Inducing Point Approximations of Kernel Matrices

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Our bunnies
(No affil)

The setup

Given (maybe noisy) evals at points $X \subset \Omega$ of

$$f : \Omega \subset \mathbb{R}^d \to \mathbb{R}$$

Want to compute $s \approx f$ via *kernel* methods. Challenges:

- How to choose the kernel?
- What are the approximation properties?
- Can we go faster than the naive costs?
  - Fitting: $O(N^3)$
  - Evaluating: $O(N)$
  - Evaluating uncertainty: $O(N^2)$

Plan for Today

- Function approximation setup
- NLA and kernel matrix approximation
- Gaussian processes and variational inference
- Norms, native spaces, and optimal recovery

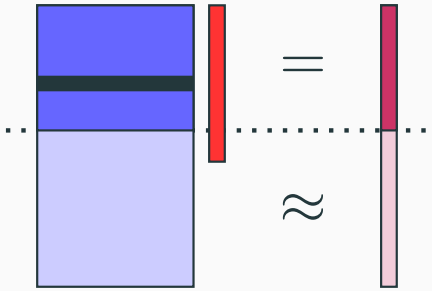
Inducing points

Idea: Organize approximation around relatively few *inducing points*. Different methods for different perspectives:

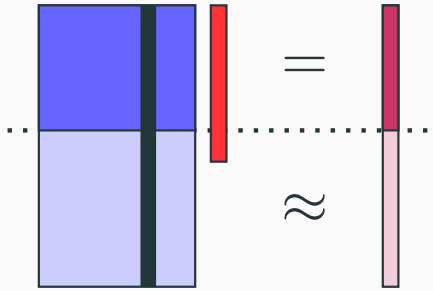
- **NLA**: Nyström, subset of regressors, FITC (see e.g. Rasmussen and Williams, Ch. 8)
- **GP**: Variational inference
- **Optimal recovery**: Norm minimization with ℓ^∞ constraints

Kernel-Based Regression: Four Stories

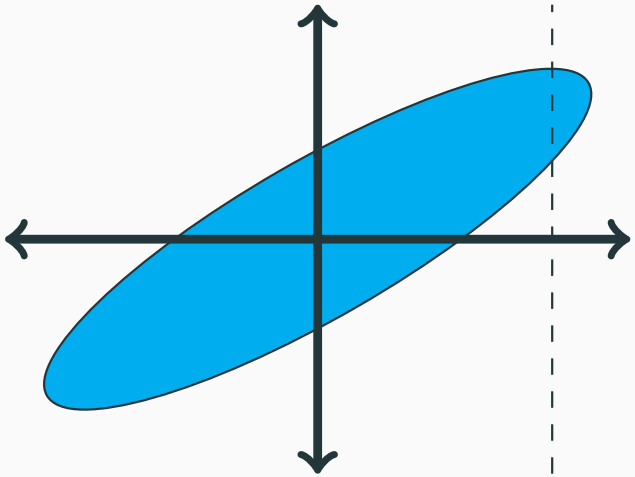
Feature map



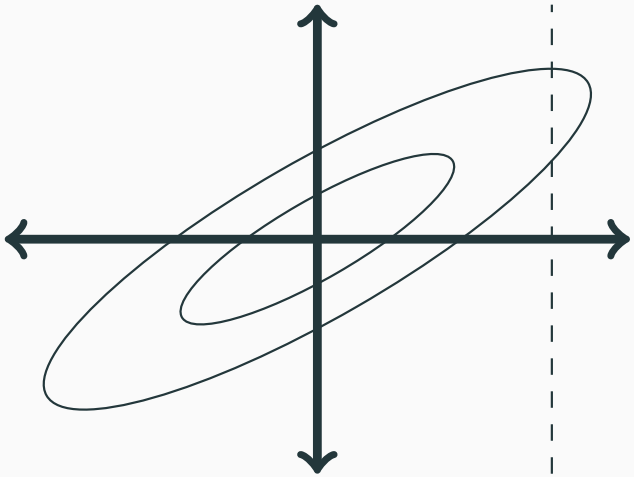
Data-dependent basis



Energy minimization



Gaussian process



Feature Maps

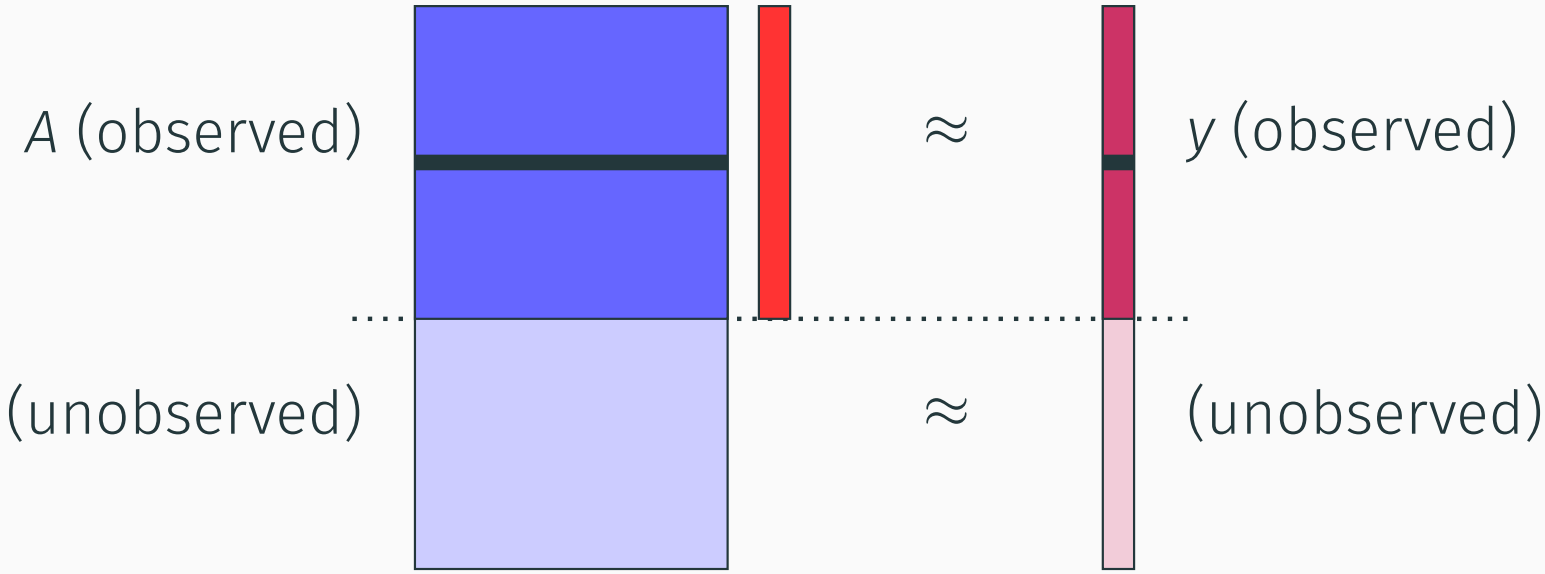
$$\begin{bmatrix} x \\ y \end{bmatrix} \mapsto \begin{bmatrix} 1 \\ x \\ y \\ x^2 \\ xy \\ y^2 \end{bmatrix}$$

Augment simple linear model ($c^T x$) with feature map:

$$f(x) \approx \langle d, \psi(x) \rangle$$

where $\psi : \Omega \to \mathcal{F}$ and $d \in \mathcal{F}$, some Hilbert space $\mathcal{F}$.

Feature Maps and Dimensionality

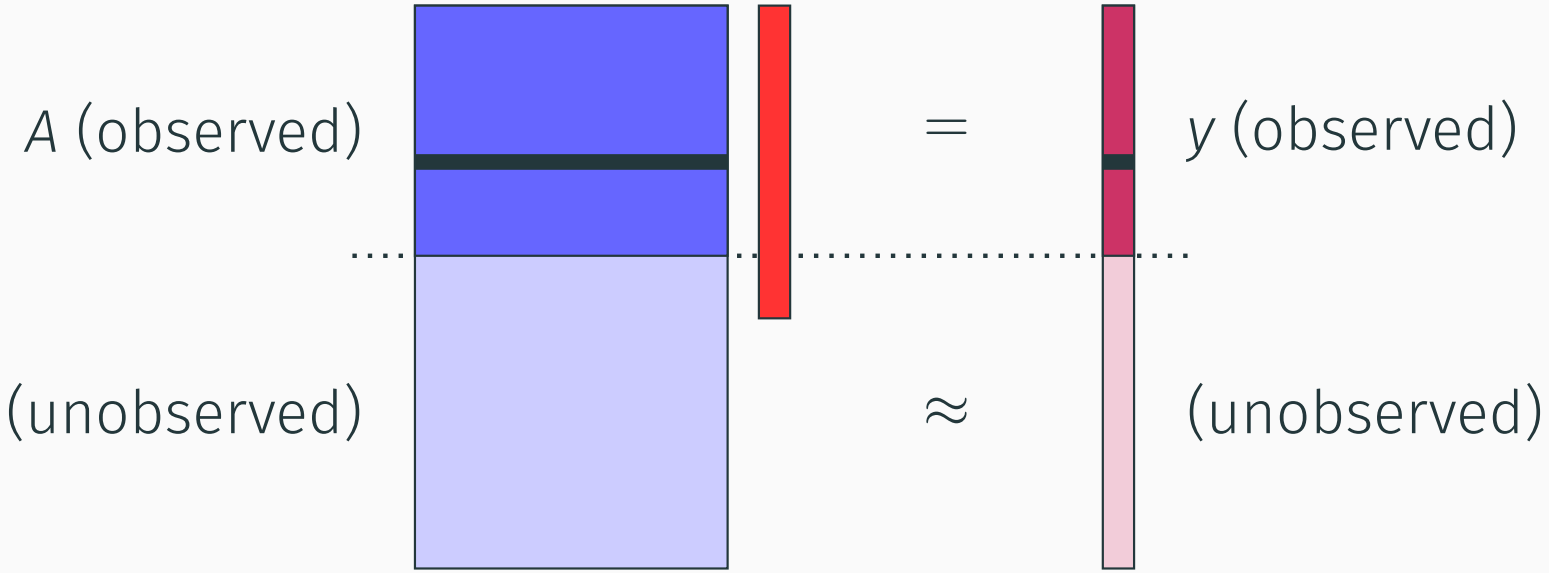


Usual idea with $A^T = \begin{bmatrix} \psi(x_1) & \dots & \psi(x_n) \end{bmatrix}^T$:

- $\dim \mathcal{F} < n$: least squares
- $\dim \mathcal{F} = n$: interpolation

May be ill-posed for general scattered (multidimensional) case (Mairhuber-Curtis theorem)

Feature Maps and Dimensionality



Underdetermined ($\dim \mathcal{F} > n$): seek *minimal norm* solution.
For standard inner product (ℓ^2):

$$d = A^\dagger y = A^T (AA^T)^{-1} y$$

$$f(x) \approx \psi(x)^T d = \psi(x)^T A^T (AA^T)^{-1} y$$

Implicit preference for some models over others.

