

Surrogate-based Simulation Optimization

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$$\max_{x \in \mathcal{X}} \{f(x) := \mathbb{E}[F(x)]\}$$

- $f(x)$ can only be evaluated via noisy, expensive samples
 - E.g., the expected profit of a complex inventory system
- SO is concerned with designing sampling algorithms to allocate the simulation budget to find a good solution
- Fu and Henderson (2017): history of SO

- Ranking and selection (R&S)
 - \mathcal{X} is a set of a relatively small number of feasible solutions with no inherent ordering defined
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- Discrete optimization via simulation (DOvS)
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- **Continuous SO**
 - $\mathcal{X} \subseteq \mathbb{R}^d$
 - Algorithms for the continuous setting can often be applied to DOvS

- Sample average approximation (Kim, Pasupathy, and Henderson, 2015)
- Stochastic approximation (Chau and Fu, 2015)
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- **Surrogate-based methods** (Barton and Meckesheimer, 2006)
 - Flexible to capture complex surface shapes
 - Capable to predict surface values where no simulation samples are observed

1. Typical Surrogates
2. Locally Convergent Algorithms
3. Globally Convergent Algorithms
4. Computation for Large Datasets
5. Concluding Remarks

- a.k.a. **metamodel**: an approximation to the response surface (simulation input-output relationship)
- Mitigate the computational burden of running simulation experiments
- Any supervised learning model may, in principle, be used

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 - Simulation samples are expensive
- Computationally easy to fit
 - Often need to be updated as more samples become available
- Yield a predictor in explicit form
 - Efficient computation of predictions
 - Facilitate theoretical analysis
 - Easy optimization of the surrogate

- Low-order polynomials
- Linear basis function models
- Gaussian processes (GPs)

- The number of terms explodes in multiple dimensions
- Polynomials with orders higher than two are seldom used

$$f(\mathbf{x}) = \beta_0 + \sum_{j=1}^d \beta_j x_j + \sum_{j=1}^d \sum_{k=1}^d \beta_{jk} x_j x_k,$$

- Suitable for approximating the surface in a **localized** region
- $\beta_0, \beta_j, \beta_{jk}$ can be estimated via ordinary least squares (OLS)

$$f(x) = \beta^T \phi(x) = \sum_{k=1}^p \beta_k \phi_k(x)$$

- $\phi(x)$: e.g., truncated power basis and radial basis
- β can be also estimated via OLS:

$$\begin{aligned}\hat{\beta} &= \underset{\beta}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^n (\bar{y}_i - \beta^T \phi(x_i))^2 \\ &= \Phi^T (\Phi \Phi^T)^{-1} \bar{y},\end{aligned}$$

where Φ is the n -by- p matrix with the i -th row being $\phi(x_i)^T$

- The prediction is given by

$$\hat{f}(x) = \hat{\beta}^T \phi(x) = (\Phi \phi(x))^T (\Phi \Phi^T)^{-1} \bar{y}$$

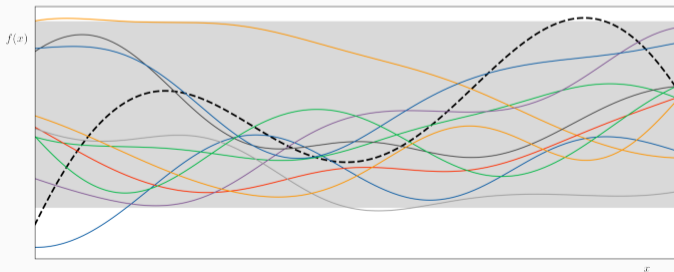
- Generalization of multivariate normal random variables
- Fully characterized by
 - Mean function $\mu : \mathcal{X} \mapsto \mathbb{R}$
 - Covariance function (kernel) $K : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$

Gaussian Processes

- Generalization of multivariate normal random variables
- Fully characterized by
 - Mean function $\mu : \mathcal{X} \mapsto \mathbb{R}$
 - Covariance function (kernel) $K : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$
- Bayesian approach: assume prior distribution of f is $\text{GP}(\mu, K)$

$$(f(\mathbf{x}_1), \dots, f(\mathbf{x}_n)) \sim \text{MVNormal}(\boldsymbol{\mu}, \mathbf{K}),$$

where $\boldsymbol{\mu} = (\mu(\mathbf{x}_1), \dots, \mu(\mathbf{x}_n))^T$ and $\mathbf{K} = (K(\mathbf{x}_i, \mathbf{x}_{i'}))_{i,i'=1}^n$



