PDE continuum limits for prediction with expert advice

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Joint work with Nadejda Drenska (UMN) and Charlie Smart (Chicago)

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Outline

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- Prediction from expert advice [Kohn & Drenska, 2020] [Drenska & Calder, 2020]
  - Generalization of the Kohn-Serfaty game

Kohn-Serfaty Game

The game is played in a convex domain $\Omega \subset \mathbb{R}^2$ starting at $x_0 \in \Omega$ and involves a small parameter $\varepsilon > 0$. The rules of the game are

1. Paul chooses a direction vector $v_k \in \mathbb{S}^1$.
2. Carol moves the token from x_k to $x_{k+1} = x_0 \pm \sqrt{2}\varepsilon v_k$.

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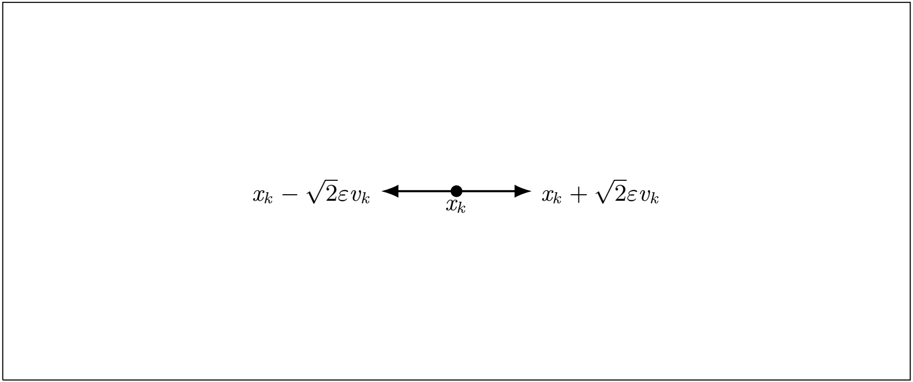

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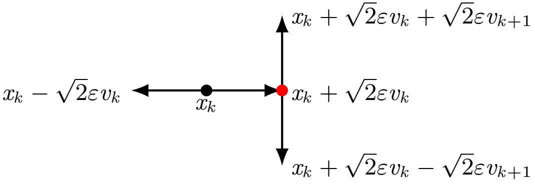

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Let us define

$$u_\varepsilon(x_0) = \varepsilon^2(\text{Number of steps for Paul to escape } \Omega)$$

given that both players play optimally and the game starts at x_0. The value function u satisfies the dynamic programming principle

$$u_\varepsilon(x) = \varepsilon^2 + \min_{|v|=1} \max_{b=\pm 1} u_\varepsilon(x + \sqrt{2}\varepsilon bv).$$

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We assume $u_\varepsilon \approx u$ where u is smooth and Taylor expand to obtain

$$u(x) \approx \varepsilon^2 + \min_{|v|=1} \max_{b=\pm 1} \left\{ u(x) + \sqrt{2}\varepsilon b \nabla u(x)^T v + \varepsilon^2 v^T \nabla^2 u(x) v \right\}.$$

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$$0 \approx 1 + \frac{(\nabla^\perp u)^T}{|\nabla u|} \nabla^2 u \frac{\nabla^\perp u}{|\nabla u|} = 1 + |\nabla u| \operatorname{div}\left(\frac{\nabla u}{|\nabla u|}\right).$$

Kohn-Serfaty Game

Kohn & Serfaty showed that $u_\varepsilon \to u$ as $\varepsilon \to 0$ where u is the viscosity solution of

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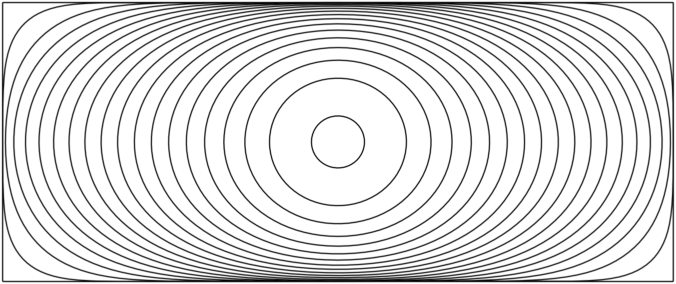

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State space: $\mathcal{X} := \{X_1, \ldots, X_n\}$

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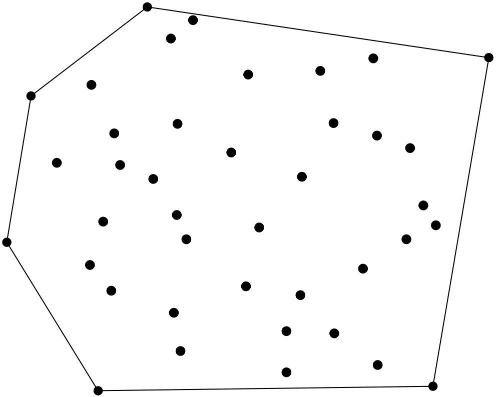

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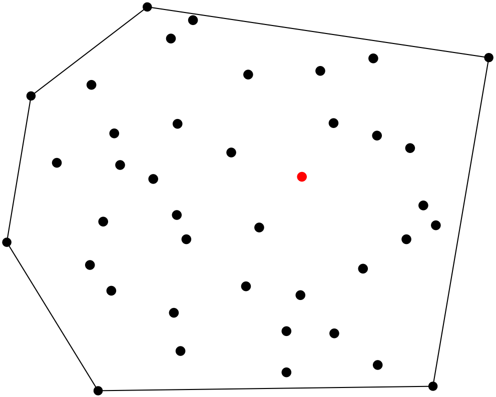

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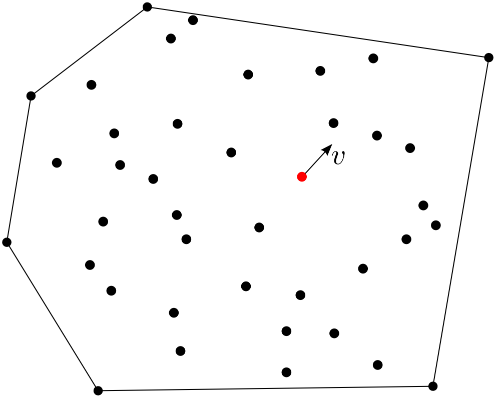

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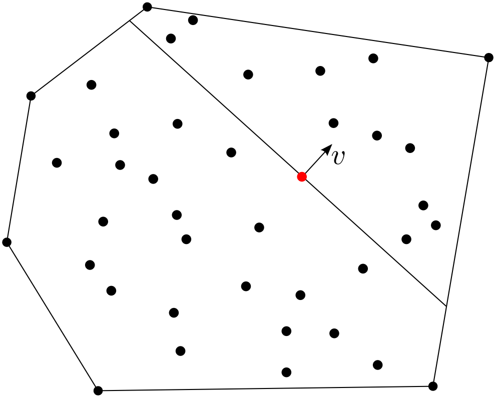

