Hyper-parameters Selection by Algorithmic Differentiation

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Joint work with






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Parametric estimators

Estimator

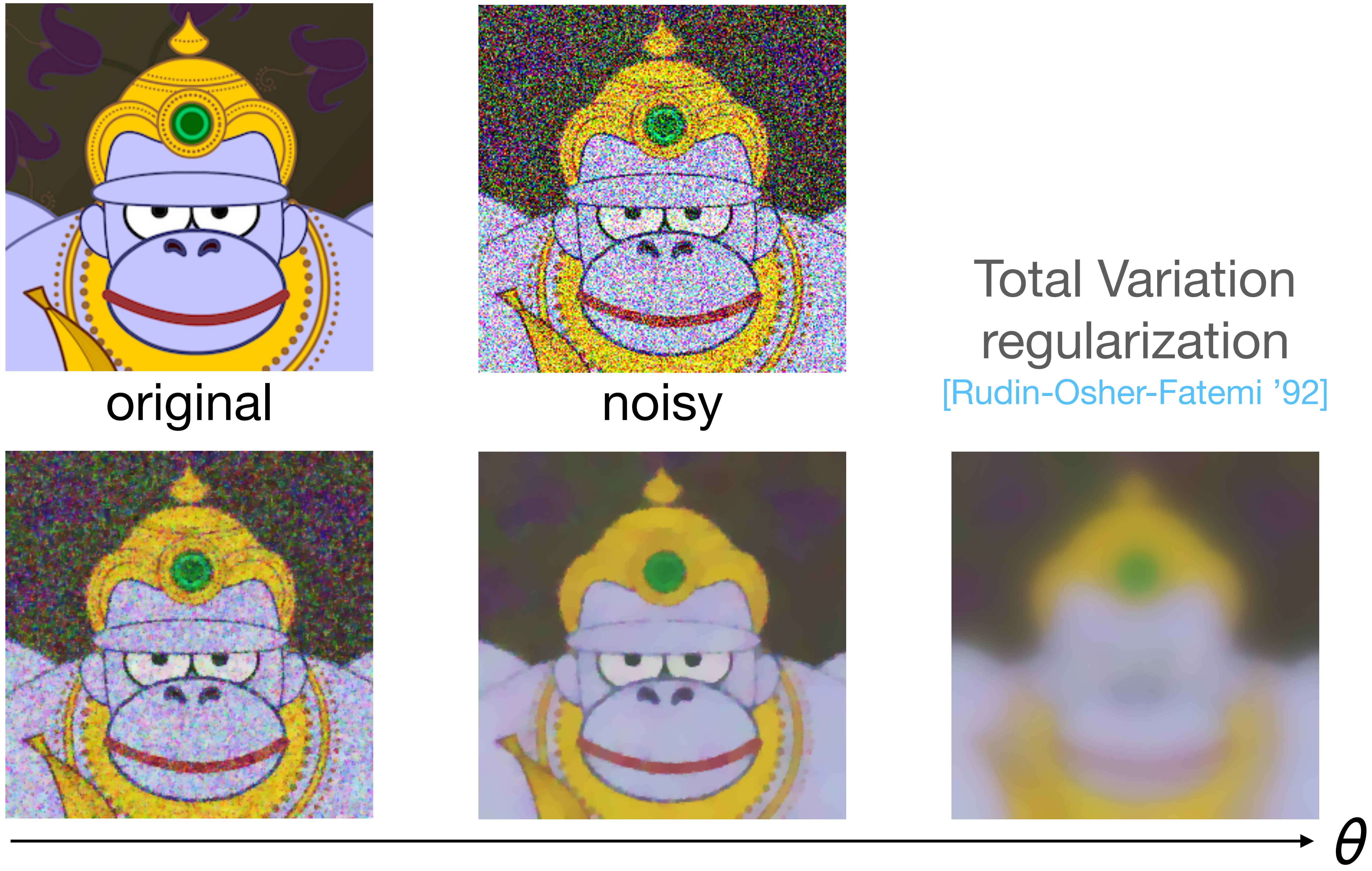
$$\hat{w}_\theta : \begin{cases} \mathbb{R}^n & \longrightarrow \mathbb{R}^p \\ y & \longmapsto \hat{w}_\theta(y) \end{cases}$$

observations

Hyper-parameters

$$\theta \in \Theta \subseteq \mathbb{R}^l$$

parameter space



Typical example

linear regression

$$y = X w_{\text{true}} + \varepsilon$$

design matrix ground truth noise

regularization *a.k.a* variational methods

$$\hat{w}_\theta(y) \in \operatorname{argmin}_w \ \text{datafit}(w, y) + \text{regularity}(w, \theta)$$

trade-off

e.g. Lasso: $\operatorname{argmin}_w \|y - Xw\|_2^2 + \theta \|w\|_1$ [Chen-Donoho '94, Tibshirani '95]

Selection criteria

Estimator

$\hat{w}_\theta : \mathbb{R}^n \longrightarrow \mathbb{R}^p$ estimator

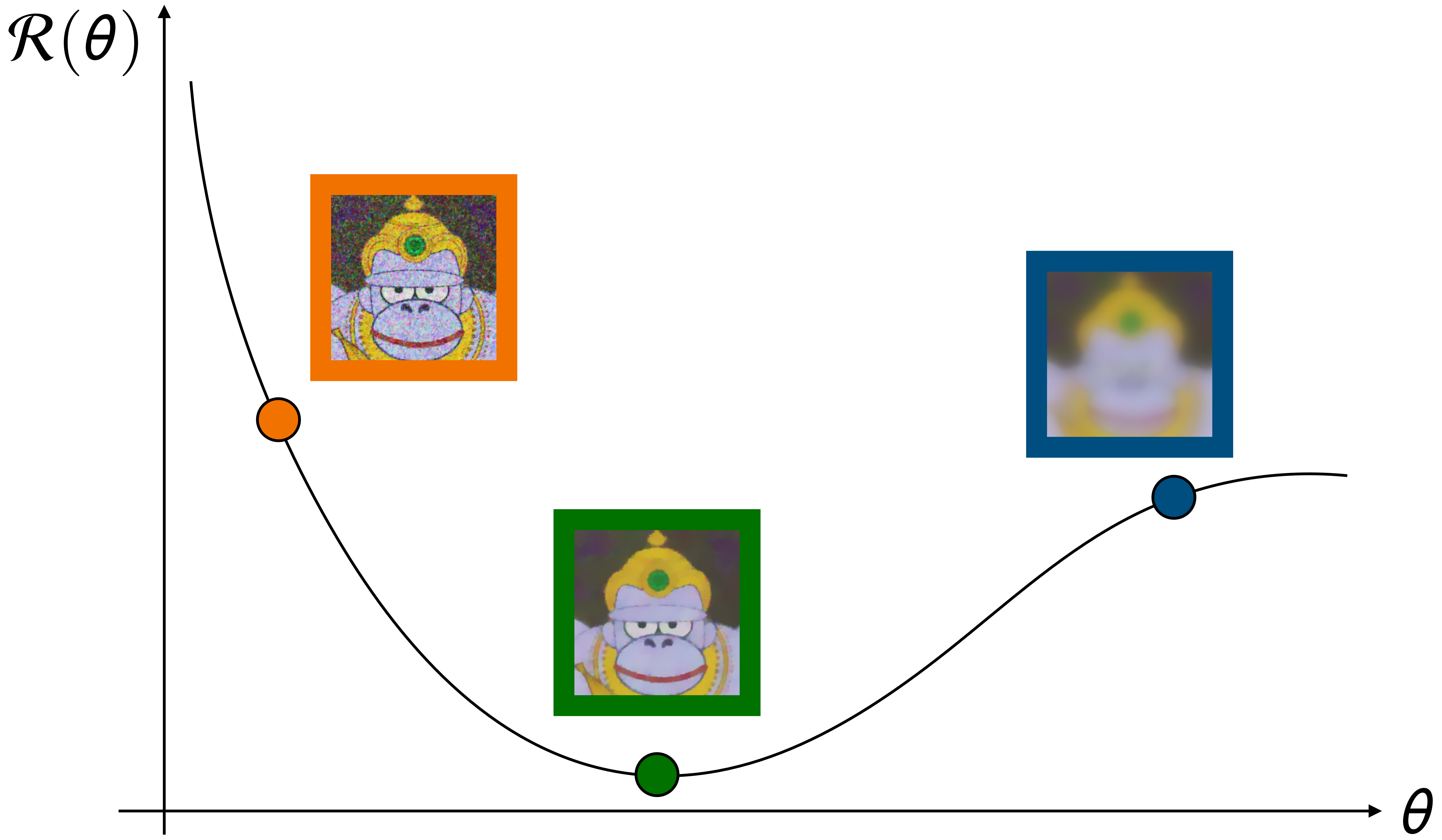
$\theta \in \Theta$ hyper-parameter

$\mathcal{R} : \Theta \longrightarrow \mathbb{R}$ criterion

Goal

Find $\theta^\star \in \operatorname*{argmin}_{\theta \in \Theta} \mathcal{R}(\theta)$

(or close to it)



Inverse problems

$y = X w_{\text{true}} + \varepsilon$

estimation risk

[Rice '86]

$$\mathcal{R}(\theta) = \mathbb{E}_\varepsilon \left(\| \hat{w}_\theta(y) - w_{\text{true}} \|_2^2 \right)$$

Machine learning

validation set: $y^{\text{val}}, X^{\text{val}}$

hold-out loss

[Stone-Ramer '65]

$$\mathcal{R}(\theta) = \| y^{\text{val}} - X^{\text{val}} \hat{w}_\theta(y) \|_2^2$$

projected risk
cross-validation
model criteria
...

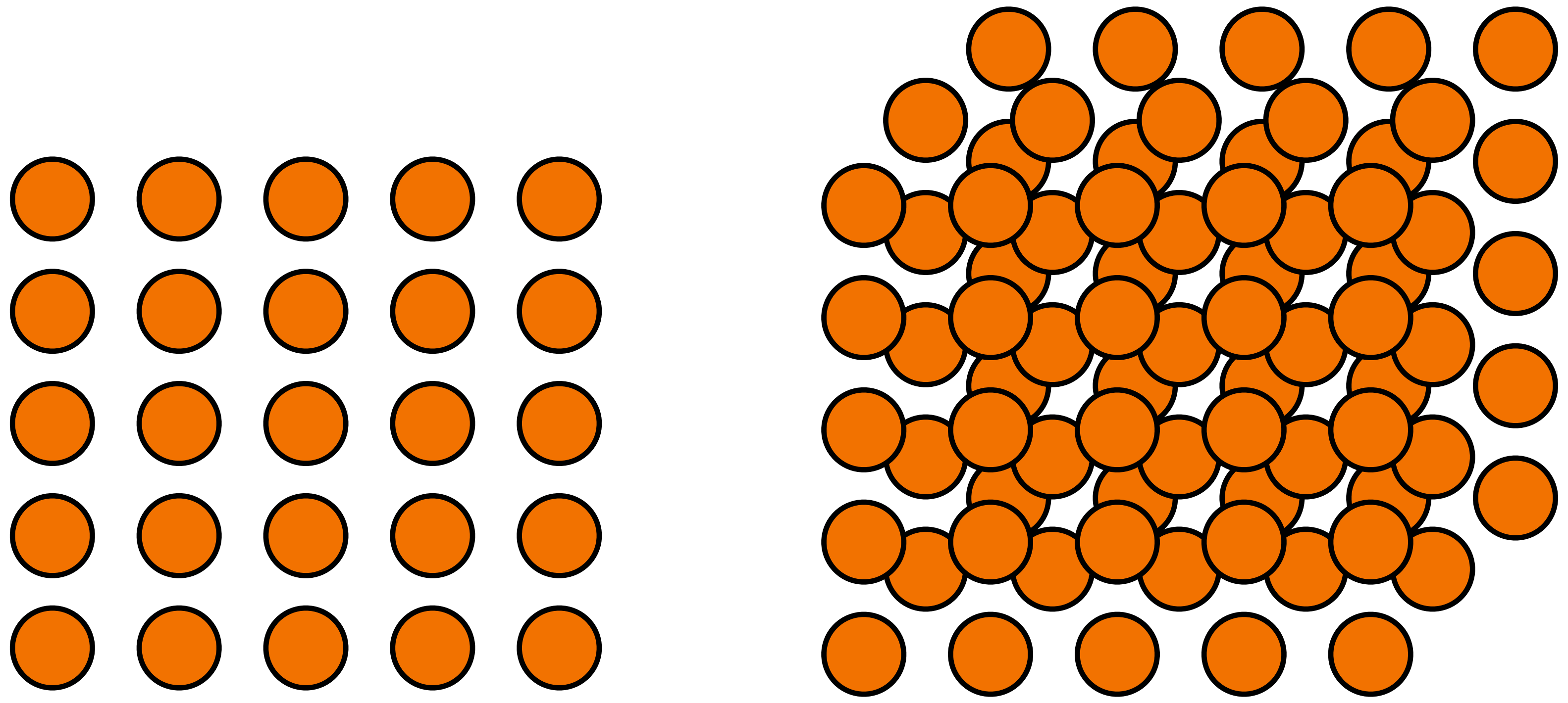
Grid search

Algorithm

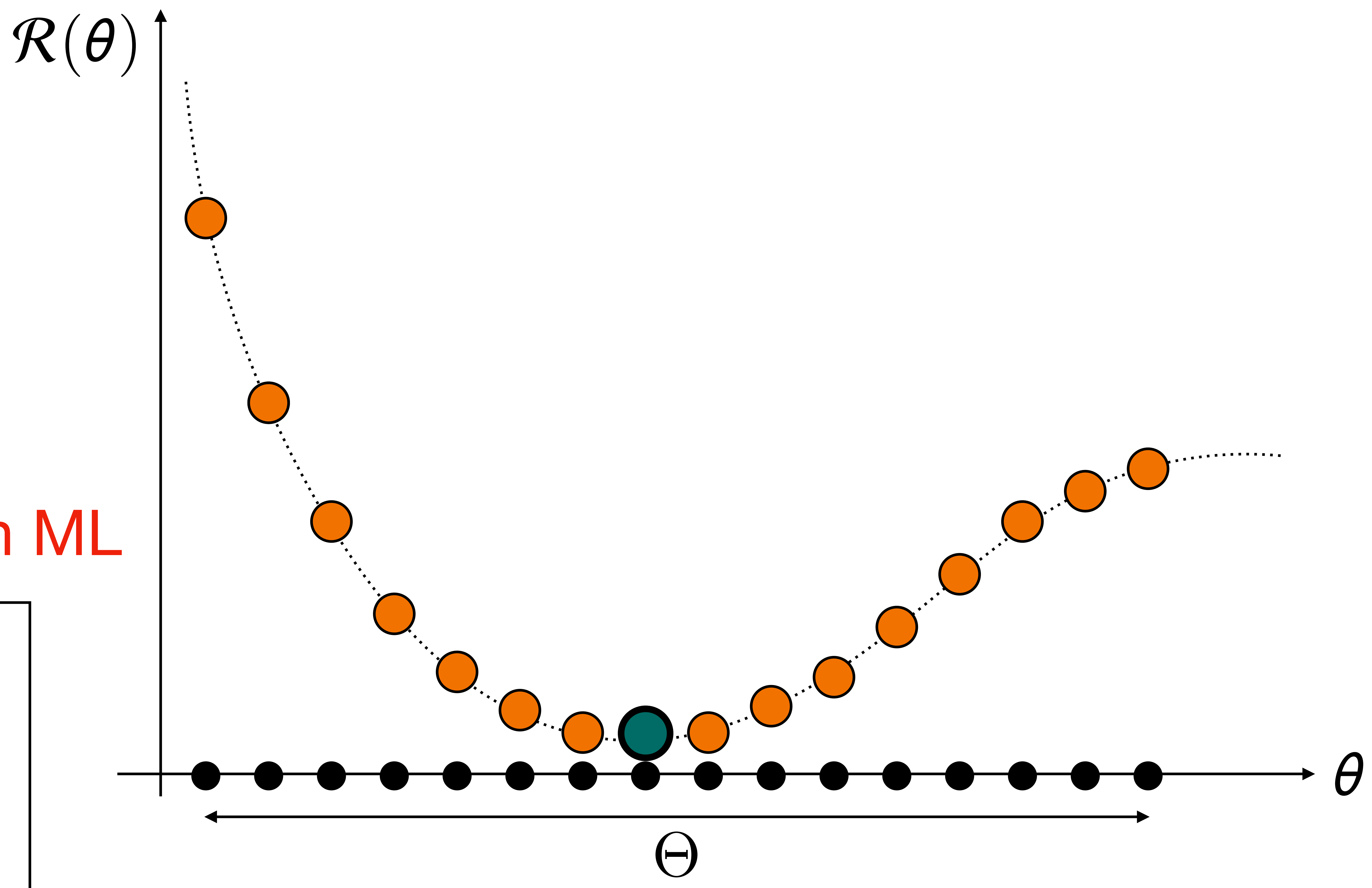
1. Choose a criterion $\mathcal{R}$
2.
3.
4.

Grid search is the standard in ML

Dimensionality issues of sampling Θ



2 parameters   3 parameters



Can be mitigated using Random Search [Bergstra-Bengio ’12]
Bayesian methods [Brochu et al. ’10]

First order methods for parameter selection

Goal

Find $\theta^\star \in \underset{\theta \in \Theta}{\operatorname{argmin}}\ \mathcal{R}(\theta)$

(or close to it)

$$\mathcal{R}(\theta) = \mathcal{C}(\hat{w}_\theta(y)) = (\mathcal{C} \circ \hat{w}_\bullet(y))\,(\theta)$$

$$\mathcal{C} : \mathbb{R}^p \to \mathbb{R}$$

$$\hat{w}_\bullet(y) : \Theta \subseteq \mathbb{R}^l \to \mathbb{R}^p$$

Chain rule

Assuming $\mathcal{C}$ and $\hat{w}_\bullet(y)$ to be differentiable

$$\nabla\mathcal{R}(\theta) = \left[\mathrm{Jac}_{\hat{w}_\bullet(y)}(\theta)\right]^\perp \nabla\mathcal{C}(\hat{w}_\theta(y))$$

and

$$\nabla\mathcal{R}(\theta^\star) = 0$$

Potential issues

- differentiability
- access to the cost
- size of the Jacobian
- approximation stability
- convergence (non-convex)

“Hyper”-gradient descent

$$\theta^{k+1} = \theta^k - \rho\nabla\mathcal{R}(\theta^k)$$

possibly **projected** gradient descent on the parameter space

First order methods for parameter selection

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Find $\theta^\star \in \underset{\theta \in \Theta}{\operatorname{argmin}}\, \mathcal{R}(\theta)$

(or close to it)

