Scalable algorithms for kernel-based surrogates in prediction and optimization

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Because Shoemaker spoke first...

Surrogate optimization idea:

- Goal: minimize f
- Know some information (e.g. $f(x_1), \ldots, f(x_n)$)
- Fit an approximation $\hat{f}$ to guide next sample

See:

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https://github.com/dme65/pySOT
https://github.com/dbindel/POAP
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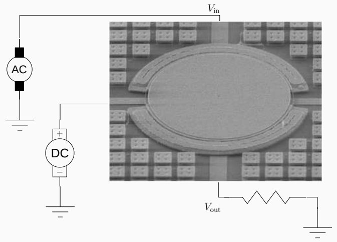
... and that is all I will say about surrogate optimization!

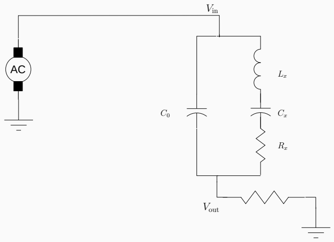
My background

- Formal training: numerical analysis at CS/math border
- Research "home base": numerical linear algebra
    - With applications from engineering and CS
    - Projections into optimization, approximation theory, HPC
- Most weeks, this means:

CG	=	Conjugate Gradients
DFT	=	Discrete Fourier Transform
LDA	=	Latent Dirichlet Allocation

My background: compact models / model reduction





Compact modeling: PDE device model $\rightarrow$ small ODE model

- May involve reduced theory
  - Solid $\rightarrow$ beam and plate theory
  - Reaction-diffusion $\rightarrow$ CSTR
  - Maxwell $\rightarrow$ basic circuit elements
- Or automated model reduction (computer driven)
- Or phenomenological (e.g. most transistor models)

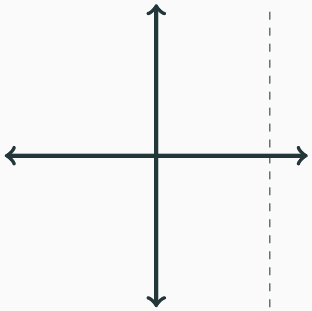
Desiderata

What makes a good reduced model depends on application:

- High accuracy
    - May not require uniform error bounds
    - May want an error indicator
- Good numerical stability
    - Careful bias/variance tradeoff
    - Regularization matters!
- Low computational expense
    - Set up fit in reasonable time?
    - More stringent demands on evaluation time
- Composability ($\implies$ structural constraints)
- Parameterized behavior

Goal today: Address first few points for kernel methods

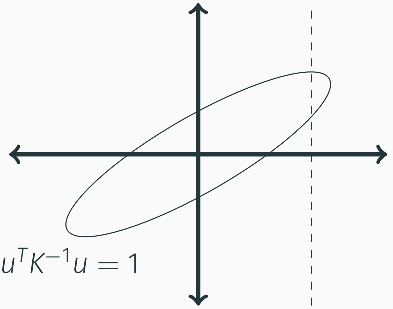
Simple and impossible



Let $u = (u_1, u_2)$. Given u_1, what is u_2?

We need an assumption! Two different standard takes.

Being Bayesian



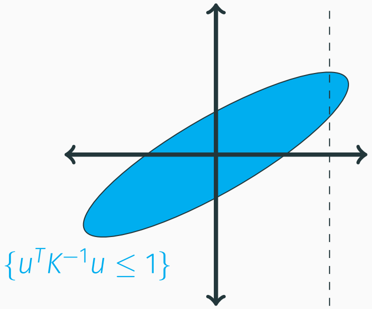
Let $U = (U_1, U_2) \sim N(0, K)$. Given $U_1 = u_1$, what is U_2?