The Kernel Trick

Formula:

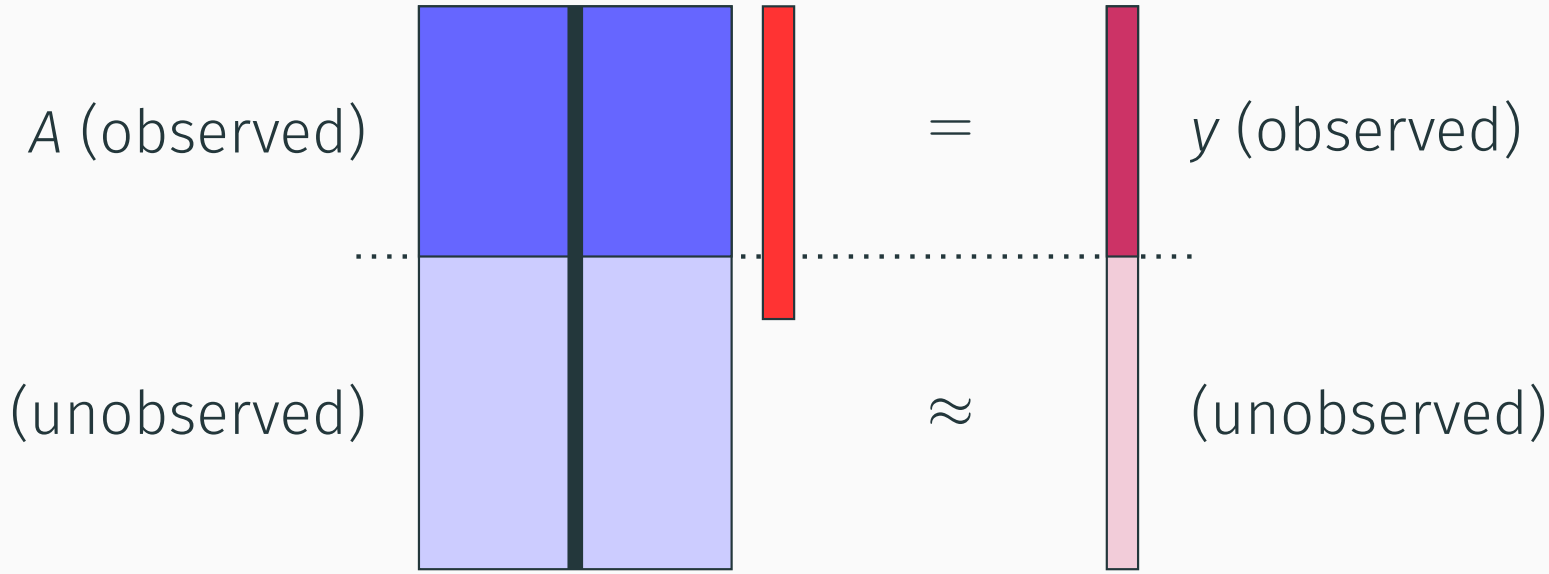
$$A^T = \begin{bmatrix} \psi(x_1) & \dots & \psi(x_n) \end{bmatrix}$$
$$f(x) \approx s(x) \equiv \left(\psi(x)^T A^T\right) \left(AA^T\right)^{-1} y$$

In terms of *kernel* $k(x, y) = \langle \psi(x), \psi(y) \rangle$:

$$(AA^T)_{ij} = k(x_i, x_j) = (K_{XX})_{ij}$$
$$K_{XX} c = y = f_X$$
$$s(x) = K_{xX} c = \sum_{j=1}^{n} k(x, x_j) c_j$$

Subscripts to denote vectors/matrices of function evaluations.

Rows or Columns?



Change perspective: feature vectors $\psi(x_i)$ to basis vectors $\psi_j(x)$

- Native space: combinations of basis (with $d \in \mathcal{F}$)
- Sampling-dependent subspace of min-norm interpolants:

$$\mathcal{S}_X = \left\{ x \mapsto \sum_{j=1}^{n} k(x, x_j) c_j \right\}$$

Feature Maps to RKHS

Basis vectors $\psi_j(x)$ form orthonormal basis for a Hilbert space:

$$s(x) = \sum_i d_i \psi_i(x), \quad \|s\|_{\mathcal{H}}^2 = \|d\|^2$$

For $x \in \Omega$, define $k_x \in \mathcal{H}$ as

$$k_x(y) = \sum_i \psi_i(x)\psi_i(y)$$

Then k_x defines a point evaluation functional in $\mathcal{H}$

$$\begin{aligned}\langle k_x, s\rangle_{\mathcal{H}} &= \sum_i \psi_i(x) \left\langle \psi_i, \sum_j d_j \psi_j \right\rangle_{\mathcal{H}} \\ &= \sum_i \psi_i(x) d_i = s(x)\end{aligned}$$

This is a *reproducing kernel Hilbert space* (RKHS).

Putting the Kernel before the Map

Start with symmetric kernel function $k : \Omega \times \Omega \to \mathbb{R}$.
k positive definite if K_{XX} spd for all samples X.

Associate integral operator with continuous spd kernel k:

$$(\mathcal{K}f)(x) = \int k(x, y) f(y)\, dy$$

$\mathcal{K}$ compact (actually Hilbert-Schmidt), so have

$$\mathcal{K} = \sum_{j=1}^{\infty} \lambda_j \psi_j \psi_j^*$$

and features are $\sqrt{\lambda_j}\psi_j(x)$.

But features are not really needed! Focus on the kernel.

Basic ingredient: Kernel functions

Call the *kernel* (or *covariance*) function k. Required (today):

- **Pos def**: K_{XX} is always positive definite

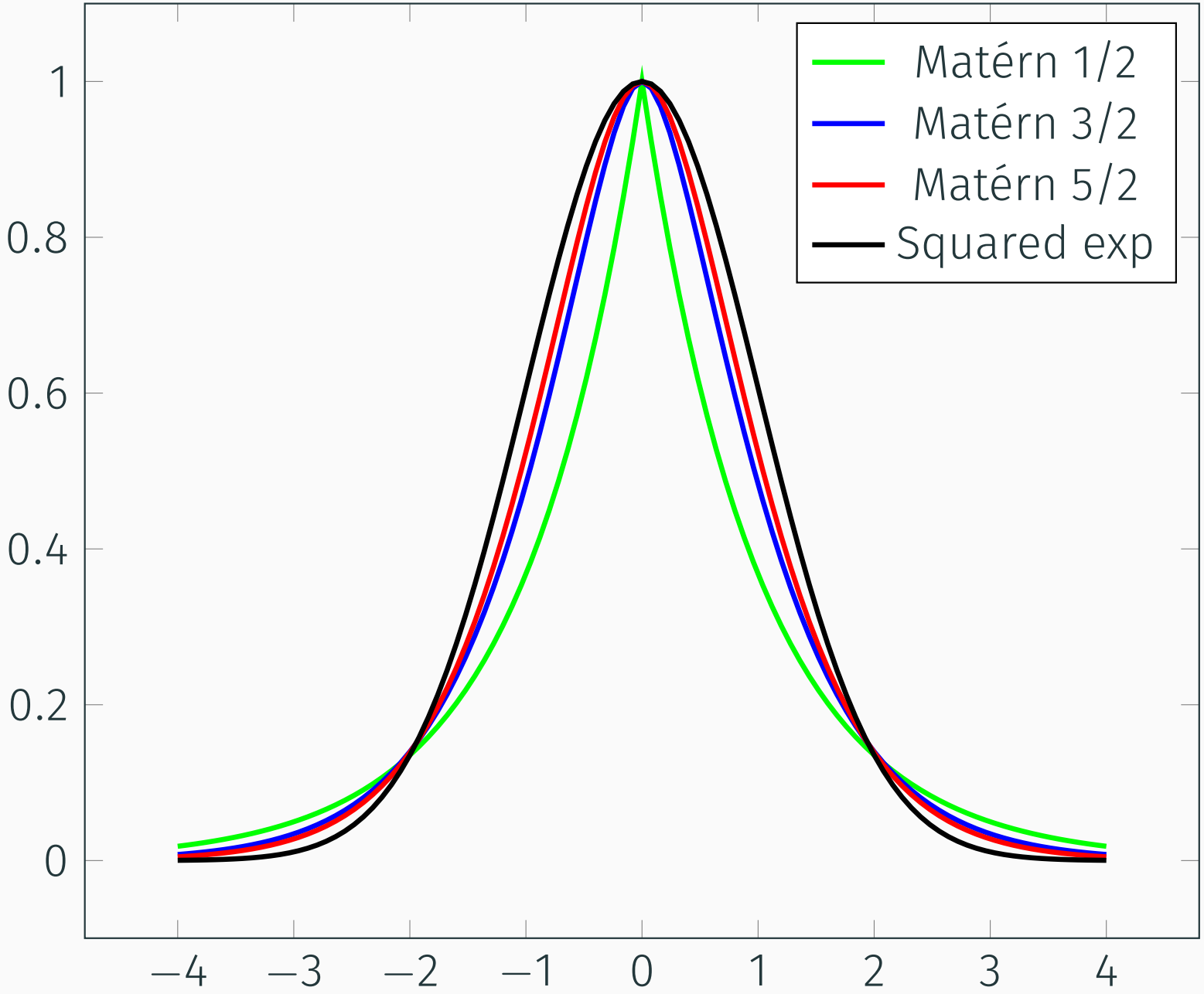
Often desirable:

- **Stationary**: $k(x, y)$ depends only on $x - y$
- **Isotropic**: $k(x, y)$ depends only on x and $\|x - y\|$

Often want both (sloppy notation: $k = k(r)$).

Common examples (e.g. Matérn, SE) also depend on *hyper-parameters* θ — suppressed in notation unless needed.

