$\leq$") or SDP.

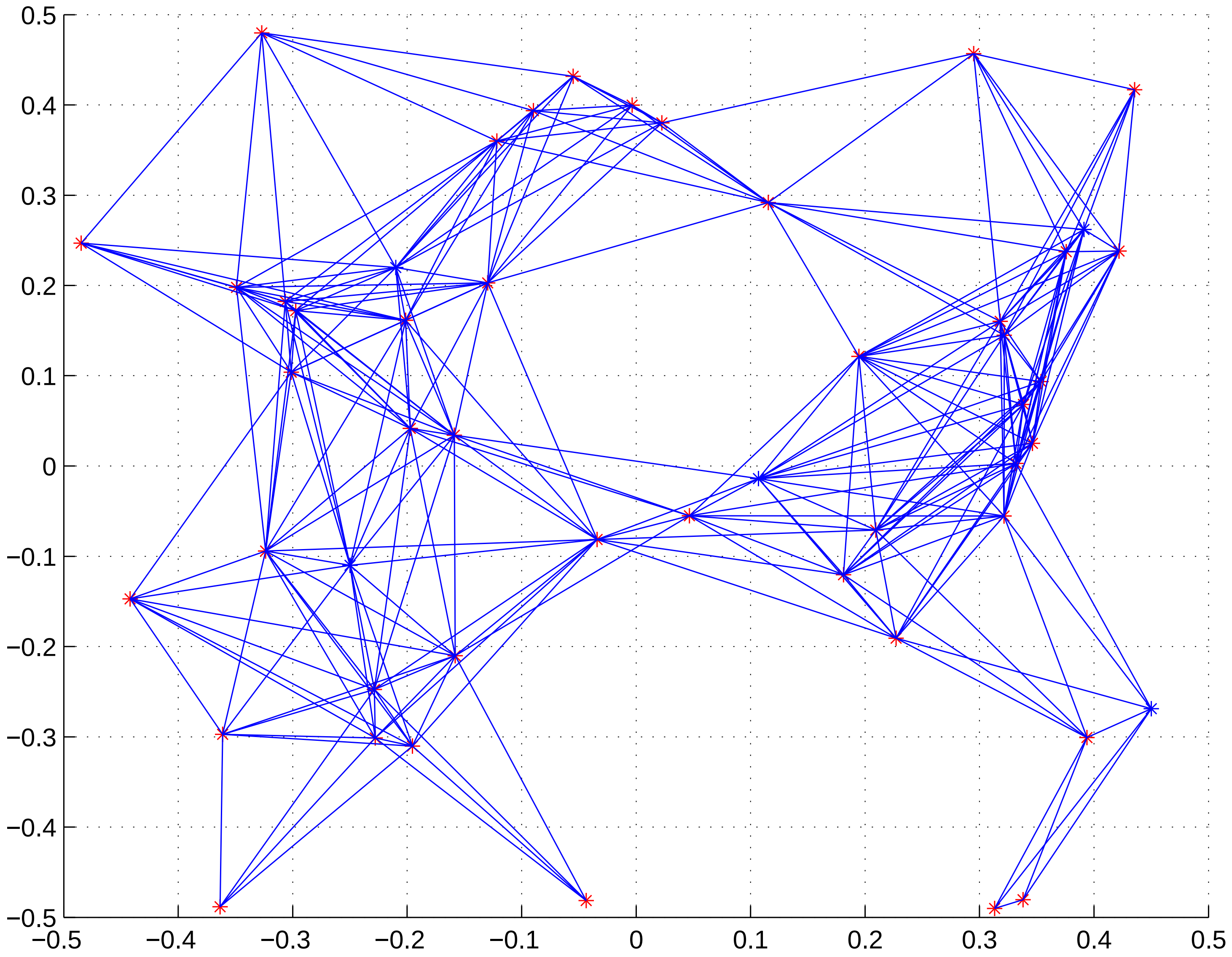


Figure 4: 50-node 2-D Sensor Localization.

Matrix Representation of SNL and SDP Relaxation

Let $X = [\mathbf{x}_1\ \mathbf{x}_2\ \ldots\ \mathbf{x}_n]$ be the $d \times n$ matrix that needs to be determined and $\mathbf{e}_j$ be the vector of all zero except 1 at the jth position. Then

$$\mathbf{x}_i - \mathbf{x}_j = X(\mathbf{e}_i - \mathbf{e}_j) \quad \text{and} \quad \mathbf{a}_k - \mathbf{x}_j = [I\ \ X](\mathbf{a}_k; -\mathbf{e}_j)$$

so that

$$\|\mathbf{x}_i - \mathbf{x}_j\|^2 = (\mathbf{e}_i - \mathbf{e}_j)^T X^T X(\mathbf{e}_i - \mathbf{e}_j)$$

$$\|\mathbf{a}_k - \mathbf{x}_j\|^2 = (\mathbf{a}_k; -\mathbf{e}_j)^T [I\ \ X]^T [I\ \ X](\mathbf{a}_k; -\mathbf{e}_j) =$$

$$(\mathbf{a}_k; -\mathbf{e}_j)^T \begin{pmatrix} I & X \\ X^T & X^T X \end{pmatrix} (\mathbf{a}_k; -\mathbf{e}_j).$$

