

Séminaire de Calcul Scientifique du CERMICS



École des Ponts
ParisTech

‘Off-the-grid’ methods

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26 juin 2018

CERMICS
June 26th, 2018

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« Off-The-Grid » methods



Orthant

$$x \geq 0$$

Vectors

- **High-Dimensional Statistics**

Orthant

$$x \geq 0$$

Vectors

SDP

$$M \succeq 0$$

Matrices

- High-Dimensional Statistics
 - Matrix completion, recovery, factorisation

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$$x \geq 0$$

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Matrices

Lasserre's hierarchies

$$\mu \geq 0$$

Measures

- **High-Dimensional Statistics**
- **Matrix completion, recovery, factorisation**
- **Global Optimization**
- **Sparse Deconvolution**
- **Computational Limits**

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Measures

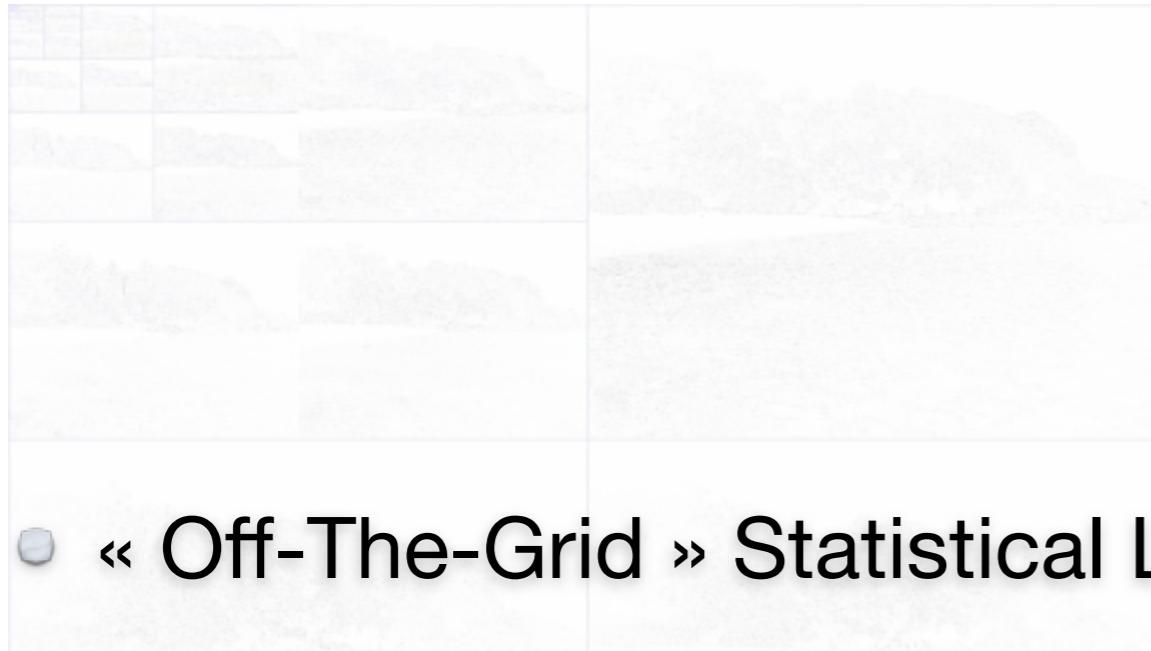
- **High-Dimensional Statistics**

- **Matrix completion, recovery, factorisation**

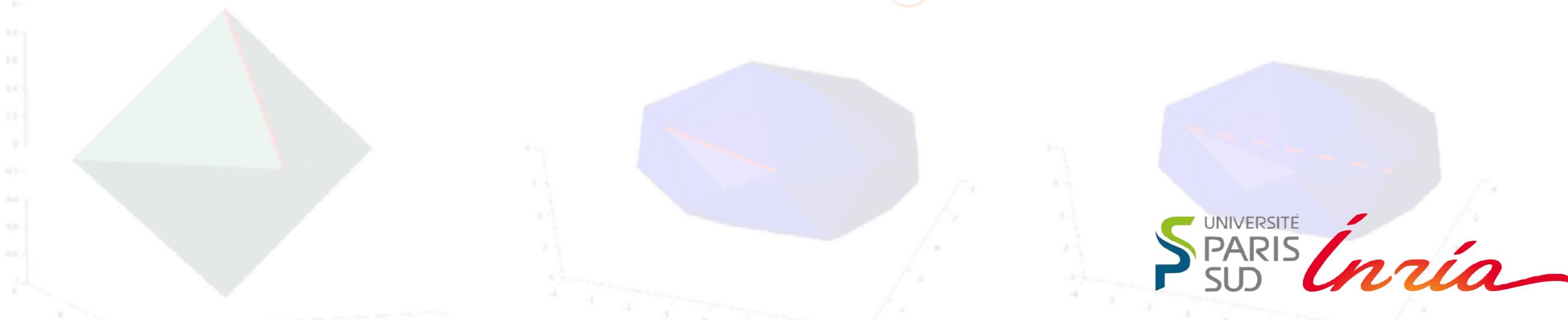
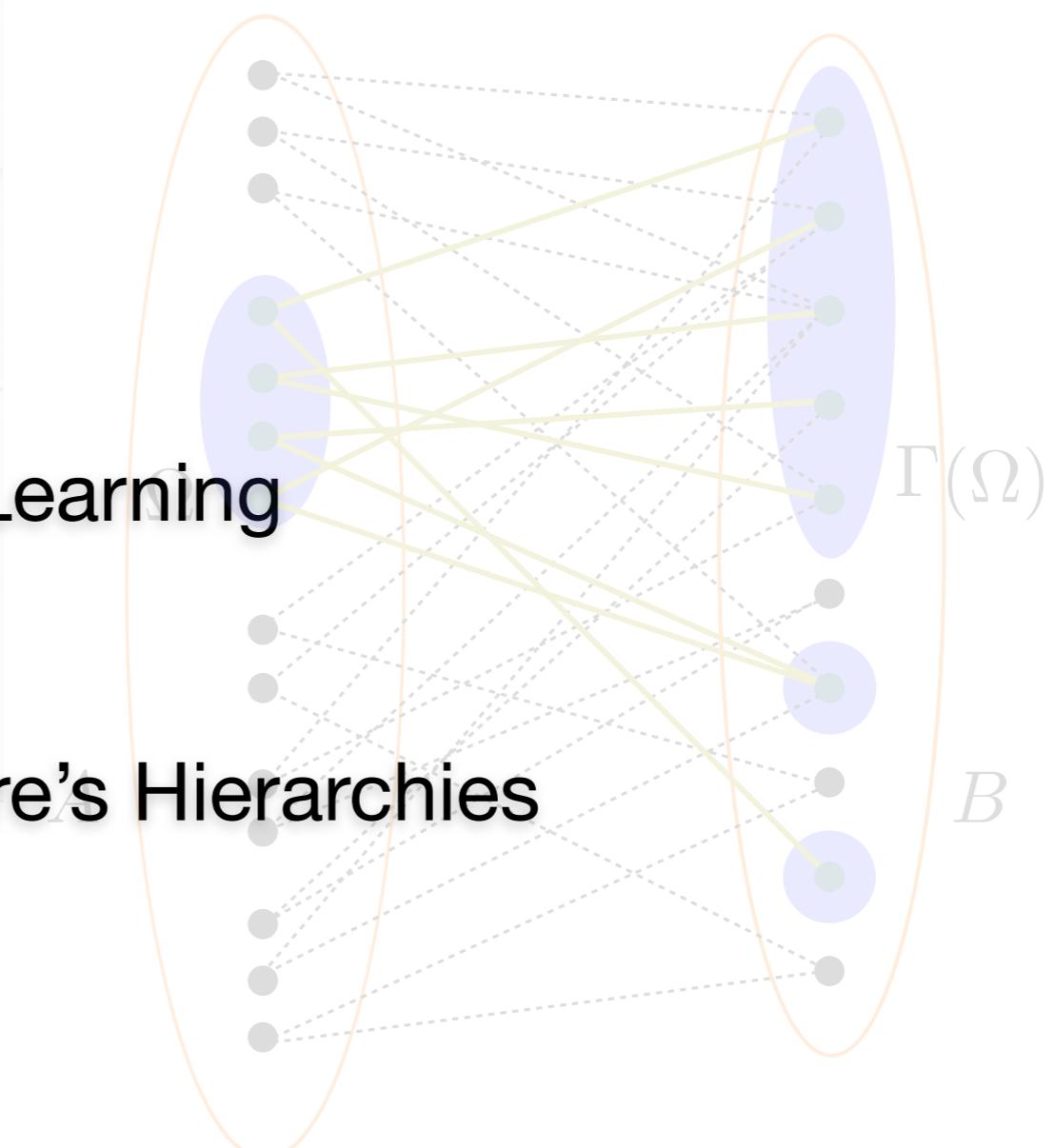
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- **Sparse Deconvolution**
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Grids

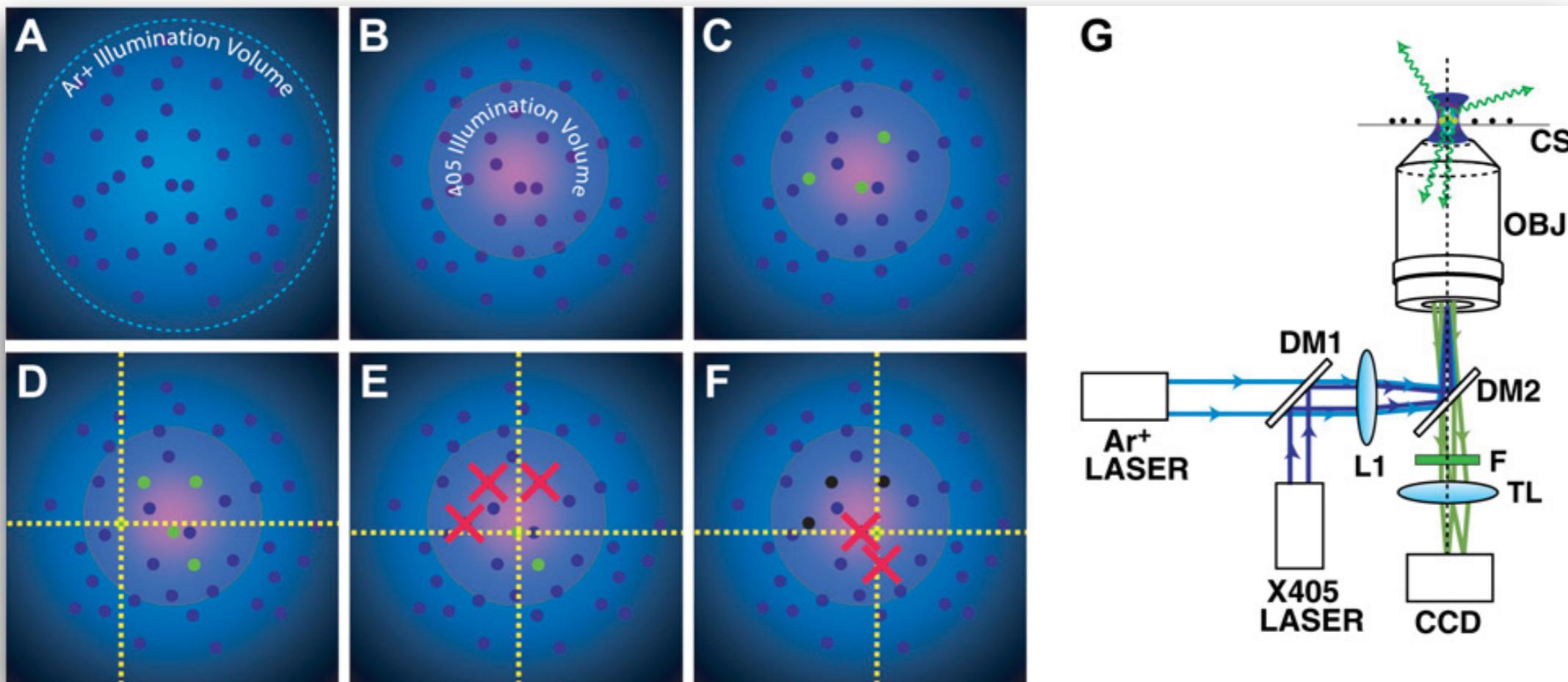
« Off-The-Grid » Methods



- « Off-The-Grid » Statistical Learning
- The Meta Algorithm: Lasserre's Hierarchies