- Encode one's prior knowledge about the overall shape of f
- Set $\mu(\mathbf{x}) \equiv c$ for some constant c : common practice
- Set $\mu(\mathbf{x}) = \boldsymbol{\beta}^\top \boldsymbol{\phi}(\mathbf{x})$, where $\boldsymbol{\phi}(\mathbf{x})$ is a vector of known basis functions and $\boldsymbol{\beta}$ is a vector of hyperparameters of compatible dimension
- Set $\mu(\mathbf{x})$ to be a function derived from a simplified model of the same stochastic system

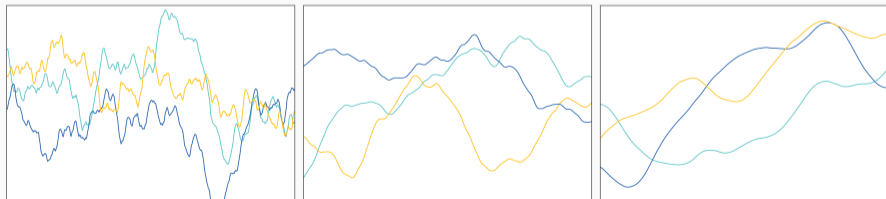
- Gaussian kernels

$$K_{\text{Gaussian}}(\mathbf{x}, \mathbf{x}') = \tau^2 \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\eta^2}\right)$$

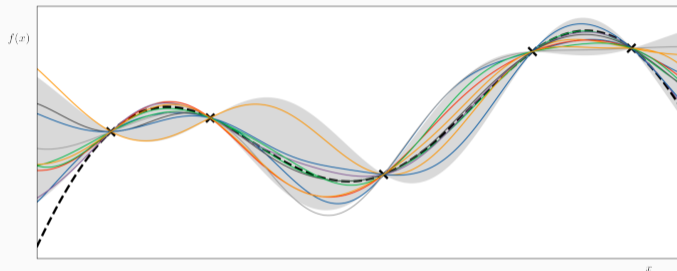
- Matérn kernels

$$K_{\text{Matern}}(\mathbf{x}, \mathbf{x}'; \nu) = \frac{\tau^2}{\Gamma(\nu)2^{\nu-1}} \left(\frac{\sqrt{2\nu}\|\mathbf{x} - \mathbf{x}'\|}{\eta}\right)^\nu K_\nu\left(\frac{\sqrt{2\nu}\|\mathbf{x} - \mathbf{x}'\|}{\eta}\right)$$

- ν : **smoothness** parameter, usually set to be $1/2, 3/2, 5/2, \dots$



- Assume simulation noise is Gaussian with **known** variance
- Posterior of f is also a GP



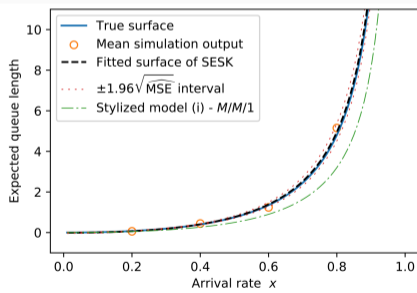
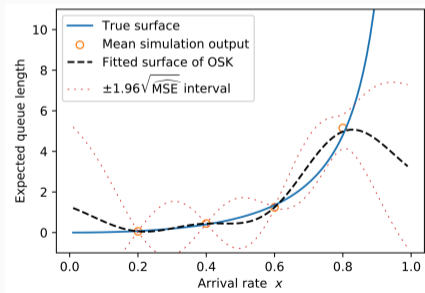
- Use the posterior mean for prediction

$$\hat{f}(x) = \mu(x) + k(x)^T (K + \Sigma)^{-1} (\bar{y} - \mu),$$

where $k(x) = (K(x, x_1), \dots, K(x, x_n))^T$ and Σ is a diagonal matrix

Enhancing Surrogates with Stylized Models

- The main features of a complex system may be captured by a stylized model that yields an analytical expression, say $\psi(x)$
 - Complicated queueing network v.s. independent nodes
- Use ψ in linear basis function models or in the mean functions of GPs
- Shen, Hong, and Zhang (2018); Lin, Matta, and Shanthikumar (2019)