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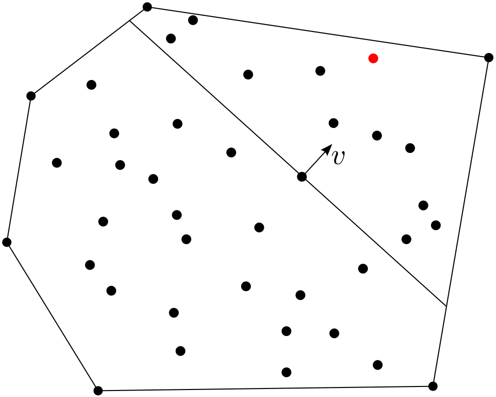

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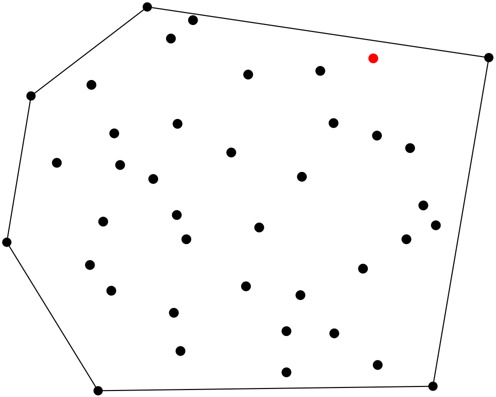

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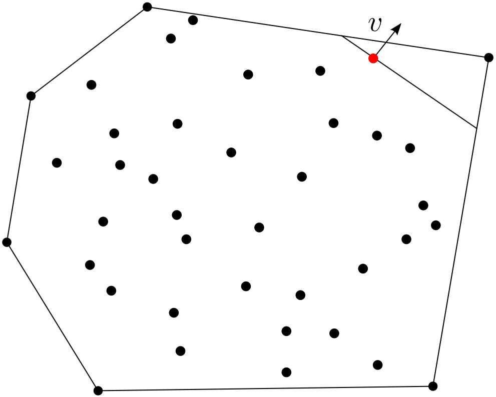

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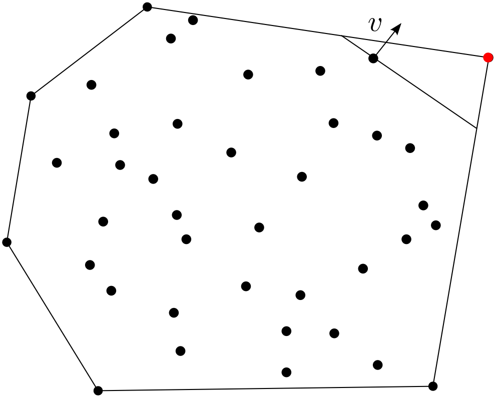

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- Used in robust statistics, machine learning, mathcing of point clouds, fingerprint identification, etc.

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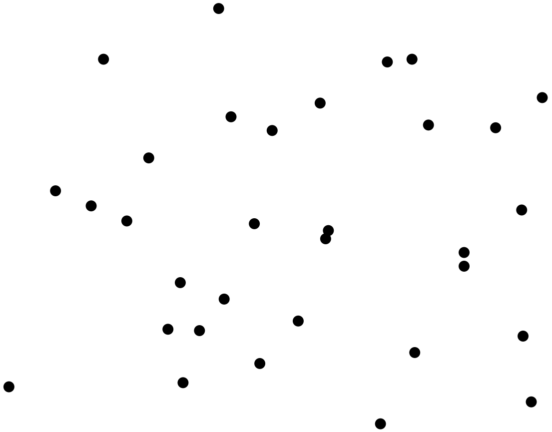

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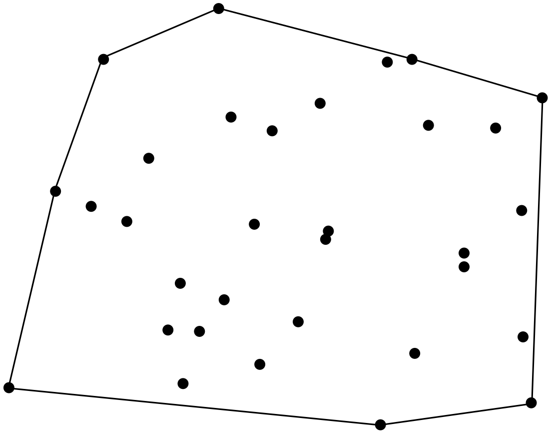

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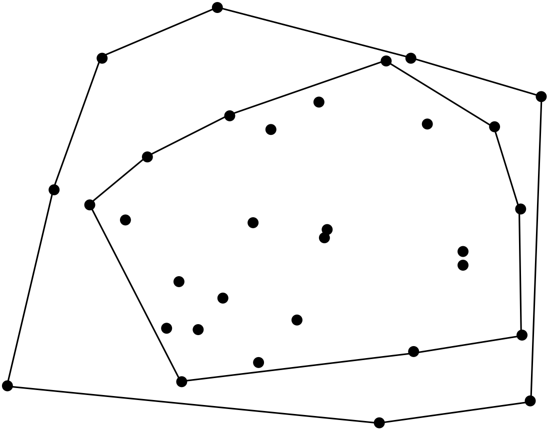

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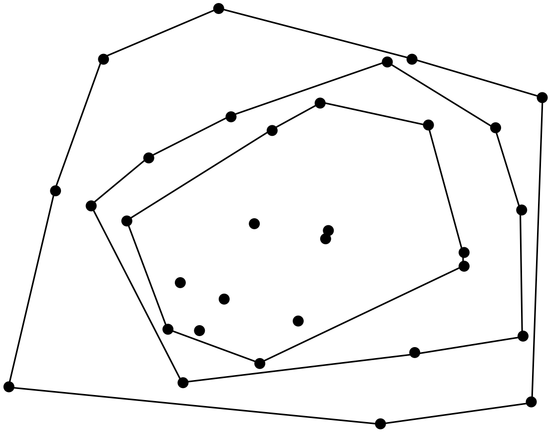

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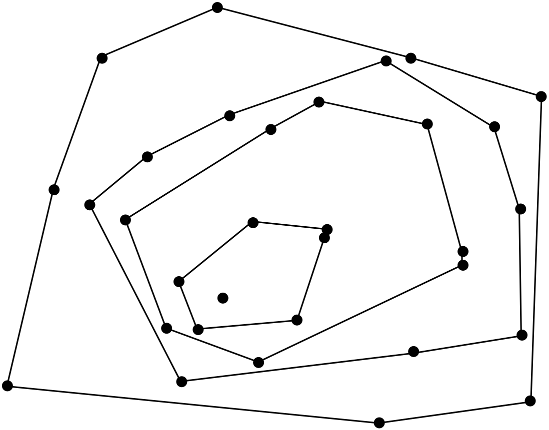

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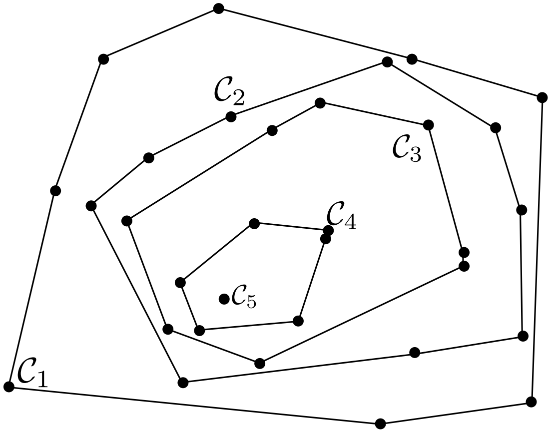