Or, equivalently,

$$
\begin{array}{l}
(\mathbf{e}_i - \mathbf{e}_j)^T Y (\mathbf{e}_i - \mathbf{e}_j) = d_{ij}^2, \ \forall\, i, j \in N_x, \ i < j, \\
(\mathbf{a}_k; -\mathbf{e}_j)^T \begin{pmatrix} I & X \\ X^T & Y \end{pmatrix} (\mathbf{a}_k; -\mathbf{e}_j) = \hat{d}_{kj}^2, \ \forall\, k, j \in N_a, \\
Y = X^T X.
\end{array}
$$

Relax $Y = X^T X$ to $Y \succeq X^T X$, which is equivalent to matrix inequality:

$$
\begin{pmatrix} I & X \\ X^T & Y \end{pmatrix} \succeq \mathbf{0}.
$$

This matrix has rank at least d; if it's d, then $Y = X^T X$, and the converse is also true.

The problem is now an SDP problem: when the SDP relaxation is exact?

Algorithm: Convex relaxation first and steepest-descent-search second strategy?

Stochastic Optimization and Learning

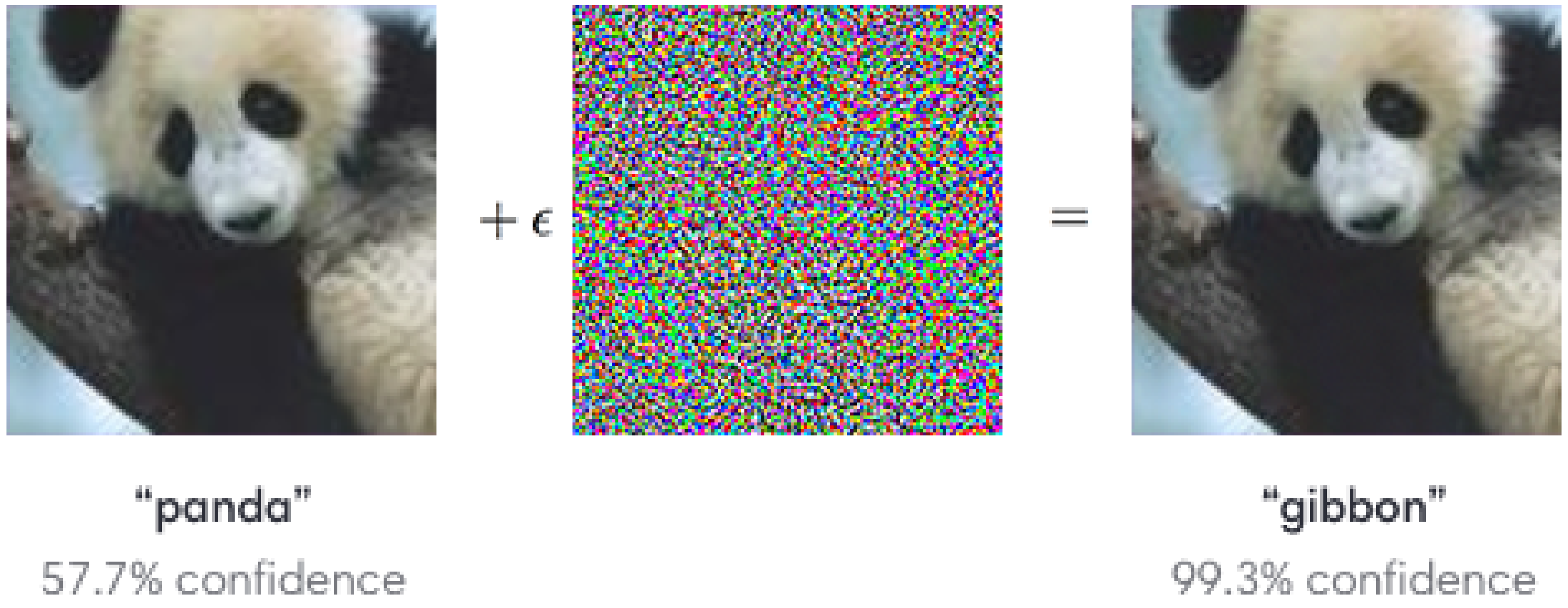
In real world, we most often do

$$\text{mimimize}_{\mathbf{x}\in X} \quad \mathbf{E}_{F_\xi}[h(\mathbf{x},\xi)] \tag{1}$$

where ξ represents random variables with the joint distribution F_ξ.

