revrand: Technical Report

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Abstract

This is a technical report on the *revrand* software library. This library implements Bayesian linear models (Bayesian linear regression), generalized linear models and approximate Gaussian processes. These algorithms have been implemented such that they can be used for large-scale learning by using stochastic variational inference. All of the algorithms in *revrand* use a unified feature composition framework that allows for easy concatenation and selective application of regression basis functions.

Contents

1. Core Algorithms

Recent developments in stochastic gradient optimisation have simplified the application of machine learning to massive datasets, in particular, modern stochastic optimisation algorithms are far more robust to initial learning rate settings. Furthermore, Bayesian machine learning algorithms have a number of well defined methods for learning model parameters and *hyperparameters* from training data, that do not involve cross validation. When used in combination, stochastically optimized Bayesian machine learning algorithms allow practitioners to learn probabilistic predictors from large data sets with minimal tuning and retraining.

We make use of some of these recent developments in stochastic gradient methods and stochastic variational inference in *revrand* for supervisd regression tasks. We outline the core algorithms implemented in *revrand* in this section.

1.1 Stochastic Gradients and Variational Objective Functions

When a machine learning objective function factorises over data,

$$f(\mathbf{X}, \theta) = \sum_{\mathbf{x} \in \mathbf{X}} f(\mathbf{x}, \theta)\,, \tag{1}$$

a regular gradient descent would perform the following iterations to minimise the function w.r.t. the parameters θ,

$$\theta_k := \theta_{k-1} - \eta_k \sum_{\mathbf{x} \in \mathbf{X}} \nabla_\theta f(\mathbf{x}, \theta)|_{\theta=\theta_{k-1}}, \tag{2}$$

where η_k is the learning rate (step size) at iteration k. Stochastic gradients proposes the following update,

$$\theta_k := \theta_{k-1} - \eta_k \sum_{\mathbf{x} \in \mathbf{B}} \nabla_\theta f(\mathbf{x}, \theta)|_{\theta=\theta_{k-1}}, \tag{3}$$

where $\mathbf{B} \subset \mathbf{X}$ is a mini-batch of the original dataset, where $|\mathbf{B}| \ll |\mathbf{X}|$. Frequently objective functions to not entirely decompose over the data, i.e.,

$$f(\mathbf{X}, \theta) = \sum_{\mathbf{x} \in \mathbf{X}} f(\mathbf{x}, \theta) + g(\theta)\,. \tag{4}$$

However, it is trivial to make these objectives work in a stochastic gradient setting. Let $M = |\mathbf{B}|$ and $N = |\mathbf{X}|$, then we divide the contribution of the constant term amongst the mini-batches in stochastic gradients,

$$\theta_k := \theta_{k-1} - \eta_k \sum_{\mathbf{x} \in \mathbf{B}} \nabla_\theta f(\mathbf{x}, \theta)|_{\theta=\theta_{k-1}} - \frac{M}{N} \eta_k \nabla_\theta g(\theta)|_{\theta=\theta_{k-1}}. \tag{5}$$

or, equivalently, boost the contribution of the mini-batch,

$$\theta_k := \theta_{k-1} - \frac{N}{M} \eta_k \sum_{\mathbf{x} \in \mathbf{B}} \nabla_\theta f(\mathbf{x}, \theta)|_{\theta=\theta_{k-1}} - \eta_k \nabla_\theta g(\theta)|_{\theta=\theta_{k-1}}. \tag{6}$$

This is particularly relevant for variational inference where the evidence lower bound objective has a component independent of the data. For example, lets consider the model,

$$\text{Likelihood:} \quad \prod_{n=1}^{N} p(y_n|\theta)\,, \tag{7}$$

$$\text{prior:} \quad p(\theta|\alpha)\,, \tag{8}$$

where we want to learn the values of the hyper-parameters, α. Minimising negative log-marginal likelihood is a good objective in this instance, since we don't care about the value(s) of θ,

$$\underset{\alpha}{\operatorname{argmin}} - \log \int \prod_{n=1}^{N} p(y_n|\theta)\, p(\theta|\alpha)\, d\theta. \tag{9}$$