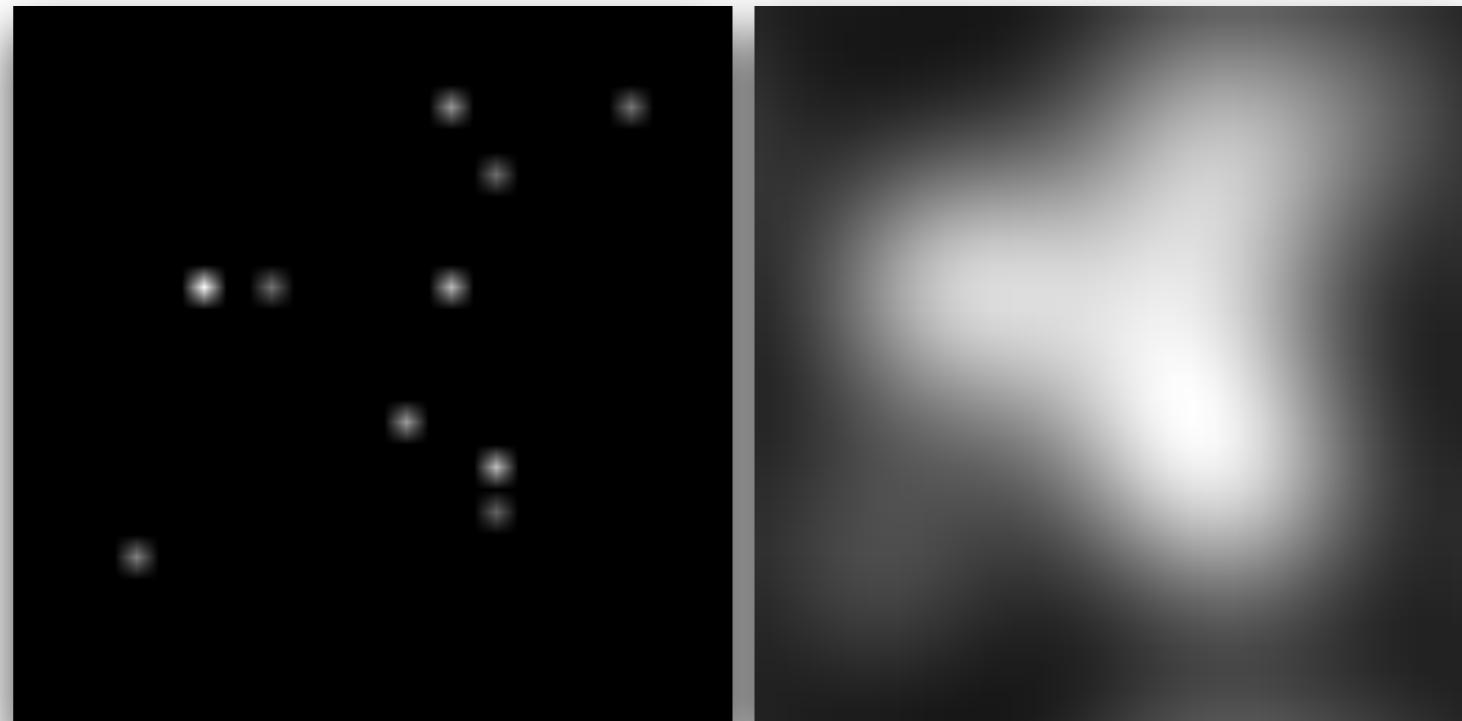


Sparse Deconvolution



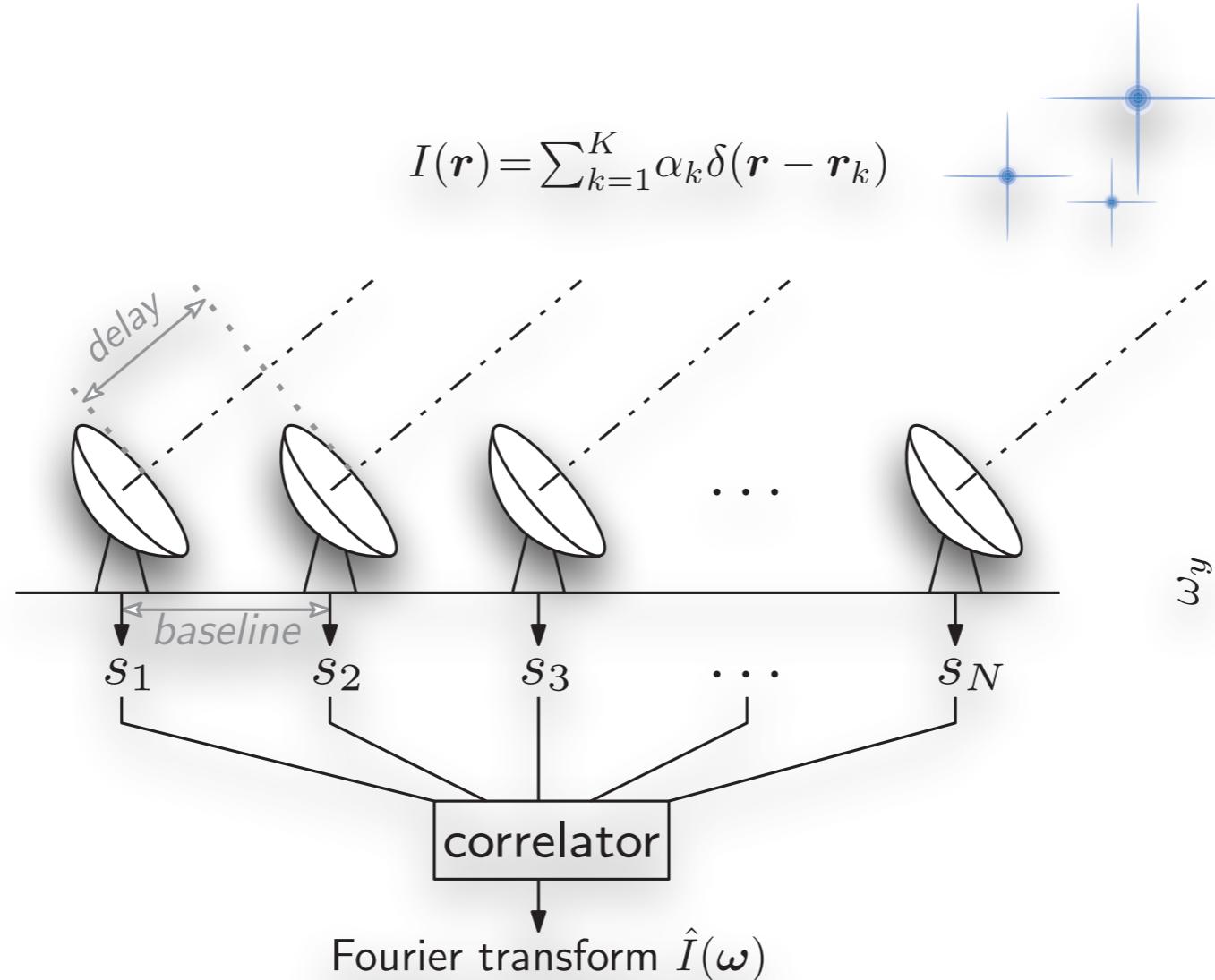
- S. Hess, T. Girirajan, M. Mason, Ultra-High Resolution Imaging by Fluorescence Photoactivation Localization Microscopy, *Biophysical Journal* (2004).

Sparse Deconvolution

(a) Heat source u_0 (b) $Au_0 = f$

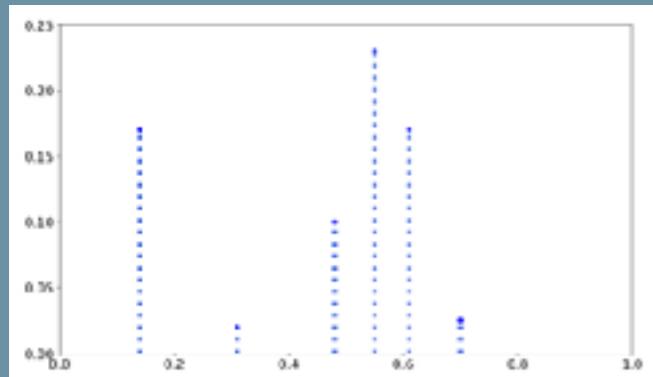
- Y. Li, S. Osher, R. Tsai, Heat Source Identification based on L1 Constrained Minimization, *Inverse Problems and Imaging* (2014).

Sparse Deconvolution



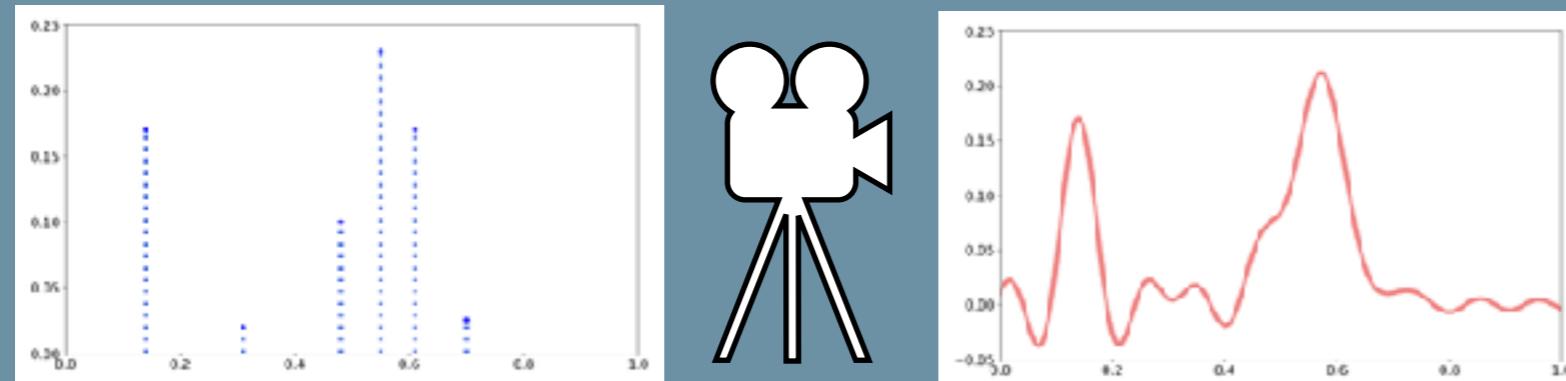
- H. Pan, T. Blu, M. Vetterli, Towards Generalized FRI Sampling With an Application to Source Resolution in Radioastronomy, *IEEE trans. on Signal Processing* (2017).

Sparse Deconvolution



x

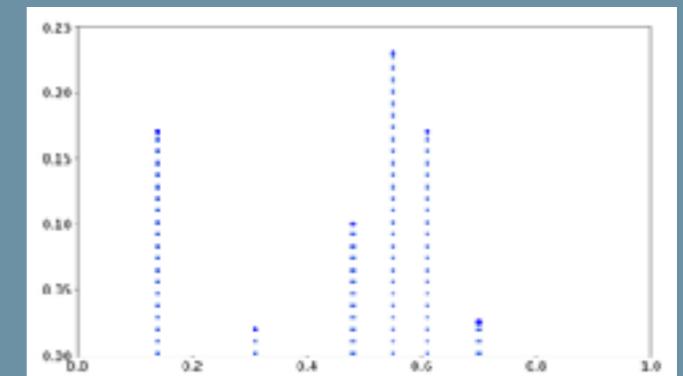
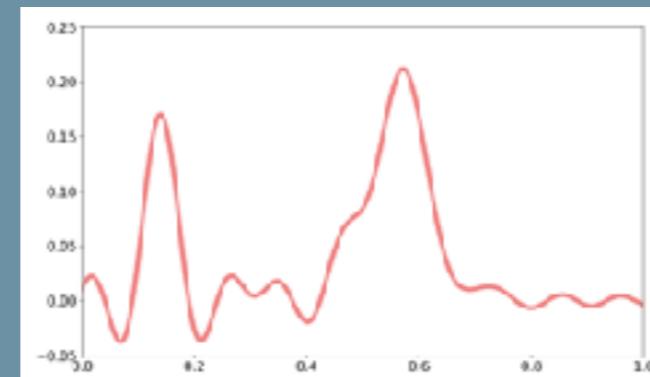
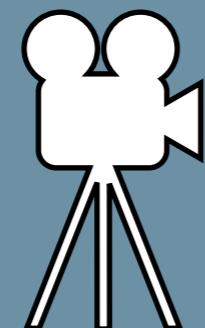
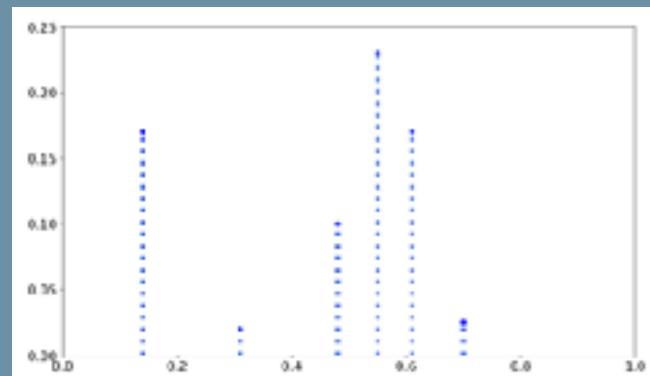
Sparse Deconvolution

 x y

$$y = \Phi(x)$$

Sparse Deconvolution

$$\|x\|_{\text{TV}} = \min_{x=x_+ - x_-, x_\pm \geq 0} \int dx_+ + \int dx_-$$



x

y

↑

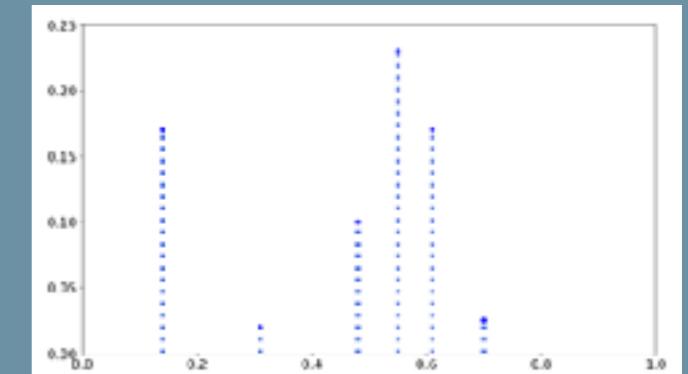
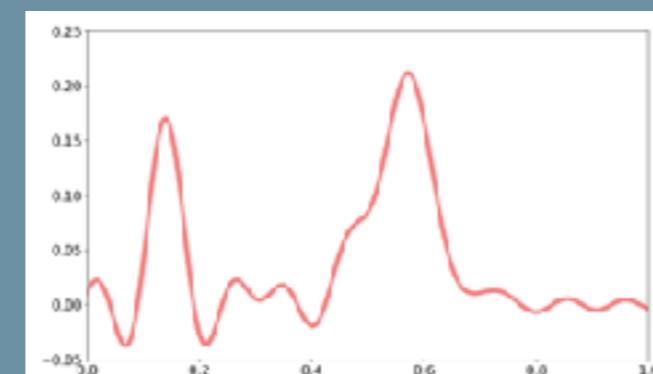
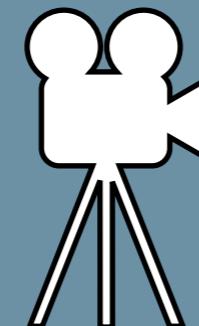
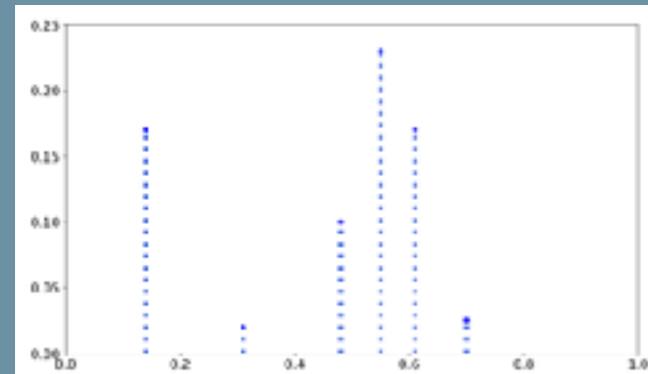
Perfect Recovery

$$y = \Phi(x)$$

$$\min_{y=\Phi(x)} \|x\|_{\text{TV}}$$

Sparse Deconvolution

$$\|x\|_{\text{TV}} = \min_{x=x_+ - x_-, x_\pm \geq 0} \int dx_+ + \int dx_-$$



x

y

Perfect Recovery

$$y = \Phi(x)$$

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Discrete Measure

Sparse Deconvolution

$$\min_{y=\Phi(x)} \|x\|_{\text{TV}} = \min_{y=\Phi(x_+) - \Phi(x_-), x_\pm \geq 0} \langle 1, x_+ \rangle + \langle 1, x_- \rangle$$

