

Bayesian Interpretations of Regularization

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Regularized least squares maps $\{(x_i, y_i)\}_{i=1}^n$ to a function that minimizes the regularized loss:

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

Can we interpret RLS from a probabilistic point of view?

Some notation

- $S = \{(x_i, y_i)\}_{i=1}^n$ is the set of observed input/output pairs in $\mathbb{R}^d \times \mathbb{R}$ (the training set).
- X and Y denote the matrices $[x_1, \dots, x_n]^T \in \mathbb{R}^{n \times d}$ and $[y_1, \dots, y_n]^T \in \mathbb{R}^n$, respectively.
- θ is a vector of parameters in \mathbb{R}^p .
- $p(Y|X, \theta)$ is the joint distribution over outputs Y given inputs X and the parameters.

Where do probabilities show up?

$$\frac{1}{2} \sum_{i=1}^n V(y_i, f(x_i)) + \frac{\lambda}{2} \|f\|_{\mathcal{H}}^2$$

becomes

$$p(Y|f, X) \cdot p(f)$$

- **Likelihood**, a.k.a. **noise model**: $p(Y|f, X)$.
 - Gaussian: $y_i \sim \mathcal{N}(f^*(x_i), \sigma_i^2)$
 - Poisson: $y_i \sim \text{Pois}(f^*(x_i))$
- **Prior**: $p(f)$.

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The estimation problem:

- Given data $\{(x_i, y_i)\}_{i=1}^N$ and model $p(Y|f, X), p(f)$.
- Find a good f to explain data.

- Maximum likelihood estimation for ERM
- MAP estimation for linear RLS
- MAP estimation for kernel RLS
- Transductive model
- Infinite dimensions get more complicated

Maximum likelihood estimation

- Given data $\{(x_i, y_i)\}_{i=1}^N$ and model $p(Y|f, X), p(f)$.
- A good f is one that maximizes $p(Y|f, X)$.

Maximum likelihood and least squares

For least squares, noise model is:

$$y_i | f, x_i \sim \mathcal{N}(f(x_i), \sigma^2)$$

a.k.a.

$$Y | f, X \sim \mathcal{N}(f(X), \sigma^2 I)$$

So

$$p(Y | f, X) = \frac{1}{(2\pi\sigma^2)^{N/2}} \exp \left\{ - \sum_{i=1}^N \frac{1}{\sigma^2} (y_i - f(x_i))^2 \right\}$$

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Maximum likelihood and least squares

Maximum likelihood: maximize

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Empirical risk minimization: minimize

$$\sum_{i=1}^N (y_i - f(x_i))^2$$

$$\sum_{i=1}^N (y_i - f(x_i))^2$$

$$e^{-\sum_{i=1}^N \frac{1}{\sigma^2} (y_i - f(x_i))^2}$$

What about regularization?

RLS:

$$\arg \min_f \frac{1}{2} \sum_{i=1}^n (y_i - f(x_i))^2 + \frac{\lambda}{2} \|f\|_{\mathcal{H}}^2$$

Is there a model of Y and f that yields RLS?

Yes.

$$e^{-\frac{1}{2\sigma_\varepsilon^2} \left(\sum_{i=1}^n (y_i - f(x_i))^2 \right) - \frac{\lambda}{2} \|f\|_{\mathcal{H}}^2}$$

$$p(Y|f, X) \cdot p(f)$$

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Posterior function estimates

- Given data $\{(x_i, y_i)\}_{i=1}^N$ and model $p(Y|f, X), p(f)$.
- Find a good f to explain data.

(If we can get $p(f|Y, X)$)

Bayes least squares estimate:

$$\hat{f}_{BLS} = \mathbb{E}_{(f|X, Y)}[f]$$

i.e. the mean of the posterior.

MAP estimate:

$$\hat{f}_{MAP}(Y|X) = \arg \max_f p(f|X, Y)$$

i.e. a mode of the posterior.

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A posterior on functions?

How to find $p(f|Y, X)$?

Bayes' rule:

$$\begin{aligned} p(f|X, Y) &= \frac{p(Y|X, f) \cdot p(f)}{p(Y|X)} \\ &= \frac{p(Y|X, f) \cdot p(f)}{\int p(Y|X, f) df} \end{aligned}$$

When is this well-defined?

A posterior on functions?

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A posterior on functions?

Functions vs. parameters:

$$\mathcal{H} \cong \mathbb{R}^p$$

Represent functions in \mathcal{H} by their coordinates w.r.t. a basis:

$$f \in \mathcal{H} \leftrightarrow \theta \in \mathbb{R}^p$$

Assume (for the moment): $p < \infty$

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Assume (for the moment): $p < \infty$

Linear function:

$$f(\mathbf{x}) = \langle \mathbf{x}, \theta \rangle$$

Noise model:

$$Y|X, \theta \sim \mathcal{N}(X\theta, \sigma_\varepsilon^2 I)$$

Add a *prior*:

$$\theta \sim \mathcal{N}(\mathbf{0}, \Lambda)$$

Posterior for linear RLS

Model:

$$Y|X, \theta \sim \mathcal{N}(X\theta, \sigma_\varepsilon^2 I), \quad \theta \sim \mathcal{N}(0, \Lambda)$$

Joint over Y and θ :

$$\begin{bmatrix} Y \\ \theta \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} X\Lambda X^T + \sigma_\varepsilon^2 I & X\Lambda \\ \Lambda X^T & \Lambda \end{bmatrix}\right)$$

Condition on Y .