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and

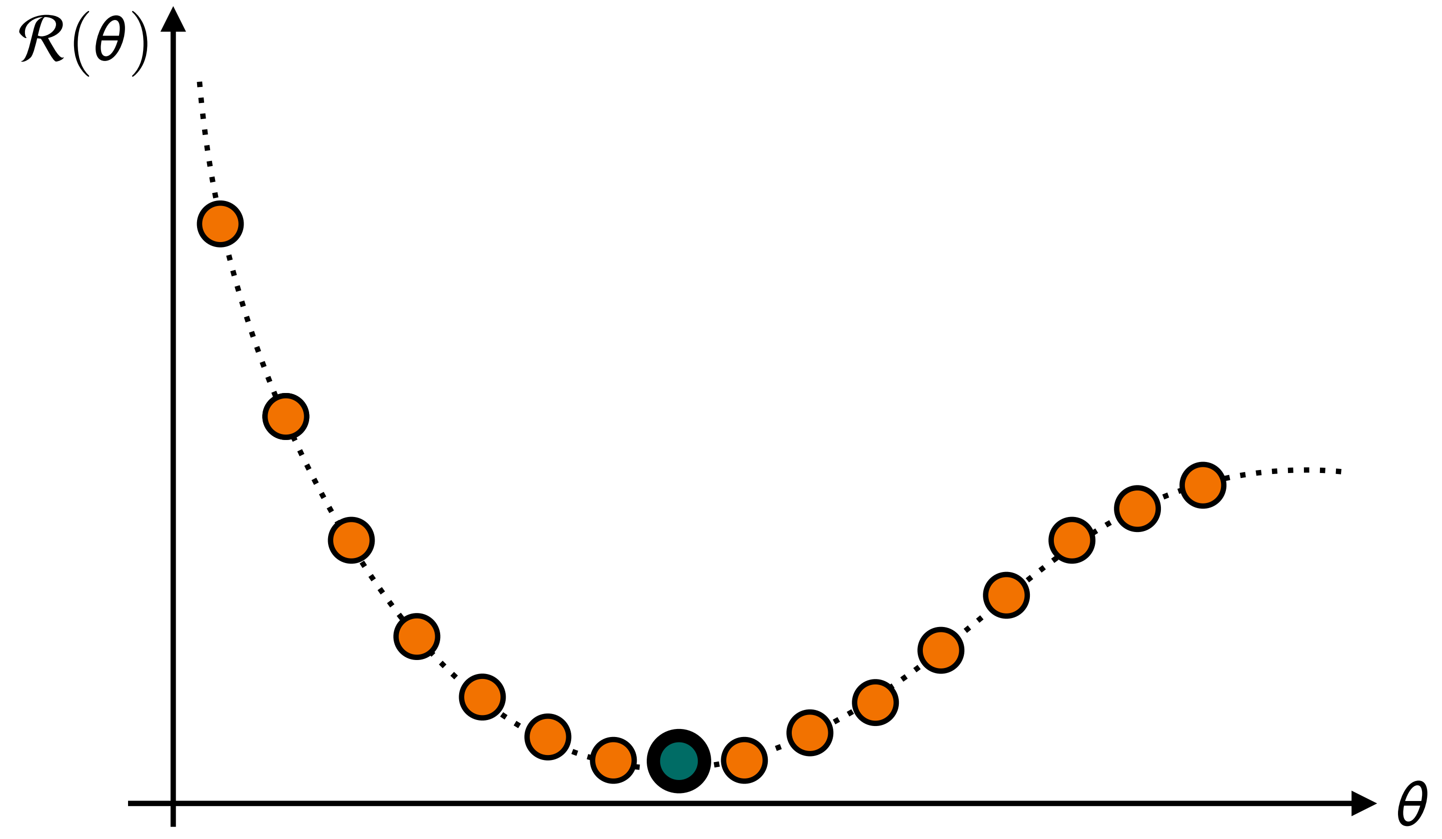
$$\nabla\mathcal{R}(\theta^\star) = 0$$

"Hyper"-gradient descent

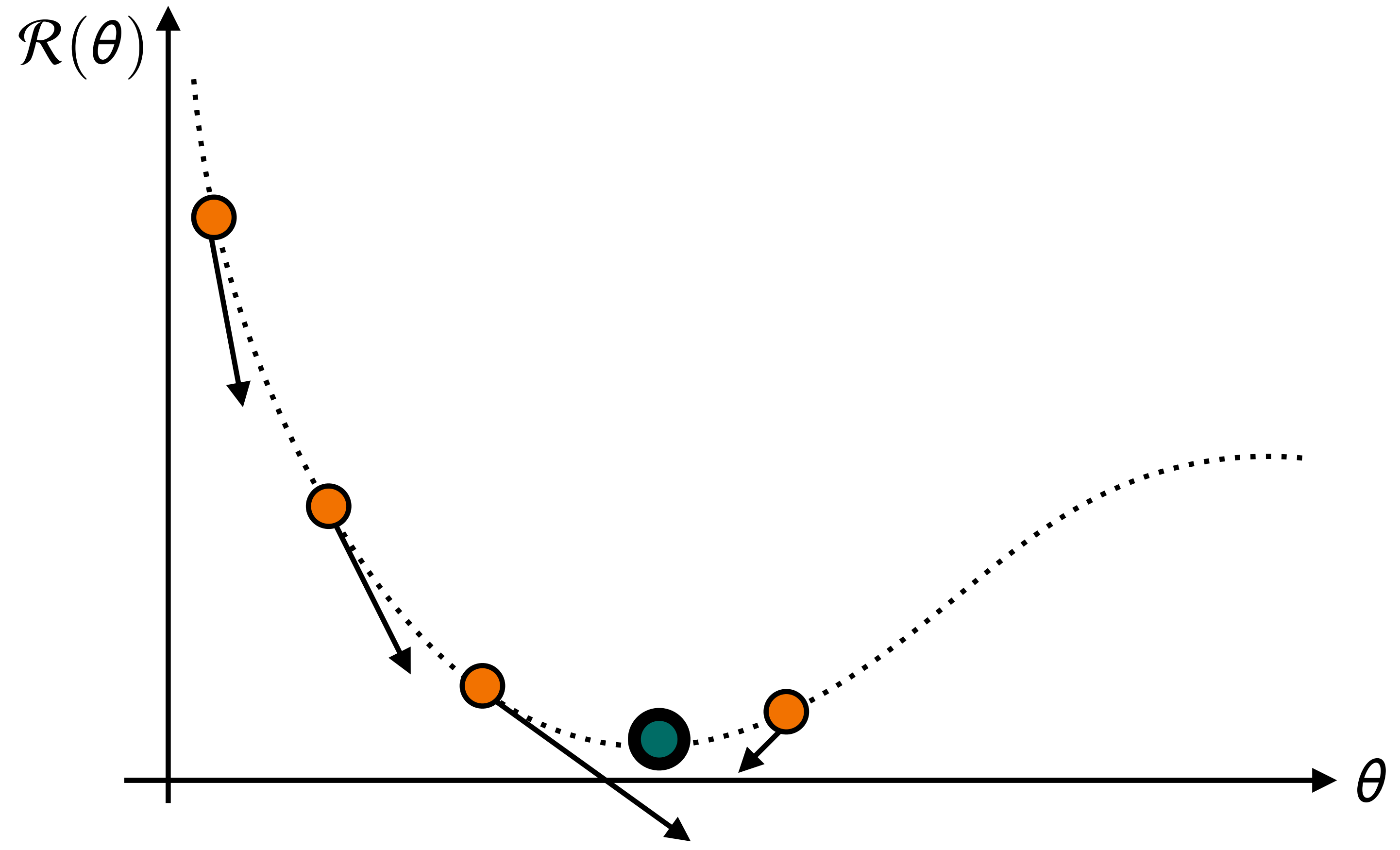
$$\theta^{k+1} = \theta^k - \rho\nabla\mathcal{R}(\theta^k)$$

possibly **projected** gradient descent on the parameter space

Grid search (a.k.a 0-order)



Gradient descent



Estimating a Jacobian

Estimator

$\hat{w}_\theta : \mathbb{R}^n \longrightarrow \mathbb{R}^p$

differentiable

Jacobian

$\mathrm{Jac}_{\hat{w}_\bullet}(y) : \Theta \longrightarrow \mathbb{R}^{p \times l}$

$\mathrm{Jac}_{\hat{w}_\theta} : \mathbb{R}^n \longrightarrow \mathbb{R}^{p \times n}$

$$\mathrm{Jac}_{\hat{w}_\theta}(y) = \begin{pmatrix} \frac{\partial(\hat{w}_\theta)_1}{\partial y_1}(y) & \cdots & \frac{\partial(\hat{w}_\theta)_1}{\partial y_n}(y) \\ \vdots & & \vdots \\ \frac{\partial(\hat{w}_\theta)_p}{\partial y_1}(y) & \cdots & \frac{\partial(\hat{w}_\theta)_p}{\partial y_n}(y) \end{pmatrix} \in \mathbb{R}^{p \times n}$$

Numerical approximation

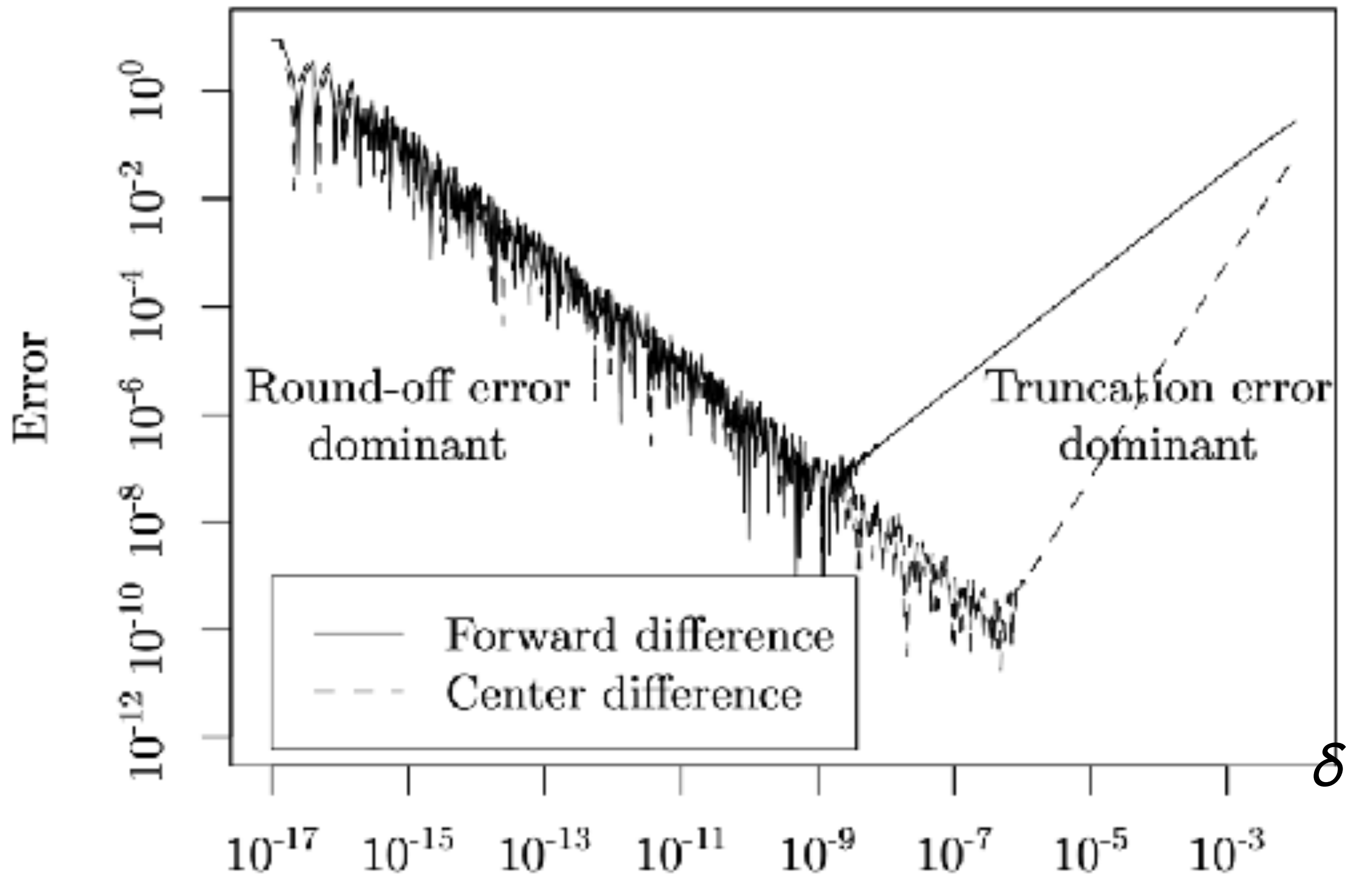
$$\mathrm{Jac}_{\hat{w}_\theta}(y) \approx \begin{pmatrix} \frac{\hat{w}_\theta(y+\delta \mathbf{e}_1)-\hat{w}_\theta(y)}{\delta} & \cdots & \frac{\hat{w}_\theta(y+\delta \mathbf{e}_n)-\hat{w}_\theta(y)}{\delta} \end{pmatrix}$$

needs $O(nT)$ operations

parameter dimension   cost of evaluating $\hat{w}_\theta(\cdot)$

Numerical errors

from [Baydin '18]



$f(x) = 64x(1-x)(1-2x)^2(1-8x+8x^2)^2$

Unstable for low **and** high precision

Symbolic differentiation

Used by Mathematica, Maple, SymPy, Maxima, Lisp

Ineffective for "complex" programs

$\longrightarrow$ expression swell

The SURE way

SV, C. Deledalle, G. Peyré, J. Fadili, C. Dossal. The Degrees of Freedom of Partly Smooth Regularizers. Ann Inst Stat Math. 69(4):791—832. 2017
SV, C. Deledalle, G. Peyré, C. Dossal, J. Fadili. Local Behavior of Sparse Analysis Regularization: Applications to Risk Estimation. Appl Comput Harmon Anal. 35(3):433—451. 2013.

Estimation and prediction risk

Goal

Find $\theta^\star \in \underset{\theta \in \Theta}{\operatorname{argmin}} \mathcal{R}(\theta)$

(or close to it)

Inverse problems

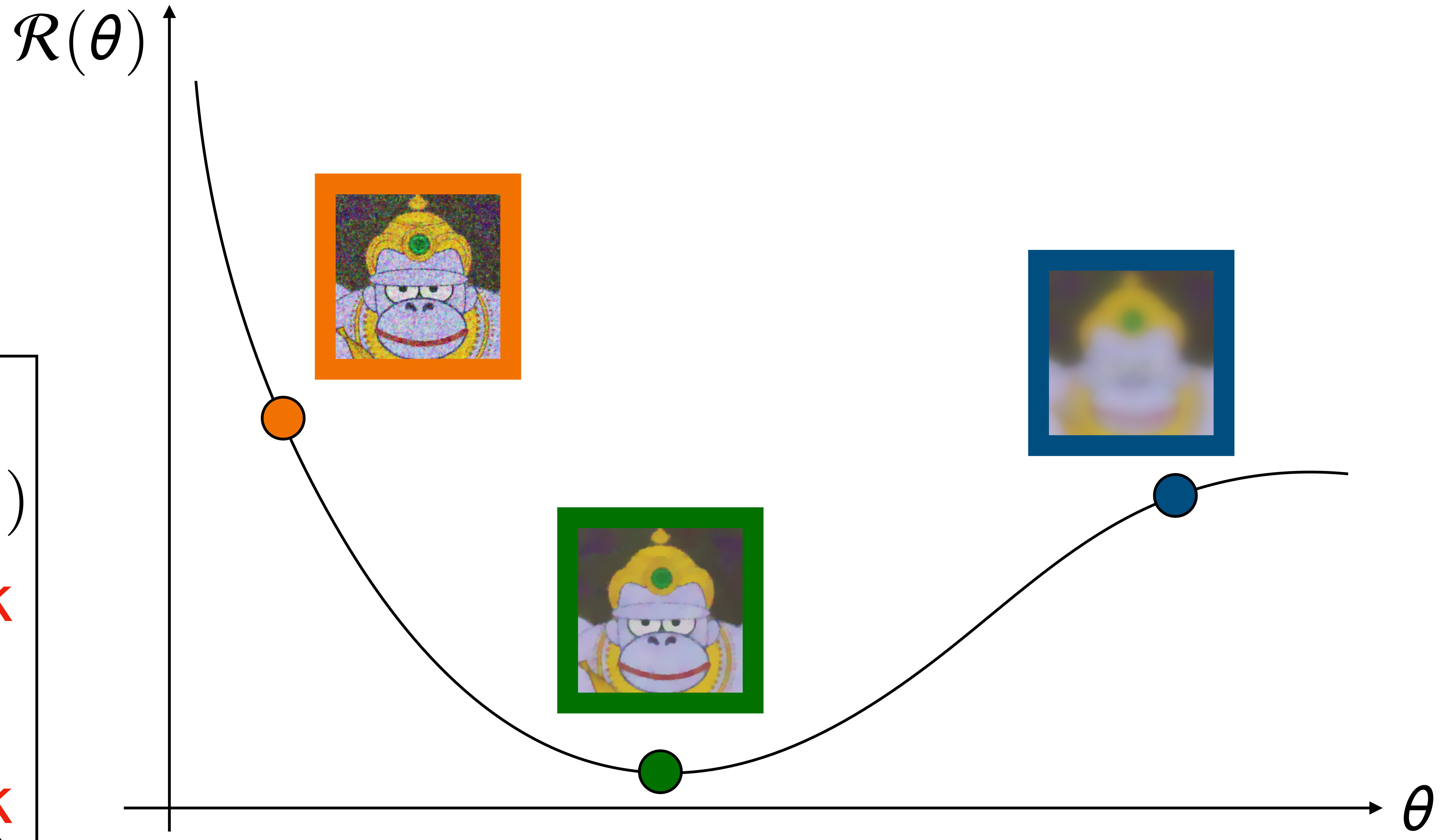
$y = X w_{\text{true}} + \varepsilon \qquad \varepsilon \sim \mathcal{N}(0, \sigma^2 \text{Id})$

estimation risk

$$\mathcal{R}(\theta) = \mathbb{E}_\varepsilon \left(\|\hat{w}_\theta(y) - w_{\text{true}}\|_2^2 \right)$$

prediction risk

$$\mathcal{R}(\theta) = \mathbb{E}_\varepsilon \left(\|X \hat{w}_\theta(y) - X w_{\text{true}}\|_2^2 \right)$$



only **one** observation $y \implies \mathbb{E}_\varepsilon$ is not computable

only one **observation** $y \implies w_{\text{true}}$ is not known

Stein Unbiased Risk Estimation — SURE

Inverse problems

$$y = X w_{\text{true}} + \varepsilon \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 \mathrm{Id})$$

Prediction

$$\hat{\mu}_\theta(y) = X \hat{w}_\theta(y)$$

Prediction risk

$$\mathcal{R}(\theta) = \mathbb{E}_\varepsilon \left(\|\hat{\mu}_\theta(y) - X w_{\text{true}}\|_2^2 \right)$$

Degrees of freedom [Efron '86]

$$\mathrm{df}_\theta(y) = \sum_{i=1}^{n} \frac{\mathrm{cov}(\hat{\mu}_\theta(y)_i, y_i)}{\sigma^2}$$

Cp [Mallows '73]
AIC [Akaike '73]
BIC [Schwarz '78]
GCV [Craven-Wahba '79]
SURE [Stein '81]

Examples

Ordinary least square

$$\mathrm{df}_\theta(y) = p$$

Lasso [Dossal et al. '13, Zou et al. '07]

$$\mathrm{df}_\theta(y) = \|\hat{w}_\theta(y)\|_0 = |\operatorname{supp}(\hat{w}_\theta(y))|$$

Stein's lemma

[Stein '81]

If $\hat{\mu}_\theta$ weakly differentiable

Empirical degrees of freedom

$$\widehat{\mathrm{df}}_\theta(y) = \mathrm{div}(\hat{\mu}_\theta(y)) = \sum_{i=1}^{n} \frac{\partial (\hat{\mu}_\theta)_i}{\partial y_i}(y)$$

$$\mathbb{E}_\varepsilon(\widehat{\mathrm{df}}_\theta(y)) = \mathrm{df}_\theta(y)$$

Stein Unbiased Risk Estimation

[Stein '81]

If $\hat{\mu}_\theta$ weakly differentiable

$$\mathrm{SURE}_\theta(y) = \|y - \hat{\mu}_\theta(y)\|_2^2 - n\sigma^2 + 2\sigma^2 \widehat{\mathrm{df}}_\theta(y)$$

$$\mathbb{E}_\varepsilon(\mathrm{SURE}_\theta(y)) = \mathcal{R}(\theta)$$

🥴 requires the noise variance

SURE for smooth regularized least square

Inverse problems

$$y = X w_{\text{true}} + \varepsilon \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 \mathrm{Id})$$

Prediction

$$\hat{\mu}_\theta(y) = X \hat{w}_\theta(y)$$

Prediction risk

$$\mathcal{R}(\theta) = \mathbb{E}_\varepsilon \left(\|\hat{\mu}_\theta(y) - X w_{\text{true}}\|_2^2 \right)$$

Degrees of freedom and SURE

$$\widehat{\mathrm{df}}_\theta(y) = \mathrm{div}(\hat{\mu}_\theta(y)) = \sum_{i=1}^{n} \frac{\partial (\hat{\mu}_\theta)_i}{\partial y_i}(y)$$

$$\mathrm{SURE}_\theta(y) = \|y - \hat{\mu}_\theta(y)\|_2^2 - n\sigma^2 + 2\sigma^2 \widehat{\mathrm{df}}_\theta(y)$$

$$\mathbb{E}_\varepsilon(\mathrm{SURE}_\theta(y)) = \mathcal{R}(\theta)$$

Smooth regularised least-square

$$\hat{w}_\theta(y) \in \underset{w \in \mathbb{R}^p}{\mathrm{argmin}} \ \frac{1}{2}\|y - X w\|_2^2 + \theta J(w)$$

First order conditions

$$X^\top (X \hat{w}_\theta(y) - y) + \theta \nabla J(\hat{w}_\theta(y)) = 0$$

Implicit function theorem

$$\Gamma_\theta(y) = X^\top X + \theta \nabla^2 J(\hat{w}_\theta(y)) \longrightarrow \mathrm{Jac}_{\hat{\mu}_\theta}(y) = X \Gamma_\theta(y)^{-1} X^\top$$

SURE for regularized least square

Inverse problems

$$y = X w_{\text{true}} + \varepsilon \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 \mathrm{Id})$$

Prediction

$$\hat{\mu}_\theta(y) = X \hat{w}_\theta(y)$$

Prediction risk

$$\mathcal{R}(\theta) = \mathbb{E}_\varepsilon \left(\| \hat{\mu}_\theta(y) - X w_{\text{true}} \|_2^2 \right)$$

Degrees of freedom and SURE

$$\widehat{\mathrm{df}}_\theta(y) = \mathrm{div}(\hat{\mu}_\theta(y)) = \sum_{i=1}^{n} \frac{\partial (\hat{\mu}_\theta)_i}{\partial y_i}(y)$$

$$\mathrm{SURE}_\theta(y) = \| y - \hat{\mu}_\theta(y) \|_2^2 - n\sigma^2 + 2\sigma^2 \widehat{\mathrm{df}}_\theta(y)$$

$$\mathbb{E}_\varepsilon(\mathrm{SURE}_\theta(y)) = \mathcal{R}(\theta)$$

~~Smooth~~ regularised least-square

$$\hat{w}_\theta(y) \in \underset{w \in \mathbb{R}^p}{\mathrm{argmin}} \ \frac{1}{2} \| y - X w \|_2^2 + \theta J(w)$$

Theorem [V. et al. '13,17]

When J is regular enough, $\mathrm{Jac}_{\hat{\mu}_\theta(y)}(y)$ is computable *a.e.* in closed form

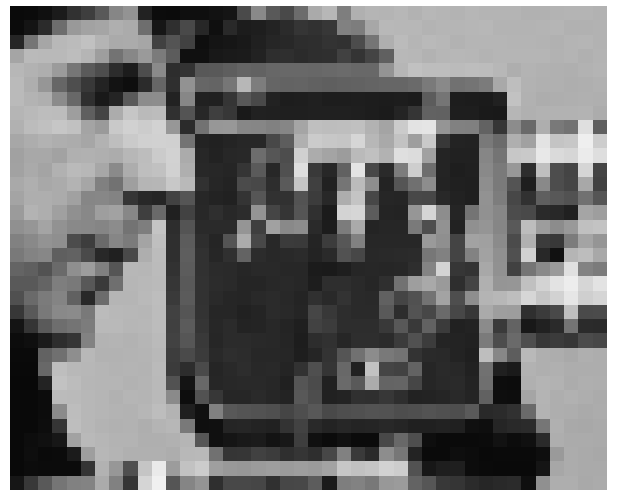
Generalizes [Yuan-Lin '06, Dossal et al. '12, Tibshirani-Taylor '12, ...]