Sparse Deconvolution

$$\min_{y=\Phi(x)} \|x\|_{\text{TV}} = \min_{y=\Phi(x_+) - \Phi(x_-), x_\pm \geq 0} \langle 1, x_+ \rangle + \langle 1, x_- \rangle$$

- **[Cone]** Moments of Nonnegative Measures
- **[Algorithms]** Lasserre's Hierarchies, Frank-Wolfe

Sparse Deconvolution

$$\min_{y=\Phi(x)} \|x\|_{\text{TV}} = \min_{y=\Phi(x_+) - \Phi(x_-), x_\pm \geq 0} \langle 1, x_+ \rangle + \langle 1, x_- \rangle$$

Linear Conic with « Moments » Constraints

- **[Cone]** Moments of Nonnegative Measures
- **[Algorithms]** Lasserre's Hierarchies, Frank-Wolfe

Robust Moment Problem

- $y = \Phi(x) + \eta :$

Robustness

$$\bar{x} \in \arg \min_v \left\{ \frac{1}{2} \|y - \Phi(v)\|_2^2 + \lambda \|v\|_{TV} \right\}$$

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[DC et al; Candès and Fernandez-Granda; Recht; ...] Spike Detection

- Analysis via « Dual Certificate » [DC, Gamboa; Candès, Tao; ...]

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- Analysis via « Dual Certificate » [DC, Gamboa; Candès, Tao; ...]
- « Minimal Separation Condition » on the support of the spikes
- Optimal error bounds

+ Support Recovery

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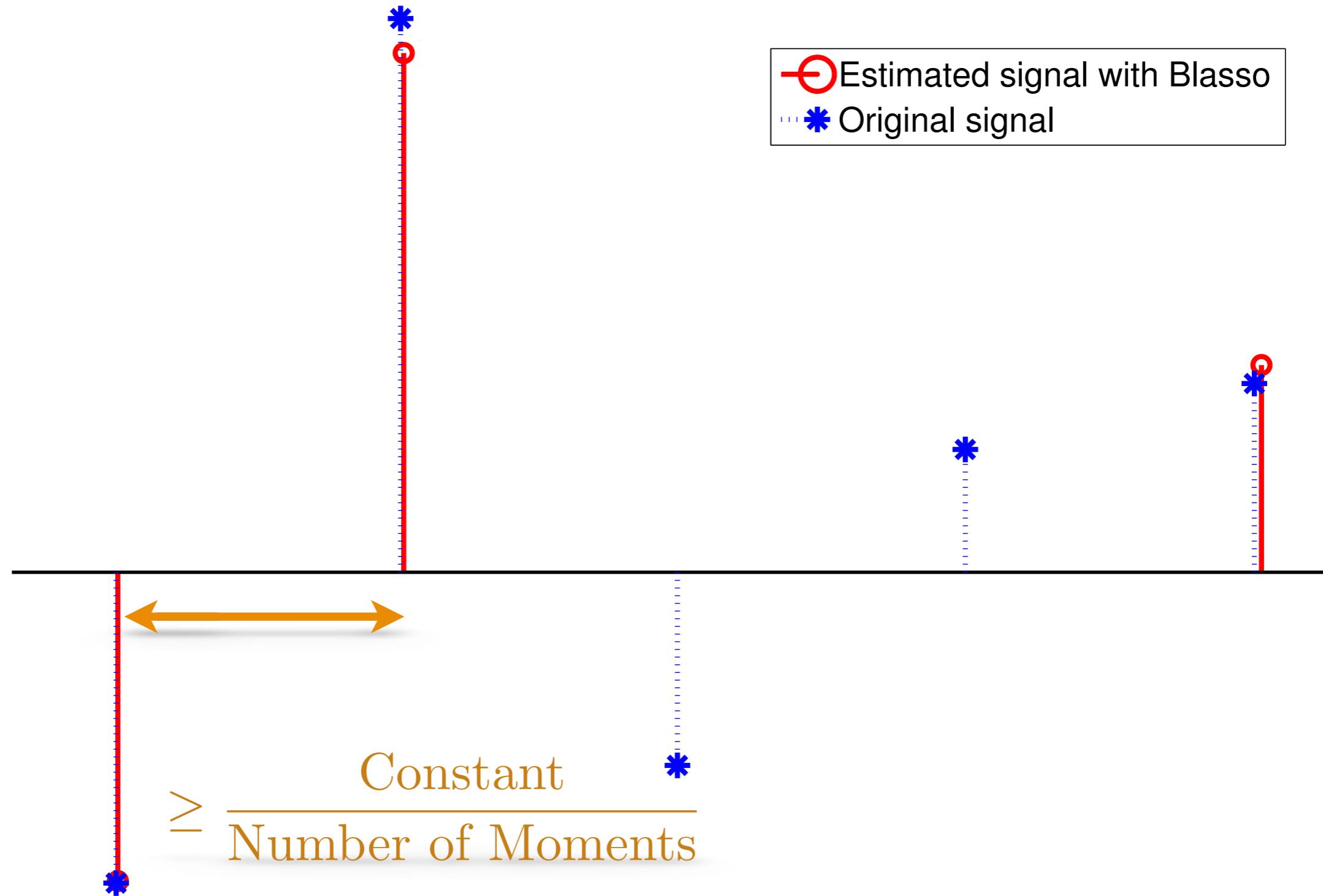
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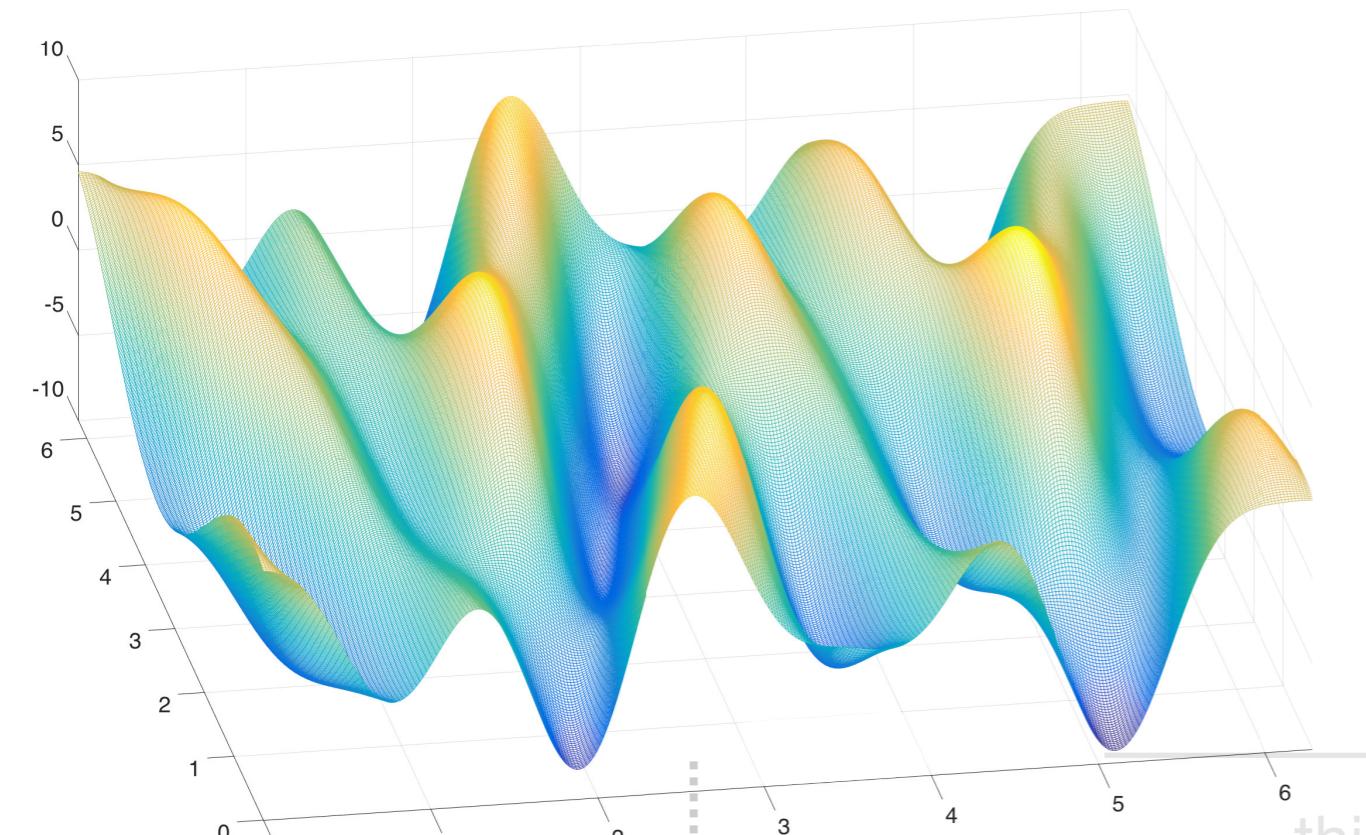
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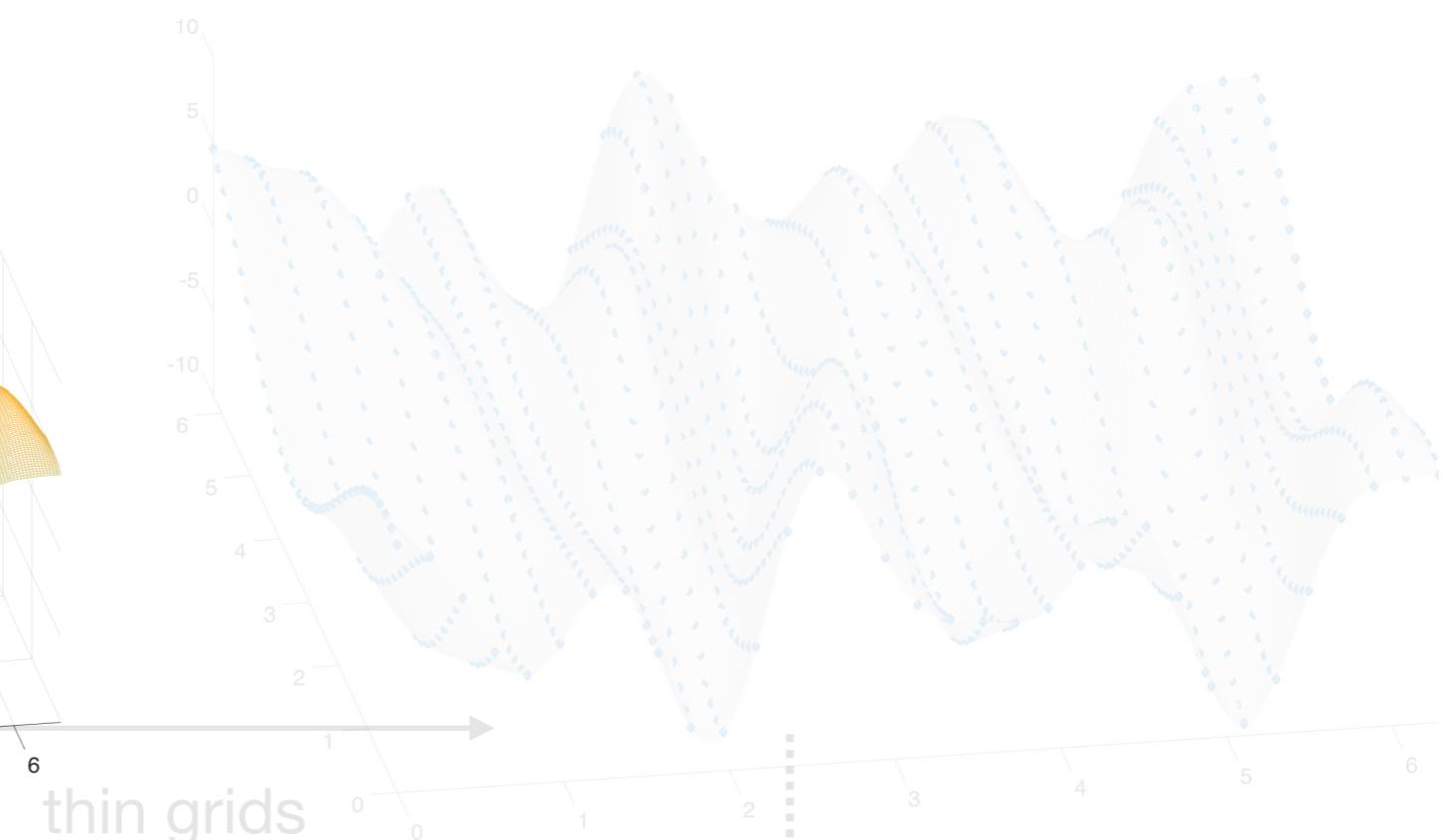


Grid vs Off-the-grid [ADCM18]



