MTRI Summer 2022 Internship Presentation

Nathan Willey

Michigan Tech Research Institute

About Me

- Rising senior at Michigan State University
    - Majoring in Mathematics and Physics with a minor in Data Science
- Planning to apply for graduate school in applied math next fall
- Worked hybrid at-home/in-office this summer

Projects

Worked with Joel on various math projects in MATLAB

Main Projects:

1. Optimization over manifolds
2. Monotonic Regression

Smaller Projects:

- Translating MATLAB implementations into Python
- Padé Splines

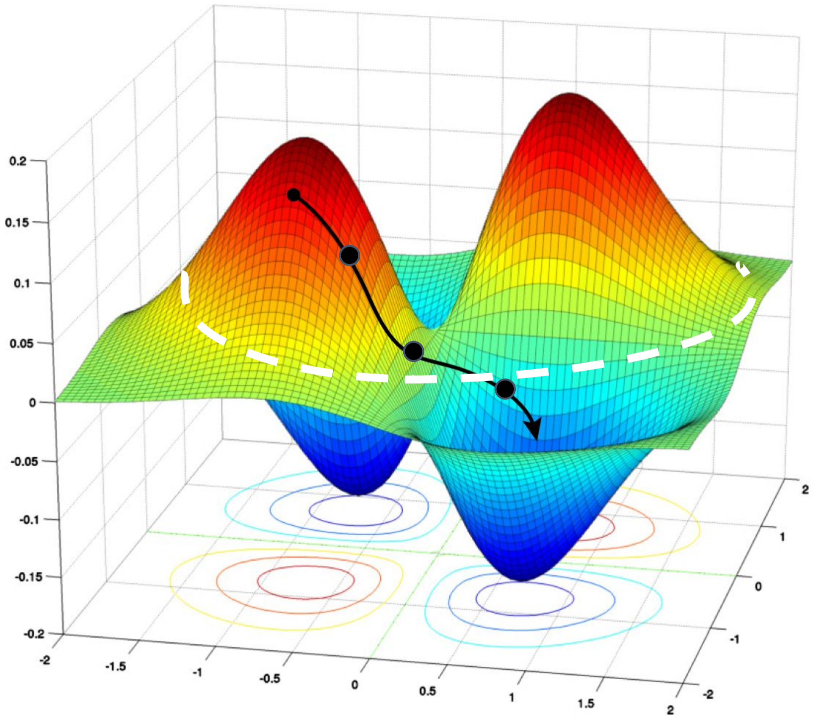
Manifold Optimization

Goal: Find the minimum of a function f(**x**), where **x** is subject to constraints s.t. **x** lies on a smooth manifold

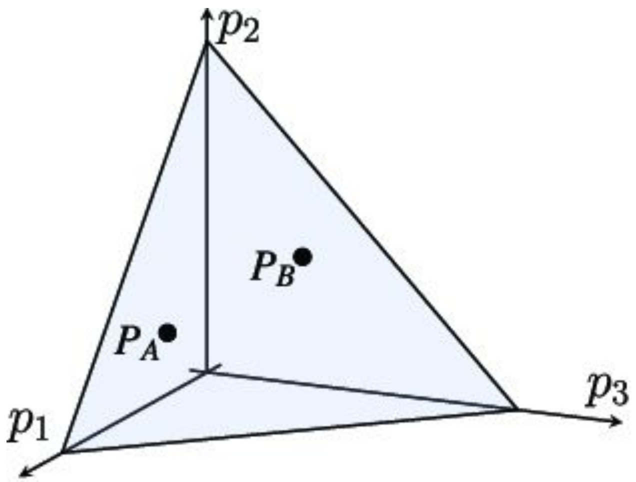
Manifold Optimization Intro

We want to solve problems of the form $\min_{x \in \mathcal{M}} f(x)$

$\mathcal{M}$ is a submanifold of real-space– i.e. sphere or *probability simplex*



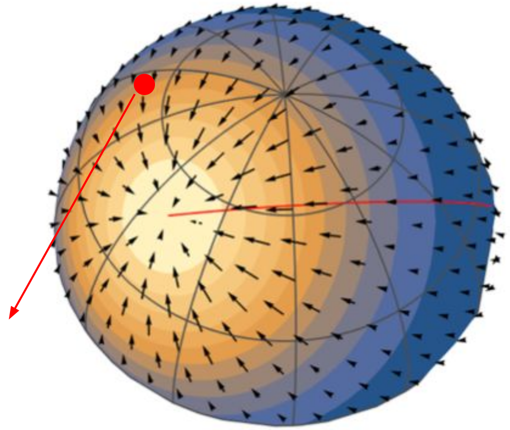
$$\{x \in \mathbb{R}^k | \sum_{i=1}^{N} x_i = 1, x_i \geq 0\}$$