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

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

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

Being bounded



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

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

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

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

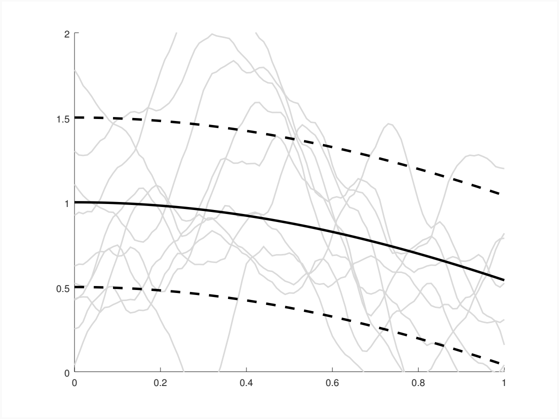
Tomato, tomato

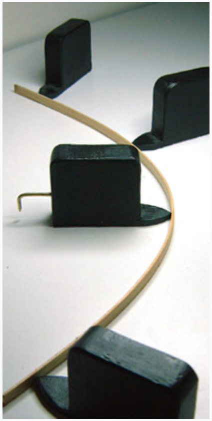
Both cases: K plays a similar fundamental role

- Predictor minimizes $\|u\|^2_{K^{-1}}$ subject to data
- Extends beyond knowing values – OK if data is any $l^* u$
- Schur complement central to error estimates

But error interpretation is very different!

Basic ingredients





Survey: Schaback and Wendland, Acta Numerica (2006)

Gaussian Processes (GPs)

Our favorite continuous distributions over

$\mathbb{R}$:	Normal(μ, σ^2),	$\mu, \sigma^2 \in \mathbb{R}$
$\mathbb{R}^n$:	Normal(μ, C),	$\mu \in \mathbb{R}^n, C \in \mathbb{R}^{n \times n}$
$\mathbb{R}^d \to \mathbb{R}$:	GP(μ, k),	$\mu : \mathbb{R}^d \to \mathbb{R}$, $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$

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

$$\forall X = (x_1, \ldots, x_n),\, x_i \in \mathbb{R}^d,$$

$$\text{have } f_X \sim N(\mu_X, K_{XX}), \text{ where}$$

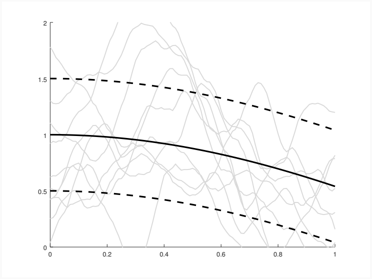
$$f_X \in \mathbb{R}^n, \quad (f_X)_i \equiv f(x_i)$$

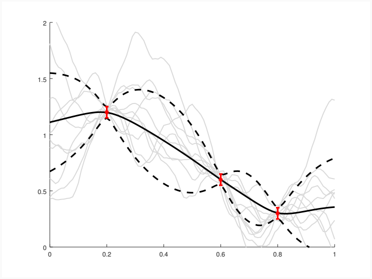
$$\mu_X \in \mathbb{R}^n, \quad (\mu_X)_i \equiv \mu(x_i)$$

$$K_{XX} \in \mathbb{R}^{n \times n}, \quad (K_{XX})_{ij} \equiv k(x_i, x_j)$$

When X is unambiguous, we will sometimes just write K.

Bayesian inference





Prior: $f \sim \mathrm{GP}(\mu, k)$, noisy measurements

$$f_X \sim y + \epsilon, \quad \epsilon \sim N(0, W), \qquad \text{typically } W = \sigma^2 I$$

Posterior: $f \sim \mathrm{GP}(\mu', k')$ with

$$\mu'(x) = \mu(x) + K_{xX} c \qquad \tilde{K} = K_{XX} + W$$

$$k'(x, x') = K_{xx'} - K_{xX} \tilde{K}^{-1} K_{Xx'} \qquad c = \tilde{K}^{-1}(y - \mu_X)$$

Cubic splines

Minimize bending energy

$$\mathcal{E}(u) = \int_\Omega |u''|^2 \, dx$$

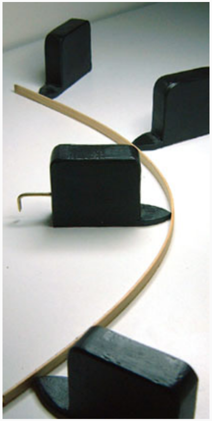
subject to constraints. Write solution as

$$s(x) = \sum_{j=1}^{n} c_j |x - x_j|^3 + a_1 x + a_2$$

where

$$\begin{bmatrix} K & P \\ P^T & 0 \end{bmatrix} \begin{bmatrix} c \\ a \end{bmatrix} = \begin{bmatrix} f_X \\ 0 \end{bmatrix}$$

with $K_{ij} = |x_i - x_j|^3$, $P_{1i} = x_i$, $P_{2i} = 1$.



