Comparing regularisation paths of (conjugate) gradient estimators in ridge regression

Laura Hucker, Markus Reiß, Thomas Stark

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Linear regression setting

Under random design

$$y_i = x_i^\top \beta_0 + \varepsilon_i, \quad i = 1, \ldots, n$$

- $\beta_0 \in \mathbb{R}^p$ unknown true coefficient vector
- i.i.d. observations (x_i, y_i) of $\mathbb{R}^p$-valued feature vectors x_i, $\mathbb{R}$-valued responses y_i
- ε_i error variables, $\mathbb{E}[\varepsilon_i \,|\, x_i] = 0$, $\mathsf{Var}(\varepsilon_i \,|\, x_i) = \sigma^2$, $\sigma > 0$
- $p \gg n$ possible (high-dim. setting)
- **short**: $y = X\beta_0 + \varepsilon$ with $y := (y_1, \ldots, y_n)^\top$, $X := (x_1, \ldots, x_n)^\top$, $\varepsilon := (\varepsilon_1, \ldots, \varepsilon_n)^\top$
- assumptions: $\beta_0 = X^+ X \beta_0$, $\sum_{j=1,\ldots,p:\, s_j = s_i} \langle X^\top y, v_j \rangle^2 > 0$, $i = 1, \ldots, p$

Penalised least squares criterion

= Ridge regression (RR) objective

$$\hat{\beta}_\lambda^{\mathrm{RR}} := \operatorname*{argmin}_{\beta \in \mathbb{R}^p} \mathscr{E}_\lambda(\beta) \quad \text{with} \quad \mathscr{E}_\lambda(\beta) := \frac{1}{2n}\|y - X\beta\|^2 + \frac{\lambda}{2}\|\beta\|^2, \quad \lambda \geqslant 0$$

- $\lambda = 0$: $\hat{\beta}_0^{\mathrm{RR}} = X^+ y$ minimum-norm solution of $y = X\beta$, $\hat{\Sigma}_0^{-1} := \hat{\Sigma}^+$ [Ali et al. 2019]
- $\lambda > 0$: $\hat{\beta}_\lambda^{\mathrm{RR}} = \hat{\Sigma}_\lambda^{-1} \cdot n^{-1} X^\top y$, where $\hat{\Sigma}_\lambda := \hat{\Sigma} + \lambda I_p$ with $\hat{\Sigma} := n^{-1} X^\top X$
- eigenvalues of $\hat{\Sigma}$: $s_1 \geqslant \ldots \geqslant s_p \geqslant 0$
- for simplicity: assume $\hat{\Sigma}_\lambda$ has p distinct eigenvalues

Penalised least squares criterion

= Ridge regression (RR) objective

$$\begin{aligned}\mathscr{E}_\lambda(\beta) &= \frac{1}{2n}\|y - X\beta\|^2 + \frac{\lambda}{2}\|\beta\|^2 \\ &= \frac{1}{2}\langle\hat{\Sigma}_\lambda\beta,\beta\rangle - \frac{1}{n}\langle X^\top y,\beta\rangle + \frac{1}{2n}\|y\|^2 \\ &= \frac{1}{2}\|\hat{\Sigma}_\lambda^{1/2}\beta - y_\lambda\|^2 + \frac{1}{2n}\|y\|^2 - \frac{1}{2}\|y_\lambda\|^2\end{aligned}$$

with

$$y_\lambda := \frac{1}{n}\hat{\Sigma}_\lambda^{-1/2}X^\top y = \hat{\Sigma}_\lambda^{1/2}\beta_\lambda + \varepsilon_\lambda, \quad \beta_\lambda := \hat{\Sigma}_\lambda^{-1}\hat{\Sigma}\beta_0, \quad \varepsilon_\lambda := \frac{1}{n}\hat{\Sigma}_\lambda^{-1/2}X^\top\varepsilon$$

normal equations: $\hat{\Sigma}_\lambda\hat{\beta}_\lambda^{\mathrm{RR}} = \hat{\Sigma}_\lambda^{1/2}y_\lambda$ s.t. $\hat{\beta}_\lambda^{\mathrm{RR}} = \beta_\lambda + \hat{\Sigma}_\lambda^{-1/2}\varepsilon_\lambda$

How to calculate the RR estimator in practice?

scikit learn

API Reference > sklearn.linear_model > Ridge

Ridge

class sklearn.linear_model.**Ridge**(*alpha=1.0*, ***, *fit_intercept=True*, *copy_X=True*, *max_iter=None*, *tol=0.0001*, *solver='auto'*, *positive=False*, *random_state=None*) [source]

Linear least squares with l2 regularization.