There are two problems with this objective however, (1) it may not factor over data and (2) the integral may be intractable, for instance, if the prior and likelihood are not conjugate. In variational inference we use Jensen's inequality to lower-bound log-marginal likelihood with a tractable objective function called the evidence lower bound (ELBO),

$$\begin{aligned}
\log p(\mathbf{y}|\alpha) &= \log \int \prod_{n=1}^{N} p(y_n|\theta)\, p(\theta|\alpha)\, d\theta \\
&= \log \int \frac{\prod_n p(y_n|\theta)\, p(\theta|\alpha)}{q(\theta)} q(\theta)\, d\theta \\
&\geq \int q(\theta) \log \left[\frac{\prod_n p(y_n|\theta)\, p(\theta|\alpha)}{q(\theta)} \right] d\theta
\end{aligned} \tag{10}$$

where $q(\theta)$ is an approximation of $p(\theta|\alpha)$ that makes inference easier. This can be re-written as,

$$\mathcal{L} = \sum_{n=1}^{N} \langle \log p(y_n|\theta) \rangle_q - \mathrm{KL}[q(\theta) \| p(\theta|\alpha)] \,, \tag{11}$$

which takes the form of Equation (4), and so if we use stochastic gradients optimisation we can weight the Kullback-Leibler term like the constant term, $g(\cdot)$, from Equation (5), or boost the expected log likelihood term like in Equation (6).

1.2 Bayesian Linear Regression – `StandardLinearModel`

The first machine learning algorithm in *revrand* is a simple Bayesian linear regressor of the following form,

$$\text{Likelihood:} \quad \prod_{n=1}^{N} \mathcal{N}\left(y_n \middle| \boldsymbol{\phi}_n^\top \mathbf{w}, \sigma^2\right), \tag{12}$$

$$\text{prior:} \quad \mathcal{N}(\mathbf{w}|\mathbf{0}, \boldsymbol{\Lambda})\,, \tag{13}$$

where $\boldsymbol{\phi}_n := \phi(\mathbf{x}_n, \theta)$ is a feature, or basis, function that maps $\phi : \mathbb{R}^d \to \mathbb{R}^D$, and $\boldsymbol{\Lambda} \in \mathbb{R}^{D \times D}$ is a diagonal matrix (i.e. it could be $\lambda \mathbf{I}_D$) that has the effect of regularising the magnitude of the weights. This is the same algorithm described in Rasmussen and Williams (2006, Chapter 2). We then:

- Optimise $\sigma^2, \boldsymbol{\Lambda}$ and θ w.r.t. log-marginal likelihood,

  $$\log p\left(\mathbf{y} \middle| \sigma^2, \boldsymbol{\Lambda}, \theta\right) = \log \mathcal{N}\left(\mathbf{y} \middle| \mathbf{0}, \sigma^2 \mathbf{I}_N + \boldsymbol{\Phi}^\top \boldsymbol{\Lambda} \boldsymbol{\Phi}\right), \tag{14}$$

  where $\boldsymbol{\Phi} \in \mathbb{R}^{N \times D}$ is the concatenation of all the features, $\boldsymbol{\phi}_n$. Note this results in the covariance of the log-marginal likelihood being $N \times N$, though we can use the Woodbury identity to simplify the corresponding matrix inversion.

- Solve analytically for the posterior over weights, $\mathbf{w}|\mathbf{y} \sim \mathcal{N}(\mathbf{m}, \mathbf{C})$ given the above hyperparameters, where,

$$\mathbf{C} = \left[\boldsymbol{\Lambda}^{\text{-}1} + \frac{1}{\sigma^2}\boldsymbol{\Phi}^\top\boldsymbol{\Phi}\right]^{\text{-}1},$$
$$\mathbf{m} = \frac{1}{\sigma^2}\mathbf{C}\boldsymbol{\Phi}^\top\mathbf{y}.$$

- Use the predictive distribution

$$p(y^*|\mathbf{y}, \mathbf{X}, \mathbf{x}^*) = \int \mathcal{N}\left(y^* \middle| \boldsymbol{\phi}^{*\top}\mathbf{w}, \sigma^2\right) \mathcal{N}(\mathbf{w}|\mathbf{m}, \mathbf{C})\, d\mathbf{w},$$
$$= \mathcal{N}\left(y^* \middle| \boldsymbol{\phi}^{*\top}\mathbf{m}, \sigma^2 + \boldsymbol{\phi}^{*\top}\mathbf{C}\boldsymbol{\phi}^*\right) \tag{15}$$

for query inputs, $\mathbf{x}^*$. This gives us the useful expectations,

$$\mathbb{E}[y^*] = \boldsymbol{\phi}^{*\top}\mathbf{m}, \tag{16}$$
$$\mathbb{V}[y^*] = \sigma^2 + \boldsymbol{\phi}^{*\top}\mathbf{C}\boldsymbol{\phi}^{*\top}. \tag{17}$$