Inference from the continuous process

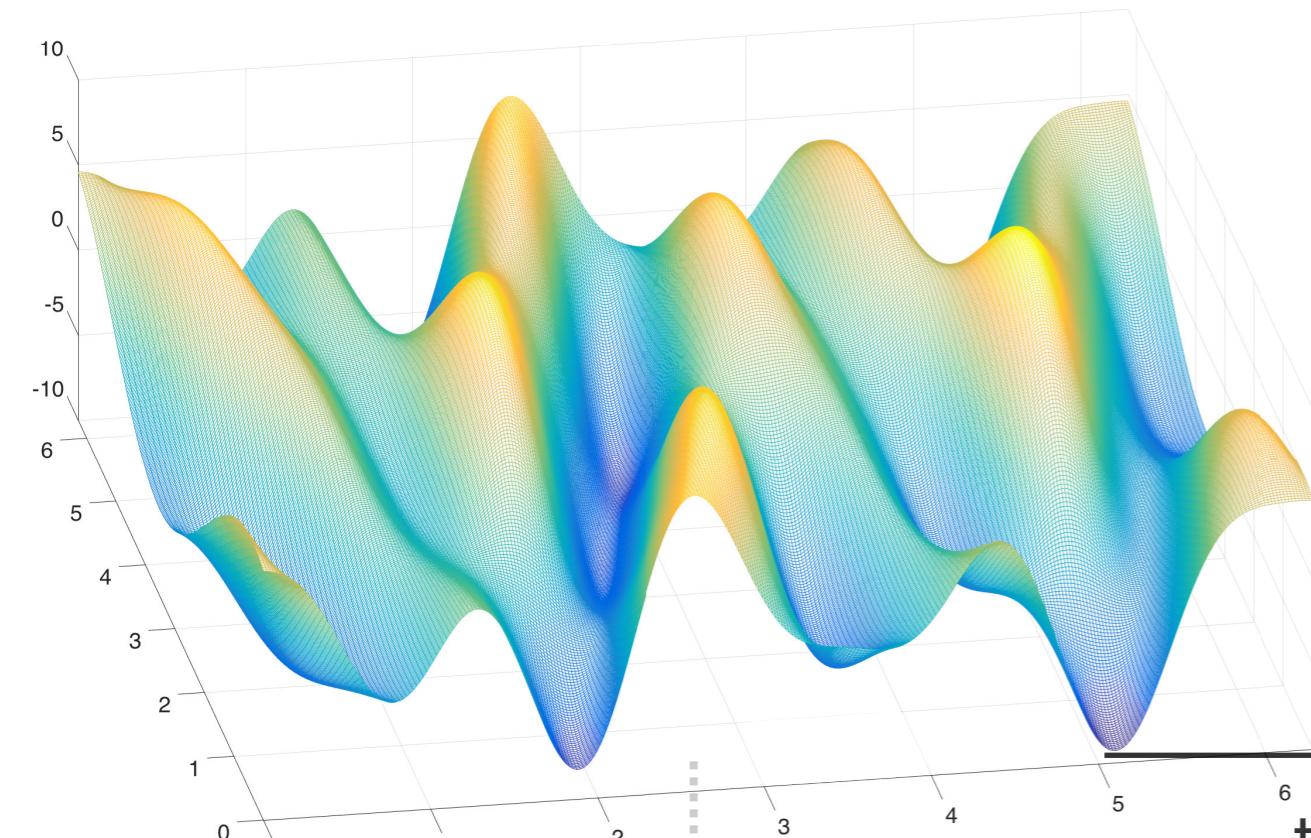
Grid-less approach



Inference from p grid points

Grid approach

Grid vs Off-the-grid [ADCM18]