Minimizes the objective function:

```
||y - Xw||^2_2 + alpha * ||w||^2_2
```

solver : *{'auto', 'svd', 'cholesky', 'lsqr', 'sparse_cg', 'sag', 'saga', 'lbfgs'}, default='auto'*

Solver to use in the computational routines:

- 'auto' chooses the solver automatically based on the type of data.
- 'svd' uses a Singular Value Decomposition of X to compute the Ridge coefficients. It is the most stable solver, in particular more stable for singular matrices than 'cholesky' at the cost of being slower.
- 'cholesky' uses the standard scipy.linalg.solve function to obtain a closed-form solution.
- 'sparse_cg' uses the conjugate gradient solver as found in scipy.sparse.linalg.cg. As an iterative algorithm, this solver is more appropriate than 'cholesky' for large-scale data (possibility to set `tol` and `max_iter`).
- 'lsqr' uses the dedicated regularized least-squares routine scipy.sparse.linalg.lsqr. It is the fastest and uses an iterative procedure.
- 'sag' uses a Stochastic Average Gradient descent, and 'saga' uses its improved, unbiased version named SAGA. Both methods also use an iterative procedure, and are often faster than other solvers when both n_samples and n_features are large. Note that 'sag' and 'saga' fast convergence is only guaranteed on features with approximately the same scale. You can preprocess the data with a scaler from sklearn.preprocessing.
- 'lbfgs' uses L-BFGS-B algorithm implemented in `scipy.optimize.minimize`. It can be used only when `positive` is True.

How to calculate the RR estimator in practice?

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used only w

By iterative solvers!

Gradient descent/flow (GD/GF)

$\eta > 0, k \in \mathbb{N}, \hat{\beta}^{\mathsf{GD}}_{\lambda,\eta,0} = 0,$

$$\begin{aligned}\hat{\beta}^{\mathsf{GD}}_{\lambda,\eta,k} &:= \hat{\beta}^{\mathsf{GD}}_{\lambda,\eta,k-1} - \eta \nabla \mathscr{E}_\lambda(\hat{\beta}^{\mathsf{GD}}_{\lambda,\eta,k-1}) \\ &= \hat{\beta}^{\mathsf{GD}}_{\lambda,\eta,k-1} - \eta(\hat{\Sigma}_\lambda \hat{\beta}^{\mathsf{GD}}_{\lambda,\eta,k-1} - \hat{\Sigma}^{1/2}_\lambda y_\lambda)\end{aligned}$$

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$$\eta_k = t/k,\ k \to \infty,\ t > 0 \quad \Big\downarrow \quad = \hat{\beta}^{\mathsf{GD}}_{\lambda,\eta,k-1} - \eta(\hat{\Sigma}_\lambda \hat{\beta}^{\mathsf{GD}}_{\lambda,\eta,k-1} - \hat{\Sigma}^{1/2}_\lambda y_\lambda)$$

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$\eta_k = t/k,\ k \to \infty,\ t > 0$

$$\hat{\beta}^{\mathsf{GF}}_{\lambda,t} \text{ satisfying } \hat{\beta}^{\mathsf{GF}}_{\lambda,0} = 0,$$

$$\frac{d}{dt}\hat{\beta}^{\mathsf{GF}}_{\lambda,t} = -(\hat{\Sigma}_\lambda \hat{\beta}^{\mathsf{GF}}_{\lambda,t} - \hat{\Sigma}^{1/2}_\lambda y_\lambda),\ t \geqslant 0$$

