Probabilistic Numerics

IV – Linear Algebra

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Yesterday:

- probabilities: a rigorous notion of uncertainty
- Gaussians provide a computationally efficient algebra of uncertainty
- classic methods for **Quadrature** and **ODEs** can be re-formulated as MAP/mean inference in Gaussian models. The associated covariances yield calibrated (worst-case) error bars
- these probabilistic formulations also provide additional functionality that would be tricky in the classic formulations

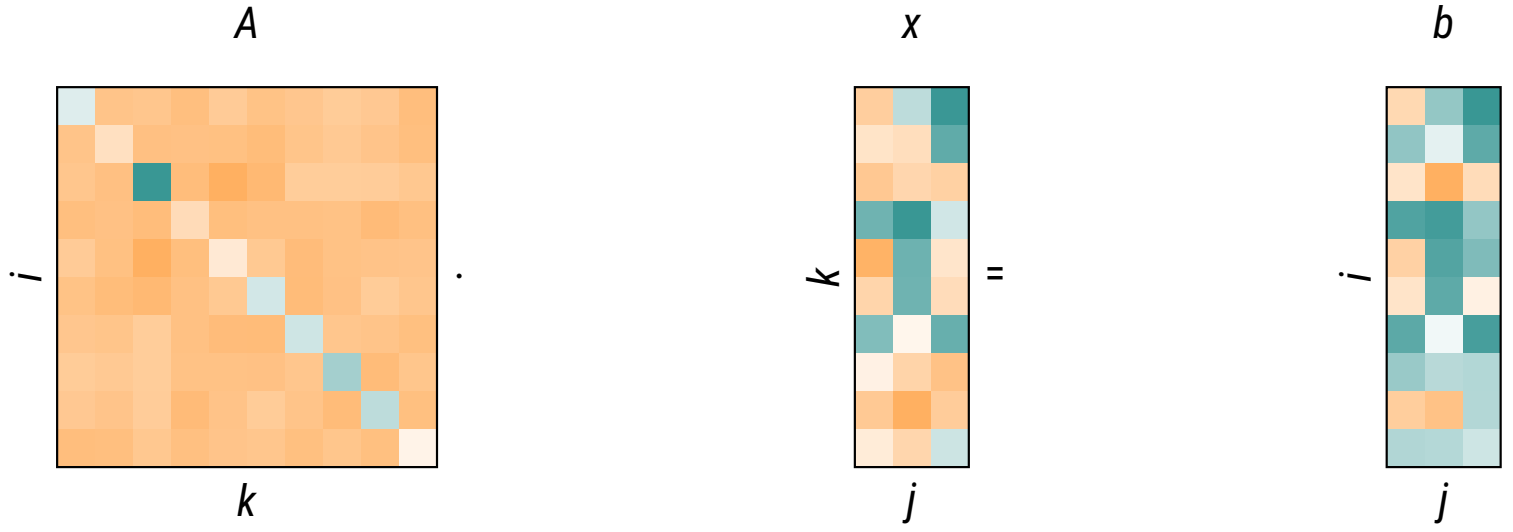
all slides from yesterday at ($x = 1, 2, 3$)
`http://tinyurl.com/Dobbiaco-Hennig-x`

Now:

- a probabilistic formulation of **iterative linear solvers**
- a connection to nonlinear optimization

Problem Setting

The least-squares problem



$$Ax = b \qquad A \in \mathbb{R}^{N \times N} \qquad b \in \mathbb{R}^{N}$$

- in machine learning and statistics:

$$A = \Phi\Phi^{\mathsf{T}} + \sigma^2 I \qquad \text{symmetric positive definite}$$

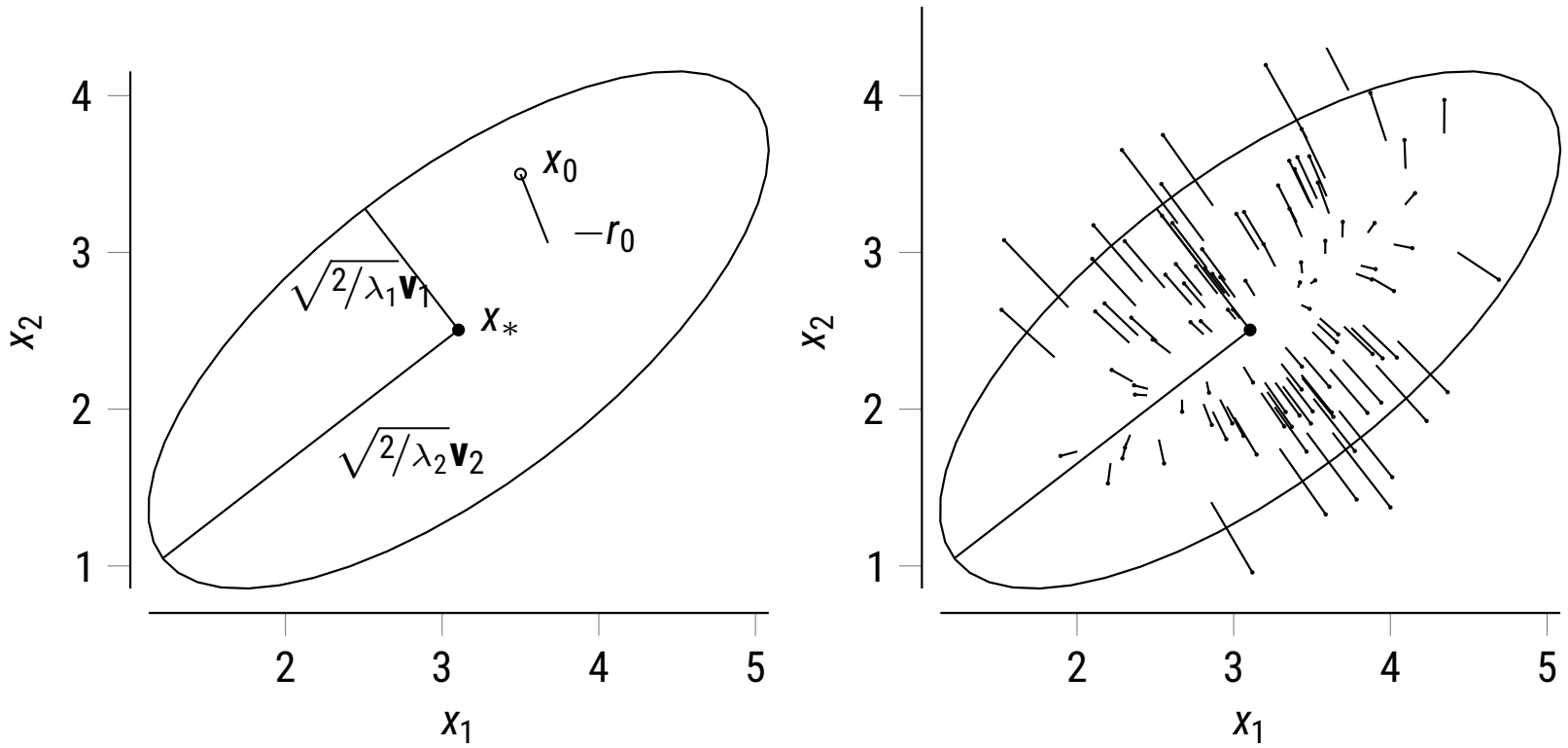
- aka. the **least-squares problem**, because then

$$x = \arg\min_{\tilde{x}} f(\tilde{x}) \qquad \text{for} \qquad f(\tilde{x}) = {}^1\!/_2 \tilde{x}^{\mathsf{T}} A \tilde{x} - \tilde{x}^{\mathsf{T}} b$$

$$\text{with} \qquad \nabla_{\tilde{x}} f = A\tilde{x} - b. \qquad \text{Define } H := A^{-1}.$$

A Pictorial View

SPD linear problems are quadratic optimization problems



$$Ax_* = b \qquad A = \begin{bmatrix}\mathbf{v}_1 & \mathbf{v}_2\end{bmatrix}\begin{bmatrix}\lambda_1 & 0\\ 0 & \lambda_2\end{bmatrix}\begin{bmatrix}\mathbf{v}_1^T\\ \mathbf{v}_2^T\end{bmatrix}$$

$$f(\tilde{x}) = {}^1\!/_2\tilde{x}^T A\tilde{x} - \tilde{x}^T b \qquad r(x_i) := Ax_i - b = \nabla f(x_i)$$

Method of Conjugate Gradients

our target for the day

Hestenes & Stiefel, 1952

1 **procedure** CG($A(\cdot)$, b, x_0)
2 $r_0 = Ax_0 - b$ // initial gradient
3 $d_0 = 0, \beta_0 = 0$ // for notational clarity
4 **for** $i = 1, \dots, N$ **do**
5 $d_i = -r_{i-1} + \beta_{i-1} p_{i-1}$ // compute direction
6 $z_i = Ad_i$ // **observe**
7 $\alpha_i = -d_i^\intercal r_{i-1} / d_i^\intercal z_i$ // optimal step-size
8 $s_i = \alpha_i d_i$ // re-scale step
9 $y_i = \alpha_i z_i$ // re-scale observation
10 $x_i = x_{i-1} + s_i$ // update estimate for x
11 $r_i = r_{i-1} + y_i$ // new gradient at x_i
12 $\beta_i = r_i^\intercal r_i / r_{i-1}^\intercal r_{i-1}$ // compute conjugate correction
13 **end for**
14 **end procedure**

- produces **iterate sequence** $x_0, x_1, \dots, x_i$, so that $x_N = x$
- cost dominated by line 6. But no required access to A per se, only $A(\cdot)$

A First Idea

a probabilistic linear solver

Idea: treat $y_i = As_i$ as **observations** of A, **infer** $H = A^{-1}$.

procedure LinSolve_Hopeful($A(\cdot)$, b, $p(A)$)
  $x_0 = H_0 b$ // initial guess
  $r_0 = Ax_0 - b$ // initial gradient
  for $i = 1, \dots, N$ **do**
    $s_i = -H_{i-1} r_{i-1}$ // compute direction
    $y_i = As_i$ // **observe**
    $x_i = x_{i-1} + s_i$ // update estimate for x
    $r_i = r_{i-1} + y_i$ // new gradient at x_i
    $H_i = \text{Infer}(H \mid Y_i, S_i, p(A))$ // estimate H. **To be expanded below**
  end for
end procedure

- why not $x_i = H_i b$? Because classic methods allow for generic x_0. Note

$$x_{i+1} = x_i - H_i(Ax_i - b) = x_i - H_i \left(\sum_{j \leq i} As_j + Ax_0 - b \right) = H_i b + (I - H_i A)x_0.$$

A Refinement

analytic step-size give our generic probabilistic iterative solver — Hennig, SIOPT 2015

1 **procedure** LINSOLVE_HOPEFUL($A(\cdot)$, b, $p(A)$)
2 $x_0 = H_0 b$ // initial guess
3 $r_0 = Ax_0 - b$ // initial gradient
4 **for** $i = 1, \dots, N$ **do**
5 $s_i = -H_{i-1} r_{i-1}$ // compute direction
6 $y_i = As_i$ // **observe**
7 $x_i = x_{i-1} + s_i$ // update estimate for x
8 $r_i = r_{i-1} + y_i$ // new gradient at x_i
9 $H_i = \text{INFER}(H \mid Y_i, S_i, p(A))$ // estimate H. **To be expanded below**
10 **end for**
11 **end procedure**

line 6 gives additional information *before* update (7), fixes step-size:

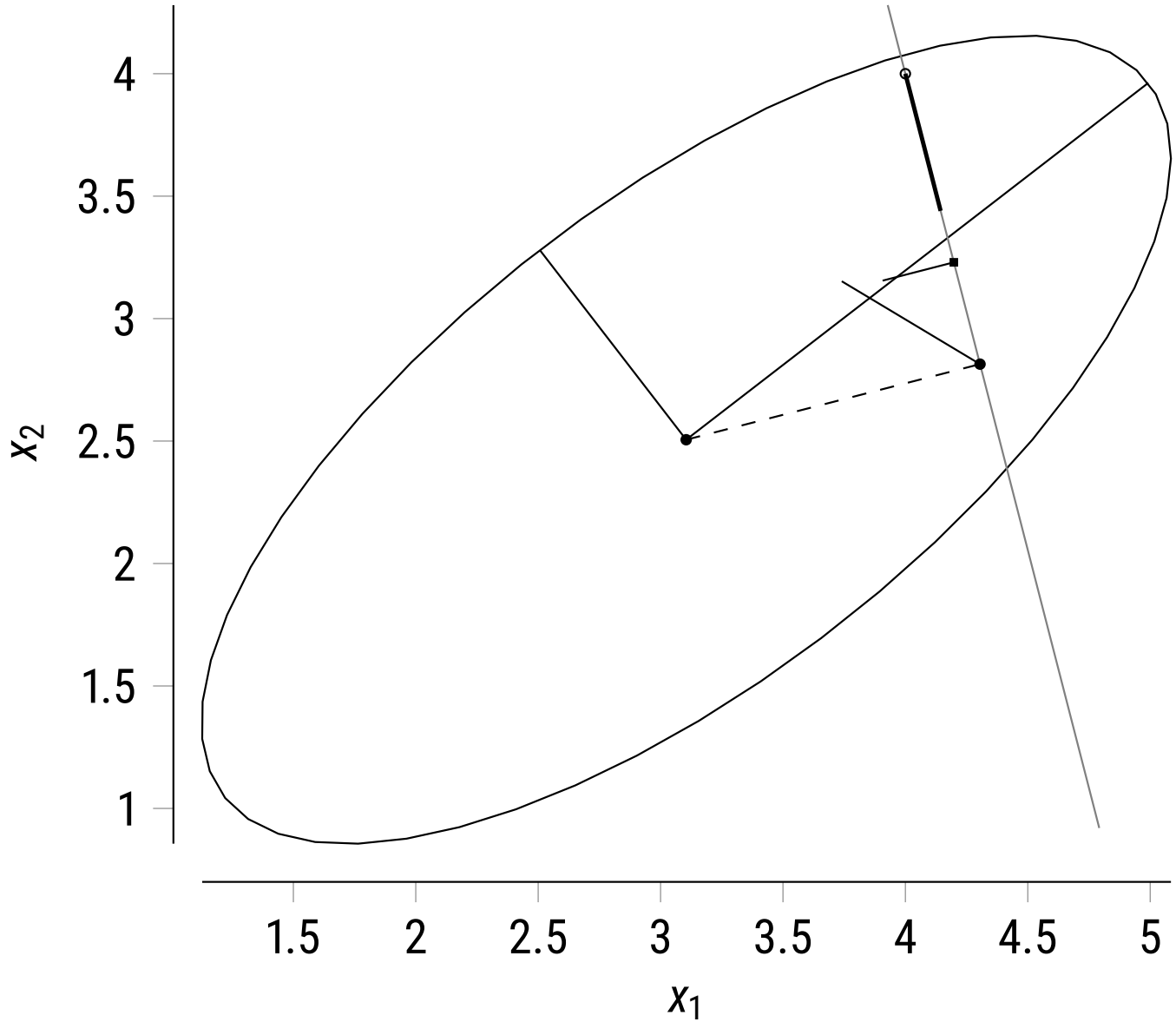
$$\frac{\partial f(x_{i-1} + \alpha_i d_i)}{\partial \alpha_i} = \alpha_i d_i^\intercal A d_i + d_i^\intercal (A x_{i-1} - b) = \alpha_i d_i^\intercal A d_i + d_i^\intercal r_{i-1}$$

$$\Rightarrow \quad \alpha_i = -\frac{d_i^\intercal r_{i-1}}{d_i^\intercal z_i}.$$

A Refinement

analytic step-size give our generic probabilistic iterative solver

Hennig, SIOPT 2015



A Refinement

analytic step-size give our generic probabilistic iterative solver

Hennig, SIOPT 2015

procedure LINSOLVE_PROB($A(\cdot)$, b, $p(A)$)

- $x_0 = H_0 b$ // initial guess
- $r_0 = A x_0 - b$ // initial gradient
- **for** $i = 1, \dots, N$ **do**
  - $d_i = -H_{i-1} r_{i-1}$ // compute direction
  - $z_i = A d_i$ // **observe**
  - $\alpha_i = -d_i^\intercal r_{i-1} / d_i^\intercal z_i$ // optimal step-size
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  - $H_i = \text{INFER}(H \mid Y_i, S_i, p(A))$ // estimate H
- **end for**

end procedure

A Refinement

analytic step-size give our generic probabilistic iterative solver

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procedure CG($A(\cdot)$, b, x_0)
  $d_0 = 0, \beta_0 = 0$ // for notational clarity
  $r_0 = Ax_0 - b$ // initial gradient
  for $i = 1, \dots, N$ **do**
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  end for
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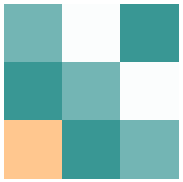
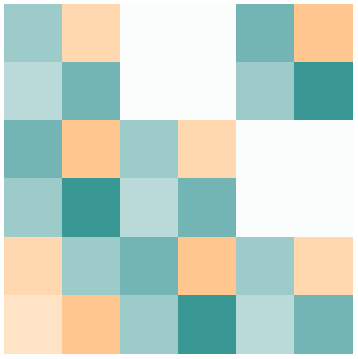
Some Notation

unfortunately, computational linear algebra is tedious and often confusing





- vectorized matrices

$$A \in \mathbb{R}^{N \times N} \quad \Rightarrow \quad \vec{A} \in \mathbb{R}^{N^2 \times 1}. \qquad [A]_{ij} = [\vec{A}]_{(ij)}$$

- the Kronecker product

$$A \in \mathbb{R}^{N_A \times M_A}, B \in \mathbb{R}^{N_B \times M_B} \Rightarrow A \otimes B \in \mathbb{R}^{N_A N_B \times M_A M_B}$$

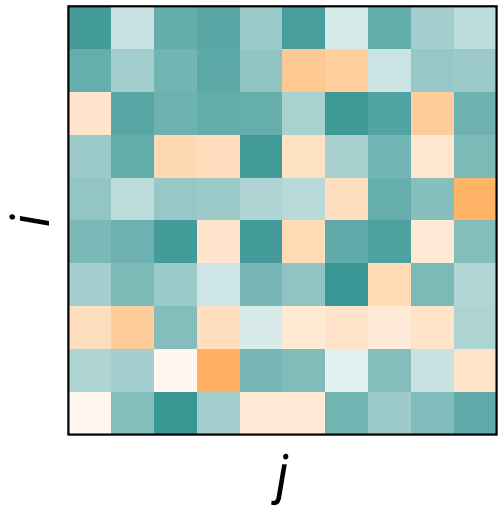
$$[A \otimes B]_{(ij),(k\ell)} = [A]_{ik} \cdot [B]_{j\ell}$$

$$(A \otimes B)\vec{C} = \sum_{k\ell} A_{ik} C_{k\ell} B_{j\ell} = \overrightarrow{ACB^{\mathsf{T}}}$$

$$(A \otimes B) \cdot (C \otimes D) = (AC) \otimes (BD) \qquad (A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$$

Inference on Matrix Elements

general Gaussians on matrix objects work in principle, but are **way** too expensive



$$p(A) = \mathcal{N}(A; A_0, \Sigma_0) = \frac{1}{\sqrt{2\pi}|\Sigma|^{D/2}} \exp\left((\overrightarrow{A - A_0})^\intercal \Sigma_0^{-1} (\overrightarrow{A - A_0})\right)$$

$$p(S, Y \mid A) = \delta(\vec{Y} - (I \otimes S^\intercal)\vec{A}) = \lim_{\beta \to 0} \mathcal{N}(Y; (I \otimes S^\intercal)\vec{A}, \beta\Lambda)$$

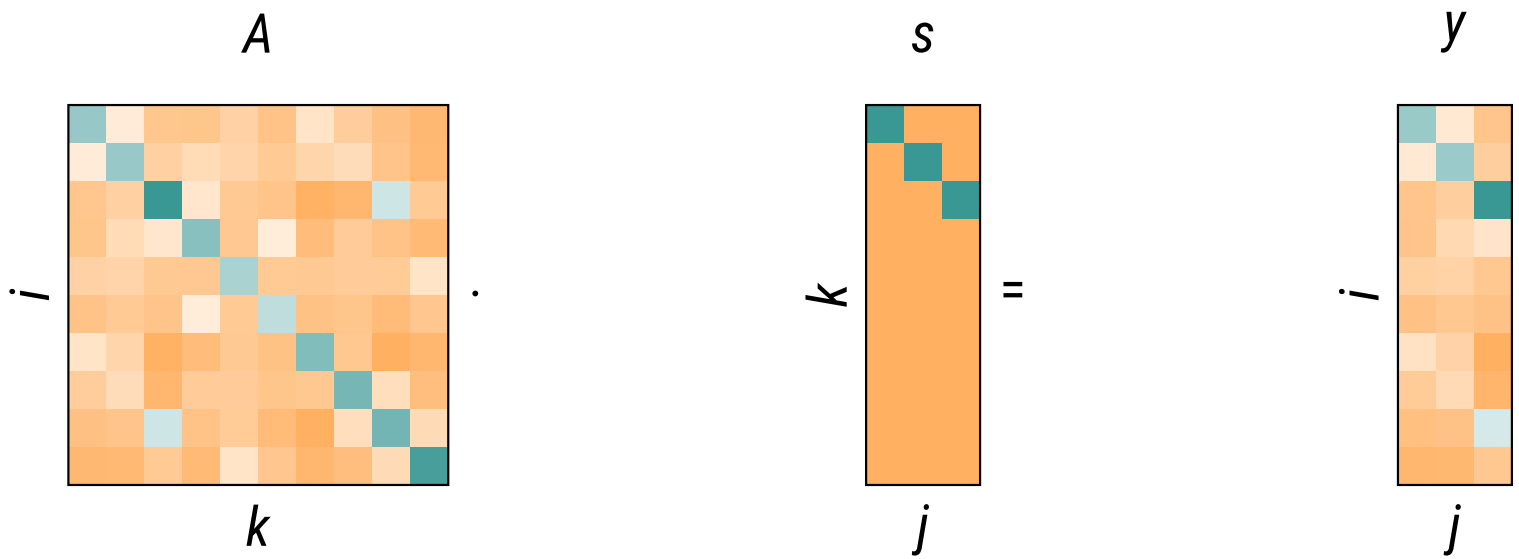
$$p_A(A \mid Y, S) = \mathcal{N}(A; A_M, \Sigma_M) \quad \text{with}$$

$$\vec{A}_M := \vec{A}_0 + \Sigma_0 (I \otimes S)\left((I \otimes S^\intercal)\Sigma_0 (I \otimes S)\right)^{-1}\left(\vec{Y} - (I \otimes S^\intercal)\vec{A}_0\right), \text{ and}$$

$$\Sigma_M := \Sigma_0 - \Sigma_0 (I \otimes S)\Big(\underbrace{(I \otimes S^\intercal)\Sigma_0 (I \otimes S)}_{:= G_M \in \mathbb{R}^{NM \times NM}}\Big)^{-1} (I \otimes S^\intercal)\Sigma_0$$