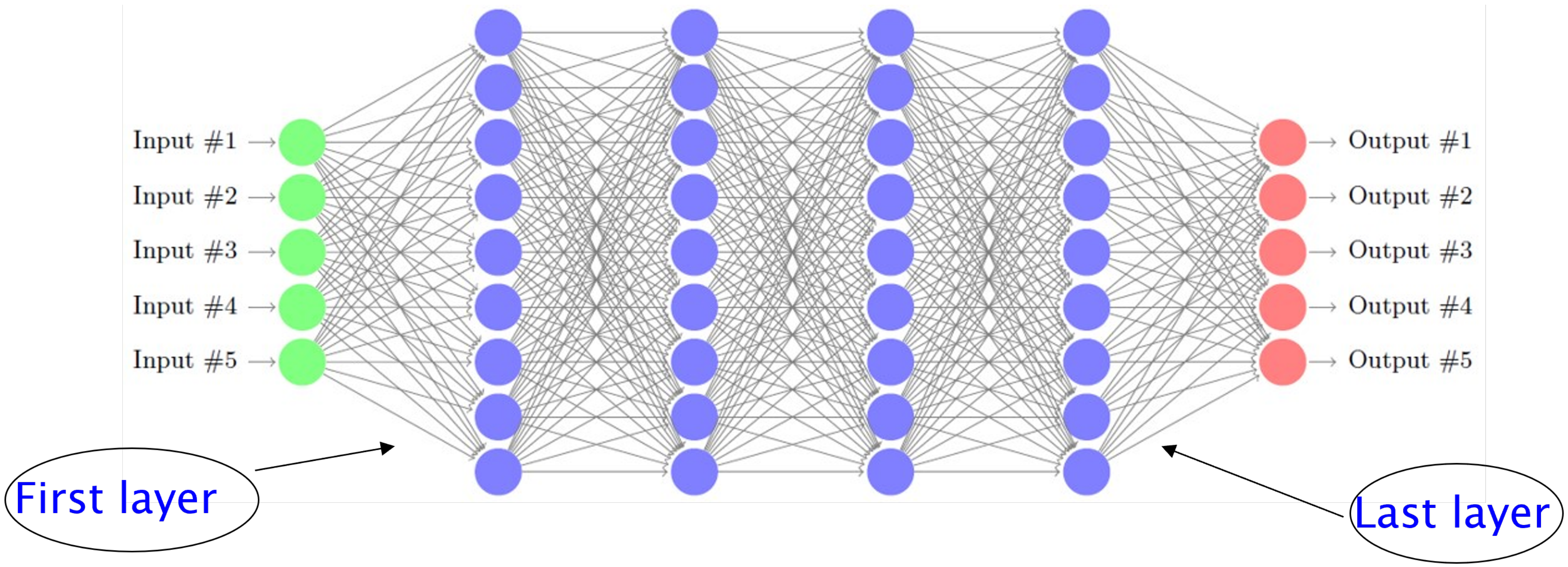
- Pros: In many cases, the expected value is a good measure of performance
- Cons: One has to know the exact distribution of ξ to perform the stochastic optimization so that we most frequently use sample distribution. Then, deviant from the assumed distribution may result in sub-optimal solutions. Even know the distribution, the solution/decision is generically risky.

Learning with Noises/Distortions



Goodfellow et al. [2014]

Deep-Learning on Neural-Network I



The input vector is denoted by $\mathbf{x}$ and the output vector of layer l is denoted by $\mathbf{y}^l$. The edge-weights of layer l are denoted by $w^l_{i,j}$ where the relation of input-output is

$$y^l_j = \max\{0,\ w^l_{0,j} + \sum_i w^l_{i,j} y^{l-1}_j\},\ \forall j,\ l = 1, ..., L.$$

where the formula is called ReLU operator/function and $\mathbf{y}^0 = \mathbf{x}$.

Deep-Learning on Neural-Network II

The Deep-Learning is to use massive sample images/inputs $\mathbf{x}$ to optimize/train (or learn edge-weights $w^l_{i,j}$ such that a (classification) sample-average error function is minimized. In other words, for this example, the outputs of images/inputs of Panda and Gibbon are distinguishable/separable, or they belong to different regions in the output space.

When all weights are determined, then the last-layer output vector of the neural-network, denoted by $\mathbf{y}^L(\mathbf{x})$, is a vector function/mapping of an input vector $\mathbf{x}$.

The neural network verification, for this example, is to find the smallest distortion of a given typical Panda image such that its output is in the output-region of normal Gibbon images, that is,

$$\begin{array}{ll} \text{minimize}_{\mathbf{x}} & \|\mathbf{x} - \hat{\mathbf{x}}\|^2 \\ \text{subject to} & \mathbf{y}^L(\mathbf{x}) \in \text{a (convex) region outside of } \mathbf{y}^L(\hat{\mathbf{x}}). \end{array}$$

A Neural-Network Verification Optimization Problem

The problem can be represented as a constrained problem:

$$\begin{array}{rl} \text{minimize}_{\{\mathbf{x},\mathbf{y}^l\}} & \|\mathbf{x}-\hat{\mathbf{x}}\|^2 \\ \text{subject to} & \mathbf{y}^L \in \text{a (convex) region outside of } \mathbf{y}^L(\hat{\mathbf{x}}), \\ & y^l_j = \max\{0,\ w^l_{0,j} + \sum_i w^l_{i,j} y^{l-1}_j\},\ \forall j,\ l=1,...,L \\ & \mathbf{y}^0 = \mathbf{x}. \end{array}$$

Convex Relaxation(?):

$$\begin{array}{rl} \text{minimize}_{\{\mathbf{x},\mathbf{y}^l\}} & \|\mathbf{x}-\hat{\mathbf{x}}\|^2 \\ \text{subject to} & \mathbf{y}^L \in \text{a (convex) region outside of } \mathbf{y}(\hat{\mathbf{x}}), \\ & y^l_j \ge w^l_{0,j} + \sum_i w^l_{i,j} y^{l-1}_j,\ \forall j,\ l=1,...,L \\ & y^l_j \ge 0,\ \forall j,\ l=1,...,L \\ & \mathbf{y}^0 = \mathbf{x}. \end{array}$$

A Neural-Network Verification Decision Problem

A related problem would be a regularized problem where $\mathbf{y}^L(\mathbf{x})$ is in a (convex) polyhedral region outside of $\mathbf{y}^L(\hat{\mathbf{x}})$?