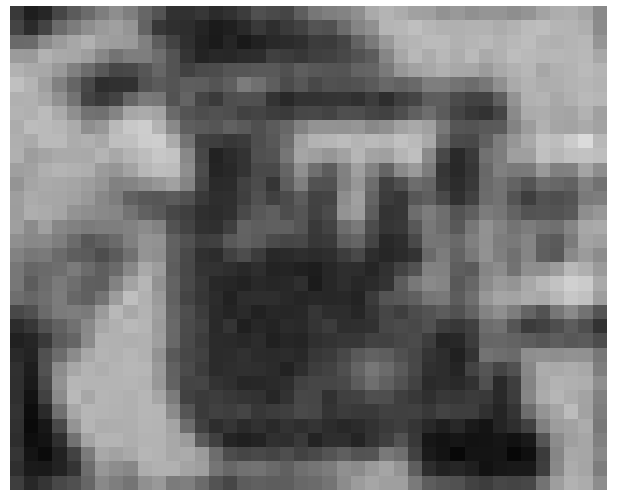
Example: SURE Grid search

Anisotropic Total Variation

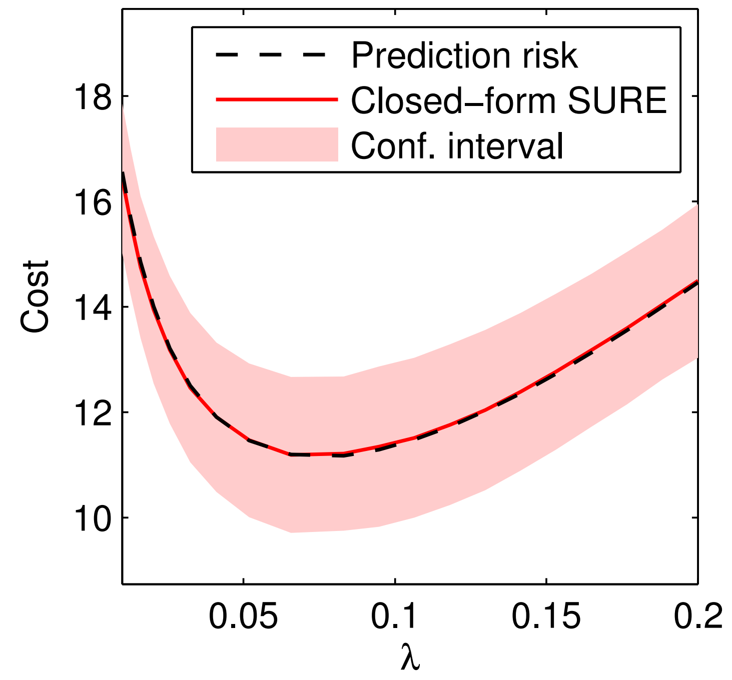
$$J(w) = \| \nabla_{2\mathrm{D}} w \|_1$$

X Gaussian convolution


original


blurred


optimal



Explicit SURE: shortcomings

Inverse problems

$$y = X w_{\text{true}} + \varepsilon \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 \mathrm{Id})$$

Prediction

$$\hat{\mu}_\theta(y) = X \hat{w}_\theta(y)$$

Prediction risk

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Degrees of freedom and SURE

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$$\mathbb{E}_\varepsilon(\mathrm{SURE}_\theta(y)) = \mathcal{R}(\theta)$$

Pb 1: expectation VS realization

only **one** observation $y \implies \mathbb{E}_\varepsilon$ is not computable

(Mostly stable because expectation of a low dimensional quantity with a high dimensional variable)

Pb 2: computational tractability

$\widehat{\mathrm{df}}_\theta(y) = \mathrm{trace}(\mathrm{Jac}_{\hat{\mu}_\theta}(y))$ potentially large

$\longrightarrow$ Monte Carlo SURE

Pb 3: convergence

$$\begin{tikzcd}
w_\theta^{(k)}(y) \arrow[r, "?"] \arrow[d, "\text{stability}"'] & \hat{w}_\theta(y) \arrow[d, dotted] \\
\mathrm{Jac}_{\hat{w}_\theta}(y) \arrow[r, "?"] & \mathrm{Jac}_{w_\theta^{(k)}}(y)
\end{tikzcd}$$

very high precision required

The SUGAR way

B. Pascal, SV, N. Pustelnik, P. Abry. Automated data-driven selection of the hyperparameters for Total-Variation based texture segmentation. 2020.
C. Deledalle, SV, J. Fadili, G. Peyré. Stein Unbiased GrAdient estimator of the Risk (SUGAR) for multiple parameter selection. SIAM J Imaging Sci. 7(4):2448—2487. 2014.
C. Deledalle, SV, G. Peyré, J. Fadili, C. Dossal. Proximal Splitting Derivatives for Risk Estimation. *NCMIP*. 2012.

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$$\hat{\mu}_\theta(y) = X \hat{w}_\theta(y)$$

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$$\mathbb{E}_\varepsilon(\text{SURE}_\theta(y)) = \mathcal{R}(\theta)$$

Practical aspect | **Estimator and algorithm** | **Theoretical aspect**

$$\begin{tikzcd}
\text{numerical algorithm} \arrow[r] & w_\theta^{(k)}(y) \arrow[r] \arrow[d] & \hat{w}_\theta(y) \arrow[d, dotted] & \text{“true” mathematical solution} \arrow[l] \\
\text{estimation error} \arrow[r] & \text{Jac}_{\hat{w}_\theta}(y) \arrow[r] & \text{Jac}_{w_\theta^{(k)}}(y) & \text{sensitivity analysis} \arrow[l]
\end{tikzcd}$$

Convergence of functions does not imply convergence of derivatives!

Estimating a Jacobian

Estimator

$\hat{w}_\theta : \mathbb{R}^n \longrightarrow \mathbb{R}^p$

differentiable

Jacobian

$$\mathrm{Jac}_{\hat{w}_{\bullet}(y)} : \Theta \longrightarrow \mathbb{R}^{p\times l}$$

$$\mathrm{Jac}_{\hat{w}_\theta} : \mathbb{R}^n \longrightarrow \mathbb{R}^{p\times n}$$

$$\mathrm{Jac}_{\hat{w}_\theta}(y) = \begin{pmatrix} \frac{\partial(\hat{w}_\theta)_1}{\partial y_1}(y) & \cdots & \frac{\partial(\hat{w}_\theta)_1}{\partial y_n}(y) \\ \vdots & & \vdots \\ \frac{\partial(\hat{w}_\theta)_p}{\partial y_1}(y) & \cdots & \frac{\partial(\hat{w}_\theta)_p}{\partial y_n}(y) \end{pmatrix} \in \mathbb{R}^{p\times n}$$

Numerical approximation

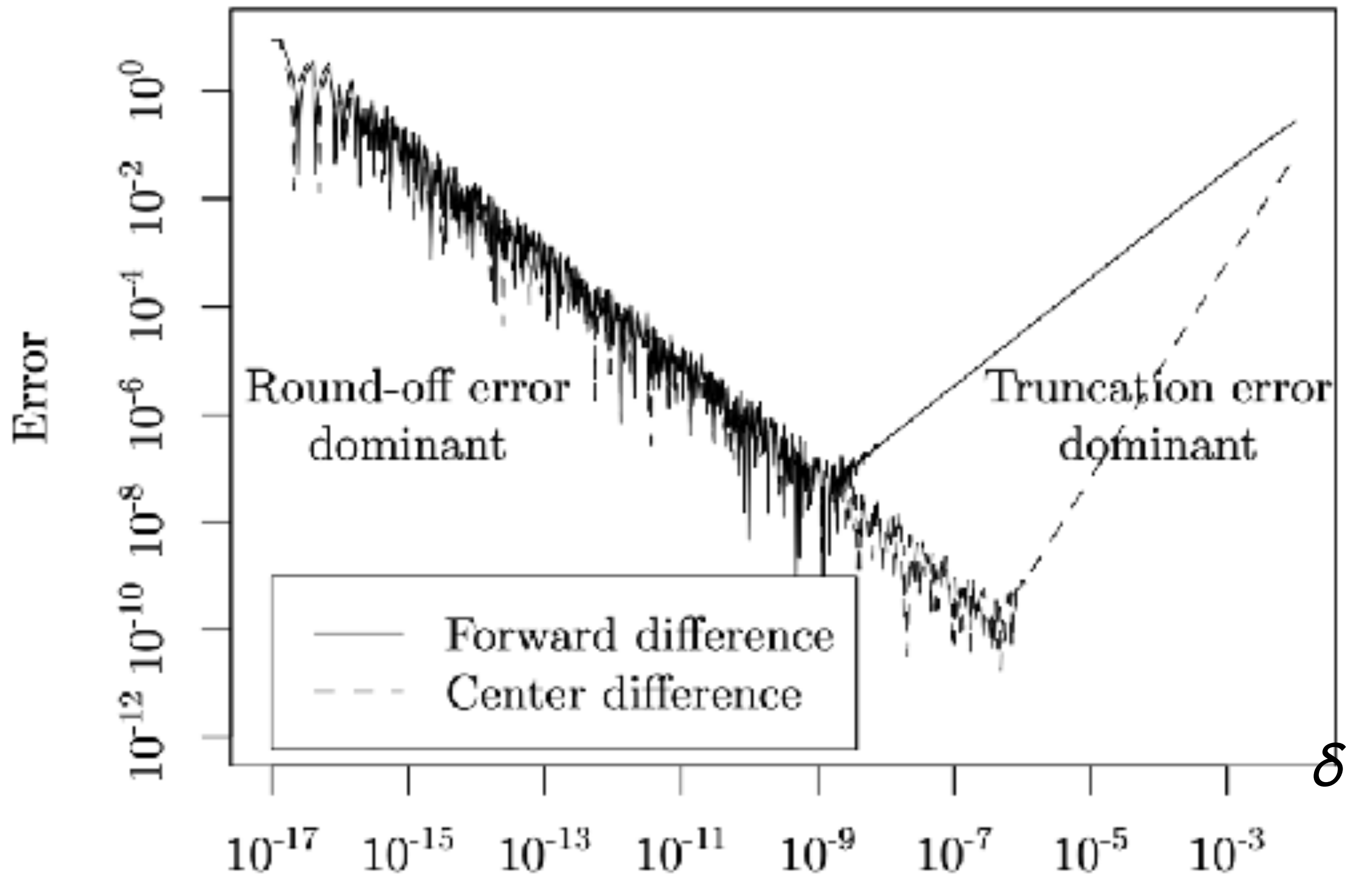
$$\mathrm{Jac}_{\hat{w}_\theta}(y) \approx \left(\frac{\hat{w}_\theta(y+\delta \mathbf{e}_1)-\hat{w}_\theta(y)}{\delta} \quad \cdots \quad \frac{\hat{w}_\theta(y+\delta \mathbf{e}_n)-\hat{w}_\theta(y)}{\delta} \right)$$

needs $O(nT)$ operations

parameter dimension   cost of evaluating $\hat{w}_\theta(\cdot)$

Numerical errors

from [Baydin '18]



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Unstable for low **and** high precision

Symbolic differentiation

Used by Mathematica, Maple, SymPy, Maxima, Lisp

Ineffective for “complex” programs

$\longrightarrow$ expression swell

Automatic differentiation: forward mode

Function

$$f : \mathbb{R}^p \longrightarrow \mathbb{R}^n$$

$$f(x_1, x_2, x_3) = \begin{pmatrix} x_1 x_2 + \exp(x_3) \\ x_1 x_2 - \log(x_1) \end{pmatrix}$$

Jacobian

$$\mathrm{Jac}_f : \mathbb{R}^p \longrightarrow \mathbb{R}^{n \times p}$$

$$\mathrm{Jac}_f(x_1, x_2, x_3) = \begin{pmatrix} x_2 & x_1 & \exp(x_3) \\ x_2 & x_1 & 1/x_3 \end{pmatrix}$$

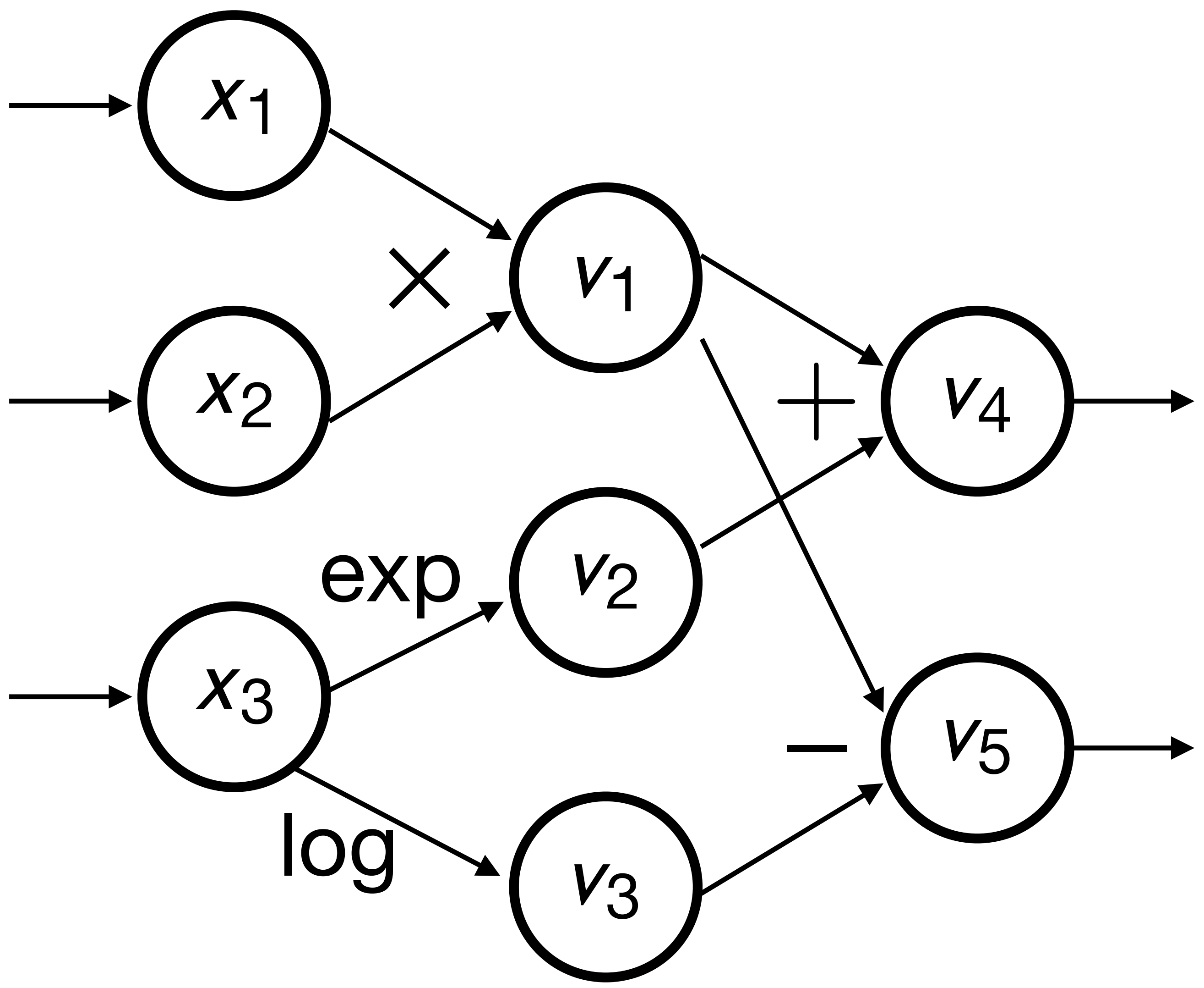
$$\frac{\partial f}{\partial x_1}(1, 2, 3) = (2, 2)^\top$$

Computer program

```python
def f(x1, x2, x3):
    v1 = x1 * x2
    v2 = exp(x3)
    v3 = log(x3)
    v4 = v1 + v2
    v5 = v1 - v3
    return (v4, v5)
```

Forward Tangent Program

Computational graph [Bauer '74]



Inspired by [Baydin '18]

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$$\frac{\partial f}{\partial x_1}(1, 2, 3) = (2, 2)^\top$$

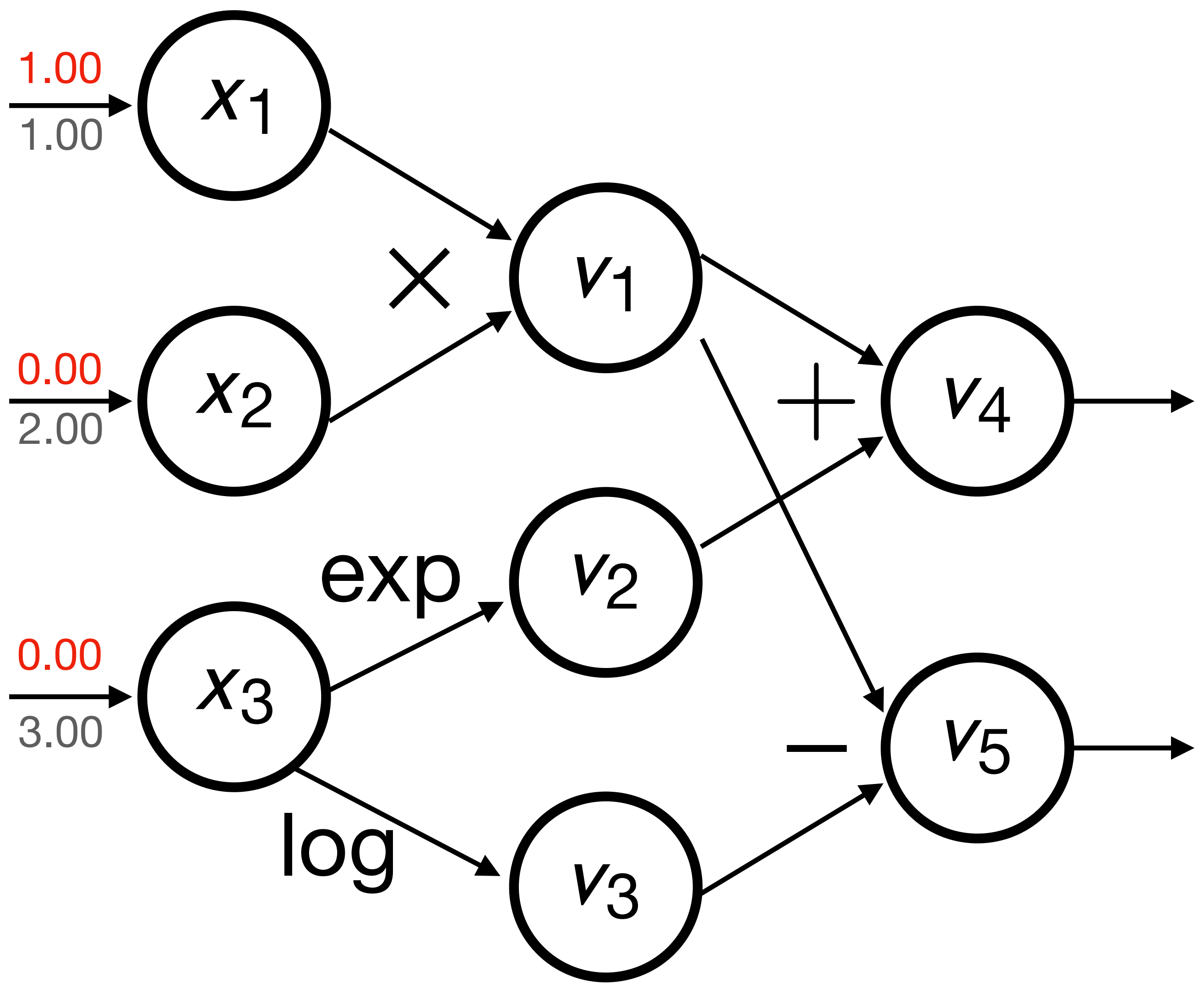
Computer program

```
        1.00  2.00  3.00
def f(x1, x2, x3):
```

Forward Tangent Program

```
         1.00   0.00   0.00
def df(dx1, dx2, dx3):
```

Computational graph [Bauer '74]



Inspired by [Baydin '18]

Automatic differentiation: forward mode

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$$\mathrm{Jac}_f(x_1, x_2, x_3) = \begin{pmatrix} x_2 & x_1 & \exp(x_3) \\ x_2 & x_1 & 1/x_3 \end{pmatrix}$$

$$\frac{\partial f}{\partial x_1}(1,2,3) = (2,2)^\top$$

Computer program

1.00 2.00 3.00

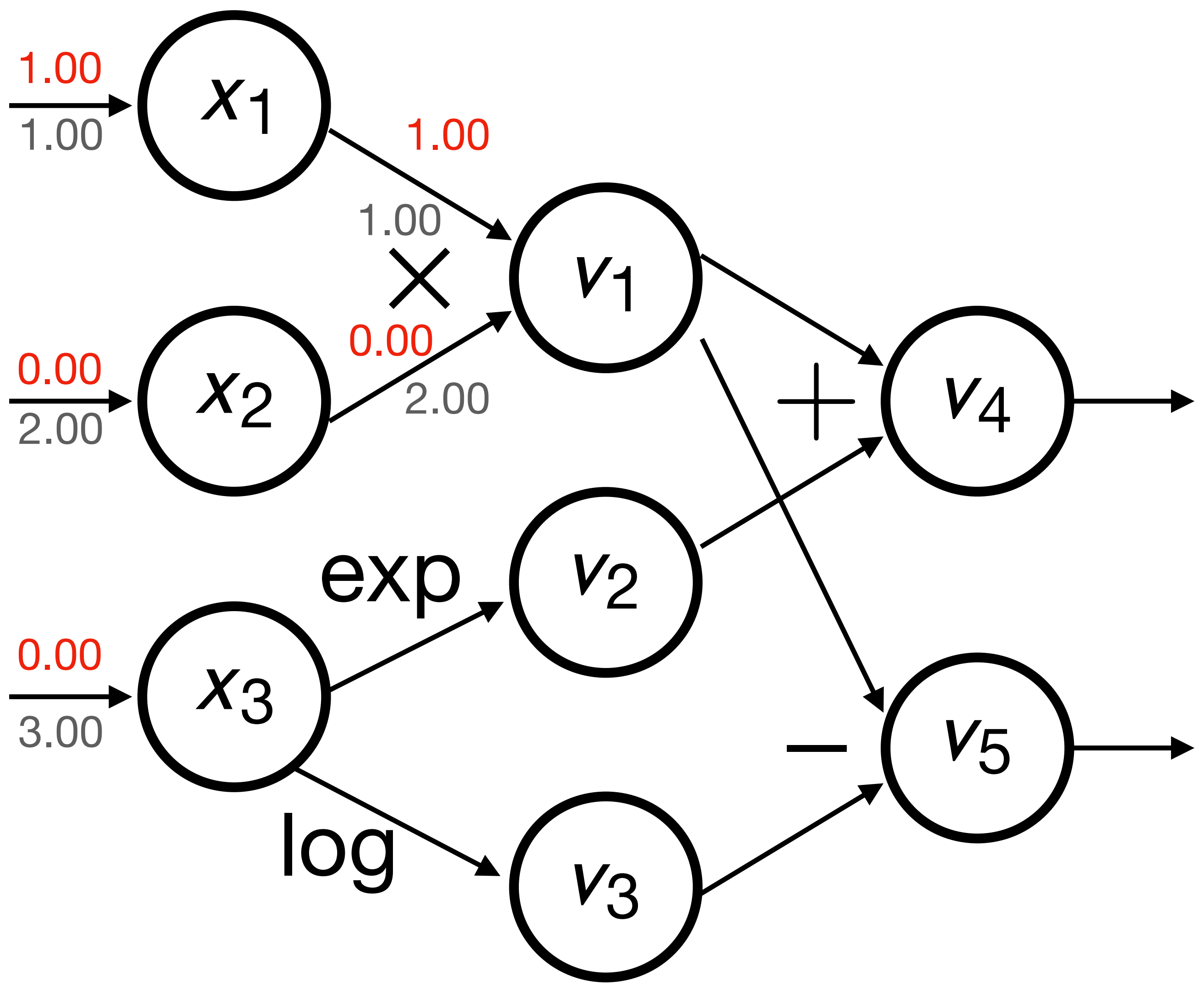
```
def f(x1, x2, x3):
    v1 = x1 * x2          2.00
```