Kronecker Products to the Rescue!

low-rank posteriors



$$p(A) = \mathcal{N}(A; A_0, V_0 \otimes W_0) \qquad p(S, Y \mid A) = \delta(\vec{Y} - (I \otimes S^\intercal)\vec{A})$$

$$p_A(A \mid Y, S) = \mathcal{N}(A; A_M, V_0 \otimes W_M) \quad \text{with}$$

$$\vec{A}_M := \vec{A}_0 + (V_0 \otimes W_0)(I \otimes S)\left((I \otimes S^\intercal)(V_0 \otimes W_0)(I \otimes S)\right)^{-1}\left(\vec{Y} - (I \otimes S^\intercal)\vec{A}_0\right)$$

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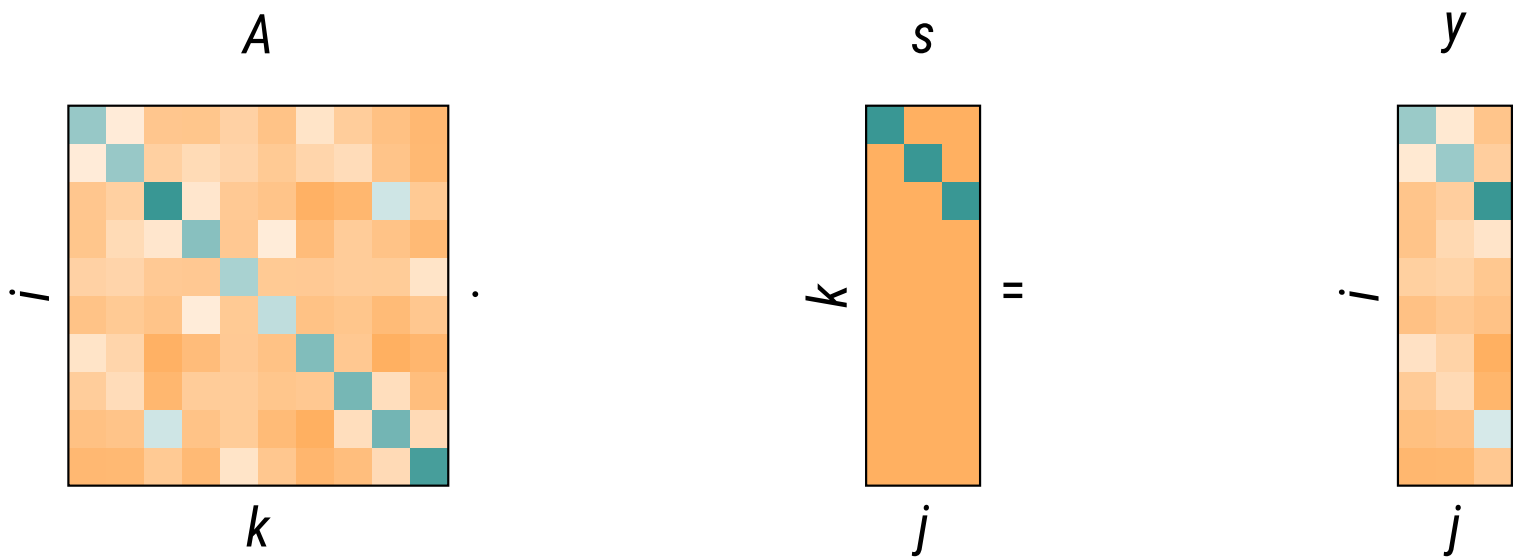

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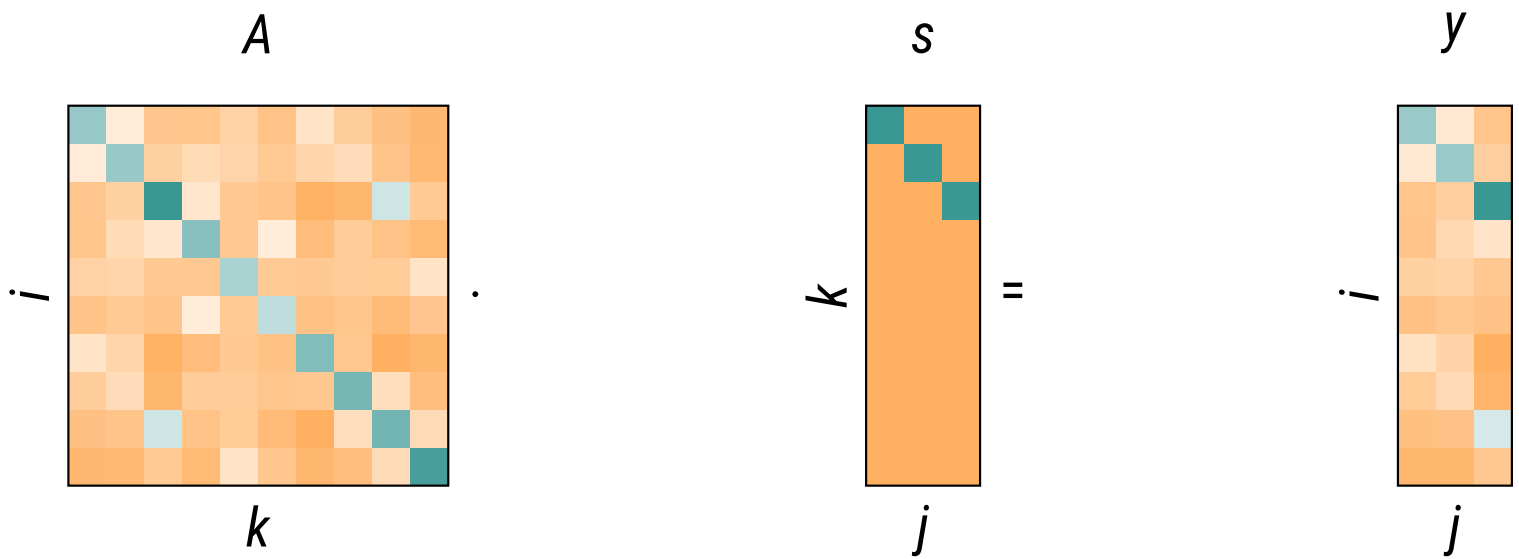

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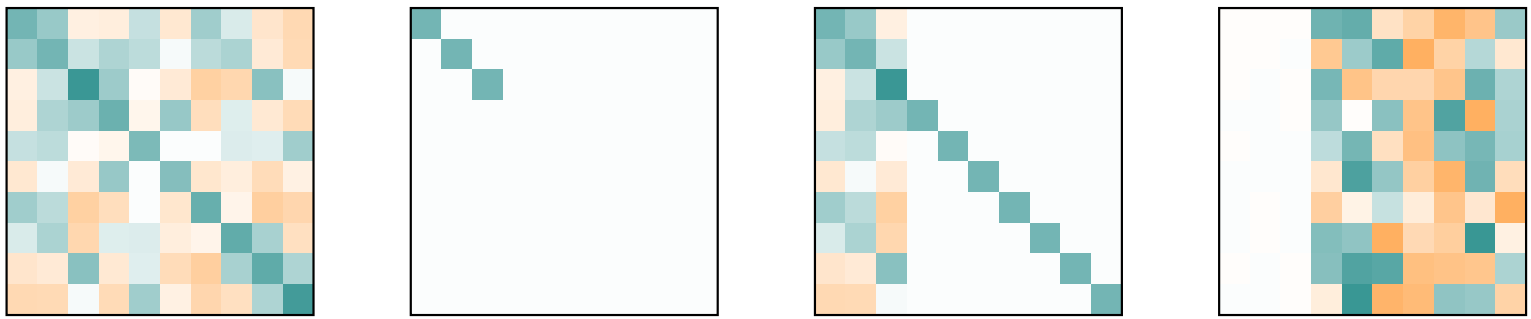
$$\vec{A}_M := \vec{A}_0 + \left(I \otimes W_0 S (S^\intercal W_0 S)^{-1}\right)\left(\vec{Y} - \overrightarrow{A_0 S}\right), \text{ and}$$

$$\Sigma_M := (V_0 \otimes W_0) - \left(V_0 \otimes W_0 S (S^\intercal W_0 S)^{-1} S^\intercal W_0\right)$$

Kronecker Products to the Rescue!

low-rank posteriors

A S $A_M(W_0 = I)$



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$$p_A(A \mid Y, S) = \mathcal{N}(A; A_M, V_0 \otimes W_M) \quad \text{with}$$

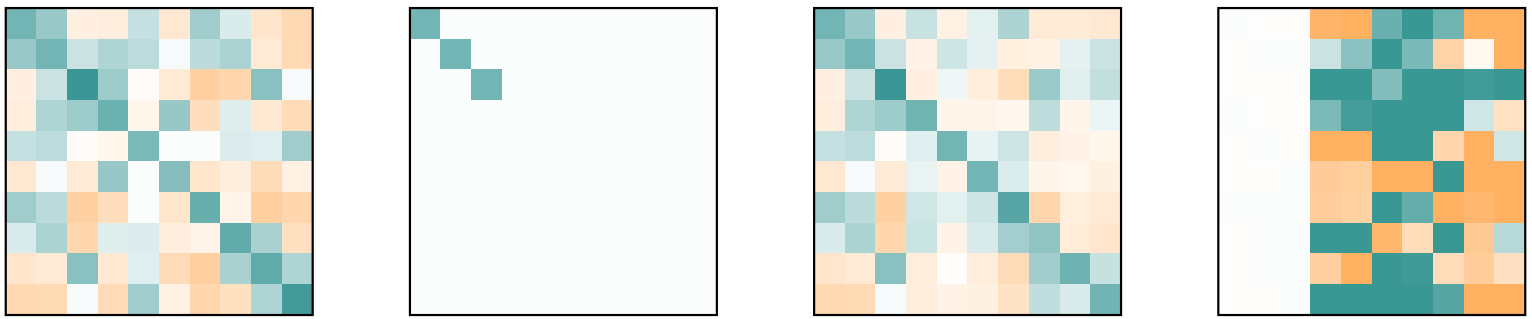
$$A_M := A_0 + (Y - A_0 S)(S^\intercal W_0 S)^{-1} S^\intercal W_0, \text{ and}$$

$$\Sigma_M := V_0 \otimes \underbrace{(W_0 - W_0 S(S^\intercal W_0 S)^{-1} S^\intercal W_0)}_{=:W_M}$$

Kronecker Products to the Rescue!