Interpret: f_X is displacements, c is forces, $c^T K c$ as energy.
“Native space” $\mathcal{H}^2(\Omega)$ of functions where energy makes sense.

Beyond cubic splines

- Define a native space (a RKHS) via kernel
    - Start with kernel $k(x, \cdot)$
    - Interpolants are linear combinations of kernels
    - Native space is closure of space of all interpolants
- Interpolation: minimize $|s|^2$ s.t. $s_X = y$
- Smoothing: minimize $\|s_X - y\|^2 + \lambda |s|^2$
- Smoothing spline $\equiv$ noisy GP

Kernels?

What is a kernel function $k(x, y)$?

- A useful basis function for interpolation
- A Green's function for a PDE (for polyharmonic splines)
- An inner product in a feature space: $k(x, y) = \langle \phi(x), \phi(y) \rangle$
- A covariance function
- A reproducing kernel in a certain RKHS

Choose whichever makes you happy...

Kernel properties

For variational interp, need:

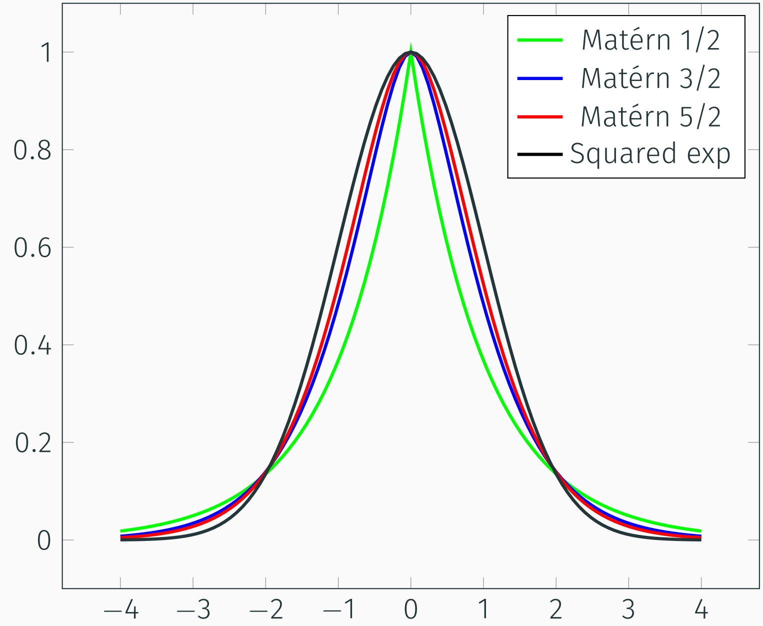
- **Pos def**: need K_{XX} positive definite *or*
- **Conditional pos def**: $c^T K_{XX} c > 0$ for $c \neq 0$ and $P^T c = 0$

Often desirable:

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

Radial basis function is both (sloppy notation: $k = k(r)$).

Matérn and SE kernels



Kernels and tails

A few ways to let physics inform kernel approximation:

- Less smooth kernels for less regular functions.
- Can always symmetrize kernel; for symmetry group G:

$$k^{\text{sym}}(x, y) = \frac{1}{|G|} \sum_{Q \in G} k(Qx, Qy)$$

- Can include known singularities in a tail term:

$$f(x) \approx \sum_{j=1}^{n} c_k k(x, x_k) + B(x)a$$

  where B is a basis for an extra space (polynomial or other).
- Can symmetrize the tail as well.