Forward Tangent Program

1.00 0.00 0.00

```
def df(dx1, dx2, dx3):
    dv1 = dx1 * x2 + dx1 * x2     2.00
```

Computational graph [Bauer '74]



Inspired by [Baydin '18]

Automatic differentiation: forward mode

Function

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$$f(x_1, x_2, x_3) = \begin{pmatrix} x_1 x_2 + \exp(x_3) \\ x_1 x_2 - \log(x_1) \end{pmatrix}$$

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$$\mathrm{Jac}_f : \mathbb{R}^p \longrightarrow \mathbb{R}^{n \times p}$$

$$\mathrm{Jac}_f(x_1, x_2, x_3) = \begin{pmatrix} x_2 & x_1 & \exp(x_3) \\ x_2 & x_1 & 1/x_3 \end{pmatrix}$$

$$\frac{\partial f}{\partial x_1}(1, 2, 3) = (2, 2)^\top$$

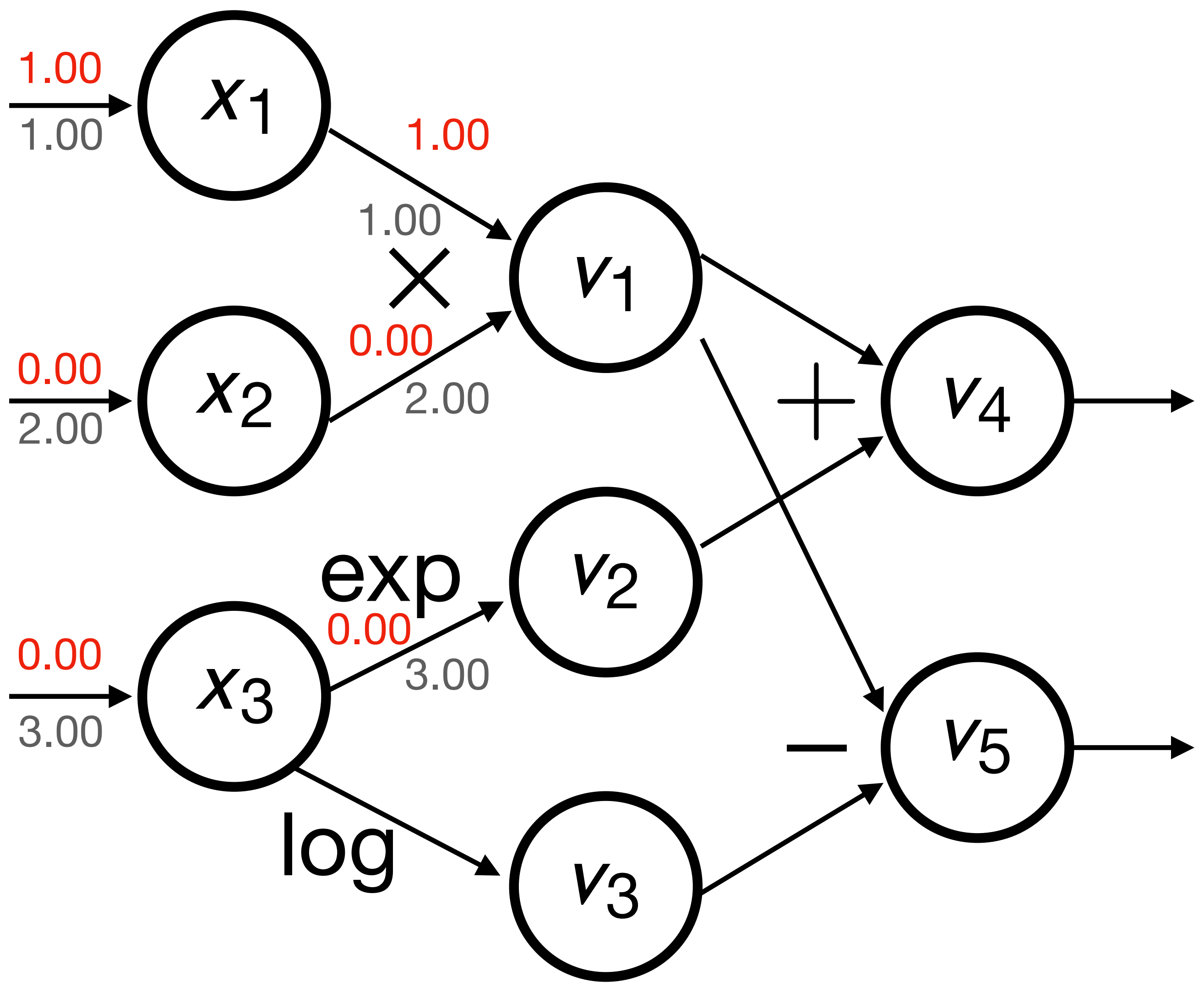
Computer program

```
          1.00  2.00  3.00
def f(x1, x2, x3):
    v1 = x1 * x2            2.00
    v2 = exp(x3)            20.08
```

Forward Tangent Program

```
           1.00  0.00  0.00
def df(dx1, dx2, dx3):
    dv1 = dx1 * x2 + dx1 * x2     2.00
    dv2 = dx3 * exp(x3)           0.00
```

Computational graph [Bauer '74]



Inspired by [Baydin '18]

Automatic differentiation: forward mode

Function

$$f : \mathbb{R}^p \longrightarrow \mathbb{R}^n$$

$$f(x_1, x_2, x_3) = \begin{pmatrix} x_1 x_2 + \exp(x_3) \\ x_1 x_2 - \log(x_1) \end{pmatrix}$$

Jacobian

$$\mathrm{Jac}_f : \mathbb{R}^p \longrightarrow \mathbb{R}^{n \times p}$$

$$\mathrm{Jac}_f(x_1, x_2, x_3) = \begin{pmatrix} x_2 & x_1 & \exp(x_3) \\ x_2 & x_1 & 1/x_3 \end{pmatrix}$$

$$\frac{\partial f}{\partial x_1}(1, 2, 3) = (2, 2)^\top$$

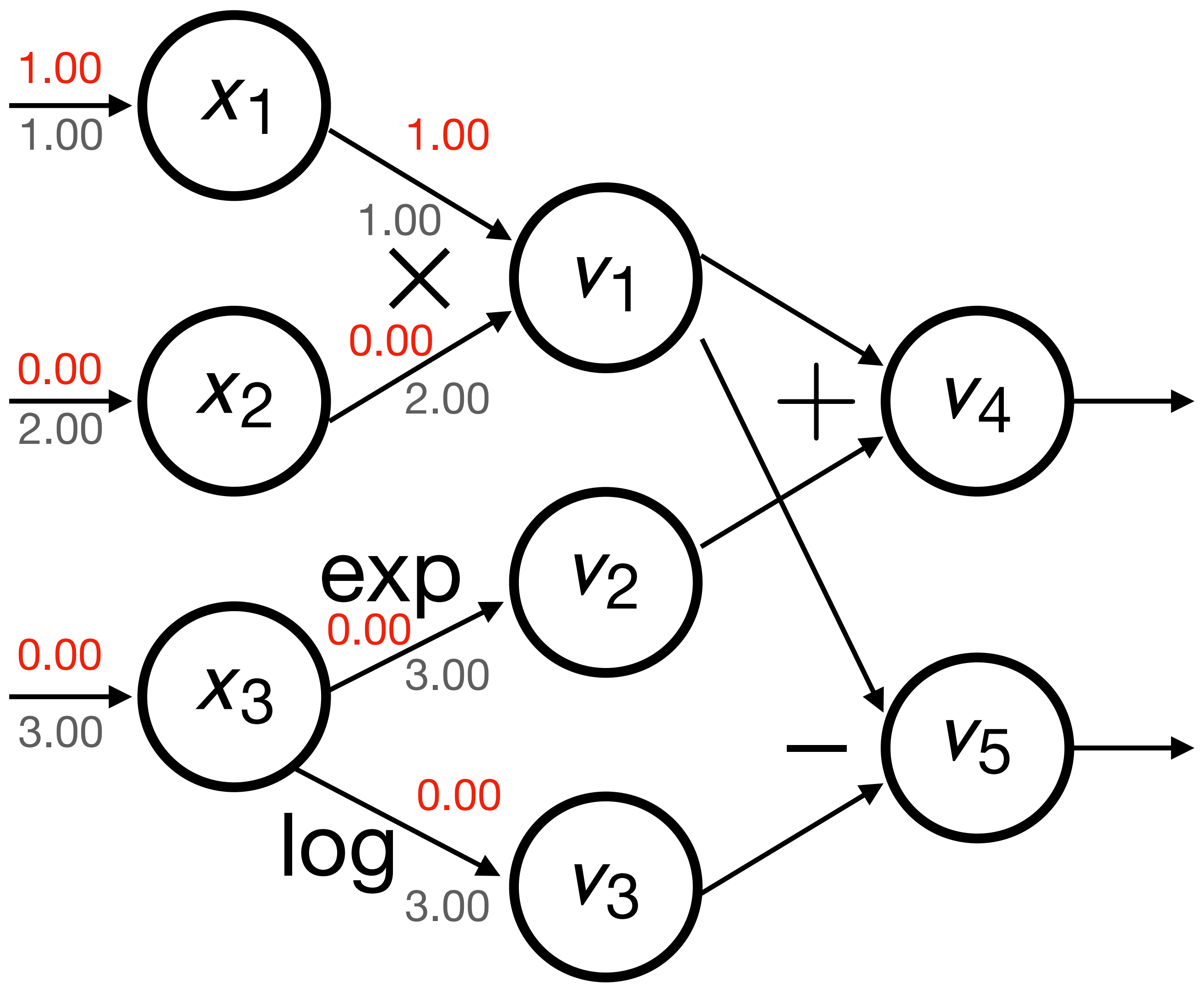
Computer program

```
        1.00  2.00  3.00
def f(x1, x2, x3):
    v1 = x1 * x2          2.00
    v2 = exp(x3)          20.08
    v3 = log(x3)          0.48
```

Forward Tangent Program

```
         1.00  0.00  0.00
def df(dx1, dx2, dx3):
    dv1 = dx1 * x2 + dx1 * x2     2.00
    dv2 = dx3 * exp(x3)           0.00
    dv3 = dx3 / x3                0.00
```

Computational graph [Bauer ’74]



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    v4 = v1 + v2          22.08
```

Forward Tangent Program

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         1.00   0.00   0.00
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    dv3 = dx3 / x3               0.00
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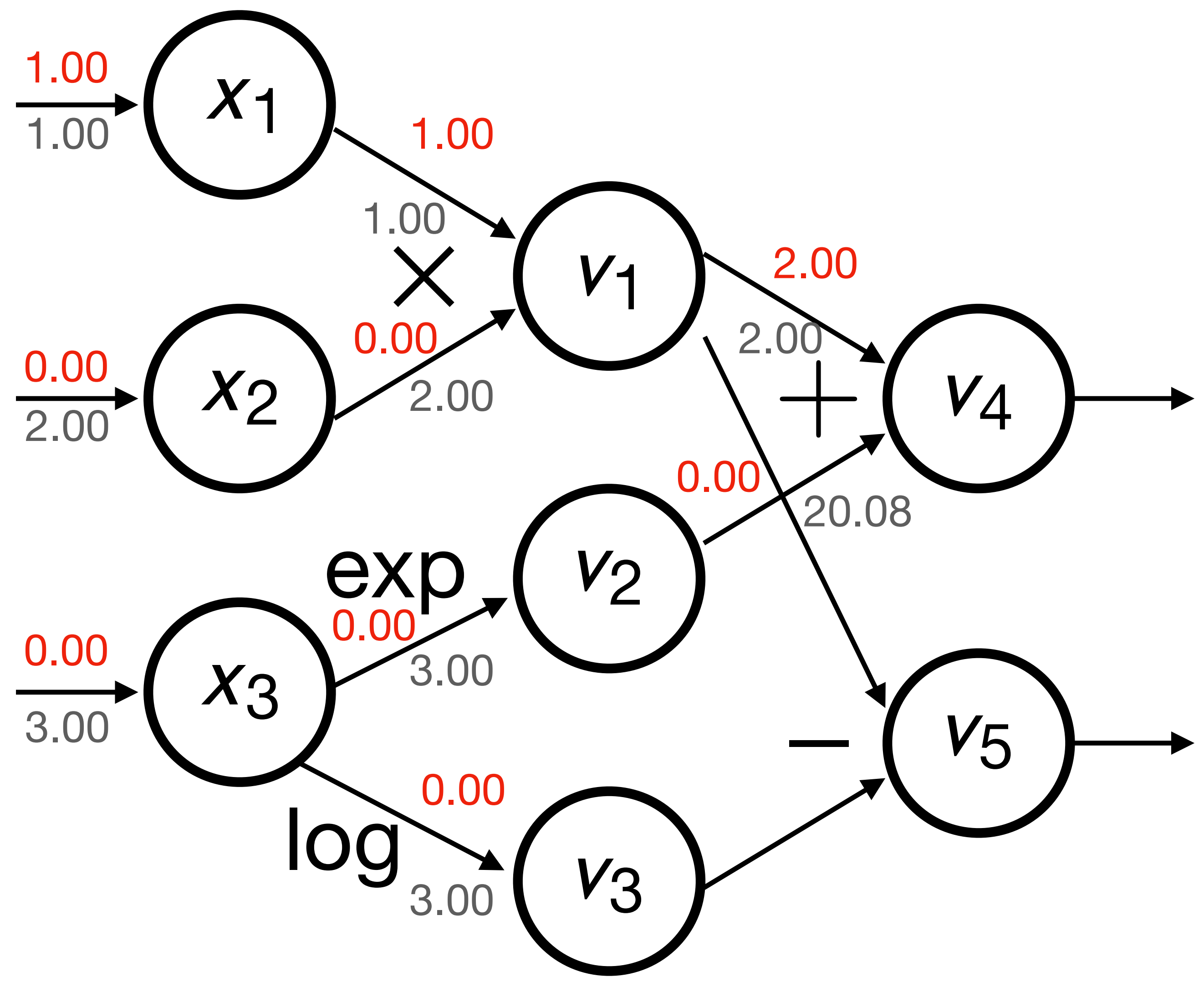
```

Computational graph [Bauer '74]



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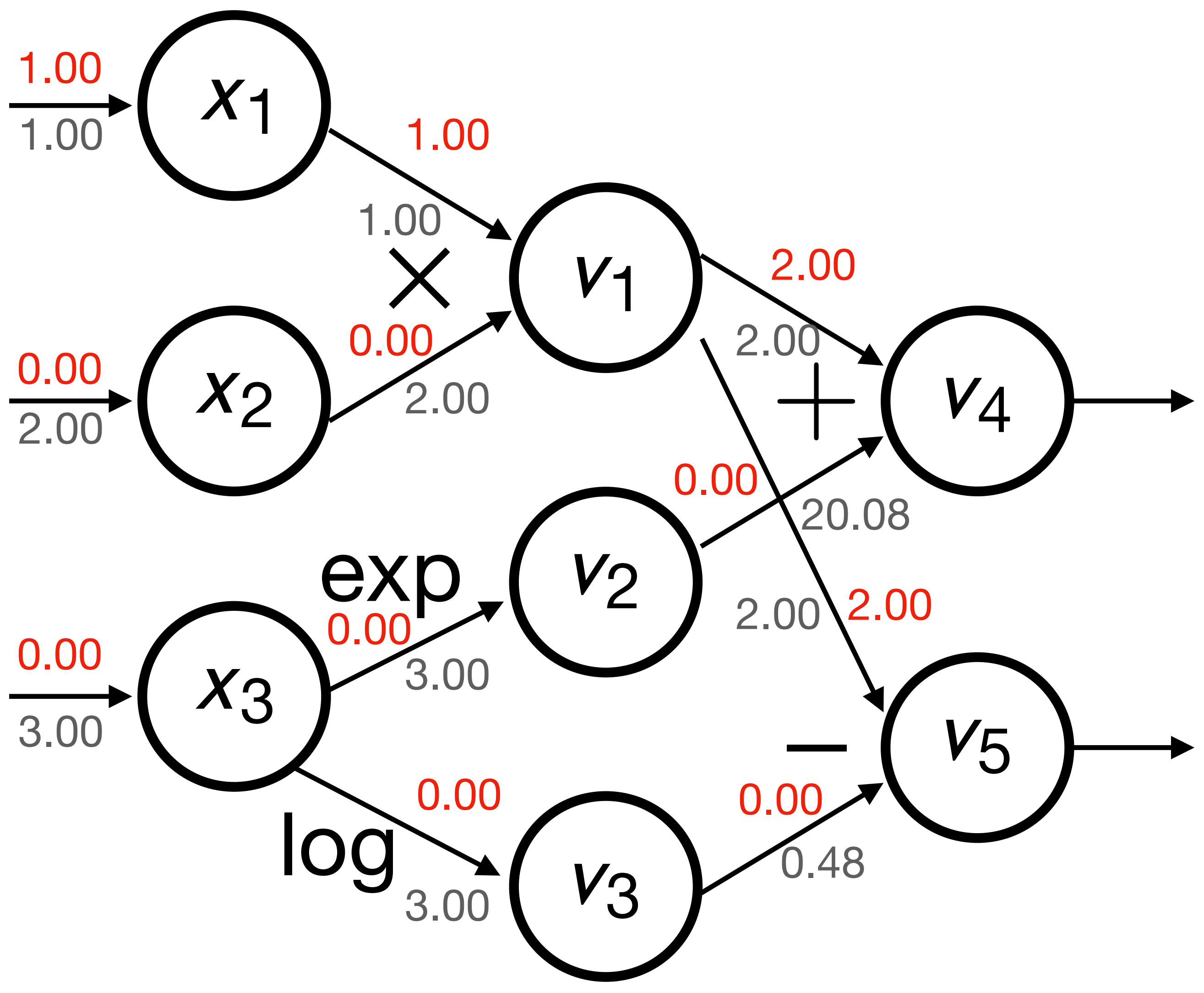
    v4 = v1 + v2         22.08
    v5 = v1 - v3         2.08
```

Forward Tangent Program

```
         1.00   0.00   0.00
def df(dx1, dx2, dx3):
    dv1 = dx1 * x2 + dx1 * x2     2.00
    dv2 = dx3 * exp(x3)           0.00
    dv3 = dx3 / x3                0.00
    dv4 = dv1 + dv2               2.00
    dv5 = dv1 - dv3               2.00
```

Computational graph [Bauer '74]



Inspired by [Baydin '18]

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    v4 = v1 + v2              22.08
    v5 = v1 - v3              2.08
    return (v4, v5) (22.08, 2.08)
```