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$$\hat{\beta}^{\mathsf{GF}}_{\lambda,t} = \hat{\Sigma}^{-1/2}_\lambda (I_p - R^{\mathsf{GF}}_t(\hat{\Sigma}_\lambda)) y_\lambda,$$

$$R^{\mathsf{GF}}_t(x) = \exp(-tx)$$

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$\eta_k = t/k,$
$k \to \infty,$
$t > 0$

$$= \hat{\beta}^{\mathsf{GD}}_{\lambda,\eta,k-1} - \eta(\hat{\Sigma}_\lambda \hat{\beta}^{\mathsf{GD}}_{\lambda,\eta,k-1} - \hat{\Sigma}^{1/2}_\lambda y_\lambda)$$

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Conjugate gradients (CG)

Algorithm 1 Penalised CG method

$\hat{\beta}^{\mathrm{CG}}_{\lambda,0} \leftarrow 0$, $q_0 \leftarrow \frac{1}{n} X^\top y$, $d_0 \leftarrow q_0$, $e_0 \leftarrow X d_0$, $k = 1$
while (no division by zero) **do**
  $a_k \leftarrow \|q_{k-1}\|^2 / (\frac{1}{n}\|e_{k-1}\|^2 + \lambda \|d_{k-1}\|^2)$
  $\hat{\beta}^{\mathrm{CG}}_{\lambda,k} \leftarrow \hat{\beta}^{\mathrm{CG}}_{\lambda,k-1} + a_k d_{k-1}$
  $q_k \leftarrow q_{k-1} - \frac{a_k}{n} X^\top e_{k-1} - \lambda a_k d_{k-1}$
  $b_k \leftarrow \|q_k\|^2 / \|q_{k-1}\|^2$
  $d_k \leftarrow q_k + b_k d_{k-1}$
  $e_k \leftarrow X d_k$
  $k \leftarrow k + 1$
end while

Gradient descent/flow (GD/GF)

$$\hat{\beta}^{\mathsf{GF}}_{\lambda,t} = \hat{\Sigma}_\lambda^{-1/2}(I_p - R^{\mathsf{GF}}_t(\hat{\Sigma}_\lambda))y_\lambda,$$

$$R^{\mathsf{GF}}_t(x) = \exp(-tx)$$

Conjugate gradients (CG)

$$\hat{\beta}^{\mathsf{CG}}_{\lambda,k} = \hat{\Sigma}_\lambda^{-1/2}(I_p - R^{\mathsf{CG}}_k(\hat{\Sigma}_\lambda))y_\lambda,$$

$$R^{\mathsf{CG}}_k := \arg\min_{P_k} \|P_k(\hat{\Sigma}_\lambda)y_\lambda\|^2$$

[Phatak and de Hoog 2002]

Gradient descent/flow (GD/GF)

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[Phatak and de Hoog 2002]

$$\Rightarrow \quad \hat{\beta}^{\mathsf{CG}}_{\lambda,p} = \hat{\beta}^{\mathsf{RR}}_\lambda$$

Gradient descent/flow (GD/GF)

$$\hat{\beta}_{\lambda,t}^{\mathsf{GF}} = \hat{\Sigma}_{\lambda}^{-1/2}(I_p - R_t^{\mathsf{GF}}(\hat{\Sigma}_{\lambda}))y_{\lambda},$$

$$R_t^{\mathsf{GF}}(x) = \exp(-tx)$$

Conjugate gradients (CG)

continuous iteration path:

$$t = k + \alpha,\ k \in [\![0, p-1]\!],\ \alpha \in (0,1],$$

$$\hat{\beta}_{\lambda,t}^{\mathsf{CG}} := \hat{\Sigma}_{\lambda}^{-1/2}(I_p - R_t^{\mathsf{CG}}(\hat{\Sigma}_{\lambda}))y_{\lambda},$$

$$R_t^{\mathsf{CG}} := (1-\alpha)R_k^{\mathsf{CG}} + \alpha R_{k+1}^{\mathsf{CG}}$$

[Hucker and Reiß 2025]