- Given a sample of $f(\mathbf{x})$, an estimate of $\nabla f(\mathbf{x})$ can often be computed with a negligible extra cost
 - Infinitesimal perturbation analysis or the likelihood ratio method (L'Ecuyer, 1990)
- Surrogate for f induces surrogate for ∇f : jointly estimate the parameters
- Chen, Ankenman, and Nelson (2013); Fu and Qu (2014); Qu and Fu (2014); Huo, Zhang, and Zheng (2018)

Part II: Locally Convergent SO Algorithms

- Global: converge to a global optimal solution
- Local: converge to a local optimal solution or a stationary point

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- Global convergence requires exploring the entire feasible region in the limit
- Local convergence only needs to explore part of the feasible region
 - Advantageous when the simulation budget is very limited

- Stage 1
 - Run a number of experiments in a local region of the current solution
 - Fit a first-order polynomial: $f(\mathbf{x}) = \beta_0 + \sum_{j=1}^d \beta_j x_j$
 - Find a better solution along the ascent direction $\nabla f(\mathbf{x}) = (\beta_1, \dots, \beta_d)^\top$
 - Repeat the process until first-order polynomials are no longer adequate

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- Stage 2
 - Fit a second-order polynomial: $f(\mathbf{x}) = \beta_0 + \sum_{j=1}^d \beta_j x_j + \sum_{j=1}^d \sum_{k=1}^d \beta_{jk} x_j x_k$
 - Maximize the polynomial

- Procedure involves human judgement
 - In each iteration, the local region over which one optimizes the surrogate is determined based human experience
 - The transition between first- and second-order surrogates relies on human experience
- Typically used for (very) expensive simulation/real experiments, so large-sample properties such as convergence are not clear

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- Chang, Hong, and Wan (2013): use the trust-region method to address the heuristic nature of RSM

- Iteration k : \mathbf{x}_k is the current solution, Δ_k is the size of the trust region
- (1) Fit a surrogate $r_k(\mathbf{x})$ around \mathbf{x}_k
 - If $\Delta_k \geq \tilde{\Delta}$, $r_k(\mathbf{x})$ is a first-order polynomial
 - Otherwise, $r_k(\mathbf{x})$ is a second-order polynomial
 - (2) Solve $\mathbf{x}_k^* = \mathop{\text{argmax}}\{r_k(\mathbf{x}) : \mathbf{x} \in \mathcal{B}(\mathbf{x}_k, \Delta_k)\}$
 - (3) Simulate a number of observations at \mathbf{x}_k^* and estimate $f(\mathbf{x}_k^*)$;
 - (4) Conduct two tests to update \mathbf{x}_{k+1} and Δ_{k+1}
 - One tests whether \mathbf{x}_k^* is significantly better than \mathbf{x}_k
 - The other tests whether the surrogate works well

- If \mathbf{x}_k^* is not significantly better than \mathbf{x}_k , then set $\mathbf{x}_{k+1} = \mathbf{x}_k$ and decrease Δ_k
- If \mathbf{x}_k^* is significantly better than \mathbf{x}_k , then compute the ratio between the observed and predicted improvements

$$\rho_k = \frac{\bar{f}_k(\mathbf{x}_k^*) - \bar{f}_k(\mathbf{x}_k)}{r_k(\mathbf{x}_k^*) - r_k(\mathbf{x}_k)}$$

- If ρ_k is large (surrogate works well), then set $\mathbf{x}_{k+1} = \mathbf{x}_k^*$ and increase Δ_k
- If ρ_k is small (surrogate works poorly), then set $\mathbf{x}_{k+1} = \mathbf{x}_k$ and decrease Δ_k
- Otherwise: set $\mathbf{x}_{k+1} = \mathbf{x}_k^*$ and keep Δ_k

- Procedure involves no human judgement
 - The local region is the trust region and its size is updated based on two tests
 - The transitions between first- and second-order surrogates are based on Δ_k
- The STRONG algorithm converges to a stationary point