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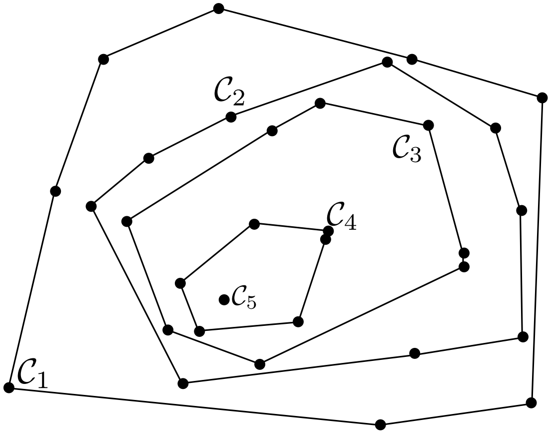
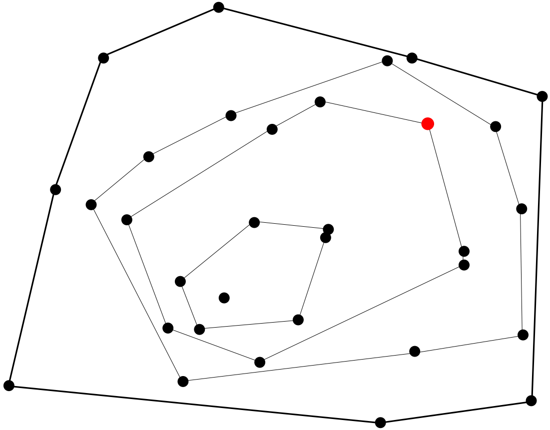


Convex hull peeling median := Centroid of final layer

Optimal strategies come from Convex Hull Peeling

Paul's optimal choice: Any halfspace supporting current convex layer

Carol's optimal choice: Any point on the previous convex layer



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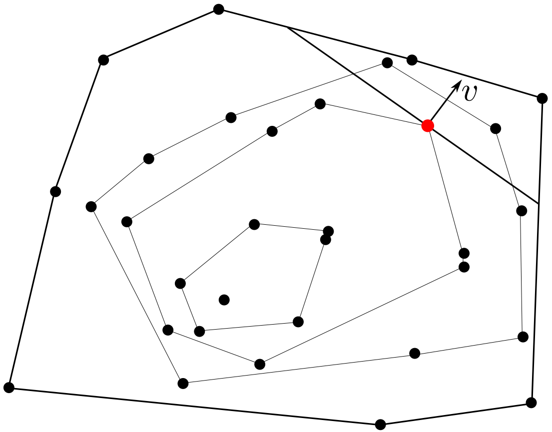

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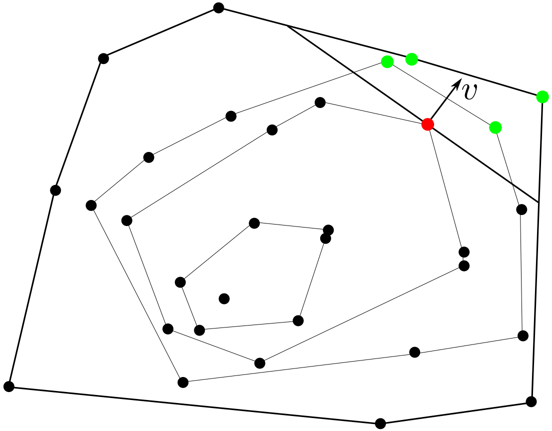

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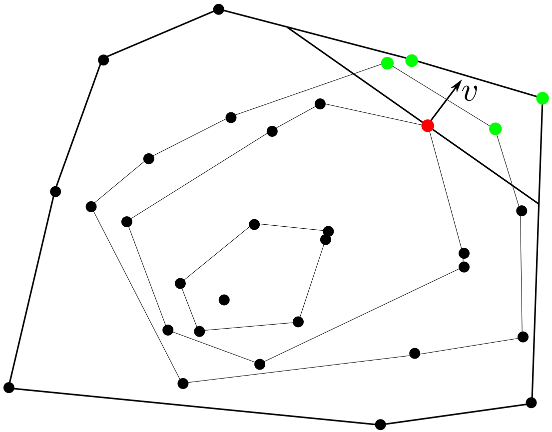
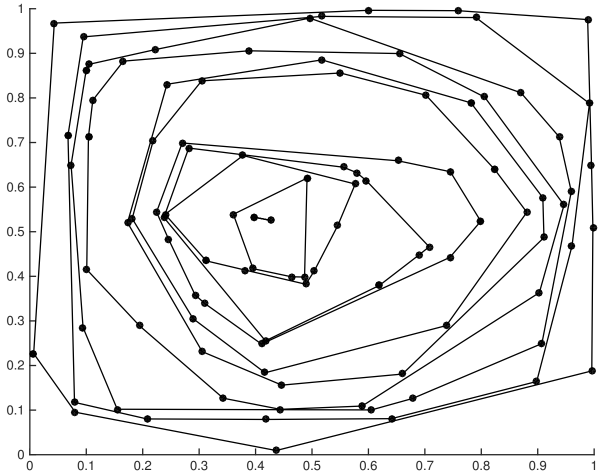


Value function $= U_n(x^0) =$ Convex depth function.

Convex hull peeling: Demo - Uniform distribution



$n = 10^2$ points

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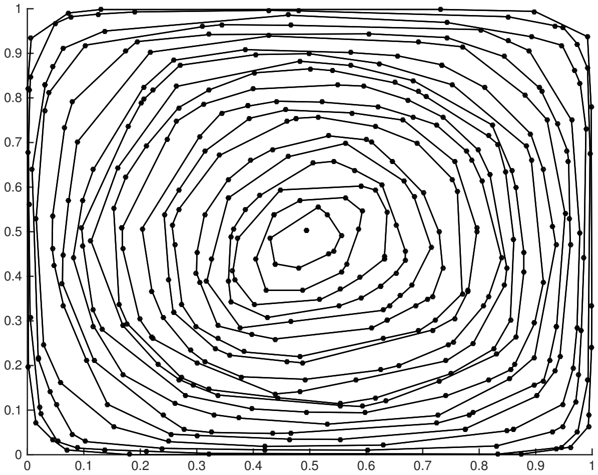

$n = 10^3$ points

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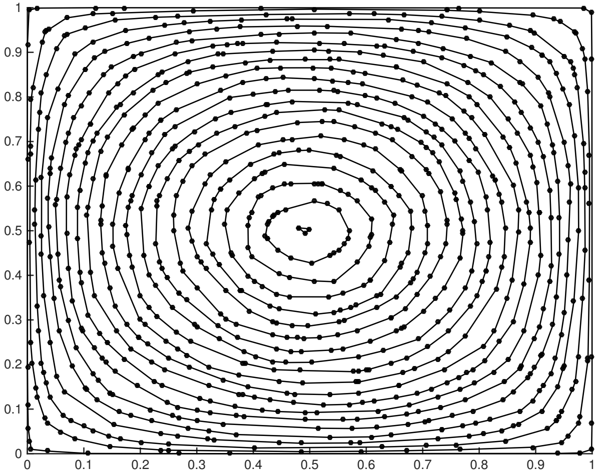