Linearly-Constrained Quadratic Minimization Problem:

$$\begin{array}{rl} \text{minimize}_{\{\mathbf{x},\mathbf{y}^l\}} & \|\mathbf{x}-\hat{\mathbf{x}}\|^2 + \mu\sum_l\sum_j y_j^l(y_j^l - w_{0,j}^l - \sum_i w_{i,j}^l y_j^{l-1}) \\ \text{subject to} & \mathbf{y}^L \in \text{a (convex) polyhedral region outside of } \mathbf{y}(\hat{\mathbf{x}}), \\ & y_j^l \geq w_{0,j}^l + \sum_i w_{i,j}^l y_j^{l-1},\ \forall j,\ l = 1, ..., L \\ & y_j^l \geq 0,\ \forall j,\ l = 1, ..., L \\ & \mathbf{y}^0 = \mathbf{x}. \end{array}$$

The is a linearly constrained quadratic optimization problem.

Is the objective function convex?

Distributionally Robust Optimization and Learning

On the other hand: Why does error occur? Believing that the sample distribution is the true distribution...

In practice, although the exact distribution of the random variables may not be known, people usually know certain observed samples or training data and other statistical information. Thus, we can consider an enlarged distribution set $\mathcal{D}$ that confidently containing the sample distribution, and do

$$\text{minimize}_{\mathbf{x}\in X} \quad \max_{F_\xi \in \mathcal{D}} \mathbf{E}_{F_\xi}[h(\mathbf{x},\xi)] \tag{2}$$

In DRO, we consider a set of distributions $\mathcal{D}$ and choose one to minimize the expected value for the worst distribution in $\mathcal{D}$. When choosing $\mathcal{D}$, we need to consider the following:

- Tractability
- Practical (Statistical) Meanings
- Performance (the potential loss comparing to the benchmark cases)

This is a nonlinear Saddle-Point Min-Max optimization/zero-sum-game problem

Reinforcement Learning: Markov Decision/Game Process

- RL/MDPs provide a mathematical framework for modeling sequential decision-making in situations where outcomes are partly random and partly under the control of a decision maker.
- Markov game processes (MGPs) provide a mathematical slidework for modeling sequential decision-making of two-person turn-based zero-sum game.
- MDGPs are useful for studying a wide range of optimization/game problems solved via dynamic programming, where it was known at least as early as the 1950s (cf. Shapley 1953, Bellman 1957).
- Modern applications include dynamic planning under uncertainty, reinforcement learning, social networking, and almost all other stochastic dynamic/sequential decision/game problems in Mathematical, Physical, Management and Social Sciences.

MDP Stationary Policy and Cost-to-Go Value

- An MDP problem is defined by a given number of states, indexed by i, where each state has a number of actions, $\mathcal{A}_i$, to take. Each action, say $j \in \mathcal{A}_i$, is associtaed with an (immeidiate) cost c_j of taking, and a probability distribution $\mathbf{p}_j$ to transfer to all possible states at the next time period.

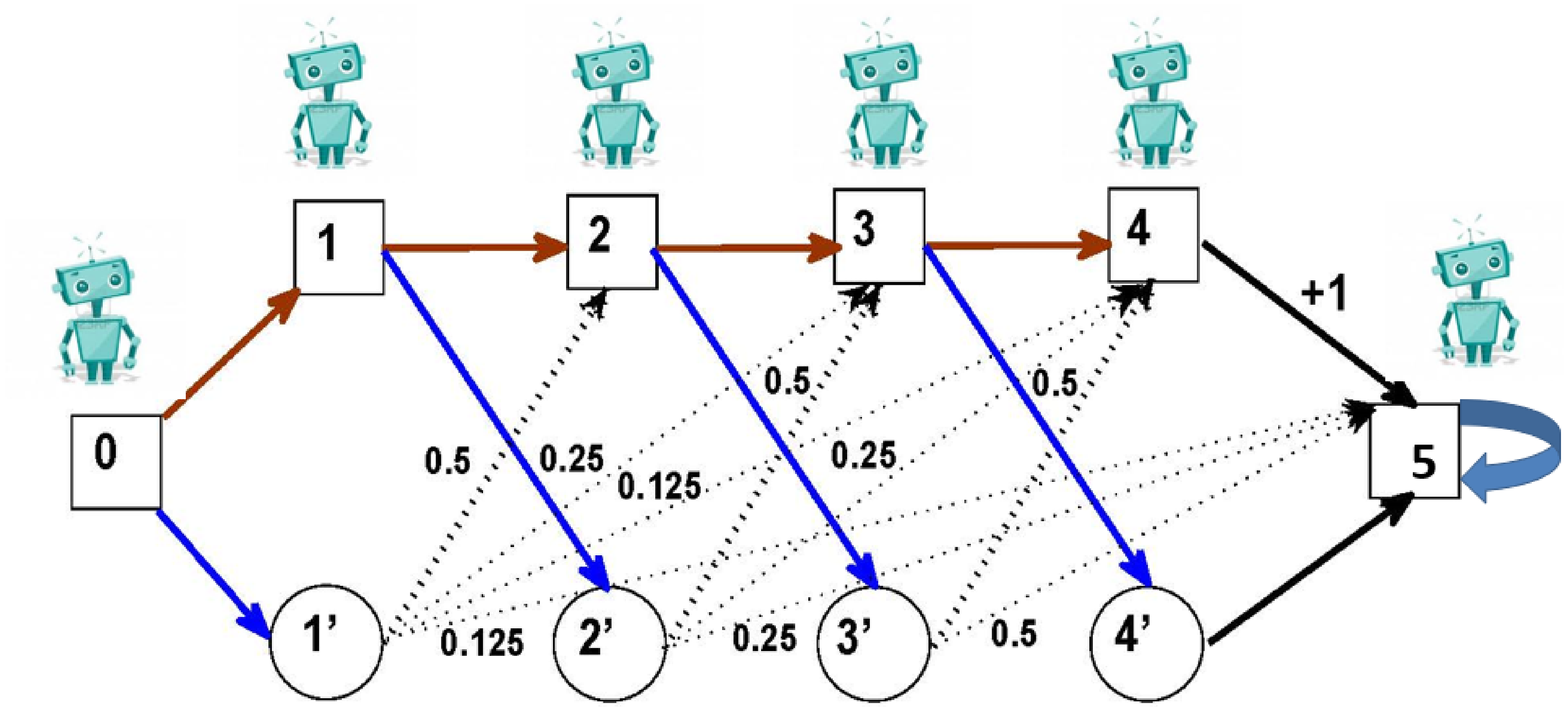
- A stationary policy for the decision maker is a function $\pi = \{\pi_1, \pi_2, \cdots, \pi_m\}$ that specifies an action in each state, $\pi_i \in \mathcal{A}_i$, that the decision maker will take at any time period; which also lead to a cost-to-go value for each state.