Part III: Globally Convergent SO Algorithms

- Select design points $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ **before** any simulation
 - Primary design principle: cover the design space as much as possible
 - E.g., space-filling designs (Santner, Williams, and Notz, 2003)
- Run simulation at each design point, possibly multiple times
- Fit a surrogate with the observations
- Optimize the predicted surface $\hat{f}(\mathbf{x})$ —a **deterministic** function—with any numerical optimization algorithms

- Design points are selected one at a time after each new sample is obtained
- Each new design point is selected based on
 - The updated surrogate reflecting the previous observations
 - Certain criterion that balances **exploration** and **exploitation**

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- Each new design point is selected based on
 - The updated surrogate reflecting the previous observations
 - Certain criterion that balances **exploration** and **exploitation**
- GPs are the favorite because of the need for uncertainty quantification
- Closely related to “Bayesian optimization” (Shahriari et al., 2016; Frazier, 2018)

- (1) Impose a GP prior on f
- (2) Select the next batch of design points subject to a prescribed “criterion”
- (3) Run simulation at each of the newly selected design points
- (4) Update the GP posterior given the new observations of f
- (5) Repeat Steps (2)–(4) until the simulation budget is exhausted
- (6) Optimize the posterior mean function and return the optimum

- Given $\mathcal{D}_n = \{(x_i, y_i) : i = 1, \dots, n\}$, the posterior $f|\mathcal{D}_n \sim \text{GP}(\mu_n, K_n)$
 - Updating equations for μ_n and K_n are in closed form
- Select $\mathbf{x}_{n+1} = \text{argmax}_{\mathbf{x} \in \mathcal{X}} \text{KG}_n(\mathbf{x})$

$$\text{KG}_n(\mathbf{x}) := \mathbb{E} \left[\underbrace{\max_{\mathbf{v} \in \mathcal{X}} \mu_{n+1}(\mathbf{v}) - \max_{\mathbf{v} \in \mathcal{X}} \mu_n(\mathbf{v})}_{\text{increment in belief about } \max_{\mathbf{v}} f(\mathbf{v})} \mid \mathcal{D}_n, \mathbf{x}_{n+1} = \mathbf{x} \right]$$

- Conditional on $\{\mathcal{D}_n, \mathbf{x}_{n+1} = \mathbf{x}\}$: $\mu_{n+1}(\mathbf{v})$ has a normal distribution that depends on \mathbf{x} , while $\mu_n(\mathbf{v})$ is a constant

- Scott, Frazier, and Powell (2011): discretization

$$\widetilde{\text{KG}}_n(\mathbf{x}) := \mathbb{E} \left[\max_{1 \leq i \leq n+1} \mu_{n+1}(\mathbf{x}_i) - \max_{1 \leq i \leq n+1} \mu_n(\mathbf{x}_i) \mid \mathcal{D}_n, \mathbf{x}_{n+1} = \mathbf{x} \right]$$

- Wu and Frazier (2016): stochastic approximation

$$\begin{aligned} \nabla_{\mathbf{x}} \text{KG}_n(\mathbf{x}) &= \nabla_{\mathbf{x}} \mathbb{E} \left[\max_{\mathbf{v} \in \mathcal{X}} \mu_{n+1}(\mathbf{v}) - \max_{\mathbf{v} \in \mathcal{X}} \mu_n(\mathbf{v}) \mid \mathcal{D}_n, \mathbf{x}_{n+1} = \mathbf{x} \right] \\ &= \mathbb{E} \left[\nabla_{\mathbf{x}} \max_{\mathbf{v} \in \mathcal{X}} \mu_{n+1}(\mathbf{v}) \mid \mathcal{D}_n, \mathbf{x}_{n+1} = \mathbf{x} \right] \end{aligned}$$

Upper Confidence Bound (UCB)

- A celebrated class of methods for multi-armed bandit (MAB) problems
 - MAB: online, maximize **cumulative** reward
 - R&S: offline, maximize **terminal** reward
- GP-UCB: Srinivas et al. (2012) generalize UCB to the continuous setting
- Selecte $\mathbf{x}_{n+1} = \operatorname{argmax}_{\mathbf{x} \in \mathcal{X}} \operatorname{UCB}_n(\mathbf{x})$

$$\operatorname{UCB}_n(\mathbf{x}) := \mu_n(\mathbf{x}) + \sqrt{\gamma_n K_n(\mathbf{x}, \mathbf{x})},$$

where $\gamma_n > 0$ is a tuning parameter that varies as a function of n

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- MAB: $\gamma_n \asymp \ln(n)$
- SO: conceivably larger due to emphasis on the terminal reward
 - More exploration is needed

	GP-UCB	KG
Max. acquisition function	easy	hard
Tuning parameter	γ_n	n.a.