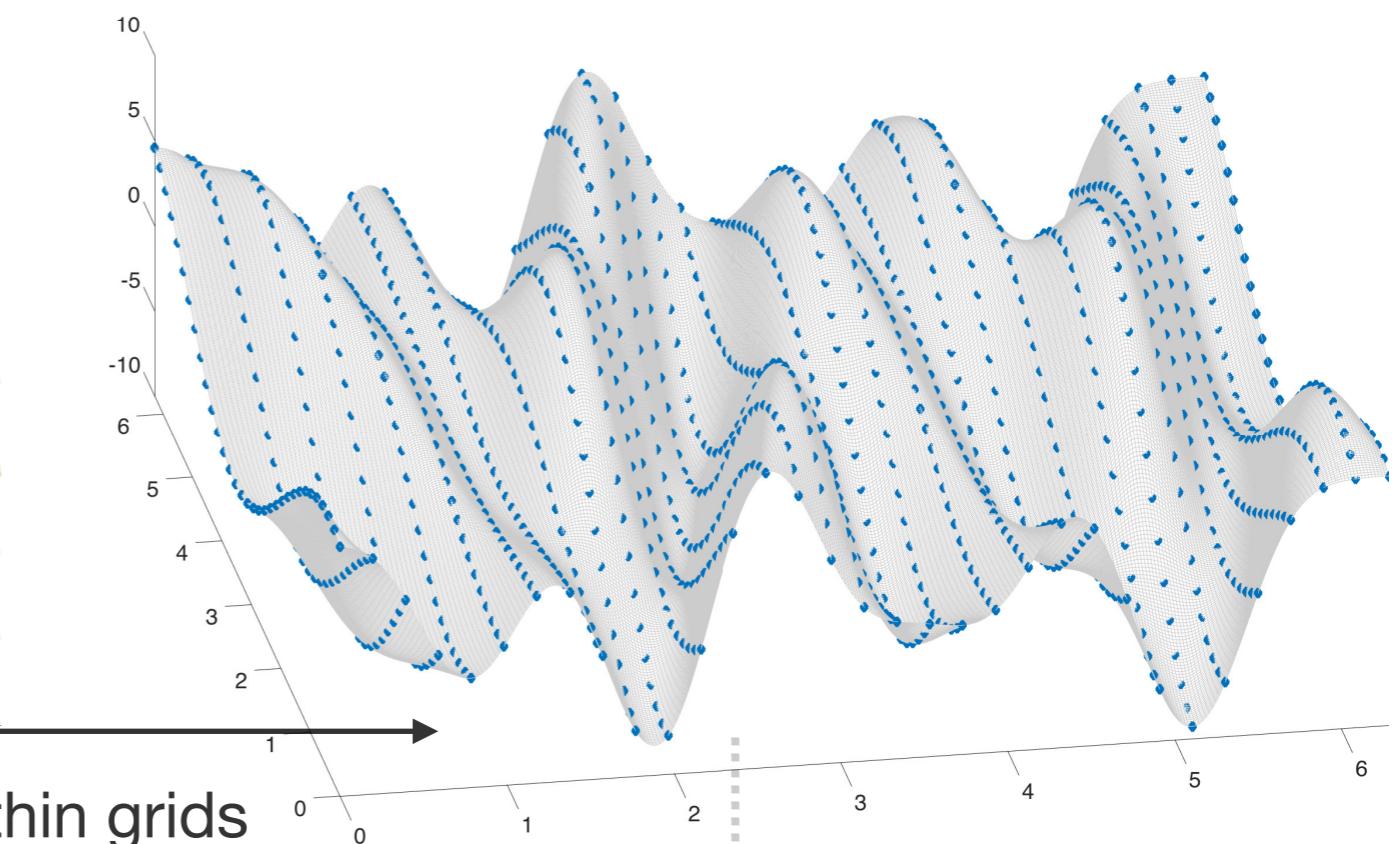


Inference from the continuous process

thin grids

thin grids

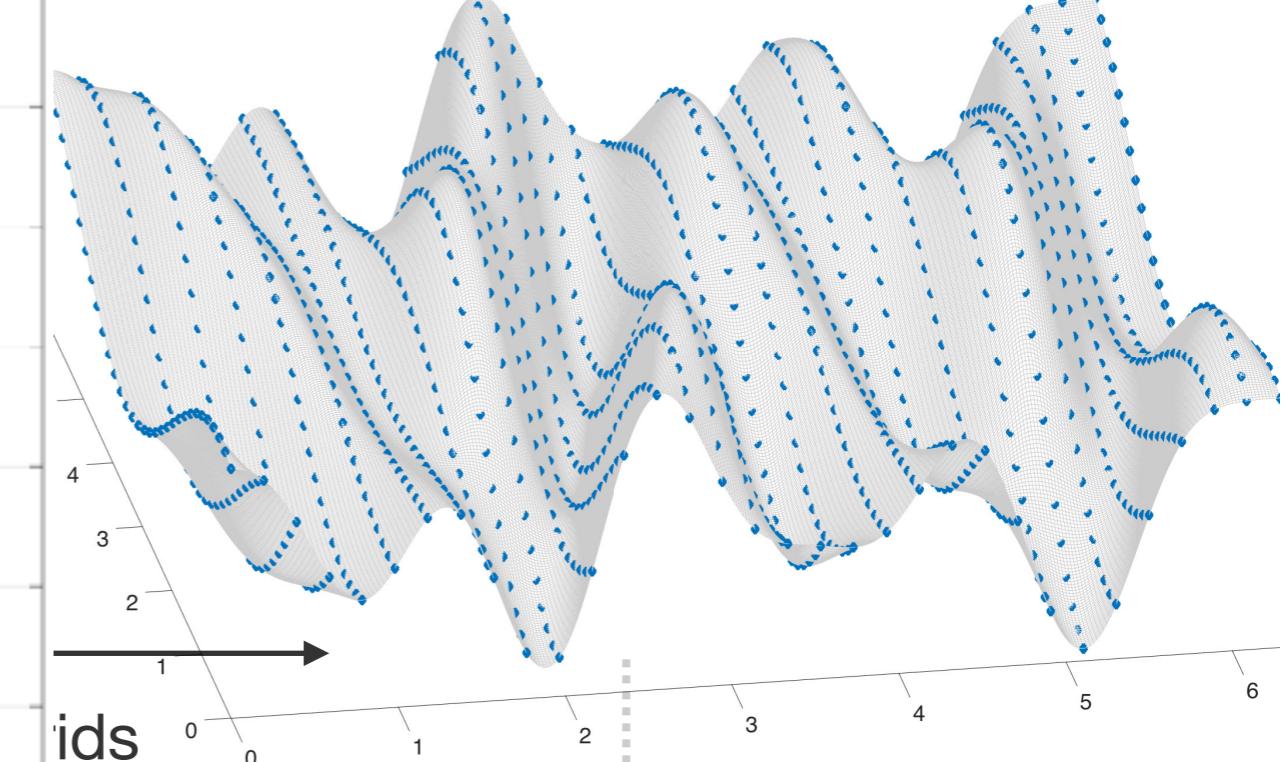
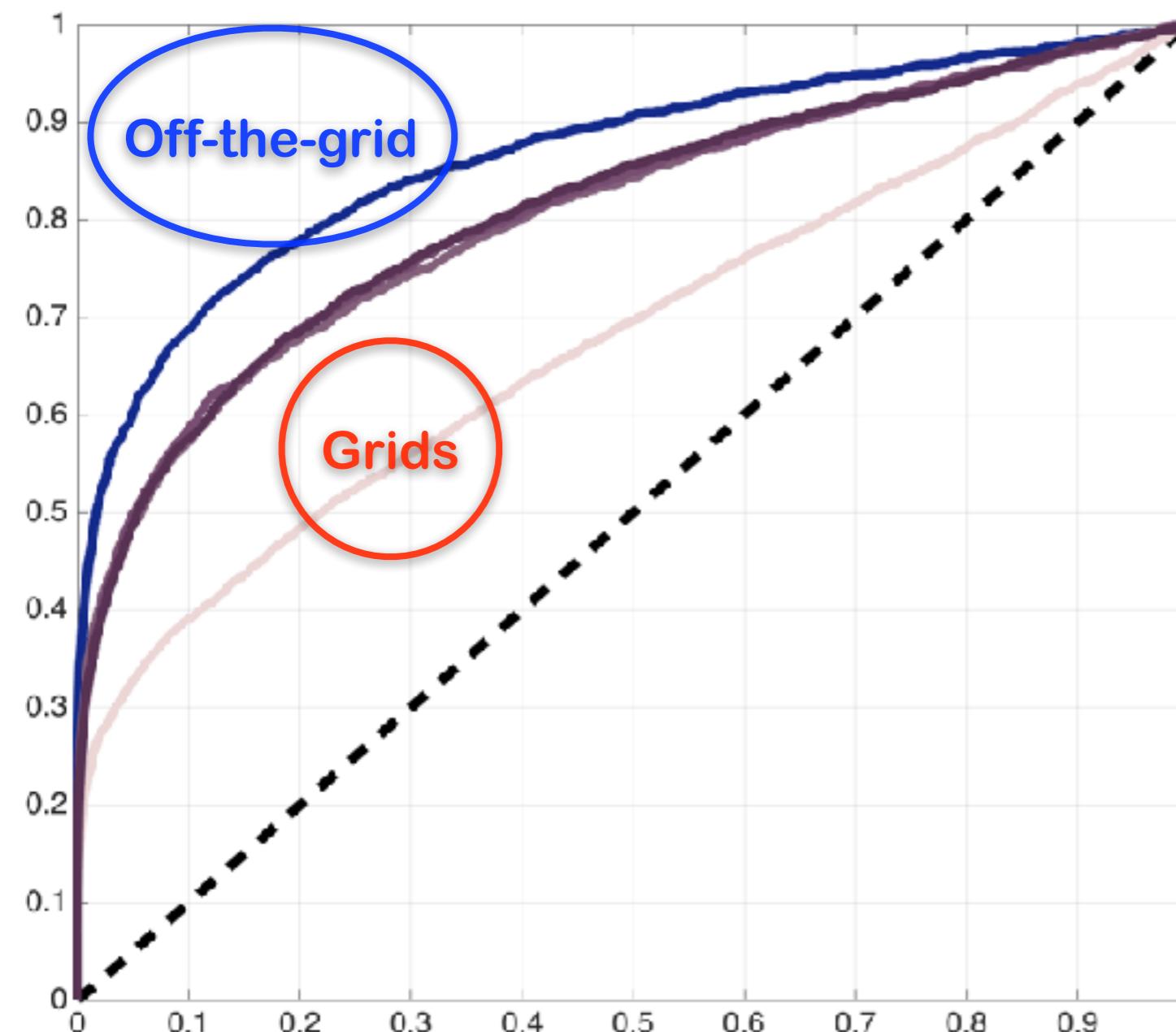
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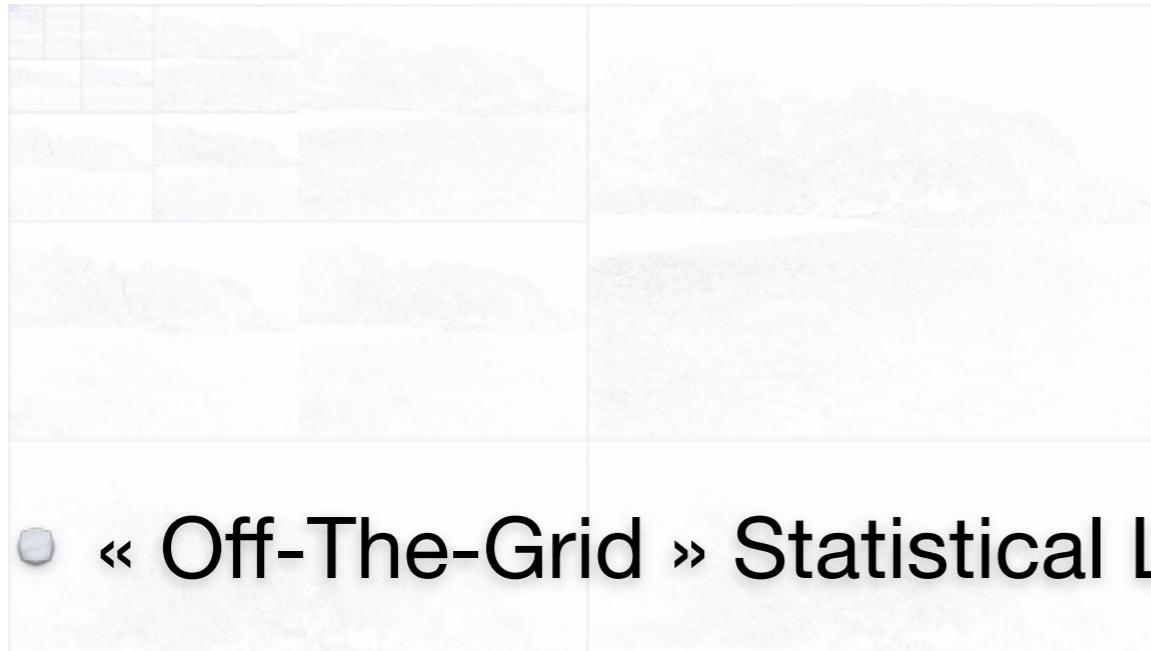
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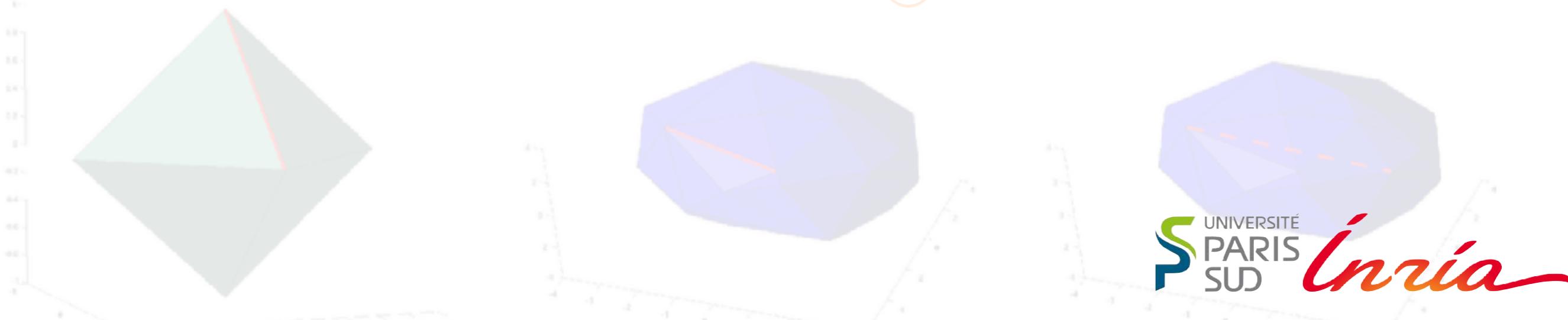
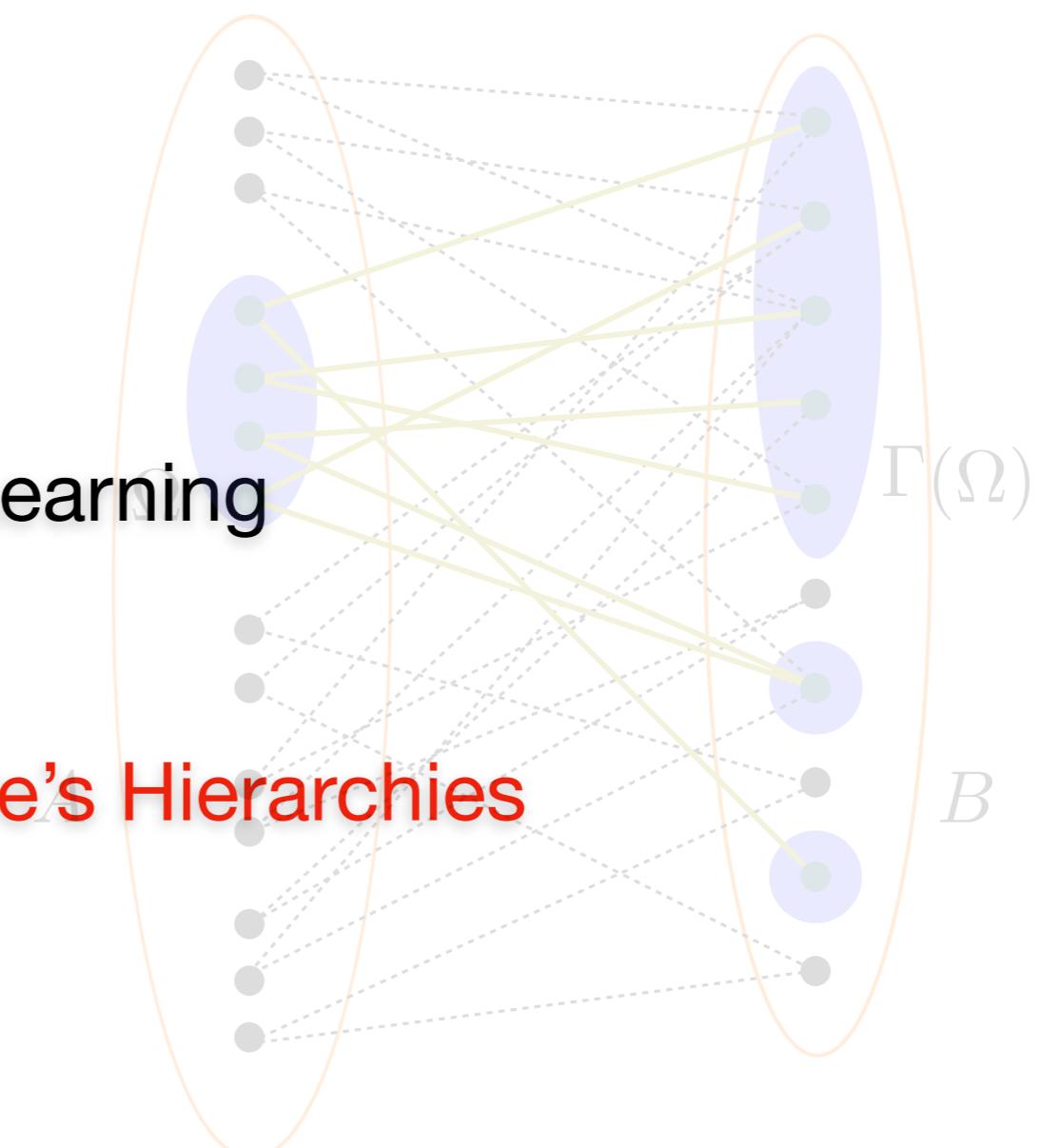
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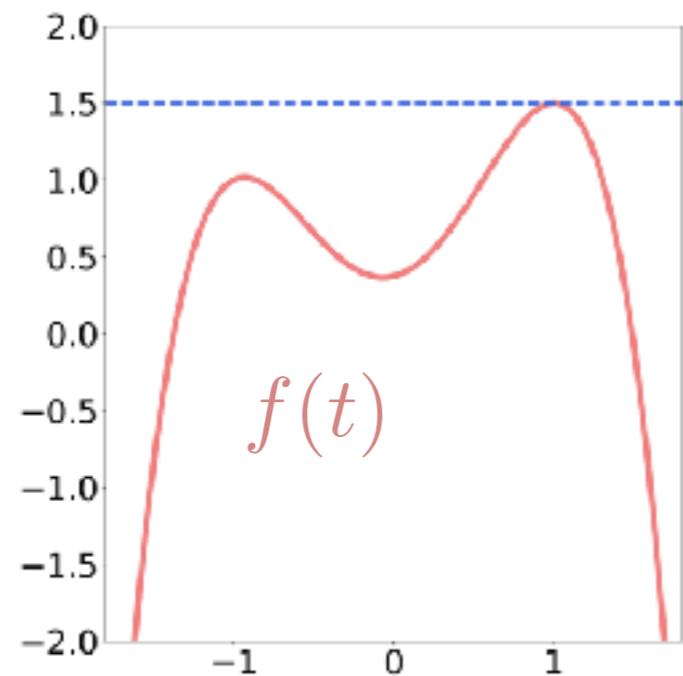
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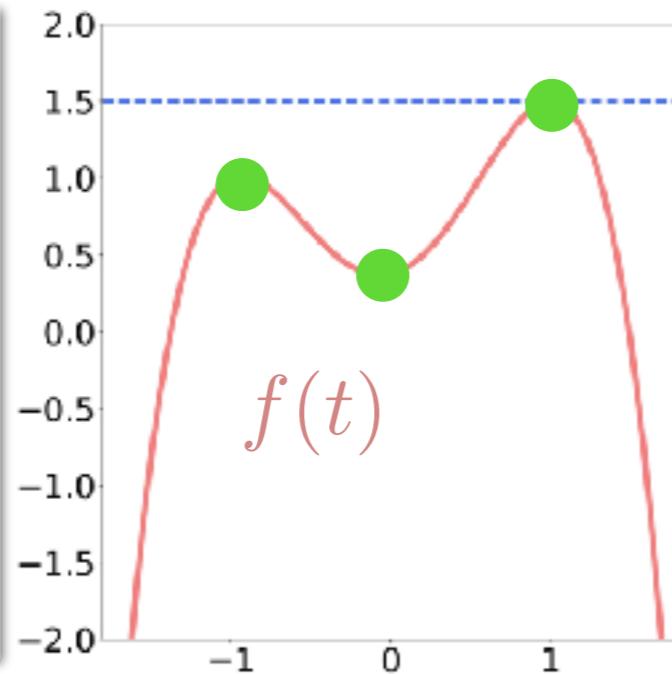
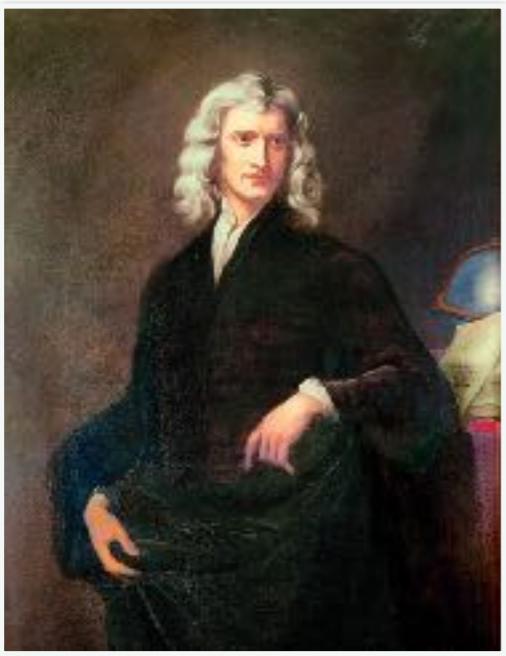
Under one Sparse alternative



- « Off-The-Grid » Statistical Learning
- The Meta Algorithm: Lasserre's Hierarchies



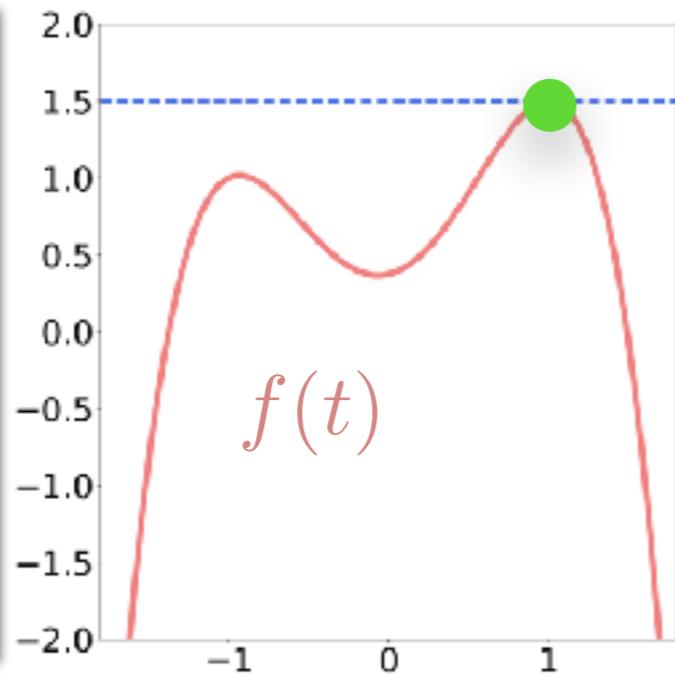
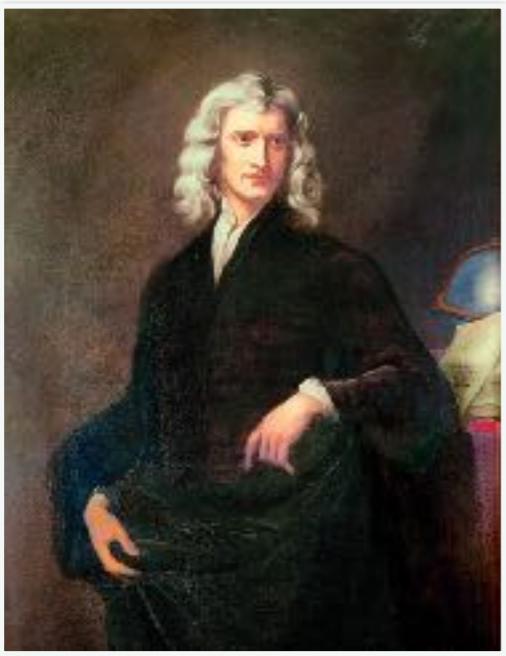