Observations on kernel matrices

Kernel is *chosen by modeler*

- Choose Matérn / SE for regularity and simplicity
- Rarely have the intuition to pick the "right" kernel
- Common choices are *universal* — can recover anything
  - … though with less data for a "good" choice
- Universality may not be needed for all kernels…

Properties of kernel matrices:

- Positive definite by design, but not well conditioned!
- Weyl: $k(r) \in C^\nu \implies |\lambda_n| = o(n^{-\nu-1/2})$
- SE case: eigenvalues decay exponentially
- Adding $\sigma^2 I$ "wipes out" small eigenvalues

Hyper-parameter MLE

How to estimate hyper-parameters (i.e. ℓ and s_f, σ^2)? Recall

$$f(y) = \frac{1}{\sqrt{\det(2\pi \tilde{K}_{XX})}} \exp\left(-\frac{1}{2} u^T \tilde{K}_{XX}^{-1} u\right)$$

Log-likelihood function for kernel hypers θ

$$\mathcal{L}(\theta|y) = \mathcal{L}_y + \mathcal{L}_{|K|} - \frac{n}{2}\log(2\pi)$$

where (again with $c = \tilde{K}^{-1}(y - \mu_X)$)

$$\mathcal{L}_y = -\frac{1}{2}(y - \mu_X)^T c, \qquad \frac{\partial \mathcal{L}_y}{\partial \theta_i} = \frac{1}{2} c^T \left(\frac{\partial \tilde{K}}{\partial \theta_i}\right) c$$

$$\mathcal{L}_{|K|} = -\frac{1}{2}\log\det\tilde{K}, \qquad \frac{\partial \mathcal{L}_{|K|}}{\partial \theta_i} = -\frac{1}{2}\operatorname{tr}\left(\tilde{K}^{-1}\frac{\partial \tilde{K}}{\partial \theta_i}\right)$$

Scalability bottlenecks

Consider n data points

- Straightforward regression: factor $\tilde{K}$ at $O(n^3)$ cost
- Kernel hyper MLE requires multiple $O(n^3)$ ops
  - To compute $\log\det\tilde{K}$ is $O(n^3)$ per step
  - To compute $\operatorname{tr}\left(\tilde{K}^{-1}\frac{\partial\tilde{K}}{\partial\theta_i}\right)$ is $O(n^3)$ per hyper per step
- GCV has similar costs (see Golub, Heath, Wahba 1979)

Two possible work-arounds

- Data-sparse factorization methods
- Methods that avoid factorization (e.g. iterative solvers)
  - Q: how to handle determinants and traces?

Today: The second approach.

Basic ingredients

- Fast MVMs with kernel matrices
- Krylov methods for linear solves and matrix functions
- Stochastic estimators: trace, diagonal, and other

Kernel approximations

Goal: Fast matrix-vector multiplication

- Low-rank approximation
  - Often phrased via *inducing points*
  - Non-smooth kernels, small length scales $\implies$ large rank
  - Only semi-definite
- Sparse approximation
  - OK with SE kernels and short length scales
  - Less good with heavy tails or long length scales
  - May again lose definiteness
- More sophisticated: fast multipole, Fourier transforms
  - Same picture as in integral eq world (FMM, PFFT)
  - Main restriction: low dimensional spaces (2-3D)
  - But... this really means “near” vs “far”
- Kernel a model choice — how does approx affect results?

Example: Structured Kernel Interpolation (SKI)

Write $K_{XX} \approx W^T K_{UU} W$ where

- U is a uniform mesh of m points (m not always small)
- Sparse W interpolates values from X to U
- K_{UU} has Toeplitz or block Toeplitz structure

Apply K_{UU} via FFTs in $O(m \log m)$ time.

The power of fast MVMs

Fast MVM with symmetric $\tilde{K} \implies$ try Lanczos!

- Incrementally computes $\tilde{K}Q = QT$ where
  - Q has orthonormal columns
  - Leading k columns span k-dim Krylov space
  - T is tridiagonal
- Building block for
  - Solving linear systems (CG)
  - Approximating eigenvalues
  - Approximating matrix functions: $f(\tilde{K})b$
  - Quadrature vs spectral measure for $\tilde{K}$
- Fast (three-term recurrence) and elegant...
- ... but not forward stable in finite precision

Function application via Lanczos

A computational kernel: $f(\tilde{K})b$

- Run Lanczos from starting vector $b/\|b\|$
- At n steps in exact arithmetic,

$$f(\tilde{K})b = Qf(T)Q^T b = \|b\|Qf(T)e_1$$

- Truncate at $k \ll n$ steps, use

$$f(\tilde{K})b \approx \|b\|Q_1 f(T_{11})e_1$$

- Error analysis hinges on quality of poly approx

$$\min_{f \in P_k} \max_{\lambda \in \Lambda(\tilde{K})} |f(\lambda) - \hat{f}(\lambda)|$$

- Compare: Chebyshev methods just use $[\lambda_{\min}, \lambda_{\max}]$

CG is a special case corresponding to $f(z) = z^{-1}$.