Matérn and SE kernels



Observations on kernel matrices

Kernel is *chosen by modeler*

- Matérn / SE for regularity and simplicity
- Rarely have the intuition to pick the "right" kernel
- Common choices are *universal* — can recover anything
  - ... with less data for "good" choice (inductive bias)
- Smoother k *implies* "prefer" smoother approximator

Intuitively, strong inductive bias $\implies$ rapid eigenvalue decay for $\mathcal{K}$ (or for K_{XX})

- Unit norm ball is close to a low-dimensional set; or
- Probability concentrates near a low-dimensional set

Eigenvalues of integral operators and kernel matrices

Weyl-Courant implies

$$\lambda_{n+1} \leq \|\mathcal{K} - \mathcal{S}\| \text{ for any } \mathbf{rank}(\mathcal{S}) = n.$$

Many decay bounds for kernels on $[0,1]^2$ (Fredholm and Weyl, Reade, Ha, Little and Reade, Chang and Hua, Wathen and Zhu):

- Tactic: polynomial interpolation to get finite rank S
- $k(r) \in C^\nu \implies |\lambda_n| = o(n^{-\nu-1/2})$
- Analytic on some region $\implies |\lambda_n| = O(\rho^{-n})$
- SE case: eigenvalues decay super-exponentially

Similar behavior for kernel matrices (see, e.g., Braun).

SoR and FITC

Approximate via inducing points $U \subset X$:

$$K_{XX} + \eta I \approx K_{XU} K_{UU}^{-1} K_{UX} + D,$$

where $D = \eta I$ (SoR) plus some additional correction (FITC).

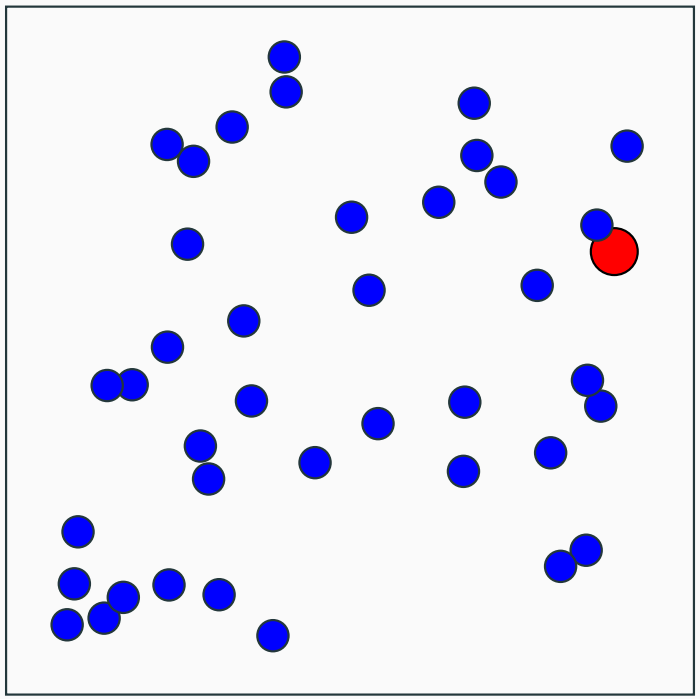
A good exercise: solve $(K_{XU} K_{UU}^{-1} K_{UX} + D)c = y$ by

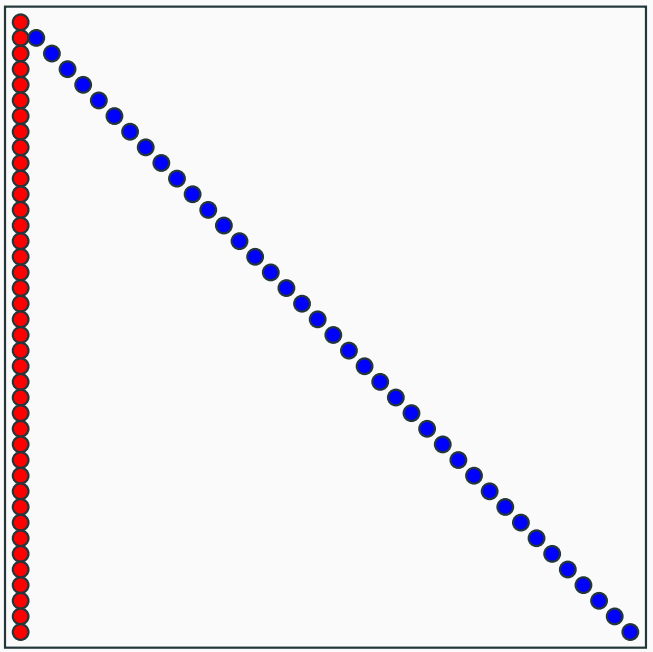
- Minimize $\left\| \begin{bmatrix} D^{-1/2} K_{XU} \\ K_{UU} \end{bmatrix} \lambda - \begin{bmatrix} D^{-1/2} y \\ 0 \end{bmatrix} \right\|$
- Recover $c = D^{-1}(y - K_{XU}\lambda)$ if desired
- Prediction $K_{xU} K_{UU}^{-1} K_{UX} c = K_{xU} \lambda$.

Can be a good preconditioner even when not great alone.
Things like log determinants are also simple to compute.

Choosing points

Greedy choice of inducing points *U* for smooth case:
Left-looking partial pivoted Cholesky





Diagonal element: 1.00e+00

Choosing points

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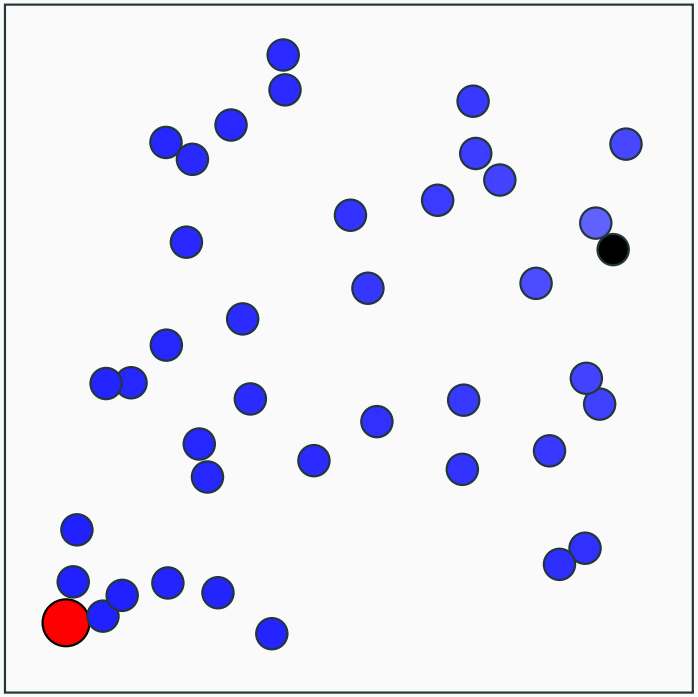

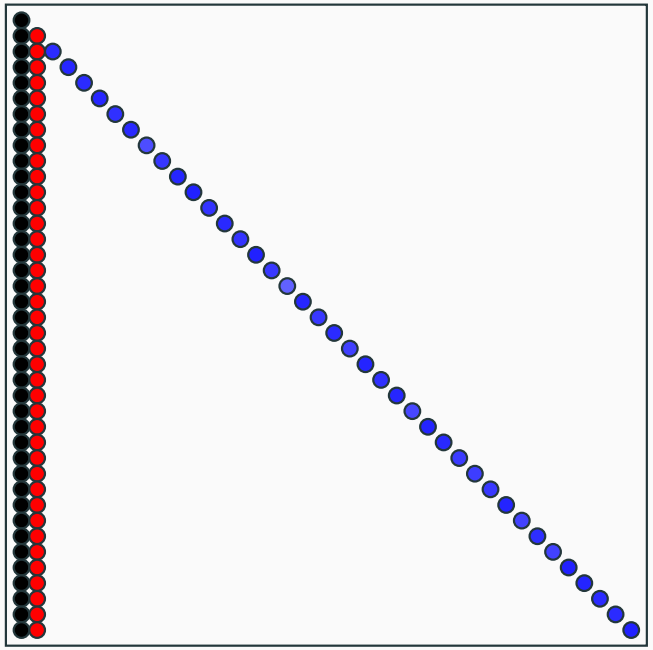

Diagonal element: 6.77e-02

Choosing points

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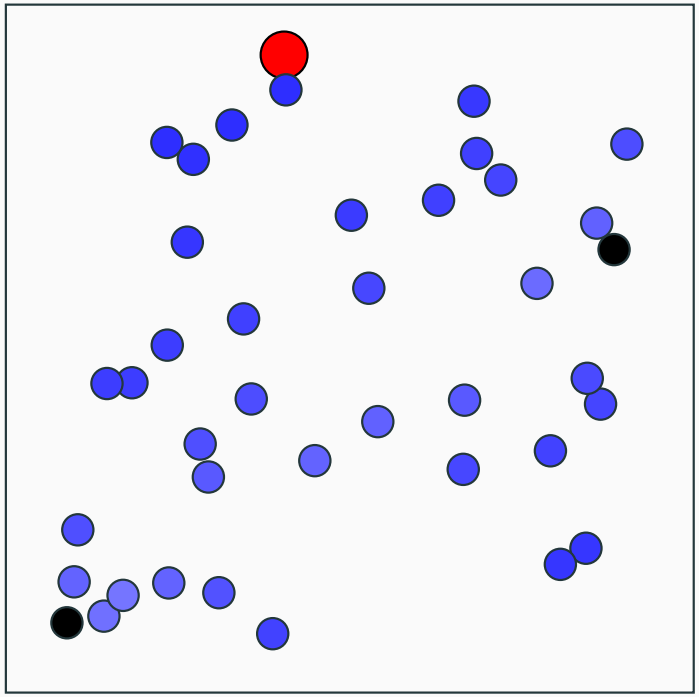