Forward Tangent Program

```
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    dv4 = dv1 + dv2              2.00
    dv5 = dv1 - dv3              2.00
    return (dv4, dv5)            (2.00, 2.00)
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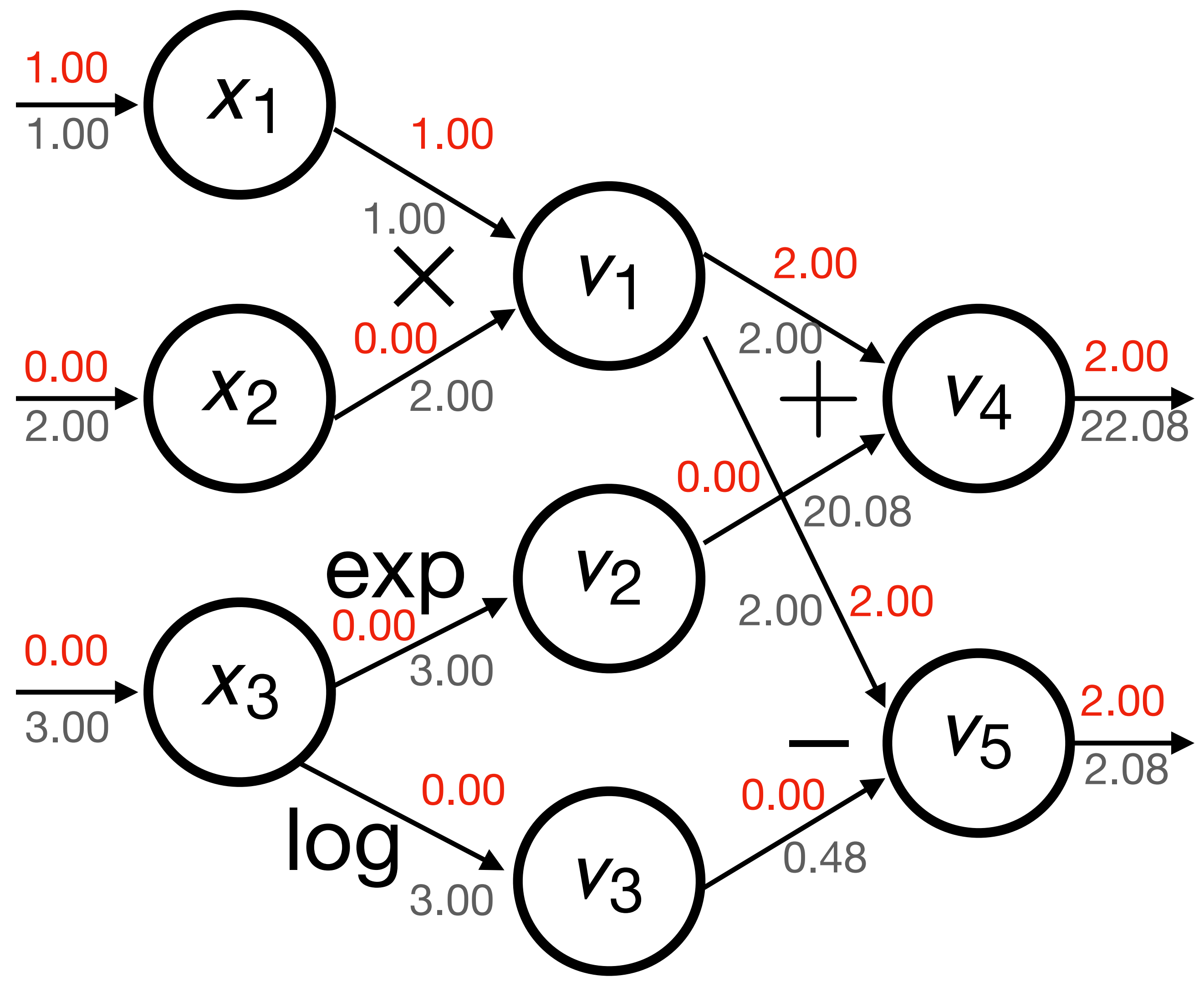
Computational graph [Bauer '74]



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$$\mathrm{Jac}_f(x_1, x_2, x_3) = \begin{pmatrix} x_2 & x_1 & \exp(x_3) \\ x_2 & x_1 & 1/x_3 \end{pmatrix}$$

$$\frac{\partial f}{\partial x_1}(1, 2, 3) = (2, 2)^\top$$

- Computing the full Jacobian requires p calls to tangent program
- No memory requirement
- Performant when $p < n$

[Wengert '64, Griewank '89]

Computer program

```
         1.00  2.00  3.00
def f(x1, x2, x3):
    v1 = x1 * x2                2.00
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```

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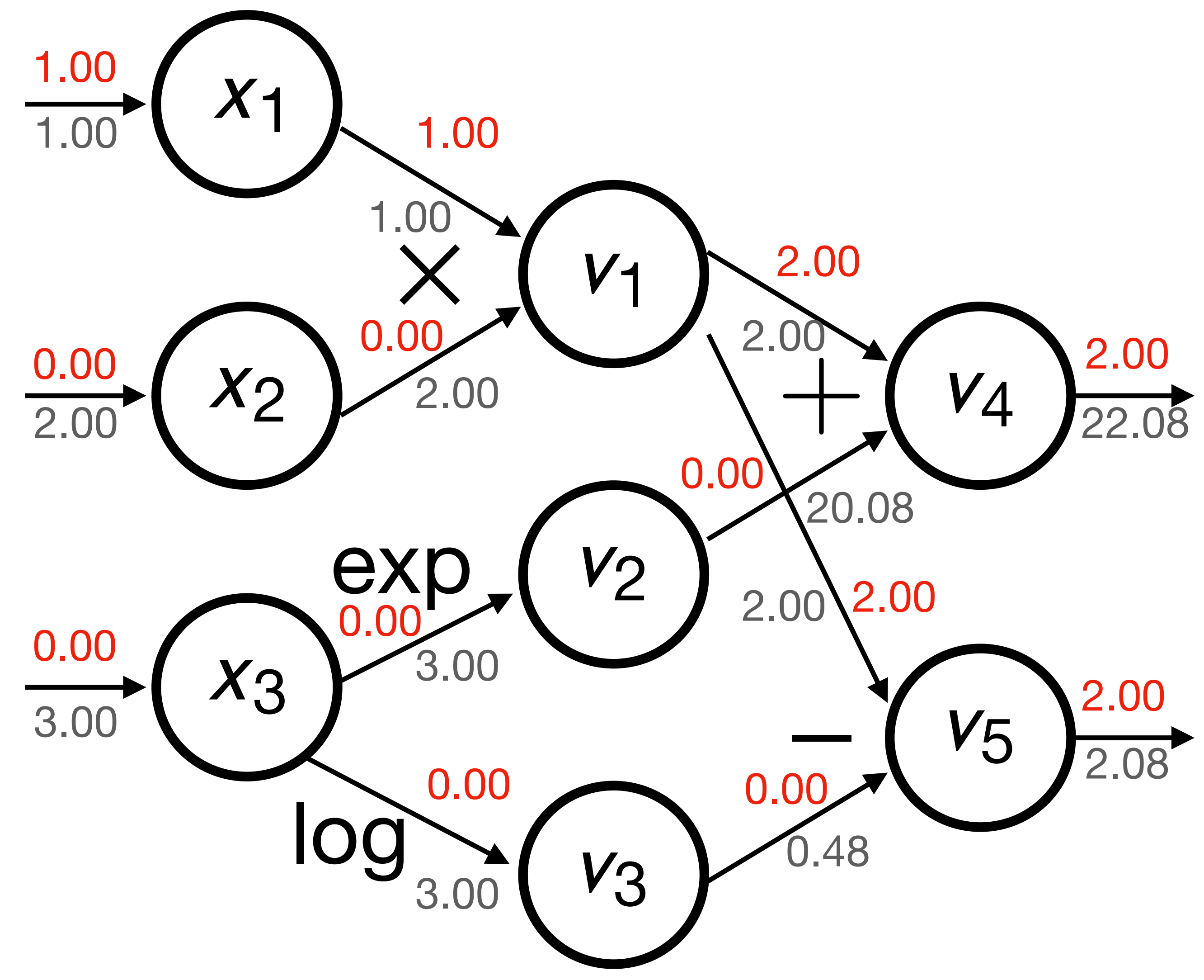
```
          1.00  0.00  0.00
def df(dx1, dx2, dx3):
    dv1 = dx1 * x2 + dx1 * x2    2.00
    dv2 = dx3 * exp(x3)          0.00
    dv3 = dx3 / x3               0.00
    dv4 = dv1 + dv2              2.00
    dv5 = dv1 - dv3              2.00
    return (dv4, dv5)     (2.00, 2.00)
```

Computational graph [Bauer '74]



Forward automatic differentiation

=

Forward derivative accumulation

=

Tangent linear mode

=

Line-to-line derivation

=

Jacobian-vector product $\mathrm{Jac}_f(x) \cdot z$

$\neq$

~~Backpropagation~~

Note that in practice the forward tangent program need to be implemented in the same function (variables accessibility)

Inspired by [Baydin '18]

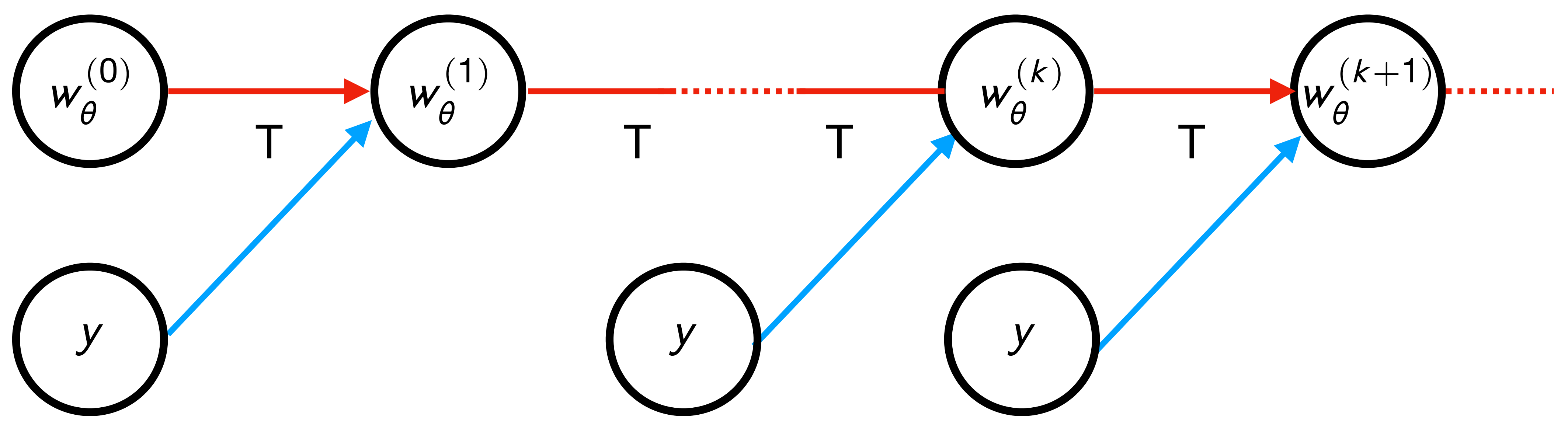
Estimating a Jacobian of iterative estimator

Iterative estimators $w_\theta^{(k)}(y)$

$$\mathrm{T} : \mathbb{R}^p \times \mathbb{R}^n \to \mathbb{R}^p$$

$$\begin{cases} w_\theta^{(k)}(y) \xrightarrow{k \to +\infty} \hat{w}_\theta(y) \\ w_\theta^{(k+1)}(y) = \mathrm{T}(w_\theta^{(k)}(y), y) \end{cases}$$

Computational graph



Chain rule

$$\mathrm{Jac}_{w_\theta^{k+1}}(y) = \partial_1 \mathrm{T}(w_\theta^k(y), y) \cdot \mathrm{Jac}_{w_\theta^k(y)}(y) + \partial_2 \mathrm{T}(w_\theta^k(y), y)$$

$p \times n$ $\quad p \times p \quad$ $p \times n$ $\quad p \times n$

Forward differentiation "Jacobian-vector product"

$$\begin{cases} w_\theta^{(k+1)}(y) &= \mathrm{T}(w_\theta^{(k)}(y), y) \\ \mathrm{d}w_\theta^{(k+1)}(y) &= \partial_1 \mathrm{T}(w_\theta^k(y), y) \cdot \mathrm{d}w_\theta^{(k+1)}(y) + \partial_2 \mathrm{T}(w_\theta^k(y), y)\delta \end{cases}$$

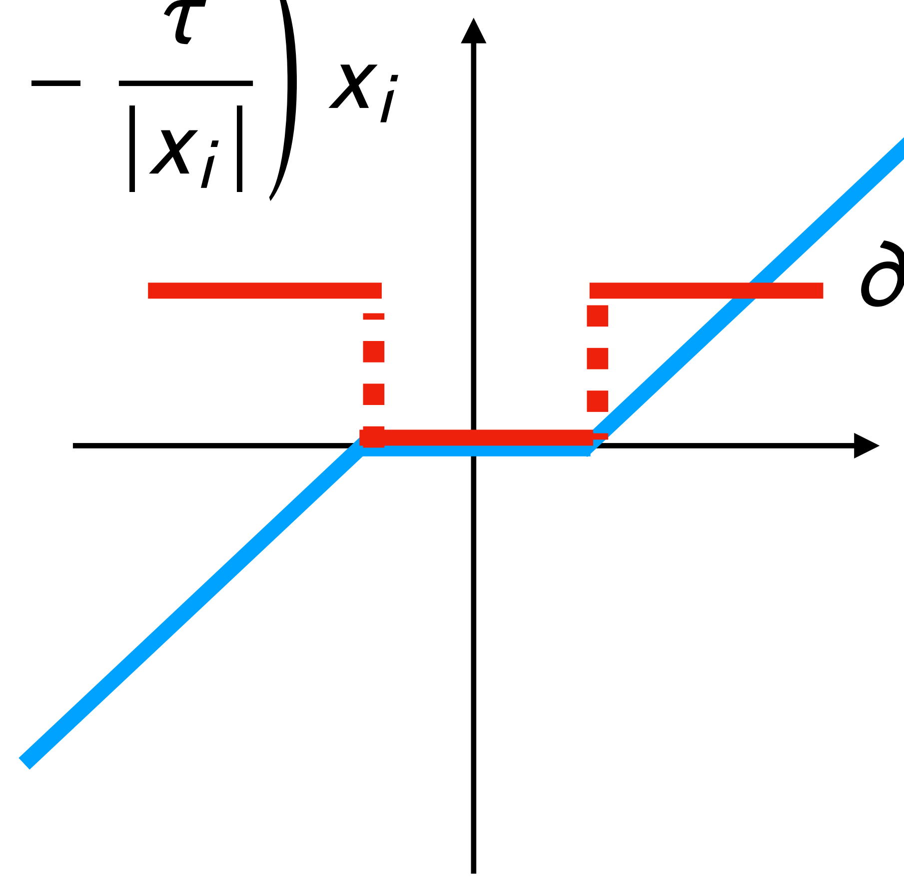
Forward differentiation of a Lasso solver

Lasso

$$\hat{w}_\theta(y) \in \underset{w \in \mathbb{R}^p}{\operatorname{argmin}} \frac{1}{2}\|y - Xw\|_2^2 + \theta\|w\|_1$$

Soft-thresholding

$$\operatorname{prox}_{\tau\|\cdot\|_1}(x)_i = \min\left(0, 1 - \frac{\tau}{|x_i|}\right) x_i$$



Iterative soft-thresholding (Forward-Backward)

$$w_\theta^{(k+1)}(y) = \operatorname{prox}_{\tau\theta\|\cdot\|_1}(w_\theta^{(k)}(y) - \tau X^\top(X w_\theta^{(k)}(y) - y))$$

If $\tau < 2/\|X\|^2$, $w_\theta^{(k)}(y) \to \hat{w}_\theta(y)$

Derivative of Forward-Backward

$$\begin{aligned}
\partial_1 \mathrm{T}(w, y) &= \operatorname{Jac}_{\operatorname{prox}_{\tau\theta\|\cdot\|_1}}(w - \tau X^\top(Xw - y)) \cdot \operatorname{Jac}_{w \mapsto w - \tau X^\top(Xw - y)}(w) \\
&= \partial\operatorname{prox}_{\tau\theta\|\cdot\|_1}(w - \tau X^\top(Xw - y)) \cdot (\mathrm{Id} - \tau X^\top X) \\
\partial_2 \mathrm{T}(w, y) &= \operatorname{Jac}_{\operatorname{prox}_{\tau\theta\|\cdot\|_1}}(w - \tau X^\top(Xw - y)) \cdot \operatorname{Jac}_{y \mapsto w - \tau X^\top(Xw - y)}(y) \\
&= \partial\operatorname{prox}_{\tau\theta\|\cdot\|_1}(w - \tau X^\top(Xw - y)) \cdot \tau X
\end{aligned}$$

Fifty shades of SURE

Closed-form SURE [Stein '81]

$$\mathrm{SURE}_\theta(y) = \|y - \hat\mu_\theta(y)\|_2^2 - n\sigma^2 + 2\sigma^2 \widehat{\mathrm{df}}_\theta(y) \qquad \widehat{\mathrm{df}}_\theta(y) = \mathrm{trace}(\mathrm{Jac}_{\hat\mu_\theta}(y))$$

Issue: dimensionality of the Jacobian

$$\mathbb{E}_z\left(\widehat{\mathrm{df}}_\theta^{\mathrm{MC}}(y)\right) = \widehat{\mathrm{df}}_\theta(y)$$

Monte-Carlo SURE [Ramani et al. '08]

$$z \sim \mathcal{N}(0, \mathrm{Id})$$

$$\mathrm{SURE}_\theta^{\mathrm{MC}}(y) = \|y - \hat\mu_\theta(y)\|_2^2 - n\sigma^2 + 2\sigma^2 \widehat{\mathrm{df}}_\theta^{\mathrm{MC}}(y) \qquad \widehat{\mathrm{df}}_\theta^{\mathrm{MC}}(y) = \langle \mathrm{Jac}_{\hat\mu_\theta}(y) z,\, z\rangle$$

Issue: accessibility of the true Jacobian

need proof
of convergence

Iterative Monte-Carlo SURE [Vonesch et al. '08, Giryes et al. '11, Ramani et al. '12, Deledalle et al. '12]

$$\mathrm{SURE}_\theta^{(k),\mathrm{MC}}(y) = \|y - \mu_\theta^{(k)}(y)\|_2^2 - n\sigma^2 + 2\sigma^2 \widehat{\mathrm{df}}_\theta^{(k),\mathrm{MC}}(y) \qquad \widehat{\mathrm{df}}_\theta^{(k),\mathrm{MC}}(y) = \langle \mathrm{d}w_\theta^{(k)},\, z\rangle$$

Fifty shades of SURE — continued

DoF, Monte-Carlo DoF and Iterative Monte-Carlo DoF

$$\widehat{\mathrm{df}}_\theta(y) = \mathrm{trace}(\mathrm{Jac}_{\hat{\mu}_\theta}(y)) \qquad \widehat{\mathrm{df}}_\theta^{\mathrm{MC}}(y) = \langle \mathrm{Jac}_{\hat{\mu}_\theta}(y) z,\ z\rangle \qquad \widehat{\mathrm{df}}_\theta^{(k),\mathrm{MC}}(y) = \langle \mathrm{d}w_\theta^{(k)},\ z\rangle$$

Finite-difference SURE [Ye '98, Shen-Ye '02, Ramani et al. '08]

$$\widehat{\mathrm{df}}_\theta^{\mathrm{FD}}(y) = \frac{1}{\delta}\sum_{i=1}^{n} (\hat{\mu}_\theta(y + \delta \mathbf{e}_i) - \hat{\mu}_\theta(y))_i$$

If $\hat{\mu}_\theta$ Lipschitz-continuous

$$\lim_{\delta \to 0} \widehat{\mathrm{df}}_\theta^{\mathrm{FD}}(y) = \widehat{\mathrm{df}}_\theta(y)$$

Issues:

- numerical instabilities
- observation dimension

Finite-difference Monte-Carlo SURE

$$\widehat{\mathrm{df}}_\theta^{\mathrm{FDMC}}(y) = \frac{1}{\delta}\langle \hat{\mu}_\theta(y + \delta z) - \hat{\mu}_\theta(y),\ z\rangle$$

$$\mathbb{E}_z\left(\widehat{\mathrm{df}}_\theta^{\mathrm{FDMC}}(y)\right) = \widehat{\mathrm{df}}_\theta^{\mathrm{FD}}(y)$$

Issue: accessibility of the true estimator!

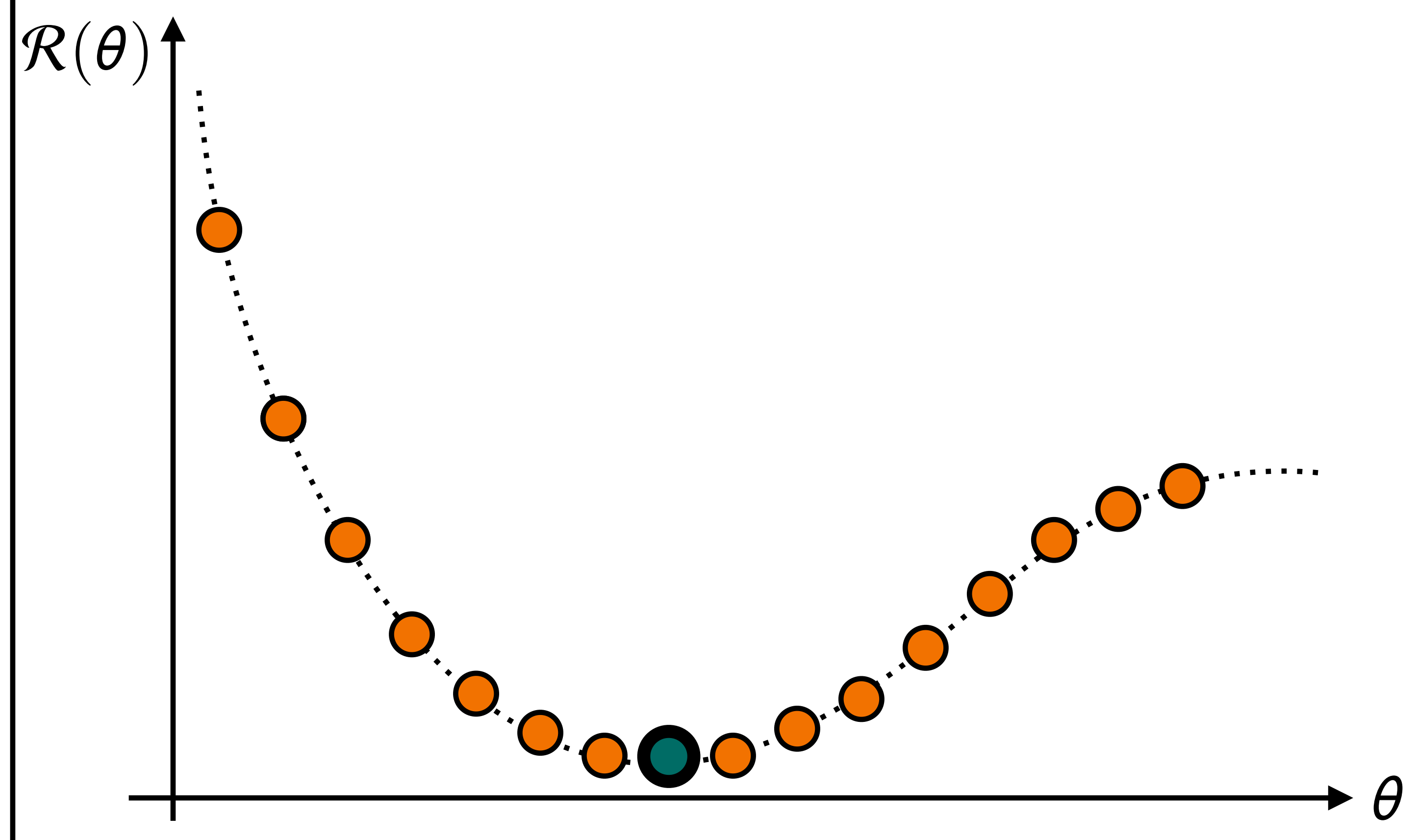
Iterative Finite-difference Monte-Carlo SURE

$$\widehat{\mathrm{df}}_\theta^{(k),\mathrm{FDMC}}(y) = \tfrac{1}{\delta}\langle \mu_\theta^{(k)}(y + \delta z) - \mu_\theta^{(k)}(y),\ z\rangle$$

