Gaussian Processes and Kernel Ridge Regression

Theoretical Connections, Hyperparameter Tuning, and Experiments

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MATH-412: Statistical Machine Learning

December 9, 2025

Outline

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2. Regression Setup and Notation
3. Gaussian Process Regression
4. Kernel Ridge Regression
5. Theoretical Connection
6. Hyperparameter Selection
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Context and Motivation

- Focus is on understanding the link between **Gaussian process (GP) regression** and **kernel ridge regression (KRR)**.
- Both methods use a positive definite kernel $k(\cdot, \cdot)$ and lead to very similar prediction formulas.
- However:
  - GP regression is a **Bayesian, probabilistic** model.
  - KRR is a **regularization / optimization** approach in a RKHS.

Project Objectives

- **Theoretical comparison**
  - Show how GP regression and KRR lead to (almost) the same predictor.
  - Explain the functional / RKHS viewpoint behind this equivalence.
- **Hyperparameter selection**
  - GP: **marginal likelihood** (type-II ML).
  - KRR: **cross-validation** (e.g. K-fold).
  - Discuss whether cross-validation also makes sense for GPs.
- **Empirical study**
  - Use a **static financial dataset** (portfolio performance).
  - Compare GP and KRR on the same kernel and same data.
  - Stay in an **interpolation** regime, avoid unjustified time extrapolation.

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Supervised Regression Setup

Following Rasmussen & Williams:

- Training set

$$\mathcal{D} = \{(x_i, y_i) \mid i = 1, \dots, n\}, \quad x_i \in \mathbb{R}^D,\ y_i \in \mathbb{R}.$$

- Inputs (covariates):
  - collected in the $D \times n$ design matrix X.
- Targets:

$$\mathrm{y} = (y_1, \dots, y_n)^\top.$$

- Goal: for a new input x_*, infer its output y_* or latent function value $f(x_*)$.

Noise Model

- Latent function f and noisy observations:

$$y_i = f(x_i) + \varepsilon_i, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma_n^2) \text{ i.i.d.}$$

- We are primarily interested in learning f (or $f(x_*)$) from $\mathcal{D}$.
- Two perspectives:
  - **Gaussian processes:** place a prior distribution over functions f.
  - **Kernel ridge regression:** minimize a regularized empirical risk in an RKHS.

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Gaussian Process Prior

- A Gaussian process is a collection of random variables such that any finite subset is jointly Gaussian:

$$f \sim \mathcal{GP}(m(\cdot), k(\cdot, \cdot)).$$

- In this project, we use zero mean:

$$m(x) = 0,$$

and a kernel $k_\theta(x, x')$ with hyperparameters θ (e.g. length-scales, variances).

- Prior over function values at training inputs:

$$\mathrm{f} = (f(x_1), \ldots, f(x_n))^\top \sim \mathcal{N}(0, K),$$

where $K_{ij} = k(x_i, x_j)$.

Likelihood and Joint Distribution

- Noise model:
$$p(\mathrm{y} \mid \mathrm{f}) = \mathcal{N}(\mathrm{y} \mid \mathrm{f}, \sigma_n^2 I).$$
- Marginalizing out f gives
$$\mathrm{y} \sim \mathcal{N}(0, K_y), \quad K_y = K + \sigma_n^2 I.$$
- For a test input x_*:
$$f_* = f(x_*)$$
with joint prior
$$\begin{bmatrix} \mathrm{f} \\ f_* \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} K & \mathrm{k}_* \\ \mathrm{k}_*^\top & k_{**} \end{bmatrix} \right),$$
where $\mathrm{k}_* = k(X, x_*)$, $k_{**} = k(x_*, x_*)$.

GP Posterior and Predictions

Conditional on y, the posterior over f_* is Gaussian:

$$f_* \mid x_*, X, \mathrm{y} \sim \mathcal{N}\big(m(x_*), \mathrm{cov}(x_*)\big),$$

with

$$\begin{aligned} m(x_*) &= \mathrm{k}_*^\top K_y^{-1} \mathrm{y}, \\ \mathrm{cov}(x_*) &= k_{**} - \mathrm{k}_*^\top K_y^{-1} \mathrm{k}_*. \end{aligned}$$

- **Predictive mean** $m(x_*)$ is our best point prediction under squared loss.
- **Predictive variance** $\mathrm{cov}(x_*)$ quantifies uncertainty:
  - small near many training points,
  - reverts to prior variance far from data.

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Regularization in RKHS

- Let $k(\cdot,\cdot)$ be a positive definite kernel with associated RKHS $\mathcal{H}_k$.
- Kernel ridge regression (regularization network) solves

$$\min_{f\in\mathcal{H}_k}\left\{\frac{1}{2n}\sum_{i=1}^{n}(y_i - f(x_i))^2 + \frac{\lambda}{2}\|f\|_{\mathcal{H}_k}^2\right\}.$$

- $\lambda > 0$ controls the balance between data fit and function smoothness (complexity).