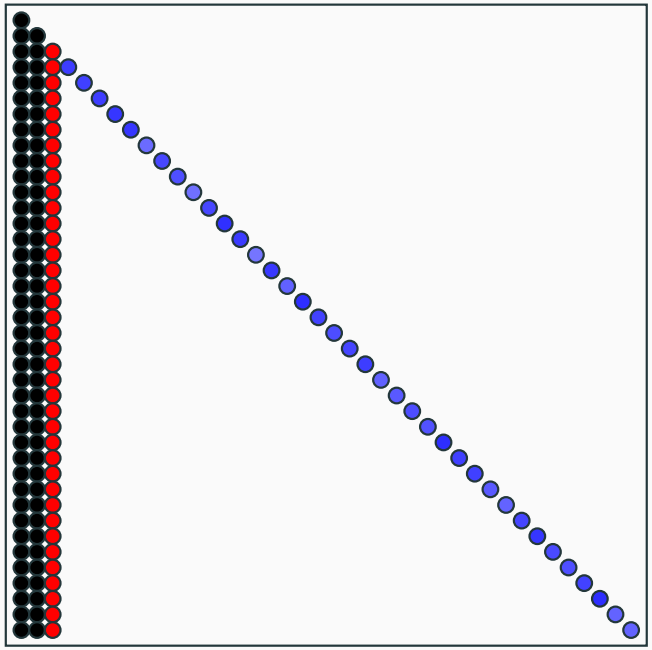

Diagonal element: 1.91e-02

Choosing points

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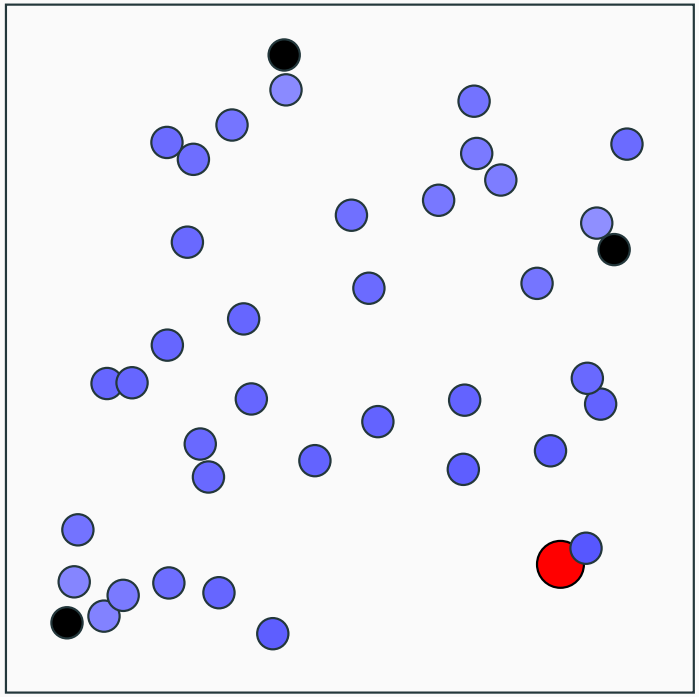

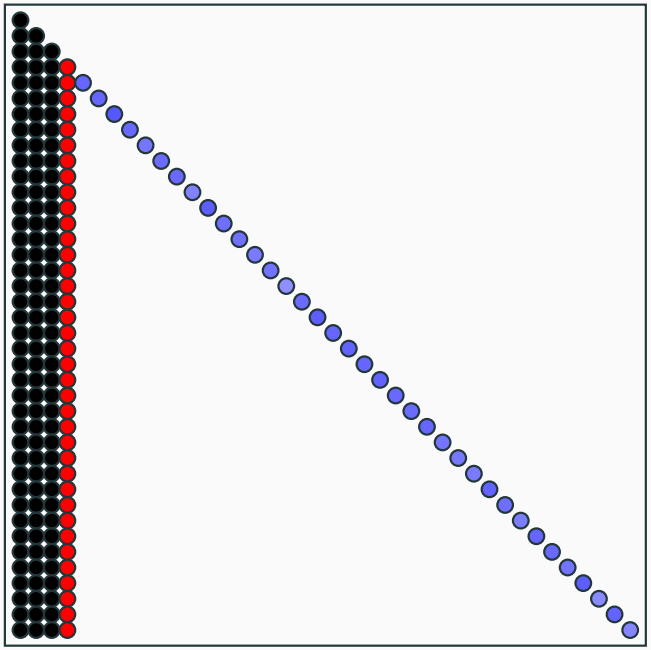

Diagonal element: 5.11e-04

Choosing points

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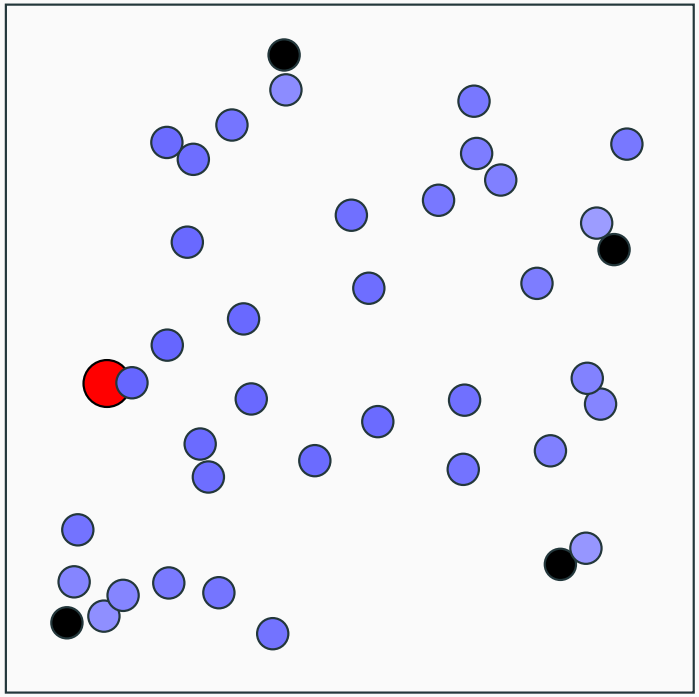

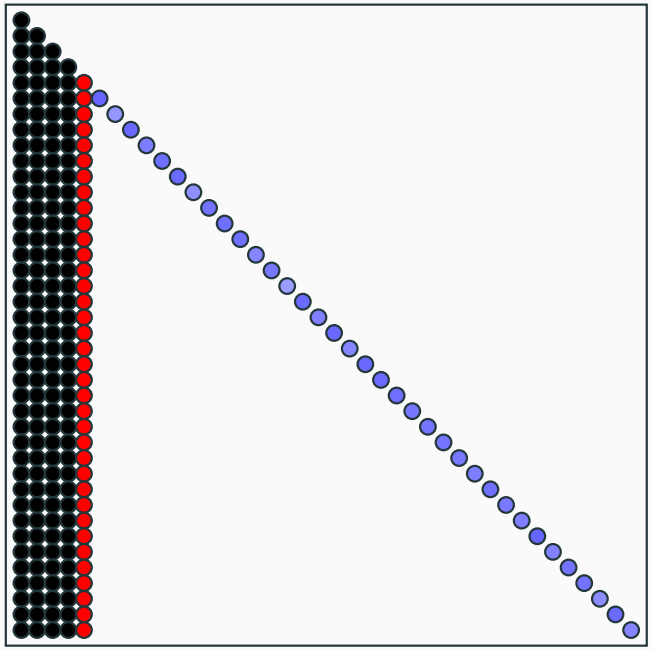

Diagonal element: 1.19e-04

Choosing points

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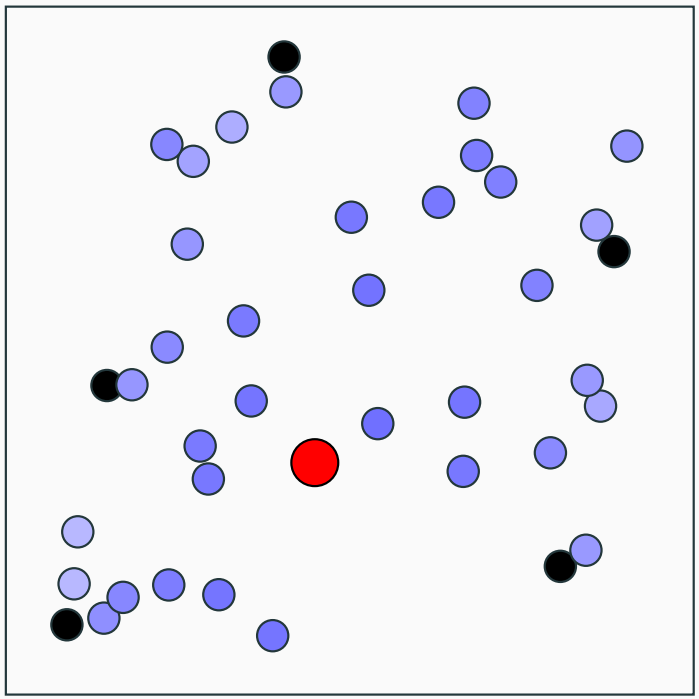
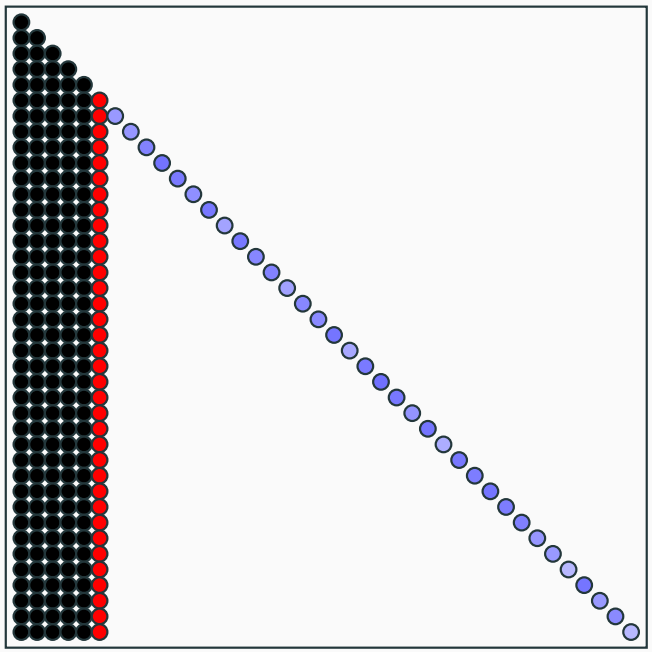
Left-looking partial pivoted Cholesky