low-rank posteriors

A S $A_M(W_0\ \mathcal{W}(I, N+1)$



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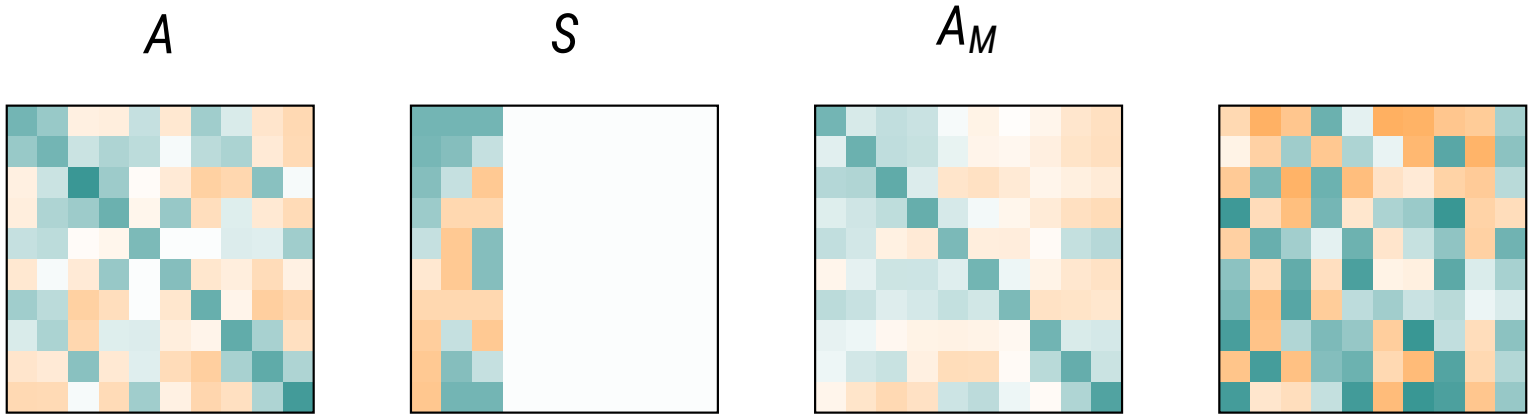
Kronecker Products to the Rescue!

low-rank posteriors



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$$\Sigma_M := V_0 \otimes \underbrace{(W_0 - W_0 S(S^\intercal W_0 S)^{-1} S^\intercal W_0)}_{=:W_M}$$

What does this prior mean?

some intuition

- full support: if V, W are spd, then this is a **weighted Frobenius norm**

$$\begin{aligned}\vec{A}^\intercal (V \otimes W)^{-1} \vec{A} &= \vec{A}^\intercal (\overrightarrow{V^{-1} A W^{-1\intercal}}) \\ &= \mathrm{tr}(A^\intercal V^{-1} A W^{-1}) \\ &= \|V^{-1/2} A W^{-1/2}\|_F^2 > 0 \ \forall A \neq 0\end{aligned}$$

$$V_0, W_0 \in \mathbb{R}^{N \times N}$$

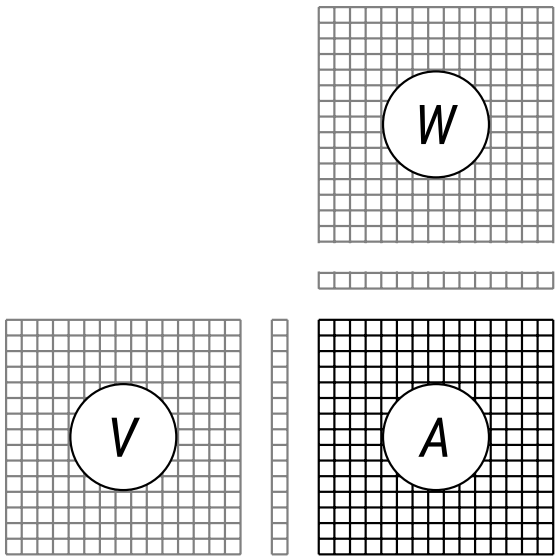
$$V_0 \otimes W_0 \in \mathbb{R}^{N^2 \times N^2}$$

- this is **not** the same as drawing columns and rows independently. Instead:

$$b_i \in \mathbb{R}^{N \times 1}, \text{ and } c_j \in \mathbb{R}^{1 \times N}, i = 1, \ldots, N$$

$$b_i \sim \mathcal{N}(0, V_0) \qquad c_j \sim \mathcal{N}(0, W_0)$$

$$A = B \odot C \quad \Rightarrow \quad \mathrm{cov}(A_{ij}, A_{k\ell}) = [V_0 \otimes W_0]_{(ij),(k\ell)}$$



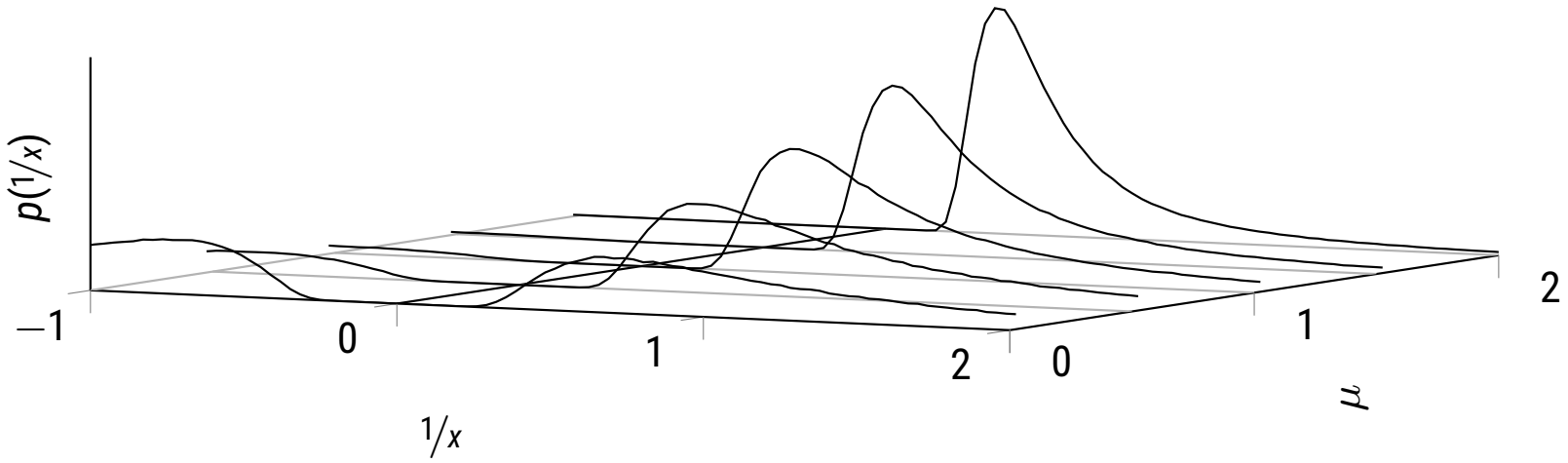
- $\mathrm{var}(A_{ij}) = V_{A0,ii} \cdot W_{A0,jj}$.

A Prior Over what?

direct and inverse models

Hennig, SIOPT 2015

If A is spd, then $Ax = b \Leftrightarrow x = Hb$. Are we inferring A or $H = A^{-1}$?



$$p(A) = \mathcal{N}(A; A_0, V_0 \otimes W_0) \qquad p(Y, S \mid A) = \delta(Y - AS)$$

$$p(A \mid Y, S) = \mathcal{N}\left(A, \underbrace{A_0 + (Y - A_0 S)(S^\intercal W_0 S)^{-1} S^\intercal W_0}_{=:A_M}, V_0 \otimes (W_0 - W_0 S(S^\intercal W_0 S)^{-1} S^\intercal W_0)\right)$$

$$A_M^{-1} = A_0^{-1} + (S - A_0^{-1} Y)(S^\intercal W_0 A_0^{-1} Y)^{-1} S^\intercal W_0 A_0^{-1}$$

$$p(H) = \mathcal{N}(H; H_0, V_0 \otimes W_0) \qquad p(Y, S \mid H) = \delta(S - HY)$$

$$p(H \mid Y, S) = \mathcal{N}\left(H, H_0 + (S - H_0 Y)(Y^\intercal W_0 Y)^{-1} Y^\intercal W_0, V_0 \otimes (W_0 - W_0 Y(Y^\intercal W_0 Y)^{-1} Y^\intercal W_0)\right)$$

It only matters a little

direct and inverse models are not equivalent, but closely related

but wait for later!

$$A_M^{-1} = A_0^{-1} + (S - A_0^{-1}Y) \cdot (S^\intercal W_0^A A_0^{-1} Y)^{-1} \cdot S^\intercal W_0^A A_0^{-1}$$
$$H_M = H_0 + (S - H_0 Y) \cdot (Y^\intercal W_0^H Y)^{-1} \cdot Y^\intercal W_0^H$$

Theorem:

Assume A_0 and W_0 are spd, and the search directions S are chosen linearly independent. Then, for spd A, the inverse A_M^{-1} exists.
Further, if $H_0 = A_0^{-1}$ we have $A_M^{-1} = H_M$ whenever $S^\intercal W_0^A A_0^{-1} = Y^\intercal W_0^H$ (e.g. if $W_0^A = A, W_0^H = A_0^{-1}$).
Proof: If A_0 is spd, its inverse exists. $Y = AS$, and products of spd matrices are spd. Thus, $W_0 A_0^{-1} A$ is spd, hence $S^\intercal W_0 A_0^{-1} AS$ invertible. The rest of the theorem follows by inspection of the above equation. □

Corollary:

If S are spd, for every **direct prior** $p(A) = \mathcal{N}(A; A_0, V_0 \otimes W_0^A)$, there exists an **equivalent inverse prior** $p(H) = \mathcal{N}(H; H_0, \tilde{V}_0 \otimes W_0^H)$, so that the probabilistic linear solver (using A_M^{-1} for line 12 in the first case) behaves identically.

Projection Methods

every Gaussian iterative solver is a projection method

1 **procedure** LINSOLVE_PROB($A(\cdot)$, b, $p(A)$)
2 $x_0 = H_0 b$ // initial guess
3 $r_0 = Ax_0 - b$ // initial gradient
4 **for** $i = 1, \dots, N$ **do**
5 $d_i = -H_{i-1} r_{i-1}$ // compute optimization direction
6 $z_i = Ad_i$ // **observe**
7 $\alpha_i = -d_i^\intercal r_{i-1} / d_i^\intercal z_i$ // optimal step-size
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10 $x_i = x_{i-1} + s_i$ // update estimate for x
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12 $H_i = \text{INFER}(H \mid Y_i, S_i, p(A))$ // estimate H
13 **end for**
14 **end procedure**

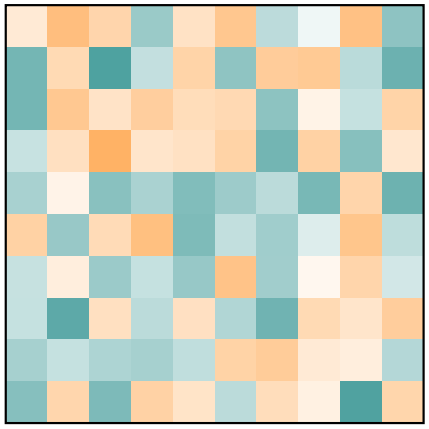
Definition:

By its general form, (regardless of line 12), LINSOLVE_PROP selects x_i within a sequence $\mathbb{K}_i = \text{span}\{d_1, \dots, d_i\}$. If $r_i \neq 0$, then for all $i > 0$, there is a non-empty space $\mathbb{L}_i$ such that $r_i \perp \mathbb{L}_i$ (by construction, $d_i \in \mathbb{L}_i$). Such an algorithm is called a **projection method**.