It is actually easier to use the ELBO form with stochastic gradients for learning the parameters of this algorithm, rather than log-marginal likelihood recast using the Woodbury identity. This is because it is plainly in the same form as Equation (4), though it would give the same result as log-marginal likelihood because the "approximate" posterior is the same form as the true posterior, i.e. $q(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{m}, \mathbf{C})$. The ELBO for this model is,

$$\mathcal{L} = \sum_{n=1}^{N} \left\langle \log \mathcal{N}\left(y_n \middle| \boldsymbol{\phi}_n^\top\mathbf{w}, \sigma^2\right)\right\rangle_q - \mathrm{KL}[\mathcal{N}(\mathbf{w}|\mathbf{m}, \mathbf{C}) \| \mathcal{N}(\mathbf{w}|\mathbf{0}, \boldsymbol{\Lambda})]\,. \tag{18}$$

More specifically,

$$\left\langle \log \mathcal{N}\left(y_n \middle| \boldsymbol{\phi}_n^\top\mathbf{w}, \sigma^2\right)\right\rangle_q = \log \mathcal{N}\left(y_n \middle| \boldsymbol{\phi}_n^\top\mathbf{m}, \sigma^2\right) - \frac{1}{2\sigma^2}\mathrm{tr}\left(\boldsymbol{\phi}_n^\top\boldsymbol{\phi}_n\mathbf{C}\right),$$
$$\mathrm{KL}[\mathcal{N}(\mathbf{w}|\mathbf{m}, \mathbf{C}) \| \mathcal{N}(\mathbf{w}|\mathbf{0}, \boldsymbol{\Lambda})] = \frac{1}{2}\left[\mathrm{tr}\left(\boldsymbol{\Lambda}^{\text{-}1}\mathbf{C}\right) + \mathbf{m}^\top\boldsymbol{\Lambda}^{\text{-}1}\mathbf{m} - \log|\mathbf{C}| + \log|\boldsymbol{\Lambda}| - D\right]$$

We have not implemented a stochastic gradient version of this algorithm since it still requires a matrix solve of a $D \times D$ matrix, and so is $\mathcal{O}(D^3)$ in complexity, per iteration. This is true even if we optimise the posterior covariance directly (or a triangular parameterisation). The GLM presented in the next section circumvents this issue, and is more suited to really large N and D problems.

1.3 Bayesian Generalized Linear Models – `GeneralizedLinearModel`

The algorithm of primary interest in *revrand* is the Bayesian generalized linear model. The general form of the model implemented by this algorithm is,

$$\text{Likelihood:} \quad \prod_{n=1}^{N} p\left(y_n \middle| g\left(\boldsymbol{\phi}_n^\top\mathbf{w}\right), \gamma\right), \tag{19}$$
$$\text{prior:} \quad \mathcal{N}(\mathbf{w}|\mathbf{0}, \boldsymbol{\Lambda}), \tag{20}$$

for an arbitrary univariate likelihood, $p(\cdot)$, with an appropriate transformation (inverse link) function, $g(\cdot)$, and parameter(s), γ.

Naturally, both calculating the exact posterior over the weights, $p(\mathbf{w}|\mathbf{y}, \mathbf{X})$, and the log-marginal likelihood, $p(\mathbf{y})$, for hyperparameter learning are intractable since we may have a non-conjugate relationship between the likelihood and prior. Therefore we must resort to approximating the true posterior and the log-marginal likelihood.

Firstly, we approximate the true posterior over weights with a mixture of K diagonal Gaussians,

$$\begin{aligned} p(\mathbf{w}|\mathbf{y}, \mathbf{X}) &\approx q(\mathbf{w}) \,, \\ &= \frac{1}{K} \sum_{k=1}^{K} \mathcal{N}(\mathbf{w}|\mathbf{m}_k, \mathbf{\Psi}_k) \,, \end{aligned} \tag{21}$$

where $\mathbf{\Psi}_k = \operatorname{diag}\big([\Psi_{k,1}, \ldots, \Psi_{k,D}]^\top\big)$, which is inspired from similar approximations made in Gershman et al. (2012); Nguyen and Bonilla (2014). This is a very flexible form for the approximate posterior, and has the nice property that our algorithm no longer has a $\mathcal{O}\big(D^3\big)$ cost associated with the number of features.