Diagonal element: 4.18e-05

Choosing points

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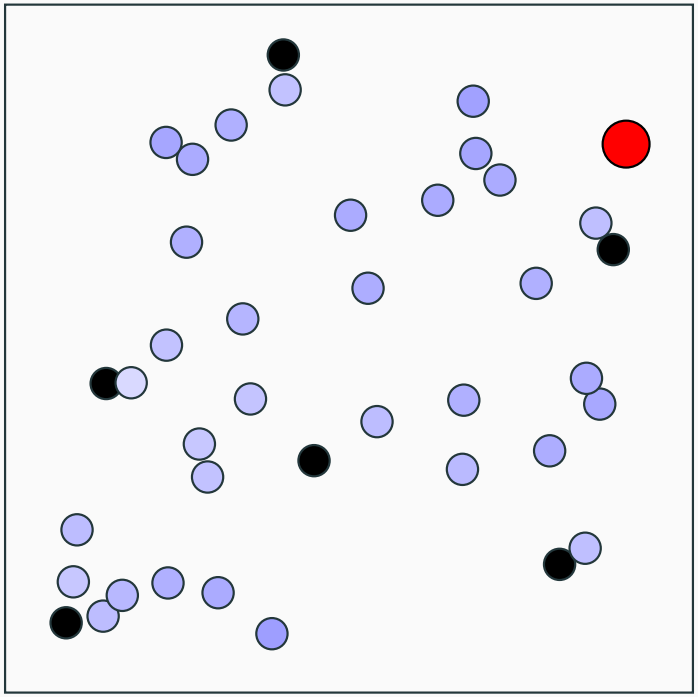

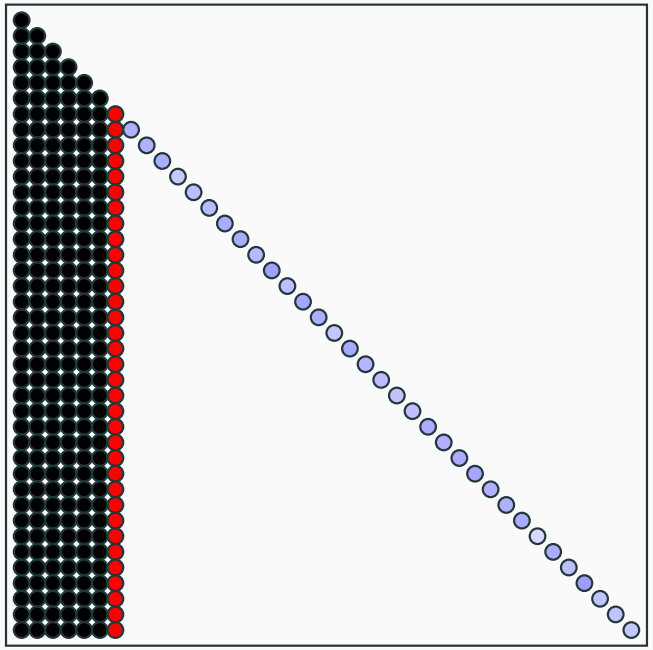

Diagonal element: 8.54e-07

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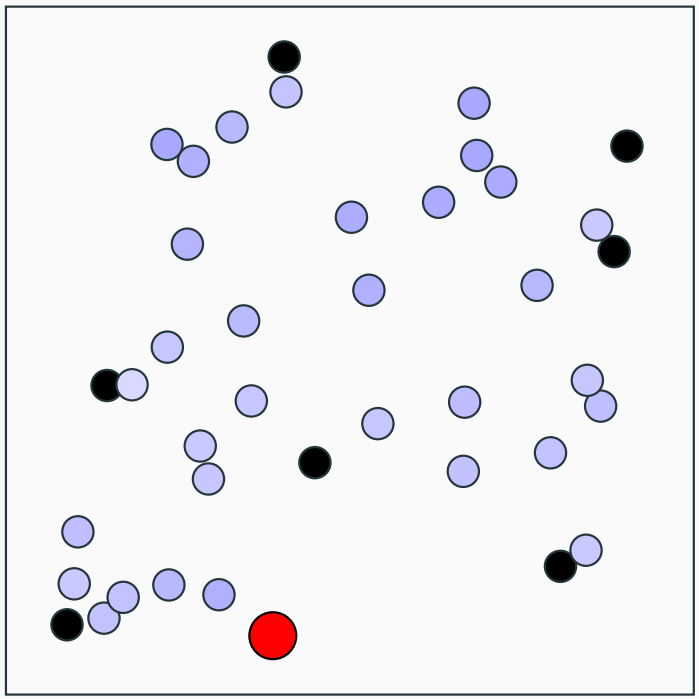

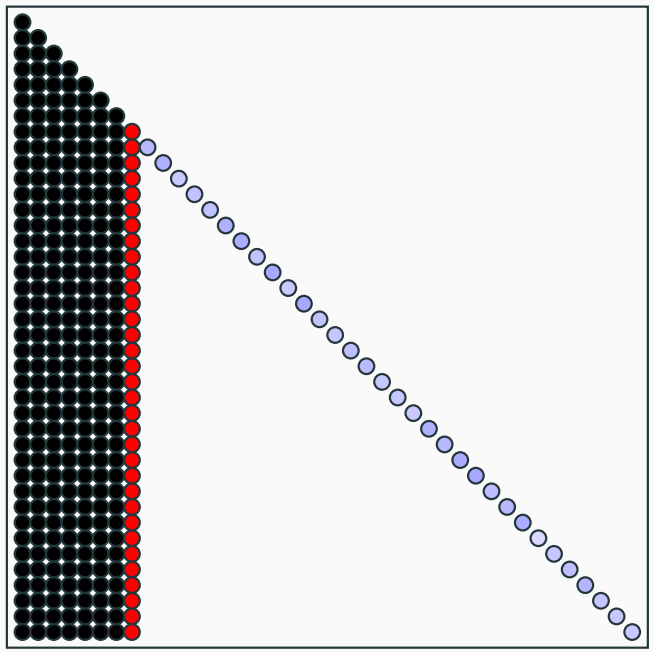

Diagonal element: 3.58e-07

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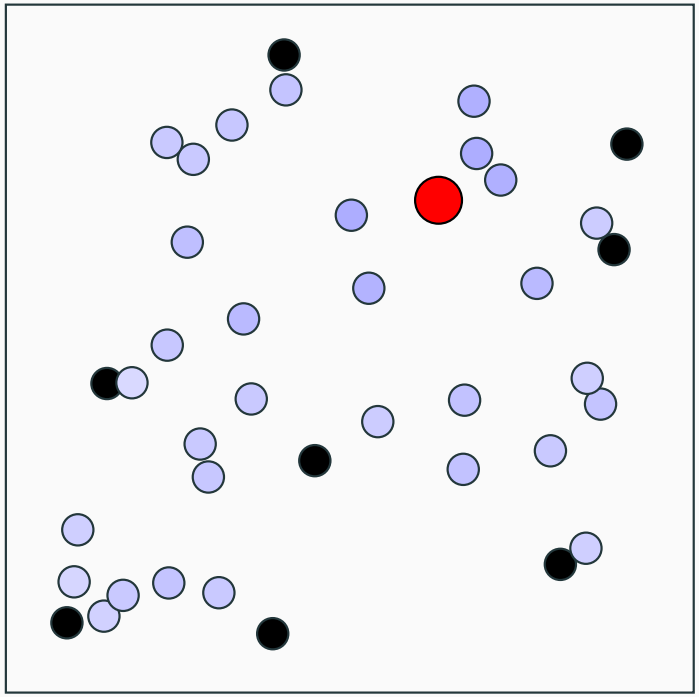
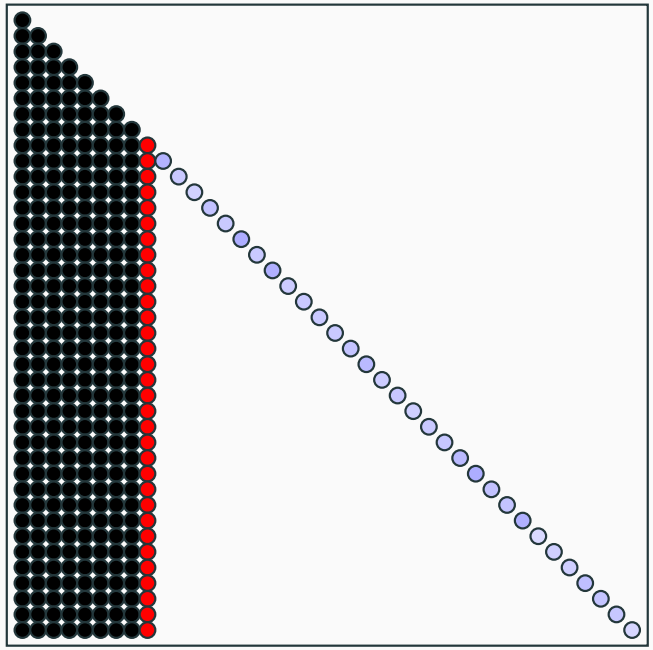
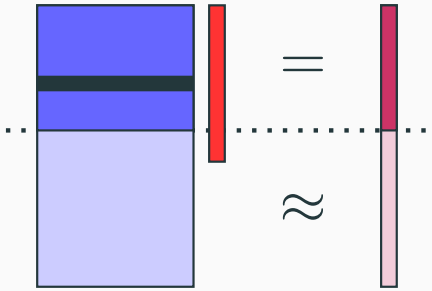




Diagonal element: 1.92e-07

Kernel-Based Regression: Four Stories

Feature map



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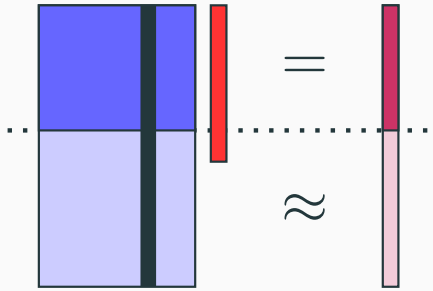