- The MDP is to find a stationary policy to minimize/maximize the expected discounted sum over the infinite horizon with a discount factor $0 \leq \gamma < 1$:

$$\sum_{t=0}^{\infty} \gamma^t E[c^{\pi_{i^t}}(i^t, i^{t+1})].$$

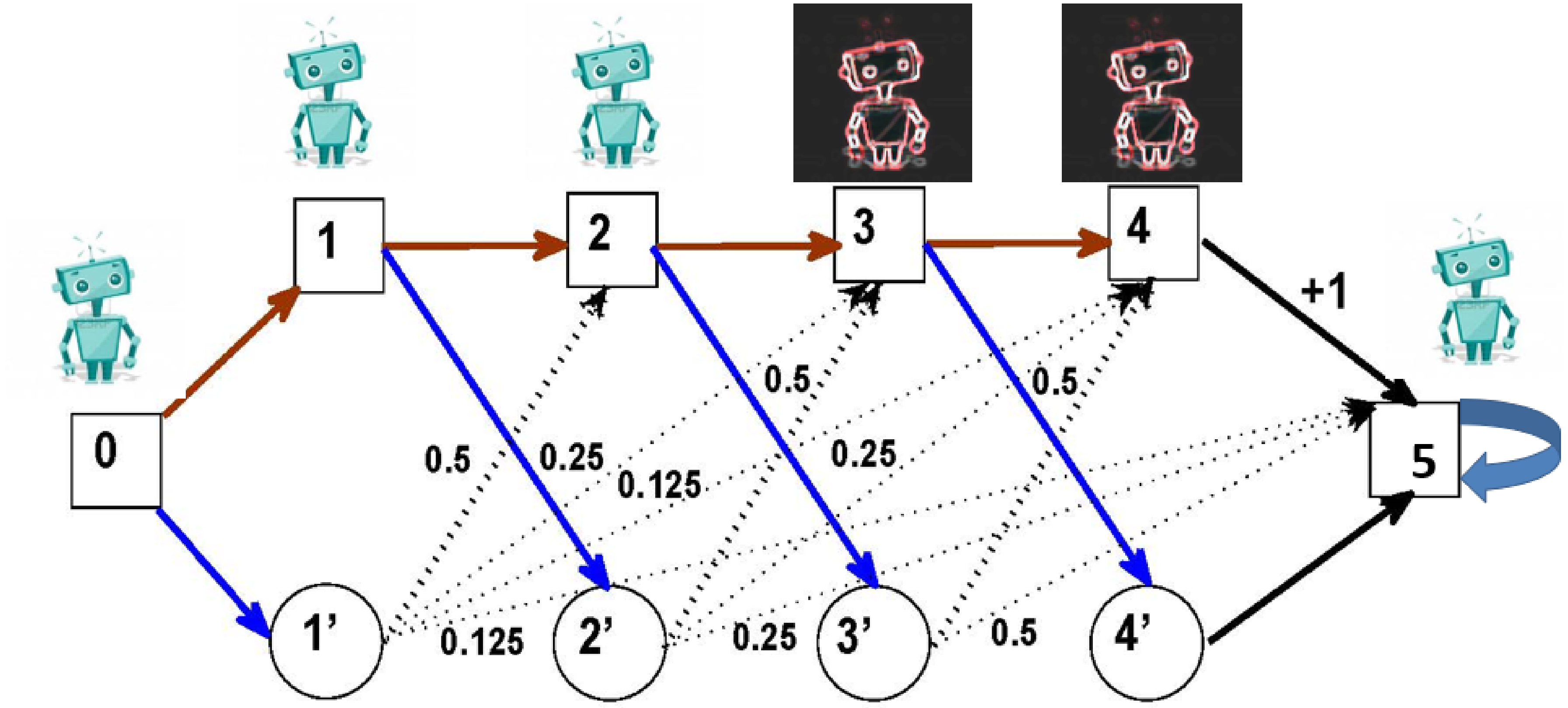
- If the states are partitioned into two sets, one is to minimize and the other is to maximize the discounted sum, then the process becomes a two-person turn-based zero-sum stochastic game.