Reminder: 0-order vs 1-order search

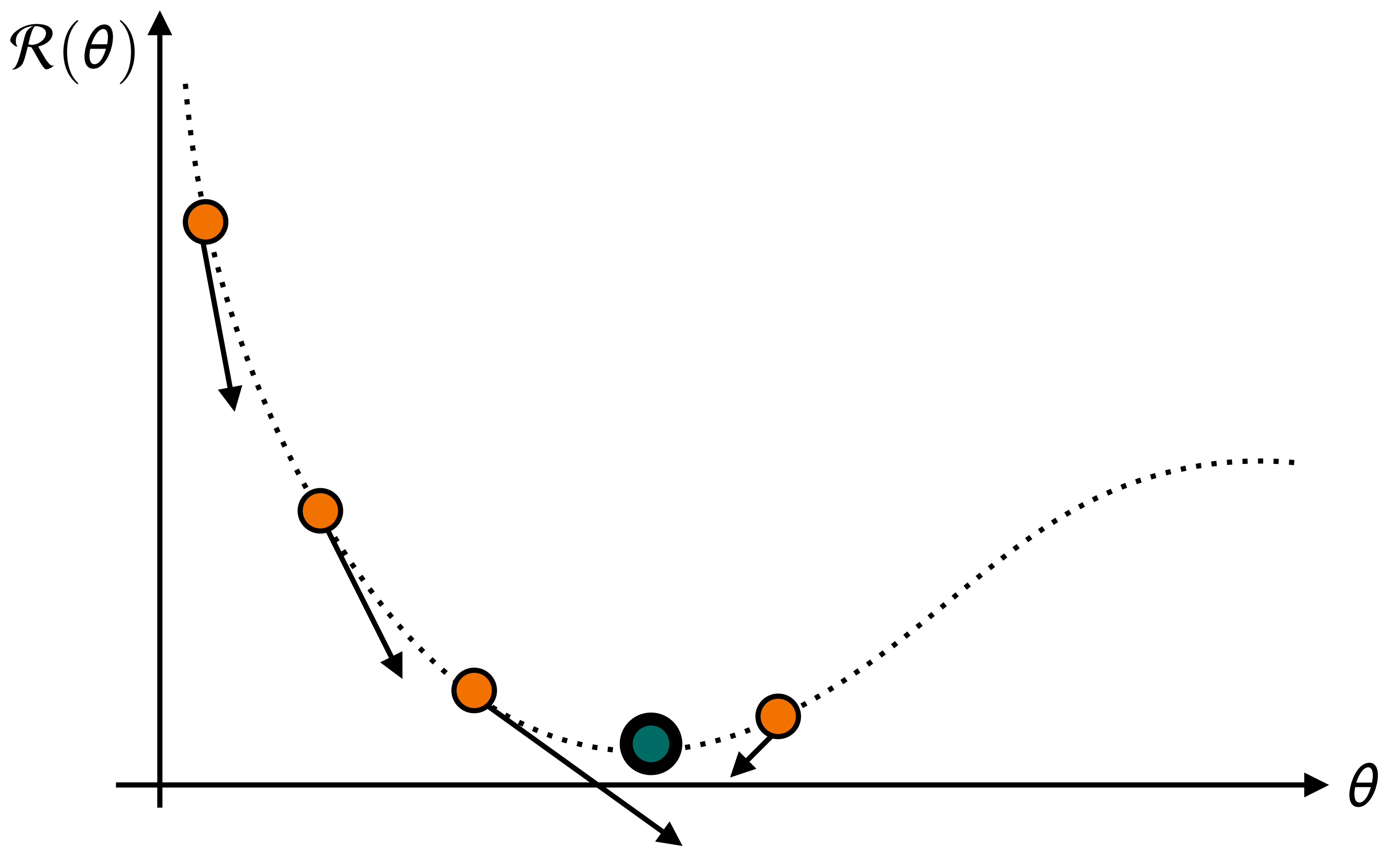
Grid search

1. Choose a criterion $\mathcal{R}$
2. Sample uniformly Θ
3. Evaluate $\mathcal{R}(\theta)$ on the grid
4. Keep the best $\theta^\star$



Hyper-gradient descent

1. Choose a criterion $\mathcal{R}$
2. Take a starting point
3. Eval. $\mathcal{R}(\theta), \nabla\mathcal{R}(\theta)$ on-the-fly
4. Keep the last iterate $\theta^\star$



BUT

$$\theta \mapsto \mathbb{E}_\varepsilon \left(\|\hat{\mu}_\theta(y) - X w_{\text{true}}\|_2^2 \right)$$

(weakly) differentiable

$$\not\Downarrow$$

$$\theta \mapsto \mathrm{SURE}_\theta(y)$$

differentiable or continuous

What about $\mathrm{SURE}_\theta^{\mathrm{FD}}(y)$, $\mathrm{SURE}_\theta^{\mathrm{FDMC}}(y)$?

From SURE to SUGAR

$$\widehat{\mathrm{df}}_\theta^{\mathrm{FD}}(y) = \frac{1}{\delta}\sum_{i=1}^{n}(\hat{\mu}_\theta(y+\delta \mathbf{e}_i) - \hat{\mu}_\theta(y))_i \qquad \widehat{\mathrm{df}}_\theta^{\mathrm{FDMC}}(y) = \frac{1}{\delta}\langle \hat{\mu}_\theta(y+\delta z) - \hat{\mu}_\theta(y),\, z\rangle$$

Proposition [Deledalle et al. '14, Pascal et al. '20]

Assume $(y,\theta) \mapsto \hat{\mu}_\theta(y)$ weakly differentiable *w.r.t* y and θ

Given $\delta > 0$, $\widehat{\mathrm{df}}_\theta^{\mathrm{FD}}(y)$, $\widehat{\mathrm{df}}_\theta^{\mathrm{FDMC}}(y)$ are also weakly differentiable

$\mathrm{SURE}_\theta^{\mathrm{FD}}(y)$, $\mathrm{SURE}_\theta^{\mathrm{FDMC}}(y)$

Stein Unbiased GrAdient estimator of the Risk (SUGAR)

$$\begin{aligned}\mathrm{SUGAR}_\theta^{\mathrm{FD/FDMC}}(y) &= \nabla_\theta(\mathrm{SURE}_\bullet^{\mathrm{FD/FDMC}}(\bullet))(y,\theta)\\ &= 2\mathrm{Jac}_{\hat{\mu}_\bullet(\theta)}(y)^\top(\hat{\mu}_\theta(y) - y) + 2\sigma^2\nabla_\theta(\widehat{\mathrm{df}}_\bullet^{\mathrm{FD/FDMC}}(\bullet))(y,\theta)\end{aligned}$$

$$\nabla_\theta(\widehat{\mathrm{df}}_\bullet^{\mathrm{FDMC}}(\bullet))(y,\theta) = \frac{1}{\delta}(\mathrm{Jac}_{\hat{\mu}_\bullet(y+\delta z)}(\theta) - \mathrm{Jac}_{\hat{\mu}_\bullet(y)}(\theta))^\top z$$

$$\nabla_\theta(\widehat{\mathrm{df}}_\bullet^{\mathrm{FD}}(\bullet))(y,\theta) = \frac{1}{\delta}\sum_{i=1}^{n}(\mathrm{Jac}_{\hat{\mu}_\bullet(y+\delta \mathbf{e}_i)}(\theta) - \mathrm{Jac}_{\hat{\mu}_\bullet(y)}(\theta))^\top \mathbf{e}_i$$

Asymptotic unbiasedness of SUGAR

Theorem [Deledalle et al. '14, Pascal et al. '20]

Assume $(y, \theta) \mapsto \hat{\mu}_\theta(y)$ Lipschitz-continuous *w.r.t* y and θ

$$\lim_{\delta \to 0} \mathbb{E}_\varepsilon \left(\mathrm{SUGAR}_\theta^{\mathrm{FD/FDMC}}(y) \right) = \nabla_\theta \mathbb{E}_\varepsilon \left(\|\hat{\mu}_\bullet(y) - X w_{\mathrm{true}}\|_2^2 \right)(\theta)$$

In practice, δ / n need to not decrease quickly to ensure numerical stability

Stein Unbiased GrAdient estimator of the Risk (SUGAR)

$$\begin{aligned} \mathrm{SUGAR}_\theta^{\mathrm{FD/FDMC}}(y) &= \nabla_\theta (\mathrm{SURE}_\bullet{}^{\mathrm{FD/FDMC}}(\bullet))(y, \theta) \\ &= 2 \mathrm{Jac}_{\hat{\mu}_\bullet(\theta)}(y)^\top (\hat{\mu}_\theta(y) - y) + 2\sigma^2 \nabla_\theta (\widehat{\mathrm{df}}_\bullet{}^{\mathrm{FD/FDMC}}(\bullet))(y, \theta) \end{aligned}$$

$$\nabla_\theta (\widehat{\mathrm{df}}_\bullet{}^{\mathrm{FDMC}}(\bullet))(y, \theta) = \frac{1}{\delta} \left(\mathrm{Jac}_{\hat{\mu}_\bullet(y + \delta z)}(\theta) - \mathrm{Jac}_{\hat{\mu}_\bullet(y)}(\theta) \right)^\top z$$

SUGAR for iterative estimators

Iterative estimators $w_\theta^{(k)}(y)$

$$\mathrm{T} : \mathbb{R}^p \times \mathbb{R}^n \to \mathbb{R}^p$$

$$\begin{cases} w_\theta^{(k+1)}(y) & = \mathrm{T}(w_\theta^{(k)}(y), y) \\ \mathrm{d}w_\theta^{(k+1)}(y) & = \partial_1 \mathrm{T}(w_\theta^k(y), y) \cdot \mathrm{d}w_\theta^{(k)}(y) + \partial_2 \mathrm{T}(w_\theta^k(y), y) z \end{cases}$$

Running time x2

Global complexity: **4x** original iterative estimator

Iterative SUGAR Finite-difference + Monte-Carlo

$$\mathrm{SUGAR}_\theta^{(k),\mathrm{FD/FDMC}}(y) = \nabla_\theta(\mathrm{SURE}_\bullet{}^{(k),\mathrm{FD/FDMC}}(\bullet))(y, \theta)$$

$$= 2\mathrm{Jac}_{\mu_\bullet{}^{(k)}(\theta)}(y)^\top(\mu_\theta^{(k)}(y) - y) + 2\sigma^2 \nabla_\theta(\widehat{\mathrm{df}}_\bullet{}^{(k),\mathrm{FD/FDMC}}(\bullet))(y, \theta)$$

$$\nabla_\theta(\widehat{\mathrm{df}}_\bullet{}^{(k),\mathrm{FDMC}}(\bullet))(y, \theta) = \frac{1}{\delta}(\mathrm{d}w_\theta{}^{(k)}(y + \delta z) - \mathrm{d}w_\theta{}^{(k)}(y))$$

Running time x2

Generalizations of SUGAR

Generalized SURE [Eldar '09, V. et al '13]

$$\text{Risk} \quad \mathcal{R}^A(\theta) = \mathbb{E}_\varepsilon \left(\| A\hat{\mu}_\theta(y) - AXw_{\text{true}} \|_2^2 \right)$$

$$\text{DoF} \quad \widehat{\text{df}}_\theta^A(y) = \text{trace}\left(A \text{Jac}_{\hat{\mu}_\theta}(y) A^\top \right)$$

$$\text{SURE}_\theta^A(y) = \| A(y - \hat{\mu}_\theta(y)) \|_2^2 - \sigma^2 \text{trace}(A^\top A) + 2\sigma^2 \widehat{\text{df}}_\theta^A(y)$$

Examples

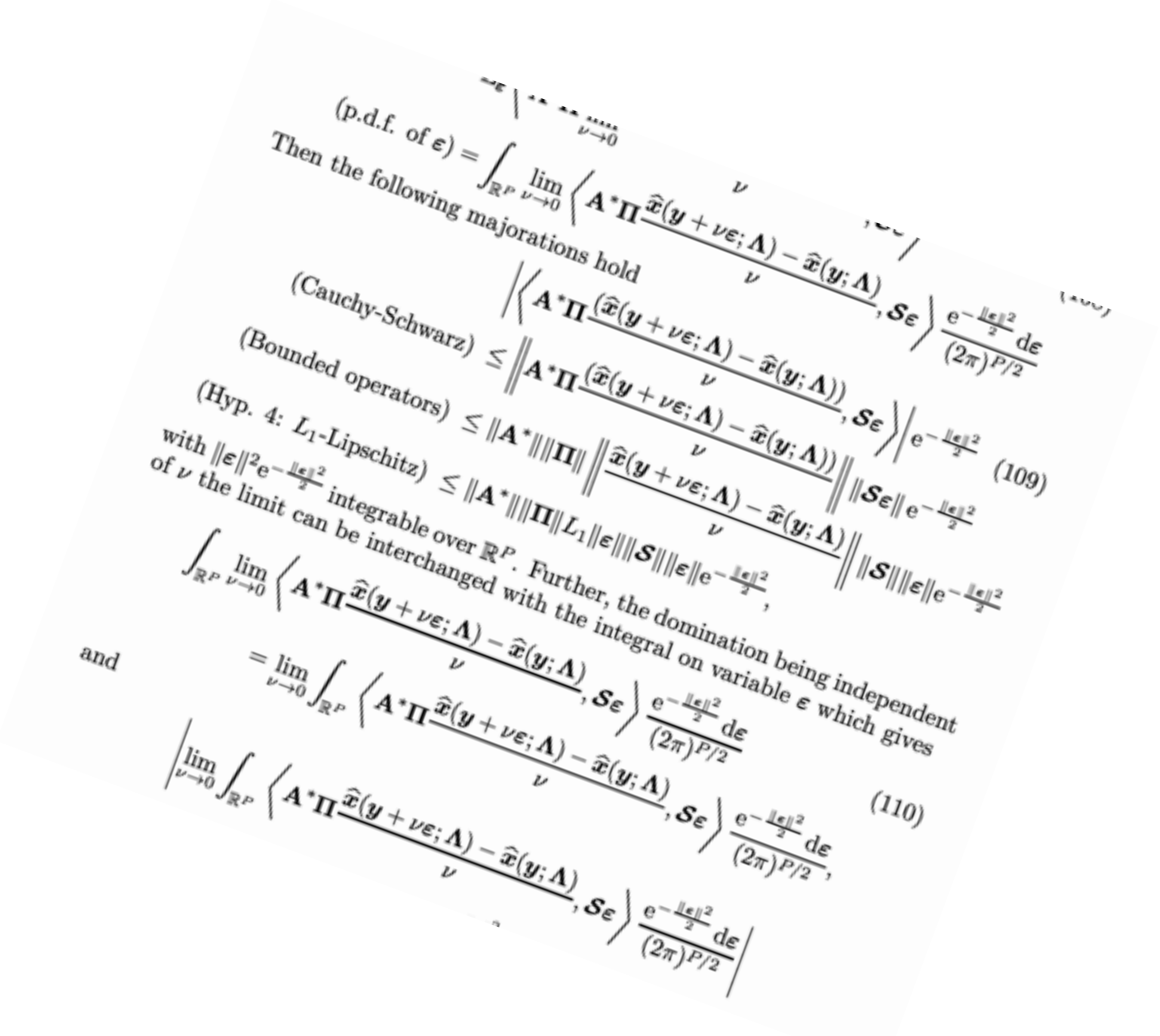
$A = \text{Id} \sim$ prediction

$A = X^\top (XX^\top)^+ \sim$ projection

$A = (X^\top X)^{-1} X^\top \sim$ estimation

Generalized SUGAR for correlated noise [Pascal et al. '20]

$$y = Xw_{\text{true}} + \varepsilon \qquad \varepsilon \sim \mathcal{N}(0, \Sigma)$$


(p.d.f. of ε) $= \int_{\mathbb{R}^P} \lim_{\nu \to 0} \left\langle A^* \Pi \frac{\widehat{x}(y+\nu\varepsilon;\Lambda) - \widehat{x}(y;\Lambda)}{\nu}, S\varepsilon \right\rangle \frac{e^{-\frac{\|\varepsilon\|^2}{2}}}{(2\pi)^{P/2}} d\varepsilon$

Then the following majorations hold

$\left| \left\langle A^* \Pi \frac{\widehat{x}(y+\nu\varepsilon;\Lambda) - \widehat{x}(y;\Lambda)}{\nu}, S\varepsilon \right\rangle \right| e^{-\frac{\|\varepsilon\|^2}{2}}$

(Cauchy-Schwarz) $\leq \left\| A^* \Pi \frac{\widehat{x}(y+\nu\varepsilon;\Lambda) - \widehat{x}(y;\Lambda)}{\nu} \right\| \|S\varepsilon\| e^{-\frac{\|\varepsilon\|^2}{2}}$

(Bounded operators) $\leq \|A^*\| |||\Pi||| \left\| \frac{\widehat{x}(y+\nu\varepsilon;\Lambda) - \widehat{x}(y;\Lambda)}{\nu} \right\| \|S\varepsilon\| e^{-\frac{\|\varepsilon\|^2}{2}}$ (109)

(Hyp. 4: L_1-Lipschitz) $\leq \|A^*\| |||\Pi||| L_1 \|\varepsilon\| |||S||| \|\varepsilon\| e^{-\frac{\|\varepsilon\|^2}{2}}$,

with $\|\varepsilon\|^2 e^{-\frac{\|\varepsilon\|^2}{2}}$ integrable over $\mathbb{R}^P$. Further, the domination being independent of ν the limit can be interchanged with the integral on variable ε which gives

$\int_{\mathbb{R}^P} \lim_{\nu \to 0} \left\langle A^* \Pi \frac{\widehat{x}(y+\nu\varepsilon;\Lambda) - \widehat{x}(y;\Lambda)}{\nu}, S\varepsilon \right\rangle \frac{e^{-\frac{\|\varepsilon\|^2}{2}}}{(2\pi)^{P/2}} d\varepsilon$

$= \lim_{\nu \to 0} \int_{\mathbb{R}^P} \left\langle A^* \Pi \frac{\widehat{x}(y+\nu\varepsilon;\Lambda) - \widehat{x}(y;\Lambda)}{\nu}, S\varepsilon \right\rangle \frac{e^{-\frac{\|\varepsilon\|^2}{2}}}{(2\pi)^{P/2}} d\varepsilon$, (110)

and

$\left| \lim_{\nu \to 0} \int_{\mathbb{R}^P} \left\langle A^* \Pi \frac{\widehat{x}(y+\nu\varepsilon;\Lambda) - \widehat{x}(y;\Lambda)}{\nu}, S\varepsilon \right\rangle \frac{e^{-\frac{\|\varepsilon\|^2}{2}}}{(2\pi)^{P/2}} d\varepsilon \right|$

Open problems

- Non-Gaussian noise

  Adapt SUGAR to MKLA/MKLS [Deledalle '17]

- Non-weakly differentiable estimators

  Heuristics? Theory?