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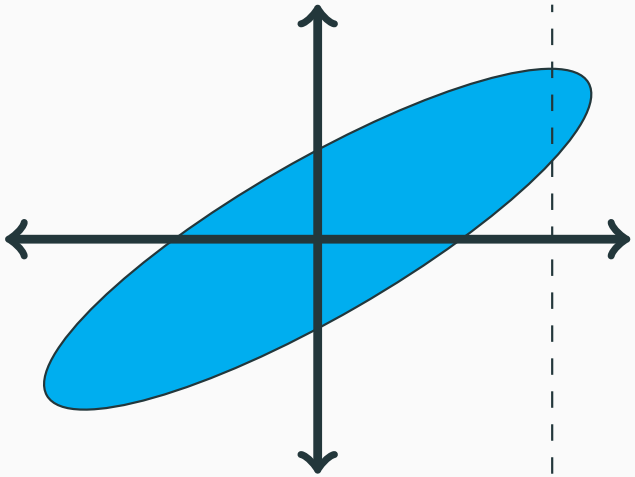
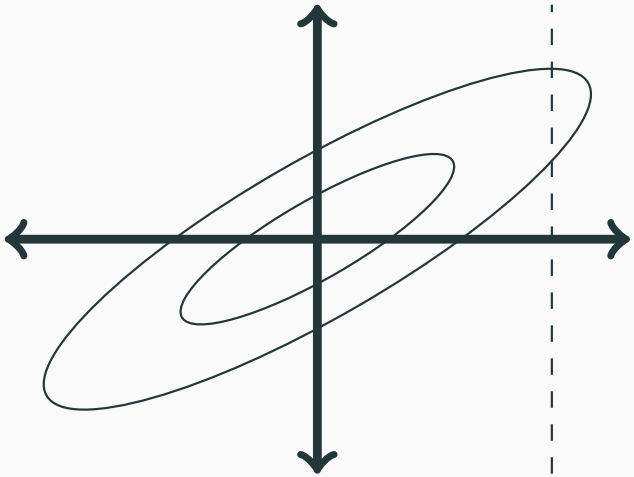


Gaussian process



From Kernels to Inner Products

To build RKHS without an explicit feature map:

- Observe that $\langle k_x, k_y \rangle_{\mathcal{H}} = k(x, y)$
- For $u(x) = \sum_{i=1}^{N} c_i k(x_i, x)$ and $v(x) = \sum_{i=1}^{N} d_i k(x_i, x)$, have

$$\langle u, v \rangle_{\mathcal{H}} = \left\langle \sum_i c_i k_{x_i}, \sum_j d_j k_{x_j} \right\rangle_{\mathcal{H}} = \sum_{i,j} c_i k(x_i, x_j) d_j = d^T K_{XX} c.$$

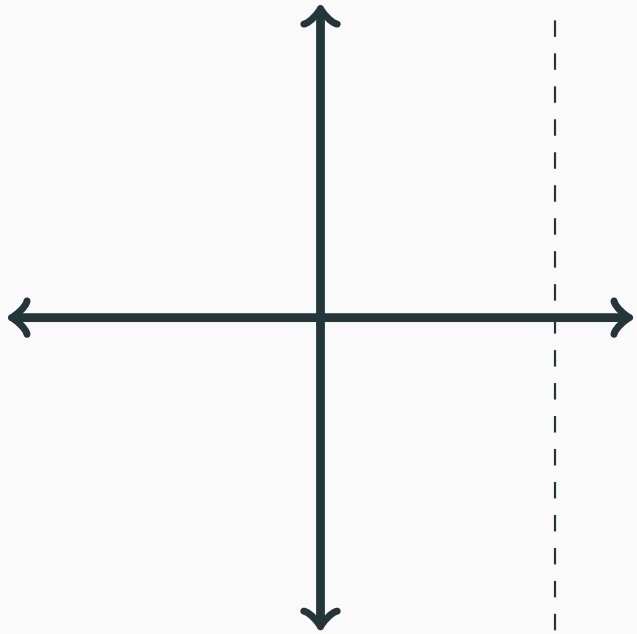
  Note:

$$\langle u, v \rangle_{\mathcal{H}} = v_X^T K_{XX}^{-1} u_X$$

- Gives pre-Hilbert structure, close to get Hilbert space.

How to reason about approximation error in terms of K_{XX}?

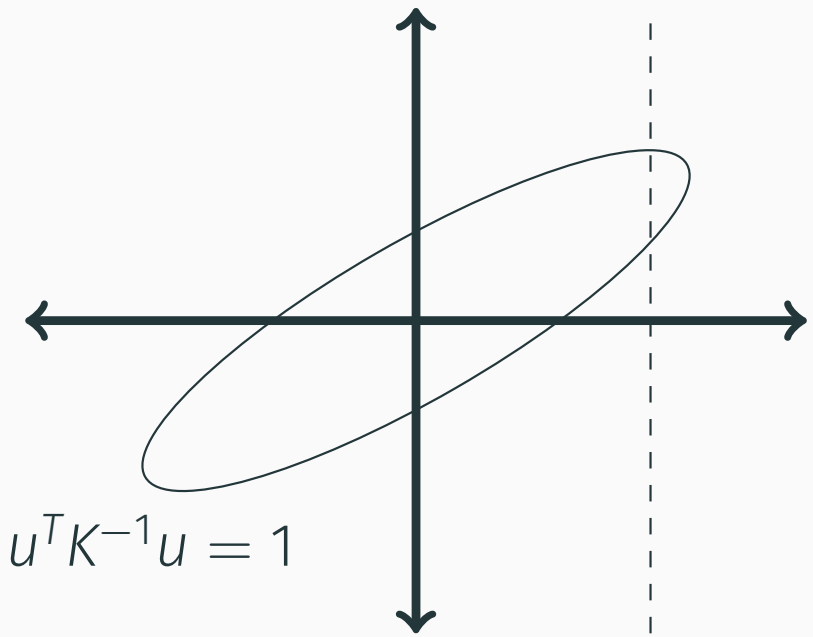
Simple and Impossible



Let $u = (u_1, u_2)$ (think $(f_X, f_{X'})$). Given u_1, what is u_2?

We need an assumption!

Being Bayesian



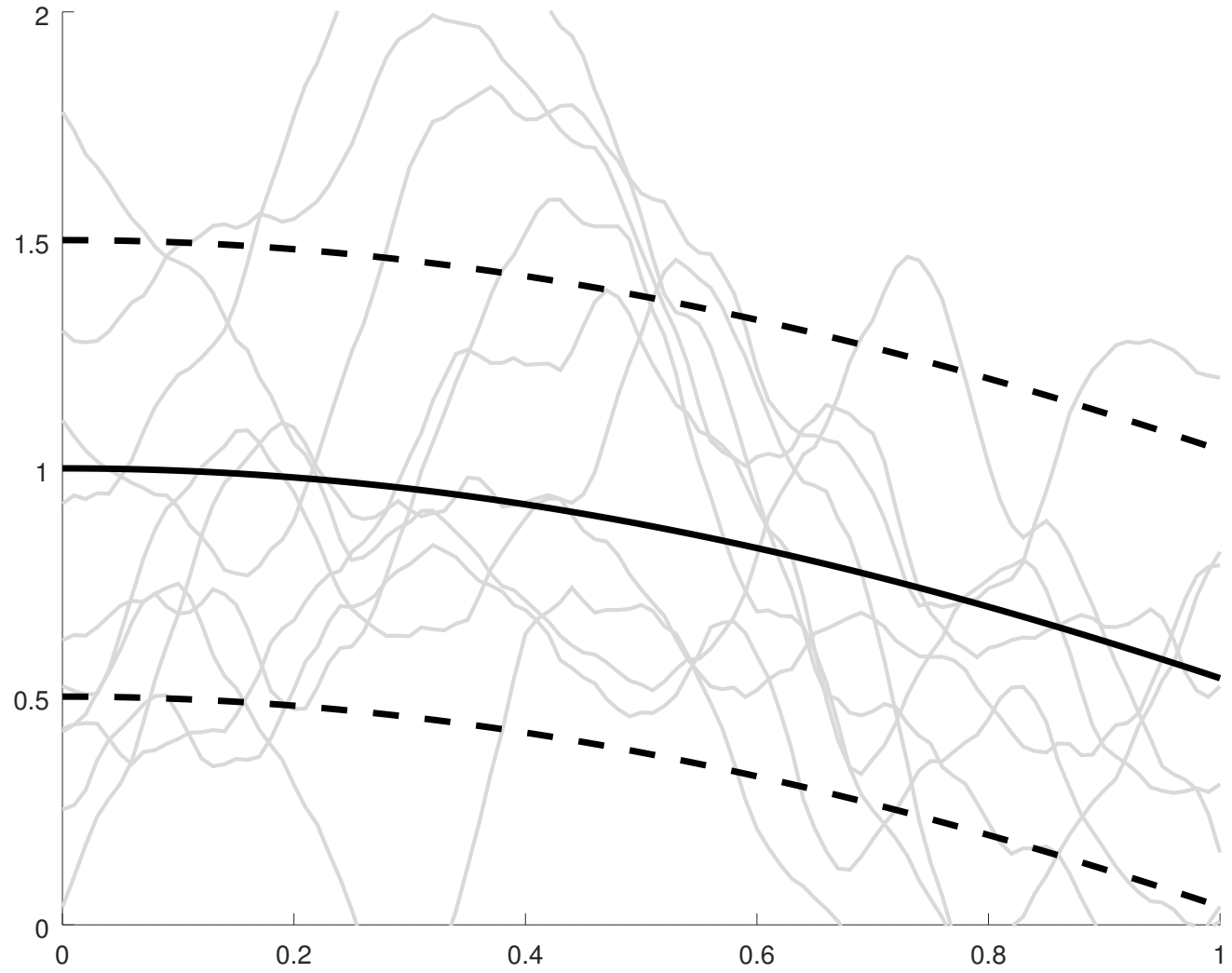
Let $U = (U_1, U_2) \sim N(0, K)$. Given $U_1 = u_1$, what is U_2?