Posterior for linear RLS

Posterior:

$$\theta|X, Y \sim \mathcal{N}(\mu_{\theta|X, Y}, \Sigma_{\theta|X, Y})$$

where

$$\begin{aligned}\mu_{\theta|X, Y} &= \Lambda X^T (X \Lambda X^T + \sigma_\varepsilon^2 I)^{-1} Y \\ \Sigma_{\theta|X, Y} &= \Lambda - \Lambda X^T (X \Lambda X^T + \sigma_\varepsilon^2 I)^{-1} X \Lambda\end{aligned}$$

This is Gaussian, so

$$\hat{\theta}_{MAP}(Y|X) = \hat{\theta}_{BLS}(Y|X) = \Lambda X^T (X \Lambda X^T + \sigma_\varepsilon^2 I)^{-1} Y$$

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Linear RLS as a MAP estimator

Model:

$$Y|X, \theta \sim \mathcal{N}(X\theta, \sigma_\varepsilon^2 I), \quad \theta \sim \mathcal{N}(0, \Lambda)$$

$$\hat{\theta}_{MAP}(Y|X) = \Lambda X^T (X \Lambda X^T + \sigma_\varepsilon^2 I)^{-1} Y$$

Recall the linear RLS solution:

$$\begin{aligned} \hat{\theta}_{RLS}(Y|X) &= \arg \min_{\theta} \frac{1}{2} \sum_{i=1}^N (y_i - \langle x_i, \theta \rangle)^2 + \frac{\lambda}{2} \|\theta\|^2 \\ &= \Lambda X^T (X X^T + \frac{\lambda}{2} I)^{-1} Y \end{aligned}$$

So what's Λ ? λ ?

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So what's Λ ? λ ?

Represent functions in \mathcal{H} by their coordinates w.r.t. a basis:

$$f \in \mathcal{H} \leftrightarrow \theta \in \mathbb{R}^p$$

Which basis?

Mercer's theorem:

$$K(x_i, x_j) = \sum_k \nu_k \psi_k(x_i) \psi_k(x_j)$$

where $\nu_k \psi_k(\cdot) = \int K(\cdot, y) \psi_k(y) dy$ for all k . The functions $\{\sqrt{\nu_k} \psi_k(\cdot)\}$ form an *orthonormal basis* for \mathcal{H}_K .

Let $\phi(\cdot) = [\sqrt{\nu_1} \psi_1(\cdot), \dots, \sqrt{\nu_p} \psi_p(\cdot)]$. Then:

$$\mathcal{H}_K = \{\phi(\cdot)\theta \mid \theta \in \mathbb{R}^p\}$$

Posterior for kernel RLS

Model for *linear* RLS:

$$Y|X, \theta \sim \mathcal{N}(X\theta, \sigma_\varepsilon^2 I), \quad \theta \sim \mathcal{N}(0, I)$$

Model for kernel RLS?

$$Y|X, \theta \sim \mathcal{N}(\phi(X)\theta, \sigma_\varepsilon^2 I), \quad \theta \sim \mathcal{N}(0, I)$$

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$$\hat{\theta}_{MAP}(Y|X) = \phi(X)^T (\phi(X)\phi(X)^T + \sigma_\varepsilon^2 I)^{-1} Y$$

Potential problem?

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$$\hat{\theta}_{MAP}(Y|X) = \phi(X)^T (K + \sigma_\varepsilon^2 I)^{-1} Y$$

Potential problem?

Problem: there's no such thing as

$$\theta \sim \mathcal{N}(0, I)$$

when $\theta \in \mathbb{R}^\infty$!

A quick recap

- **Empirical risk minimization is ML.**

$$p(Y|f, X) \propto e^{-\frac{1}{2} \sum_{i=1}^N (y_i - f(x_i))^2}$$

- **Linear RLS is MAP.**

$$p(Y, f|X) \propto e^{-\frac{1}{2} \sum_{i=1}^N (y_i - \langle x_i, \theta \rangle)^2} \cdot e^{-\frac{\lambda}{2} \theta^T \theta}$$

- **Kernel RLS is also MAP.**

$$p(Y, f|X) \propto e^{-\frac{1}{2} \sum_{i=1}^N (y_i - f(x_i))^2} \cdot e^{-\frac{\lambda}{2} \|f\|_{\mathcal{H}}^2}$$

But these aren't well-defined for infinite dimensional function spaces...