Then we approximate the log marginal likelihood using auto-encoding variational Bayes (Kingma and Welling, 2014). The exact lower bound on log marginal likelihood is,

$$\mathcal{L} = \sum_{n=1}^{N} \left\langle \log p\Big(y_n \Big| g\Big(\boldsymbol{\phi}_n^\top \mathbf{w}\Big), \gamma\Big) \right\rangle_q - \mathrm{KL}\left[\tfrac{1}{K} \textstyle\sum_k \mathcal{N}(\mathbf{w}|\mathbf{m}_k, \mathbf{\Psi}_k) \middle\| \mathcal{N}(\mathbf{w}|\mathbf{0}, \mathbf{\Lambda})\right]. \tag{22}$$

This can be expanded,

$$\begin{aligned} \mathcal{L} = \frac{1}{K} \sum_{k=1}^{K} \sum_{n=1}^{N} \left\langle \log p\Big(y_n \Big| g\Big(\boldsymbol{\phi}_n^\top \mathbf{w}\Big), \gamma\Big) \right\rangle_{q_k} + \frac{1}{K} \sum_{k=1}^{K} \left\langle \log \mathcal{N}(\mathbf{w}|\mathbf{0}, \mathbf{\Lambda}) \right\rangle_{q_k} \\ + \mathbb{H}\left[\tfrac{1}{K} \textstyle\sum_k \mathcal{N}(\mathbf{w}|\mathbf{m}_k, \mathbf{\Psi}_k)\right], \end{aligned} \tag{23}$$

but unfortunately there are two intractable integrals here, the expected log likelihood, and the entropy of the Gaussian mixture. We can use the lower bound on the entropy term also used in Gershman et al. (2012); Nguyen and Bonilla (2014),

$$\mathbb{H}\left[\tfrac{1}{K} \textstyle\sum_k \mathcal{N}(\mathbf{w}|\mathbf{m}_k, \mathbf{\Psi}_k)\right] \geq -\frac{1}{K} \displaystyle\sum_{k=1}^{K} \log \sum_{j=1}^{K} \frac{1}{K} \mathcal{N}(\mathbf{m}_k|\mathbf{m}_j, \mathbf{\Psi}_k + \mathbf{\Psi}_j) \,. \tag{24}$$

We can then use the reparameterisation trick in auto-encoding variational Bayes (Kingma and Welling, 2014) to sample the expected log likelihood,

$$\sum_{n=1}^{N} \left\langle \log p\Big(y_n \Big| g\Big(\boldsymbol{\phi}_n^\top \mathbf{w}\Big), \gamma\Big) \right\rangle_{q_k} \approx \frac{1}{L} \sum_{l=1}^{L} \sum_{n=1}^{N} \log p\Big(y_n \Big| g\Big(\boldsymbol{\phi}_n^\top \hat{\mathbf{w}}_k^{(l)}\Big), \gamma\Big) \tag{25}$$

where,

$$\hat{\mathbf{w}}_k^{(l)} = f_k\Big(\mathbf{m}_k, \mathbf{\Psi}_k, \boldsymbol{\epsilon}^{(l)}\Big) = \mathbf{m}_k + \sqrt{\mathbf{\Psi}_k} \odot \boldsymbol{\epsilon}^{(l)}, \qquad \boldsymbol{\epsilon}^{(l)} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_D) \,. \tag{26}$$

Here $\odot$ is the element-wise product. We can also use this trick to compute approximate derivatives, $\frac{\partial}{\partial \alpha} \langle \log p(y|\alpha) \rangle_{q(\alpha)} \approx \frac{1}{L} \sum_{l=1}^{L} \frac{\partial}{\partial \alpha} \log p\big(y \big| f\big(\alpha, \boldsymbol{\epsilon}^{(l)}\big)\big)$, which simplifies the implementation greatly! The final auto-encoding variational Bayes objective for our GLM is,

$$\mathcal{L} \approx \frac{1}{K} \sum_{k=1}^{K} \Bigg[\frac{1}{L} \sum_{l=1}^{L} \sum_{n=1}^{N} \log p\Big(y_n \Big| g\Big(\boldsymbol{\phi}_n^\top \hat{\mathbf{w}}_k^{(l)}\Big), \gamma\Big) + \log \mathcal{N}(\mathbf{m}_k | \mathbf{0}, \boldsymbol{\Lambda}) - \frac{1}{2} \mathrm{tr}\big(\boldsymbol{\Lambda}^{-1} \boldsymbol{\Psi}_k\big) - \log \sum_{j=1}^{K} \frac{1}{K} \mathcal{N}(\mathbf{m}_k | \mathbf{m}_j, \boldsymbol{\Psi}_k + \boldsymbol{\Psi}_j) \Bigg]. \tag{27}$$