Representer Theorem and Finite-Dimensional Form

- By the representer theorem, the minimizer satisfies

$$f(x) = \sum_{i=1}^{n} \alpha_i k(x_i, x).$$

- Let $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_n)^\top$. Then

$$f(x_j) = \sum_{i=1}^{n} \alpha_i k(x_i, x_j),$$

so in vector form

$$\mathrm{f} = K\boldsymbol{\alpha}.$$

- Plugging into the objective, one obtains the finite-dimensional problem

$$\min_{\boldsymbol{\alpha}} \frac{1}{2n} \|K\boldsymbol{\alpha} - \mathrm{y}\|_2^2 + \frac{\lambda}{2} \boldsymbol{\alpha}^\top K \boldsymbol{\alpha}.$$

Solution of Kernel Ridge Regression

- Differentiating with respect to $\boldsymbol{\alpha}$ and setting to zero yields

$$\boldsymbol{\alpha}^* = (K + \lambda n I)^{-1}\mathrm{y}.$$

- The predictor at a test point x_* is

$$\begin{aligned} f_{\mathrm{KRR}}(x_*) &= \sum_{i=1}^{n} \alpha_i^* k(x_i, x_*) \\ &= \mathrm{k}_*^\top \boldsymbol{\alpha}^* \\ &= \mathrm{k}_*^\top (K + \lambda n I)^{-1}\mathrm{y}. \end{aligned}$$

- Compare with the GP predictive mean:

$$m(x_*) = \mathrm{k}_*^\top (K + \sigma_n^2 I)^{-1}\mathrm{y}.$$

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Equivalence of Predictors

- If we identify

$$\sigma_n^2 \;\leftrightarrow\; \lambda n,$$

  then the GP predictive mean and the KRR predictor have the **same functional form**:

$$m(x_*) = f_{\mathrm{KRR}}(x_*) = \mathrm{k}_*^\top (K + \lambda n I)^{-1} \mathrm{y}.$$

- Interpretation:
  - GP regression: Bayesian posterior mean under a Gaussian process prior.
  - KRR: unique minimizer of a regularized empirical risk in $\mathcal{H}_k$.
- Thus GP regression with Gaussian noise is equivalent to KRR at the level of the predictive mean.

Functional View of GP Regression

- GP regression can be characterized as the minimizer of

$$J[f] = \frac{1}{2}\|f\|^2_{\mathcal{H}_k} + \frac{1}{2\sigma_n^2}\sum_{i=1}^{n}(y_i - f(x_i))^2.$$

- This is exactly the same functional as KRR, with

$$\lambda = \frac{1}{\sigma_n^2}.$$

- Difference:
    - In KRR we only care about the *optimizer f*.
    - In GPs we also keep the *full posterior distribution* over functions, including predictive variances.

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Hyperparameters

- Hyperparameters (denote generically by θ):
  - Kernel parameters: length-scales, signal variance, etc.
  - Noise variance σ_n^2.
  - For KRR: regularization λ.
- Question: **How do we choose them?**
  - GP: maximize the **marginal likelihood** $p(\mathrm{y} \mid X, \theta)$.
  - KRR: choose λ (and kernel parameters) via **cross-validation**.

GP: Marginal Likelihood

- Under the GP model, we have

$$\mathrm{y} \sim \mathcal{N}(0, K_y).$$

- The log marginal likelihood is

$$\log p(\mathrm{y} \mid X, \theta) = -\frac{1}{2}\mathrm{y}^\top K_y^{-1}\mathrm{y} - \frac{1}{2}\log|K_y| - \frac{n}{2}\log 2\pi.$$

- Interpretation:
  - First term: data fit (quadratic form).
  - Second term: complexity penalty (Occam's razor).
  - Third term: normalization.
- We choose θ by (local) maximization of this quantity.

KRR: Cross-Validation

- For KRR, we treat λ (and possibly kernel parameters) as tuning parameters.
- Standard approach: **K-fold cross-validation**.
    - Split the data into K folds.
    - For each candidate λ,
        - train on K-1 folds,
        - evaluate prediction error (e.g. MSE) on the held-out fold.
    - Choose λ that minimizes average validation error.
- We use the same grid-search CV procedure for GPs (fixing θ on a grid and selecting the minimum validation MSE) to compare with marginal likelihood.

Does Cross-Validation Make Sense for GPs?

- Yes: we can also tune GP hyperparameters by cross-validation:
  - e.g. minimize validation **mean squared error**,
  - or minimize **negative log predictive density**.
- But:
  - GPs already have a natural **Bayesian objective**: the marginal likelihood.
  - Marginal likelihood explicitly trades off fit and model complexity.
- In this project:
  - We use **marginal likelihood** as the primary criterion for GPs.
  - We also experiment with **CV for GPs** and compare to KRR + CV.