Error analysis

For in-sample prediction errors

- pure prediction error: $n^{-1}\|X(\hat{\beta} - \beta_0)\|^2 = \|\hat{\Sigma}^{1/2}(\hat{\beta} - \beta_0)\|^2$
- population risk:
  $\beta \mapsto \mathbb{E}[\mathscr{E}_\lambda(\beta) \,|\, X] = \frac{1}{2}\|\hat{\Sigma}_\lambda^{1/2}(\beta - \beta_\lambda)\|^2 + \frac{1}{2}\sigma^2 + \frac{1}{2}\|\hat{\Sigma}^{1/2}\beta_0\|^2 - \frac{1}{2}\|\hat{\Sigma}_\lambda^{1/2}\beta_\lambda\|^2$
- excess penalised prediction error:
  $\|\hat{\Sigma}_\lambda^{1/2}(\hat{\beta} - \beta_\lambda)\|^2 = n^{-1}\|X(\hat{\beta} - \beta_\lambda)\|^2 + \lambda\|\hat{\beta} - \beta_\lambda\|^2 =: \mathscr{E}^{\text{in}}_{\lambda,\beta_\lambda}(\hat{\beta})$
- regularised in-sample prediction loss:
  $\mathscr{E}^{\text{in}}_{\lambda,\gamma}(\hat{\beta}) := \|\hat{\Sigma}_\lambda^{1/2}(\hat{\beta} - \gamma)\|^2 = n^{-1}\|X(\hat{\beta} - \gamma)\|^2 + \lambda\|\hat{\beta} - \gamma\|^2$
- prediction risk: $\mathscr{R}^{\text{in}}_{\lambda,\gamma}(\hat{\beta}) := \mathbb{E}[\mathscr{E}^{\text{in}}_{\lambda,\gamma}(\hat{\beta}) \,|\, X]$

Standard prediction error decomposition
(Useful for linear regularisation methods)

Consider for any residual filter function $R : [0,\infty) \to \mathbb{R}$ the estimator $\hat{\beta} = \hat{\Sigma}_\lambda^{-1/2}(I_p - R(\hat{\Sigma}_\lambda))y_\lambda$.

Then the penalised prediction loss satisfies $\mathscr{E}^{\text{in}}_{\lambda,\gamma}(\hat{\beta}) = A_{\lambda,\gamma}(R) + S_\lambda(R) - 2C_{\lambda,\gamma}(R)$

with approximation, stochastic and cross term errors

$$A_{\lambda,\gamma}(R) = \|\hat{\Sigma}_\lambda^{1/2}(R(\hat{\Sigma}_\lambda)\beta_\lambda + (\gamma - \beta_\lambda))\|^2,$$

$$S_\lambda(R) = \|(I_p - R(\hat{\Sigma}_\lambda))\varepsilon_\lambda\|^2,$$

$$C_{\lambda,\gamma}(R) = \langle \hat{\Sigma}_\lambda^{1/2}(R(\hat{\Sigma}_\lambda)\beta_\lambda + (\gamma - \beta_\lambda)), (I_p - R(\hat{\Sigma}_\lambda))\varepsilon_\lambda \rangle .$$

If R is deterministic, then $\mathscr{R}^{\text{in}}_{\lambda,\gamma}(\hat{\beta}) = A_{\lambda,\gamma}(R) + \frac{\sigma^2}{n}\text{trace}((I_p - R(\hat{\Sigma}_\lambda))^2\hat{\Sigma}_\lambda^{-1}\hat{\Sigma})$.

Prediction error decomposition for CG

[Hucker and Reiß 2025, Proposition 5.2]

- denote by $x_{1,t}$ the smallest zero on $[0,\infty)$ of R_t^{CG}, $t \in (0,p]$
- for $x \geqslant 0$, $R_{t,<}^{\mathsf{CG}}(x) := R_t^{\mathsf{CG}}(x)\mathbf{1}(x < x_{1,t})$, $R_{t,>}^{\mathsf{CG}}(x) := R_t^{\mathsf{CG}}(x)\mathbf{1}(x > x_{1,t})$