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$$p(Y, f|X) \propto e^{-\frac{1}{2} \sum_{i=1}^N (y_i - f(x_i))^2} \cdot e^{-\frac{\lambda}{2} \|f\|_{\mathcal{H}}^2}$$

But these aren't well-defined for infinite dimensional function spaces...

Transductive setting

We hinted at problems if $\dim \mathcal{H}_K = \infty$.

Idea: Forget about estimating θ (i.e. f).

Instead: Estimate *predicted outputs*

$$Y^* = [y_1^*, \dots, y_M^*]^T$$

at test inputs

$$X^* = [x_1^*, \dots, x_M^*]^T$$

Need the joint distribution over Y^* and Y .

Transductive setting

Say Y^* and Y are *jointly Gaussian*:

$$\begin{bmatrix} Y \\ Y^* \end{bmatrix} = \mathcal{N} \left(\begin{bmatrix} \mu_Y \\ \mu_{Y^*} \end{bmatrix}, \begin{bmatrix} \Lambda_Y & \Lambda_{YY^*} \\ \Lambda_{Y^*Y} & \Lambda_{Y^*} \end{bmatrix} \right)$$

Want: kernel RLS.

General form for the posterior:

$$Y^*|X, Y \sim \mathcal{N}(\mu_{Y^*|X, Y}, \Sigma_{Y^*|X, Y})$$

where

$$\mu_{Y^*|X, Y} = \mu_{Y^*} + \Lambda_{YY^*}^T \Lambda_Y^{-1} (Y - \mu_Y)$$

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$$\Sigma_{Y^* | X, Y} = \Lambda_{Y^*} - \Lambda_{YY^*}^T \Lambda_Y^{-1} \Lambda_{YY^*}$$

$$\text{Set } \Lambda_Y = K(X, X) + \sigma^2 I, \Lambda_{YY^*} = K(X, X^*), \Lambda_{Y^*} = K(X^*, X^*).$$

Posterior:

$$Y^* | X, Y \sim \mathcal{N}(\mu_{Y^* | X, Y}, \Sigma_{Y^* | X, Y})$$

where

$$\mu_{Y^* | X, Y} = \mu_{Y^*} + K(X^*, X)(K(X, X) + \sigma^2 I)^{-1}(Y - \mu_Y)$$

$$\Sigma_{Y^* | X, Y} = K(X^*, X^*) - K(X^*, X)(K(X, X) + \sigma^2 I)^{-1}K(X, X^*)$$

$$\text{So: } \hat{Y}_{MAP}^* = \hat{f}_{RLS}(X^*).$$

Transductive setting

Model:

$$\begin{bmatrix} Y \\ Y^* \end{bmatrix} = \mathcal{N} \left(\begin{bmatrix} \mu_Y \\ \mu_{Y^*} \end{bmatrix}, \begin{bmatrix} K(X, X) + \sigma_\varepsilon^2 I & K(X, X^*) \\ K(X^*, X) & K(X^*, X^*) \end{bmatrix} \right)$$

MAP estimate (posterior mean) = RLS function *at every point* x^* , regardless of $\dim \mathcal{H}_K$.

Are the prior and posterior (*on points!*) consistent with a distribution on \mathcal{H}_K ?

Transductive setting

Strictly speaking, θ and f don't come into play here at all:

Have: $p(Y^*|X, Y)$

Do not have: $p(\theta|X, Y)$ or $p(f|X, Y)$

But, *if \mathcal{H}_K is finite dimensional*, the joint over Y and Y^* is consistent with:

- $Y = f(X) + \varepsilon$,
- $Y^* = f(X)$, and
- $f \in \mathcal{H}_K$ is a random trajectory from a **Gaussian process** over the domain, with mean μ and covariance K .
- (Ergo, people call this “Gaussian process regression.”)
(Also “Kriging,” because of a guy.)

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(Also “Kriging,” because of a guy.)

- **Empirical risk minimization** is the maximum likelihood estimator when:

$$y = x^T \theta + \varepsilon$$

- **Linear RLS** is the MAP estimator when:

$$y = x^T \theta + \varepsilon, \quad \theta \sim \mathcal{N}(0, I)$$

- **Kernel RLS** is the MAP estimator when:

$$y = \phi(x)^T \theta + \varepsilon, \quad \theta \sim \mathcal{N}(0, I)$$

in finite dimensional \mathcal{H}_K .

- **Kernel RLS** is the MAP estimator *at points* when:

$$\begin{bmatrix} Y \\ Y^* \end{bmatrix} = \mathcal{N} \left(\begin{bmatrix} \mu_Y \\ \mu_{Y^*} \end{bmatrix}, \begin{bmatrix} K(X, X) + \sigma_\varepsilon^2 I & K(X, X^*) \\ K(X^*, X) & K(X^*, X^*) \end{bmatrix} \right)$$

in possibly infinite dimensional \mathcal{H}_K .

Is this useful in practice?

- Want confidence intervals + believe the posteriors are meaningful = yes
- Maybe other reasons?