An MDGP Toy Example: Maze Robot Runners (Simplified)



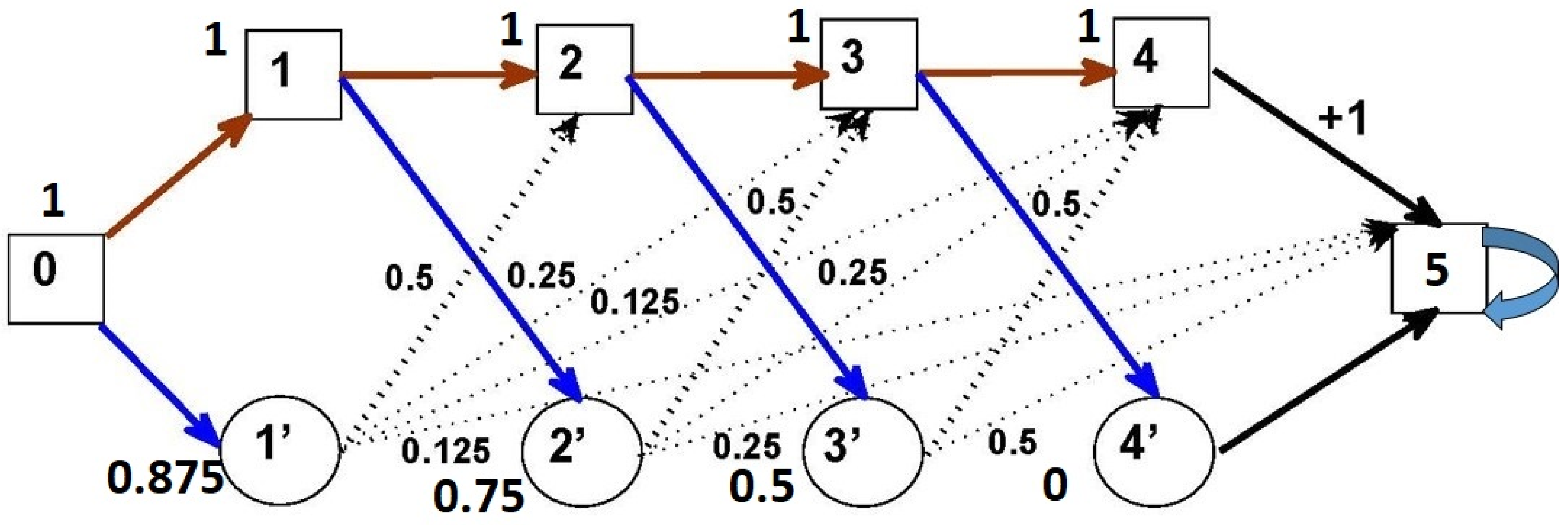
Actions are in red, blue and black; and all actions have zero cost except the state 4 to the exit/termination state 5. Which actions to take from every state to minimize the total cost (called optimal policy)?

Toy Example: Game Setting



States $\{0, 1, 2, 5\}$ minimize, while States $\{3, 4\}$ maximize.

The Cost-to-Go Values of the States



Cost-to-go values on each state when actions in red are taken: the current policy is not optimal since there are better actions to choose to minimize the cost.

The Optimal Cost-to-Go Value Vector

Let $\mathbf{y} \in \mathbf{R}^m$ represent the cost-to-go values of the m states, ith entry for ith state, of a given policy.

The MDP problem entails choosing an optimal policy where the corresponding cost-to-go value vector $\mathbf{y}^*$ satisfying:

$$y_i^* = \min\{c_j + \gamma \mathbf{p}_j^T \mathbf{y}^*, \ \forall j \in \mathcal{A}_i\}, \ \forall i,$$

with optimal policy

$$\pi_i^* = \arg\min\{c_j + \gamma \mathbf{p}_j^T \mathbf{y}^*, \ \forall j \in \mathcal{A}_i\}, \ \forall i.$$

In the Game setting, the conditions becomes:

$$y_i^* = \min\{c_j + \gamma \mathbf{p}_j^T \mathbf{y}^*, \ \forall j \in \mathcal{A}_i\}, \ \forall i \in I^-,$$

and

$$y_i^* = \max\{c_j + \gamma \mathbf{p}_j^T \mathbf{y}^*, \ \forall j \in \mathcal{A}_i\}, \ \forall i \in I^+.$$

They both are fix-point or saddle-point optimization problems. The MDP problem can be cast as a linear program; see next page.