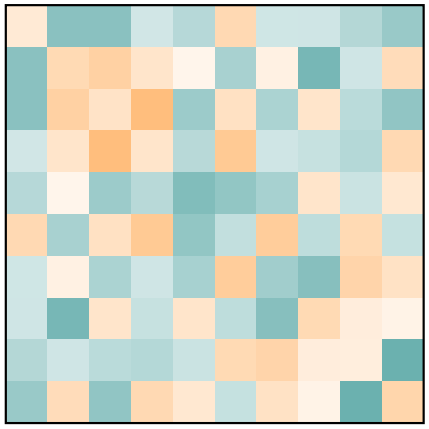
Encoding Symmetry – The Symmetric Kronecker Product

We **know** $A = A^\intercal$. But the prior does not reflect it!

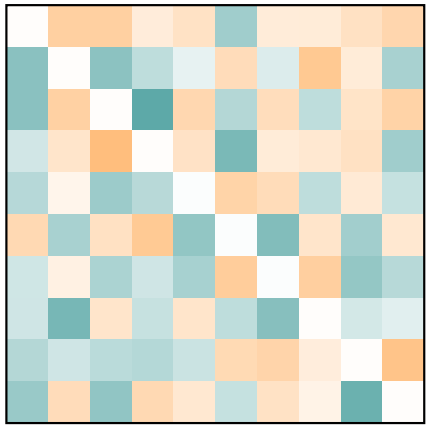
$p(A)$



$p(A \mid A = A^\intercal)$



$p(A \mid A = -A^\intercal)$



$A - A^\intercal = 0$ is an "observation" of a linear projection of A!

Symmetric Kronecker Products

van Loan 2000. *The ubiquitous Kronecker product.* J of Computational and Applied Mathematics **123**, 85–100

- define $\Pi_\ominus, \Pi_\oplus : \mathbb{R}^{N^2} \to \mathbb{R}^{N^2}$ by their elements

$$\Pi_{\ominus\,(ij),(k\ell)} := \tfrac{1}{2}(\delta_{ik}\delta_{j\ell} + \delta_{i\ell}\delta_{jk}) \qquad \Pi_{\oplus\,(ij),(k\ell)} := \tfrac{1}{2}(\delta_{ik}\delta_{j\ell} - \delta_{i\ell}\delta_{jk})$$

- thus

$$\Pi_\ominus \vec{X} = \overrightarrow{\tfrac{1}{2}(X + X^\mathsf{T})} \qquad \Pi_\oplus \vec{X} = \overrightarrow{\tfrac{1}{2}(X - X^\mathsf{T})}$$

- $\Pi_\oplus, \Pi_\ominus$ are **orthogonal projections**: $\Pi_\oplus^\mathsf{T} = \Pi_\oplus, \quad \Pi_\ominus^\mathsf{T} = \Pi_\ominus$

$$\Pi_\ominus\Pi_\ominus = \Pi_\ominus, \quad \Pi_\oplus\Pi_\oplus = \Pi_\oplus, \quad \Pi_\ominus\Pi_\oplus = \Pi_\oplus\Pi_\ominus = \mathbf{0}, \quad \Pi_\ominus + \Pi_\oplus = I$$

- $\forall W : \left[\Pi_\ominus(W \otimes W)\Pi_\oplus\right]_{(ij),(k\ell)} = \frac{1}{4}(W_{ik}W_{j\ell} - W_{i\ell}W_{jk} - W_{ik}W_{j\ell} + W_{i\ell}W_{jk}) = 0.$
- Thus define the **symmetric (antisymmetric) Kronecker product** $\circledast$ ($\circledcirc$):

$$W \otimes W = \underbrace{\Pi_\ominus(W \otimes W)\Pi_\ominus}_{=:W\circledast W} + \underbrace{\Pi_\oplus(W \otimes W)\Pi_\oplus}_{=:W\circledcirc W}$$

$$[W\circledast W]_{(ij),(k\ell)} = \tfrac{1}{2}(W_{ik}W_{j\ell} + W_{i\ell}W_{jk})$$

$$(W\circledast W)\vec{X} = \tfrac{1}{2}(WXW^\mathsf{T} + WX^\mathsf{T}W^\mathsf{T})$$

Symmetric Gaussian Priors

encoding symmetry in the prior

Hennig, SIOPT 2015

- condition on symmetry

$$p(\ominus \mid A) = \delta(\Pi_{\oplus} A - 0) = \lim_{\beta \to 0} \mathcal{N}(0; \Pi_{\oplus} A, \beta I)$$

- generic Gaussian posterior from above, choosing $\Sigma = W \otimes W$,

$$p(A \mid \ominus) = \mathcal{N}(A; \vec{A}_0 - \Sigma_0 \Pi_{\oplus}^{\intercal} (\Pi_{\oplus} \Sigma_0 \Pi_{\oplus}^{\intercal})^{-1} (-\Pi_{\oplus} \vec{A}_0),$$
$$\Sigma_0 - \Sigma_0 \Pi_{\oplus}^{\intercal} (\Pi_{\oplus} \Sigma_0 \Pi_{\oplus}^{\intercal})^{-1} \Pi_{\oplus} \Sigma_0)$$

$$\mathbb{E}(A) = \vec{A}_0 - (\Pi_{\oplus} + \Pi_{\ominus}) \Sigma_0 \Pi_{\oplus} (\Pi_{\oplus} \Sigma_0 \Pi_{\oplus})^{-1} \Pi_{\oplus} \vec{A}_0$$
$$= (\Pi_{\oplus} + \Pi_{\ominus}) \vec{A_0} - \Pi_{\oplus} \vec{A_0} = \Pi_{\ominus} \vec{A}_0$$

$$\mathrm{cov}(A) = \Sigma_0 - \Sigma_0 \Pi_{\oplus}^{\intercal} (\Pi_{\oplus} \Sigma_0 \Pi_{\oplus}^{\intercal})^{-1} \Pi_{\oplus} \Sigma_0 = \Pi_{\ominus} \Sigma_0 \Pi_{\ominus} = W \otimes\!\!\!\!\ominus W$$

$$\Rightarrow \quad p(A \mid \ominus) = \mathcal{N}(A; \Pi_{\ominus} \vec{A}_0, W \otimes\!\!\!\!\ominus W)$$

- with likelihood $p(Y, S \mid A) = \delta(Y - AS)$ get **rank-2M** posterior update

$$A_M = A_0 + (Y - A_0 S)(S^{\intercal} W S)^{-1} S^{\intercal} W + W S (S^{\intercal} W S)^{-1} (Y - A_0 S)^{\intercal}$$
$$- W S (S^{\intercal} W S)^{-1} S^{\intercal} (Y - A_0 S)(S^{\intercal} W S)^{-1} S^{\intercal} W$$

$$\Sigma_M = W_M \otimes\!\!\!\!\ominus W_M \quad \text{with (again)} \quad W_M := W_0 - W_0 S (S^{\intercal} W_0 S) S^{\intercal} W.$$

Conjugate Direction Methods

every symmetric Gaussian iterative solver is a CD method

1 **procedure** LINSOLVE_PROB($A(\cdot)$, b, $p(A)$)
2 $x_0 = H_0 b$ // initial guess
3 $r_0 = Ax_0 - b$ // initial gradient
4 **for** $i = 1, \ldots, N$ **do**
5 $d_i = -H_{i-1} r_{i-1}$ // compute optimization direction
6 $z_i = Ad_i$ // **observe**
7 $\alpha_i = -d_i^\intercal r_{i-1} / d_i^\intercal z_i$ // optimal step-size
8 $s_i = \alpha_i d_i$ // re-scale step
9 $y_i = \alpha_i z_i$ // re-scale observation
10 $x_i = x_{i-1} + s_i$ // update estimate for x
11 $r_i = r_{i-1} + y_i$ // new gradient at x_i
12 $H_i = \text{INFER}(H \mid Y_i, S_i, p(A))$ // estimate H
13 **end for**
14 **end procedure**

Theorem: (proof on next slide)

If A is symmetric, and line 12 produces a **symmetric** estimator H_i, then LINSOLVE_PROB is a **conjugate directions method**. That is, $s_i^\intercal A s_j = 0$ if $i \neq j$.

Conjugate directions methods converge to the correct $\boldsymbol{x}$ in at most $\boldsymbol{N}$ steps [Nocedal & Wright, Thm. 5.1] (they are *linearly consistent*). They also ensure $\boldsymbol{r_k} \perp \boldsymbol{s_{j<k}}$ [op.cit., Thm. 5.2]. (they are *orthogonal projection methods*).

Proof of Theorem

by induction

📖 Hennig, Osborne, Girolami, upcoming

By induction: For the base case[1] $i = 2$, i.e. after the first iteration of the loop, we have (recall that $\alpha_1 = -d_1^\intercal r_0 / d_1^\intercal A d_1$. The symmetry of the estimator H_i is used at $\star$

$$
\begin{aligned}
d_1^\intercal A d_2 &= -d_1^\intercal A(H_1 r_1) && = -d_1^\intercal A(H_1(y_1 + r_0)) && = -d_1^\intercal A(s_1 + H_1 r_0) \\
&= -\alpha_1 d_1^\intercal A d_1 - d_1^\intercal A H_1 r_0 && = d_1^\intercal r_0 - \alpha_1^{-1} s_1^\intercal A H_1 r_0 && = d_1^\intercal r_0 - \alpha_1^{-1} y_1^\intercal H_1 r_0 \\
&\overset{\star}{=} d_1^\intercal r_0 - \alpha_1^{-1} s_1^\intercal r_0 && = d_1^\intercal r_0 - d_1^\intercal r_0 = 0.
\end{aligned}
$$

For the inductive step, assume $\{d_0, \dots, d_{i-1}\}$ are pairwise A-conjugate. Consider any $k < i$, and use this assumption *twice* to find

$$
\begin{aligned}
d_k^\intercal A d_i &= -d_k^\intercal A(H_i r_i) && = -d_k^\intercal A H_i \left(\sum_{j \leq i} y_j + r_0 \right) \\
&= -d_k^\intercal A \left(\sum_{j \leq i} s_j + H_i r_0 \right) && = -d_k^\intercal A \left(\sum_{j \leq i} \alpha_j d_j + H_i r_0 \right) \\
&= -\alpha_k d_k^\intercal A d_k - d_k^\intercal A(H_i r_0) && = d_k^\intercal r_{k-1} - d_k^\intercal r_0 \\
&= d_k^\intercal \left(\sum_{j<k} y_j + r_0 \right) - d_k^\intercal r_0 = 0 && = \sum_{j<k} \alpha_j d_k^\intercal A d_j = 0.
\end{aligned}
$$

[1] For this proof, it does not actually matter how the first direction d_1 is chosen.

Connection to Conjugate Gradients

main result of this lecture

📖 Hennig, Osborne, Girolami, upcoming

Theorem: (proof only on request)

Assume A is spd, H_i is symmetric for all $i \geq 0$, and LinSolve_Prob does not terminate before step $k < N$. Then, if

$$d_i = -H_{i-1} r_{i-1} \in \text{span}\{s_1, \dots, s_{i-1}, y_1, \dots, y_{i-1}, r_{i-1}\}.$$

it holds that

$$r_i \perp r_j \qquad \forall\, 0 \leq i \neq j \leq k,$$

and there exist $\gamma_i \in \mathbb{R}_{\setminus 0}$ for all $i < k$ so that line 12 of LinSolve_Prob is

$$d_i = -H_{i-1} r_{i-1} = \gamma_i \left(-r_{i-1} + \frac{\beta_i}{\gamma_{i-1}} d_{i-1} \right), \quad \text{with} \quad \beta_i := \frac{r_{i-1}^\intercal r_{i-1}}{r_{i-2}^\intercal r_{i-2}}.$$

Then, LinSolve_Prob **is equivalent to the method of conjugate gradients** (with $x_0 = H_0 b$).