Posterior distribution: $(U_2 | U_1 = u_1) \sim N(w, S)$ where

$$w = K_{21} K_{11}^{-1} u_1$$

$$S = K_{22} - K_{21} K_{11}^{-1} K_{12}$$

Basic ingredient: Gaussian Processes (GPs)



Basic ingredient: Gaussian Processes (GPs)

Our favorite continuous distributions over

$$\begin{array}{lll} \mathbb{R}: & \text{Normal}(\mu, \sigma^2), & \mu, \sigma^2 \in \mathbb{R} \\ \mathbb{R}^n: & \text{Normal}(\mu, C), & \mu \in \mathbb{R}^n, C \in \mathbb{R}^{n \times n} \\ \mathbb{R}^d \to \mathbb{R}: & \text{GP}(\mu, k), & \mu : \mathbb{R}^d \to \mathbb{R},\ k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R} \end{array}$$

More technically, define GPs by looking at finite sets of points:

$$\begin{aligned} \forall X = (x_1, \ldots, x_n),\ x_i \in \mathbb{R}^d, & \\ \text{have } f_X \sim N(\mu_X, K_{XX}), & \text{ where} \\ f_X \in \mathbb{R}^n, \quad & (f_X)_i \equiv f(x_i) \\ \mu_X \in \mathbb{R}^n, \quad & (\mu_X)_i \equiv \mu(x_i) \\ K_{XX} \in \mathbb{R}^{n \times n}, \quad & (K_{XX})_{ij} \equiv k(x_i, x_j) \end{aligned}$$

Being Bayesian

Consider a (zero-mean) GP prior with kernel k:

$$f \sim \mathrm{GP}(0, k)$$

Measure at X, apply Bayes to get posterior:

$$(f \mid f_X = y) \sim \mathrm{GP}(\mu, \tilde{k})$$

where

$$\begin{aligned} \mu(x) &= k_{xX} c \\ \tilde{k}(x, y) &= k(x, x) - k_{xX} K_{XX}^{-1} k_{Xy} \end{aligned}$$

Specifically, posterior for $f(x)$ at given x is

$$N(k_{xX} c, k(x, x) - k_{xX} K_{XX}^{-1} k_{Xx})$$

Sparse GPs and variational inference

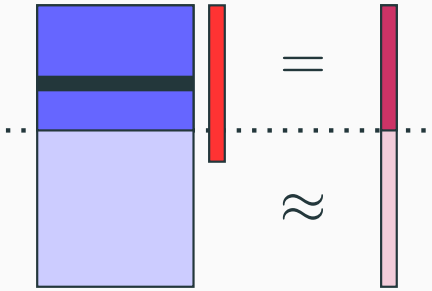
Idea:

- Take a Bayesian perspective – want to approximate the posterior distribution conditioned on observations.
- As approximating family, consider GP conditioned on inducing values at inducing locations ($U \not\subset X$).
- Maximize the evidence lower bound (ELBO) / minimize the KL divergence between the approximating GP and the true posterior.

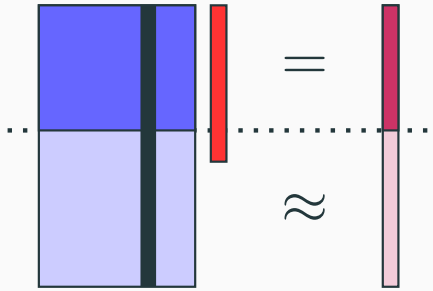
Optimization via SGD variants. Several variations on this. Also useful with non-Gaussian likelihoods.

Kernel-Based Regression: Four Stories

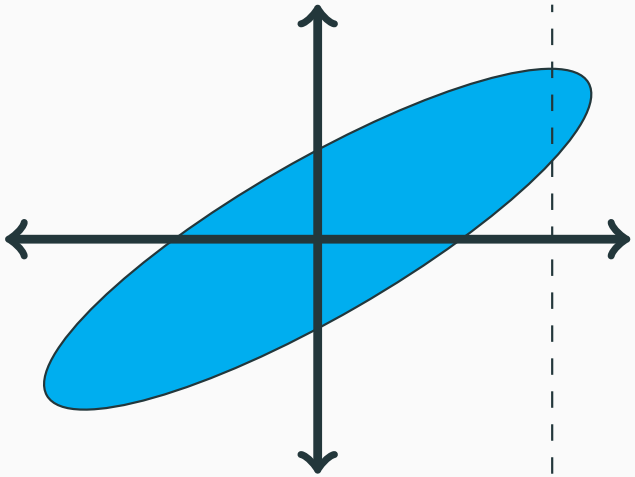
Feature map



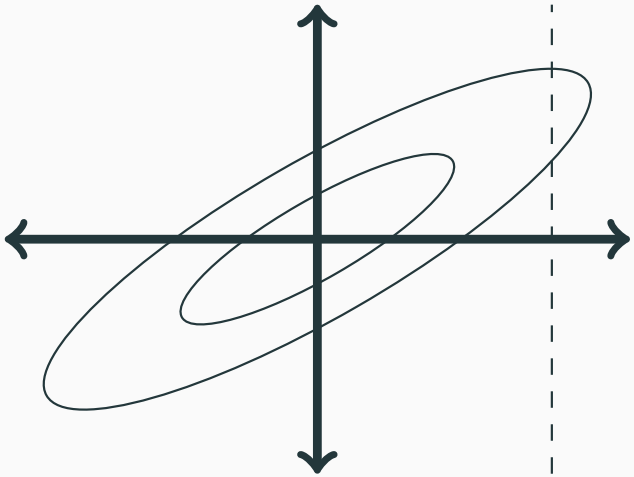
Data-dependent basis



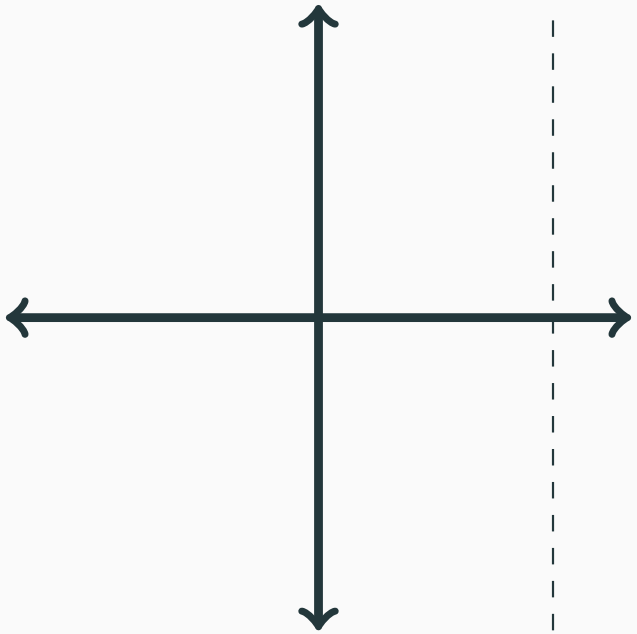
Energy minimization



Gaussian process



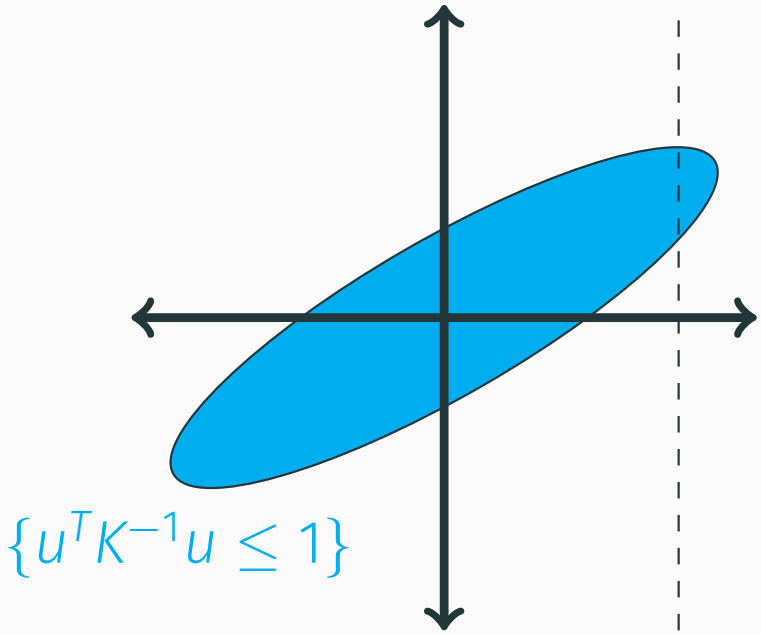
Simple and Impossible



Let $u = (u_1, u_2)$ (think $(f_X, f_{X'})$). Given u_1, what is u_2?

We need an assumption!

Being Bounded



Let $u = (u_1, u_2)$ s.t. $\|u\|^2_{K^{-1}} \leq 1$. Given u_1, what is u_2?

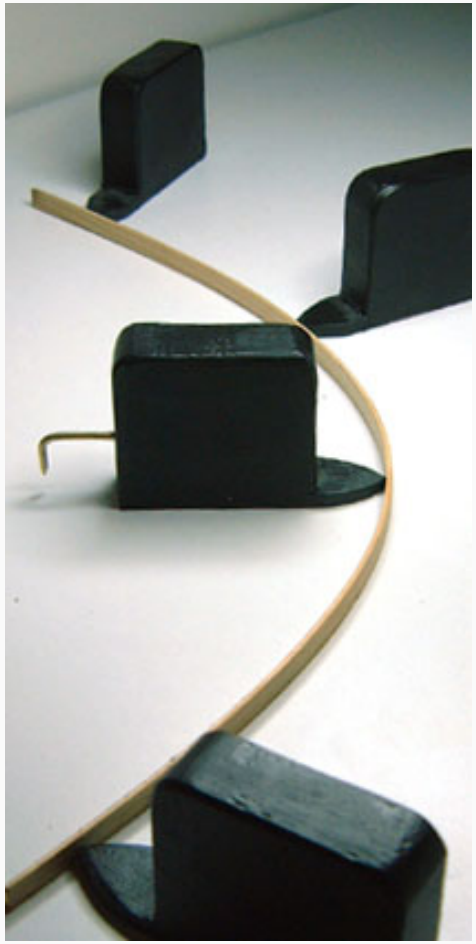
Optimal recovery: $\|u_2 - w\|^2_{S^{-1}} \leq 1 - \|u_1\|^2_{(K_{11})^{-1}}$

$$w = K_{21} K_{11}^{-1} u_1$$

$$S = K_{22} - K_{21} K_{11}^{-1} K_{12}$$

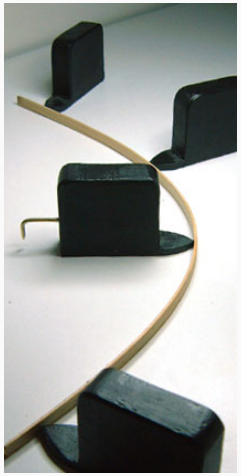
Minimizes $\|u\|_{K^{-1}}$ subject to data constraints.