$n = 10^4$ points

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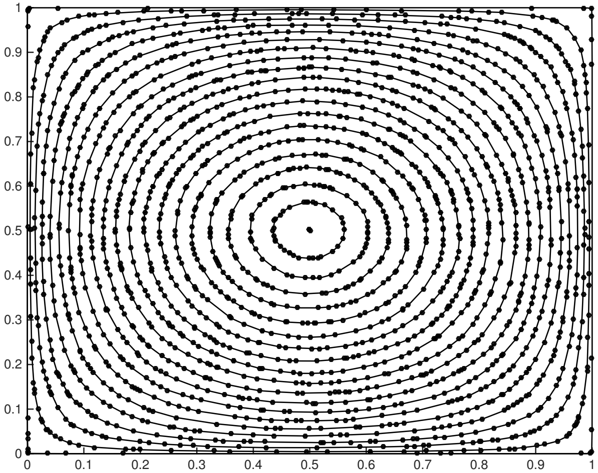
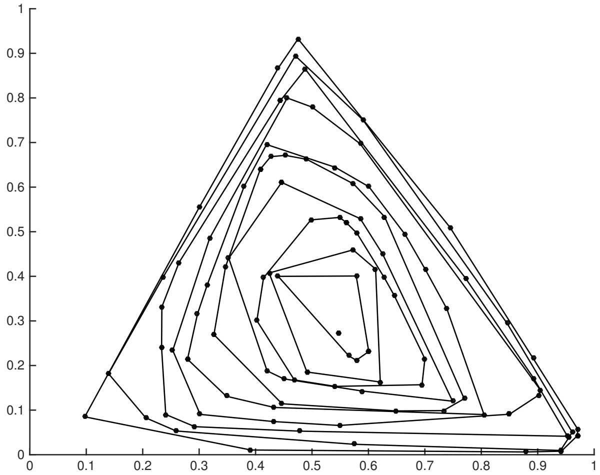


$n = 10^5$ points

Convex hull peeling: Demo - Triangle distribution



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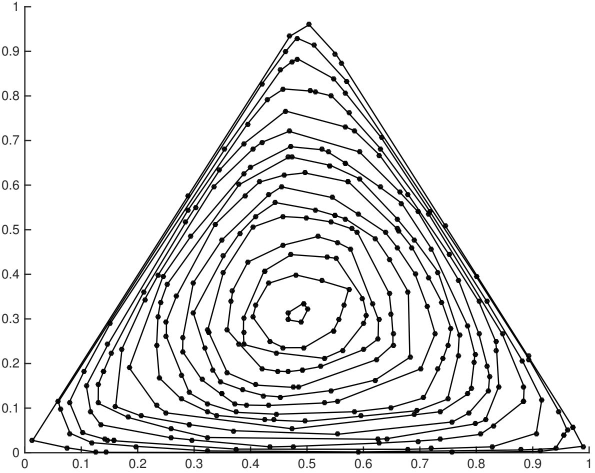

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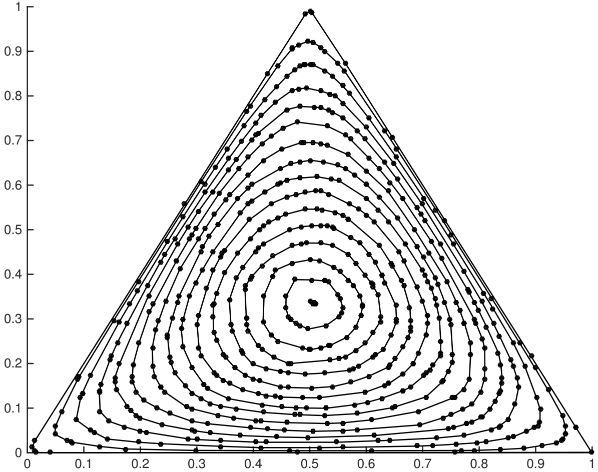
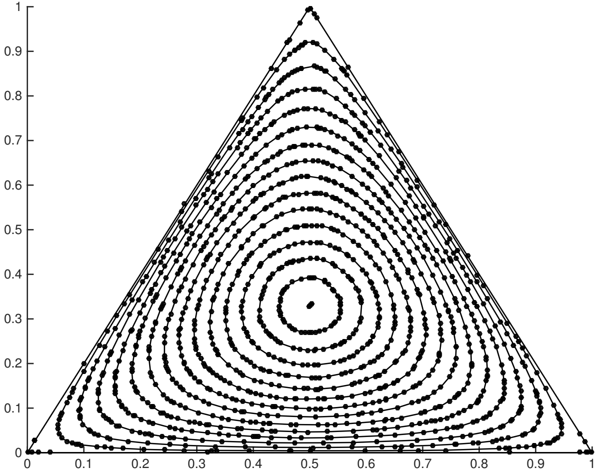