Probabilistic Conjugate Gradients

main result of this lecture

📖 Hennig, Osborne, Girolami, upcoming

Theorem:

Consider a prior $p(H) = \mathcal{N}(H; H_0, W_H \otimes W_H)$. For all choices of (H_0, W_H) with $H_0 = \alpha I$ and $W_H = \beta I + \gamma H$, for $\alpha \in \mathbb{R}\ \beta, \gamma \in \mathbb{R}_+$, LinSolve_Prob is equivalent to the method of conjugate gradients, in the sense that it produces the exact same sequence $\{x_i\}$. The same is true for MAP inference using $p(A) = \mathcal{N}(A; A_0, W_A \otimes W_A)$ with scalar $A_0 = \alpha I$ and $W_A = \beta I + \gamma A$.

Proof:

Use theorems on previous slides. First: conjugate directions by symmetry. Then to show: H_i resulting from the above models satisfies assumption of theorem on previous slide., i.e. r_{i-1} is mapped to $s_i = -H_{i-1} r_{i-1}$ in the span of $\{S, Y, r_{i-1}\}$. Consider the image of H_i as defined above. For the model on H, if $S_{:i-1}$ denotes $(s_1, \dots, s_{i-1})$ and analogously for $Y_{:i-1}$, then H_{i-1} maps $v \in \mathbb{R}^N$ to $\mathbf{span}\{H_0 v, S_{:i-1}, H_0 Y_{:i-1}, W_H Y_{:i-1}\}$. Hence, if H_0 is scalar and $W_H = \beta I + \gamma H$, then (since $HY = S$), r_{i-1} is mapped to $\mathbf{span}\{r_{i-1}, S_{:i-1}, Y_{:i-1}\}$. For models on A, H_{i-1} maps r_{i-1} to $\mathbf{span}\{A_0^{-1} r_{i-1}, A_0^{-1} W_A S_{:i-1}, A_0^{-1} Y_{:i-1}, S_{:i-1}\}$. For a scalar A_0 and $W_A = \beta I + \gamma A$, using $AS = Y$, this is the span of $\{r_{i-1}, Y_{:i-1}, S_{:i-1}\}$. □

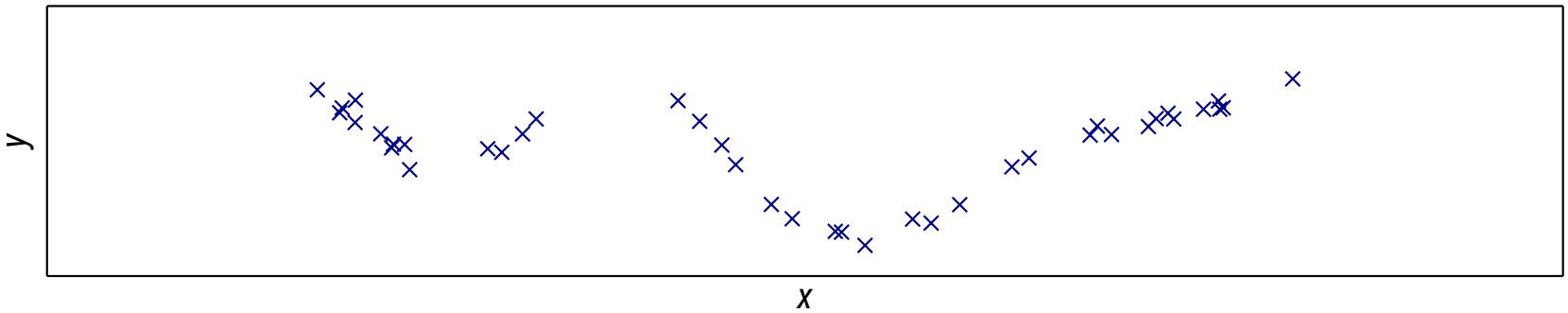
The big picture:

- Gaussian measures on matrices can be used to construct **projection methods** by MAP estimation
- **Symmetry** can be encoded analytically, and gives **conjugate direction methods**
- There is a nontrivial subset of symmetric priors that give **conjugate gradients**

Uncertainty Calibration for Iterative Solvers

an example of statistically calibrated error estimates

Bartels & Hennig, AISTATS 2016



- $\Rightarrow \mu(x) = k_{xX} k_{XX}^{-1} Y = \arg\min_{f \in \mathcal{H}_k} [\|Y - f_X\|^2 + \|f\|_k^2]$ where

$$[k_{XX}]_{ij} = k(x_i, x_j) \qquad \text{e.g.} \qquad k(a,b) = \exp\left(-\frac{(a-b)^2}{2\lambda^2}\right)$$

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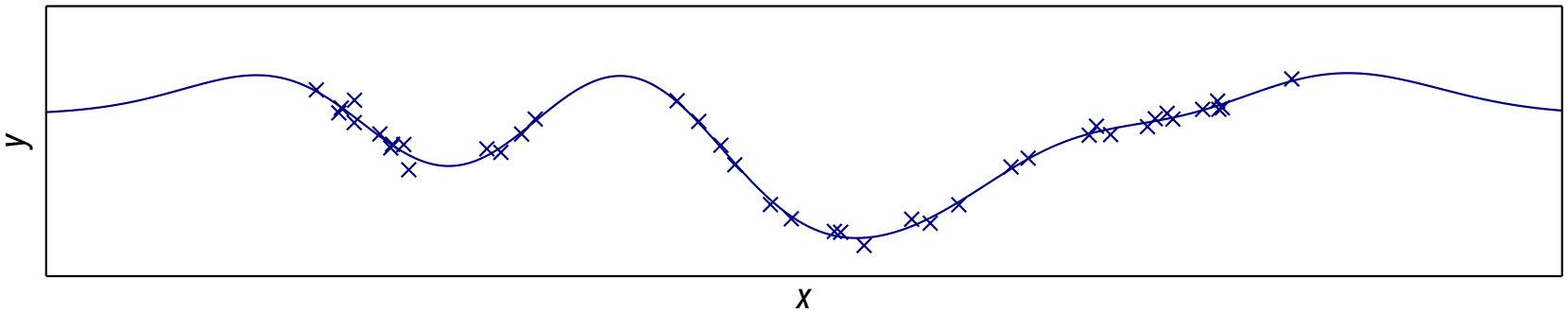

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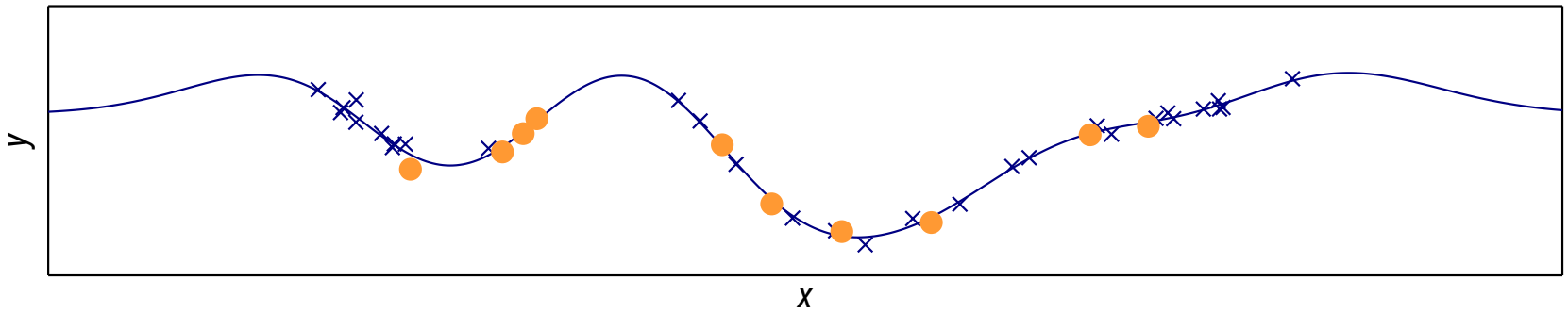

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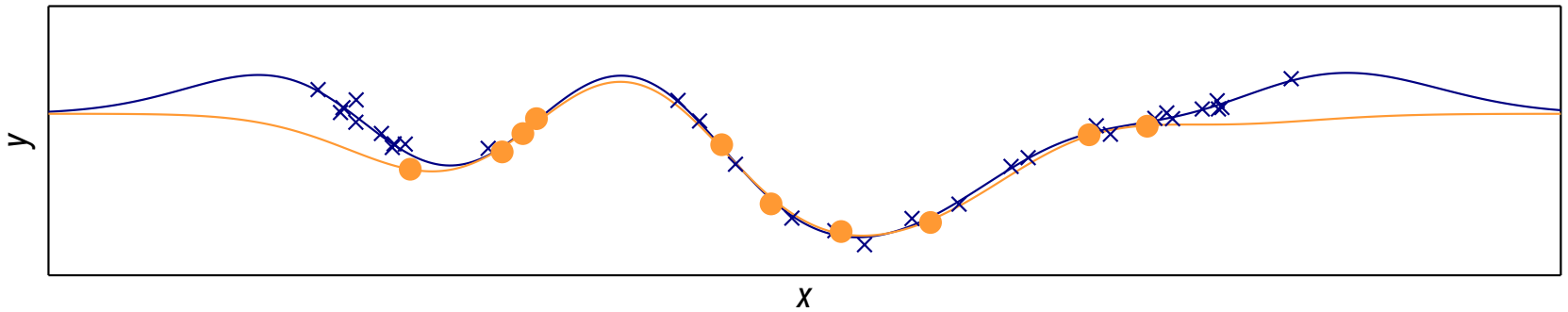

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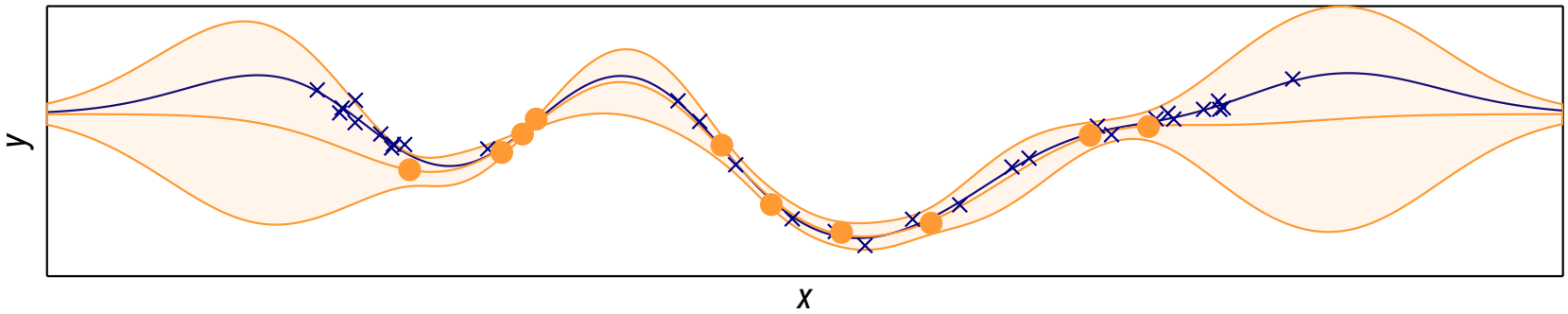

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- choose $p(k_{XX}^{-1}) = \mathcal{N}(\alpha_0 I, \beta^2 I \otimes I)$. Use statistical regularity assumptions to get calibrate posterior to get upper bound on approximation error $|\mu - \tilde{\mu}|$