We can straight forwardly use this objective within a stochastic gradients setting using with the tactic in Equations (5) or (6).

The most simple and accurate method for approximating the predictive distribution, $p(y^*|\mathbf{y}, \mathbf{X}, \mathbf{x}^*)$ is to Monte-Carlo sample the integral,

$$p(y^*|\mathbf{y}, \mathbf{X}, \mathbf{x}^*) \approx \int p\Big(\mathbf{y} \Big| g\Big(\boldsymbol{\phi}^{*\top} \mathbf{w}\Big), \gamma\Big) \frac{1}{K} \sum_{k=1}^{K} \mathcal{N}(\mathbf{w} | \mathbf{m}_k, \boldsymbol{\Psi}_k) \, d\mathbf{w}. \tag{28}$$

However, this integral is not particularly useful unless we wish to evaluate known $\mathbf{y}^*$ under the model. For prediction, it is more useful to compute (using Monte-Carlo integration) the predictive expectation,

$$\begin{aligned} \mathbb{E}[y^*] &\approx \int \frac{1}{K} \sum_{k=1}^{K} \mathcal{N}(\mathbf{w} | \mathbf{m}_k, \boldsymbol{\Psi}_k) \int y^* p\Big(y^* \Big| g\Big(\boldsymbol{\phi}^{*\top} \mathbf{w}\Big), \gamma\Big) \, dy^* d\mathbf{w} \\ &= \int \mathbb{E}\Big[p\Big(y^* \Big| g\Big(\boldsymbol{\phi}^{*\top} \mathbf{w}\Big), \gamma\Big)\Big] \frac{1}{K} \sum_{k=1}^{K} \mathcal{N}(\mathbf{w} | \mathbf{m}_k, \boldsymbol{\Psi}_k) \, d\mathbf{w}. \end{aligned} \tag{29}$$

Often we find $\mathbb{E}\big[p\big(y^* \big| g\big(\boldsymbol{\phi}^{*\top} \mathbf{w}\big), \gamma\big)\big] = g\big(\boldsymbol{\phi}^{*\top} \mathbf{w}\big)$, however this is only true with with right choice and usage of the activation function. Furthermore, it is useful to compute quantiles of the predictive density in order to ascertain the predictive uncertainty. We start by sampling the predictive cumulative density function, $P(\cdot)$,

$$\begin{aligned} &P(y^* \leq \alpha | \mathbf{y}, \mathbf{X}, \mathbf{x}^*) \\ &\quad \approx \int \frac{1}{K} \sum_{k=1}^{K} \mathcal{N}(\mathbf{w} | \mathbf{m}_k, \boldsymbol{\Psi}_k) \int_{-\infty}^{\alpha} p\Big(y^* \Big| g\Big(\boldsymbol{\phi}^{*\top} \mathbf{w}\Big), \gamma\Big) \, dy^* d\mathbf{w} \\ &\quad = \int P\Big(y^* \leq \alpha \Big| g\Big(\boldsymbol{\phi}^{*\top} \mathbf{w}\Big), \gamma\Big) \frac{1}{K} \sum_{k=1}^{K} \mathcal{N}(\mathbf{w} | \mathbf{m}_k, \boldsymbol{\Psi}_k) \, d\mathbf{w}. \end{aligned} \tag{30}$$