SUGAR in practice: image deblurring

Total variation deblurring

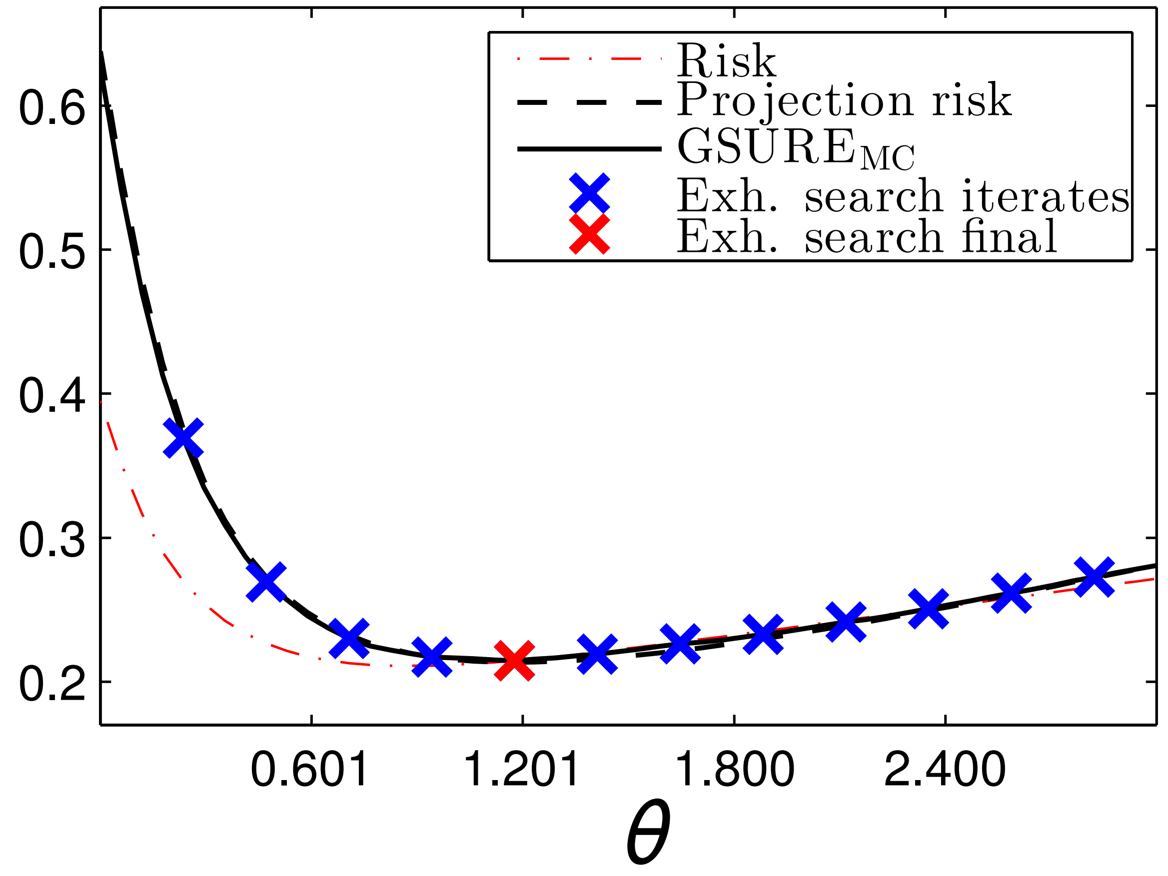
$$y = X w_{\mathrm{true}} + \varepsilon$$

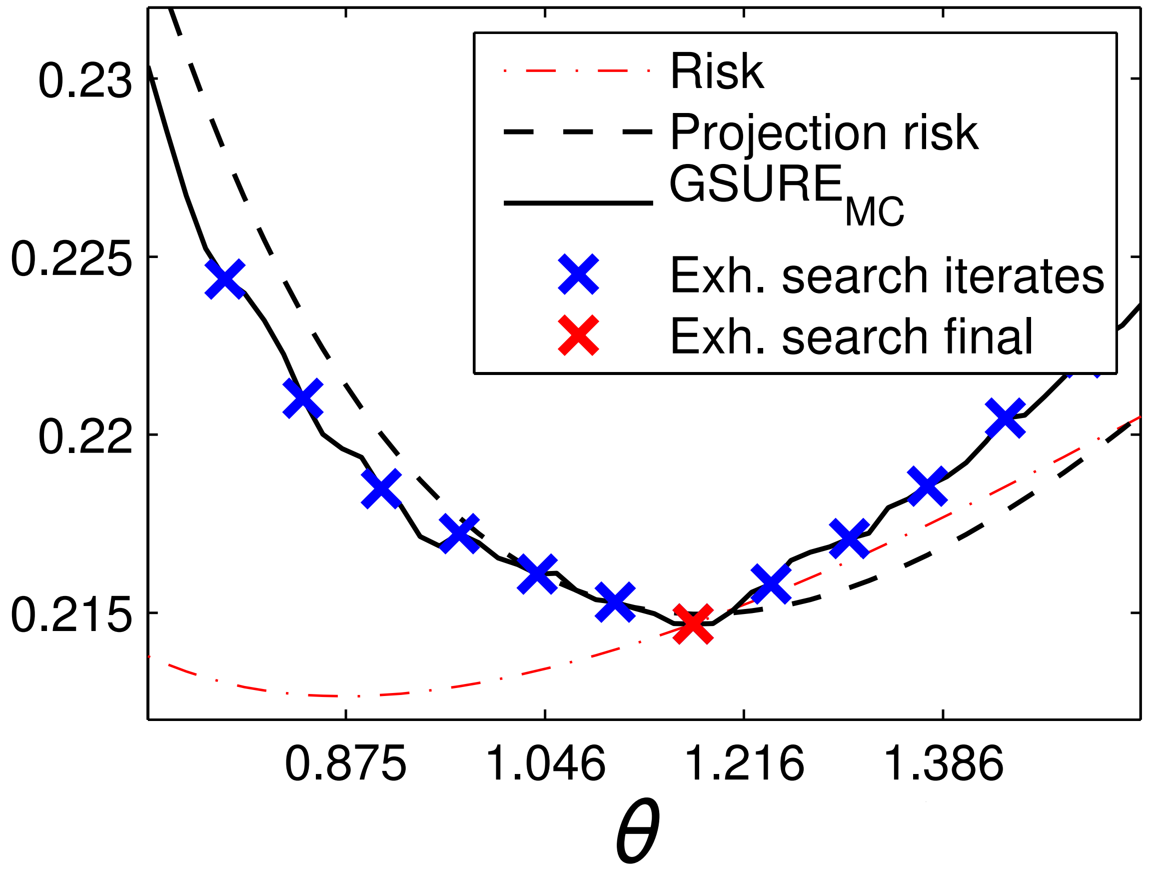
$$\hat{w}_\theta(y) \in \underset{w}{\operatorname{argmin}} \frac{1}{2}\|y - X w_{\mathrm{true}}\|_2^2 + \theta \|\nabla_{2D} w\|_{1,2}$$

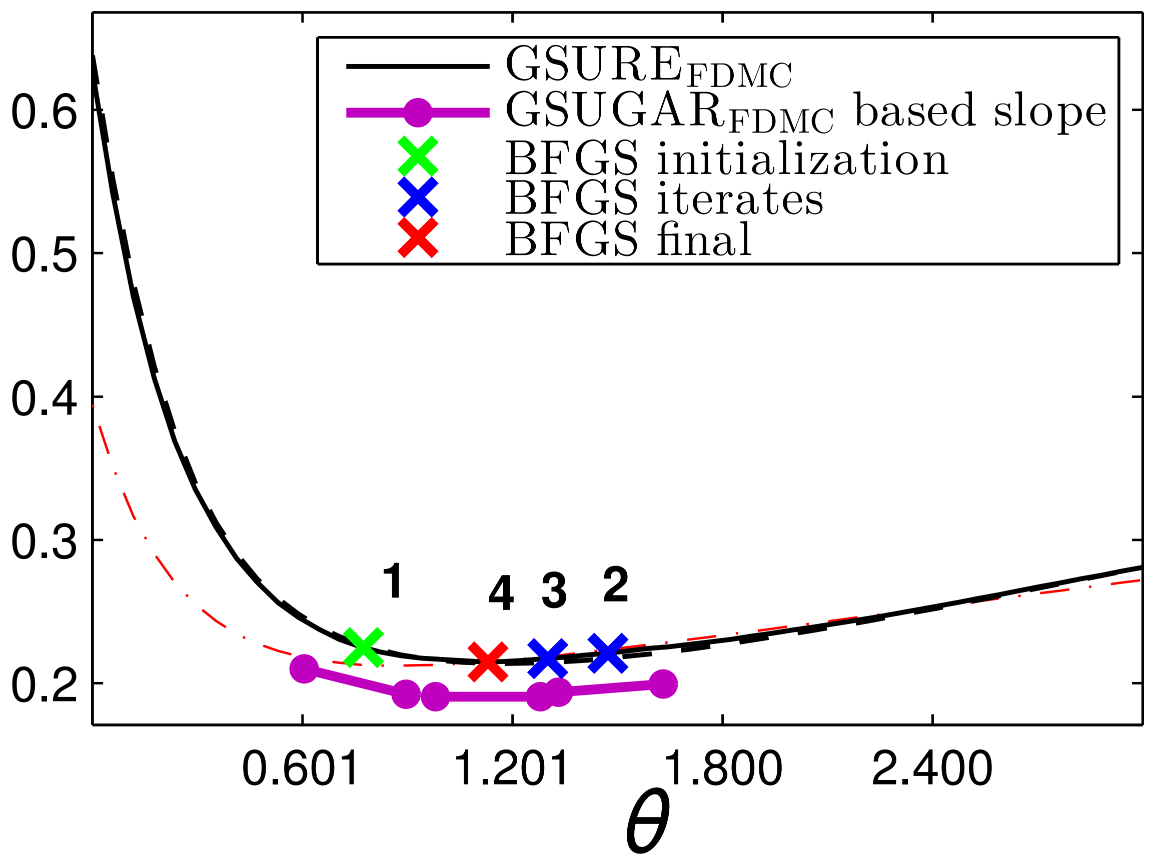
[Chambolle-Pock ’11]

$w_\theta^{(k)}(y)$ computed with a differentiated Primal-Dual algorithm

$$\theta^{(t+1)} = \theta^{(t)} - B^{(t)} \mathrm{SUGAR}_{\theta^{(t)}}^{(k),\mathrm{FDMC}}(y)$$







w_{true}

y

$\hat{w}_{\theta^\star}$

SUGAR in practice: compressed sensing

Multiscale compressed sensing

two-orientation wavelet transform enforces smooth images w/ sharp discontinuities

$$\hat{w}_\theta(y) \in \underset{w}{\operatorname{argmin}} \ \frac{1}{2}\|y - Xw\|_2^2 + \sum_{j=1}^{J} \theta_j \Big(\underbrace{\|\Psi_j^{\rightarrow} w\|_1}_{\text{horizontal}} + \underbrace{\|\Psi_j^{\uparrow} w\|_1}_{\text{vertical}} \Big)$$

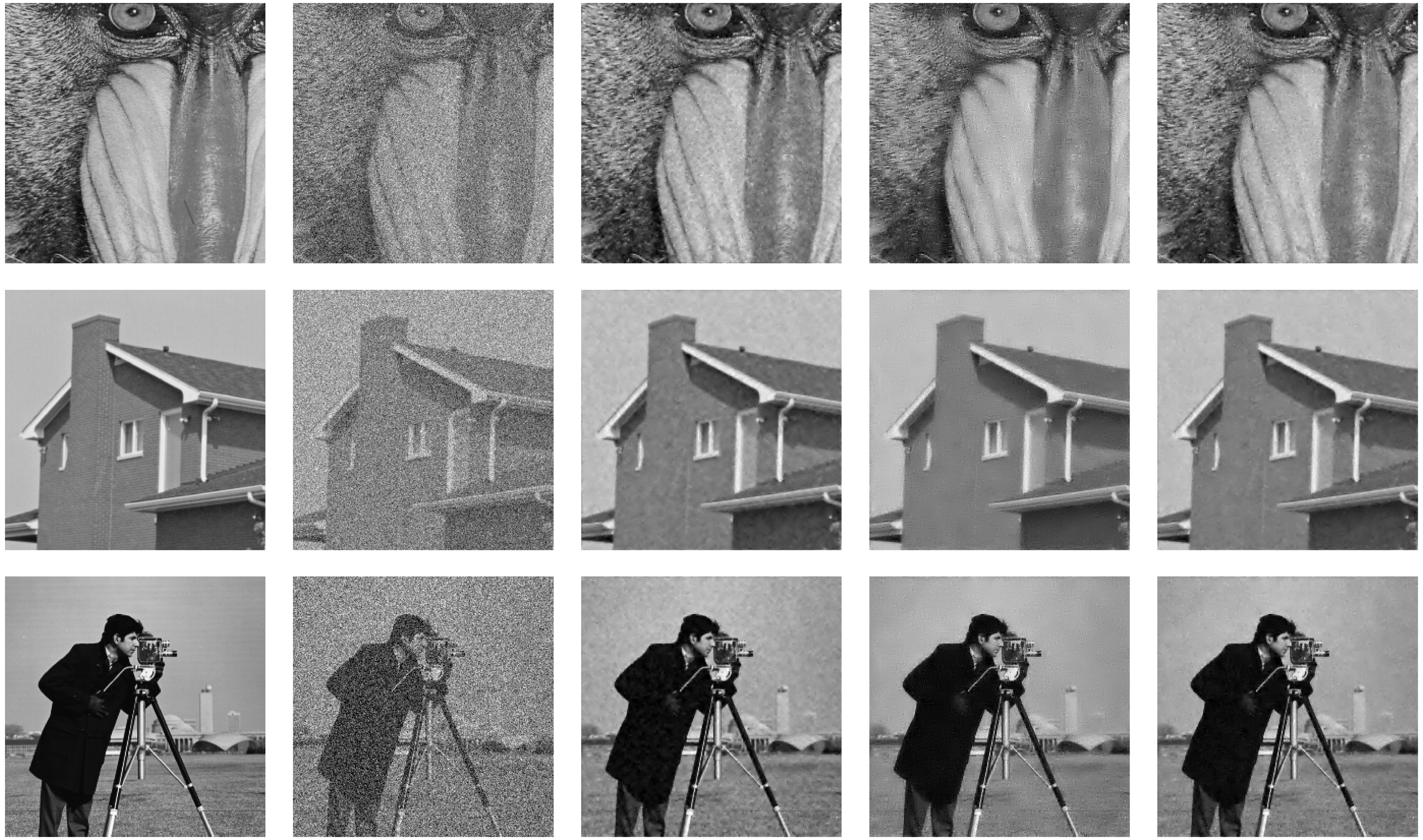
$$y = X w_{\text{true}} + \varepsilon$$

Gaussian measurement matrix $n \ll p$

[Chambolle-Pock '11]

Same primal-dual algorithm

Input		Optimal parameters			SURE/PSNR		
Image	PSNR	J	$\dim \Lambda$	λ^*	$0.75\lambda^*$	λ^*	$1.25\lambda^*$
Mandrill	17.37	1	1	(7.58)	7.53/24.84	**7.39**/24.90	7.43/**24.94**
		2	1	(5.63)	7.60/24.85	**7.45**/24.88	7.58/**24.89**
		3	1	(4.54)	7.87/24.04	**7.71/24.10**	7.83/**24.10**
		2	2	(5.94, 4.24)	7.49/25.02	**7.30**/25.06	7.38/**25.07**
		3	3	(7.51, 1.07, 0.99)	7.37/25.12	**7.22**/25.18	7.33/**25.20**
House	17.65	1	1	(18.38)	3.69/**31.16**	**3.51**/31.15	3.68/30.55
		2	1	(11.11)	3.72/31.31	**3.51/31.40**	3.81/31.05
		3	1	(8.73)	4.30/30.18	**4.08/30.31**	4.43/30.13
		2	2	(14.47, 5.20)	3.53/31.51	**3.34/31.57**	3.55/31.05
		3	3	(15.00, 2.50, 2.83)	3.52/31.55	**3.27/31.63**	3.44/31.14
Cameraman	15.13	1	1	(13.50)	5.29/28.61	**5.09/28.73**	5.35/28.64
		2	1	(8.78)	5.34/28.75	**5.09/28.83**	5.38/28.72
		3	1	(7.14)	5.84/28.03	**5.60/28.06**	5.88/27.99
		2	2	(10.98, 3.74)	5.16/28.91	**4.90/29.04**	5.09/28.96
		3	3	(11.56, 3.31, 0.97)	5.07/29.00	**4.86/29.11**	5.13/28.99



original | least-square solution | 1 level | 3 levels 1 parameters | 3 levels 3 parameters

The direct way

Q. Bertrand, Q. Klopfenstein, M. Blondel, SV, A. Gramfort, J. Salmon. Implicit differentiation of Lasso-type models for hyperparameter optimization. *ICML*. 2020.

First order methods for parameter selection

Goal

Find $\theta^\star \in \underset{\theta \in \Theta}{\operatorname{argmin}} \mathcal{R}(\theta)$

(or close to it)

$$\mathcal{R}(\theta) = \mathcal{C}(\hat{w}_\theta(y)) = (\mathcal{C} \circ \hat{w}_\bullet(y))(\theta)$$

$$\mathcal{C} : \mathbb{R}^p \to \mathbb{R}$$

$$\hat{w}_\bullet(y) : \Theta \subseteq \mathbb{R}^l \to \mathbb{R}^p$$

Chain rule

Assuming $\mathcal{C}$ and $\hat{w}_\bullet(y)$ to be differentiable

$$\nabla \mathcal{R}(\theta) = \left[\mathrm{Jac}_{\hat{w}_\bullet(y)}(\theta)\right]^\perp \nabla \mathcal{C}(\hat{w}_\theta(y))$$

and

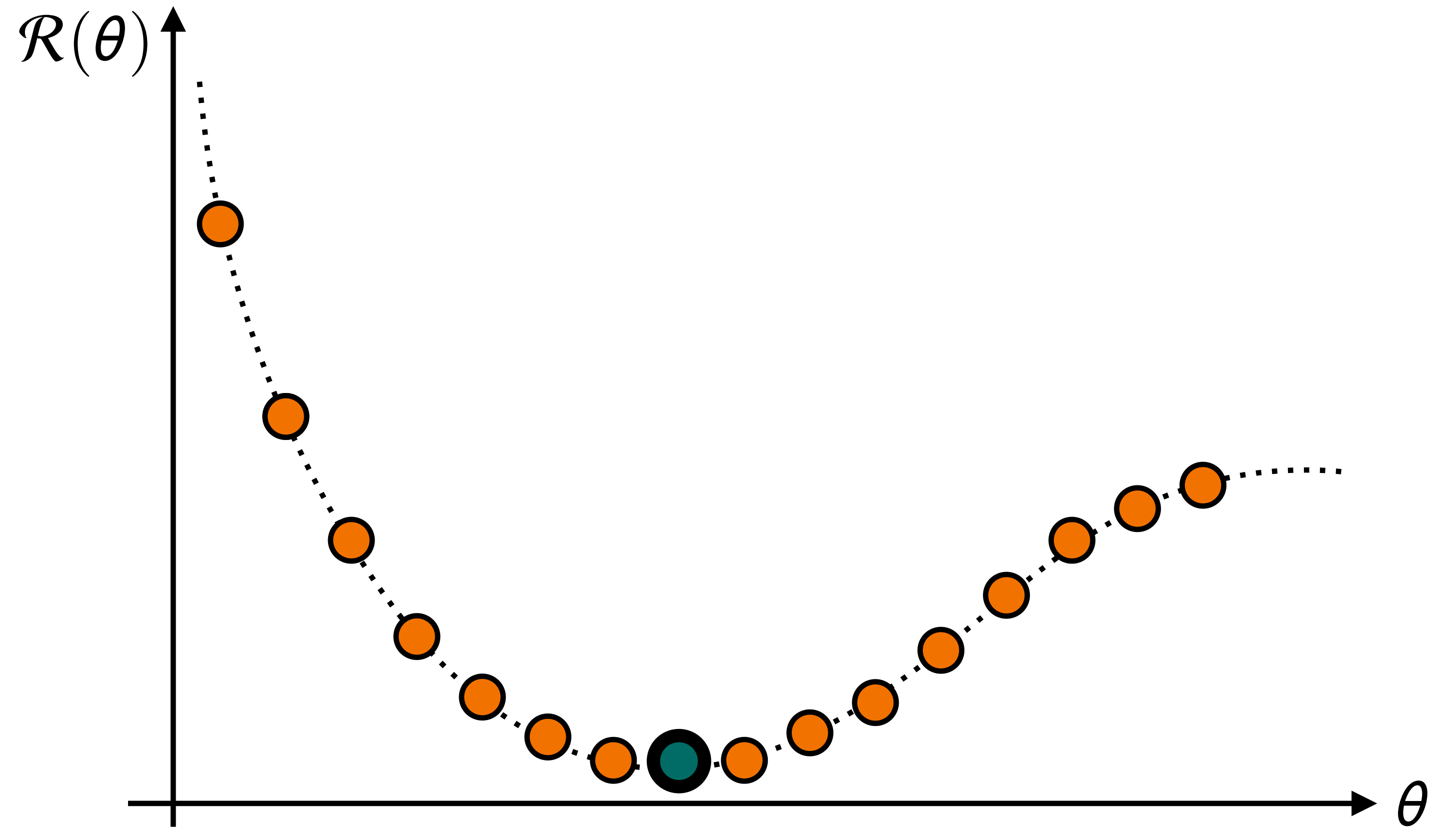
$$\nabla \mathcal{R}(\theta^\star) = 0$$

"Hyper"-gradient descent

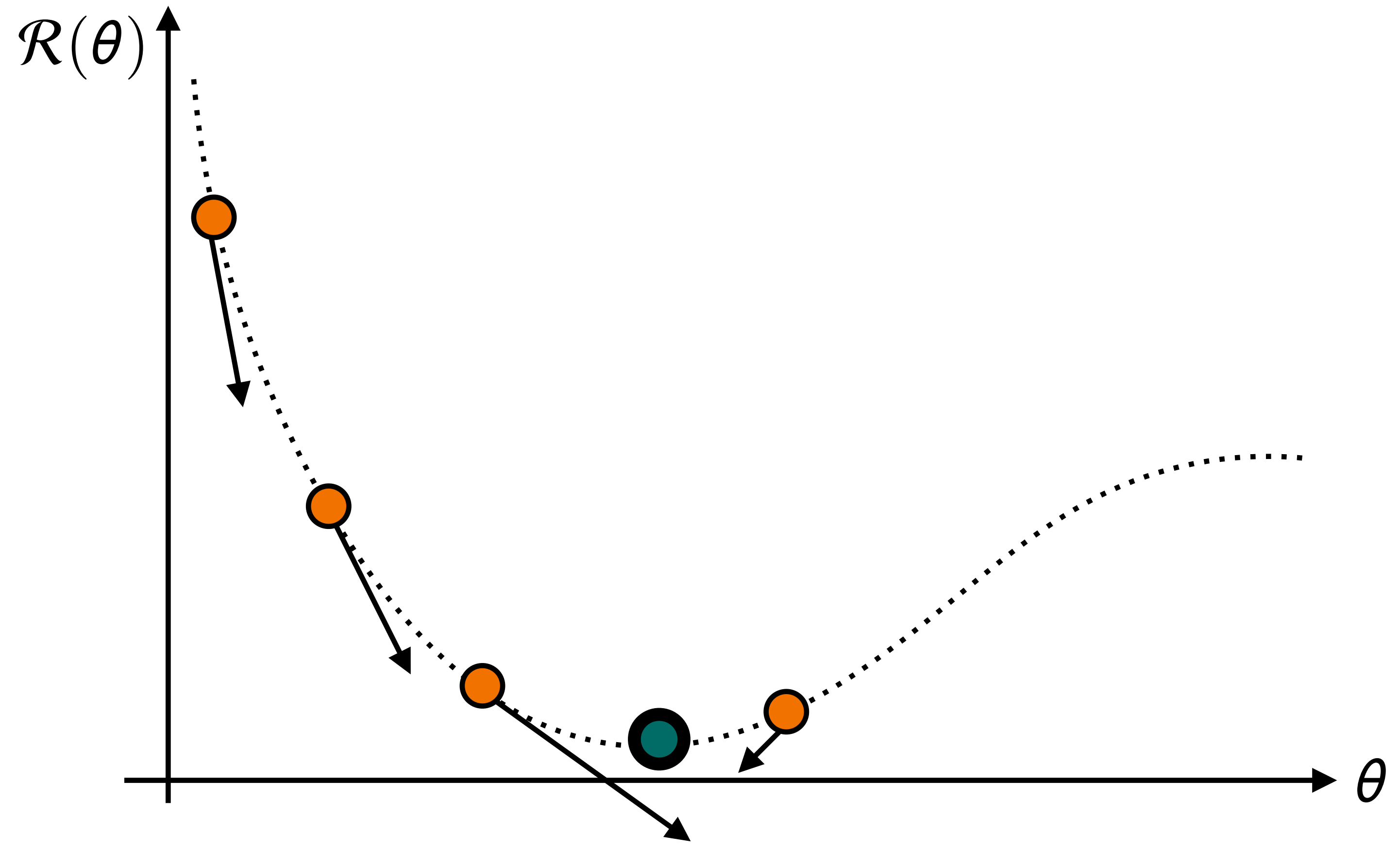
$$\theta^{k+1} = \theta^k - \rho \nabla \mathcal{R}(\theta^k)$$

possibly **projected** gradient descent on the parameter space

Grid search (a.k.a 0-order)