The Equivalent LP Formulation for MDP

This model can be reformulated as an LP:

$$\begin{array}{lrcl}
\text{maximize}_{\mathbf{y}} & \sum_{i=1}^m y_i & & \\
\text{subject to} & y_1 - \gamma \mathbf{p}_j^T \mathbf{y} & \leq & c_j,\ j \in \mathcal{A}_1 \\
& & \vdots & \\
& y_i - \gamma \mathbf{p}_j^T \mathbf{y} & \leq & c_j,\ j \in \mathcal{A}_i \\
& & \vdots & \\
& y_m - \gamma \mathbf{p}_j^T \mathbf{y} & \leq & c_j,\ j \in \mathcal{A}_m.
\end{array}$$

Theorem 1 *When $\mathbf{y}$ is maximized, there must be at least one inequality constraint in $\mathcal{A}_i$ that becomes equal for every state i, that is, maximal $\mathbf{y}$ is a fixed point solution.*

The Maze Runner Example

The Fixed-Point formulation:

$$\begin{aligned}
y_0 &= \min\{0+\gamma y_1, 0+\gamma(0.5y_2+0.25y_3+0.125y_4+0.125y_5)\}\\
y_1 &= \min\{0+\gamma y_2, 0+\gamma(0.5y_3+0.25y_4+0.25y_5)\}\\
y_2 &= \min\{0+\gamma y_3, 0+\gamma(0.5y_4+0.5y_5)\}\\
y_3 &= \min\{0+\gamma y_4, 0+\gamma y_5\}\\
y_4 &= 1+\gamma y_5\\
y_5 &= 0\ (\text{or } y_5 = 0+\gamma y_5)
\end{aligned}$$

The LP formulation:

$$\begin{array}{ll}
\text{maximize}_{\mathbf{y}} & y_0+y_1+y_2+y_3+y_4+y_5\\[2em]
\text{subject to} & \text{change each equality above into inequality}
\end{array}$$

The Interpretations of the LP Formulation

The LP variables $\mathbf{y} \in \mathbf{R}^m$ represent the expected present cost-to-go values of the m states, respectively, for a given policy.

The LP problem entails choosing variables in $\mathbf{y}$, one for each state i, that maximize $\mathbf{e}^T\mathbf{y}$ so that it is the fixed point

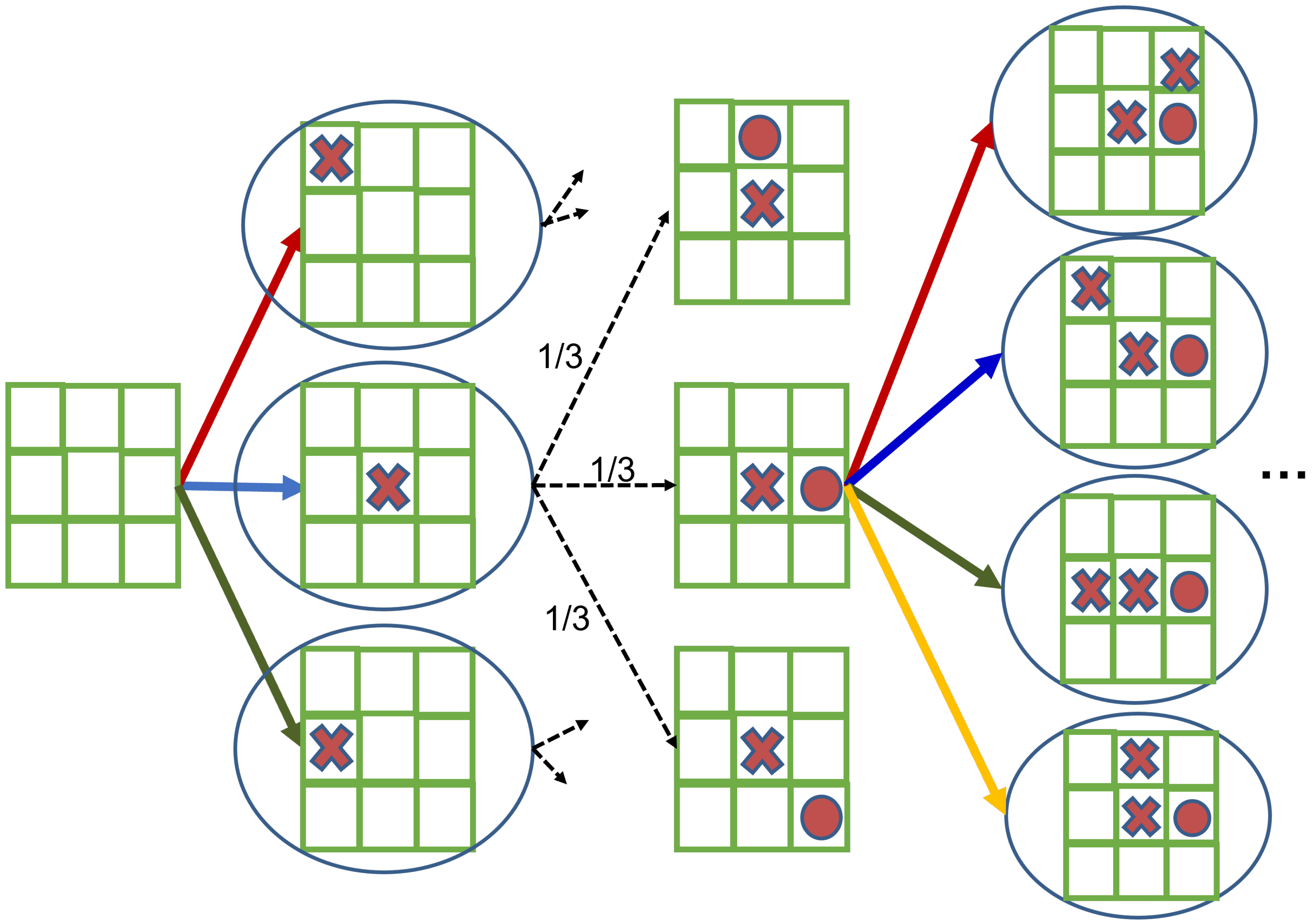
$$y_i^* = \min_{j \in \mathcal{A}_i} \{\mathbf{c}_{j_i} + \gamma \mathbf{p}_{j_i}^T \mathbf{y}\}, \ \forall i,$$