Once we have obtained sufficient samples from the (mixture) posterior we can obtain quantiles, α, for some chosen level of probability, p, using root finding techniques. Specifically, we use root finding techniques to solve the following for α,

$$P(y^* \leq \alpha | \mathbf{y}, \mathbf{X}, \mathbf{x}^*) - p = 0. \tag{31}$$

1.4 Large Scale Gaussian Process Approximation

In *revrand* we approximate Gaussian Processes (Rasmussen and Williams, 2006) with our standard and generalized linear models by using random feature functions such as those of Rahimi and Recht (2007; 2008) and Le et al. (2013). They use Bochner's theorem regarding the relationship between a kernel and the Fourier transform of a non-negative measure (e.g. a probability measure) that establishes the duality of the covariance function of a stationary process and its spectral density,

$$k(\boldsymbol{\tau}) = \int p_{\boldsymbol{\omega}}(\boldsymbol{\omega}) e^{i\boldsymbol{\omega}^\top \boldsymbol{\tau}} d\boldsymbol{\omega}, \tag{32}$$

$$p_{\boldsymbol{\omega}}(\boldsymbol{\omega}) = \int k(\boldsymbol{\tau}) e^{-i\boldsymbol{\omega}^\top \boldsymbol{\tau}} d\boldsymbol{\tau}. \tag{33}$$

where $k(\cdot)$ is a kernel function, and $p_{\boldsymbol{\omega}}(\cdot)$ its spectral density. Rahimi and Recht's main insight (2007) is that we can approximate the kernel by constructing 'suitable' random features and Monte Carlo averaging over samples from $p_{\boldsymbol{\omega}}(\boldsymbol{\omega})$ for *shift invariant* kernels,

$$k(\mathbf{x} - \mathbf{x}') = k(\boldsymbol{\tau}) \approx \frac{1}{D} \sum_{i=1}^{D} \phi_i(\mathbf{x})^\top \phi_i(\mathbf{x}'), \tag{34}$$

$\phi_i(\mathbf{x})$ corresponds to the ith sample from the feature map. An example of a radial basis kernel feature vector construction using the above approximation is,

$$\begin{aligned} [\phi_i(\mathbf{x}), \phi_{D+i}(\mathbf{x})] &= \frac{1}{\sqrt{D}} \left[\cos(\boldsymbol{\omega}_i^T \mathbf{x}), \sin(\boldsymbol{\omega}_i^T \mathbf{x})\right], \\ \text{with } \boldsymbol{\omega}_i &\sim \mathcal{N}\left(\boldsymbol{\omega}_i \middle| \mathbf{0}, l_\phi^{-1} \mathbf{I}_d\right), \end{aligned} \tag{35}$$

for $i = 1, \ldots, D$, which in fact is a mapping into a $2D$-dimensional feature space. See Table 1 for some of the random kernel approximations we use in *revrand*.

Table 1: Kernels and the corresponding Fourier weight ($\boldsymbol{\omega}_i$) sampling distributions for the Rahimi and Recht (2007)-style random bases in *revrand*. Here GAL refers to a multivariate Laplace distribution Kozubowski et al. (2013).

Kernel	$k(\mathbf{x} - \mathbf{x}')$	$p_{\boldsymbol{\omega}}(\boldsymbol{\omega})$
RBF	$\exp\left(-\frac{\lVert\mathbf{x}-\mathbf{x}'\rVert^2}{2l_\phi^2}\right)$	$\boldsymbol{\omega}_i \sim \mathcal{N}\left(\mathbf{0}, l_\phi^{-1}\mathbf{I}_d\right)$,
Laplace	$\exp\left(-\frac{\lVert\mathbf{x}-\mathbf{x}'\rVert}{l_\phi}\right)$	$\boldsymbol{\omega}_i \sim \prod_d \text{Cauchy}\left(l_\phi^{-1}\right)$
Cauchy	$\frac{1}{1+\left(\lVert\mathbf{x}-\mathbf{x}'\rVert/l_\phi\right)^2}$	$\boldsymbol{\omega}_i \sim \text{GAL}\left(1, \mathbf{0}, l_\phi^{-1}\mathbf{I}_d\right)$
Matern 3/2	$\left(1 + \frac{\sqrt{3}\lVert\mathbf{x}-\mathbf{x}'\rVert}{l_\phi}\right)\exp\left(-\frac{\sqrt{3}\lVert\mathbf{x}-\mathbf{x}'\rVert}{l_\phi}\right)$	$\boldsymbol{\omega}_i \sim \text{t}_{\nu=3}\left(\mathbf{0}, l_\phi^{-1}\mathbf{I}_d\right)$
Matern 5/2	$\left(1 + \frac{\sqrt{5}\lVert\mathbf{x}-\mathbf{x}'\rVert}{l_\phi} + \frac{5\lVert\mathbf{x}-\mathbf{x}'\rVert^2}{3l_\phi^2}\right)\exp\left(-\frac{\sqrt{5}\lVert\mathbf{x}-\mathbf{x}'\rVert}{l_\phi}\right)$	$\boldsymbol{\omega}_i \sim \text{t}_{\nu=5}\left(\mathbf{0}, l_\phi^{-1}\mathbf{I}_d\right)$