(a)

Reparametrization of Constraints

Consider spherical restrictions: $$\sum_{i=1}^{k} \beta_k^2 = 1$$



If you minimize over $\mathbb{R}^k$ you have a *constrained* optimization problem

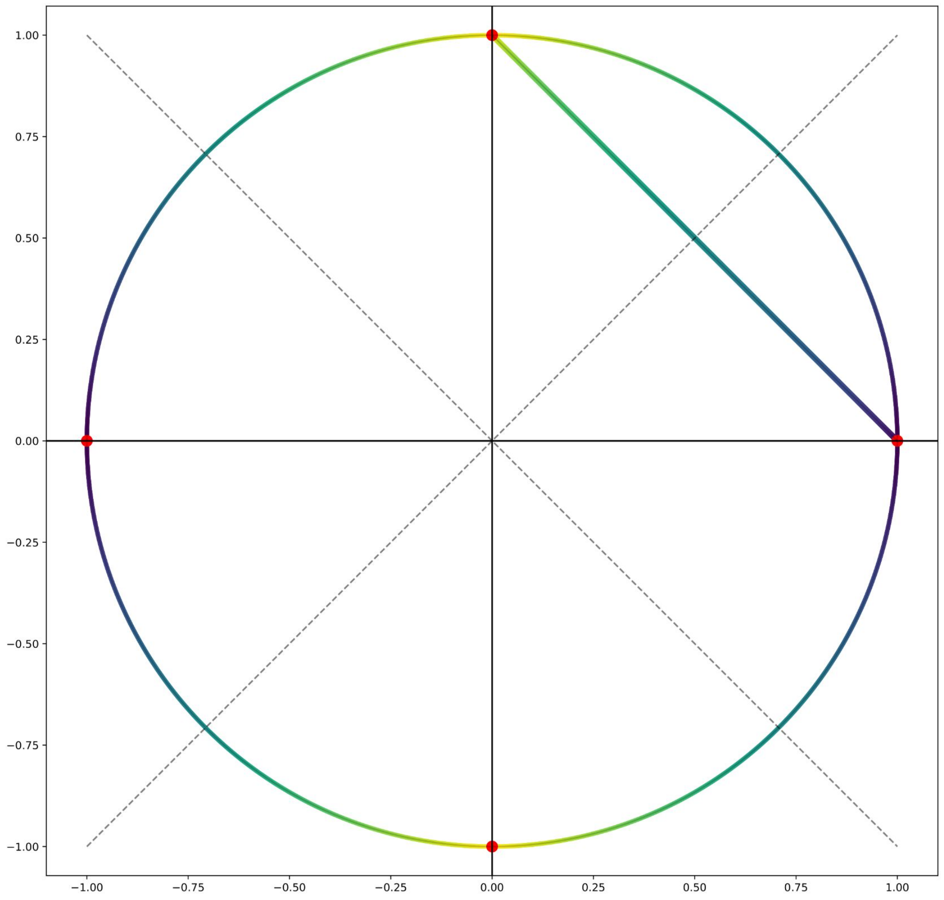
We can use spherical coordinates to always stay within constraints!

We can do a similar parametrization for the probability simplex:

Spherical		Cartesian		Probability Simplex
$\vec{\alpha}$	$\longrightarrow$	$\vec{x}$	$\longrightarrow$	$\vec{x} \odot \vec{x}$

Simplex via Spherical Coordinates

- Best conditioned on diagonals where the tangent spaces are parallel ("isometry points")
- Conditioning gets worse towards the axes
  - Mapping has gradient **0** on any axis



We would *like* to always be minimizing the function near the isometry point x_{isometry}