- Given $\mathcal{D}_n = \{(\mathbf{x}_i, y_i) : i = 1, \dots, n\}$, the posterior $f|\mathcal{D}_n \sim \text{GP}(\mu_n, K_n)$
- Use **probability of improvement** to devise a sampling distribution

$$h_n(\mathbf{x}) \propto \Pr(\text{Normal}(\mu_n(\mathbf{x}), K_n(\mathbf{x}, \mathbf{x})) > f_n^*),$$

where f_n^* is the current estimated optimal value

- Draw the next batch of design points from $h_n(\cdot)$

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 - Sun, Hong, and Hu (2014): Markov chain Monte Carlo
 - Sun, Hu, and Hong (2018): Gaussian mixture approximation

	GPS	KG/GP-UCB
Criterion	sampling distribution	acquisition function
# points determined	batch	one at a time

Part IV: Computation for Large Datasets

- Many computations involve matrix inversion

Linear basis function model: $\hat{f}(x) = (\Phi\phi(x))^T(\Phi\Phi^T)^{-1}\bar{y}$

GP regression: $\hat{f}(x) = \mu(x) + k(x)^T(K + \Sigma)^{-1}(\bar{y} - \mu)$

- Surrogates become computationally challenging when n is large
 - Time complexity: $\mathcal{O}(n^3)$
 - Space complexity: $\mathcal{O}(n^2)$

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- Surrogates become computationally challenging when n is large
 - Time complexity: $\mathcal{O}(n^3)$
 - Space complexity: $\mathcal{O}(n^2)$
- Vast literature on GP approximations
 - Nyström method
 - Random features

- **Goal:** approximate $(K + \Sigma)^{-1}$, where Σ is a diagonal matrix
- Consider a rank- m matrix of the form $\tilde{K} = UCV$, where $U \in \mathbb{R}^{n \times m}$, $C \in \mathbb{R}^{m \times m}$, and $V \in \mathbb{R}^{m \times n}$ with $m < n$
- Woodbury formula:

$$(K + \Sigma)^{-1} \approx (\tilde{K} + \Sigma)^{-1} = \Sigma^{-1} - \Sigma^{-1}U \underbrace{(C^{-1} + V\Sigma^{-1}U)}_{m \times m}^{-1}V\Sigma^{-1}$$

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- Construct another kernel $\tilde{K}(\cdot, \cdot)$ that yields a **low-rank** \tilde{K}

- Smola and Schölkopf (2000); Rudi et al. (2015); Lu et al. (2020)
- Select m design points out of $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$
 - $I = \{1, \dots, n\}$
 - $A \subset I$ is the selected indices
- Let $\mathbf{k}_m(\mathbf{x}) = (K(\mathbf{x}_i, \mathbf{x}))_{i \in A}$ and $\mathbf{K}_{m,m} := (K(\mathbf{x}_i, \mathbf{x}_{i'}))_{i \in A, i' \in A}$

$$\tilde{K}(\mathbf{x}, \mathbf{x}') := \mathbf{k}_m(\mathbf{x})^\top \mathbf{K}_{m,m}^{-1} \mathbf{k}_m(\mathbf{x}')$$

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$$\tilde{K}(\mathbf{x}, \mathbf{x}') := \mathbf{k}_m(\mathbf{x})^\top \mathbf{K}_{m,m}^{-1} \mathbf{k}_m(\mathbf{x}')$$