Gradient descent



Bilevel problem: implicit differentiation

Goal

Find $\theta^\star \in \underset{\theta \in \Theta}{\operatorname{argmin}}\, \mathcal{R}(\theta)$

(or close to it)

$$\mathcal{R}(\theta) = \mathcal{C}(\hat{w}_\theta(y))$$

- $\mathcal{C}$, $\nabla \mathcal{C}$ easy to compute
- $\hat{w}_\theta$ variational estimator
- $\mathcal{F}$ convex smooth

Bilevel optimization

outer problem

$$\theta^\star \in \underset{\theta \in \Theta}{\operatorname{argmin}}\, \mathcal{C}(\hat{w}_\theta(y))$$

subject to $\quad \hat{w}_\theta(y) \in \underset{w \in \mathbb{R}^p}{\operatorname{argmin}}\, \mathcal{F}(w, \theta)$

inner problem

$$\nabla \mathcal{R}(\theta) = \left[\mathrm{Jac}_{\hat{w}_\bullet(y)}(\theta)\right]^\perp \nabla \mathcal{C}(\hat{w}_\theta(y))$$

Smooth case

Kernel-based
[Chapelle et al. '02]
Weighted ridge
[Foo et al. '08]
Image restoration
[Kunish-Pock '13]
Noisy stability
[Pedregosa '16]

Non-smooth

Elastic-net
[Mairal et al. '12]
Lasso
[Dossal et al. '13,
Zou et al. '07]
Generalized Lasso
[V. et al. '13
Tibshirani-Taylor '11]
Partly smooth
[V. et al. '17]
Constrained quad
[Amos-Kolter '17]
Simplex constrained
[Niculae-Blondel '17]

[Larsen et al. '96] **Fixed point equation** $\quad \nabla_w \mathcal{F}(\hat{w}_\theta(y), \theta) = 0$

$$\xrightarrow{\frac{\partial}{\partial \theta}}$$

$$\nabla^2_{w,\theta} \mathcal{F}(\hat{w}_\theta(y), \theta) + \left[\mathrm{Jac}_{\hat{w}_\bullet(y)}(\theta)\right]^\perp \nabla^2_w \mathcal{F}(\hat{w}_\theta(y), \theta) = 0$$

assuming invertibility

$$\left[\mathrm{Jac}_{\hat{w}_\bullet(y)}(\theta)\right]^\perp = -\nabla^2_{w,\theta} \mathcal{F}(\hat{w}_\theta(y), \theta) \left(\nabla^2_w \mathcal{F}(\hat{w}_\theta(y), \theta)\right)^{-1}$$

invert $p \times p$ system

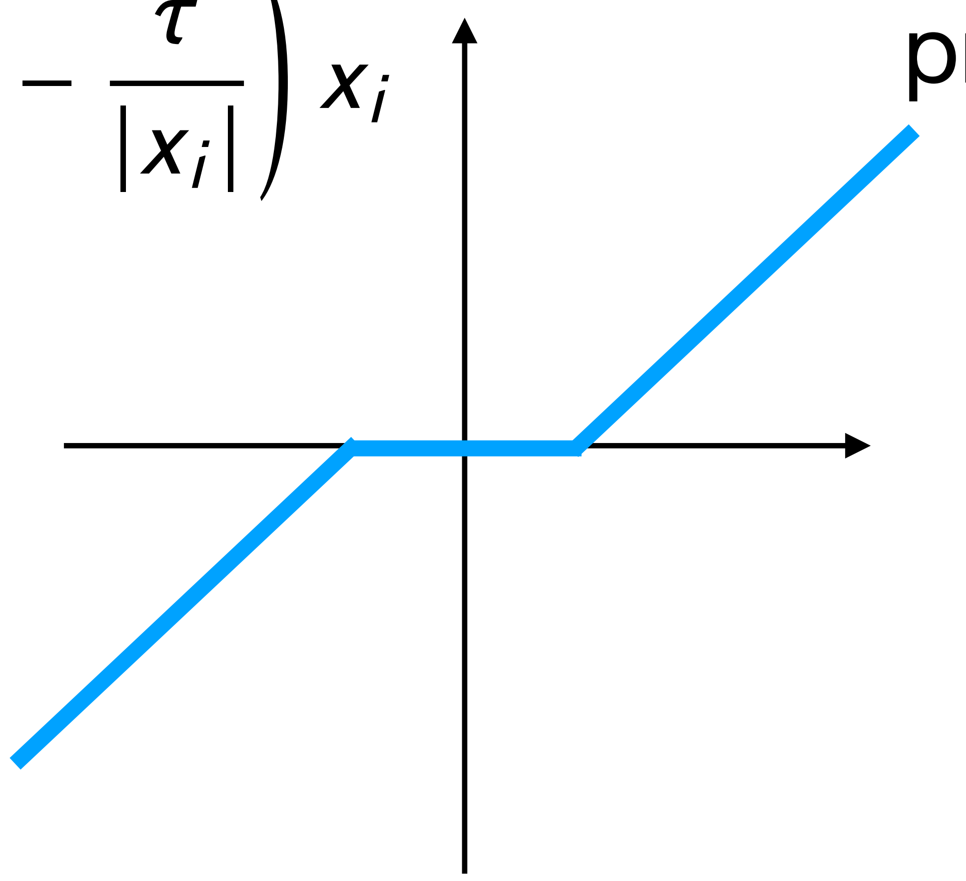
A focus on the Lasso

Lasso

$$\hat{w}_\theta(y) \in \underset{w \in \mathbb{R}^p}{\operatorname{argmin}} \frac{1}{2}\|y - Xw\|_2^2 + \theta\|w\|_1$$

Soft-thresholding

$$\operatorname{prox}_{\tau\|\cdot\|_1}(x)_i = \min\left(0, 1 - \frac{\tau}{|x_i|}\right) x_i$$



Fixed-point equation

$j \in [p], \alpha > 0$

$$(\hat{w}_\theta(y))_j = \operatorname{prox}_{\frac{\theta}{\alpha}\|\cdot\|_1}\left((\hat{w}_\theta(y))_j - \frac{1}{\alpha} X_{j,:}^\top (X\hat{w}_\theta(y) - y)\right)$$

Proximal Coordinate Descent [Tseng '09]

For $k = 1$ to $n_{\mathtt{epochs}}$

For $j = 1$ to p

$$(w_\theta^{k+1}(y))_j = \operatorname{prox}_{\frac{\theta}{\|X_{:,j}\|^2}|\cdot|}\left(((w_\theta^k(y))_j - \frac{1}{\|X_{j,:}\|^2} X_{:,j}^\top (X(w_\theta^k(y))_j - y)\right)$$

Implicit differentiation

[Vaiter '13]

$\frac{\partial}{\partial \theta}$

$$[\mathrm{Jac}_{\hat{w}_{\cdot}(y)}(\theta)]_{\hat{S}} = -\theta (X_{\hat{S}}^\top X_{\hat{S}})^{-1} \operatorname{sign}(\hat{w}_\theta(y))_{\hat{S}}$$

$$[\mathrm{Jac}_{\hat{w}_{\cdot}(y)}(\theta)]_{\hat{S}^c} = 0$$

$\hat{S} = \operatorname{supp}(\hat{w}_\theta(y))$

$X_{\hat{S}}$ full rank

Issue: Jacobian size

$p \times p$

Fixed-point equation

$j \in [p], \alpha > 0$

$$(\hat{w}_\theta(y))_j = \operatorname{prox}_{\frac{\theta}{\alpha}\|\cdot\|_1}\left((\hat{w}_\theta(y))_j - \frac{1}{\alpha} X_{j,:}^\top (X\hat{w}_\theta(y) - y)\right)$$

Issue: Inversion

$(X_{\hat{S}}^\top X_{\hat{S}})^{-1}$

Proximal Coordinate Descent [Tseng '09]

For $k = 1$ to $n_{\mathtt{epochs}}$

For $j = 1$ to p

$$(w_\theta^{k+1}(y))_j = \operatorname{prox}_{\frac{\theta}{\|X_{:,j}\|^2}|\cdot|}\left(((w_\theta^k(y))_j - \frac{1}{\|X_{j,:}\|^2} X_{:,j}^\top (X(w_\theta^k(y))_j - y)\right)$$

Forward Iterative Differentiation

Chain rule

$$\mathrm{Jac}_{w_{\bullet}^{k+1}(y)}(\theta) = \partial_1 \mathrm{T}(w_\theta^k(y), \theta) \cdot \mathrm{Jac}_{w_{\bullet}^{k}(y)}(\theta) + \partial_2 \mathrm{T}(w_\theta^k(y), \theta)$$

$$\frac{\partial}{\partial \theta}$$

Fixed-point equation $j \in [p], \alpha > 0$

$$(\hat{w}_\theta(y))_j = \mathrm{prox}_{\frac{\theta}{\alpha}\|\cdot\|_1}\left((\hat{w}_\theta(y))_j - \frac{1}{\alpha} X_{j,:}^\top (X \hat{w}_\theta(y) - y)\right)$$

Proximal Coordinate Descent [Tseng '09]

For $k = 1$ to n_{epochs}

For $j = 1$ to p

$$(w_\theta^{k+1}(y))_j = \mathrm{prox}_{\frac{\theta}{\|X_{:,j}\|^2}|\cdot|}\left(((w_\theta^k(y))_j - \frac{1}{\|X_{j,:}\|^2} X_{:,j}^\top (X(w_\theta^k(y))_j - y)\right)$$

Numerical experiments

Machine learning

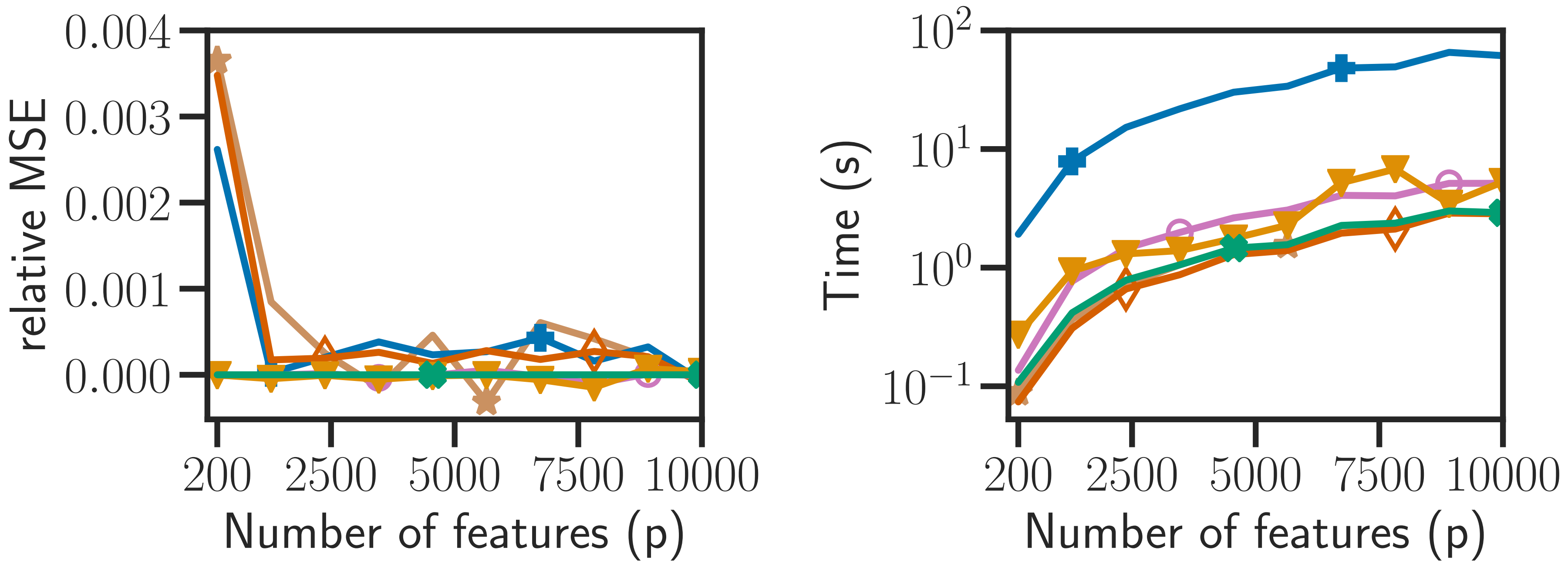
validation set: $y^{\text{val}}, X^{\text{val}}$

hold-out loss

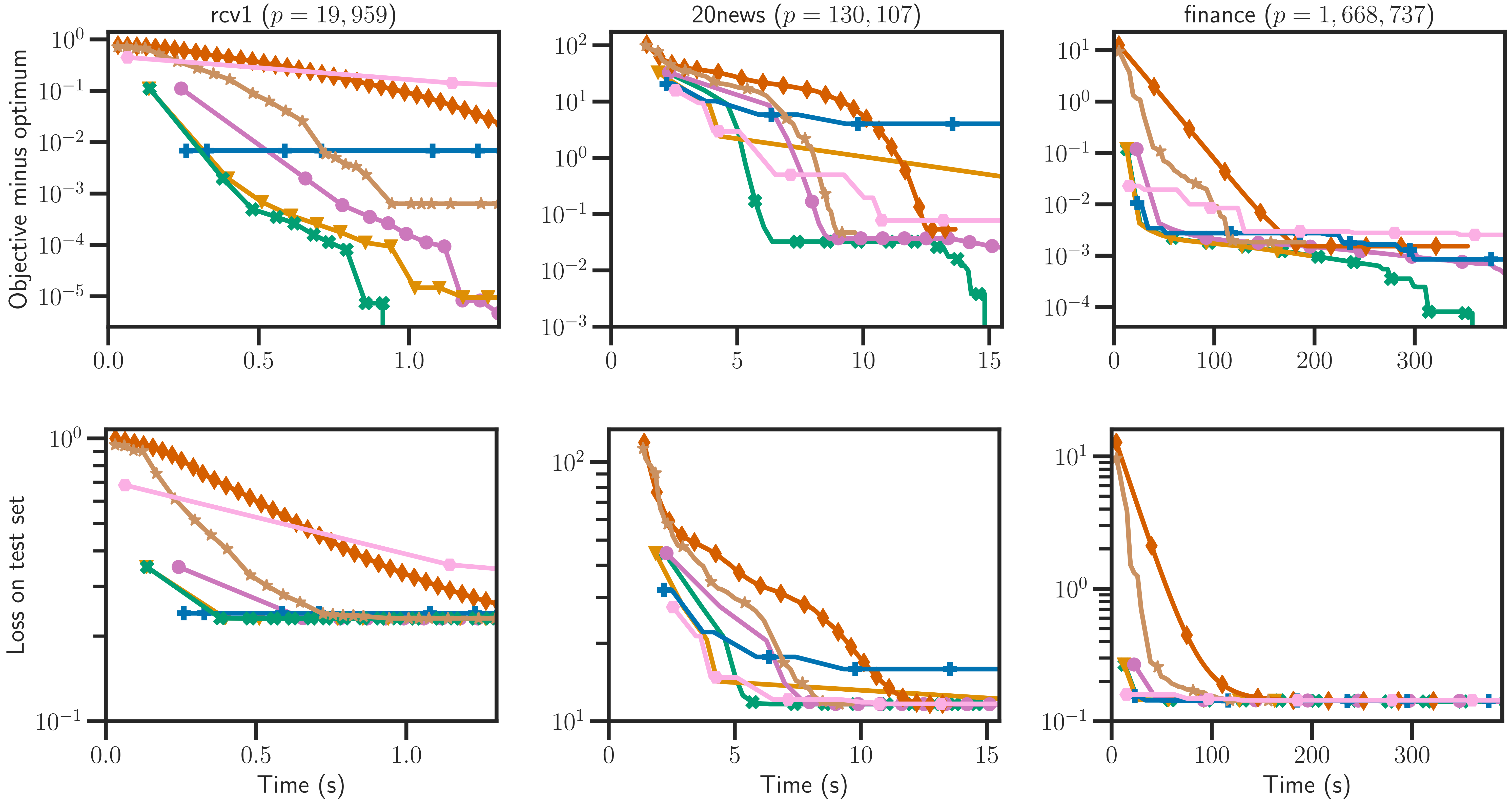
[Stone-Ramer '65]

$$\mathcal{R}(\theta) = \|y^{\text{val}} - X^{\text{val}} \hat{w}_\theta(y)\|_2^2$$

$\hat{w}_\theta(y)$: Lasso



Estimation performance



Computation time

Summary

Estimator

$\hat{w}_\theta : \mathbb{R}^n \longrightarrow \mathbb{R}^p$ estimator

$\theta \in \Theta$ hyper-parameter

$\mathcal{R} : \Theta \longrightarrow \mathbb{R}$ criterion

Goal

$$\text{Find } \theta^\star \in \operatorname*{argmin}_{\theta \in \Theta} \mathcal{R}(\theta)$$

(or close to it)

Estimator and algorithm

$$\begin{tikzcd}
w_\theta^{(k)}(y) \arrow[r] \arrow[d] & \hat{w}_\theta(y) \arrow[d, dotted] \\
\mathrm{Jac}_{\hat{w}_\theta}(y) \arrow[r] & \mathrm{Jac}_{w_\theta^{(k)}}(y)
\end{tikzcd}$$

Iterative estimators

$$\mathrm{T} : \mathbb{R}^p \times \mathbb{R}^n \longrightarrow \mathbb{R}^p$$

$$\begin{cases} w_\theta^{(k)}(y) \xrightarrow{k \to +\infty} \hat{w}_\theta(y) \\ w_\theta^{(k+1)}(y) = \mathrm{T}(w_\theta^{(k)}(y), y) \end{cases}$$

Chain rule

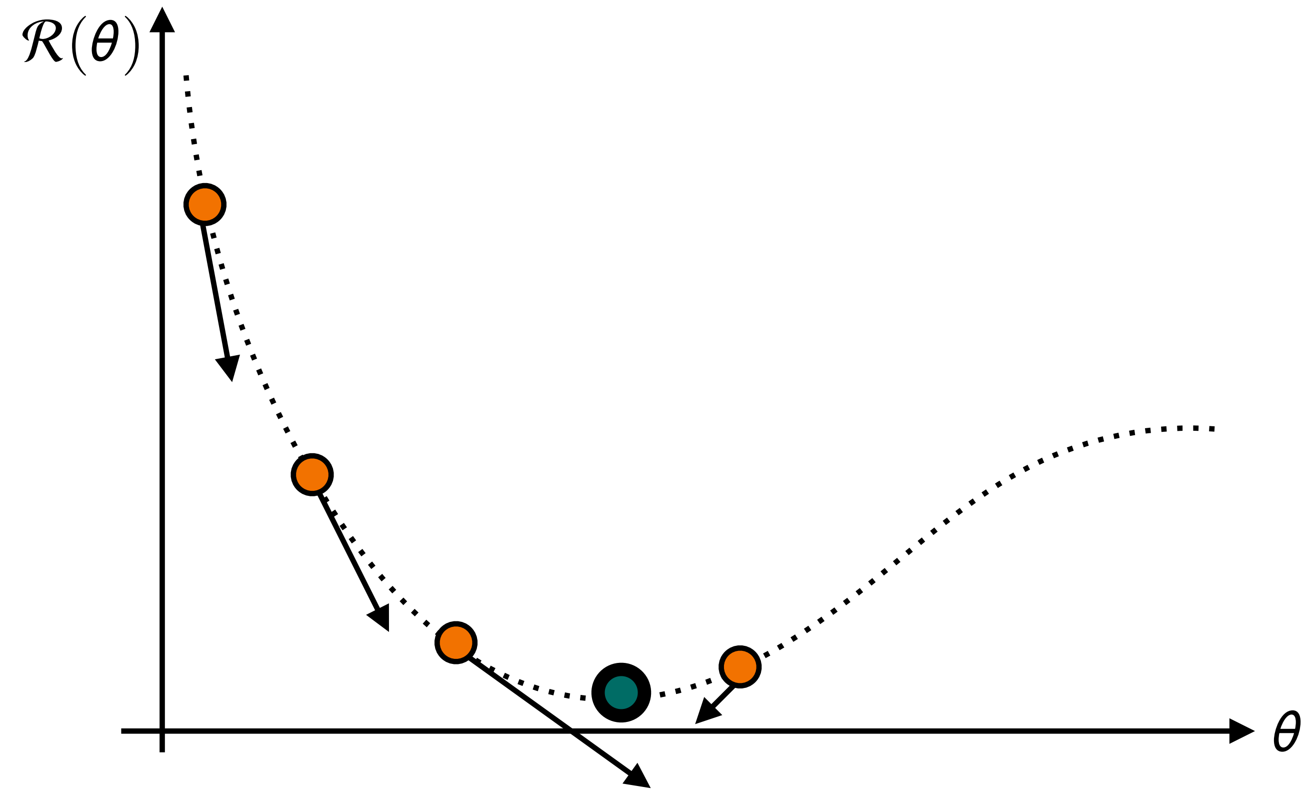
$$\mathrm{Jac}_{w_\theta^{k+1}}(y) = {\color{red}\partial_1}\mathrm{T}({\color{red}w_\theta^k(y)}, y) \cdot \mathrm{Jac}_{w_\theta^k(y)}(y) + {\color{blue}\partial_2}\mathrm{T}(w_\theta^k(y), {\color{blue}y})$$

“Hyper”-gradient descent

$$\theta^{k+1} = \theta^k - \rho \nabla \mathcal{R}(\theta^k)$$

Several strategies:

- Implicit differentiation
- Risk estimation (SUGAR)
- Direct Jacobian estimation



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Thanks!

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