Newton's approach

- Search through **local** optima
- Well suited for **convex** functions
- BUT simple non-convex function may have an exponential number of bad optima, e.g.

$$f(t_1) + \dots + f(t_n)$$

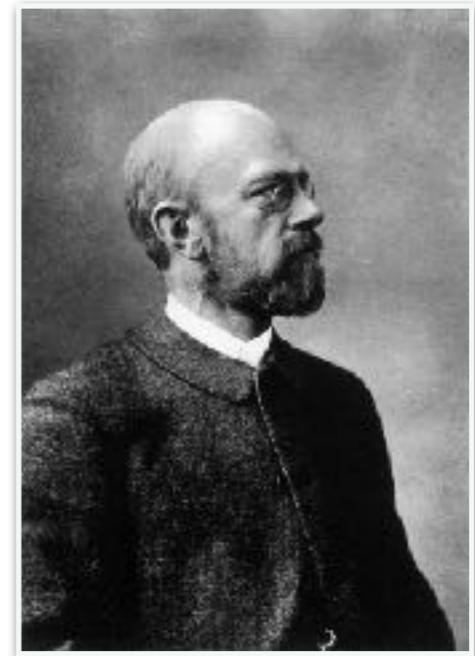


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$$f(t) = \frac{3}{2} - \frac{(t-1)^2}{8} - (t^2 - 1)^2$$



Hilbert's approach

- Globally** decompose the function into simple pieces
- Lasserre's hierarchy algorithm: **find decomposition efficiently**
- Strongest provable guarantees for **LOTS** of ML problems

Global Optimization

$$\min_{t \in \Omega} f(t) = \min_{\mu \geq 0, \mu(\Omega)=1} \int_{\Omega} f(t) \mu(dt)$$

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Framework

$$\Omega = \left\{ t \in \mathbb{R}^D : \sum g_{\alpha,m} t^\alpha \geq 0, 1 \leq m \leq M \right\}$$

Semi-Algebraic

$$f(t) = \sum f_\alpha t^\alpha$$

Polynomial

Global Optimization

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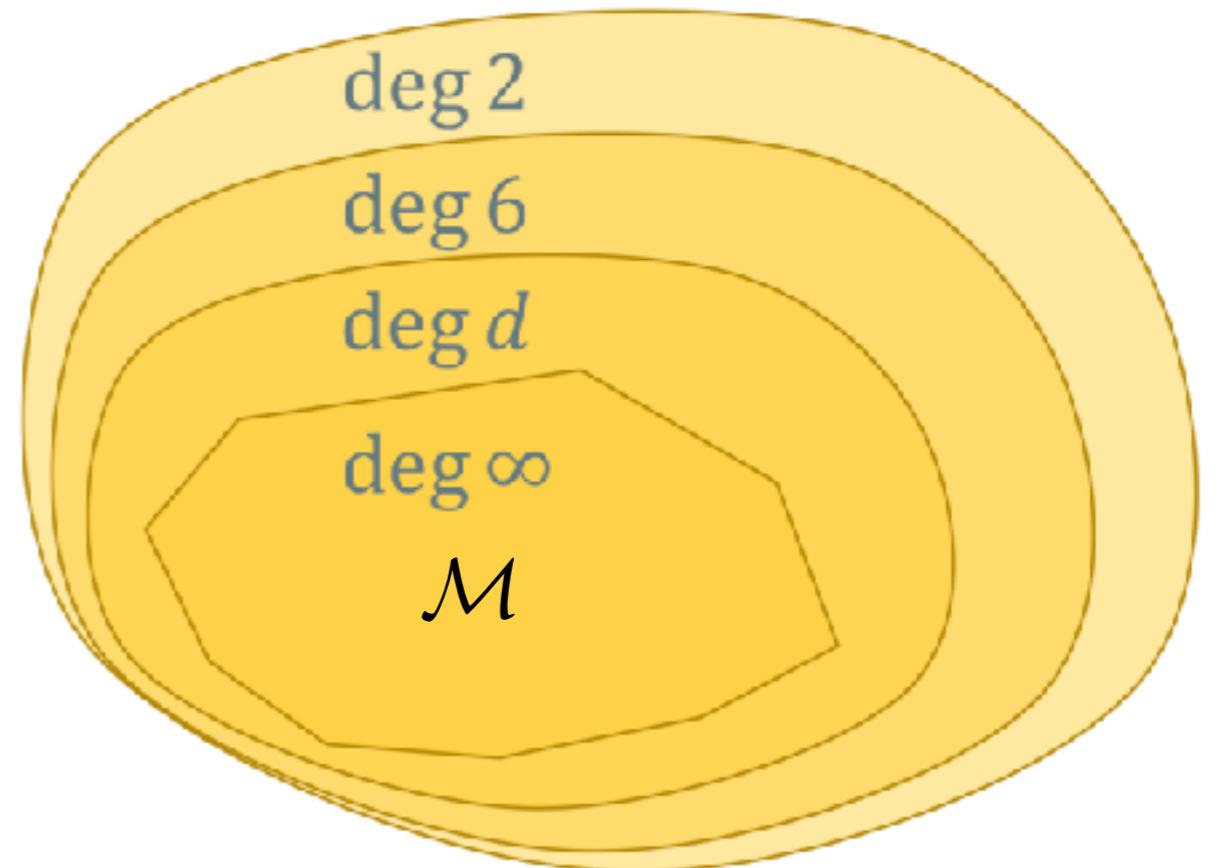
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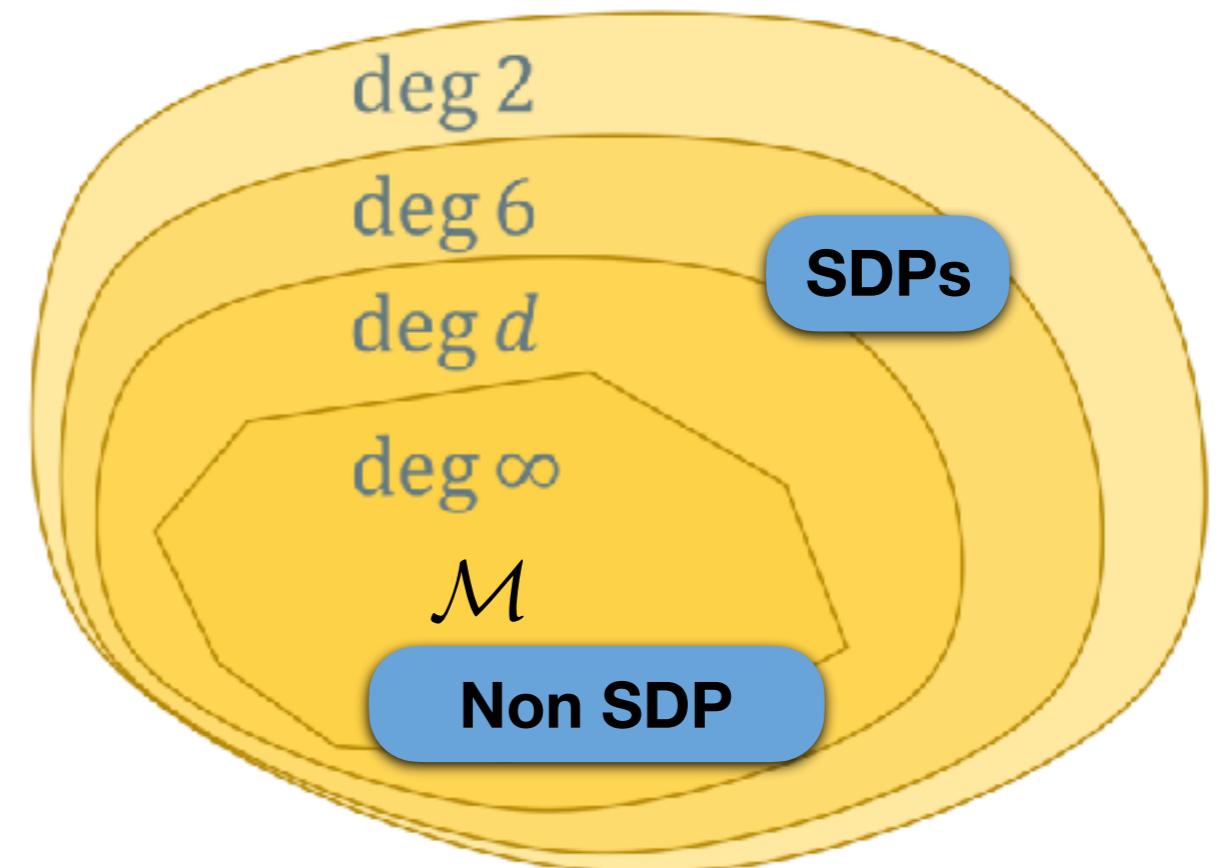
$$\mathcal{M} = \liminf_d \mathcal{M}^{\text{SOS}(d)} \subseteq \dots \subseteq \mathcal{M}^{\text{SOS}(d)} \subseteq \mathcal{M}^{\text{SOS}(d-2)} \subseteq \dots \subseteq \mathcal{M}^{\text{SOS}(2)}$$



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Lasserre's hierarchies give
a sequence of nested OUTER
SDP approximations
of the cone of moments
of nonnegative measures



$$\min_{t \in \Omega} \sum f_\alpha t^\alpha = \min_{\mu \geq 0, \mu(\Omega)=1} \sum f_\alpha \int_{\Omega} t^\alpha \mu(dt) = \min_{(m_\alpha) \in \mathcal{M}} \sum f_\alpha m_\alpha$$

Optimality of Lasserre's hierarchies?

Under Khot's Unique Game Conjecture:

NP-hard to achieve better approximation guarantees than Lasserre's hierarchies for class of worst-case discrete optimization problems
[Khot'02, Raghavendra'08]

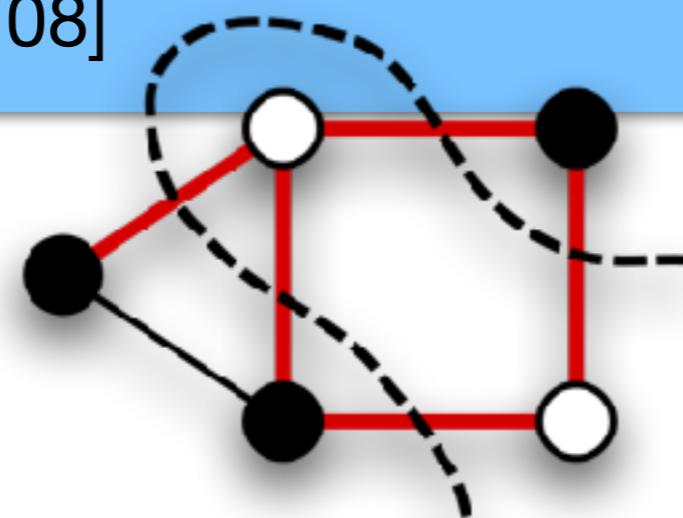
- Max Cut problem
- Stable Set problem
- Planted Clique problem
- Deg. 4 on the Sphere
- Tensor PCA
- LOTS of problems