At $t \in [0,p]$, the penalised CG estimator satisfies for $\gamma = \beta_\lambda$

$$\ell_{\lambda,\beta_\lambda}^{\mathsf{in}}(\hat{\beta}_{\lambda,t}^{\mathsf{CG}}) = A_{\lambda,\beta_\lambda,t}^{\mathsf{CG}} + S_{\lambda,t}^{\mathsf{CG}} - 2C_{\lambda,\beta_\lambda,t}^{\mathsf{CG}} \leqslant 2A_{\lambda,\beta_\lambda,t}^{\mathsf{CG}} + 2S_{\lambda,t}^{\mathsf{CG}}$$

with approximation, stochastic and cross term errors given by

$$A_{\lambda,\beta_\lambda,t}^{\mathsf{CG}} := \|\hat{\Sigma}_\lambda^{1/2} R_{t,<}^{\mathsf{CG}}(\hat{\Sigma}_\lambda)^{1/2}\beta_\lambda\|^2 + \|R_t^{\mathsf{CG}}(\hat{\Sigma}_\lambda)y_\lambda\|^2 - \|R_{t,<}^{\mathsf{CG}}(\hat{\Sigma}_\lambda)^{1/2}y_\lambda\|^2 \leqslant \|\hat{\Sigma}_\lambda^{1/2} R_{t,<}^{\mathsf{CG}}(\hat{\Sigma}_\lambda)^{1/2}\beta_\lambda\|^2,$$

$$S_{\lambda,t}^{\mathsf{CG}} := \|(I_p - R_{t,<}^{\mathsf{CG}}(\hat{\Sigma}_\lambda))^{1/2}\varepsilon_\lambda\|^2, \quad C_{\lambda,\beta_\lambda,t}^{\mathsf{CG}} := \langle R_{t,>}^{\mathsf{CG}}(\hat{\Sigma}_\lambda)y_\lambda, \varepsilon_\lambda\rangle .$$

$$\rho_t := |(R_t^{\mathsf{CG}})'(0)|,$$

$$(1-\rho_t x)_+ \leqslant R_t^{\mathsf{CG}}(x) \leqslant \exp(-\rho_t)x, \quad x \in [0, x_{1,t}]$$

[Hucker and Reiß 2025, Lemma 4.7]