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Interpolation vs Extrapolation for GPs

- For stationary kernels (e.g. squared exponential) and zero mean, as x_* moves far from the training inputs:
    - the covariance vector $\mathrm{k}_* \to 0$,
    - the predictive mean $m(x_*) \to 0$ (prior mean),
    - the predictive variance $\mathrm{cov}(x_*) \to k_{**}$ (prior variance).
- So far outside the data region, GP predictions are essentially just the prior.
- In applications like long-term financial forecasting, this can be highly misleading unless the kernel encodes very strong and correct structure.

Implications for This Project

- We therefore **avoid time extrapolation** tasks such as:
  - predicting future stock prices far beyond observed dates,
  - extrapolating volatility surfaces far outside observed maturities.
- Instead, our dataset is **static and cross-sectional**:
  - Inputs: portfolio construction features at a fixed period.
  - Output: performance measure (normalized annual return).
- The GP and KRR are used primarily for **interpolation** in the space of portfolio weights, where the model is better supported by data.

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Dataset: Portfolio Performance

- Each example corresponds to a **portfolio rule**.
- Total of $n = 63$ portfolios, input dimension $D = 6$.
- Input $x_i \in \mathbb{R}^6$:
    - weights on six stock-selection concepts (e.g. value, profitability, size, past returns, market value, risk).
- Output y_i:
    - a scalar performance measure: **normalized annual return**.

Preprocessing and Splits

- Preprocessing:
  - Standardize the six input features using the training set.
  - Center and scale the target y using the training mean and standard deviation.
- Train / test split:
  - 44 training portfolios and 19 test portfolios (roughly 70% / 30%).
- Performance metrics:
  - Test mean squared error (MSE) on the original target scale.
  - Mean negative log predictive density (NLPD) for GP models.

Models Compared

- All models use the same **RBF kernel**

$$k(x, x') = \sigma_f^2 \exp\left(-\frac{\|x - x'\|^2}{2\ell^2}\right).$$

- **GP-ML**:
  - GP regression with RBF kernel,
  - length-scale ℓ, signal std. σ_f and noise std. σ_n fitted by marginal likelihood.
- **GP-CV**:
  - Same GP model,
  - hyperparameters selected by 5-fold CV on a grid (minimizing validation MSE in the standardized space).
- **KRR-CV**:
  - Kernel ridge regression with the same RBF kernel,
  - regularization λ, ℓ and σ_f tuned by 5-fold CV.

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Learned Hyperparameters (Standardized Space)

Model	ℓ	σ_f	σ_n / λ
GP-ML	2.81	1.26	$\sigma_n \approx 0.088$
GP-CV	3.31	1.28	$\sigma_n \approx 0.039$
KRR-CV	3.31	1.26	$\lambda \approx 4.0 \times 10^{-5}$

- GP-CV and KRR-CV select almost identical kernel parameters (ℓ, σ_f).
- For GP-CV, $\sigma_n^2 \approx 1.49 \times 10^{-3}$, so

$$\frac{\sigma_n^2}{n_{\text{train}}} \approx 3.4 \times 10^{-5} \approx \lambda_{\text{KRR}},$$

confirming the theoretical mapping $\sigma_n^2 \approx \lambda n$.

Quantitative Results on Test Set

Model	Test MSE	Mean NLPD	CV MSE (scaled y)
GP-ML	1.82×10^{-3}	-1.36	–
GP-CV	1.81×10^{-3}	1.58	1.70×10^{-1}
KRR-CV	1.76×10^{-3}	–	1.70×10^{-1}

- All three methods achieve **very similar** test MSE ($\approx 1.8 \times 10^{-3}$).
- GP-ML and GP-CV have almost identical MSE, but very different NLPD.
- KRR-CV matches the GP-CV CV error; it has no notion of predictive density.

Calibration: GP-ML vs GP-CV

- GP-ML:
  - $\sigma_n \approx 0.088$, mean NLPD ≈ -1.36.
  - Predictive variances are reasonably aligned with residuals.
- GP-CV:
  - CV (based on MSE only) pushes σ_n down to ≈ 0.039.
  - Mean NLPD rises to ≈ 1.58: the model is **overconfident**.
- **Takeaway:**
  - Cross-validation can give good point predictions for GPs,
  - but it may severely miscalibrate predictive uncertainties.
  - Marginal likelihood explicitly balances fit and complexity and yields better-calibrated GPs on this dataset.