Tractable traces

CG solves systems with $\tilde{K}$; problem terms are

$$\mathcal{L}_{|K|} = -\frac{1}{2}\,\mathrm{tr}\left(\log \tilde{K}\right) \qquad \frac{\partial \mathcal{L}_{|K|}}{\partial \theta_i} = -\frac{1}{2}\,\mathrm{tr}\left(\tilde{K}^{-1}\frac{\partial \tilde{K}}{\partial \theta_i}\right)$$

Q: How do we parley fast MVMs into trace computations?

Tractable traces

Stochastic trace estimation trick:

- $z \in \mathbb{R}^n$ has independent random entries
- $\mathbb{E}[z_i] = 0$ and $\mathbb{E}[z_i^2] = 1$

Then

$$\mathbb{E}[z^T A z] = \sum_{i,j} a_{ij} \mathbb{E}[z_i z_j] = \operatorname{tr}(A).$$

NB: $\mathbb{E}[z \odot Az] = \operatorname{diag}(A)$.

Standard choices for the probe vector z:

- Hutchinson: $z_i = \pm 1$ with probability 0.5
- Gaussian: $z_i \sim N(0, 1)$

See Avron and Toledo review, JACM 2011.

Putting it together

For each probe vector z until error bars small enough:

- Run Lanczos from $z/\|z\|$
- Use Lanczos to estimate $\tilde{K}^{-1}z$ and $\log(\tilde{K})z$
- Dot products yield estimators:

$$\mathcal{L}_{|K|} = -\frac{1}{2}\mathbb{E}\left[z^T \log(\tilde{K})z\right]$$

$$\frac{\partial \mathcal{L}_{|K|}}{\partial \theta_i} = -\frac{1}{2}\mathbb{E}\left[(\tilde{K}^{-1}z)^T \left(\frac{\partial \tilde{K}}{\partial \theta_i} z\right)\right]$$

Cost per probe:

- One Lanczos process
- One matvec per parameter with derivative

This is quite effective in practice!

Hessian estimators

- For Hessian of $\mathcal{L}_y$, exploit $\mathbb{E}[zz^T] = I$:

$$\frac{\partial^2 \mathcal{L}_y}{\partial\theta_i \partial\theta_j} = \frac{1}{2} c^T \left(\frac{\partial^2 K}{\partial\theta_i \partial\theta_j} - 2 \, \frac{\partial K}{\partial\theta_i} \tilde{K}^{-1} \frac{\partial K}{\partial\theta_j} \right) c$$
$$= \frac{1}{2} \mathbb{E} \left[c^T \left(\frac{\partial^2 K}{\partial\theta_i \partial\theta_j} - 2 \, \frac{\partial K}{\partial\theta_i} zz^T \tilde{K}^{-1} \frac{\partial K}{\partial\theta_j} \right) c \right]$$

- Tackle Hessian of $\mathcal{L}_{|K|}$ with independent probe $\check{z}$:

$$\frac{\partial^2 \mathcal{L}_{|K|}}{\partial\theta_i \partial\theta_j} = \frac{1}{2} \operatorname{tr} \left(\tilde{K}^{-1} \frac{\partial K}{\partial\theta_i} \tilde{K}^{-1} \frac{\partial K}{\partial\theta_j} - \tilde{K}^{-1} \frac{\partial^2 K}{\partial\theta_i \partial\theta_j} \right)$$
$$= \frac{1}{2} \mathbb{E} \left[z^T \left(\tilde{K}^{-1} \frac{\partial K}{\partial\theta_i} \check{z}\check{z}^T \tilde{K}^{-1} \frac{\partial K}{\partial\theta_j} - \tilde{K}^{-1} \frac{\partial^2 K}{\partial\theta_i \partial\theta_j} \right) z \right]$$