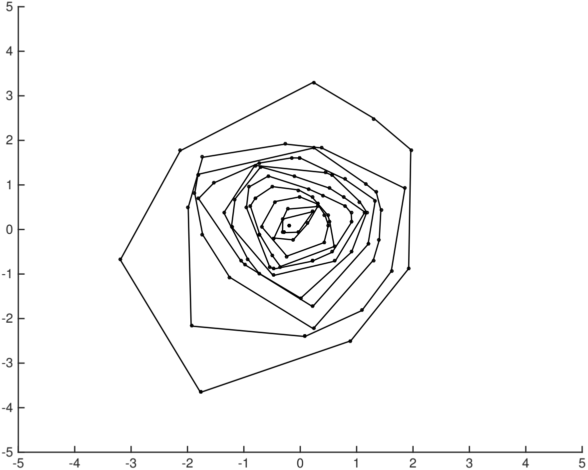
$n = 10^4$ points

Convex hull peeling: Demo - Triangle distribution



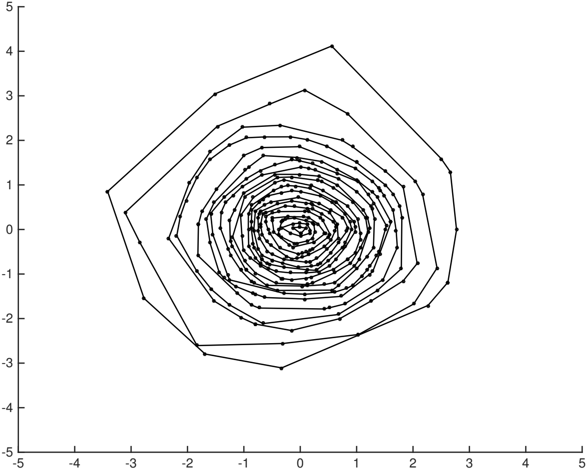
$n = 10^5$ points

Convex hull peeling: Demo - Gaussian distribution



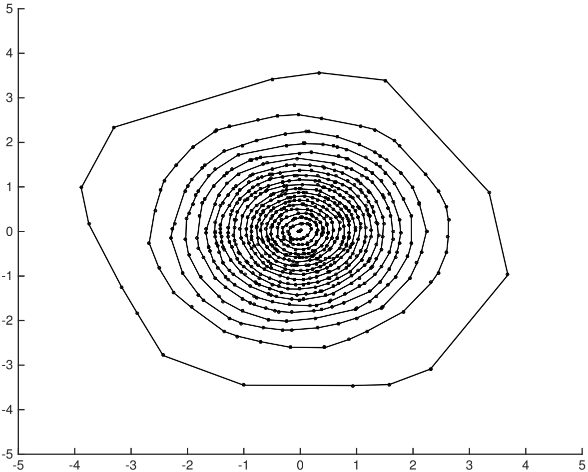
$n = 10^2$ points

Convex hull peeling: Demo - Gaussian distribution



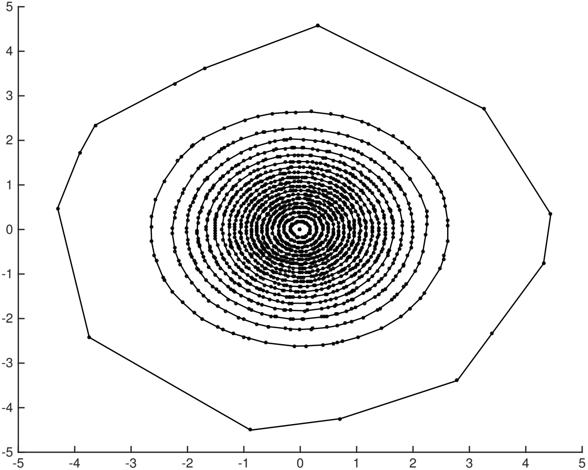
$n = 10^3$ points

Convex hull peeling: Demo - Gaussian distribution



$n = 10^4$ points

Convex hull peeling: Demo - Gaussian distribution

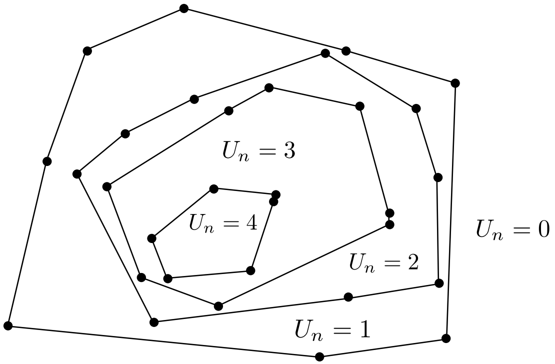


$n = 10^5$ points

A PDE continuum limit for convex hull peeling

Let $X_1, \ldots, X_n$ be i.i.d. with a continuous density ρ on a convex set $\Omega \subset \mathbb{R}^d$.

Let U_n be the function that 'counts' the associated convex layers.



Partial differential equation (PDE) continuum limit

Theorem (Calder & Smart, 2020)

There exists a universal constant α_d *such that with probability one*

$$n^{-\frac{2}{d+1}} U_n \longrightarrow \alpha_d u \quad \textit{uniformly on } \Omega,$$

where $u \in C(\overline{\Omega})$ *is the unique viscosity solution of*

$$\begin{cases} \nabla u^T \mathrm{cof}(-\nabla^2 u) \nabla u = \rho^2 & \textit{in } \Omega \\ u = 0 & \textit{on } \partial\Omega. \end{cases} \tag{2}$$

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This is just motion by a power of Gauss curvature

$$\frac{dS}{dt} = \rho^{-2/(d+1)} \kappa_G^{1/(d+1)} \mathbf{n}.$$

Known as affine invariant curvature motion when $\rho \equiv 1$.

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U_n satisfies a dynamic programming principle arising from the two player game

$$U_n(x) = \inf_{p \in \mathbb{R}^d \setminus \{0\}} \sup_{p^T(y-x)>0} [\mathbb{1}_{\{X_1,\dots,X_n\}}(y) + U_n(y)].$$

- Proof requires more than Taylor expansion and reading off the optimal strategies.
- Involves analyzing the scaling limit of the game after a large number of steps (locally), which has connections to stochsatic growth models.

Calder, J., and Smart, C.K. The limit shape of convex hull peeling. Duke Mathematical Journal, 169.11 (2020): 2079-2124.

A PDE continuum limit for convex hull peeling

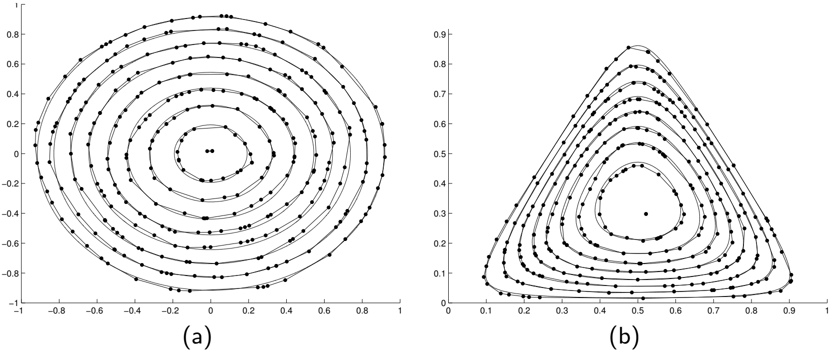
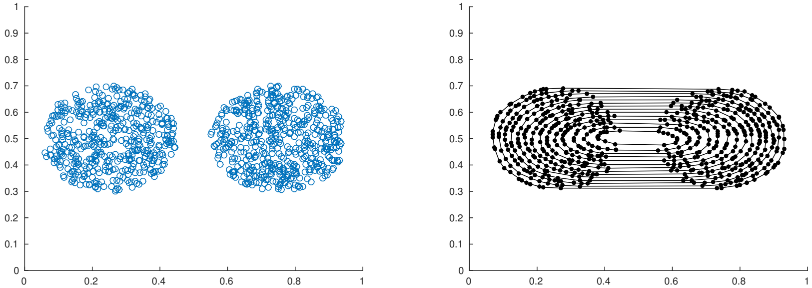


Figure: Convex layers vs continuum limit for $n = 5 \times 10^3$.

A nonconvex example

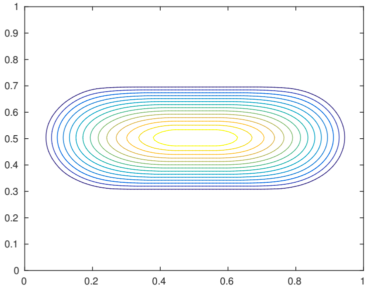


(a) Samples

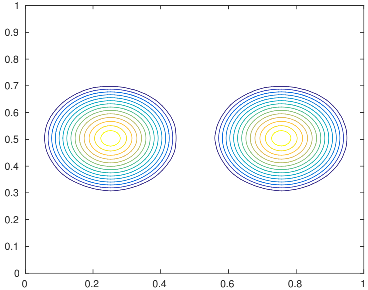
(b) Convex layers

Figure: Convex layers corresponding to disjoint clusters.