From Energy to Error



http://www.duckworksmagazine.com/03/r/articles/splineducks/splineDucks.htm

Cubic Splines



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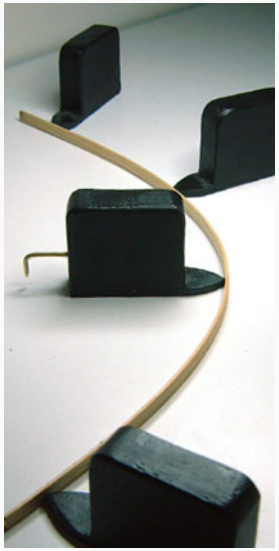
- $\phi(r) = r^3$ is conditionally positive definite of order 2
- Squared (semi-)norm is bending energy:

$$\|s\|_{\mathcal{H}}^2 \propto \frac{1}{2} \int_{\Omega} s''(x)^2 \, dx$$

- Linear polynomial tail = rigid body modes

Force, Displacement, Stiffness



Target function $f \in \mathcal{H}^2$, known bending energy

$$E[f] = \frac{1}{2} \int_\Omega f''(x)^2 \, dx$$

Cubic spline minimizes $E[s]$ s.t. $s(x_i) = f(x_i)$, so

$$E[s] \leq E[f]$$

- $f(x_i)$ as displacement, c_i as corresponding force
- Kernel matrix K_{XX} is compliance (force $\mapsto$ displacement)
- Residual compliance (inverse stiffness) at x is $P_X(x)^{-2}$
- Energy bound for error at X

$$P_X(x)^{-2} \left(s(x) - f(x)\right)^2 \leq E[f] - E[s]$$

General Picture

Interpolant is

$$s(x) = K_{xX}c + b(x)^T\lambda$$

Can compute *power function* $P_X(x)$ from factorization; SPD case:

$$P_X(x)^2 = \phi(0) - K_{xX}K_{XX}^{-1}K_{Xx}$$

Bound is

$$|s(x) - f(x)| \leq P_X(x)\sqrt{\|f\|_{\mathcal{H}}^2 - \|s\|_{\mathcal{H}}^2}$$

Only thing that is hard to compute generally: $\|f\|_{\mathcal{H}}^2$.

Beyond optimal recovery

Optimal recovery perspective on kernel interpolation:

$$\text{minimize } \|s\|_{\mathcal{H}}^2 \text{ s.t. } s_X = f_X$$

Representer theorem says kernel interpolator is the minimizer.

What if we relax interpolation?

$$\text{minimize } \|s\|_{\mathcal{H}}^2 \text{ s.t. } \|s_X - f_X\|_\infty \leq \epsilon$$

Variation on representer theorem: solution is a kernel approximation with a subset of points X.

Incorporating bounds

Continuous problem:

$$\text{minimize } \|s\|_{\mathcal{H}}^2 \text{ s.t. } \|s_X - f_X\|_\infty \leq \epsilon$$

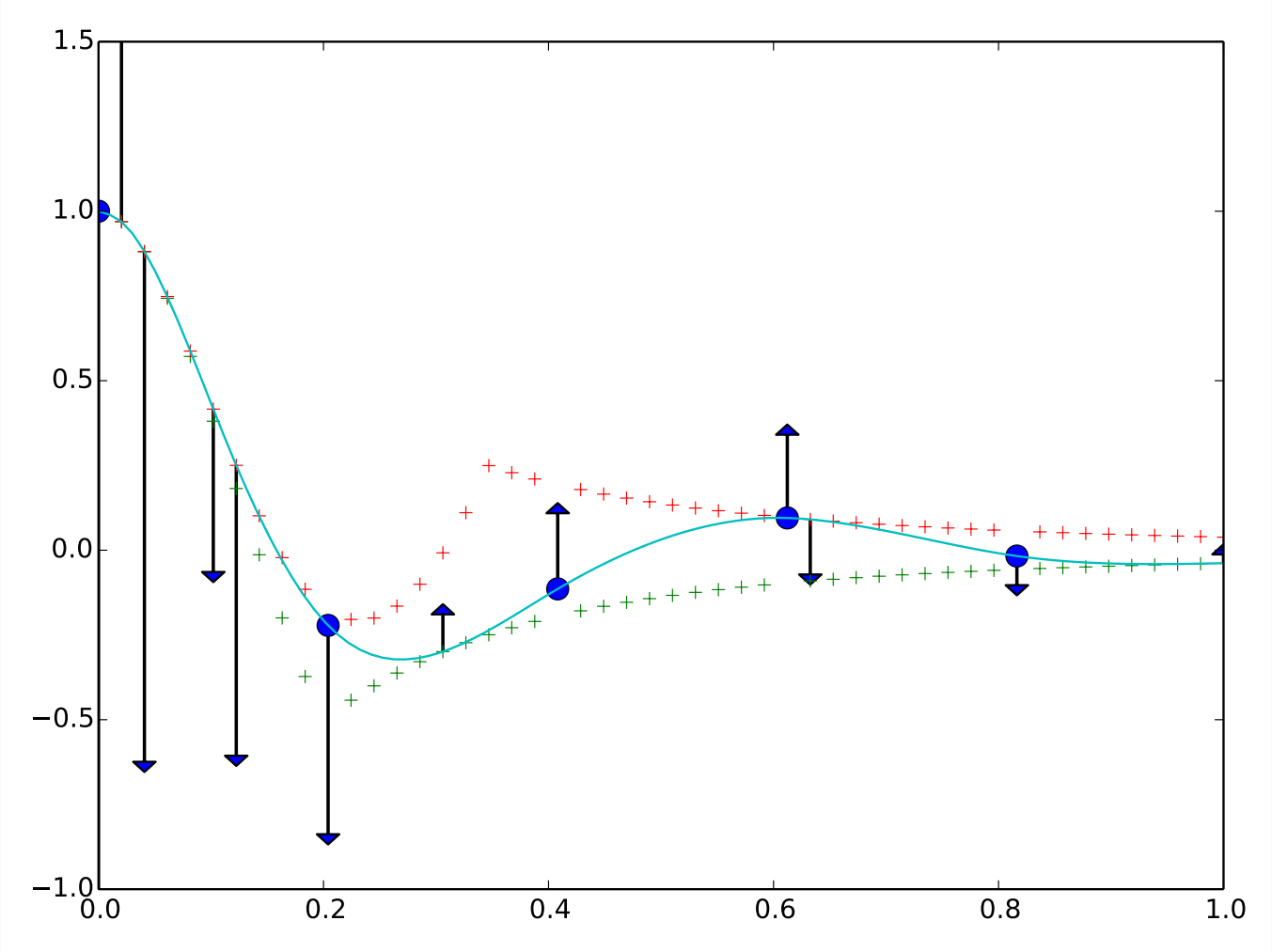
Becomes a nice quadratic program

$$\text{minimize } s_X^T K_{XX}^{-1} s_X \text{ s.t. } \|s_X - f_X\|_\infty \leq \epsilon.$$

Generalize to $\ell \leq s_X \leq u$; KKT conditions: $K_{XX}c = s_X$,

$$\begin{aligned} s(x_i) = \ell_i &\implies c_i \geq 0 \\ s(x_i) = u_i &\implies c_i \leq 0 \\ \ell_i < s(x_i) < u_i &\implies c_i' = 0. \end{aligned}$$

Incorporating bounds



Why do this?

- Has an adjustable cost/accuracy knob
- No local minimizers (problem for VI methods)
- Can build on standard RBF error bounds

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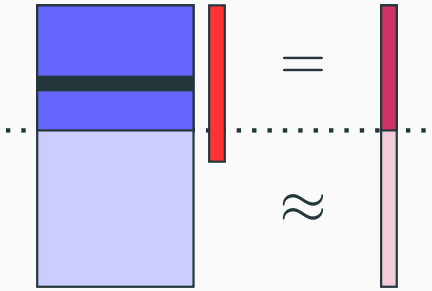

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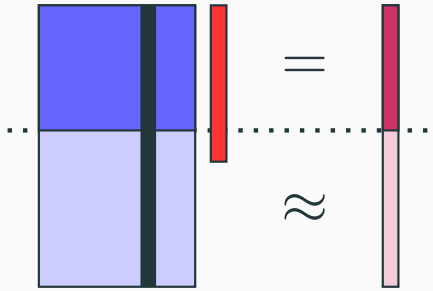

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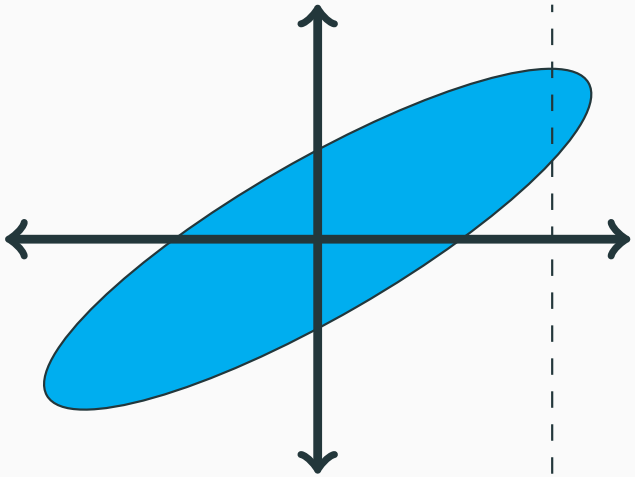

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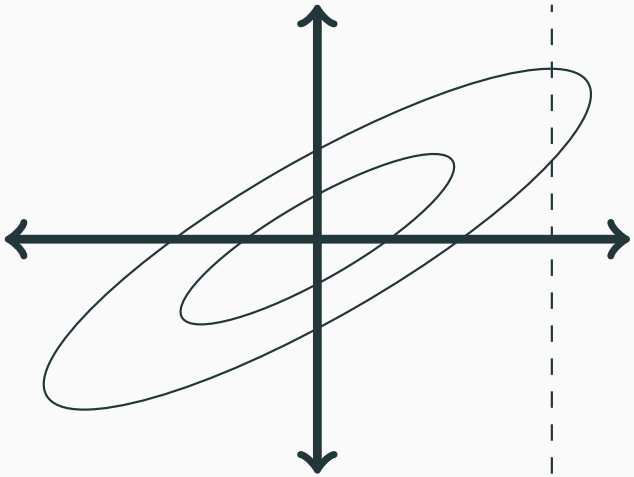

Summary

Three flavors of inducing point methods from three different perspectives:

- **Matrix perspective**: Diagonal + low-rank approximation of the kernel matrix. Use alone or as a preconditioner.
- **Bayesian variational inference**: Use inducing points (and values) to define a candidate family. Maximize the evidence lower bound over that family / minimize KL divergence to true posterior.
- **Optimization perspective**: Inducing points arise naturally from minimizing norm subject to inequality bounds (vs subject to interpolation constraints).

Unlike interpolation, get *fundamentally different* methods from these perspectives.