- The covariance matrix associated with evaluating \tilde{K} at $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ is

$$\tilde{K} = \mathbf{K}_{n,m} \mathbf{K}_{m,m}^{-1} \mathbf{K}_{m,n}$$

$$\mathbb{E}[\tilde{f}(x)|\mathcal{D}_n] = \mu(x) + \mathbf{k}_m(x)^\top \underbrace{(\mathbf{K}_{m,m} + \mathbf{K}_{m,n}\Sigma^{-1}\mathbf{K}_{n,m})}_{m \times m}^{-1} \mathbf{K}_{m,n}\Sigma^{-1}(\bar{\mathbf{y}} - \boldsymbol{\mu})$$
$$\text{Cov}[\tilde{f}(x), \tilde{f}(x')|\mathcal{D}_n] = K(x, x') - \mathbf{k}_m(x)^\top \underbrace{(\mathbf{K}_{m,m} + \mathbf{K}_{m,n}\Sigma^{-1}\mathbf{K}_{n,m})}_{m \times m}^{-1} \mathbf{k}_m(x')$$

- Both can be computed with time complexity $\mathcal{O}(m^2n)$

- Rahimi and Recht (2007): random Fourier features (RFF)
- Bochner's theorem: if K is **stationary** (e.g., Gaussian and Matérn), then

$$\begin{aligned}K(\mathbf{x}, \mathbf{x}') &= K(\mathbf{0}, \mathbf{0}) \int_{\mathbb{R}^d} e^{i\boldsymbol{\omega}^\top(\mathbf{x}-\mathbf{x}')} p(d\boldsymbol{\omega}) \\ &= K(\mathbf{0}, \mathbf{0}) \int_{\mathbb{R}^d} \cos(\boldsymbol{\omega}^\top(\mathbf{x} - \mathbf{x}')) p(d\boldsymbol{\omega}) \\ &= K(\mathbf{0}, \mathbf{0}) \mathbb{E}_{\boldsymbol{\omega}} [\cos(\boldsymbol{\omega}^\top(\mathbf{x} - \mathbf{x}'))],\end{aligned}$$

where $p(\cdot)$ is a probability measure on \mathbb{R}^d

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where $p(\cdot)$ is a probability measure on \mathbb{R}^d

- If K is Gaussian, then $p(\cdot)$ is multivariate normal
- If K is Matérn, then $p(\cdot)$ is multivariate Student's T

Monte Carlo Approximation

- Straightforward calculation shows: if $b \sim \text{Unif}[0, 2\pi]$, then

$$\mathbb{E}_{\omega} [\cos(\omega^T(x - x')))] = \mathbb{E}_{\omega, b} [\sqrt{2} \cos(\omega^T x + b) \sqrt{2} \cos(\omega^T x' + b)]$$

- Draw ω_t from $p(\cdot)$ and b_t from $\text{Unif}[0, 2\pi]$

$$\begin{aligned} K(x, x') &\approx K(\mathbf{0}, \mathbf{0}) \cdot \frac{1}{m} \sum_{t=1}^m \sqrt{2} \cos(\omega_t^T x + b_t) \sqrt{2} \cos(\omega_t^T x' + b_t) \\ &:= \sum_{t=1}^m \phi_t(x) \phi_t(x') := \tilde{K}(x, x'), \end{aligned}$$

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- $\phi_m(\mathbf{x}) = (\phi_1(\mathbf{x}), \dots, \phi_m(\mathbf{x}))^{\top}$ is a vector of basis functions (i.e., **features**)
- The covariance matrix associated with evaluating \tilde{K} at $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ is

$$\tilde{K} = \begin{pmatrix} \phi_m(\mathbf{x}_1)^{\top} \\ \vdots \\ \phi_m(\mathbf{x}_n)^{\top} \end{pmatrix} \begin{pmatrix} \phi_m(\mathbf{x}_1) & \cdots & \phi_m(\mathbf{x}_n) \end{pmatrix} := \Phi_m \Phi_m^{\top}.$$

	RFF	Nyström
Data-dependent?	No	Yes
Kernel-dependent?	Yes	No

- Low-order polynomials, linear basis function models, and GPs
- Enhancement via stylized models and/or gradient observations

- Locally convergent: RSM, STRONG
- Globally convergent: KG, GP-UCB, GPS

- Scalable GP computations: the Nyström method, random features

- Integrate local search and global search
- Leverage structural info (convexity/smoothness) to accelerate convergence
- Deeper theoretical understanding of SO algorithms
- Parallel computing

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