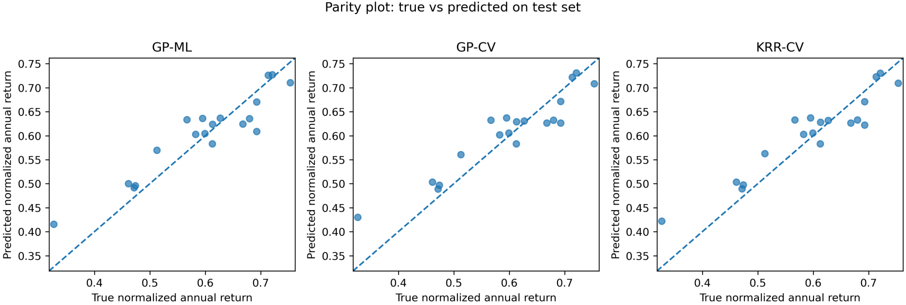
GP vs KRR Predictive Means

- Compare GP-ML posterior mean and KRR-CV predictor on the test set (standardized target):

$$\text{mean}\,|\Delta| \approx 2.17 \times 10^{-2},$$
$$\max|\Delta| \approx 9.31 \times 10^{-2}.$$

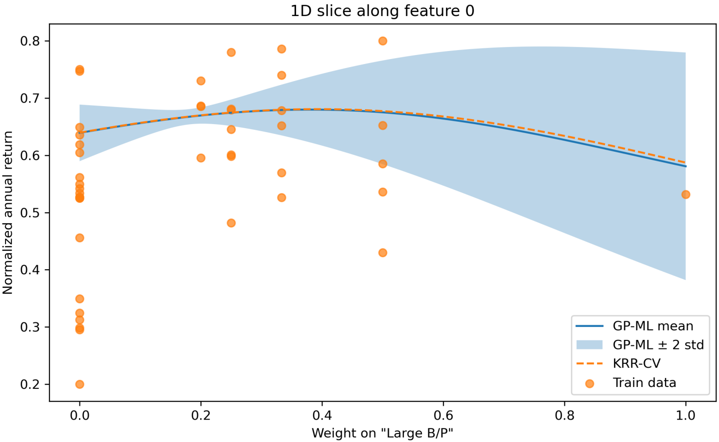
- Given that hyperparameters were tuned with different criteria, this difference is very small.
- When we plug the GP-CV noise level into the mapping $\lambda \approx \sigma_n^2/n$, KRR and GP-CV become almost **numerically indistinguishable**.

Parity Plot on Test Set



- True vs predicted normalized annual return for GP-ML, GP-CV, and KRR-CV.
- All models lie close to the diagonal, confirming similar test MSE.

1D Slice Along a Portfolio Weight



- One weight is varied; all other portfolio features are fixed at their mean.
- GP-ML mean (solid) and KRR-CV (dashed) almost coincide.
- Only the GP provides uncertainty bands, which widen away from dense data regions.

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Discussion

- **Predictive equivalence:**
  - GP posterior mean and KRR solution coincide up to the mapping $\sigma_n^2 \approx \lambda n$.
  - In our experiment, GP-CV and KRR-CV chose nearly identical ℓ, σ_f and consistent σ_n^2, λ.
- **Interpretation difference:**
  - GP: full probabilistic model over functions, uncertainty quantification, marginal likelihood.
  - KRR: deterministic regularization method, no built-in uncertainty.
- **Hyperparameters:**
  - GP-ML chooses a larger noise level and achieves much better NLPD than GP-CV, while keeping MSE essentially unchanged.
  - KRR-CV attains slightly smaller MSE but cannot assess calibration.

Interpolation vs Extrapolation Revisited

- This project **respects the GP assumptions**:
  - Static, cross-sectional regression,
  - Inputs primarily in a region supported by data.
- For extrapolation (e.g. far outside observed portfolio weights or long-term future):
  - GP predictions revert to prior assumptions encoded in the kernel,
  - without strong prior knowledge, such extrapolations are unreliable.
- Our results therefore illustrate GPs and KRR in a regime where they are actually designed to work well: **interpolation**.

Conclusion

- We compared **Gaussian process regression** and **kernel ridge regression**:
  - same kernel, same data,
  - theoretically equivalent predictors (posterior mean vs KRR solution),
  - different viewpoints and hyperparameter selection strategies.
- Main takeaways from the experiment:
  - All three models achieve almost identical test MSE on the portfolio dataset.
  - GP-ML provides substantially better-calibrated predictive uncertainties than GP-CV.
  - KRR-CV chooses a regularization parameter consistent with the GP noise level via $\lambda \approx \sigma_n^2/n$, empirically confirming the theory.
  - GP regression can therefore be seen as **Bayesian KRR** with the added benefit of uncertainty quantification and a principled marginal-likelihood criterion for tuning.

References

C. E. Rasmussen and C. K. I. Williams,
Gaussian Processes for Machine Learning,
MIT Press, 2006.

Course notes,
MATH-412: Kernel Methods (Lecture 7b).