Improving Conditioning

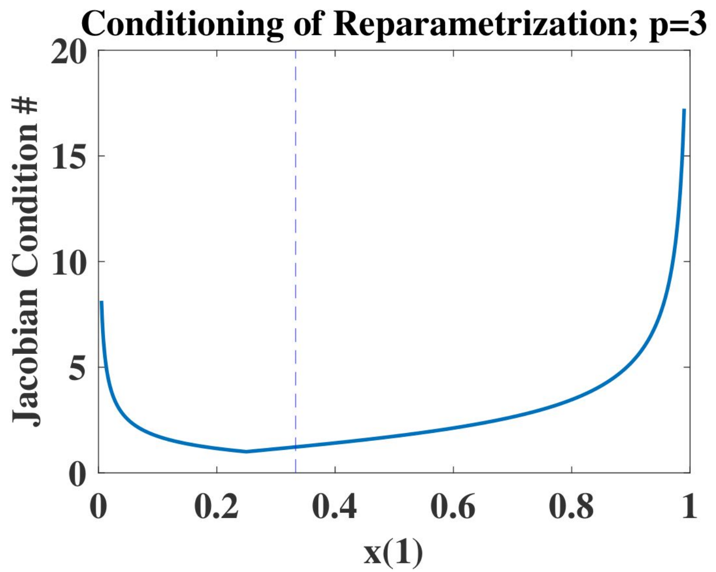
One option explored:

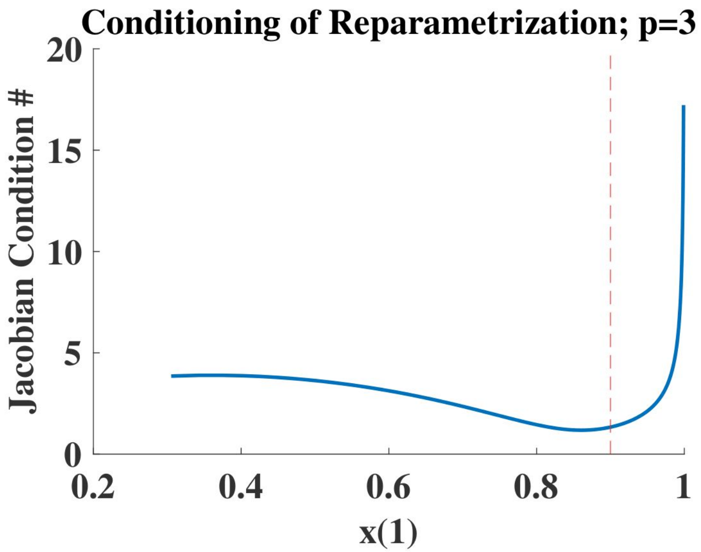
Define another intermediate mapping **T** s.t. $T(x_{isometry}) \cong x_i$

Uses Padé splines to shift coordinates

Spherical — Cartesian — Probability Simplex — Remap to x_i

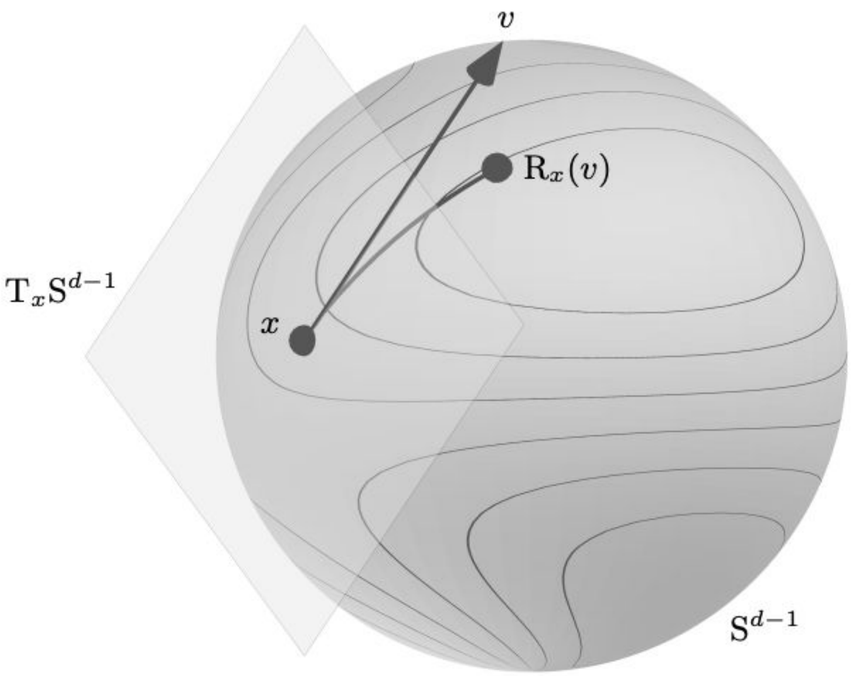
$$\vec{\alpha}_{isom} \rightarrow \vec{x} \rightarrow \vec{x} \odot \vec{x} \rightarrow T(\vec{x} \odot \vec{x})$$