All of the kernel functions in Table 1 have length scale hyperparameters, and in *revrand* these can be isotropic or anisotropic length scales that are learned alongside the other hyperparameters. We have also implemented a few other variants of these random basis functions, namely the Fastfood (Le et al., 2013) and A la Carte (Yang et al., 2014) basis functions that improve scalability and representational flexibility respectively. In Figure 1 we compare the basis approximations with their corresponding kernels. We refer the reader to our demo notebooks for further discussion and experiments comparing these approximate basis functions and the kernels they approximate.

An important feature of *revrand* is that we can combine these random features (and non-random features) to build even more expressive features. In particular, we support basis *concatenation* while still allowing basis function hyperparameter learning,

$$\mathbf{\Phi}_{\text{cat}} = \left[\phi_1(\mathbf{X}, \theta_1)\,, \phi_2(\mathbf{X}, \theta_2)\,, \ldots, \phi_P(\mathbf{X}, \theta_P)\right]. \tag{36}$$

In the following manner this approximates kernel addition,

$$\lambda_1 k_1(\mathbf{X}, \mathbf{X}, \theta_1) + \lambda_2 k_2(\mathbf{X}, \mathbf{X}, \theta_2) + \ldots + \lambda_P k_P(\mathbf{X}, \mathbf{X}, \theta_P) \approx \mathbf{\Phi}_{\text{cat}} \mathbf{\Lambda} \mathbf{\Phi}_{\text{cat}}^\top, \tag{37}$$

where $\mathbf{\Lambda} = \text{diag}([\lambda_1 \mathbf{1}, \lambda_2 \mathbf{1}, \ldots, \lambda_P \mathbf{1}])$ and each vector of $\mathbf{1}$ is the same dimension as the corresponding basis. That is, the regression regularizer, or weight prior variance in Equations (13) and (20), acts as a kernel mixing/amplitude parameter. Kernel products also have an equivalent representation with basis functions (outer product of bases), however we have not yet implemented this.

We also support *partial application* of basis functions to certain dimensions of the inputs, $\mathbf{X}$, while also allowing concatentation, e.g,

$$\phi(\mathbf{X}, \boldsymbol{\theta}) = \left[\phi_1(\mathbf{X}_{1:10}, \theta_1)\,, \phi_2(\mathbf{X}_{5:D}, \theta_2)\,, \ldots, \phi_P(\mathbf{X}, \theta_P)\right] \tag{38}$$

Where the subscript of $\mathbf{X}$ denotes (arbitrary) column slices. See *revrand*'s documentation for how to use this features.

2. Experiments

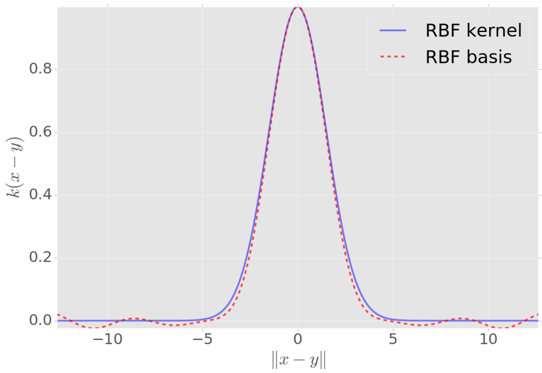
2.1 Boston Housing Regression

Algorithm	**R-square**	**MSLL**
SLM	0.9018 (0.0134)	-1.504 (0.1191)
GLM	0.8411 (0.0491)	-0.9209 (0.1530)
GP	**0.9027 (0.0137)**	**-1.1792 (0.1581)**
RF	0.8467 (0.0709)	N/A
SVR	0.6295 (0.0863)	N/A