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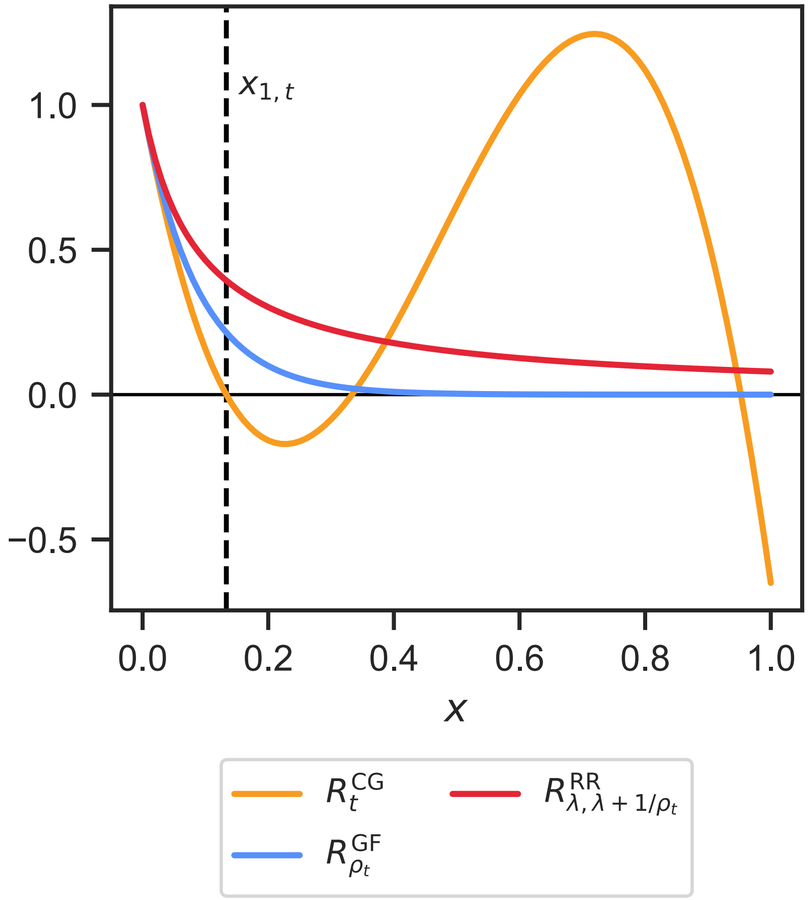
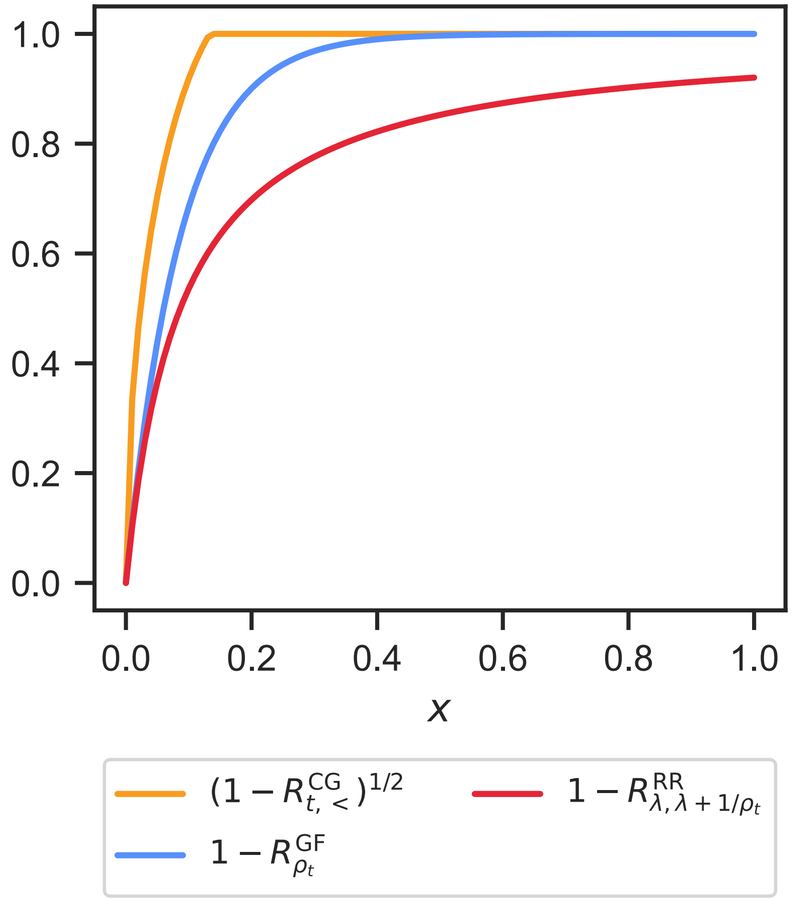
[Hucker and Reiß 2025, Lemma 4.7]





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[Hucker and Reiß 2025, Lemma 4.7]

Let $t \in [0,p]$. Assume that $\gamma \in \mathbb{R}^p$ satisfies the condition (CROSS)

$$\langle \hat{\Sigma}_\lambda \exp(-\rho_t \hat{\Sigma}_\lambda/2)\beta_\lambda, \gamma - \beta_\lambda \rangle \geqslant 0.$$

Then the regularised in-sample prediction loss for the CG estimator is bounded by

$$\ell^{\mathsf{in}}_{\lambda,\gamma}(\hat{\beta}^{\mathsf{CG}}_{\lambda,t}) \leqslant 4\overline{A}^{\mathsf{CG}}_{\lambda,\gamma,t} + 2\overline{S}^{\mathsf{CG}}_{\lambda,t}$$

with γ-dependent approximation and stochastic error bounds

$$\overline{A}^{\mathsf{CG}}_{\lambda,\gamma,t} := \|\hat{\Sigma}_\lambda^{1/2}(\beta_\lambda - \exp(-\rho_t\hat{\Sigma}_\lambda/2)\beta_\lambda - \gamma)\|^2, \quad \overline{S}^{\mathsf{CG}}_{\lambda,t} := \|(\rho_t\hat{\Sigma}_\lambda \wedge 1)^{1/2}\varepsilon_\lambda\|^2.$$