Direct Manifold Optimization

- I also looked into and created a write-up on a method for optimizing directly on manifolds being done in the MATLAB package manOpt
- Involves projecting the function’s unbound gradient onto the tangent space of a manifold



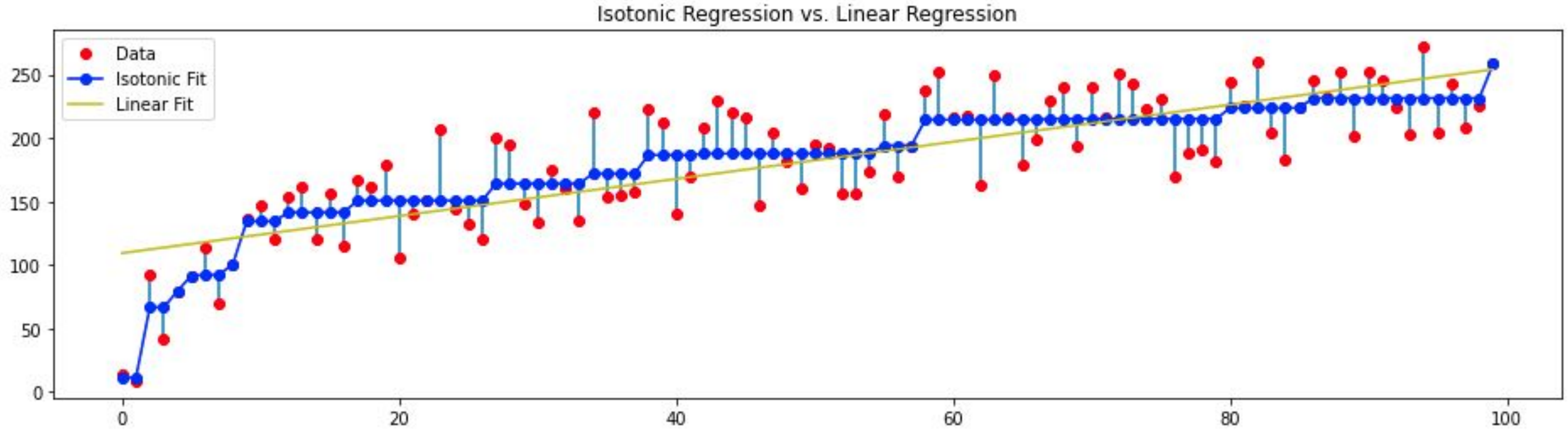
Monotonic Regression

Goal: Fit 1D data with a *nondecreasing,* non-parametric function

Monotonic Regression Intro

Purpose: Estimation of non-decreasing physical parameters or cumulative probability density functions

This is most commonly/easily done with PAVA algorithm:



I looked into recent research in the area to find and implement smooth monotone regression splines