A nonconvex example



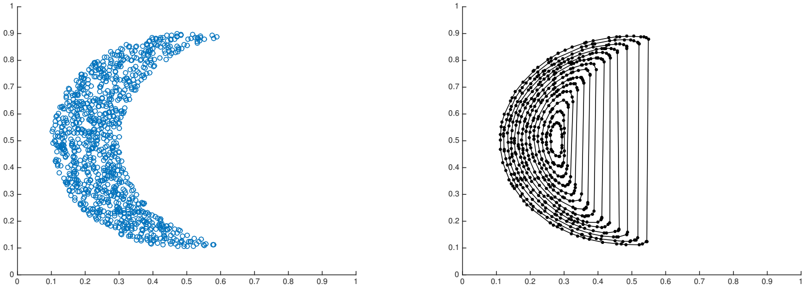
(a) One solution



(b) Another solution

Figure: Two different solutions continuum PDE.

The halfmoon



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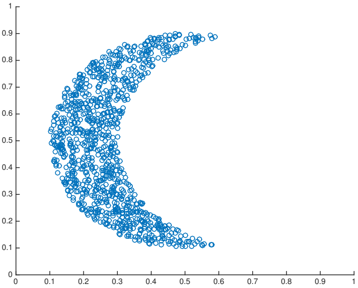
(b) Convex layers

Figure: Convex layers corresponding to the halfmoon distribution.

The halfmoon



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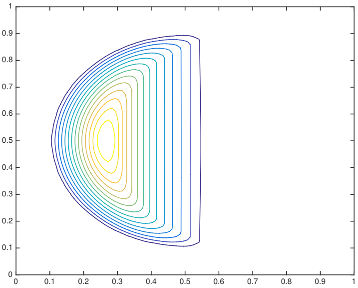

(b) PDE

Figure: Solution of PDE for the halfmoon example.

Outline

Prediction with expert advice

- One of the oldest online machine learning problems [Cover, 1966].
- We are given a stream of data $b_1, b_2, b_3, \ldots$.
- A pool of "experts" makes predictions about future values b_k.
- The player must use the expert advice to make their own prediction.
- The player's performance is measured by regret

$$\text{Regret to expert } i := \text{Expert } i\text{'s performance} - \text{Player's performance.}$$

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Applications: Financial math, weather prediction, click prediction,. . .

Example: Weather prediction

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Possible Experts:

1. The Weather Network
2. AccuWeather
3. Weather Underground
4. Your own deep neural network
5. It will rain today if it rained yesterday
6. It always rains
7. It never rains
8. Toss a coin
9. Red sky in the morning

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- $n = 2, 3$ experts [Gravin et al., 2016, Abbasi et al., 2017].
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- Connection to PDEs for $n \geq 2$ experts
  - [Zhu, 2014, Drenska, 2017, Drenska and Kohn, 2019b]

Problem setup: History dependent experts

- Daily stock price movements $b_1, b_2, b_3, \ldots, b_k, \ldots$ with $b_k \in \mathcal{B} := \{-1, 1\}$.

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- We have n experts predicting b_i based on d-days of history

$$m^i := (b_{i-d}, b_{i-d+1}, \ldots, b_{i-1}) \in \mathcal{B}^d.$$

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  2. The market chooses $b_i \in \mathcal{B}$.
  3. Investor accumulates regret $q_j(m^i)b_i - f_i b_i$ with respect to expert j.

Problem setup: History dependent experts

- After N steps of the game, the accumulated regret is

$$R_N := \sum_{i=1}^{N} b_i(q(m^i) - f_i \mathbb{1}), \qquad \mathbb{1} = (1, \ldots, 1).$$

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- Common choice for payoff is

$$g(x) = \max\{x_1, x_2, \ldots, x_n\},$$

where x_i = regret with respect to expert i.

Drenska, N., and Kohn R.V. A PDE approach to the prediction of a binary sequence with advice from two history-dependent experts. arXiv preprint:2007.12732 (2020).

Problem setup: History dependent experts

- Notation: For $m = (m_1, \ldots, m_d) \in \mathcal{B}^d$ and $b \in \mathcal{B}$ we denote

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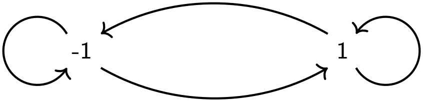
Definition (Value function)

Let $g : \mathbb{R}^n \to \mathbb{R}$. Given $N \in \mathbb{N}$, $m \in \mathcal{B}^d$, and $1 \leq \ell \leq N$, the value function $V_N(x, \ell; m)$ is defined by $V_N(x, \ell; m) = g(x)$ for $\ell = N$, and

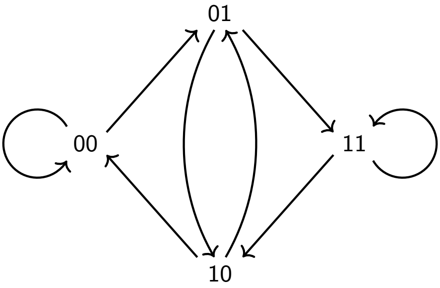
$$(4) \qquad V_N(x, \ell; m) = \min_{|f_\ell| \leq 1} \max_{b_\ell = \pm 1} \cdots \min_{|f_{N-1}| \leq 1} \max_{b_{N-1} = \pm 1} g\left(x + \sum_{i=\ell}^{N-1} b_i(q(m^i) - f_i \mathbb{1})\right)$$

for $1 \leq \ell \leq N - 1$, where $m^\ell = m$ and $m^{i+1} = m^i|b_i$ for $i = \ell, \ldots, N-1$.

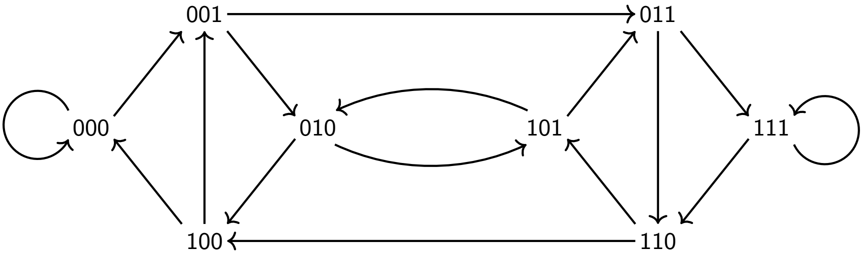
De Bruijn graph $d = 1$



De Bruijn graph $d = 2$



De Bruijn graph $d = 3$



Assumptions

- For $T > 0, N \in \mathbb{N}$, define $\varepsilon > 0$ by $T = \varepsilon^2 N$ and set

$$u_N(x,t;m) := \frac{1}{\sqrt{N}} V_N(\sqrt{N}x, \lceil Nt \rceil; m),$$

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- We assume $g \in C^4(\mathbb{R}^n)$ with uniformly bounded derivatives of order up to 4 over $\mathbb{R}^n$, there exists $\theta > 0$ such that

$$\nabla g(x)^T \mathbb{1} \geq \theta \quad \text{for all } x \in \mathbb{R}^n, \tag{5}$$

and that g is positively 1-homogeneous, that is

$$g(sx) = sg(x) \ \text{ for all } x \in \mathbb{R}^n, s > 0. \tag{6}$$

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- We also assume the expert strategies $q = (q_1, \ldots, q_n)$ satisfy

$$q : \mathcal{B}^d \to [-\mu, \mu]^n \quad \text{for some } \mu \in (0, 1). \tag{7}$$

Our main result

Let u be the viscosity solution of

$$\begin{cases} u_t + \frac{1}{2^{d+1}} \sum_{m \in \mathcal{B}^d} \eta(m)^T \nabla^2 u \, \eta(m) = 0, & \text{in } \mathbb{R}^n \times (0,1) \\ u = g, & \text{on } \mathbb{R}^n \times \{t = 1\}, \end{cases} \tag{8}$$

where

$$\eta(m) = q(m) - \frac{\nabla u^T q(m)}{\nabla u^T \mathbb{1}} \mathbb{1}. \tag{9}$$

Theorem (Drenska & Calder, 2020)

There exists $C_1, C_2 > 0$, depending on u, n and θ, such that

$$|u_N(x,t;m) - u(x,t)| \leq C_1 d(1 - t + \varepsilon)\varepsilon \tag{10}$$

holds for all $N \geq C_2 d^2/\mu^2$, $(x,t) \in \mathbb{R}^n \times [0,1]$ and $m \in \mathcal{B}^d$, where $\varepsilon = N^{-1/2}$.