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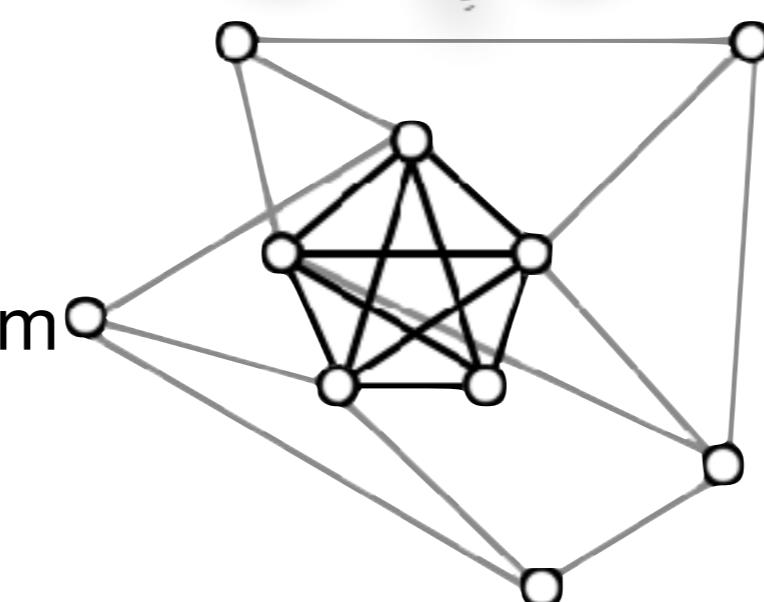
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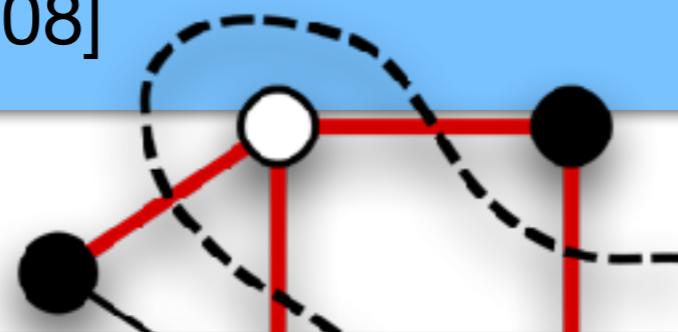
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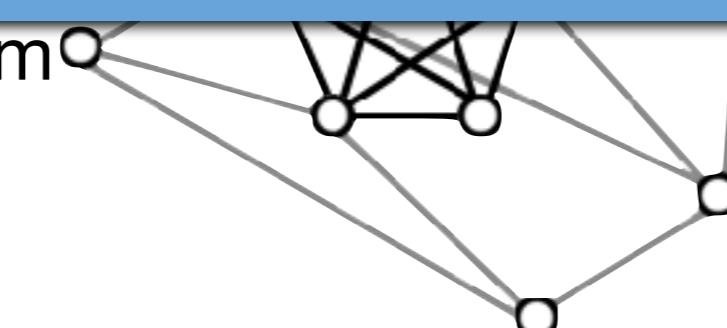
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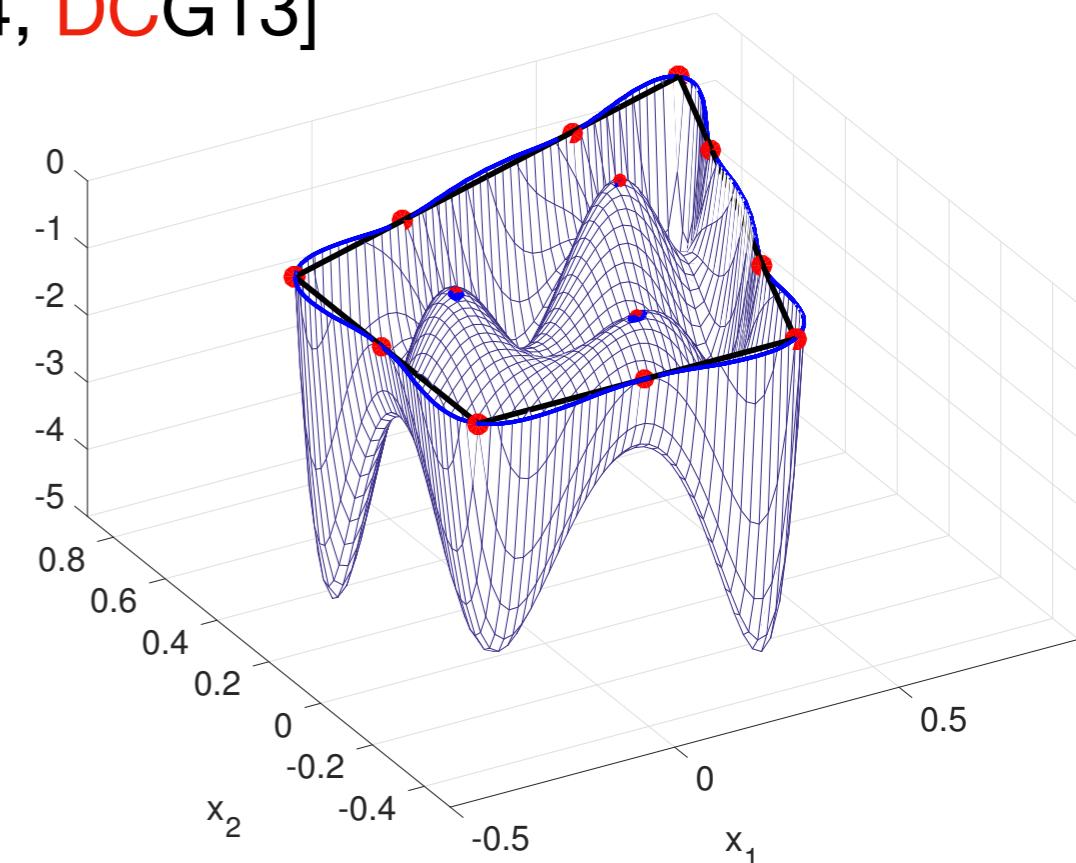
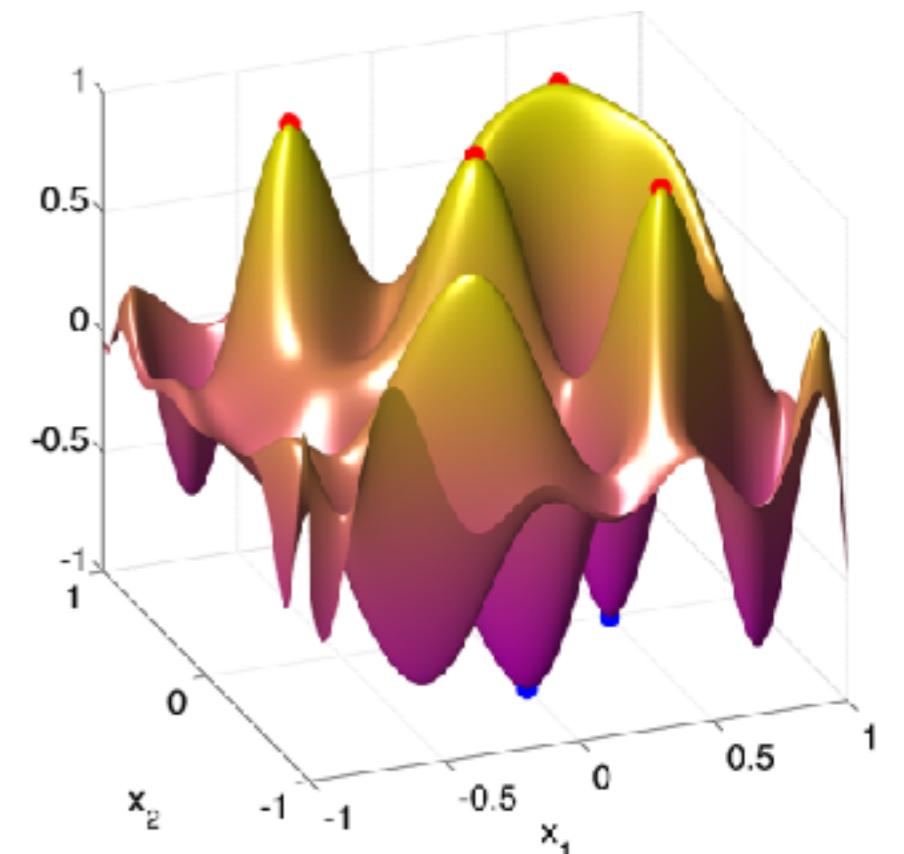
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In Theoretical Computer Science
Lasserre = Computational Limit



ML Applications

- Combinatorial Optimization on Graphs
- Tensor Decompositions
- Sparse Deconvolution [DCGHL16, ADCG14, DCG13]
- Gaussian Mixtures [DCGMM18+]
- Optimal Designs [DCGHHL18]



Step by Step Sketch of Proof in Convex Duality



Convex Objective

$$\inf_{(m_\alpha) \in \mathcal{M}} \sum_{\alpha=0}^{s-1} f_\alpha m_\alpha \longrightarrow \inf_{(m_\alpha) \in \mathcal{M}} F\left(\sum_{\alpha=0}^{s-1} m_\alpha H_\alpha\right)$$

- Convex objective: F
- Symmetric matrices: H_0, \dots, H_{s-1}
- Moment matrix: $M_s(m_\alpha) : (m_\alpha) \mapsto \sum_{\alpha=0}^{s-1} m_\alpha H_\alpha$

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Primal

$$\inf_{(m_\alpha)} \{F(M_s(m_\alpha)) : m = (m_\alpha) \in \mathcal{M}, Am = b\}.$$

Fenchel Dual

$$F^*(W) := \sup_{X \in \mathbb{S}_d} \{ \langle X, W \rangle - F(X) \}$$

Key Property 1

$$\forall W, \exists X_W \text{ s.t. } \nabla F(X_W) = W, \quad F^*(W) = \langle X_W, W \rangle - F(X_W)$$

$$\forall X, \exists W_X \text{ s.t. } \nabla F^*(W_X) = X, \quad F(X) = \langle X, W_X \rangle - F^*(W)$$

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Dual Cone

$$\mathcal{M}^* := \left\{ c \in \mathbb{R}^s : \forall m = (m_\alpha)_{\alpha=0}^{s-1} \in \mathcal{M}, \langle m, c \rangle \geq 0 \right\}$$

Key Property 2

$$c \in \mathcal{M}^* \Leftrightarrow \sum_{\alpha} c_{\alpha} t^{\alpha} \geq 0 \text{ on } \Omega$$

$$\mathcal{M}^* = \limsup_d \mathcal{M}^{*, \text{SOS}(d)} \supseteq \dots \supseteq \mathcal{M}^{*, \text{SOS}(d)} \supseteq \dots \supseteq \mathcal{M}^{*, \text{SOS}(2)}$$

INNER SDP approximations
of nonnegative polynomials

Dual Cone

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$$\langle m, c \rangle = \int_{\Omega} (\sum c_\alpha t^\alpha) d\mu(t)$$



Key Property 2

$$c \in \mathcal{M}^* \Leftrightarrow \sum_{\alpha} c_\alpha t^\alpha \geq 0 \text{ on } \Omega$$

$$\mathcal{M}^* = \limsup_d \mathcal{M}^{*, \text{SOS}(d)} \supseteq \dots \supseteq \mathcal{M}^{*, \text{SOS}(d)} \supseteq \dots \supseteq \mathcal{M}^{*, \text{SOS}(2)}$$

INNER SDP approximations
of nonnegative polynomials

Dual Cone

$$\mathcal{M}^* := \left\{ c \in \mathbb{R}^s : \forall m = (m_\alpha)_{\alpha=0}^{s-1} \in \mathcal{M}, \langle m, c \rangle \geq 0 \right\}$$

$$\langle m, c \rangle = \int_{\Omega} (\sum c_\alpha t^\alpha) d\mu(t)$$



Key Property 2

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**INNER SDP approximations
of nonnegative polynomials**

Lagrangian Analysis

Primal

$$\inf_{(m_\alpha)} \{ F(M_s(m_\alpha)) : m = (m_\alpha) \in \mathcal{M}, Am = b \}.$$

$$\mathcal{L} = F(X) - \langle W, X - M_s(m) \rangle + \langle z, Am - b \rangle - \langle m, c \rangle \quad (1)$$

$$= F(X) - \langle W, X \rangle - \langle z, b \rangle + \sum_{\alpha=0}^{s-1} m_\alpha (\underbrace{\langle W, H_\alpha \rangle}_{\text{Primal}} + \underbrace{(A^\top z)_\alpha - c_\alpha}_{\text{Dual}}) \quad (2)$$

$$(1) \xrightarrow{\hspace{1cm}} \inf_{X,m} \sup_{W,c,z} \mathcal{L} =$$

Primal

Lagrangian Analysis

Primal

$$\inf_{(m_\alpha)} \{ F(M_s(m_\alpha)) : m = (m_\alpha) \in \mathcal{M}, Am = b \}.$$

$$\mathcal{L} = F(X) - \underbrace{\langle W, X - M_s(m) \rangle}_{\text{blue bar}} + \underbrace{\langle z, Am - b \rangle}_{\text{orange bar}} - \underbrace{\langle m, c \rangle}_{\text{purple bar}} \quad (1)$$

$$= F(X) - \langle W, X \rangle - \langle z, b \rangle + \sum_{\alpha=0}^{s-1} m_\alpha \left(\langle W, H_\alpha \rangle + (A^\top z)_\alpha - c_\alpha \right) \quad (2)$$

$$(1) \xrightarrow{\text{orange arrow}} \inf_{X,m} \sup_{W,c,z} \mathcal{L} =$$

Primal

Lagrangian Analysis

Dual

$$\sup_{W \in \mathbb{S}_d, z \in \mathbb{R}^m} \left\{ \langle z, b \rangle - F^\star(W) : (\langle W, H_\alpha \rangle)_\alpha + A^\top z \in \mathcal{M}^\star \right\}.$$

$$\mathcal{L} = F(X) - \underbrace{\langle W, X - M_s(m) \rangle}_{\text{blue bar}} + \underbrace{\langle z, Am - b \rangle}_{\text{orange bar}} - \underbrace{\langle m, c \rangle}_{\text{purple bar}} \quad (1)$$

$$= F(X) - \langle W, X \rangle - \langle z, b \rangle + \sum_{\alpha=0}^{s-1} m_\alpha \left(\langle W, H_\alpha \rangle + (A^\top z)_\alpha - c_\alpha \right) \quad (2)$$

$$(2) \xrightarrow{\text{orange arrow}} \sup_{W, c, z} \inf_{X, m} \mathcal{L} = \boxed{\text{Dual}}$$

Primal

$$\inf_{(m_\alpha)} \left\{ F(M_s(m_\alpha)) : m = (m_\alpha) \in \mathcal{M}, Am = b \right\}.$$

Dual

$$\sup_{W \in \mathbb{S}_d, z \in \mathbb{R}^m} \left\{ \langle z, b \rangle - F^*(W) : (\langle W, H_\alpha \rangle)_\alpha + A^\top z \in \mathcal{M}^* \right\}.$$

When no duality gap: $\langle z^*, b \rangle - F^*(W^*) = F(M_s(m^*))$

Complementarity leads to:

$$\langle W^*, M_s(m^*) \rangle - \langle z^*, b \rangle = \sum_{\alpha=0}^{s-1} m_\alpha^* (\langle W^*, H_\alpha \rangle + (A^\top z^*)_\alpha) = 0$$

$$\langle W^*, M_s(m^*) \rangle = \langle z^*, b \rangle = F(M_s(m^*)) + F^*(W^*) \quad \text{and} \quad W^* = \nabla F(M_s(m^*)).$$

Primal

$$\inf_{(m_\alpha)} \left\{ F(M_s(m_\alpha)) : m = (m_\alpha) \in \mathcal{M}, Am = b \right\}.$$

Dual

$$\sup_{W \in \mathbb{S}_d, z \in \mathbb{R}^m} \left\{ \langle z, b \rangle - F^*(W) : (\langle W, H_\alpha \rangle)_\alpha + A^\top z \in \mathcal{M}^* \right\}.$$

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Primal

$$\inf_{(m_\alpha)} \left\{ F(M_s(m_\alpha)) : m = (m_\alpha) \in \mathcal{M}, Am = b \right\}.$$

Dual

$$\sup_{W \in \mathbb{S}_d, z \in \mathbb{R}^m} \left\{ \langle z, b \rangle - F^\star(W) : (\langle W, H_\alpha \rangle)_\alpha + A^\top z \in \mathcal{M}^\star \right\}.$$