- Too much variance to be useful without help

Control variates

If unsatisfied with estimator, use *control variates*:

$$\begin{aligned} \mathbb{E}[X] &\text{ desired} \\ \mathbb{E}[Y] &= 0 \\ \mathbb{E}[X - \alpha Y] &= E[X] \\ \operatorname{Var}[X - \alpha Y] &= \operatorname{Var}[X] - 2\alpha \operatorname{Cov}[X, Y] + \alpha^2 \operatorname{Var}[Y] \end{aligned}$$

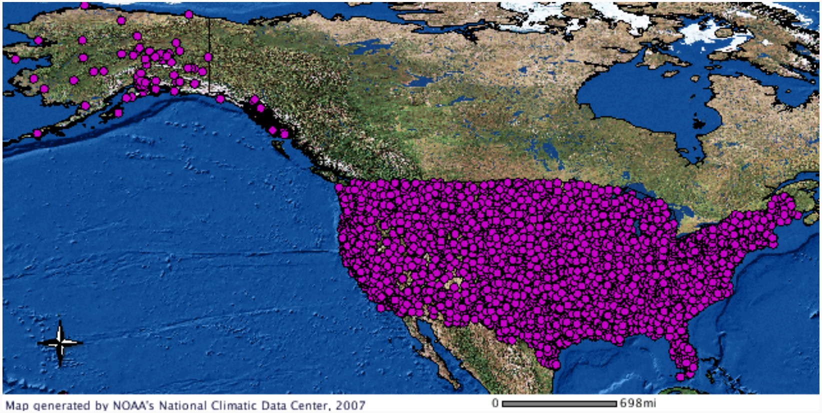
Optimal choice is

$$\alpha_* = \operatorname{Cov}[X, Y] / \operatorname{Var}[Y], \quad \operatorname{Var}[X - \alpha_* Y] = \operatorname{Var}[X] - \frac{\operatorname{Cov}[X, Y]^2}{\operatorname{Var}[Y]}.$$

Idea: Crude kernel approximants to construct control variates.

So where are we now?

Have you ever seen the rain?



Have you ever seen the rain?

- Data: Hourly precipitation data at 5500 weather stations
- Aggregate into daily precipitation
- Total data: $628K$ entries
- Train on $100K$ data points, test on remainder
- Use SKI with 100 points per spatial dim, 300 in time
- Reference comparisons:
  - Scaled eigenvalue approximation for log det
  - Smaller exact computation ($12K$ entries)

The rain, revisited

Method	n	m	MSE	Time [min]
Lanczos	528k	3M	0.613	14.3
Scaled eigenvalues	528k	3M	0.621	15.9
Exact	12k	-	0.903	11.8

So should we just stick to scaled eigs?

Hickory data

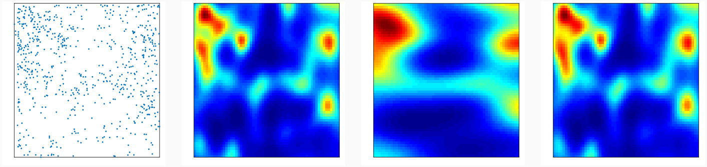
- Log-Gaussian Cox process model
    - Poisson conditional on intensity function
    - Log intensity drawn from a GP
- Laplace approximation for posterior
- Data set is point pattern of 703 hickory trees in Michigan

Hickory data

Method	s_f	ℓ_1	ℓ_2	$-\log p(y\|\theta)$	Time [s]
Exact	0.696	0.063	0.085	1827.56	465.9
Lanczos	0.693	0.066	0.096	1828.07	21.4
Scaled eigs	0.543	0.237	0.112	1851.69	2.5

Table 1: Hyper-parameters recovered by different methods

Hickory data



(a) Points (b) Exact (c) Scaled eigs (d) Lanczos

Figure 1: Prediction by different methods on the Hickory dataset.

Conclusions (?)

"Scalable Log Determinants for GP Kernel Learning"
K. Dong, D. Eriksson, H. Nickisch, D. Bindel, A. G. Wilson
NIPS 2017 (and will appear on arXiV r.s.n.)

Still pursuing connections!

- Variance reduction (esp. for Hessian info)
- Fast large-scale posterior variance
- Connections to Bayesian optimization

Would love to add some chemical applications to the list.