Optimal strategies

An $O(\varepsilon)$ asymptotically optimal investor strategy is

$$f^* = \frac{\nabla u^T q}{\nabla u^T \mathbb{1}} + \frac{\varepsilon}{2}\left(\frac{\mathcal{H}(m_+) - \mathcal{H}(m_-)}{\nabla u^T \mathbb{1}}\right),$$

where $\mathcal{H}$ satisfies the graph Poisson equation

$$\Delta_{\mathcal{B}^d}\mathcal{H} = h - \frac{1}{2^d}\sum_{m\in\mathcal{B}^d} h(m)$$

where

$$\Delta_{\mathcal{B}^d}\mathcal{H}(m) = \mathcal{H}(m) - \frac{1}{2}\mathcal{H}(m_+) - \frac{1}{2}\mathcal{H}(m_-),$$

and

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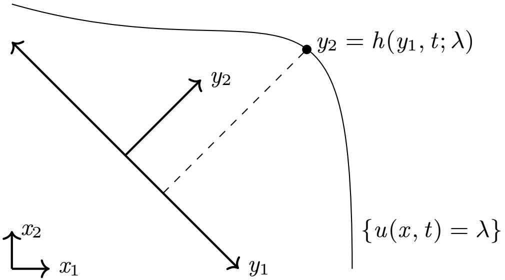
An asymptotically optimal market strategy is

$$b^* = \mathrm{sign}(f^* - f),$$

Underlying linear heat equation

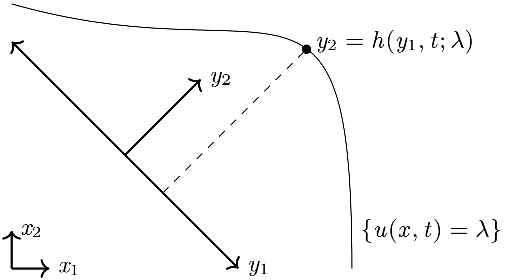


Change coordinates so $y_n = x_1 + \cdots + x_n$, $y_i = x_i - x_n$ and define h by

$$v(y_1, \ldots, y_{n-1}, h(y_1, \ldots, y_{n-1}, t; \lambda), t) = \lambda,$$

where $v(y,t) = u(x,t)$.

Underlying linear heat equation



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$$v(y_1, \ldots, y_{n-1}, h(y_1, \ldots, y_{n-1}, t; \lambda), t) = \lambda,$$

where $v(y,t) = u(x,t)$. We find h satisfies a linear heat equation

$$h_t + \frac{1}{2^{d+1}} \sum_{m \in \{-1,1\}^d} r(m)^T \nabla^2 h \, r(m) = 0, \tag{11}$$

where $r_i(m) := q_i(m) - q_n(m)$. The condition $g \in C^4$ ensures u is smooth.

Dynamic programming principle (DPP)

Recall the value function

$$V_N(x,\ell;m) = \min_{|f_\ell|\leq 1} \max_{b_\ell=\pm 1} \cdots \min_{|f_{N-1}|\leq 1} \max_{b_{N-1}=\pm 1} g\left(x + \sum_{i=\ell}^{N-1} b_i(q(m^i) - f_i\mathbb{1})\right)$$

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Proposition (1-Step Dynamic Programming Principle)

For $\ell \leq N-1$ *and* $m \in \{-1,1\}^d$

(12) $$V_N(x,\ell;m) = \min_{|f|\leq 1}\max_{b=\pm 1} V_N(x + b(q(m) - f\mathbb{1}), \ell+1; m|b).$$

Dynamic programming principle (DPP)

Recall the value function

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$$V_N(x,\ell;m) = \min_{|f|\leq 1} \max_{b=\pm 1} V_N(x + b(q(m) - f\mathbb{1}), \ell+1; m|b). \tag{12}$$

Note: The DPP is a coupled set of 2^d equations.

Dynamic programming principle

Let us assume that

$$u_N(x,t;m) = \frac{1}{\sqrt{N}} V_N(\sqrt{N}x, \lceil Nt \rceil; m) \approx u(x,t),$$

for some $u \in C^3$.

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$$\begin{aligned} u(x,t) &= \min_{|f|\le 1} \max_{b=\pm 1} u(x + \varepsilon b(q(m) - f\mathbb{1}), t + \varepsilon^2) \\ &= \min_{|f|\le 1} \max_{b=\pm 1} \Big\{ u(x,t) + \varepsilon^2 u_t + \varepsilon b \nabla u^T (q(m) - f\mathbb{1}) \\ &\qquad + \frac{\varepsilon^2}{2} (q(m) - f\mathbb{1})^T \nabla^2 u \, (q(m) - f\mathbb{1}) \Big\} + O(\varepsilon^3) \end{aligned}$$

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$$u_t + \min_{|f|\leq 1} \max_{b=\pm 1} \Big\{ \varepsilon^{-1} b \nabla u^T (q(m) - f\mathbb{1}) + \frac{1}{2} (q(m) - f\mathbb{1})^T \nabla^2 u \, (q(m) - f\mathbb{1}) \Big\} = O(\varepsilon).$$

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Investor (player) may wish to choose f to cancel out ε^{-1} term:

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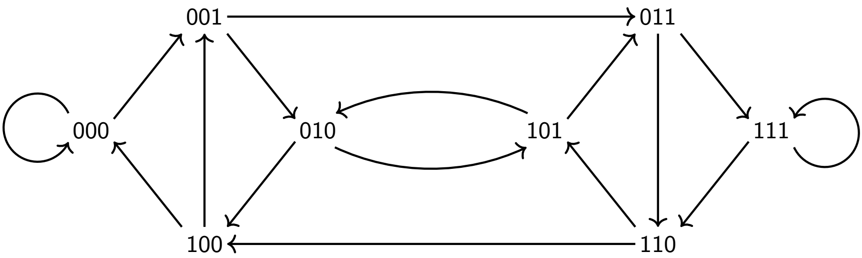
where $\eta(m) = q(m) - \frac{\nabla u^T q(m)}{\nabla u^T \mathbb{1}} \mathbb{1}$.