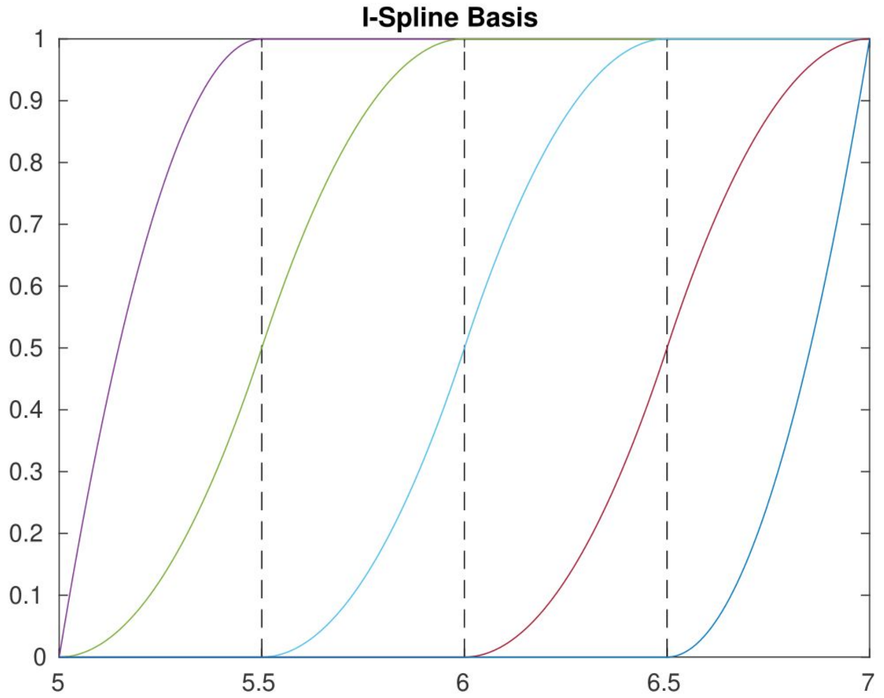
I-Splines

- Basis of non-decreasing polynomial functions
- Polynomial monotone regression splines are the result of linear combination with non-negative β

$$f(x) = \sum_{i=1}^{k} \beta_i I_i(x),\ \ \beta_i \geq 0$$

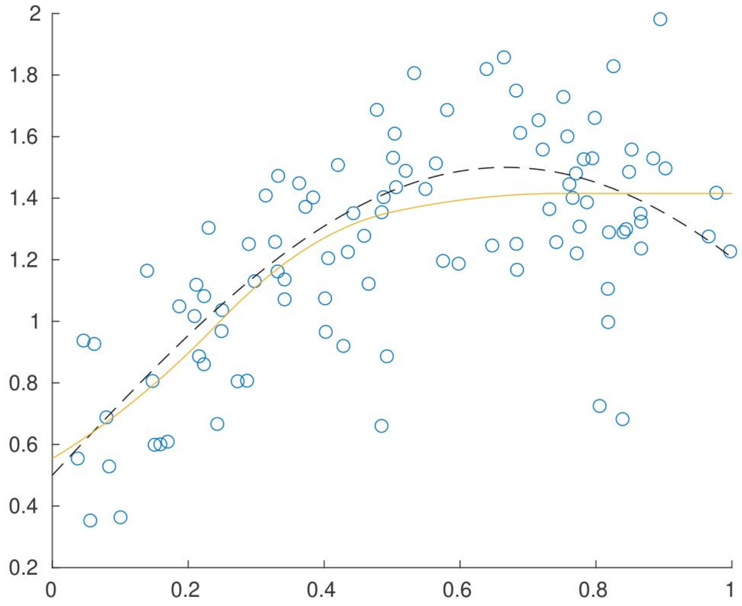
- Since each I-Spline basis function covers [0,1] we can directly fit probability curves if we fit $\boldsymbol{\beta}$ as a mixture problem

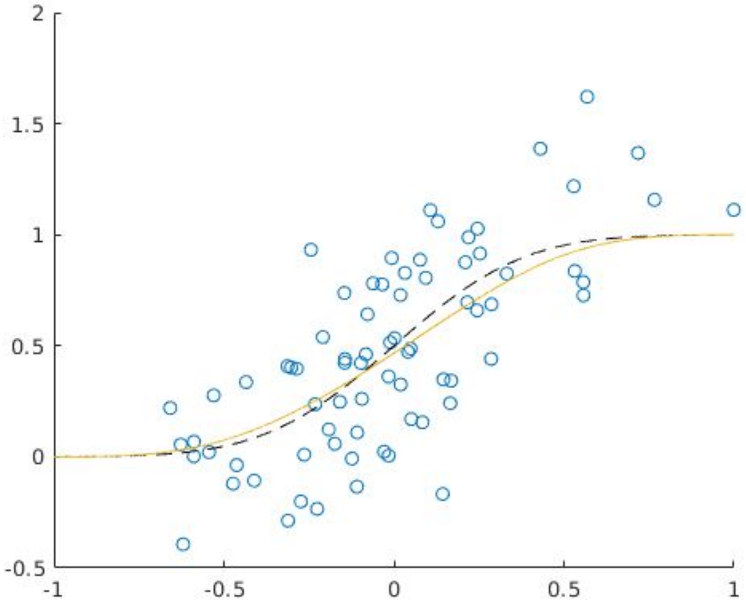
$$\sum_{i=1}^{k} \beta_i = 1$$



I-Spline Examples

5 knot cubic regression splines





$$sin(\frac{3*\pi}{4}x), x \in [0,1]$$

$$\text{normalcdf}(x; \mu = 0, \sigma = 0.3), x \in [-1, 1]$$

P-Splines

P-Splines refer to the idea of adding a discrete difference penalty on spline coeff. to enforce smoothness

$$\min_{\beta \succeq \vec{0}} \Big(\sum_{j=1}^{N} (y_j - f(x_j))^2 + \lambda \sum_{i=1}^{k} \Delta^{\ell}(\beta_i) \Big)$$