Uncertainty Calibration for Iterative Solvers

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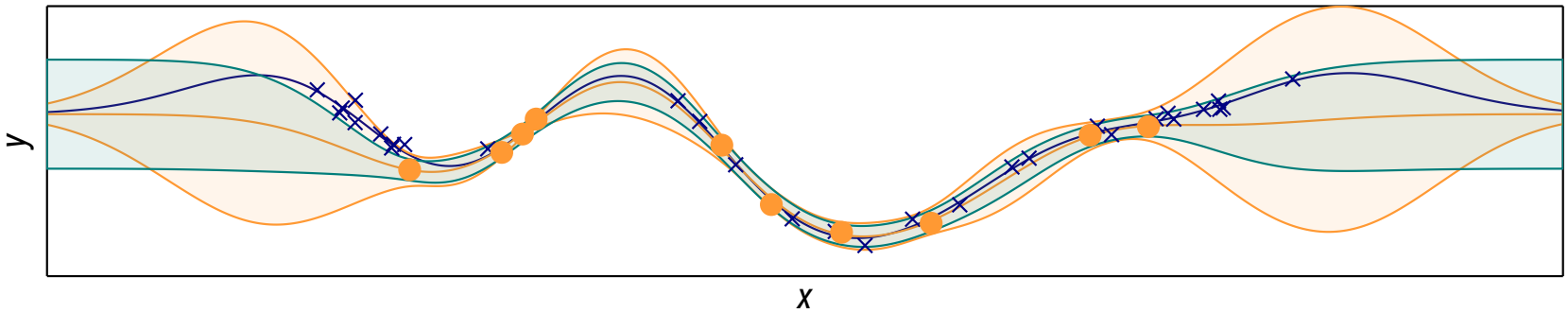

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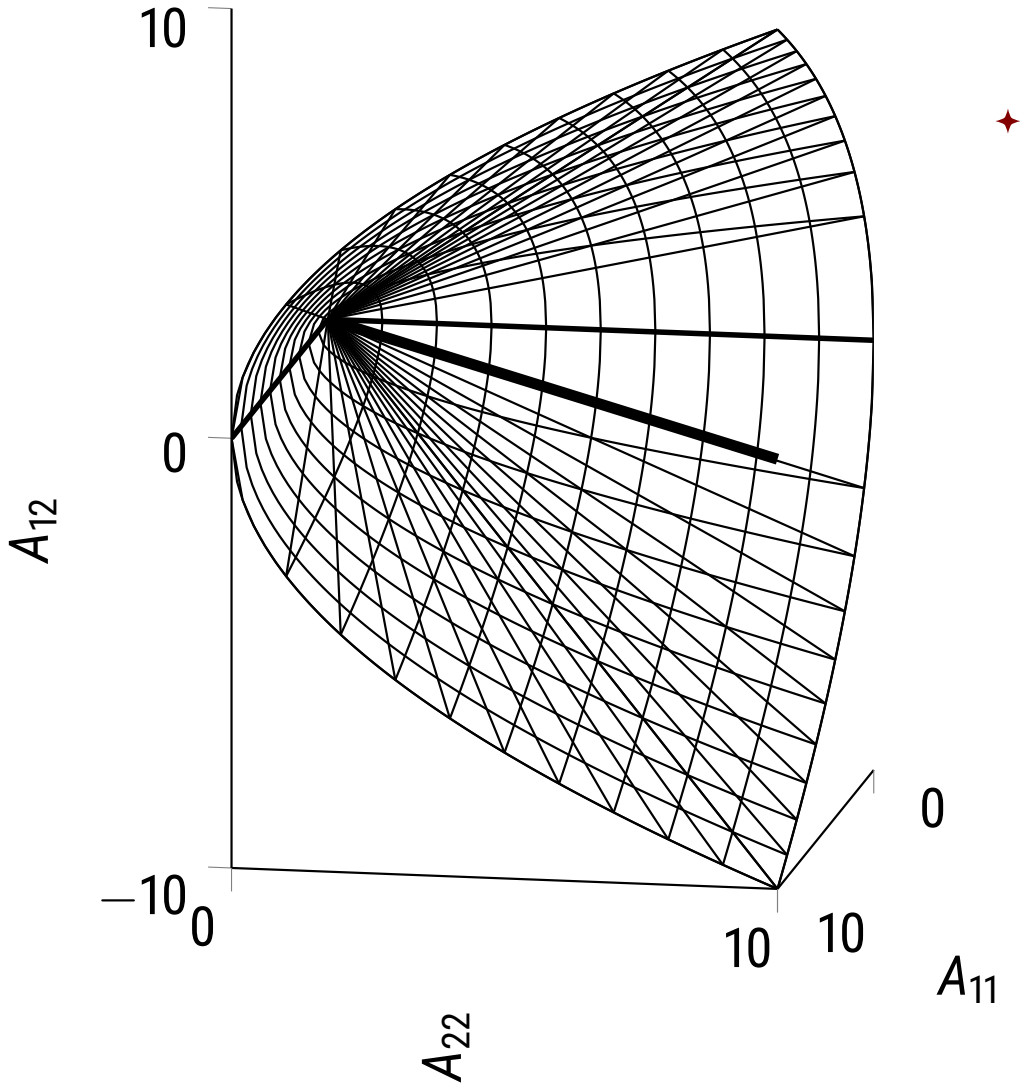
- not the same as GP posterior variance!

What about Positive Definiteness

positive definites can only be modelled approximately

📖 Hennig, Osborne, Girolami, CUP, upcoming



- the positive definite cone is not a linear sub-space of $\mathbb{R}^{N^2}$

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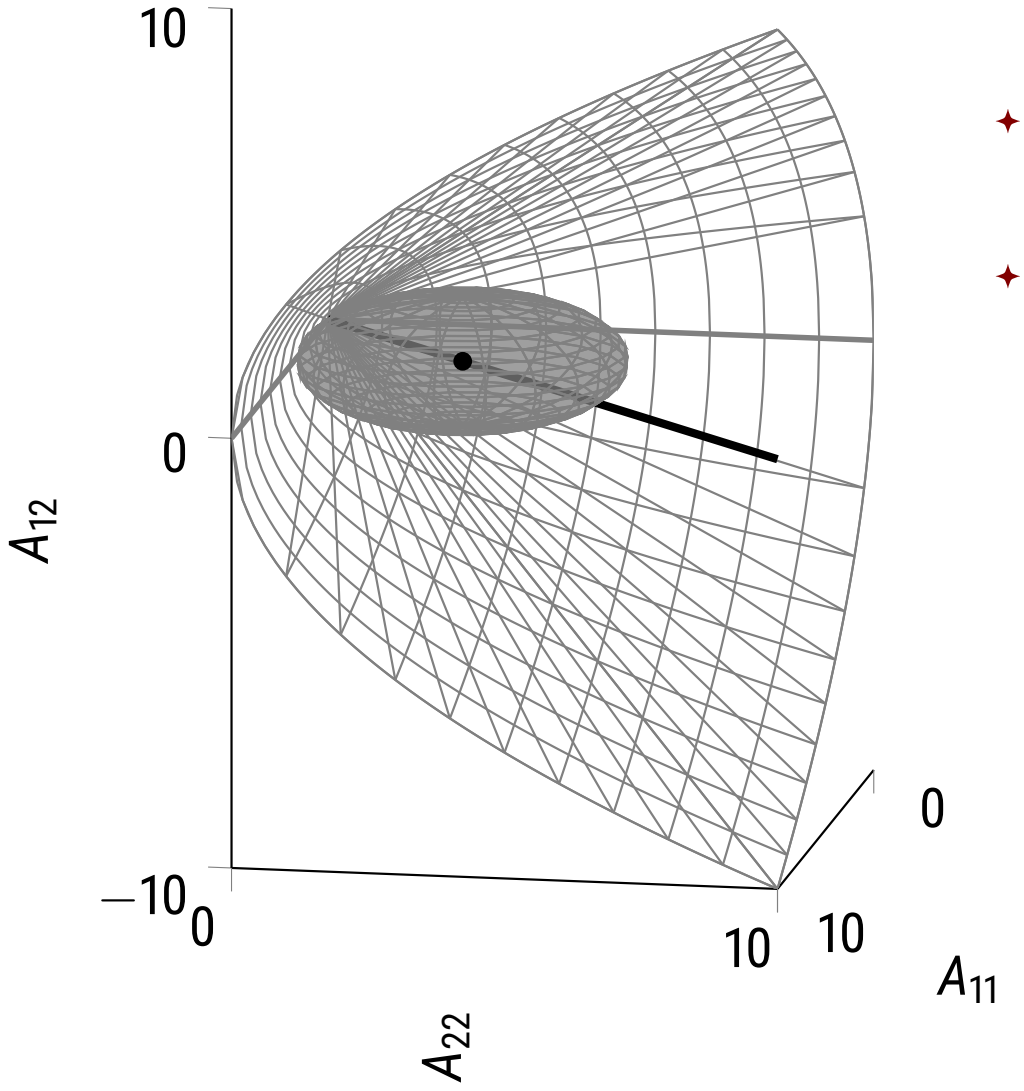

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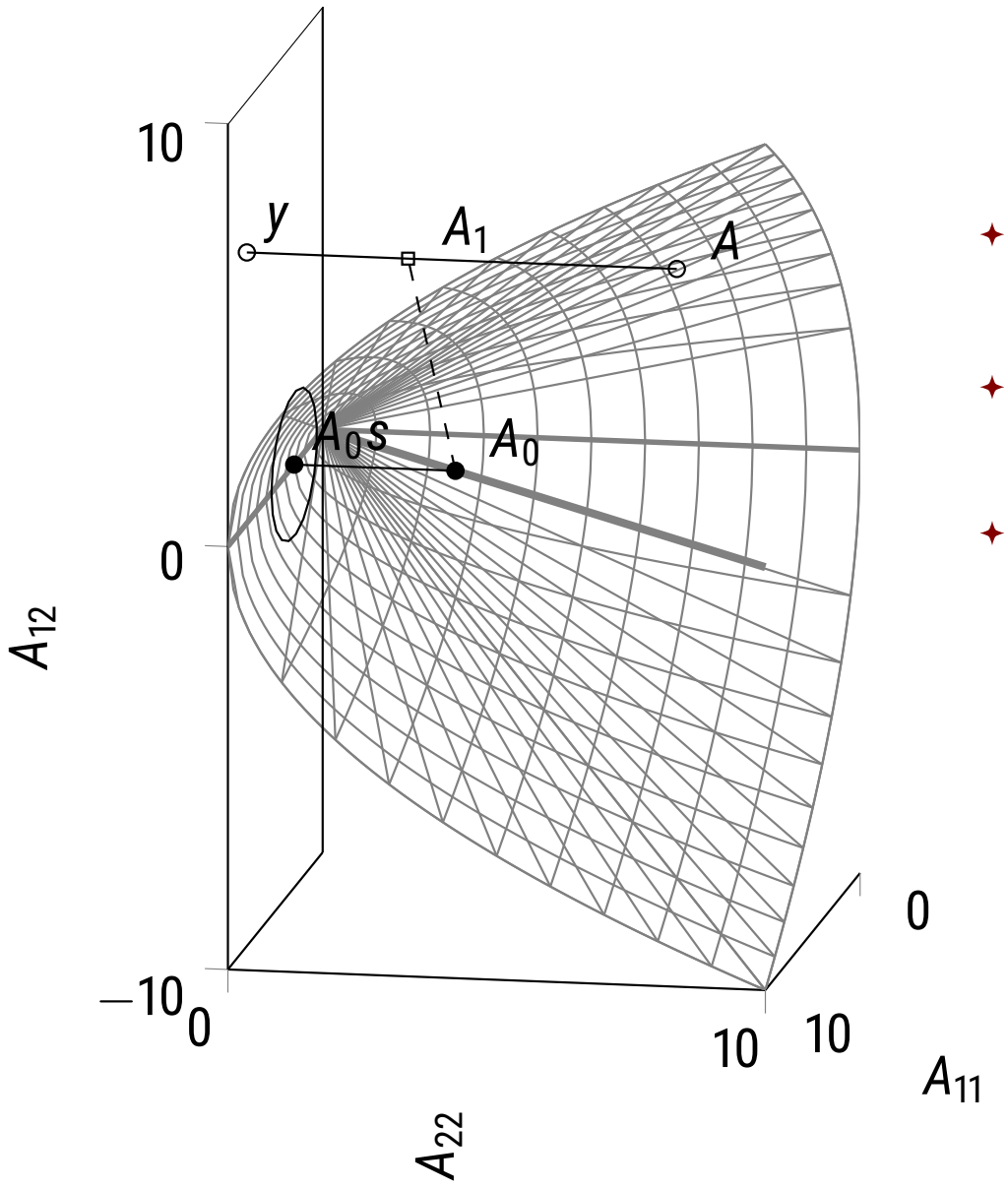

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- **Theorem** (proof on request): For $p(A) = \mathcal{N}(\beta I, \alpha^2 I \otimes I)$, the posterior mean A_M may lie outside the cone. But for any y, there is an α^2 so A_M is spd.