Main result

Compare CG and GF errors up to a random time shift

- inverting $t \mapsto \rho_t/2$ leads to the random times
  $\tau_t := \inf\{\tilde{t} \in [0,p] \,|\, |(R^{\mathsf{CG}}_{\tilde{t}})'(0)| \geqslant 2t\} \wedge p, \quad t \geqslant 0$
- under (CROSS), $\mathscr{R}^{\mathsf{in}}_{\lambda,\gamma}(\hat{\beta}^{\mathsf{CG}}_{\lambda,\tau_t}) \leqslant 4A_{\lambda,\gamma}(R^{\mathsf{GF}}_t) + \frac{4\sigma^2}{n}\mathsf{trace}((2t \wedge \hat{\Sigma}_\lambda^{-1})\hat{\Sigma})$
- remains to compare stochastic errors of CG and GF

For $t \geqslant \frac{1}{2(s_1+\lambda)}$ set $C_{t,\lambda} := \big(\sum_{j \geqslant i_t} s_j\big)\big(\sum_{j<i_t} \frac{(s_{i_t}+\lambda)s_j}{s_j+\lambda} + \sum_{j \geqslant i_t} \frac{(s_j+\lambda)s_j}{s_{i_t-1}+\lambda}\big)^{-1}\mathbf{1}\big(t < \frac{1}{2}(s_p+\lambda)^{-1}\big)$

with $i_t := \min\{j \,|\, s_j < (2t)^{-1} - \lambda\}$. Then $C_{t,\lambda} \leqslant C_{t,0}$ holds, and under (CROSS) for γ we have

$$\forall t \geqslant \frac{1}{2\|\hat{\Sigma}_\lambda\|} : \quad \mathscr{R}^{\mathsf{in}}_{\lambda,\gamma}(\hat{\beta}^{\mathsf{CG}}_{\lambda,\tau_t}) \leqslant \frac{4(1+C_{t,\lambda})}{(1-e^{-1/2})^2}\mathscr{R}^{\mathsf{in}}_{\lambda,\gamma}(\hat{\beta}^{\mathsf{GF}}_{\lambda,t}) \,.$$

Examples

Polynomial and geometric decay of the eigenvalues

For $t \geqslant \frac{1}{2(s_1+\lambda)}$ set

$$C_{t,\lambda} := \Big(\sum_{j \geqslant i_t} s_j\Big)\Big(\sum_{j<i_t} \frac{(s_{i_t}+\lambda)s_j}{s_j+\lambda} + \sum_{j \geqslant i_t} \frac{(s_j+\lambda)s_j}{s_{i_t-1}+\lambda}\Big)^{-1} \mathbf{1}\Big(t < \frac{1}{2}(s_p+\lambda)^{-1}\Big)$$

with $i_t := \min\{j \mid s_j < (2t)^{-1} - \lambda\}$.

Suppose for some $C > 0$, $\alpha > 1$, $\quad \forall\, 2 \leqslant i \leqslant j \leqslant p : \ s_j/s_i \leqslant C(j/i)^{-\alpha}$.

Then all $C_{t,\lambda}$ are uniformly bounded:

$$C_{t,\lambda} \leqslant C_{t,0} \leqslant \frac{C\sum_{j \geqslant i_t}(j/i_t)^{-\alpha}}{i_t - 1} \leqslant \frac{C(\alpha+1)}{\alpha-1}.$$

Simulated data

solid lines:

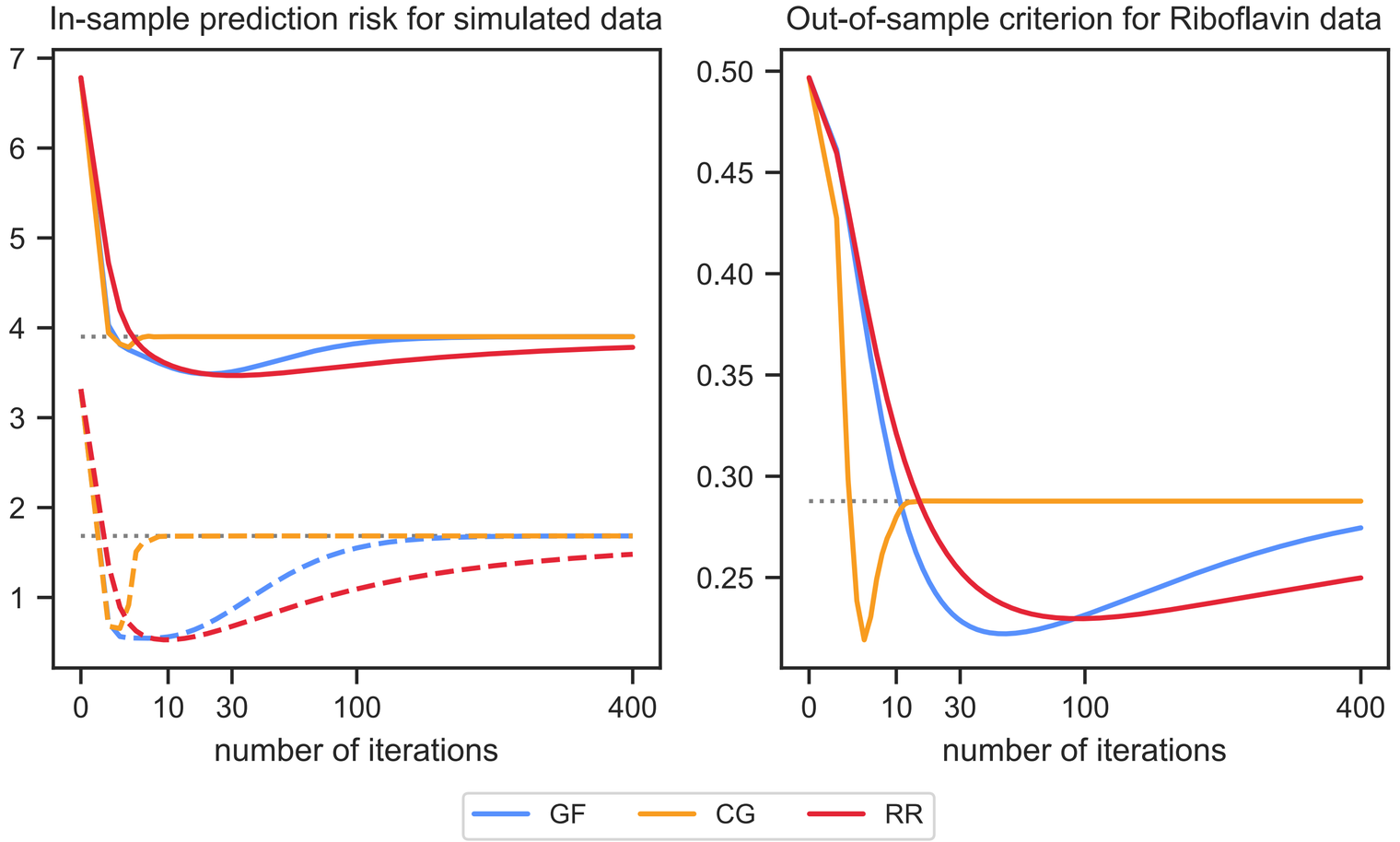
$\gamma = \beta_0$

dashed lines:

$\gamma = \beta_\lambda$

grey lines:

$\hat{\beta}_\lambda^{\mathrm{RR}}$



Real data

solid lines:

$\mathscr{E}_\lambda(\hat{\beta})$

grey line:

$\hat{\beta}_\lambda^{\mathrm{RR}}$

- $n = 400, p = 500, \lambda = 3$, 1000 Monte Carlo runs
- $\beta_0 \sim \mathcal{N}(0, p^{-1} I_p)$
- $x_i \sim \mathcal{N}(0, \Sigma)$, $\lambda_1 = \ldots = \lambda_{20} = 100, \lambda_{21} = \ldots = \lambda_{500} = 1$
- $\varepsilon_i \sim \mathcal{N}(0, 6)$

- *Riboflavin* data from R package hdi
- $n = 71, p = 2n, \lambda = 0.1$
- 1000 splits: 50 training observations, 21 test data points
- ridge criterion $\mathscr{E}_\lambda(\hat{\beta})$ evaluated on test set

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Thanks a lot for your attention!

Some further references

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