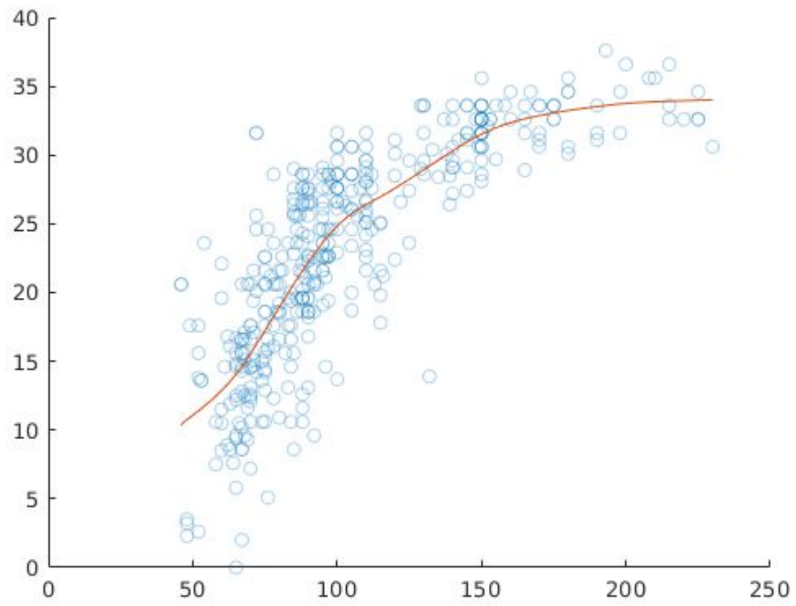
$\boldsymbol{\lambda}$ is a user-chosen smoothing parameter

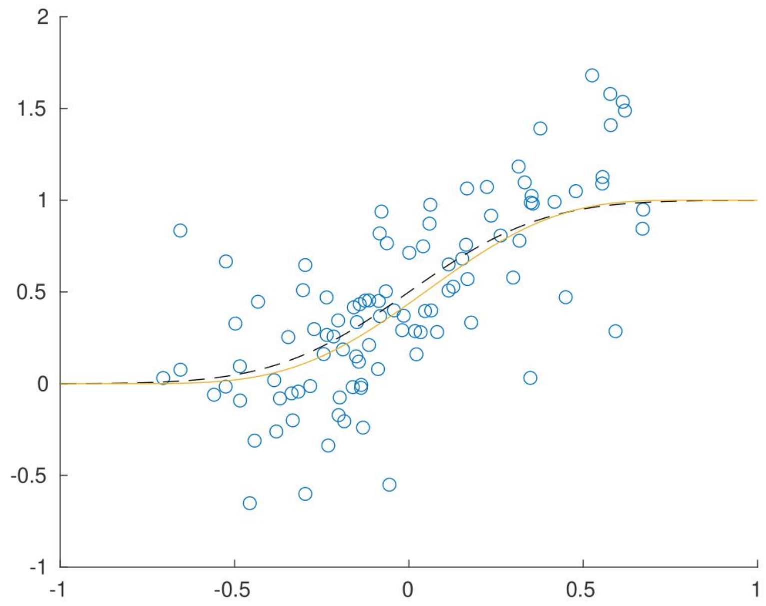
Reduces importance of knot placement

Penalized Monotone Splines

By applying a penalty to i-splines we are able to get smooth nonparametric monotone splines

- Can enforce c.d.f. restrictions





Internship Takeaways

Skills gained:

- MATLAB
- Computational optimization methods
- Splines
- Mercurial/ File Sync.
- Reading papers
- LaTeX write-ups

Questions?

References:

Ramsay, James O. ”Monotone regression splines in action.” Statistical science (1988): 425-441.

Eilers, P. H., Marx, B. D. (1996). Flexible smoothing with B-splines and penalties. Statistical science, 11(2), 89-121.

Hastie, T., Tibshirani, R., Friedman, J. H., Friedman, J. H. (2009). The elements of statistical learning: data mining, inference, and prediction (Vol.2, pp. 1-758). New York: springer.

Nicolas Boumal, An Introduction to Optimization on Smooth Manifolds, 2020