with an optimal policy

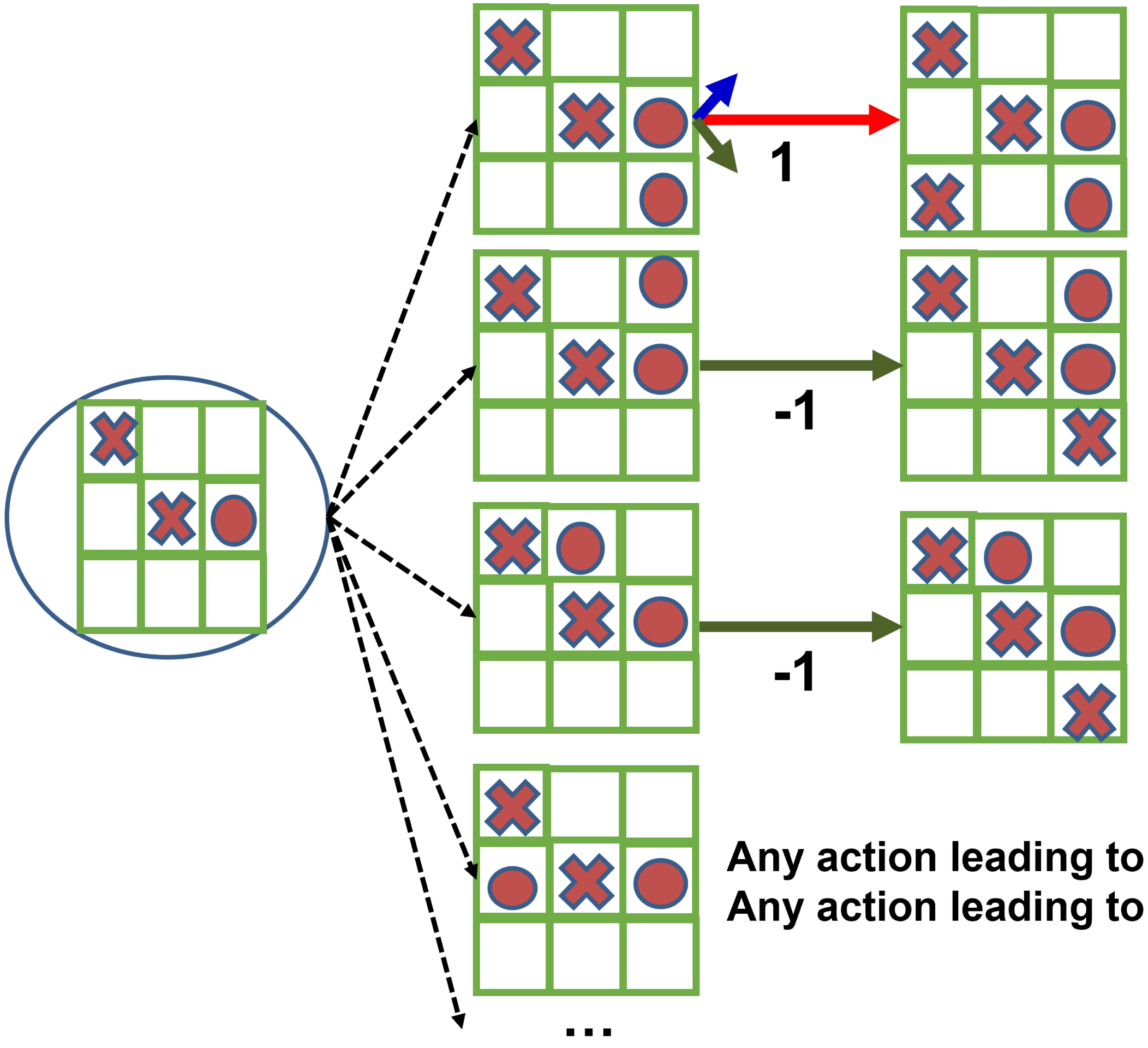
$$\pi_i^* = \arg\min\{\mathbf{c}_j + \gamma \mathbf{p}_j^T \mathbf{y}, \ j \in \mathcal{A}_i\}, \ \forall i.$$

It is well known that there exist a unique optimal stationary policy value vector $\mathbf{y}^*$ where, for each state i, y_i^* is the minimum expected present cost that an individual in state i and its progeny can incur.

States/Actions in the Tic-Tac-Toe Game



Action Costs in the Tic-Tac-Toe Game



Any action leading to win has cost -1
Any action leading to lose has cost 1