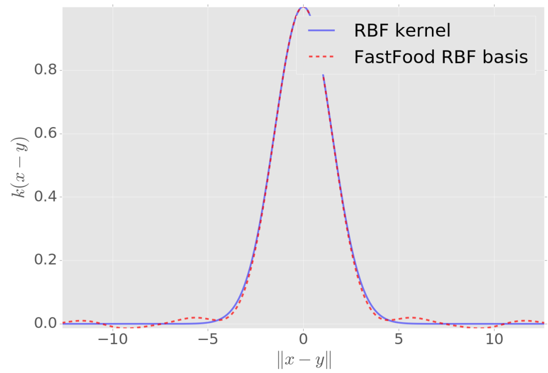
2.2 Handwritten Digits Classification

2.3 SARCOS Regression

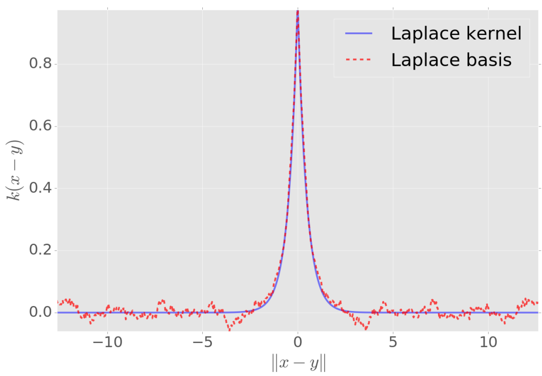
1 million iterations



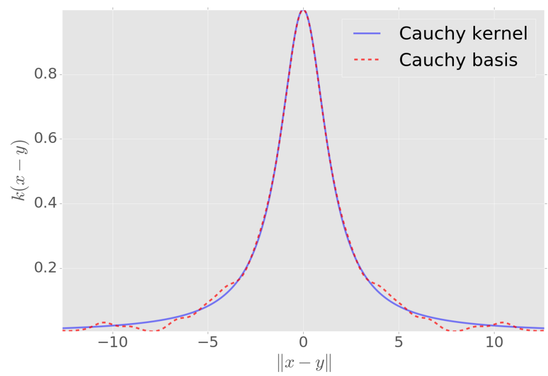
(a) RBF



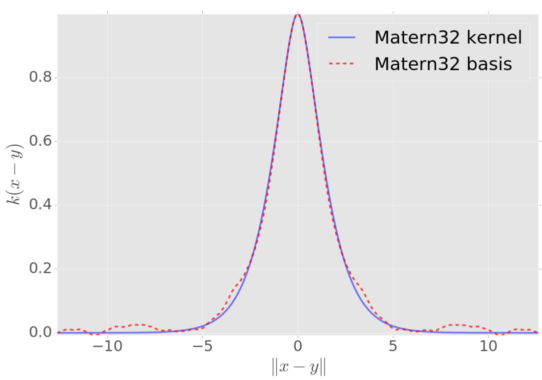
(b) RBF Fastfood



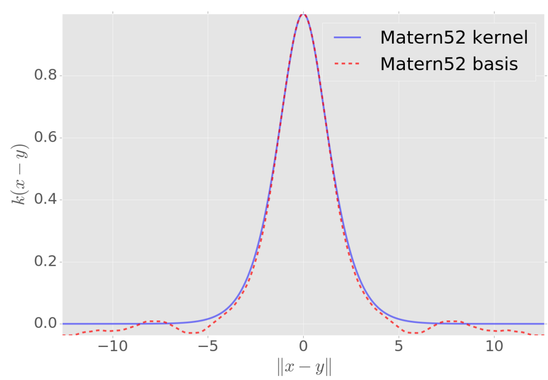
(c) Laplace



(d) Cauchy



(e) Matern 3/2



(f) Matern 5/2

Figure 1: Comparison of various kernels and their basis approximations. In each of these figures 1500 random bases have been used, and the inputs to the kernels are 10 dimensional, $\mathbf{x} \in \mathbb{R}^{10}$.

References

Samuel Gershman, Matt Hoffman, and David Blei. Nonparametric variational inference. In *Proceedings of the 29th International Conference on Machine Learning (ICML)*, July

Algorithm	Log-loss	Error (%)
GLM	0.1138	**2.07**
Logistic	0.1734	3.62
SVC	**0.1003**	6.99
GPC	0.1405	2.59
RF	0.1368	2.72

Algorithm	Approximation size	SMSE	MSLL
GLM	256	0.0358	-1.6644
	512	0.0252	-1.8397
	1024	0.0207	-1.9341
	2048	0.0171	-2.0243
	8192	0.0152	-1.9804

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