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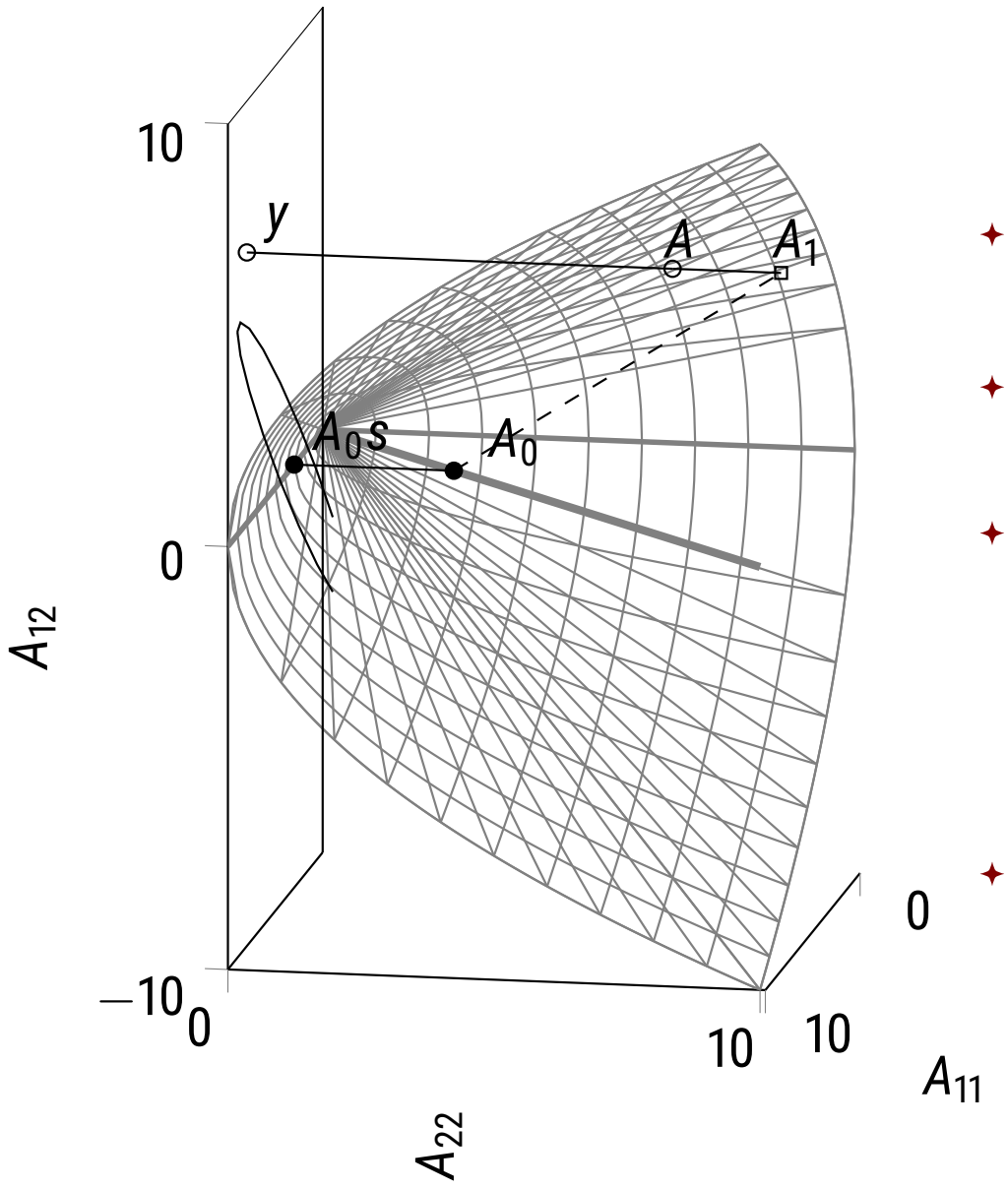
Hennig, Osborne, Girolami, CUP, upcoming



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- **Theorem** (proof on request): For $p(A) = \mathcal{N}(I, \beta I, A \otimes A)$, the posterior mean A_M always lies in the cone.

What else?

In linear algebra, PN is tightly constrained by complexity

more in 📖 Hennig, Osborne, Girolami, upcoming

Some things one may want to try

- ✦ noise on matrix elements $p(Y \mid A, S) = \mathcal{N}(Y; AS, \Lambda)$?
- ⟶ breaks Kronecker structure of covariance, requires nontrivial extensions
- ✦ hierarchical inference on scale/structure of prior?
- ⟶ possible using Gauss-Gamma prior.
  But CG does not produce iid. observations. More on request

PN affords a (one) unifying view of linear algebra methods, but significant additional functionality typically requires serious work.
There can be a trade-off between different desired probabilistic functionality: calibrated uncertainty is easier if the point-estimate is not efficient. Noisy observations require approximate inference. Etc.

The big picture:

- Gaussian measures on matrices can be used to construct **projection methods** by MAP estimation
- **Symmetry** can be encoded analytically, and gives **conjugate direction methods**
- There is a nontrivial subset of symmetric priors that give **conjugate gradients**
- There are many **cumbersome restrictions** imposed by the extremely high-dimensional space of matrix elements and the tight restrictions on computational **complexity**.

in **nonlinear Optimization**, many symmetries are broken.

$$f : \mathbb{R}^N \to \mathbb{R} \qquad \nabla f(x_*) \stackrel{!}{=} 0$$

- local approximation to second order, assuming Hessian $[B(x)]_{ij} := \dfrac{\partial^2 f(x)}{\partial x_i \partial x_j}$:

$$f(x - x_i) = f(x_i) + (x - x_i)^\intercal \nabla f(x_i) + \frac{1}{2}(x - x_i)^\intercal B(x_i)(x - x_i) + \mathcal{O}(\|x - x_i\|^3)$$

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- if B is spd (i.e. f is convex), efficient local optimization by **Newton iteration**

$$x_{i+1} \approx \arg\min f(x - x_i) = x_i - B^{-1}(x_i)\nabla f(x_i)$$

$$f : \mathbb{R}^N \to \mathbb{R} \qquad \nabla f(x_*) \stackrel{!}{=} 0$$

- local approximation to second order, assuming Hessian $[B(x)]_{ij} := \dfrac{\partial^2 f(x)}{\partial x_i \partial x_j}$:

$$f(x - x_i) = f(x_i) + (x - x_i)^\intercal \nabla f(x_i) + \frac{1}{2}(x - x_i)^\intercal B(x_i)(x - x_i) + \mathcal{O}(\|x - x_i\|^3)$$

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- accessible: $\{\nabla f(x_i)\}_{i=0,\dots}$

Quasi Newton Methods

cf. 🗎 Dennis & Moré, *Quasi-Newton Methods, motivation and theory*, SIREV 1977

- ensure **secant equation**

$$y_i := \nabla f(x_i) - \nabla f(x_{i-1}) = \hat{B}_i(x_i - x_{i-1}) =: \hat{B}_i s_i \qquad \text{or} \qquad \hat{H}_i y_i = s_i$$

- many options! E.g. The **Dennis family** (1971) of direct symmetric updates:

$$B_{i+1} = B_i + \frac{(y_i - B_i s_i)c_i^\mathsf{T} + c_i(y_i - B_i s_i)^\mathsf{T}}{c_i^\mathsf{T} s_i} - \frac{c_i s_i^\mathsf{T}(y_i - B_i s_i)c_i^\mathsf{T}}{(c_i^\mathsf{T} s_i)^2}$$

with members [cf. 🗎 Hennig, SIOPT 2015]

Symmetric Rank-1 (SR1)[Davidon, 1959]	$c = y - B_{i-1}s$
Powell[1970] **S**ymmetric **B**royden[1965]	$c = s$
Greenstadt[1970]	$c = B_{i-1}s$
Davidon[1959] **F**letcher **P**owell[1963]	$c = y$
Broyden[1969] **F**letcher[1970] **G**oldfarb[1970] **S**hanno[1970]	$c = y + \sqrt{\frac{y^\mathsf{T}s}{s^\mathsf{T}B_{i-1}s}}B_{i-1}s$

- direct models: $p(B \mid B_{i-1}) = \mathcal{N}(B, B_i, W_i \otimes W_i)$ and $p(y_i \mid s_i, B_i) = \delta(y_i - B_i s_i)$:

Symmetric Rank-1 (SR1)[Davidon, 1959]	$W_i = \alpha(\bar{B} - B_i)$
Powell[1970] **S**ymmetric **B**royden[1965]	$W_i = \alpha I$
Greenstadt[1970]	$c = B_{i-1}s$
Davidon[1959] **F**letcher **P**owell[1963]	$W_i = \alpha \bar{B}$

where $\bar{B} = \int_0^1 B(x_{i-1} + ts_i)\, dt$, $\alpha > 0$.

- inverse models: $p(H \mid H_{i-1}) = \mathcal{N}(H, H_i, V_i \otimes V_i)$ and $p(y_i \mid s_i, H_i) = \delta(s_i - H_i y_i)$:

Broyden[1969] **F**letcher[1970] **G**oldfarb[1970] **S**hanno[1970]	$V_i = \alpha \bar{H}$

Equivalence in the Linear Case

[cf. Nazareth, SINUM 1979]

Theorem (simplified, Nazareth, 1979)

If f is a convex (positive definite) quadratic function, **all** members of the Dennis family are equivalent to the method of conjugate gradients.

- Gaussian models can be used to infer matrix elements
- the potential model spaces are severely limited by computational considerations
- nevertheless, class of priors consistent with existing methods is surprisingly large
- algebraic constraints also make desirable functionality hard to achieve
- **nonlinear** optimization methods are closely related, but many **symmetries are broken**

These slides can be found at
`http://tinyurl.com/Dobbiaco-Hennig-4`

Beyond classics, let's build new functionality for contemporary challenges!