When no duality gap: $\langle z^\star, b \rangle - F^\star(W^\star) = F(M_s(m^\star))$

Complementarity leads to:

$$\langle W^\star, M_s(m^\star) \rangle - \langle z^\star, b \rangle = \sum_{\alpha=0}^{s-1} m_\alpha^\star (\langle W^\star, H_\alpha \rangle + (A^\top z^\star)_\alpha) = 0$$

$$\langle W^\star, M_s(m^\star) \rangle = \langle z^\star, b \rangle = F(M_s(m^\star)) + F^\star(W^\star) \quad \text{and} \quad W^\star = \nabla F(M_s(m^\star)).$$

Key Property 1

Primal

$$\inf_{(m_\alpha)} \left\{ F(M_s(m_\alpha)) : m = (m_\alpha) \in \mathcal{M}, Am = b \right\}.$$

Dual

Key Property 2

$$\sup_{W \in \mathbb{S}_d, z \in \mathbb{R}^m} \left\{ \langle z, b \rangle - F^*(W) : (\langle W, H_\alpha \rangle)_\alpha + A^\top z \in \mathcal{M}^* \right\}.$$

When no duality gap: $\langle z^*, b \rangle - F^*(W^*) = F(M_s(m^*))$

Complementarity leads to:

$$\langle W^*, M_s(m^*) \rangle - \langle z^*, b \rangle = \sum_{\alpha=0}^{s-1} m_\alpha^* (\langle W^*, H_\alpha \rangle + (A^\top z^*)_\alpha) = 0$$

Key Property 3

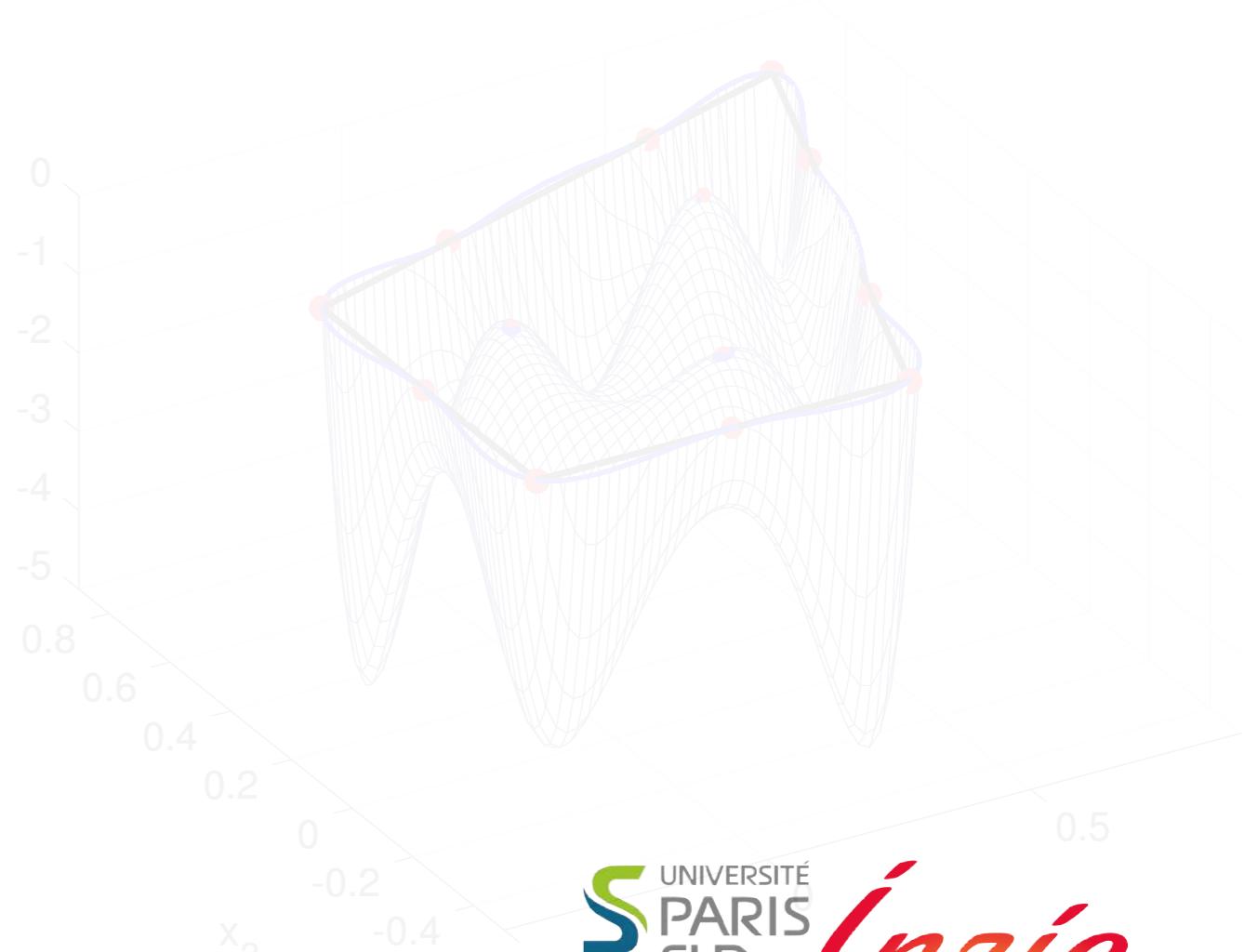
$$\int_{\Omega} P(t) \, d\mu(t) = 0$$

$$\geq 0 \quad \geq 0$$

An Example: Optimal Designs

$$\inf_{(m_\alpha)} \left\{ -\log \det(M_s(m_\alpha)) : m = (m_\alpha) \in \mathcal{M}, m_0 = 1 \right\}.$$

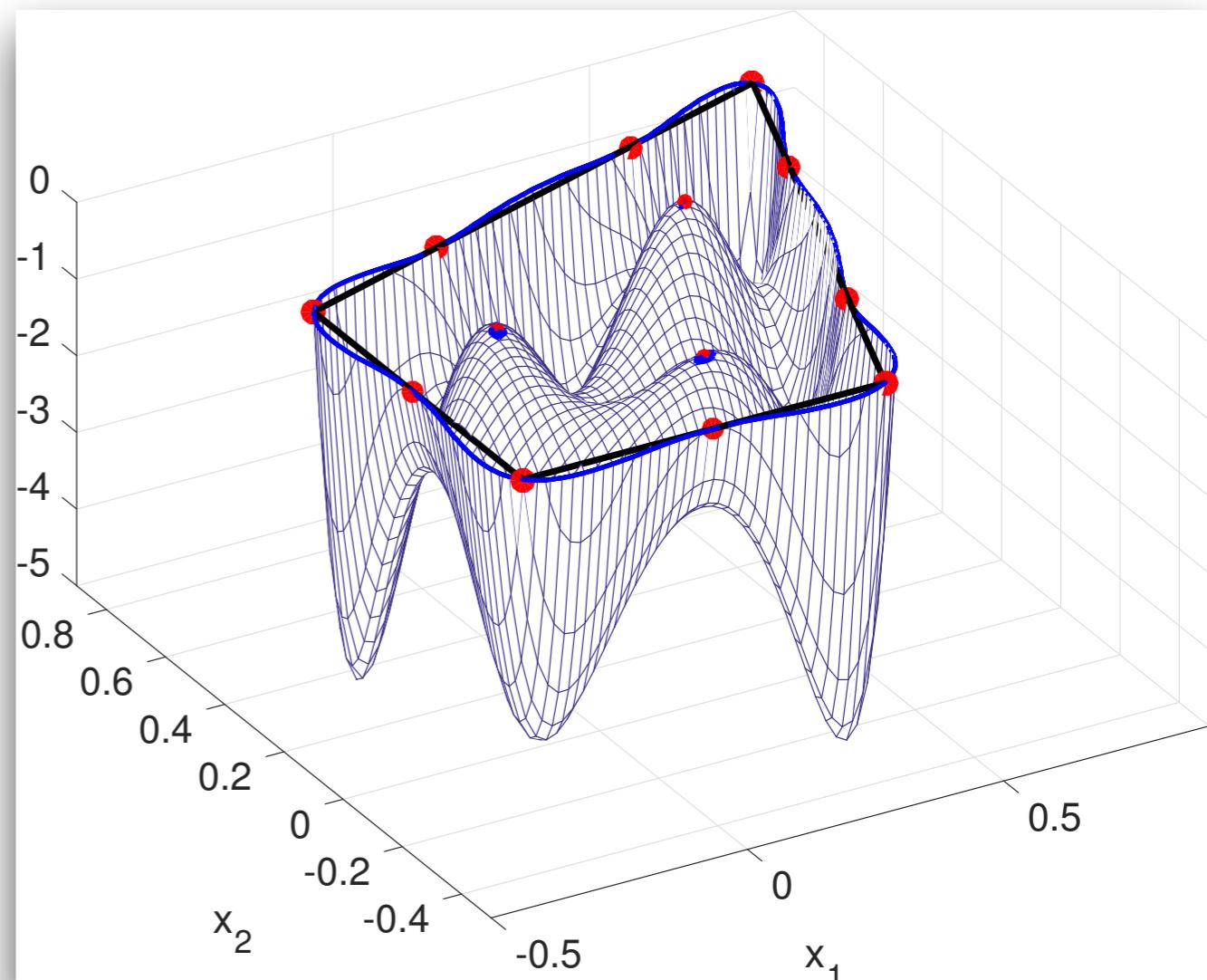
- $F^\star(W) = -s - \log \det(-W)$ and $\nabla F(X) = -X^{-1}$
- $W^\star = -M_s(m^\star)^{-1}$
- $p^\star(t) = \sum_{\alpha=0}^{s-1} \langle M_s(m^\star)^{-1}, H_\alpha \rangle t^\alpha$
- $\int_{\Omega} (s - p^\star(t)) d\mu^\star(t) = 0$



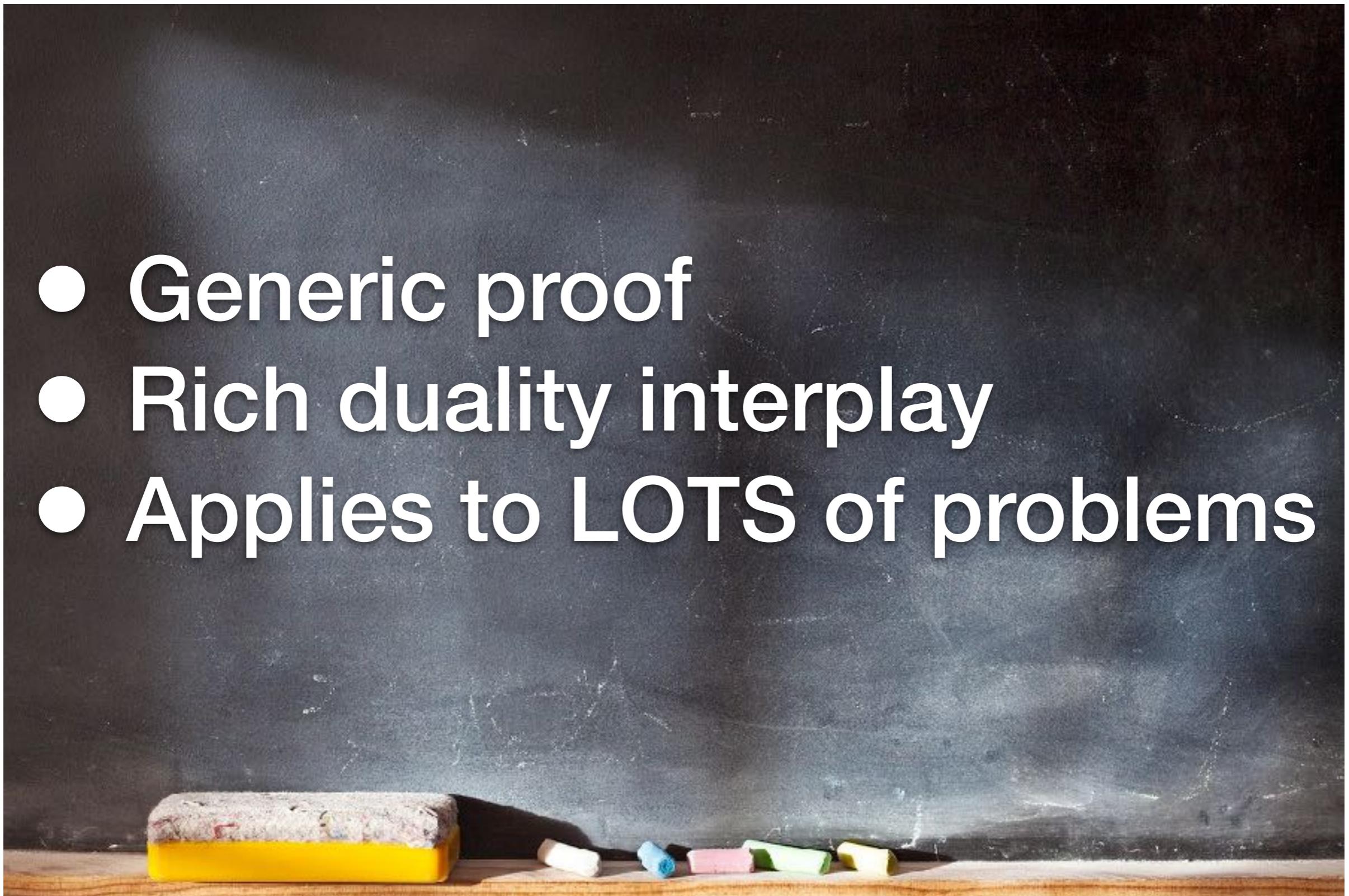
An Example: Optimal Designs

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- $F^\star(W) = -s - \log \det(-W)$ and $\nabla F(X) = -X^{-1}$
- $W^\star = -M_s(m^\star)^{-1}$
- $p^\star(t) = \sum_{\alpha} \langle M_s(m^\star)^{-1}, H_\alpha \rangle t^\alpha$
- $\int_{\Omega} (s - p^\star(t)) d\mu^\star(t) = 0$



- Generic proof
- Rich duality interplay
- Applies to LOTS of problems



THANK YOU

Yohann DE CASTRO