De Bruijn graph $d = 3$



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where $\eta(m) = q(m) - \frac{\nabla u^T q(m)}{\nabla u^T \mathbb{1}}\mathbb{1}$. [Drenska and Kohn, 2019a]

k-step Dynamic Programming Principle

Proposition (Dynamic Programming Principle)

For any $N \geq 1$, $x \in \mathbb{R}^n$, $m \in \mathcal{B}^d$, $k \geq 1$ and $\ell \leq N-k$ it holds that

$$V_N(x,\ell;m) = \min_{|f_1|\leq 1} \max_{b_1=\pm 1} \cdots \min_{|f_k|\leq 1} \max_{b_k=\pm 1} V_N\left(x + \sum_{i=1}^{k} b_i(q(m^i) - \mathbb{1} f_i), \ell + k; m^{k+1}\right),$$

where $m^1 = m$ and $m^{i+1} = m^i | b_i$ for $i = 1, \ldots, k$.

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The equivalent DPP for u_N is

$$u_N(x, t; m) = \min_{|f_1| \leq 1} \max_{b_1 = \pm 1} \cdots \min_{|f_k| \leq 1} \max_{b_k = \pm 1} u_N\left(x + \varepsilon \sum_{i=1}^{k} b_i(q(m^i) - \mathbb{1} f_i), t + \varepsilon^2 k; m^{k+1}\right).$$

The local problem

Assume $u_N(x, t; m) \approx u(x, t)$ for smooth u.

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and so

$$u_t + \frac{1}{k} \min_{|f_1|\le 1} \max_{b_1=\pm 1} \cdots \min_{|f_k|\le 1} \max_{b_k=\pm 1} \left\{ \varepsilon^{-1} \nabla u^T \Delta x + \frac{1}{2} \Delta x^T \nabla^2 u \Delta x \right\} \approx 0.$$

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$$\approx \min_{|f_1|\le 1} \max_{b_1=\pm 1} \cdots \min_{|f_k|\le 1} \max_{b_k=\pm 1} \left\{ u + k\varepsilon^2 u_t + \varepsilon \nabla u^T \Delta x + \frac{\varepsilon^2}{2}\Delta x^T \nabla^2 u \Delta x \right\},$$

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Definition (Local Problem)

The local problem is defined by

$$\mathcal{L}(\varepsilon, k, X, p, m) := \min_{|f_1|\le 1} \max_{b_1=\pm 1} \cdots \min_{|f_k|\le 1} \max_{b_k=\pm 1} \left\{ \varepsilon^{-1} p^T \Delta x + \frac{1}{2}\Delta x^T X \Delta x \right\}$$

where $m_1 = m$, $m_{i+1} = m_i | b_i$, and $\Delta x := \sum_{i=1}^k b_i(q(m_i) - \mathbb{1} f_i)$.

The local problem

Theorem (Local problem)

Let $X \in \mathbb{S}(n)$, $p \in (0,\infty)^n$, $m \in \mathcal{B}^d$, $k \geq d+1$, $\varepsilon > 0$, *and set* $\gamma_p = \min_{1\leq i\leq n} p_i$. *Then there exists* $C, c > 0$, *depending only on* n, *such that whenever* $\|X\|k\varepsilon \leq c\,\vartheta_q\gamma_p$ *we have*

$$\left|\frac{1}{k}\mathcal{L}_{k,\varepsilon}(X,p,m) - \frac{1}{2^{d+1}}\sum_{m\in\mathcal{B}^d}\eta(m)^T X\eta(m)\right| \leq C\|X\|\left(\frac{d}{k} + \|X\|\gamma_p^{-1}k\varepsilon\right). \tag{13}$$

Drenska, N., and Calder J. Online Prediction With History-Dependent Experts: The General Case. To appear in Communications on Pure and Applied Mathematics (CPAM), (2021).

Back to the dynamic programming principle

With $\varepsilon = N^{-1/2}$, the dynamic programming principle (DPP) becomes

$$u_t + \min_{|f|\leq 1} \max_{b=\pm 1} \left\{ \varepsilon^{-1} b \nabla u^T (q(m) - f\mathbb{1}) + \frac{1}{2}(q(m) - f\mathbb{1})^T \nabla^2 u \, (q(m) - f\mathbb{1}) \right\} = O(\varepsilon).$$

Investor (player) can choose a strategy of the form

$$f = \frac{\nabla u^T q(m) + \frac{\varepsilon}{2} f^{\#}(m)}{\nabla u^T \mathbb{1}} \quad \text{and} \quad \boxed{u_t + h(m) - \frac{b(m)}{2} f^{\#}(m) = O(\varepsilon),}$$

where $\eta(m) = q(m) - \frac{\nabla u^T q(m)}{\nabla u^T \mathbb{1}} \mathbb{1}$ and $h(m) = \frac{1}{2}\eta(m)^T \nabla^2 u \, \eta(m)$.

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Question: How to choose $f^{\#}(m)$ so the equation averages out to

$$u_t + (h)_{\mathcal{B}^d} = 0 \quad \text{where } (h)_{\mathcal{B}^d} := \frac{1}{2^d} \sum_{m \in \mathcal{B}^d} h(m)$$

over many steps?

Optimal investor strategy

Why not choose $f^{\#}(m)$ so that

$$h(m) - \frac{b(m)}{2} f^{\#}(m) = (h)_{\mathcal{B}^d}?$$

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This would violate the rules, since $f^{\#} = \frac{2}{b(m)}(h(m) - (h))$ depends on b.

Optimal investor strategy

It turns out a small correction on this choice is possible. We choose $f^{\#}(m)$ to satisfy

$$h(m) - \frac{b(m)}{2} f^{\#}(m) = (h)_{\mathcal{B}^d} + \mathcal{H}(m) - \mathcal{H}(m|b(m)),$$

for a potential $\mathcal{H}$ to be determined.

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$$f^{\#} = 2b\left[h(m) - (h)_{\mathcal{B}^d} + \mathcal{H}(m|b) - \mathcal{H}(m)\right].$$

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Introducing the De Bruijn graph Laplacian

$$\Delta_{\mathcal{B}^d}\mathcal{H}(m) = \mathcal{H}(m) - \frac{1}{2}\mathcal{H}(m_+) - \frac{1}{2}\mathcal{H}(m_-),$$

where $m_\pm = m|\pm 1$, we can write

$$f^{\#} = 2b\Big[h(m) - (h)_{\mathcal{B}^d} - \Delta_{\mathcal{B}^d}\mathcal{H}(m)\Big] + b\left(\mathcal{H}(m|b) - \mathcal{H}(m|-b)\right).$$

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If $\Delta_{\mathcal{B}^d}\mathcal{H}(m) = h(m) - (h)_{\mathcal{B}^d}$ then

$$f^{\#} = b\left(\mathcal{H}(m|b) - \mathcal{H}(m|-b)\right) = \mathcal{H}(m_+) - \mathcal{H}(m_-).$$

Poisson equation

The equation

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The solution is unique up to an additive constant, and the optimal strategy

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It is possible to extend these ideas slightly to other directed graphs.

Calder, J., and Drenska, N. Asymptotically optimal strategies for online prediction with history-dependent experts. Journal of Fourier Analysis and Applications 27.2 (2021): 1-20.

Outline

Future work

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2. Generalizations to other games (e.g., Markov Decision Processes in adversarial settings).

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2. Generalizations to other games (e.g., Markov Decision Processes in adversarial settings).
3. Prediction with mixed (randomized) strategies.

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Outline

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